New Variants of Variable Neighbourhood Search for 0-1 Mixed Integer Programming and Clustering

A thesis submitted for the degree of

Doctor of Philosophy

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List of Abbreviations

2SSP	:	two-stage stochastic problem
B&B	:	branch-and-bound
B&C	:	branch-and-cut
CIQ	:	colour image quantization
FP	:	feasibility pump
GCMH	:	genetic C-Means heuristic
GLS	:	guided local search
GRASP	:	greedy randomised adaptive search
ILS	:	iterated local search
IRH	:	iterative relaxation based heuristic
IIRH	:	iterative independent relaxation based heuristic
LB	:	local branching
LP	:	linear programming
LPA	:	linear programming-based algorithm
MIP	:	mixed integer programming
MIPs	:	mixed integer programming problems
MKP	:	multidimensional knapsack problem
MP	:	mathematical programming
PD-VNS	:	primal-dual variable neighbourhood search
PSO	:	particle-swarm-optimisation
RCL	:	restricted candidate list
RINS	:	relaxation induced neighbourhood search
RS	:	reactive search
RVNS	:	reduced variable neighbourhood search
SA	:	simulated annealing
TS	:	tabu search
VNB	:	variable neighbourhood branching
VND	:	variable neighbourhood descent
VNDM	:	variable nighbourhood descent with memory
VND-MIP	:	variable neighbourhood descent for mixed integer programming
VNDS	:	variable neighbourhood decomposition search
VNDS-MIP	:	variable neighbourhood decomposition search for mixed integer programming
VNP	:	variable neighbourhood pump
VNS	:	variable neighbourhood search

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Related Publications

- **Published papers**
  - J. Lazić, S. Hanafi, N. Mladenović and D. Urošević. Variable Neighbourhood Decomposition Search for 0-1 Mixed Integer Programs. Computers and Operations Research, 37 (6): 1055-1067, 2010.
  - S. Hanafi, J. Lazić and N. Mladenović. Variable Neighbourhood Pump Heuristic for 0-1 Mixed Integer Programming Feasibility. Electronic Notes in Discrete Mathematics 36 (C): 759–766, 2010, Elsevier.
  - S. Hanafi, J. Lazić, N. Mladenović, C. Wilbaut and I. Crévits. Hybrid Variable Neighbourhood Decomposition Search for 0-1 Mixed Integer Programming Problem. Electronic Notes in Discrete Mathematics 36 (C): 883–890, 2010, Elsevier.
  - J. Lazić, S. Hanafi, N. Mladenović and D. Urošević. Solving 0-1 Mixed Integer Programs with Variable Neighbourhood Decomposition Search. A Proceedings volume from the 13th Information Control Problems in Manufacturing International Symposium, 2009. ISBN: 978-3-902661-43-2, DOI: 10.3182/20090603-3-RU-2001.0502
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  - P. Hansen, J. Lazić and N. Mladenović. Variable neighbourhood search for colour image quantization. IMA Journal of Management Mathematics 18 (2): 207-221, 2007.
- **Papers submitted for publication**
  - S. Hanafi, J. Lazić, N. Mladenović, C. Wilbaut and I. Crévits. Variable Neighbourhood Decomposition Search with pseudo-cuts for Multidimensional Knapsack Problem. Submitted to Computers and Operations Research, special issue devoted to Multidimensional Knapsack Problem, 2010.
  - S. Hanafi, J. Lazić, N. Mladenović, C. Wilbaut and I. Crévits. Different Variable Neighbourhood Search Diving Strategies for Multidimensional Knapsack Problem. Submitted to Journal of Mathematical Modelling and Algorithms, 2010.
  - T. Davidović, J. Lazić, V. Maraš and N. Mladenović. MIP-based Heuristic Routing of Barge Container Ships. Submitted to Transportation Science, 2010.
  - J. Lazić, S. Hanafi and N. Mladenović. Variable Neighbourhood Search Diving for 0-1 MIP Feasibility. Submitted to Matheuristics 2010, the 3rd international workshop on model-based heuristics.

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Abstract

Many real-world optimisation problems are discrete in nature. Although recent rapid developments in computer technologies are steadily increasing the speed of computations, the size of an instance of a hard discrete optimisation problem solvable in prescribed time does not increase linearly with the computer speed. This calls for the development of new solution methodologies for solving larger instances in shorter time. Furthermore, large instances of discrete optimisation problems are normally impossible to solve to optimality within a reasonable computational time/space and can only be tackled with a heuristic approach.

In this thesis the development of so called *matheuristics*, the heuristics which are based on the mathematical formulation of the problem, is studied and employed within the variable neighbourhood search framework. Some new variants of the variable neighbourhood search metaheuristic itself are suggested, which naturally emerge from exploiting the information from the mathematical programming formulation of the problem. However, those variants may also be applied to problems described by the combinatorial formulation. A unifying perspective on modern advances in local search-based metaheuristics, a so called *hyper-reactive* approach, is also proposed. Two NP-hard discrete optimisation problems are considered: 0-1 mixed integer programming and clustering with application to colour image quantisation. Several new heuristics for 0-1 mixed integer programming problem are developed, based on the principle of variable neighbourhood search. One set of proposed heuristics consists of improvement heuristics, which attempt to find high-quality near-optimal solutions starting from a given feasible solution. Another set consists of constructive heuristics, which attempt to find initial feasible solutions for 0-1 mixed integer programs. Finally, some variable neighbourhood search based clustering techniques are applied for solving the colour image quantisation problem. All new methods presented are compared to other algorithms recommended in literature and a comprehensive performance analysis is provided. Computational results show that the methods proposed either outperform the existing state-of-the-art methods for the problems observed, or provide comparable results.

The theory and algorithms presented in this thesis indicate that hybridisation of the CPLEX MIP solver and the VNS metaheuristic can be very effective for solving large instances of the 0-1 mixed integer programming problem. More generally, the results presented in this thesis suggest that hybridisation of exact (commercial) integer programming solvers and some metaheuristic methods is of high interest and such combinations deserve further practical and theoretical investigation. Results also show that VNS can be successfully applied to solving a colour image quantisation problem.

Chapter 1

Introduction

1.1 Combinatorial Optimisation

Combinatorial optimisation, also known as discrete optimisation, is the field of applied mathematics which deals with solving combinatorial (or discrete) optimisation problems. Formally, an *optimisation problem* P can be specified as finding

$$\nu(P) = \min\{f(x) \mid x \in X, X \subseteq \mathcal{S}\} \tag{1.1}$$

where $\mathcal{S}$ denotes the *solution space*, X denotes the *feasible region* and $f : \mathcal{S} \to \mathbb{R}$ denotes the *objective function.* If $x \in X$, we say that x is a *feasible solution* of the problem (1.1). Solution $x \in \mathcal{S}$ is said to be *infeasible* if $x \notin X$. Optimisation problem P is *feasible* if there is at least one feasible solution of P. Otherwise, problem P is *infeasible*.

Formulation (1.1) assumes that the problem defined is a *minimisation* problem. A *maximisation* problem can be defined in the analogous way. However, it is obvious that any maximisation problem can easily be reformulated as a minimisation one, by setting the objective function to $F : \mathcal{S} \to \mathbb{R}$, with $F(x) = -f(x)$, $\forall x \in \mathcal{S}$, where f is the objective function of the original maximisation problem and $\mathcal{S}$ is the solution space.

If $\mathcal{S} = \mathbb{R}^n, n \in \mathbb{N}$, problem (1.1) is called a *continuous optimisation* problem. Otherwise, if $\mathcal{S}$ is finite, or infinite but enumerable, problem (1.1) is called *combinatorial* or *discrete optimisation* problem. Although in some research literature combinatorial and discrete optimisation problems are defined in different ways and do not necessarily represent the same type of problems (see, for instance, [33, 145]), in this thesis these two terms will be treated as synonymous and will be used interchangeably. Some special cases of combinatorial optimisation problems are the *integer optimisation* problem when $\mathcal{S} = \mathbb{Z}^n, n \in \mathbb{N}$, the 0-1 *optimisation problem* when $\mathcal{S} = \{0, 1\}^n, n \in \mathbb{N}$, and the *mixed integer optimisation problem* when $\mathcal{S} = \mathbb{Z}^{n_1} \times \mathbb{R}^{n_2}, n_1, n_2 \in \mathbb{N}$. A particularly important special case of the combinatorial optimisation problem (1.1) is a *mathematical programming* problem, in which $\mathcal{S} \subseteq \mathbb{R}^n$ and the feasible set X is defined as:

$$X = \{x \mid g(x) \leq b\}, \tag{1.2}$$

where $b \in \mathbb{R}^m$, $g : \mathbb{R}^n \to \mathbb{R}^m$, $g = (g_1, g_2, \ldots, g_m)$, $g_i : \mathbb{R}^n \to \mathbb{R}$, $i \in \{1, 2, \ldots, m\}$, with $g_i(x) \leq b_i$ being the ith *constraint.* If C is a set of constraints, the problem obtained by adding all constraints in C to the mathematical programming problem P will be denoted as $(P \mid C)$. In other words, if P is an optimisation problem defined by (1.1), with feasible region X as in (1.2), then $(P \mid C)$ is the problem of finding:

$$\min\{f(x) \mid x \in X, x \text{ satisfies all constraints from } C\}. \tag{1.3}$$

An optimisation problem Q, defined with $\min\{\hat{f}(x) \mid x \in \hat{X}, \hat{X} \subseteq \mathcal{S}\}$, is a *relaxation* of the optimisation problem P, defined with (1.1), if and only if $X \subseteq \hat{X}$ and $\hat{f}(x) \leq f(x)$ for all $x \in X$. If Q is a relaxation of P, then P is a *restriction* of Q. Relaxation and restriction for maximisation problems are defined analogously.

Solution $x^* \in X$ of the problem (1.1) is said to be *optimal*, if

$$f(x^*) \leq f(x),\ \forall x \in X. \tag{1.4}$$

An optimal solution is also called *optimum*. In case of a minimisation problem, an optimal solution is also called a *minimal solution* or simply a *minimum*. For a maximisation problem, the optimality condition (1.4) has the form: $f(x^*) \geq f(x),\ \forall x \in X$. An optimal solution of a maximisation problem is also called a *maximal solution* or a *maximum*. The *optimal value* $\nu(P)$ of an optimisation problem P defined by (1.1) is the objective function value $f(x^*)$ of its optimal solution x^* (the optimal value of a minimisation/maximisation problem is also called the minimal/maximal value). Values $l, u \in \mathbb{R}$ are called a *lower* and an *upper* bound, respectively, for the optimal value $\nu(P)$ of the problem P, if $l \leq \nu(P) \leq u$. Note that if Q is a relaxation of P (and P and Q are minimisation problems), then the optimal value $\nu(Q)$ of Q is not greater than the optimal value $\nu(P)$ of P. In other words, the optimal value $\nu(Q)$ of problem Q is a lower bound for the optimal value $\nu(P)$ of P. Solving the problem (1.1) *exactly* means either finding an optimal solution $x^* \in X$ and proving the optimality (1.4) of x^*, or proving that the problem has no feasible solutions, i.e. that $X = \emptyset$.

Many real-world (industrial, logistic, transportation, management, etc.) problems may be modelled as combinatorial optimisation problems. They include various assignment and scheduling problems, location problems, circuit and facility layout problems, set partitioning/covering, vehicle routing, travelling salesman problem and many more. Therefore, a lot of research has been done in the development of efficient solution techniques in the field of discrete optimisation. In general, all combinatorial optimisation solution methods can be classified as either *exact* or *approximate*. An exact algorithm is the algorithm which solves an input problem exactly. Most commonly used exact solution methods are branch-and-bound, dynamic programming, Lagrangian relaxation based methods, and linear programming based methods such as branch-and-cut, branch-and-price and branch-and-cut-and-price. Some of them will be discussed in more details in Chapter 4 devoted to 0-1 mixed integer programming. However, a great number of practical combinatorial optimisation problem instances is proven to be NP-hard [115], which means that they are not solvable by any polynomial time algorithm (in terms of the size of the input instance), unless P = NP holds[1]. Moreover, for the majority of problems which can be solved by a polynomial time algorithm, the power of that polynomial may be so large that the solution cannot be obtained within a reasonable timeframe. This is the reason why a lot of research has been carried out in designing efficient approximate solution techniques for high complexity optimisation problems.

An approximate algorithm is an algorithm which does not necessarily provide an optimal solution of an input problem, or the proof of infeasibility in case that the problem is infeasible. Approximate solution methods can be classified as either *approximation algorithms* or *heuristics*. An approximation algorithm is an algorithm which, for a given input instance P of an optimisation problem (1.1), always returns a feasible solution $x \in X$ of P (if one exists), such that the ratio $f(x)/f(x^*)$, where x^* is an optimal solution of the input instance P, is within a given approximation ratio $\alpha \in \mathbb{R}$. More details on approximation algorithms can be found, for instance, in [47, 312].

[1]For more details on complexity classes P and NP, the reader is referred to Appendix A.

Approximation algorithms can be viewed as methods which are guaranteed to provide solutions of a certain quality. However, there is a number of NP-hard optimisation problems which cannot be approximated arbitrarily well (i.e. for which an efficient approximation algorithm does not exist), unless P = NP [16]. In order to tackle these problems, one must employ methods which do not provide any guarantees regarding either the solution quality, or the execution time limitations. Such methods are usually referred to as *heuristic methods* or simply *heuristics*. In [275], the following definition of a heuristic is proposed: "A heuristic is a method which seeks good (i.e. near-optimal) solutions at a reasonable computational cost without being able to guarantee optimality, and possibly not feasibility. Unfortunately, it may not even be possible to state how close to optimality a particular heuristic solution is.". Since there is no guarantee regarding the solution quality, a certain heuristic may have a very poor performance for some (bad) instances of a given problem. Nevertheless, a heuristic is usually considered good if it outperforms good approximation algorithms on a majority of instances of a given problem. Moreover, a good heuristic may even outperform an exact algorithm regarding the computational time (i.e. usually provides a solution of a better quality than the exact algorithm, if observed after a predefined execution time which is shorter than the total running time needed for the exact algorithm to provide an optimal solution). However, one should always bare in mind the so called *No Free Lunch* theorem (NFLT) [330], which basically states that there can be no optimisation algorithm which outperforms all the others on all problems. In other words, if an optimisation algorithm performs well on a particular sub class of problems, then the specific features of that algorithm, which exploit the characteristics of that sub class, may prevent it from performing well on problems outside that class.

According to the general principle used for generating a solution of a problem, heuristic methods can be classified as follows:

1) constructive methods
2) local search methods
3) inductive methods
4) problem decomposition/partitioning
5) methods that reduce the solution space
6) evolutionary methods
7) mathematical programming based methods

The heuristic types listed here are the most common ones. However, the concept of heuristics allows for introducing new solution strategies, as well as combining the existing ones in different ways. Therefore, there is a number of other possible categories and it is hard (if possible) to make a complete classification of all heuristic methods. Comprehensive surveys on heuristic solution methods can be found, for instance, in [96, 199, 296, 336]. A brief description of each of the heuristic types stated above will be provided next. Some of these basic types will be discussed in more details later in this thesis.

Constructive methods. Normally, only one (initial) feasible solution is generated. The solution is constructed step by step, using the information from the problem structure. The two most common approaches used are *greedy* and *look-ahead*. In a greedy approach (see [139] for example), the next solution candidate is always selected as the best candidate among the current set of possible choices, according to some local criterion. At each iteration of a look-ahead approach, the consequences of possible choices are estimated and solution candidates which can lead to a bad final solution are discarded (see [27] for example).

Local search methods. Local search methods, also known as improvement methods, start from a given feasible solution and gradually improve it in an iterative process, until a local optimum is reached. For each solution x, a *neighbourhood* of x is defined as a set of all feasible solutions which are in a vicinity of x according to some predefined distance measure in the solution space of the problem. At each iteration, a neighbourhood of the current candidate solution is explored and the current solution is replaced with a better solution from its neighbourhood, if one exists. If there are no better solutions in the observed neighbourhood, local optimum is reached and the solution process terminates.

Inductive methods. The solution principles valid for small and simple problems are generalised for the larger and harder problems of the same type.

Problem decomposition/partitioning. The problem is decomposed into a number of smaller/ simpler to solve subproblems and each of them is solved separately. The solution processes for the subproblems can be either independent or intertwined in order to exchange the information about the solutions of different subproblems.

Methods that reduce the solution space. Some parts of the feasible region are discarded from further consideration in such a way that the quality of the final solution is not significantly affected. Most common ways of reducing the feasible region include the tightening of the existing constraints or introducing new constraints.

Evolutionary methods. As opposed to *single-solution* heuristics (sometimes also called *trajectory* heuristics), which only consider one solution at a time, *evolutionary* heuristics operate on a *population* of solutions. At each iteration, different solutions from the current population are combined, either implicitly or explicitly, to create new solutions which will form the next population. The general goal is to make each created population better than the previous one, according to some predefined criterion.

Mathematical programming based methods. In this approach, a solution of a problem is generated by manipulating the mathematical programming (MP) formulation (1.1)-(1.2) of the problem. The most common ways of manipulating the mathematical model are the aggregation of parameters, the modification of the objective function, and changing the nature of constraints (including modification, addition or deletion of particular constraints). A typical example of parameter aggregation is the case of replacing a number of variables with a single variable, thus obtaining a much smaller problem. This small problem is then solved either exactly or approximately, and the solution obtained is used to retrieve the solution of the original problem. Other possible ways of aggregation include aggregating a few stages of a multistage problem into a single stage, or aggregating a few dimensions of a multidimensional problem into a single dimension. A widely used modification of the objective function is Lagrangian relaxation [25], where one or more constraints, multiplied by Lagrange multipliers, are incorporated into the objective function (and removed from the original formulation). This can also be viewed as an example of changing the nature of constraints. There are numerous other ways of manipulating the constraints within a given mathematical model. One possibility is to weaken the original constraints by replacing several constraints with their linear combination [121]. Another is to discard several constraints and solve the resulting model. The obtained solution, even if not feasible for the original problem, may provide some useful information for the solution process. Probably the most common approach regarding the modification of constraints is the constraint relaxation, where a certain constraint is replaced with one which defines a region containing the region defined by the original constraint. A typical example is linear programming relaxation of integer optimisation problems, where integer variables are allowed to take real values.

The heuristic methods were first initiated in the late 1940s (see [262]). For several decades, only so called *special heuristics* were being designed. Special heuristics are heuristics which rely on the structure of the specific problem and therefore cannot be applied to other problems. In the 1980s, a new approach for building heuristic methods has emerged. These more general solution schemes, named *metaheuristics* [122], provide high level frameworks for building heuristics for broader classes of problems. In [128], metaheuristics are described as "solution methods that orchestrate an interaction between local improvement procedures and higher level strategies to create a process capable of escaping from local optima and performing a robust search of a solution space". Some of the main concepts which can be distinguished in the development of metaheuristics are the following:

1) diversification vs. intensification
2) randomisation
3) recombination
4) one vs. many neighbourhood structures
5) large neighbourhoods vs. small neighbourhoods
6) dynamic parameter adjustment
7) dynamic vs. static objective function
8) memory usage
9) hybridisation
10) parallelisation

Diversification vs. intensification. The term *diversification* refers to a shifting of the actual area of search to a part of the search space which is far (with respect to some predefined distance measure) from the current solution. In contrast, *intensification* refers to a more focused examination of the current search area, by exploiting all the information available from the search experience. Diversification and intensification are often referred to as *exploration* and *exploitation*, respectively. For a good metaheuristic, it is very important to find and keep an adequate balance between the diversification and intensification during the search process.

Randomisation. *Randomisation* allows the use of a random mechanism to select one or more solutions from a set of candidate solutions. Therefore, it is closely related to the diversification operation discussed above and represents a very important element of most metaheuristics.

Recombination. The *recombination* operator is mainly associated with evolutionary metaheuristics (such as genetic algorithm [138, 243, 277]). It combines the attributes of two or more different solutions in order to form new (ideally better) solutions. In a more general sense, adaptive memory [123, 124, 301] and path relinking [133] strategies can be viewed as an implicit way of recombination in single-solution metaheuristics.

One vs. many neighbourhood structures. As mentioned previously, the concept of a neighbourhood plays a vital role in the construction of a local search method. However, most metaheuristics employ local search methods in different ways. The way neighbourhood structures are defined and explored may distinguish one metaheuristic from the other. Some metaheuristics, such as simulated annealing [4, 173, 196] or tabu search [131] for example (but also many others), work only with a single neighbourhood structure. Others, such as numerous variants of variable neighbourhood search (VNS) [159, 161, 163, 162, 164, 166, 167, 168, 237], operate on a set of different neighbourhood structures. Obviously, multiple neighbourhood structures usually provide better means for both diversification and intensification. Consequently, it yields more flexibility in exploring the search space, which normally results in a higher overall efficiency of a metaheuristic. Although neighbourhood structures are usually not explicitly defined within an evolutionary framework, one can observe that recombination and mutation (self-modification) operators define solution neighbourhoods in an implicit way.

Large neighbourhoods vs. small neighbourhoods. As noted above, when designing a neighbourhood search type metaheuristic, a choice of neighbourhood structure, i.e. the way the neighbourhoods are defined, is essential for the efficiency and the effectiveness of the method. Normally, as the size of a neighbourhood increases, the higher is the quality of the local optima and the more accurate is the final solution. On the other hand, exploring large neighbourhoods is usually computationally extensive and demands longer execution times. Nevertheless, a number of methods which successfully deal with very large-scale neighbourhoods[2] has been developed [10, 233, 235]. They can be classified according to the techniques used to explore the neighbourhoods. In variable depth methods, heuristics are used to explore the neighbourhoods [211]. Another group of methods are those in which network flow or dynamic programming techniques are used for searching the neighbourhoods [64, 305]. Finally, there are methods in which large neighbourhoods are defined using the restrictions of the original problem, so that they are solvable in polynomial time [135].

Dynamic parameter adjustment. It is convenient if a metaheuristic framework provides a form of an automatic parameter tuning, so that it is not necessary to perform extensive preliminary experiments in order to adjust the parameters for each particular problem, when deriving a problem-specific heuristic from a given metaheuristic. A number of so called *reactive* approaches, with an automatic (dynamic) parameter adjustment, has been proposed so far (see, for example, [22, 23, 44]).

Dynamic vs. static objective function. Whereas most metaheuristics deal with the same objective function during the whole solution process and use different diversification mechanisms in order to escape from local optima, there are some approaches which dynamically change the objective function during the search, in that way changing the search landscape and avoiding the stalling in a local optimum. Some of the methods which use a dynamic objective function are guided local search [319] or reactive variable neighbourhood search [44].

Memory usage. The term *memory* (also referred to as *search history*) in a metaheuristic context refers to a storage of the relevant information during the search process (such as visited solutions, relevant solution properties, number of relevant iterations, etc.) and exploiting the collected information in order to further guide the search process. Although it is explicitly used only in tabu search [123, 131], there is a number of other metaheuristics which incorporate the memory usage in an implicit way. In genetic algorithm [277] and scatter search [133, 201], the population of solutions

[2]With the size usually exponential of the size of the input problem.

can be viewed as an implicit form of memory. The pheromone trails in Ant Colony Optimisation [88, 89] represent another example of implicit memory usage. In fact, a unifying approach for all metaheuristics with (implicit or explicit) memory usage was proposed in [301], called Adaptive Memory Programming (AMP). According to AMP, each memory-based metaheuristic in some way memorises the information from a set of solutions and uses this information to construct new provisional solutions during the search process. When combined with some other search method, AMP can be regarded as a higher-level metaheuristic itself, which uses the search history to guide the subordinate method (see [123, 124]).

Hybridisation. Naturally, each metaheuristic has its own advantages and disadvantages in solving a certain class of problems. This is why numerous hybrid schemes were designed, which combine the algorithmic principles of several different metaheuristics [36, 265, 272, 302]. These hybrid methods usually outperform the original methods they were derived from (see, for example, [29]).

Parallelisation. Parallel implementations are aimed at further speed-up of the computation process and the improvement of solution space exploration. They are based on a simultaneous search space exploration by a number of concurrent threads, which may or may not communicate among each other. Different parallel schemes may be derived depending on the subproblem/search space partition assigned to each thread and the communication scheme used. More theory on metaheuristic parallelisation can be found in [70, 71, 72, 74].

For comprehensive reviews and bibliography on metaheuristic methods, the reader is referred to [37, 117, 128, 252, 253, 276, 282, 317]. For a given problem, it may be the case that one heuristic is more efficient for a certain set of instances, whereas some other heuristic is more efficient for another set of instances. Moreover, when solving one particular instance of a given input problem, it is possible that one heuristic is more efficient in one stage of the solution process, and some other heuristic in another stage. Lately, some new classes of higher-level heuristic methods have emerged, such as *hyper-heuristics* [48], *formulation space search* [239, 240], *variable space search*[175] or *cooperative search* [97]. A hyper-heuristic is a method which searches the space of heuristics in order to detect the heuristic method which is most efficient for a certain subset of problem instances, or certain stages of the solution process for a given instance. As such, it can be viewed as a response to limitations of optimisation algorithms imposed by the No Free Lunch theorem. The most important distinction between a hyper-heuristic and a heuristic for a particular problem instance is that hyper-heuristic operates on the space comprised of heuristic methods, rather than on the solution space of the original problem. Some metaheuristic methods can also be utilised as hyper-heuristics. Formulation space search [239, 240] is based on the fact that a particular optimisation problem can often be formulated in different ways. As a consequence, different problem formulations induce different solution spaces. Formulation space search is a general framework for alternating between various problem formulations, i.e. switching between various solution spaces of the problem during the search process. The neighbourhood structures and other search parameters are defined/adjusted separately for each solution space. The similar idea is exploited in the variable space search [175], where several search spaces for the graph colouring problem are considered, with different neighborhood structures and objective functions. Like hyper-heuristics, cooperative search strategies also exploit the advantages of several heuristics [97]. However, cooperative search is usually associated with parallel algorithms (see, for instance, [177, 306]).

Another state of the art stream in the development of metaheuristics arises from a hybridisation of metaheuristics and mathematical programming (MP) techniques. The resulting hybrid methods are called *matheuristics* (short from math-heuristics). Since new solutions in the search process are generated by manipulating the mathematical model of the input problem, matheuristics are also called *model-based* heuristics. They became particularly popular with the boost in development of general-purpose MP solvers, such as IBM ILOG CPLEX, Gurobi, XPRESS, LINDO or FortMP. Often, an exact optimisation method is used as the subroutine of the metaheuristics for solving a smaller subproblem. However, the hybridisation of a metaheuristic and an MP method can be realised in two directions: either by exploiting an MP method within a metaheuristic framework (using some general-purpose MP solver as a search component within metaheuristic is one very common example) or by using a metaheuristic to improve an MP method. The first type of hybridisation is much more exploited so far. In [266, 268], a structural classification of possible hybridisations between metaheuristics and exact methods is provided, as in Figure 1.1. Two main classes of possible hybridisation types are distinguished, namely *collaborative combinations* and *integrative combinations*. Collaborative combinations refer to algorithms which do communicate to each other during the execution process, but none of them contains the other as an algorithmic component. On the other hand, in integrative combinations, one algorithm (either exact or metaheuristic) is a subordinate part of the other. In a more complex environment, there can be one master algorithm (again, either exact or metaheuristic), and more integrated slave algorithms of the other type. According to [268], some most common methodologies in combining metaheuristics and MP techniques are: a) metaheuristics for finding high-quality incumbents and bounds in branch-and-bound, b) relaxations for guiding metaheuristic search, c) exploiting the primal-dual relationship in metaheuristics, d) following the spirit of local search in branch-and-bound, e) MP techniques for exploring large neighbourhoods, etc.

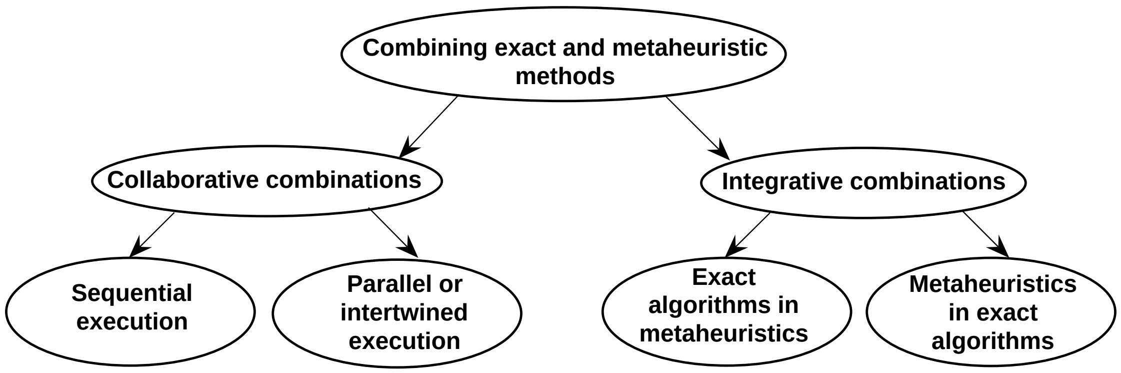

Combining exact and metaheuristic methods
Collaborative combinations
Integrative combinations
Sequential execution
Parallel or intertwined execution
Exact algorithms in metaheuristics
Metaheuristics in exact algorithms

Figure 1.1: Structural classification of hybridisations between metaheuristics and exact methods.

At present, many existing general-purpose MP solvers contain a variety of heuristic solution methods in addition to exact optimisation techniques. Therefore, any optimisation method available through a call to a general-purpose MP solver can be used as the subproblem subroutine within a given metaheuristic, which may yield in a multi-level matheuristic framework. For example, local branching [104], feasibility pump [103] or relaxation induced neighbourhood search [75] are only a few of well-known MIP matheuristic methods which are now embedded in the commercial IBM ILOG CPLEX MIP solver. If the CPLEX MIP solver is then used as a search component within some matheuristic algorithm, a multi-level (or even recursive) matheuristic scheme is obtained.

Although the term "matheuristic" is still recent, a number of methods for solving optimisation problems which can be considered as matheuristics have emerged over the last decades. Hard variable fixing (i.e. setting some variables to particular values) to generate smaller subproblems, easier to solve than the original problem, is probably one of the oldest approaches in a matheuristic design. One of the first methods which employs this principle is a convergent algorithm for pure 0-1 integer programming proposed in [298]. It solves a series of small subproblems generated by exploiting information obtained by exactly solving a series of linear programming (LP) relaxations. Several enhanced versions of this algorithm have been proposed (see [154, 326]). In [268, 269], methods of this type are also referred to as *core methods*. Usually, an LP relaxation of the original problem is used to guide the fixation process. In general, exploiting the pieces of information contained in the solution of the LP relaxation can be a very powerful tool for tackling MP problems. In [57, 271], the solutions of the LP relaxation and its dual were used to conduct the mutation and recombination process in hybrid genetic algorithms for the multi-constrained knapsack problem. Local search based metaheuristics proved to be very effective when combined with exact optimisation techniques, since it is usually convenient to search the neighbourhoods by means of some exact algorithm. Large neighbourhood search (LNS) introduced in [294], very large-scale neighbourhood search in [10], or dynasearch [64] are some well-known matheuristic examples of this type. In [155, 156], the dual relaxation solution is used within VNS in order to systematically tighten the bounds during the solution process. The resulting primal-dual variable neighbourhood search methods were successful in solving the simple plant location problem [155] and large p-median clustering problems [156]. With the rapid development of the commercial MP solvers, the use of a generic ready-made MP solver as a black-box search component is becoming increasingly popular. Some existing neighbourhood search type matheuristics which exploit generic MIP solvers for neighbourhood search are local branching (LB) [104] and VNS branching [169]. Another popular approach in matheuristics development is improving the performance of the branch-and-bound (B&B) algorithm by means of some metaheuristic methods. The genetic algorithm was successfully incorporated within a B&B search in [198] for example. Guided dives and relaxation induced neighbourhood search (RINS), proposed in [75], explore some neighbourhood of the incumbent integer solution in order to choose the next node to be processed in the B&B tree. In [124], an adaptive memory projection (AMP) method for pure and mixed integer programming was proposed, which combines the principle of projection techniques with the adaptive memory processes of tabu search to set some explicit or implicit variables to some particular values. This philosophy can be used for unifying and extending a number of other procedures: LNS [294], local branching [104], the relaxation induced neighbourhood search [75], VNS branching [169], or the global tabu search intensification using dynamic programming (**TS-DP**) [327]. For more details on matheuristic methods the reader is referred to [40, 219, 266, 268].

1.2 The 0-1 Mixed Integer Programming Problem

The *linear programming* (LP) problem consists of minimising or maximising a linear function, subject to some equality or inequality linear constraints.

$$(1.5) \qquad (\mathrm{LP}) \quad \left[\begin{array}{lll} \min \sum_{j=1}^{n} c_j x_j & & \\ \text{s.t.} \quad \sum_{j=1}^{n} a_{ij} x_j \geq b_i & & i = 1..m \\ \qquad x_j \geq 0 & & j = 1..n \end{array} \right.$$

Obviously, the LP problem (1.5) is a special case of an optimisation problem (1.1) and, more specifically, of a mathematical programming problem, where all functions $g_i : \mathbb{R}^n \to \mathbb{R}$, $i \in \{1, 2, \ldots, m\}$, from (1.2) are linear. When all variables in the LP problem (1.5) are required to be integer, the resulting optimisation problem is called a *(pure) integer linear programming* problem. If only some of the variables are required to be integer, the resulting problem is called a *mixed* *integer linear programming* problem, or simply a *mixed integer programming* problem. In further text, any linear programming problem in which the set of integer variables is non-empty will be referred to as a mixed integer programming (MIP) problem. Furthermore, if some of the variables in a MIP problem are required to be binary (i.e. either 0 or 1), the resulting problem is called a 0-1 MIP problem. In general, a 0-1 MIP problem can be expressed as:

$$(1.6) \qquad (0-1\text{ MIP}) \quad \left[\begin{array}{ll} \min \sum_{j=1}^{n} c_j x_j & \\ \text{s.t.} \quad \sum_{j=1}^{n} a_{ij} x_j \geq b_i & \forall i \in M = \{1, 2, \ldots, m\} \\ \qquad x_j \in \{0,1\} & \forall j \in \mathcal{B} \neq \emptyset \\ \qquad x_j \in \mathbb{Z}_0^+ & \forall j \in \mathcal{G}, \mathcal{G} \cap \mathcal{B} = \emptyset \\ \qquad x_j \geq 0 & \forall j \in \mathcal{C}, \mathcal{C} \cap \mathcal{G} = \emptyset, \mathcal{C} \cap \mathcal{B} = \emptyset \end{array}\right.$$

where the set of indices $N = \{1, 2, \ldots, n\}$ of variables is partitioned into three subsets $\mathcal{B}, \mathcal{G}$ and $\mathcal{C}$ of binary, general integer and continuous variables, respectively, and $\mathbb{Z}_0^+ = \{x \in \mathbb{Z} \mid x \geq 0\}$. If the set of general integer variables in a 0-1 MIP problem is empty, the resulting 0-1 MIP problem is referred to as a *pure* 0-1 MIP. Furthermore, if all variables in a pure 0-1 MIP are required to be integer, the resulting problem is called *pure 0-1 integer programming* problem.

If P is a given 0-1 MIP problem, a *linear programming relaxation* LP(P) of problem P is obtained by dropping all integer requirements on the variables from P:

$$(1.7) \qquad \text{LP}(0-1\text{ MIP}) \quad \left[\begin{array}{ll} \min \sum_{j=1}^{n} c_j x_j & \\ \text{s.t.} \quad \sum_{j=1}^{n} a_{ij} x_j \geq b_i & \forall i \in M = \{1, 2, \ldots, m\} \\ \qquad x_j \in [0,1] & \forall j \in \mathcal{B} \neq \emptyset \\ \qquad x_j \geq 0 & \forall j \in \mathcal{C} \cup \mathcal{G} \end{array}\right.$$

The theory of linear programming as a maximisation/minimisation of a linear function subject to some linear constraints was first conceived in the 1940s. At that time, mathematicians George Dantzig and George Stigler were independently working on different problems, both nowadays known to be the problems of linear programming. George Dantzig was engaged with the different planning, scheduling and logistical supply problems for the USA Air Force. As a result, in 1947 he formulated the planning problem with the linear objective function subject to satisfying a system of linear equalities/inequalities, thus formalising the concept of a linear programming problem. He also proposed the simplex solution method for the linear programming problems [76]. Note that the term "programming" is not related to computer programming, as one could assume, but rather to the planning of military operations (deployment, logistics, etc.), as used in military terminology. At the same time, George Stigler was working on the problem of the minimal cost of subsistence. He formulated a diet problem — achieving the minimal subsistence cost by fulfilling a number of nutritional requirements — as a linear programming problem [299]. For more details on the historical development of linear programming, the reader is referred to [79, 290].

Numerous combinatorial optimisation problems, including a wide range of practical problems in business, engineering and science can be modelled as 0-1 MIP problems (see [331]). Several special cases of the 0-1 MIP problem, such as knapsack, set packing, network design, protein alignment, travelling salesman and some other routing problems, are known to be NP-hard [115]. Complexity results prove that the computational resources required to optimally solve some 0-1 MIP problem instances can grow exponentially with the size of the problem instance. Over several decades many contributions have led to successive improvements in exact methods such as branch-and-bound, cutting planes, branch-and-cut, branch-and-price, dynamic programming, Lagrangian relaxation and linear programming. For a more detailed review on exact MIP solution methods, the reader is referred to [223, 331], for example. However, many MIP problems still cannot be solved within acceptable time and/or space limits by the best current exact methods. As a consequence, metaheuristics have attracted attention as possible alternatives or supplements to the more classical approaches.

Branch-and-Bound. *Branch-and-bound* (B&B) (see, for instance, [118, 204, 236, 331]) is probably the most commonly used solution technique for MIPs. The basic idea of B&B is the "divide and conquer" philosophy. The original problem is divided into smaller subproblems (also called *candidate problems*), which are again divided into even smaller subproblems and so on, as long as the obtained subproblems are not easy enough to be solved.

More formally, if the original MIP problem P is given in the form $\min_{x \in X} c^{\mathrm{T}} x$ (i.e. the feasible region of P is the set X), then the following candidate problems are created: $P_i = \min_{x \in X_i} c^{\mathrm{T}} x, i = 1, 2, \ldots, k,\ X_i \subseteq X, \forall i \in \{1, 2, \ldots, k\}$. Ideally, the feasible sets of the candidate problems should be collectively exhaustive: $\bigcup_{i=1}^{k} X_i = X$, so that the optimal solution of P is the optimal solution of at least one of the subproblems $P_i,\ i \in \{1, 2, \ldots, k\}$. Also, it is desirable that the feasible sets of the candidate problems are mutually exclusive, i.e. $X_i \cap X_j = \emptyset$, for $i \neq j$, so that no area of solution space is explored more than once. Note that the original problem P is a relaxation of the candidate problems $P_1, P_2, \ldots, P_k$.

In a B&B solution process, a candidate problem is selected from the *candidate list* (the current list of candidate problems of interest) and, depending on its properties, the problem considered is either removed from the candidate list, or used as a parent problem to create new candidate problems to be added to the list. The process of removing a candidate problem from the candidate list is called *fathoming*. Normally, candidate problems are not solved directly, but some relaxations of candidate problems are solved instead. The relaxation to be used should be selected in such a way that it is easy to solve and *tight*. A relaxation of an optimisation problem P is said to be tight, if its optimal value is very close (or equal) to the optimal value of P. Most often, the LP relaxation is used for this purpose [203]. However, the use of other relaxations is also possible. Apart from the LP relaxation, a so called *Lagrangian relaxation* [171, 172, 223] is probably most widely used.

Let P_i be the current candidate problem considered and x^* the incumbent best solution of P found so far. The optimal value $\nu(\mathrm{LP}(P_i))$ of the LP relaxation $\mathrm{LP}(P_i)$ is a lower bound of the optimal value $\nu(P_i)$ of P_i. The following possibilities can be distinguished:

Case 1 There are no feasible solutions for the relaxed problem $\mathrm{LP}(P_i)$. This means that the problem P_i itself is infeasible and does not need to be considered further. Hence, P_i can be removed from the candidate list.

Case 2 The solution of $\mathrm{LP}(P_i)$ is feasible for P. If $\nu(\mathrm{LP}(P_i))$ is less then the incumbent best value $z_{UB} = c^{\mathrm{T}} x^*$, the solution of $\mathrm{LP}(P_i)$ becomes the new incumbent x^*. The candidate problem P_i can be dropped from further consideration and removed from the candidate list.

Case 3 The optimal value $\nu(\mathrm{LP}(P_i)$ of $\mathrm{LP}(P_i)$ is greater than the incumbent best value $z_{UB} = c^{\mathrm{T}} x^*$. Since $\nu(\mathrm{LP}(P_i)) \leq \nu(P_i)$, this means that also $\nu(P_i) > c^{\mathrm{T}} x^*$ and P_i can be removed from the candidate list.

Case 4 The optimal value $\nu(\mathrm{LP}(P_i))$ of $\mathrm{LP}(P_i)$ is less than the incumbent best value $z_{UB} = c^{\mathrm{T}} x^*$, but the solution of $\mathrm{LP}(P_i)$ is not feasible for P. In this case, there is a possibility that the optimal solution of P_i is better than x^*, so the problem P_i needs to be further considered. Thus, P_i is added to the candidate list.

The difference between the optimal value $\nu(P)$ of a given MIP problem P and the optimal value $\nu(\mathrm{LP}(P))$ of its LP relaxation $\mathrm{LP}(P)$ is called the *integrality gap*. An important issue for the performance of B&B is the candidate problems selection strategy. In practice, the efficiency of a B&B method is greatly influenced by the integrality gap values of the candidate problems. A large integrality gap may lead to a very large candidate list, causing B&B to be very computationally expensive. A common candidate problem selection strategy is to choose the problem with the smallest optimal value of the LP relaxation.

The steps of the B&B method for a given MIP problem P can be presented as below:

1) Initialisation. Set the incumbent best upper bound z_{UB} to infinity: $z_{UB} = +\infty$. Solve the LP relaxation LP(P) of P. If LP(P) is infeasible, then P is infeasible as well. If the solution $\overline{x}$ of LP(P) is feasible for P, return $\overline{x}$ as an optimal solution of P. Otherwise, add LP(P) to the list of candidate problems and go to **2**.

2) Problem selection. Select a candidate problem $P_{candidate}$ from the list of candidate problems and go to **3**.

3) Branching. The current candidate problem $P_{candidate}$ has at least one fractional variable x_i, with $i \in \mathcal{B} \cup \mathcal{G}$.

a) Select a fractional variable $x_i = n_i + f_i$, $i \in \mathcal{B} \cup \mathcal{G}$, $n_i \in \mathbb{Z}$, $f_i \in (0, 1)$, for the purpose of branching.

b) Create two new candidate problems $(P \mid x_i \geq n_i + 1)$ and $(P \mid x_i \leq n_i)$ (recall (1.3)).

c) For each of the two new candidate problems created, solve the LP relaxation of the problem and update the candidate list according to cases 1-4 above.

4) Optimality test. Remove from the candidate list all candidate problems P_j with $\nu(\text{LP}(P_j)) \geq z_{UB}$. If the candidate list is empty, then the original input problem is either infeasible (in case $z_{UB} = +\infty$) or has the optimal solution z_{UB}, and algorithm stops. Otherwise, go to **2**.

Different variants of B&B can be obtained by choosing different strategies for candidate problem selection (step 2 in the above algorithm), the branching variable selection (step 3a)) and creating more then two candidate problems in each branching step. For more details on some advanced B&B developments, the reader is referred to [223, 331], for example. From the purely theoretical point of view, B&B will always find an optimal solution, if one exists. However, in practice, available computational resources will not allow B&B to find an optimum within a reasonable time/space. This is why alternative MIP solution methods are sought.

Cutting Planes. The use of cutting planes for MIP was first proposed by Gomory in the late 1950s [140, 141]. The basic idea of the cutting planes method for a given MIP problem P is to add constraints to the problem during the search process, and thus produce relaxations which are tighter than the standard LP relaxation LP(P). In other words, the added constraints should discard those areas of the feasible region of the LP relaxation LP(P), which do not contain any points with imposed integrality constraints in the original MIP problem P.

More formally, if $X = \{x \in \mathbb{R}^n \mid x_j \in \{0, 1\}, j \in \mathcal{B}, x_j \in \mathbb{N} \cup \{0\}, j \in \mathcal{G}, x_j \geq 0, j \in \mathcal{C}\}$ is the feasible region of a MIP problem P, where $\mathcal{B} \cup \mathcal{G} \neq \emptyset, \mathcal{B} \cup \mathcal{G} \cup \mathcal{C} = \{1, 2, \ldots, n\}$, then the convex hull of X is defined by:

$$\text{conv}(X) = \{\lambda_1 x_1 + \lambda_2 x_2 + \ldots + \lambda_n x_n \mid \sum_{i=1}^{n} \lambda_i = 1, \lambda_i \geq 0 \text{ for all } i \in \{1, 2, \ldots, n\}\} \tag{1.8}$$

and the feasible region of LP(P) is defined by

$$\overline{X} = \{x \in \mathbb{R}^n \mid x_j \in [0, 1], j \in \mathcal{B}, x_j \geq 0, j \in \mathcal{G} \cup \mathcal{C}, \mathcal{B} \cup \mathcal{G} \neq \emptyset\}. \tag{1.9}$$

The idea is to add a constraint/set of constraints C to the problem P, so that the feasible region X' of the problem $(P \mid C)$ is between $\text{conv}(X)$ and $\overline{X}$ [223], i.e.: $\text{conv}(X) \subseteq X' \subseteq \overline{X}$.

Definition 1.1 *Let $X \subseteq \mathbb{R}^n$, $n \in \mathbb{N}$. A* valid inequality *of X is an inequality $(\alpha)^{\mathrm{T}}x \leq \beta$, such that $(\alpha)^{\mathrm{T}}x \leq \beta$ holds for all $x \in X$. A valid inequality is also called a* cutting plane *or a* cut*.*

According to the *mixed integer finite basis theorem* (see [223], for example), if X is the feasible region of a MIP problem, then the convex hull $\text{conv}(X)$ of X is a *polyhedron*, i.e. can be represented in the form $\text{conv}(X) = \{x \in \mathbb{R}^n \mid (\alpha^i)^{\mathrm{T}}x \leq \beta_i, i = 1, 2, \ldots, q, \alpha^i \in \mathbb{R}^n, \beta_i \in \mathbb{R}\}$. Cutting planes added to the original MIP problem during the search process should ideally form the subset of the system of inequalities $(\alpha^i)^{\mathrm{T}}x \leq \beta_i, i = 1, 2, \ldots, q$ which define $\text{conv}(X)$.

Given a system of equalities $\sum_{j=1}^{n} a_{ij}x_j = b_i$, $i = 1, 2, \ldots, m$, an *aggregate constraint*

$$\sum_{j=1}^{n}\left(\sum_{i=1}^{m} u_i a_{ij}\right) x_j = \sum_{i=1}^{m} u_i b_i \tag{1.10}$$

can be generated by multiplying the original system of equalities by each of the given multipliers u_i, $i = 1, 2, \ldots, m$ and summing up the resulting systems of equalities. In a MIP case, all the variables are required to be nonnegative, so a valid cut is obtained by rounding the aggregate constraint (1.10):

$$\sum_{j=1}^{n}\left\lfloor\left(\sum_{i=1}^{m} u_i a_{ij}\right)\right\rfloor x_j \leq \sum_{i=1}^{m} u_i b_i \tag{1.11}$$

In a pure integer case, when all variables in the original MIP problem are required to be integer, the right-hand side of the cut (1.11) can be further rounded down, yielding:

$$\sum_{j=1}^{n}\left\lfloor\left(\sum_{i=1}^{m} u_i a_{ij}\right)\right\rfloor x_j \leq \left\lfloor\sum_{i=1}^{m} u_i b_i\right\rfloor. \tag{1.12}$$

The cutting plane (1.12) is called a *Chávatal-Gomory* (C-G) cut [223]. In a pure integer case, the C-G cut is normally generated starting from the solution $\overline{x}$ of the LP relaxation LP(P) of the original MIP problem P. For more theory on C-G cuts and the procedures for deriving C-G cuts, the reader is referred to [52, 140, 141].

At the time when it was proposed, the cutting plane method was not effective enough. The main drawbacks were a significant increase in the number of non-zero coefficients and roundoff problems with the cuts used, resulting in a very slow convergence. In addition, an extension to a mixed integer case (when not all of the variables are required to be integer) is not straightforward, since the inequality (1.11) does not imply the inequality (1.12) if some of the variables x_j, $j = 1, 2, \ldots, n$ are allowed to be continuous. For these reasons, the cutting plane methods were not popular for a long time after they were first introduced. They regained popularity in the 1980s, when the development of the polyhedral theory led to the design of more efficient cutting planes [73]. Additional resources on the cutting planes theory can be found in [223, 331], for example. It appears that the use of cutting planes is particularly effective when combined with the B&B method, which is discussed in the next subsection.

Branch-and-Cut. The *branch-and-cut* method (B&C) combines the B&B and cutting planes MIP solution methods, with the aim to bring together the advantages of both (see, for instance, [223]). Indeed, it seems promising to first tighten the problem by adding cuts and thus reduce the amount of enumeration to be performed by B&B. Furthermore, adding cuts before performing the branching can be very effective in reducing the integrality gap [73]. The basic steps of the B&C method for a given MIP problem P can be represented as below:

1) Initialisation. Set the incumbent best upper bound z_{UB} to infinity: $z_{UB} = +\infty$. Set the lower bound z_{LB} to infinity: $z_{LB} = -\infty$. Initialise the list of candidate problems: $L = \emptyset$.

2) LP relaxation. Solve the LP relaxation LP(P) of P. If LP(P) is infeasible or $\nu(\text{LP}(P)) > z_{UB}$, then go to step **4**. Update the lower bound $z_{LB} = \min\{z_{LB}, \nu(\text{LP}(P))\}$. If the solution $\overline{x}$ of LP(P) is feasible for P, return $\overline{x}$ as an optimal solution of P. Otherwise, replace the last added problem in L with LP(P) (or simply add LP(P) to L if $L = \emptyset$) and go to **3**.

3) Add cuts. Add cuts to P and go to step **2**.

4) Problem selection. If $L = \emptyset$ go to **6**. Otherwise, select a candidate problem $P_{candidate} \in L$ and go to **5**.

5) Branching. The current candidate problem $P_{candidate}$ has at least one fractional variable x_i, with $i \in \mathcal{B} \cup \mathcal{G}$. Select a variable x_i for the branching purposes, and branch on x_i as in *B&B*. Go to step **6**.

6) Optimality test. Remove from the candidate list all candidate problems P_j with $\nu(\text{LP}(P_j)) \geq z_{UB}$. If the candidate list is emptied, then the original input problem is either infeasible (in case $z_{UB} = +\infty$) or has the optimal solution z_{UB}, and algorithm stops. Otherwise, go to **4**.

The above algorithm is a simple variant of B&C, in which cutting planes are only added before the initial branching is performed, i.e. only at the root node of a B&B tree. In more sophisticated variants of B&C, cutting planes are added at each node of the B&B tree, i.e. to each of the candidate problems produced in step **5)** above. In that case, it is important that each cut added at a certain node of a B&B tree is also valid at all other nodes of that B&B tree. Also, if cutting planes are added at more than one node of a B&B tree, the value of the lower bound z_{LB} is used to update the candidate list in the branching step (step **5)** in the algorithm above).

B&C is nowadays a standard component in almost all generic MIP solvers. It is often used in conjunction with various heuristics for determining the initial upper bound at each node. For more details on the theory and performance of B&C, the reader is referred to, for example, [17, 67, 91, 142, 223].

Branch-and-Price. In the *column generation* approach (see, for example [85]), a small subset of variables is selected and the corresponding restricted LP relaxation is solved. The term "column generation" comes from the fact that selected variables actually represent columns in matrix notation of the original MIP problem. Then variables which are not yet included are evaluated in order to include those which lead to the best improvement of the current solution. This subproblem is called a *pricing problem*. After adding a new variable, the process is iterated until there are no more variables to add. The column generation approach can be viewed as a dual approach to cutting planes, because the variables in the primal LP problem correspond to the inequalities in the dual LP problem. *Branch-and-price* method is obtained if column generation is performed at each node of the branch-and-bound tree.

Heuristics for 0-1 Mixed Integer Programming. Although exact methods can successfully solve to optimality problems with small dimensions (see, for instance, [298]), for large-scale problems they cannot find an optimal solution with reasonable computational effort, hence the need to find near-optimal solutions.

The 0-1 MIP solution space is especially convenient for the local search based exploration. Some successful applications of tabu search for 0-1 MIPs can be found in [213, 147], for example. An application of simulated annealing for a special case of 0-1 MIP problem was proposed in [195]. A number of other approaches for tackling MIPs has been proposed over the years. Examples of pivoting heuristics, which are specifically designed to detect MIP feasible solutions, can be found in [19, 20, 94, 214]. For more details about heuristics for 0-1 MIP feasibility, including more recent approaches such as feasibility pump [103], the reader is referred to Chapter 6. Some other local search approaches for 0-1 MIPs can be found in [18, 129, 130, 176, 182, 212]. More recently, some hybridisatons with general-purpose MIP solvers have arisen, where either local search methods are integrated as node heuristics in the B&B tree within a solver [32, 75, 120], or high-level heuristics employ a MIP solver as a black-box local search tool [103, 105, 106, 104, 169]. For more details on local search in the 0-1 MIP solution space, the reader is referred to Chapter 2.

Population based heuristics can also be successfully employed for tackling the 0-1 MIP problem. Scatter search [132, 133] for 0-1 MIPs was proposed in [134]. Some applications of genetic algorithms include [39, 194, 216, 225]. In [284], an evolutionary algorithm was integrated within a B&B search tree. Some other interesting applications of evolutionary algorithms for mixed integer programming can be found in [55, 335].

1.3 Clustering

Clustering is a process of partitioning a given set of objects into a number of different categories/groups/subsets, which are referred to as *clusters*. The partitioning should be done in such a way that objects belonging to the same cluster are similar (according to some predefined criteria), whereas objects which are not in the same cluster should be different (the criteria for measuring the level of difference does not necessarily need to be the same as the criteria for measuring the level of similarity). For detailed listings of possible similarity and dissimilarity measures, the reader is referred to [157, 333].

The two most commonly studied types of clustering are *hierarchical* clustering and *partitional* clustering. Consider a set $E = \{x_1, \ldots, x_N\}$, $x_j = (x_{1j}, \ldots, x_{qj})$, of N entities (or points) in Euclidean space $\mathbb{R}^q$. Then the task of partitional clustering is to find a partition $P_M = \{C_1, C_2, \ldots, C_M\}$ of E into M clusters, such that:

- $C_j \neq \emptyset$, $j = 1, 2, \ldots, M$
- $C_i \cap C_j = \emptyset$, $i, j = 1, 2, \ldots, M$, $i \neq j$
- $\bigcup_{i=1}^{M} C_i = E$.

Conversely, the task of hierarchical clustering is to find a hierarchy $H = \{P_1, P_2, \ldots, P_r\}$, $r \leq N$, of partitions $P_1, P_2, \ldots, P_r$ of E, such that $C_i \in P_k$, $C_j \in P_\ell$ and $k > \ell$ imply $C_i \subset C_j$ or $C_i \cap C_j = \emptyset$, for all $k, \ell = 1, 2, \ldots, r$ and $i \neq j$. There is a number of possible intermediate clustering problems between these two extremes [157]. Hierarchical clustering methods are further classified as either *agglomerative* or *divisive*. Agglomerative methods begin with N clusters, each containing exactly one object, and merge them successively, until the final hierarchy is reached. Divisive methods start from a single cluster, consisting of all the data, and perform a sequence of dividing operations as long as the final hierarchy is not reached.

General surveys of clustering techniques can be found in [30, 100, 333], for example. A mathematical programming approach to clustering was studied in [157]. Combinatorial optimisation concepts in clustering are comprehensively reviewed in [231].

1.4 Thesis Overview

In this thesis, novel variable neighbourhood search [237] based heuristics for 0-1 mixed integer programming problems and clustering are presented. The major part of the reported research is dedicated to the development of matheuristics for 0-1 mixed integer programming problems, based on the variable neighbourhood search metaheuristic framework. Neighbourhood structures are implicitly defined and updated according to the set of parameters acquired from the mathematical formulation of the input problem. However, the purpose of this thesis is beyond the design of specific heuristics for specific problems. Some new variants of the VNS metaheuristic itself are also proposed, as well as a new unifying view on modern developments in metaheuristics. The subsequent chapters of this thesis are organised as follows.

In Chapter 2, an overview of the local search based metaheuristic methods (also known as *explorative* metaheuristics) is provided. Most theoretical and practical aspects of neighbourhood search are covered, from the simplest local search to the highly modern techniques, involving large-scale neighbourhood search, reactive approaches and formulation space search. The concept of local search for 0-1 mixed integer programming is explained and three existing state-of-the-art local search-based MIP heuristics are described. Apart from outlining the existing concepts and components of neighbourhood search in combinatorial optimisation, the aim of Chapter 2 is also to point out the possible future trends in the developments of explorative methods. A new unifying perspective on modern advances in metaheuristics is proposed, called *hyper-reactive* optimisation.

Chapter 3 is based on [158] and deals with the colour image quantisation problem, as a special case of a clustering problem. Colour image quantisation is a data compression technique that reduces the total set of colours in a digital image to a representative subset. This problem is first expressed as a large M-Median one. The advantages of this model over the usual minimum sum-of-squares model are discussed first and then some heuristics based on the VNS metaheuristic are applied to solve it. Computational experience proves that this approach compares favourably with two other recent state-of-the-art heuristics, based on genetic and particle swarm searches. Whereas Chapter 3 is mainly concerned with applications of existing variable neighbourhood search schemes, the subsequent chapters are devoted to the development of a new sophisticated solution methodology for 0-1 mixed integer programming.

In Chapter 4, a new matheuristic for solving 0-1 MIP problems (0-1 MIPs) is proposed, based on [206, 207], which follows the principle of variable neighbourhood decomposition search [168] (VNDS for short). It performs systematic hard variable fixing (or diving) according to the rules of VNDS, by exploiting the information obtained from the linear programming relaxation of the original problem. The general-purpose CPLEX MIP solver is used as a black-box for solving subproblems generated in this way. Extensive analysis of the computational results is performed, including the use of some non-parametric statistical tests, in order to compare the proposed method with other recent algorithms recommended in the literature and with the general-purpose CPLEX MIP solver itself as an exact method. With this approach, the best known published results were improved for 8 out of 29 instances from a well-known class of very difficult 0-1 MIP problems. Moreover, experimental results show that the proposed method outperforms the CPLEX MIP solver and all other recent most successful MIP solution methods which were used for comparison purposes.

Chapter 5 is devoted to applications of the VNDS matheuristic from Chapter 4 to some specific 0-1 MIPs, as in [80, 149, 150, 151, 152, 208]. Three different problems are considered: the multidimensional knapsack problem (MKP), the problem of barge container ships routing and two-stage stochastic mixed integer programming problem (2SSP). Some improved versions of VNDS matheuristic are proposed. Improved heuristics are constructed by adding new constraints (so called pseudo-cuts) to the problem during the search process, in order to produce a sequence of not only upper (lower in case of maximisation), but also lower (upper in case of maximisation) bounds, so that the integrality gap is reduced. Different heuristics are obtained depending on the relaxations used and the number and the type of constraints added during the search process. For the MKP, we also propose the use of a second level of decomposition in VNDS. The MKP is tackled by decomposing the problem in several subproblems, where the number of items to choose is fixed at a given integer value. For each of the three problems considered, exhaustive computational study proves that the proposed approach is comparable with the current state-of-the-art heuristics and the exact CPLEX MIP solver on a corresponding representative benchmark, with outstanding performance on some of the instances. In case of MKP, a few new lower bound values were obtained. In case of mixed integer 2SSP, VNDS based heuristic performed much better than CPLEX applied to a deterministic equivalent for the hardest instances which contain hundreds of thousands of binary variables in the deterministic equivalent.

All methods presented in Chapters 4 and 5 are improvement methods, i.e. require an initial feasible solution to start from and iteratively improve it until the fulfilment of the stopping criteria. However, finding a feasible solution of a 0-1 MIP problem is proven to be NP-complete [331] and for a number of instances it remains a hard problem in practice. This calls for the development of efficient constructive heuristics which can attain feasible solutions in a short time (or any reasonable time for very hard instances). In Chapter 6 two new heuristics for 0-1 MIP problems are proposed, based on [148, 205]. The first heuristic, called variable neighbourhood pump (VNP), combines ideas of variable neighbourhood branching [169] for 0-1 MIPs and a well-known feasibility pump [103] heuristic for constructing initial solutions for 0-1 MIPs. The second proposed heuristic is a modification of the VNDS based heuristic from Chapter 4. It relies on the observation that a general-purpose MIP solver can be used not only for finding (near) optimal solutions of a given input problem, but also for finding an initial feasible solution. The two proposed heuristics were tested on an established set of 83 benchmark problems (proven to be difficult to solve to feasibility) and compared with the IBM ILOG CPLEX 11.1 MIP solver (which already includes standard feasibility pump as a primal heuristic). A thorough performance analysis shows that both methods significantly outperform the CPLEX MIP solver.

Finally, in Chapter 7, the results and contributions of the thesis are summarised. Concluding remarks are provided, together with a perspective on possible future innovations and developments in the field of metaheuristics for combinatorial optimisation problems and matheuristics in particular.

Chapter 2

Local Search Methodologies in Discrete Optimisation

As mentioned in Chapter 1, one possible classification of heuristic methods distinguishes between *constructive* methods and *local search* methods. Whereas constructive methods build up a single solution step by step, using the information from the problem structure, local search methods start from a given feasible solution and gradually improve it in an iterative process, until a local optimum is reached. The local search approach can be seen as the basic principle underlying a number of optimisation techniques. Its appeal stems from the wide applicability and low empirical complexity in most cases [189]. Moreover, with the rapid development of metaheuristics which manipulate different local search procedures as subordinate low-level search components, the significance of a local search concept became even more evident.

This chapter focuses on the algorithmic aspects of local search and high-level metaheuristic methods which employ local search as low-level search components. In Section 2.1, the basic local search framework is explained in detail, with its variants and drawbacks. Some of the most important local search based metaheuristics are described in Section 2.2. As the research reported in this thesis is mainly based on variable neighbourhood search, this metaheuristic is thoroughly discussed in Section 2.3, where some new variable neighbourhood search schemes are also proposed. The concept of local search in the area of 0-1 mixed integer programming is discussed in Section 2.4. In Section 2.5, a unifying view on local search-based metaheuristics is proposed, along with a possible future trend in their further development.

2.1 Basic Local Search

A *local search* algorithm for solving a combinatorial optimisation problem (1.1) starts from a given initial solution and iteratively replaces the current best solution with its *neighbouring solution* which has a better objective function value, until no further improvement in the objective value can be made [2]. The concept of a *neighbourhood structure* is formally introduced in definition 2.1.

Definition 2.1 *Let P be a given optimisation problem. A* neighbourhood structure *for problem P is a function $\mathcal{N} : S \to \mathcal{P}(S)$, which maps each solution $x \in S$ from the solution space S of P into a* neighbourhood *$\mathcal{N}(x) \subseteq S$ of x. A* neighbour *(or a* neighbouring solution*) of a solution $x \in S$ is any solution $y \in \mathcal{N}(x)$ from the neighbourhood of x.*

The concept of *locally* optimal solutions naturally arises from the definition of neighbourhood structures.

Definition 2.2 *Let $\mathcal{N}$ be a neighbourhood structure for a given optimisation problem P as defined by (1.1). A feasible solution $x \in X$ of P is a* locally optimal *solution (or a* local optimum*) with respect to $\mathcal{N}$, if $f(x) \leq f(y)$, $\forall y \in \mathcal{N}(x) \cap X$.*

A local optimum for a maximisation problem is defined in an analogous way. A local optimum for a minimisation/maximisation problem is also called *local minimum/local maximum*.

When defining a neighbourhood structure for a given optimisation problem P, it is desirable to satisfy the following conditions:

- the neighbourhood of each solution should be *symmetric*, i.e. the following condition should hold: $(\forall x \in S)\, y \in \mathcal{N}(x) \Leftrightarrow x \in \mathcal{N}(y)$
- for any two solutions $x, y \in S$, there should exist a sequence of solutions $x_1, x_2, \ldots, x_n \in S$, such that $x_1 \in \mathcal{N}(x)$, $x_2 \in \mathcal{N}(x_1)$,$\ldots$, $x_n \in \mathcal{N}(x_{n-1}), y \in \mathcal{N}(x_n)$
- for a given solution $x \in S$, generating neighbours $y \in \mathcal{N}(x)$ should be of a polynomial complexity
- the size of a neighbourhood should be carefully determined: a neighbourhood should not be too large so that it can be easily explored, but also not too small so that it contains neighbours with a better objective function value.

The pseudo-code of the basic local search algorithm is provided in Figure 2.1. Input parameters for the basic local search are a given optimisation problem P and an initial feasible solution $x \in S$ of P. The algorithm returns the best solution found by iterative improvement.

```
Procedure LocalSearch($P, x$)
1  Select a neighbourhood structure $\mathcal{N} : S \to \mathcal{P}(S)$;
2  repeat
3      $x' = $ Improvement($P, x, \mathcal{N}(x)$);
4      if ($f(x') < f(x)$) then
5          $x = x'$;
6      endif
7  until ($f(x') \geq f(x)$);
8  return $x$;
```

Figure 2.1: Basic local search.

The procedure Improvement($P, x, \mathcal{N}(x)$) attempts to find a better solution within the neighbourhood $\mathcal{N}(x)$ of the current solution x. This procedure can be either a best improvement procedure or a first improvement procedure. The pseudo-code of the best improvement procedure is given in Figure 2.2. It completely explores the neighbourhood $\mathcal{N}(x)$ and returns the solution with the best (lowest in case of minimisation) value of the objective function. The pseudo-code of the first improvement procedure is given in Figure 2.3. In case of a first improvement, solutions $x_i \in \mathcal{N}(x)$ are enumerated systematically and a *move* (i.e. the change of the current solution: $x = x'$) is made as soon as a better solution is encountered.

```
Procedure BestImprovement($P, x, \mathcal{N}(x)$)
1   $x' = \text{argmin}_{y \in \mathcal{N}(x) \cap X} f(y)$;
2   return $x'$;
```

Figure 2.2: Best improvement procedure.

By applying the best improvement procedure, local search obviously ends in a local optimum, which is not necessarily the case with the first improvement. However, exploring the neighbourhoods completely can often be time-consuming. As a result, the first improvement can sometimes be a better choice in practice. Furthermore, when a local search method is used within a higher level metaheuristic framework, a first improvement variant can even lead to better results quality-wise. Alternatively, one can opt for a neighbourhood exploration strategy which is between the first and the best improvement. It is possible to generate a sample of neighbours (either randomly or by means of some learning strategy) and choose the best neighbour from the observed sample, rather than the best one in the whole neighbourhood [22]. For a detailed study on the use of best improvement vs. first improvement within a local search algorithm, the reader is referred to [165].

```
Procedure FirstImprovement($P, x, \mathcal{N}(x)$)
1   repeat
2       $x' = x$; $i = 0$;
3       repeat
4           $i = i + 1$;
5           $x' = \text{argmin}\{f(x), f(x_i)\}$, $x_i \in \mathcal{N}(x) \cap X$;
6       until ($f(x) < f(x_i)$ || $i == |\mathcal{N}(x) \cap X|$);
7   until ($f(x) \geq f(x')$);
8   return $x'$;
```

Figure 2.3: First improvement procedure.

In the local search procedure with the best improvement strategy, a move is only made to a neighbour with the lowest objective function value. Therefore, this variant of local search is also known as *steepest descent* (or *hill climbing* in case of a maximisation problem). More generally, in any variant of a classical local search, a move is only allowed to a neighbour with a lower objective function value. Consequently, once a local optimum is reached, further improvement cannot be achieved by moving to a neighbouring solution and the search process stops without being able to detect the global optimum. This phenomenon is illustrated in Figure 2.4. In order to overcome this major drawback of basic local search, a number of metaheuristic frameworks which include mechanisms for escaping from local optima during the search process has been developed. The most important metaheuristics of this type are described in the subsequent sections of this chapter.

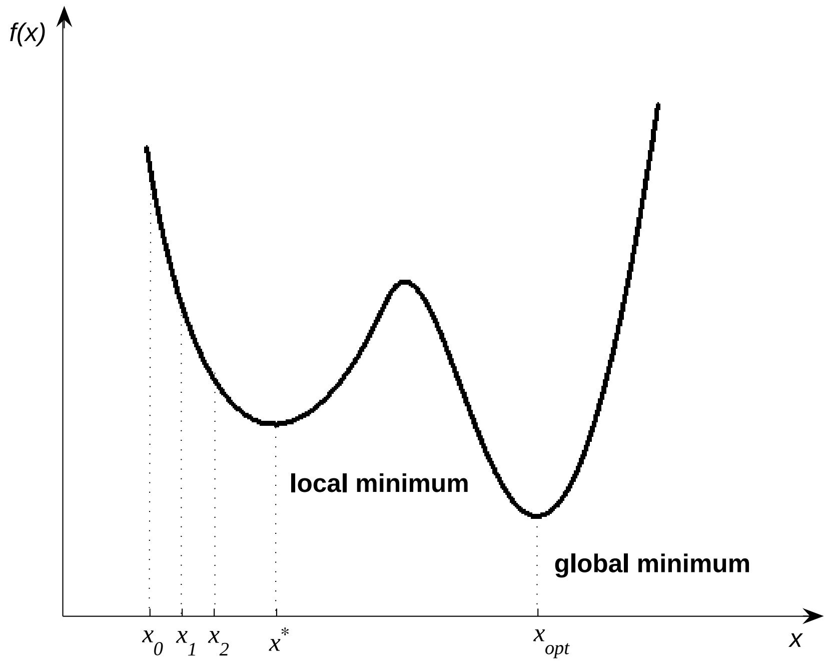


Figure 2.4: Local search: stalling in a local optimum.

2.2 A Brief Overview of Local Search Based Metaheuristics

In this section some of the most important local search based metaheuristics are presented: simulated annealing (in Subsection 2.2.1), tabu search (in Subsection 2.2.2), greedy randomised adaptive search (in Subsection 2.2.3), guided local search (in Subsection 2.2.4) and iterated local search (in Subsection 2.2.5). As the research reported in this thesis is mainly based on variable neighbourhood search, this metaheuristic is thoroughly discussed in the next section, where some new variable neighbourhood search schemes are also proposed.

2.2.1 Simulated Annealing

Simulated annealing (SA) is a metaheuristic which combines the principles of the basic local search and the probabilistic Monte Carlo approach [143]. It is one of the oldest metaheuristic methods, originally proposed in [196] and [50]. In each iteration of SA, a neighbour of the current solution is generated at random and a move is made to this neighbouring solution depending on its objective function value and the Metropolis criterion. If the selected neighbour has a better objective function value than the current solution, it is automatically accepted and becomes the new current solution. Otherwise, the new solution is accepted according to the Metropolis criterion, i.e. with a certain probability, which is systematically updated during the search process. The acceptance of worse solutions provides the mechanism for avoiding the stalling in the local optima.

The motivation for the SA approach in combinatorial optimisation comes from the Metropolis algorithm in static thermodynamics [228]. The original Metropolis algorithm was used to simulate the process of a solid material annealing: increasing the temperature of the material until it is melted and then progressively reducing the temperature to recover a solid state of a lower energy. The appropriate cooling strategy is crucial for the success of the annealing process. If the cooling is done too fast, it can cause irregularities in the material structure, which normally results in a high energy state. On the other hand, when cooling is done systematically, through a number of levels so that the temperature is held long enough at each level to reach equilibrium, the more regular structures with low-energy states are obtained. In the context of combinatorial optimisation, a solution of the problem corresponds to a state of the material, objective function value corresponds to its energy, and a move to a neighbouring solution corresponds to the change of the energy state. The general SA pseudo-code is provided in Figure 2.5.

```
Procedure SA($P$)
 1  Choose initial solution $x$;
 2  Select a neighbourhood structure $\mathcal{N} : S \to \mathcal{P}(S)$;
 3  Set $n = 0$; Set $proceed$ = true;
 4  while ($proceed$) do
 5      Choose $x' \in \mathcal{N}(x)$ at random;
 6      if ($f(x') < f(x)$) then
 7          $x = x'$;
 8      else
 9          Choose $p \in [0, 1]$ at random;
10          if ($p < \exp((f(x) - f(x'))/t_n)$) then
11              $x = x'$;
12          endif
13      endif
14      $n = n + 1$;
15      Update $proceed$;
16  endwhile
17  return $x$;
```

Figure 2.5: Simulated annealing.

The initial solution (line 1 in pseudo-code from Figure 2.5) is normally generated at random or by means of some constructive heuristic (possibly problem-specific). Stopping criteria for the algorithm are represented by the variable *proceed* (initialised in line 3 of SA pseudo-code). Most often, the stopping criteria include the maximum running time allowed, the maximum number of iterations, or the maximum number of iterations without improvements. Variable p represents the probability of acceptance and is determined in analogy to the physical annealing of solids, where a state change occurs with probability $e^{-\Delta E/kt}$, ΔE being the change in energy, t the current temperature, and k the Boltzmann constant. In the SA algorithm, the values of a so-called "temperature" parameter are defined by a sequence of positive numbers (t_n), such that $t_0 \geq t_1 \geq \ldots$ and $\lim_{n \leftarrow \infty} t_n = 0$. The sequence (t_n) is called a *cooling schedule*. The temperature parameter is used to control the diversification during the search process. Large temperature values in the beginning result in almost certain acceptance, therefore sampling the search space and avoiding the local optima traps. Conversely, small temperature values near the end of the search result in a very intensified exploration, rejecting almost all non-improving solutions. The most common cooling schedule is a geometric sequence, where $t_n = \alpha t_{n-1}$, for $0 < \alpha < 1$. This cooling schedule corresponds to an exponential decrease of the temperature values. A more robust algorithm can be obtained if the temperature is changed only after each L iterations, where $L \in \mathbb{N}$ is a predefined parameter (usually determined according to the empirical experience) as in Figure 2.6. In that case, $t_n = \alpha^k t_0$, for $kL \leq n < (k+1)L$, $k \in \mathbb{N} \cup \{0\}$.

Over the years, more advanced SA schemes have been developed (see, for instance, [1, 3,

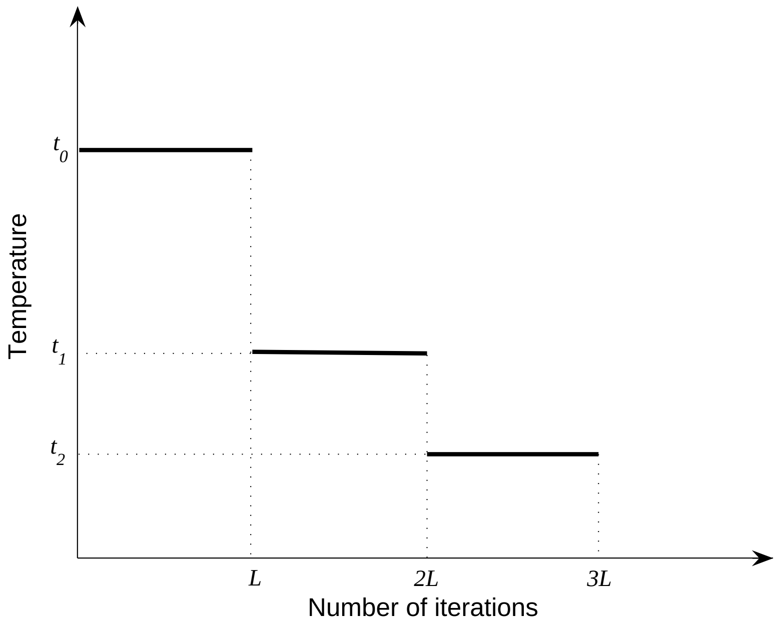


Figure 2.6: Geometric cooling scheme for Simulated annealing.

4, 173, 251]). Some of them include more general forms of acceptance than the Metropolis one, different forms of static and dynamic cooling schedules, or hybridisations with other metaheuristics (genetic algorithms or neural networks, for example). In [90], a deterministic variant of SA is proposed, where a move is made whenever the objective function value is not decreased more than a certain predefined value. There is also a number of parallel implementations of SA (for instance, [56, 226, 313]). Fixing different parts of the solution during the search process, due to frequent occurrences in previously generated solutions, was proposed in [51].

2.2.2 Tabu Search

Tabu search (TS) is another widespread metaheuristic framework, with a mechanism for avoiding the stalling in poor local optima. The basic method was proposed in [122]. As opposed to SA, the mechanism for escaping local optima is of a deterministic nature, rather than of a stochastic one.

The essential component of a TS algorithm is a so called *adaptive memory*, which contains information about the search history. In the most basic version of TS, only a *short term memory* is used, which is implemented as a so called *tabu list*. Tabu list contains the most recently visited solutions and is used to ensure that those solutions are not revisited. In each iteration, the neighbourhood of the current solution is explored (completely or partially) and a move is made to the best found solution not belonging to the tabu list. In addition, the tabu list is updated according to the first-in-first-out principle, so that the current solution is added to the list and the oldest solution in the list is removed from it. The fact that a move is made regardless of the objective function value (allowing the acceptance of a worse solution) provides the mechanism for escaping from local optima. The best known solution during the whole search is memorised separately.

Clearly, the crucial parameter which controls the extent of the diversification and intensification is the length of the tabu list. If the tabu list is short, the search concentrates on small areas of the solution space. Conversely, a long tabu list forbids a larger number of solutions and thus ensures the exploration of larger regions. In a more advanced framework, the length of the tabu list can be varied during the search, resulting in a more robust algorithm.

An implementation of the tabu list which keeps complete solutions is often inefficient. It is obviously space consuming, but also requires a long time for browsing the list. This drawback is usually overcome by storing only a set of preselected *solution attributes* instead of a complete solution. However, storing only a set of attributes may result in a loss of information, since the prohibition of a single attribute usually forces more than one solution to be added to the tabu list. This way, unvisited solutions of a good quality may be excluded from the further search. The most common solution to this problem is to introduce the set of so called *aspiration criteria*, so that a move to a solution in the tabu list is permitted whenever the solution satisfies some aspiration criterion. The simplest example of an aspiration criterion is the one which permits solutions better than the currently best known solution. This criterion is defined by $f(x) < f(x^*)$ for a given solution x, where x^* is the currently best solution. The basic form of the tabu search algorithm is provided in Figure 2.7, where P is an input optimisation problem as defined by (1.1).

```
Procedure TS($P$)
 1  Choose initial solution $x$;
 2  Memorise best solution so far: $x^* = x$;
 3  Select a neighbourhood structure $\mathcal{N} : S \to \mathcal{P}(S)$;
 4  Initialise tabu list $TL$;
 5  Initialise the set of aspiration criteria $AC$;
 6  Set $proceed$ = true;
 7  while ($proceed$) do
 8      Choose the best
            $x' \in \mathcal{N}(x) \cap \{x \in X \mid x \notin TL$ or $x$ satisfies at least one criterion from $AC\}$;
 9      $x = x'$;
10      if ($f(x) < f(x^*)$) then $x^* = x$; endif;
11      Update $TL$; Update $AC$;
12      Update $proceed$;
13  endwhile
14  return $x^*$;
```

Figure 2.7: Tabu search.

A variety of extensions and enhancements of the basic TS scheme has been proposed since it was first originated in 1986. One of the most significant and widespread improvements is the use of a *long term memory* [131]. Normally, the long term memory is based on (some of) the following four principles: recency, frequency, quality and influence [37]. Recency-based memory keeps track of the most recent relevant iteration for each solution. Frequency-based memory stores the number of times each solution was visited. The quality-based memory records the information about the good solutions/solution attributes visited during the search process. Lastly, influence-based memory keeps track of critical choices made during the search and is normally exploited to indicate the choices of interest. By using a long term memory, a much better control over the processes of diversification and intensification can be achieved than by means of a short term memory. Diversification is enforced by generating solutions with combinations of attributes significantly different from those previously encountered. On the other hand, intensification is propagated by incorporating the attributes of good-quality solutions (so called *elite* solutions) stored in the memory. Another interesting approach is the integration of TS and path relinking [131, 132], where new solutions are created by exploring the paths between elite solutions. In probabilistic TS [131], candidate solutions are selected at random from an appropriate neighbourhood, rather than deterministically as in the classical TS. This speeds up the neighbourhood exploration and at the same time increases the level of diversification. An especially interesting class of advanced TS algorithms are so called *reactive* techniques, which provide a mechanism for a dynamic adjustment of parameters during the search process [23, 227, 323]. In this context, the parameter of the greatest interest is usually the length of the tabu list. Finally, numerous hybridisations of TS with other metaheuristics have been developed. There are known hybrids with genetic algorithms [126], memetic algorithms [217], ant colony optimisation [15], etc. (the stated references are only few possible examples).

2.2.3 Greedy Randomised Adaptive Search

Greedy randomised adaptive search (GRASP) is a multi-start (i.e. iterative) algorithm, where a new solution is generated in a two-stage process at each restart (iteration), and the best overall solution is returned as a result. The two-stage process involves construction as the first phase and local search improvement as the second phase. The basic algorithm was proposed in [102], followed by enhanced versions in [260, 280].

The pseudo-code of the basic GRASP algorithm is provided in Figure 2.8. In the construction stage (lines 6–12), a new solution is constructed progressively, by adding one new component in each iteration. First, all candidate elements for the next component of the current solution x are evaluated (line 7 of the pseudo-code from Figure 2.8). The evaluation is performed according to a candidate's contribution to the objective function value, if inserted into the current partial solution x. Then, a so called *restricted candidate list* (RCL) is formed, so that it contains the best α component candidates (lines 8–9 of the pseudo-code from Figure 2.8). The next solution component x_k is chosen at random from the so obtained restricted candidate list, and added to the current partial solution. This process is iterated as long as the current solution x is not complete. The construction stage is essentially a greedy randomised procedure: it considers the best α candidates (a greedy approach) and employs randomization to select one of them. Obviously, the RCL length α is the crucial parameter for the algorithm, since it controls the level of randomization and therefore the level of diversification during the search process. If $\alpha = 1$, the best element is added, so the construction is equivalent to a deterministic greedy heuristic. Conversely, when $\alpha = n$, the construction is entirely random. The second stage of the algorithm consists of a local search procedure, with the constructed solution x as an initial solution (line 13 of the pseudo-code from Figure 2.8). This local search procedure may be the basic LS algorithm from Section 2.1, or a more advanced technique, such as simulated annealing, tabu search, variable neighbourhood search, etc. The two stages of GRASP are iterated as long as the stopping criteria, represented by the variable *proceed*, are not fulfilled.

The main drawback of the basic GRASP algorithm is that the solution processes in different restarts are completely independent, and the information from previous restarts is not available at a certain point of search. A number of GRASP enhancements have been developed which addresses this issue. The use of a long term memory within GRASP was proposed in [107]. Another possibility to incorporate memory within the GRASP search process is a reactive approach, in which the parameter α is selected from a set of values depending on the solution values from the previous restarts [13, 263, 264]. A variety of other enhancements of GRASP has also been designed. The employment of path relinking as an intensification strategy within GRASP was proposed in [200]. Some examples of parallel implementations, where the restarts are distributed over multiple

```
Procedure GRASP($P$)
 1  Select a neighbourhood structure $\mathcal{N} : S \to \mathcal{P}(S)$;
 2  Set $n$ to the number of solution components;
 3  Set $proceed$ = true;
 4  while ($proceed$) do
 5      $x = \emptyset$;
 6      for ($k = 1;\ k <= n;\ k + +$) do
 7          Evaluate the candidate components;
 8          Determine the length $\alpha$ of the restricted candidate list;
 9          Build the restricted candidate list $RCL_\alpha$ for $x$;
10          Select $x_k \in RCL_\alpha$ at random;
11          $x = x \cup \{x_k\}$;
12      endfor
13      $x'$ = LocalSearch($P, x$);
14      if (($x^*$ not yet assigned) || ($f(x') < f(x^*)$)) then
15          $x^* = x'$;
16      endif;
17      Update $proceed$;
18  endwhile
19  return $x^*$;
```

Figure 2.8: Greedy randomised adaptive search.

processors, can be found in [244, 256, 257]. Due to its simplicity, the GRASP algorithm is usually very fast and produces reasonable-quality solutions in a short time. Therefore, it is especially convenient for integration with other metaheuristics. A hybridisation with variable neighbourhood search [224] can be distinguished as one interesting example.

2.2.4 Guided Local Search

All metaheuristics discussed so far provide a mechanism for escaping from local optima through an intelligent construction of search trajectories for a fixed problem structure. In contrast, *guided local search* (GLS) metaheuristic guides the search away from local optima by changing the objective function of the problem, i.e. modifying the search landscape itself [318, 319]. The GLS strategy exploits so called *solution features* to discriminate between solutions and thus appropriately augment the objective function value in order to reposition the local optima. The general scheme is illustrated in Figure 2.9.

The pseudo-code of the basic GLS framework is provided in Figure 2.10. After the initial solution and the neighbourhood structure are selected (lines 1–2 in Figure 2.10), the vector of *penalties* $\mathbf{p} = (p_1, p_2, \ldots, p_k)$ is initialised, where k is the number of solution features considered (line 3 in Figure 2.10). Penalties represent the feature weights: the higher the penalty value p_i, the higher the importance of feature i. Stopping criteria are defined by the variable *proceed* (line 4 in Figure 2.10). In each iteration of the algorithm, the objective function is increased with respect to the current penalty values (line 6 in Figure 2.10), according to the formula:

$$f'(x) = f(x) + \lambda \sum_{i=1}^{k} p_i I_i(x). \tag{2.1}$$

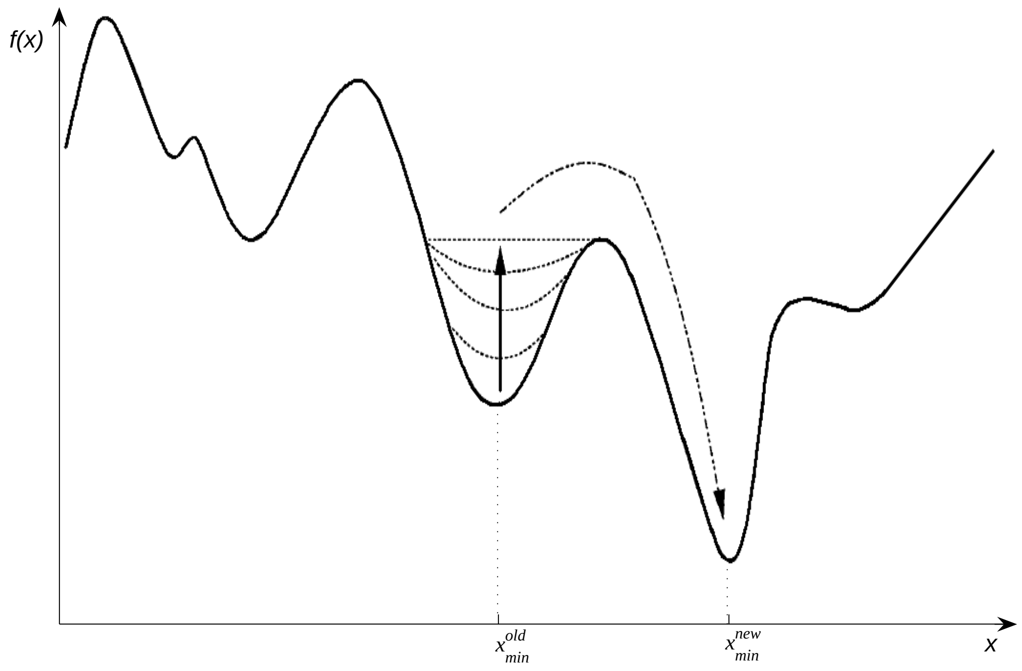


Figure 2.9: GLS: escaping from local minimum by increasing the objective function value.

Function $I_i(x)$ indicates whether the ith feature is present in the current solution x:

$$I_i(x) = \begin{cases} 1 & \text{if the } i\text{th feature is present in } x, \\ 0 & \text{otherwise.} \end{cases} \tag{2.2}$$

Parameter λ, also known as *regularisation parameter*, adjusts the overall weight given to the penalties with respect to the original objective function. The input problem P is then modified so that the original objective function f is replaced with the new objective function f' as in (2.1) (see line 7 in Figure 2.10). A local search based algorithm is applied to the so modified problem P', starting from the current solution x as an initial solution (line 8 in Figure 2.10), and the current solution is updated if necessary (line 9). Finally, the values of penalties are updated (line 10) and the whole process is reiterated as long as the stopping criteria are not fulfilled.

```
Procedure GLS($P$)
 1  Choose an initial feasible solution $x$;
 2  Select a neighbourhood structure $\mathcal{N} : S \to \mathcal{P}(S)$;
 3  Initialise vector of penalties $\mathbf{p}$;
 4  Set $proceed$ = true;
 5  while ($proceed$) do
 6      Determine the modified objective function $f'$ from $f$ and $\mathbf{p}$;
 7      Let $P'$ be the problem $\min_{x \in X} f'(x)$;
 8      $x'$ = LocalSearch($P', x$);
 9      if ($f'(x') < f'(x)$) then $x = x'$; endif;
10      Update $\mathbf{p}$;
11      Update $proceed$;
12  endwhile
13  return $x$;
```

Figure 2.10: Guided local search.

Normally, the penalties are updated according to the following incrementing rule: the penalties p_i of all features with the maximum *utility* value $I_i(x) \cdot \frac{c_i}{1+p_i}$ are increased by 1, where c_i is the *cost* of the ith feature. The cost of a feature represents the measure of importance of that feature (usually heuristically determined). The higher the cost of a feature, the higher the utility of penalising it. The goal is to penalise "bad" features, which are most often involved in local optima.

Some interesting developments of GLS include the applications for Travelling salesman problem [318], SAT problem [229], Quadratic assignment problem [230], three-dimensional bin-packing problem [101], vehicle routing problem [193, 337], capacitated arc-routing problem [34], team orienteering problem [309] and many others.

2.2.5 Iterated Local Search

Iterated local search (ILS) generates new solutions in the search space by iterating the following two operators: a local search operator to reach local optima and a perturbation operator to escape from bad local optima. Although the term "iterated local search" was proposed in [215], the concept of ILS was first introduced in [188]. A similar search strategy was also independently proposed in [45], where it was named *fixed neighbourhood search*. The formal description of the ILS pseudo-code is provided in Figure 2.11.

The key components of the ILS algorithm are listed below:

- a local search operator
- a perturbation operator

```
Procedure ILS($P$)
 1  Choose initial solution $x$;
 2  Initialise the best solution to date $x^* =$ LocalSearch($P, x$);
 3  Set $proceed =$ true;
 4  while ($proceed$) do
 5      Select a neighbourhood structure $\mathcal{N} : S \to \mathcal{P}(S)$;
 6      $x =$ Perturb($\mathcal{N}(x^*), history$);
 7      $x' =$ LocalSearch($P, x$);
 8      $x^* =$ AcceptanceCriterion($x^*, x', history$);
 9      Update $proceed$;
10  endwhile
11  return $x^*$;
```

Figure 2.11: Iterated local search.

- search history implemented as short/long term memory
- acceptance criterion.

A local search operator is used to locate the closest local optimum and thus to refine the current solution. Since the ILS algorithm itself provides a mechanism for escaping from local optima, a basic local search scheme (as described in Section 2.1) is quite effective, as it is faster than more elaborate metaheuristic schemes, such as SA or TS. A perturbation operator performs a change of a number of solution components, in order to generate a solution far enough[1] from the current local optimum. In the original work about ILS [215], it was emphasised that the method does not explicitly use any neighbourhood structures (apart from the one associated with the local search operator). However, it can be observed that the perturbation itself implies a selection of a neighbourhood structure (the number of components to change) and a selection of an appropriate solution within the selected neighbourhood (new component values). For this reason, the neighbourhood structure was explicitly incorporated in the ILS pseudo-code description in Figure 2.11. The implementation of a perturbation operator is crucial for the overall efficiency of the ILS algorithm. The smaller the size of the neighbourhood, the more likely that a stalling in local optima will occur. On the other hand, if the neighbourhood is too large, the sampling of the solution space is too randomised and the overall procedure behaves like a random restart (see Subsection 2.2.3). The size of the neighbourhood may be fixed for the entire search process, or may be adapted during the run (either in each iteration, or after a certain number of iterations). Note, however, that in each iteration only a single neighbourhood is considered. A more sophisticated search technique can be obtained if a number of neighbourhoods of different sizes is considered in each iteration, so that the levels of intensification and diversification are appropriately balanced (see Section 2.3 about variable neighbourhood search). The concept of perturbation operator was successfully exploited in [285] for location problems and in [146] for the 0-1 multidimensional knapsack problem.

The effectiveness of the algorithm can be further increased if the search history is used to select the next neighbourhood and/or the candidate solution within a neighbourhood, possibly in a similar way as in tabu search. For a more detailed discussion on possibilities to employ the search history into a metaheuristic framework, the reader is referred to Subsection 2.2.2 about TS. More importantly for ILS, the search history can be used within the acceptance operator in order to decide whether the current solution should be updated.

[1]In terms of some predefined distance function.

The acceptance criterion has a great impact on the behaviour of the ILS search process. In particular, the balance between the diversification and intensification largely depends on the acceptance rule. For instance, the criterion which accepts the new local optimum only if it is better than the currently best solution, obviously favours the intensification. Conversely, always accepting the new local optimum, regardless of the objective function value, leads to an extremely diversified search. One possible intermediate choice between these two extremes is the use of an SA-type acceptance criterion: accepting the new local optimum if it is better than the currently best one and otherwise applying the Metropolis criterion (see Subsection 2.2.1). Another interesting possibility is to use a non-monotonic cooling schedule within the SA-type criterion explained above, together with the search history: instead of constantly decreasing the temperature, it is increased when more diversification is required.

Some of the interesting developments and applications of the ILS algorithm can be found in [181, 300, 303, 304].

2.3 Variable Neighbourhood Search

All local search based metaheuristics discussed so far deal only with a single neighbourhood structure in each iteration, which may or may not be updated from one iteration to another. However, the selection of the neighbourhood structure is essential for the effectiveness of the search process, as was already mentioned in Subsection 2.2.5. Therefore, the solution process can be significantly improved if more than one neighbourhood of the currently observed solution is explored and thus a few new candidate solutions are generated in each iteration. This is the basic idea of the variable neighbourhood search metaheuristic [159, 161, 162, 164, 166, 167, 237].

Variable neighbourhood search (VNS) was first proposed in 1997 (see [237]) and has led to many developments and applications since. The idea for a systematic change of neighbourhoods, performed by VNS, is based on the following facts (see [167]):

Fact 1 A local optimum with respect to one neighbourhood structure is not necessarily a local optimum with respect to another neighbourhood structure.

Fact 2 A global optimum is a local optimum with respect to any neighbourhood structure.

Fact 3 Local optima with respect to one or several neighbourhood structures are relatively close to each other.

The last fact relies on the empirical experience: extensive experimental analysis for a huge variety of different problems suggests that local optima frequently contain some information about the global optimum. For example, it appears that some variables usually have the same values in both local and global optima.

VNS has a number of specific variants, depending on the selection of neighbourhood structures, neighbourhood change scheme, selection of candidate solutions within a neighbourhood, updating the incumbent solution, etc. In the remainder of this section, the most significant variants of VNS are described in detail. Subsection 2.3.1 is devoted to the well-established VNS schemes. Subsection 2.3.2 aims to provide an insight into more elaborate solution methodologies, with some notable contributions to the metaheuristics development in general. Some new VNS schemes are also proposed.

2.3.1 Basic Schemes

Variable neighbourhood search deals with a set of more than one neighbourhood structures at each iteration, rather than with a single neighbourhood structure (see Figure 2.12). Furthermore, in a nested VNS framework, where some VNS scheme is used as a local search operator within another VNS scheme, different sets of neighbourhood structures may be used for the two schemes. In further text, $\{\mathcal{N}_k : S \to \mathcal{P}(S) \mid 1 \leq k_{min} \leq k \leq k_{max}\}$, $k_{min}, k_{max} \in \mathbb{N}$, will denote the set of preselected neighbourhood structures for the main VNS scheme of interest.

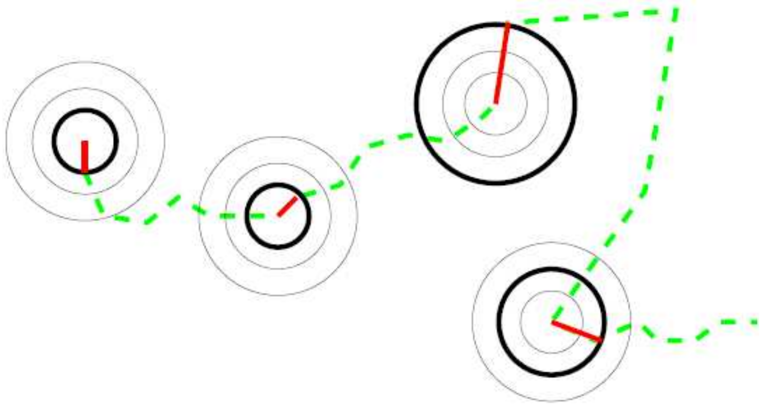


Figure 2.12: The change of the used neighbourhood in some typical VNS solution trajectory.

Usually, neighbourhood structures $\mathcal{N}_k, 1 \leq k_{min} \leq k \leq k_{max}$ are induced by one or more metric (or quasi-metric[2]) functions of the form $\rho : S^2 \to \mathbb{R}^+$, defined in the solution space S:

$$\mathcal{N}_k(x) = \{y \in X \mid \rho(x, y) \ \leq \ k\}. \tag{2.3}$$

Definition (2.3) implies that the neighbourhoods are nested, i.e. $\mathcal{N}_k(x) \subset \mathcal{N}_{k+1}(x)$, for any $x \in S$ and appropriate value of k. There are, however, other possibilities to define distance-induced neighbourhood structures. If the solution space S is discrete, condition $\rho(x, y) \ \leq \ k$ in definition (2.3) can be replaced with $\rho(x, y) \ = \ k$. If the solution space S is continuous, condition $\rho(x, y) \ \leq \ k$ is commonly replaced with $k - 1 \leq \rho(x, y) \ < \ k$. The choice of neighbourhood structures depends on the problem of interest and the final requirement (whether the most important issue for the end user is the execution time, solution quality, etc.). In a more advanced environment, the neighbourhood structures to be used can even be changed from one iteration to another.

In order to solve problem (1.1) by exploring several neighbourhoods in each iteration, facts 1 to 3 can be combined in three different ways to balance between diversification and intensification: (i) deterministic; (ii) stochastic; (iii) both deterministic and stochastic. The resulting VNS variants are described in the subsequent subsections.

Variable Neighbourhood Descent

Variable neighbourhood descent (VND) is obtained if all neighbourhoods generated during the search are explored completely [159]. The VND pseudo-code is provided in Figure 2.13, with procedure `BestImprovement`$(P, x, \mathcal{N}_k(x))$ as in Figure 2.2 in Section 2.1. The input parameters for the VND algorithm are an optimisation problem P as defined in (1.1), the initial solution x and the maximum number k_{vnd} of neighbourhoods (of a single solution) to explore. The best solution found is returned as the result.

[2]Where the symmetry requirement is dropped.

```
Procedure VND($P, x, k_{vnd}$)
1   Select a set of neighbourhood structures $\mathcal{N}_k : S \to \mathcal{P}(S)$, $1 \le k \le k_{vnd}$;
2   Set $stop$ = false;
3   repeat
4       Set $k = 1$;
5       repeat
6           $x'$ = BestImprovement($P, x, \mathcal{N}_k(x)$);
7           if ($f(x') < f(x)$) then
8               $x = x'$, $k = 1$; // Make a move.
9           else $k = k + 1$; // Next neighbourhood.
10          endif
11          Update $stop$;
12      until ($k == k_{vnd}$ or $stop$);
13  until ($f(x') \ge f(x)$ or $stop$);
14  return $x$.
```

Figure 2.13: VND pseudo-code.

If no additional stopping criteria are imposed (variable *stop* is set to `false` throughout the search process), k_{vnd} neighbourhoods of the current solution are explored in each iteration, thus generating the k_{vnd} candidate solutions, among which the best one is chosen as the next incumbent solution. The process is iterated until no improvement is reached. Since performing such an exhaustive search can be too time consuming, additional stopping criteria are usually imposed, such as maximum running time or the maximum number of outer loop iterations. The final solution should be a local minimum with respect to all k_{vnd} neighbourhoods. This is why the chances to reach the global minimum are greater with VND than with a basic local search with a single neighbourhood structure. However, because the complete neighbourhood exploration requires a lot of computational time, the diversification process is rather slow, whereas intensification is enforced. Therefore, VND is normally used as a local search operator within some other metaheuristic framework. In case that the other metaheuristic framework is the basic VNS variant, the General VNS scheme is obtained. Some interesting applications of VND can be found in [53, 113, 174, 248]. Note that the principle of VND is similar to the multi-level composite heuristic proposed in [286], where level k corresponds to the kth neighbourhood in VND.

Reduced Variable Neighbourhood Search

Reduced variable neighbourhood search (RVNS) is a variant of VNS in which new candidate solutions are chosen at random from appropriate neighbourhoods, without any attempt to improve them by means of some local search operator [159]. The RVNS pseudo-code is provided in Figure 2.14. The input parameters for the RVNS algorithm are an optimisation problem P as defined in (1.1), the initial solution x, the minimum neighbourhood size k_{min}, the neighbourhood size increase step k_{step} and the maximum neighbourhood size k_{max}. The best solution found is returned as the result. In order to reduce the number of parameters, k_{step} is usually set to the same value as k_{min}. In addition, k_{min} is commonly set to 1. The stopping criteria, represented by the variable *stop*, are usually chosen as the maximum running time and/or the maximum number of iterations between two improvements.

```
Procedure RVNS($P, x, k_{min}, k_{step}, k_{max}$)
1   Select a set of neighbourhood structures $\mathcal{N}_k : S \to \mathcal{P}(S)$, $k_{min} \le k \le k_{max}$;
2   Set $stop$ = false;
3   repeat
4       Set $k = k_{min}$;
5       repeat
6           Select $x' \in \mathcal{N}_k(x)$ at random; //Shaking.
7           if $(f(x') < f(x))$ then
8               $x = x'$, $k = k_{min}$; // Make a move.
9           else $k = k + k_{step}$; // Next neighbourhood.
10          endif
11          Update $stop$;
12      until ($k \ge k_{max}$ or $stop$);
13  until ($stop$);
14  return $x$.
```

Figure 2.14: RVNS pseudo-code.

As opposed to VND, which enforces intensification, RVNS obviously enforces diversification, as new candidate solutions are obtained in an entirely stochastic way. Therefore, RVNS is useful for very large instances, when applying local descent has a high computational cost. Some successful applications of RVNS are described in [160, 238, 278, 293].

Basic Variable Neighbourhood Search

The *Basic variable neighbourhood search* (BVNS) [237] aims to provide a balance between the intensification and diversification. Recall that VND completely explores the current neighbourhood, thus requiring a large amount of computational effort, whereas RVNS only chooses the next candidate solution from an appropriate neighbourhood at random, thus completely discarding the solution quality. BVNS chooses the next candidate solution from an appropriate neighbourhood by first selecting an element from the neighbourhood at random and then applying some local search technique in order to improve the selected solution. The resulting solution is then taken as the next candidate solution from the observed neighbourhood. This way, the complete exploration of neighbourhood is avoided, while still providing a reasonable-quality solution. This idea is illustrated in Figure 2.15.

The steps of BVNS are provided in Figure 2.16 (the meaning of all parameters is the same as for previously described VNS variants). The `Improvement` operator is usually chosen as the `FirstImprovement` operator, described in Section 2.1 (see Figure 2.3). However, the `BestImprovement` (Figure 2.2) can also be applied, as well as some intermediate improvement operator between the two extremes. For example, it is possible to explore only a subset of an observed neighbourhood and choose the best candidate solution from that subset.

General Variable Neighbourhood Search

If variable neighbourhood descent is used as an improvement (i.e. local search) operator within the basic VNS (see line 7 in Figure 2.16), a so called *General variable neighbourhood search* (GVNS) scheme is obtained. The GVNS pseudo-code is given in Figure 2.17. An additional input parameter

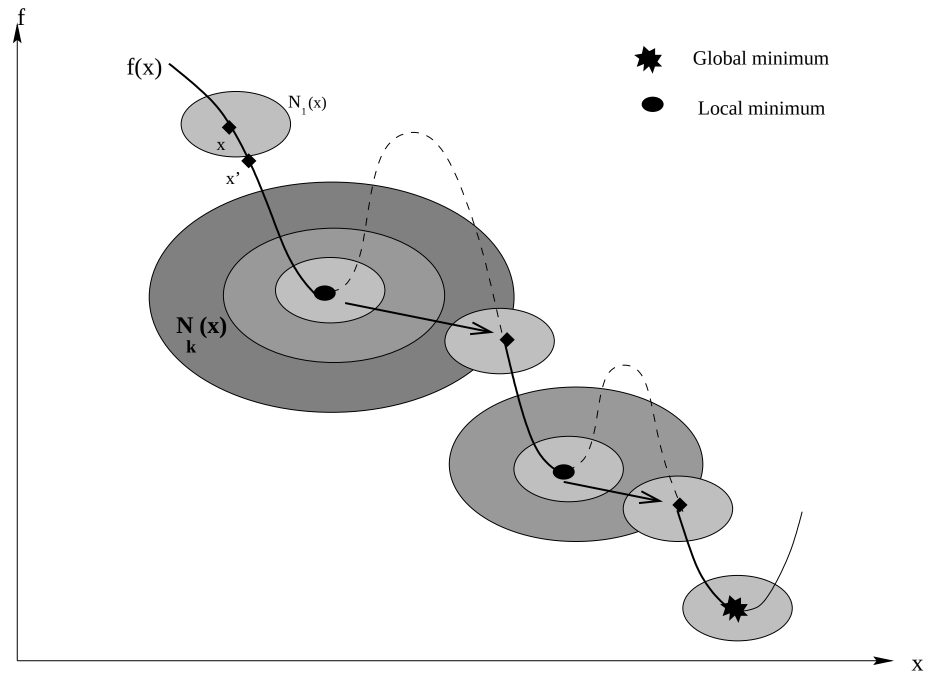


Figure 2.15: The basic VNS scheme.

```
Procedure BVNS($P, x, k_{min}, k_{step}, k_{max}$)
 1   Select a set of neighbourhood structures $\mathcal{N}_k : S \to \mathcal{P}(S)$, $k_{min} \leq k \leq k_{max}$;
 2   Set $stop$ = false;
 3   **repeat**
 4       Set $k = k_{min}$;
 5       **repeat**
 6           Select $x' \in \mathcal{N}_k(x)$ at random; //Shaking.
 7           $x''$ = Improvement($P, x', \mathcal{N}_k(x)$);
 8           **if** ($f(x'') < f(x)$) **then**
 9               $x = x''$, $k = k_{min}$; // Make a move.
10           **else** $k = k + k_{step}$; // Next neighbourhood.
11           **endif**
12           Update $stop$;
13       **until** ($k \geq k_{max}$ **or** $stop$);
14   **until** ($stop$);
15   **return** $x$.
```

Figure 2.16: The Basic VNS pseudo-code.

for the GVNS procedure is the maximum neighbourhood size k_{vnd} within the VND procedure (see line 7 in Figure 2.16). The GVNS scheme appears to be particularly successful. Few representative application examples can be found in [14, 45, 49, 160, 169, 283].

```
Procedure GVNS($P, x, k_{min}, k_{step}, k_{max}, k_{vnd}$)
 1   Select a set of neighbourhood structures $\mathcal{N}_k : S \to \mathcal{P}(S)$, $k_{min} \leq k \leq k_{max}$;
 2   Set $stop$ = false;
 3   repeat
 4       Set $k = k_{min}$;
 5       repeat
 6           Select $x' \in \mathcal{N}_k(x)$ at random; //Shaking.
 7           $x''$ = VND($P, x', k_{vnd}$);
 8           if ($f(x'') < f(x)$) then
 9               $x = x''$, $k = k_{min}$; // Make a move.
10           else $k = k + k_{step}$; // Next neighbourhood.
11           endif
12           Update $stop$;
13       until ($k \geq k_{max}$ or $stop$);
14   until ($stop$);
15   return $x$.
```

Figure 2.17: General VNS.

Skewed Variable Neighbourhood Search

The *Skewed variable neighbourhood search* (SVNS) introduces a more flexible acceptance criterion in order to successfully explore large valleys in the search landscape [163]. In case that an observed local optimum is a local optimum for large area of the solution space (i.e. in the case of a large valley), it would be necessary to explore large neighbourhoods of the incumbent solution in order to escape from that optimum, by using the standard acceptance criterion. However, a systematic exploration of a number of preceding smaller neighbourhoods usually requires a significant amount of computational time, so reaching the global optimum is likely to be very time consuming. Even for problems where the exploration of neighbourhoods is fast enough, successive jumps to large neighbourhoods would result in a random restart-like behaviour.

In order to avoid the stalling in large valleys, SVNS allows the moves to solutions worse than the incumbent solution. Note that the diversification in some other metaheuristics, such as SA or TS, is based on the same underlying idea. A distance function $\rho : S^2 \leftarrow \mathbb{R}^+$ is employed to measure the distance between the local optimum found x'' and the incumbent solution x. The function ρ may or may not be the same as the distance function $\delta : S^2 \leftarrow \mathbb{R}^+$ used to define neighbourhood structures $\mathcal{N}_k$. A move from x to x'' is then made if $f(x'') - f(x) < \alpha\delta(x'', x)$, where $\alpha \in \mathbb{R}^+$ is a parameter which controls the level of diversification. It must be large enough in order to accept the exploration of valleys far away from x when $f(x'')$ is larger than $f(x)$, but not too large (otherwise one will always leave x). The best value for α is determined either empirically or through some learning process. The acceptance criterion for SVNS can be viewed as as an example of *threshold accepting*, which was introduced in [90] and extensively exploited in many heuristics and metaheuristics thereafter. The pseudo-code of the SVNS scheme is provided in Figure 2.18.

Few interesting applications of SVNS can be found in [46, 81].

Variable Neighbourhood Decomposition Search

Variable neighbourhood decomposition search (VNDS) is a two-level VNS scheme for solving opti-

```
Procedure SVNS($P, x, k_{min}, k_{step}, k_{max}, k_{vnd}$)
1   Select a set of neighbourhood structures $\mathcal{N}_k : S \to \mathcal{P}(S)$, $k_{min} \leq k \leq k_{max}$;
2   Set $stop$ = false;
3   repeat
4       Set $k = k_{min}$;
5       repeat
6           Select $x' \in \mathcal{N}_k(x)$ at random; //Shaking.
7           $x''$ = VND($P, x', k_{vnd}$);
8           if $(f(x'') - f(x) < \alpha\delta(x'', x))$ then
9               $x = x''$, $k = k_{min}$; // Make a move.
10          else $k = k + k_{step}$; // Next neighbourhood.
11          endif
12          Update $stop$;
13      until ($k \geq k_{max}$ or $stop$);
14  until ($stop$);
15  return $x$.
```

Figure 2.18: Skewed VNS.

misation problems, based upon the decomposition of the problem [168]. The motivation for this variant of VNS comes from the difficulty to solve large instances of combinatorial optimisation problems, where basic VNS fails to provide solutions of good quality in reasonable computational time. The basic idea of VNDS is to restrict the search process to only a subspace of the entire search space (usually defined by some subset of solution attributes), which can be efficiently explored.

Let $\mathcal{A}$ be the set of all solution attributes, $J \subseteq \mathcal{A}$ an arbitrary subset of $\mathcal{A}$ and $x(J) = (x_j)_{j \in J}$ the sub-vector associated with the set of solution attributes J and solution x. If P is a given optimisation problem, as defined by (1.1), then the *reduced problem* $P(x^0, J)$, associated with the arbitrary feasible solution $x^0 \in X$ and the subset of solution attributes $J \subseteq \mathcal{A}$, can be defined as:

$$\min\{f(x) \mid x \in X, x_j = x_j^0, \forall j \in J\}. \tag{2.4}$$

The steps of the VNDS method are presented in Fig. 2.19.

At each iteration, VNDS chooses randomly a subset of solution attributes $J_k \subseteq \mathcal{A}$ with cardinality k. Then a local search is applied to the subproblem $P(x, \overline{J}_k)$, $\overline{J}_k = \mathcal{A} \setminus J_k$, where variables containing attributes from $\overline{J}_k$ are fixed to values of the current incumbent solution x. The operator `LocalSearch`$(P(x, \overline{J}_k), x(J_k))$ (line 6 in Figure 2.19) can be the basic local search method as described in Section 2.1, but also any other local search based metaheuristic method. Other VNS schemes are most commonly used for this purpose. The local search starts from the current solution $x(J_k)$, to obtain the final solution x' and it operates only on the sub-vector $x(J_k)$ (i.e., on the free variables indexed by J_k). If an improvement occurs, a local search is performed on the complete solution, starting from x', in order to refine the obtained local optimum x'. Again, the local search applied at this stage is usually some other VNS scheme. For the purpose of refinement, it is necessary to intensify the search. Therefore, the VND variant is the best choice in the majority of cases. The whole process is iterated until the fulfilment of stopping criteria. As in the previously described VNS variants, stopping criteria normally represent the running time limitations, the total number of iterations or the number of iterations between two improvements.

The VNDS approach is becoming increasingly popular, with a number of successful applications arising [68, 158, 207, 209, 308].

```
Procedure VNDS($P, x, k_{min}, k_{step}, k_{max}$)
1  repeat
2      Set $k = k_{min}$; Set $stop$ = false;
3      repeat
4          Choose randomly $J_k \subseteq \mathcal{A}$ such that $| J_k |= k$;
5          $\overline{J}_k = \mathcal{A} \setminus J_k$; $x'(\overline{J}_k) = x(\overline{J}_k)$;
6          $x'(J_k)$ = LocalSearch($P(x, \overline{J}_k), x(J_k)$);
7          if ($f(x') < f(x)$) then
8              $x$ = LocalSearch($P, x'$); //  Make a...
9              $k = k_{min}$;                  //  ...  move.
10         else $k = k + k_{step}$; // Neighbourhood change.
11         endif
12         Update $proceed$;
13     until ($k == k_{max}$ or $stop$);
14 until $stop$;
15 return $x$;
```

Figure 2.19: Variable neighbourhood decomposition search.

2.3.2 Advanced Schemes

In the previous subsection, the standard VNS schemes were described. However, there are numerous hard combinatiorial optimisation problems for which standard metaheuristic methods are not effective enough. In order to tackle these hard problems, more sophisticated mechanisms are required. This subsection aims to provide an insight into more elaborate solution methodologies, with some notable contributions to the metaheuristics development in general. Some new VNS schemes are also proposed.

2.3.3 Variable Neighbourhood Formulation Space Search

Standard optimisation techniques attempt to solve a given combinatorial optimisation problem P by considering its formulation and searching the feasible region X of P. However, it is often possible to formulate one problem in different ways, resulting in different search landscapes (local optima, valleys) for different formulations. Nevertheless, the global optima are the same in all formulations. This naturally leads to an idea of switching between different formulations during the search process, in order to escape from local optima in specific formulations and thus reach a global optimum more easily.

Let P be a given combinatorial optimisation problem and ϕ, ϕ' two different formulations of P. One possible way to incorporate the formulation change into the standard VNS framework is provided in Figure 2.20. In the provided pseudo-code, ϕ_{cur} denotes the currently active formulation. For the sake of code simplicity, we introduce formulation $\phi'' = \phi$, so that the statement in line 11 represents the formulation change. Other examples of integration between VNS and formulation changes are also possible (see [167]). Different variants can be obtained depending on the number of formulations, whether the same parameter settings are used in all formulations, whether the search is performed completely in one formulation before switching to another one, or the formulation is changed after each improvement, and so on.

VNS formulation space search has been successfully applied in [175, 239, 240].

```
Procedure VNS-FSS($P, \phi, \phi', x, k_{min}, k_{step}, k_{max}$)
1   Set $stop$ = false, $\phi_{cur} = \phi$;
2   Select neighbourhood structures $\mathcal{N}_{k,\phi} : S_\phi \to \mathcal{P}(S_\phi)$, $k_{min} \le k \le k_{max}$;
3   Select neighbourhood structures $\mathcal{N}_{k,\phi'} : S_{\phi'} \to \mathcal{P}(S_{\phi'})$, $k_{min} \le k \le k_{max}$;
4   repeat
5       Set $k = k_{min}$;
6       repeat
7           Select $x' \in \mathcal{N}_{k,\phi_{cur}}(x)$ at random;
8           $x''$ = Improvement($P, x', \mathcal{N}_{k,\phi_{cur}}(x)$);
9           if ($f(x'', \phi_{cur}) < f(x, \phi_{cur})$) then
10              $x = x''$, $k = k_{min}$; // Make a move.
11              if ($\phi_{cur} == \phi$) then // Change formulation.
12                  ($\phi_{cur} = \phi'$)
13              else ($\phi_{cur} = \phi$)
14              endif
15          else $k = k + k_{step}$; // Next neighbourhood.
16          Update $stop$;
17      until ($k \ge k_{max}$ or $stop$);
18  until ($stop$);
19  return $x$.
```

Figure 2.20: VNS formulation space search.

2.3.4 Primal-dual VNS

As already discussed in Chapter 1, heuristic methods cannot guarantee the solution optimality and often cannot provide the information about how close to optimality a particular heuristic solution is. In case of mathematical programming, the standard approach is to relax the integrality constraints on the primal variables, in order to determine the lower[3] bound for the optimal solution. Yet, for very large problem instances, even the relaxed problem could be impossible to solve to optimality using standard commercial solvers. Hence, one must look for alternatives for gaining the guaranteed bounds for the optimal solution of the original primal problem. One promising possibility is to solve dual relaxed problems heuristically as well and thus iterate the solution processes for primal and dual problems. This approach has been successfully combined with VNS for solving the large-scale simple plant location problems [155]. The resulting primal-dual VNS (PD-VNS) iterates the following three stages:

1) find an initial dual solution (generally infeasible), using the primal heuristic solution and complementary slackness conditions

2) improve the solution by applying VNS to the unconstrained nonlinear form of the dual

3) solve the dual exactly

For more details on PD-VNS, the reader is referred to [155, 167].

[3]In the context of minimisation.

2.3.5 Dynamic Selection of Parameters and/or Neighbourhood Structures

Any local search based metaheuristic method is characterised by the following three components, apart from the initial solution supplied: 1) problem formulation, 2) definition of neighbourhood structures and 3) set of method-specific parameters. In standard optimisation techniques, these components are kept fixed during the search process. However, the behaviour of the search process changes with time, as the solution approaches the optimum, and the initial settings of the above mentioned components are usually not so effective in the middle or near the end of the search process. Moreover, it normally takes a great amount of preliminary tests to determine the best settings at the beginning. Therefore, an appropriate on-the-way update of these components during the search process can be highly beneficial. Possibilities for switching between different problem formulations were already discussed in a previous subsection.

The amendment of neighbourhood structures can be twofold: either only restricting the existing neighbourhood structures to a subspace of interest, or switching to the intrinsically different types of neighbourhood structures. In the first case, it makes sense to update the neighbourhood structures once we are sure that some solutions are not longer of any interest and should be discarded from further examination. This can be viewed as modifying the solution space S, so that the new solution space becomes $S\backslash\overline{S}$, where $\overline{S}$ denotes the set of solutions that should be discarded. Then, any neighbourhood structure $\mathcal{N} : S \rightarrow \mathcal{P}(S)$ should accordingly be modified as: $\mathcal{N}' : S\backslash\overline{S} \rightarrow \mathcal{P}(S\backslash\overline{S})$, so that $\mathcal{N}'(x) = N\backslash\overline{S}$, $x \in S$, $\mathcal{N}(x) = N$. The information about the search history is thus contained in the search space itself. The analogy with tabu search (see Subsection 2.2.2) is obvious, with $\overline{S}$ being the counterpart of tabu list in TS. The iterated local search (see Subsection 2.2.5) also exploits a similar strategy. The VND variant is especially convenient for this approach, since the neighbourhoods are explored completely and therefore do not need to be revisited. The VNS scheme resulting from incorporating the search history within VND in previously described way, called *variable neighbourhood descent with memory*, is presented in Figure 2.21.

```
Procedure VNDM($P, x, k_{vnd}$)
1   Select a set of neighbourhood structures $\mathcal{N}_k : S \rightarrow \mathcal{P}(S)$, $1 \leq k \leq k_{vnd}$;
2   Set $stop$ = false;
3   repeat
4       Set $k = 1$;
5       repeat
6           $x'$ = BestImprovement($P, x, \mathcal{N}_k(x)$);
7           $S = S\backslash\mathcal{N}_k(x)$;
8           Update neighbourhood structures $\mathcal{N}_k : S \rightarrow \mathcal{P}(S)$, $1 \leq k \leq k_{vnd}$;
9           if ($f(x') < f(x)$) then
10              $x = x'$, $k = 1$; // Make a move.
11          else $k = k + 1$; // Next neighbourhood.
12          endif
13          Update $stop$;
14      until ($k == k_{vnd}$ or $stop$ or $S == \emptyset$);
15  until ($f(x') \geq f(x)$ or $stop$);
16  return $x$.
```

Figure 2.21: Variable neighbourhood descent with memory.

Successful applications of VNDM are known in the area of mathematical programming [104, 148, 169, 205, 207], where solution space modification (see line 7 in Figure 2.21) can be easily accomplished by adding an appropriate constraint to the existing mathematical formulation of the problem. In case of a combinatorial formulation, the implementation of VNDS requires an integration of short/long term memory.

It is also possible to switch between inherently different neighbourhood structures during the search. An example of this type of update can be found in [179], where different algorithms which alternate between the four different types of neighbourhood structures for the Generalised minimum edge-biconnected network problem are presented. The formulation space search can also be viewed as a framework for this type of updating the neighbourhood structures, since neighbourhood structures in different iterations are defined for different formulations. Another interesting possibility is to keep the neighbourhood structures in use fixed, but dynamically change the order in which they are examined during the search process [180, 267].

An ad-hoc automatic parameter tuning during the search process is referred to as *reactive search* (RS). According to [22], RS advocates the integration of machine learning techniques into local search heuristics for solving complex optimization problems. The term “reactive” refers to a ready response to events during the search. In RS, the search history is used to automatically adjust paremeters based on the feed-back from previous search and therefore to keep an appropriate balance between the diversification and intensification. The reactive approach was first introduced for tabu search [23] and has had many applications since then. Successful applications of reactive VNS can be found in [44, 255, 279].

Possibilities to integrate RS with an automatic update of other metaheuristic components (i.e. formulation space search and dynamic change of neighbourhoods) will be further discussed in Section 2.5.

2.3.6 Very Large-scale VNS

When designing a neighbourhood structure for a local search-based method, it is desirable that the number of steps required to completely explore the induced neighbourhoods is a polynomial with respect to the size of an input instance. However, this condition cannot always be fulfilled, which may result in neighbourhoods whose size is an exponential function of the size of the input instance. Neighbourhoods of this type are usually referred to as the *very large neighbourhoods*. When dealing with very large neighbourhoods, special techniques are required for the neighbourhood exploration.

Variable neighbourhood search can be successfully combined with a very large scale neighbourhood search. This approach was originally proposed for the general assignment problem (GAP) [234] and the multi-resource GAP [235]. However, it can easily be deduced for 0-1 mixed integer programs in general [233]. Algorithms proposed in [234, 235] are special cases of a k-exchange algorithm [2, 10, 11, 12]. As opposed to standard k-exchange heuristics, VNS algorithms from [234, 235] use very large values for k, which often results in very large neighbourhoods. These large neighbourhoods are then explored approximately, by solving a sequence of smaller GAPs (either exactly or heuristically). Instead of searching an entire k-exchange neighbourhood, only a so called *restricted k-exchange neighbourhood* is explored. The restricted k-exchange neighbourhood is obtained from the original k-exchange neighbourhood by fixing a certain set of solution attributes. In the original papers [234, 235], this set is referred to as a *binding set*. Different heuristics are then induced by different choices of the binding set. A number of possible selection strategies for the binding set is proposed in [234, 235], leading to a few effective GAP solution methods.

2.3.7 Parallel VNS

The main goal of parallelisation is to speed up the computations by engaging several processors and dividing the total amount of work between them [70, 71, 72, 74]. The benefits are manifold: 1) the search process for the same solution quality is accelerated as compared to a single processor performance 2) the solution quality within the same amount of time can be improved by allowing more processors to run 3) sharing the search information between the processors (i.e. coopearative search) can lead to a more robust solution method. The coarse classification of parallelisation strategies is based on the control of the search process and distinguishes between the two main groups: *single walk* and *multiple walks* parallelism. A single walk parallelisation assumes that a unique search trajectory is generated and only required calculations are performed in parallel. In a multiple walk parallelisation, different search trajectories are explored by different processors.

A few strategies for the parallelisation of VNS are known in the literature [70, 114, 166, 241, 242, 334]. The most simple parallelisation strategies do not involve any cooperation (i.e. the exchange of information between the processors), but consist of a number of independent search processes, run on different processors. One possible strategy of this type is a so called *Synchronous parallel VNS*, in which the local search in the sequential VNS is parallelised [114]. Another simple variant of a parallel VNS is a so called *Replicated parallel VNS*, in which an independent VNS procedure is run on each processor [241]. In a more advanced parallelisation environment, some cooperation mechanisms are employed in order to enhance the performance. In the so called *Replicated-shaking VNS*, a sequential VNS is run on the master processor and the solution so obtained is sent to each slave processor which then performs the diversification [114]. The master processor uses the solutions provided by the slaves to choose the next candidate solution and the whole process is iterated. Another interesting cooperative variant of parallel VNS was proposed in [70]. It employs the cooperative multi-search method to the VNS metaheuristic and is therefore named *Cooperative neighbourhood VNS*. In the Cooperative neighbourhood VNS, few independent VNS procedures asynchronously exchange the information about the best solution to date. The individual VNS procedures cooperate exclusively through the master processor – no communication between the individual VNS procedures is allowed. Some other interesting parallelisation strategies for VNS can be found in [242, 334].

2.4 Local Search for 0-1 Mixed Integer Programming

Let P be a given 0-1 MIP problem as defined in (1.6), with the solution space S. Let $x, y \in S$ be two arbitrary integer feasible solutions of P and $J \subseteq \mathcal{B}$. The distance between x and y can be defined as:

$$\delta(x,y) = \sum_{j \in \mathcal{B}} \mid x_j - y_j \mid \tag{2.5}$$

and can be linearised as (see [104]):

$$\delta(x,y) = \sum_{j \in \mathcal{B}} x_j(1-y_j) + y_j(1-x_j). \tag{2.6}$$

In other words, if $\mathbf{w} = (w_1, w_2, \dots, w_n)$ is the vector defined by

$$w_j = \begin{cases} 2x_j - 1 & j \in \mathcal{B} \\ 0 & j \notin \mathcal{B}, \end{cases} \tag{2.7}$$

then the following equivalences hold:

$$\delta(x,y) \lesseqqgtr k \iff \mathbf{w}^{\mathrm{T}}y \gtreqqless \left(\sum_{j\in\mathcal{B}} x_j\right) - k. \tag{2.8}$$

Note that, in case that x and y are pure binary vectors, the distance defined in (2.5) is equivalent to the *Hamming distance* [144], which represents the number of components having different values in x and y.

More generally, let $\hat{x} \in \mathbb{R}^n$ be an arbitrary n-dimensional vector, not necessarily an integer feasible solution of P. Let further $B(\hat{x}) \subseteq \mathcal{B}$ denote the set of indices of binary variables in P, which have binary values in $\hat{x}$:

$$B(\hat{x}) = \{j \in \mathcal{B} \mid \hat{x}_j \in \{0,1\}\}. \tag{2.9}$$

The distance between $\hat{x}$ and an integer feasible solution $y \in S$ of P can then be defined as

$$\delta(\hat{x},y) = \sum_{j\in B(\hat{x})} \hat{x}_j(1-y_j) + y_j(1-\hat{x}_j). \tag{2.10}$$

If $\widehat{\mathbf{w}} = (\hat{w}_1, \hat{w}_2, \ldots, \hat{w}_n)$ is the vector defined by

$$\hat{w}_j = \begin{cases} 2\hat{x}_j - 1 & j \in B(\hat{x}) \\ 0 & j \notin B(\hat{x}), \end{cases} \tag{2.11}$$

then the following equivalences hold:

$$\delta(\hat{x},y) \lesseqqgtr k \quad \Leftrightarrow \quad \widehat{\mathbf{w}}^{\mathrm{T}}y \gtreqqless \left(\sum_{j\in B(\hat{x})} \hat{x}_j\right) - k. \tag{2.12}$$

Note that, when $\hat{x}$ is an integer feasible solution of P, then $B(\hat{x}) = \mathcal{B}$, so (2.10) reduces to (2.6) and (2.12) reduces to (2.8).

The *partial distance* between x and y, relative to $J \subseteq \mathcal{B}$, is defined as

$$\delta(J,x,y) = \sum_{j\in J} \mid x_j - y_j \mid. \tag{2.13}$$

Obviously, $\delta(\mathcal{B},x,y) = \delta(x,y)$. The partial distance defined in (2.13) can be linearised in the same way as the distance defined in (2.5), by performing the summation in (2.6) over the indices in J, rather than in $\mathcal{B}$. The partial distance can also be defined more generally, by allowing the first vector to be any n-dimensional vector $\hat{x} \in \mathbb{R}^n$ and taking $J \subseteq B(\hat{x})$:

$$\delta(J,\hat{x},y) = \sum_{j\in J} \mid x_j - y_j \mid. \tag{2.14}$$

In this general case, the linearisation can still be performed similarly as in (2.6):

$$\delta(J,\hat{x},y) = \sum_{j\in J} \hat{x}_j(1-y_j) + y_j(1-\hat{x}_j). \tag{2.15}$$

Now the following subproblem notation for $k \in \mathbb{N} \cup \{0\}$ and $\hat{x} \in \mathbb{R}^n$ can also be introduced:

$$P(k,\hat{x}) = (P \mid \delta(\hat{x},x) \leq k). \tag{2.16}$$

The neighbourhood structures $\{\mathcal{N}_k \mid 1 \leq k_{min} \leq k \leq k_{max} \leq \mid \mathcal{B} \mid\}$ can be defined knowing the distance $\delta(x, y)$ between any two solutions $x, y \in S$ from the solution space of a given 0-1 MIP problem P. The set of all solutions in the kth neighbourhood of $x \in S$, denoted as $\mathcal{N}_k(x)$, can be defined as in (2.3), with $\rho = \delta$. Again, from the definition of $\mathcal{N}_k(x)$ it follows that $\mathcal{N}_k(x) \subset \mathcal{N}_{k+1}(x)$, $k \in \{k_{min}, k_{min} + 1, \ldots, k_{max} - 1\}$, since $\delta(x, y) \leq k$ implies $\delta(x, y) \leq k + 1$. It is trivial that, if we completely explore neighbourhood $\mathcal{N}_{k+1}(x)$, it is not necessary to explore neighbourhood $\mathcal{N}_k(x)$.

Introducing the neighbourhood structures into the 0-1 MIP solution space S makes possible the employment of a classical local search in order to explore S. The pseudo-code of the corresponding local search procedure, named `LocalSearch-MIP`, is presented in Figure 2.22. The `LocalSearch-MIP` explores the solution space of the input 0-1 MIP problem P, starting from the given initial solution x' and the initial neighbourhood $\mathcal{N}_k(x')$ of x' of the given size k, and returns the best solution found. The neighbourhood $\mathcal{N}_k(x')$ of x' is defined as a subproblem $P(k, x')$. Statement $y =$ `MIPSolve`(P, x) denotes a call to a generic MIP solver for a given input problem P, where x is a given starting solution and y is the best solution found, returned as the result. The variable `status` denotes the solution status as obtained from the MIP solver. Procedure `UpdateNeighbourhood`(&*proceed*, &k, k^*, `status`) updates the current neighbourhood size k and the stopping criterion *proceed* with respect to k^* and the MIP solution status. As in the standard local search, the stopping criterion, represented by the variable *proceed*, usually includes the maximum running time, the maximum number of iterations or the maximum number of iterations between the two improvements.

```
LocalSearch-MIP($P, x', k^*$)
 1  $proceed$ = true; $k = k^*$;
 2  while ($proceed$) do
 3      $x''$ = MIPSolve($P(k, x'), x'$);
 4      if (status == ``optimalSolFound'' ||
 5          status == ``provenInfeasible'') then
 6          $P = (P \mid \delta(x', x) > k)$; endif;
 7      if ($c^t x'' < c^t x'$) then
 8          $x' = x''$; endif;
 9      Update $proceed$;
10      UpdateNeighbourhood(&$proceed$, &$k$, $k^*$, status);
11  endwhile
12  return $x'$.
```

Figure 2.22: Local search in the 0-1 MIP solution space.

Since we have shown that a distance function and neighbourhood structures can be introduced in the 0-1 MIP solution space, all local search metaheuristic frameworks discussed so far can possibly be adjusted for tackling the 0-1 MIP problem. Some successful applications of tabu search for 0-1 MIPs can be found in [213, 147], for example. An application of simulated annealing for a special case of 0-1 MIP problem was proposed in [195]. A number of other approaches for tackling MIPs has been proposed over the years. Examples of pivoting heuristics, which are specifically designed to detect MIP feasible solutions, can be found in [19, 20, 94, 214]. For more details about heuristics for 0-1 MIP feasibility, including more recent approaches such as feasibility pump [103], the reader is referred to Chapter 6. Some other local search approaches for 0-1 MIPs can be found in [18, 129, 130, 176, 182, 212]. More recently, some hybridisatons with general-purpose

MIP solvers have arisen, where either local search methods are integrated as node heuristics in the B&B tree within a solver [32, 75, 120], or high-level heuristics employ a MIP solver as a black-box local search tool [103, 105, 106, 104, 169].

In this section, we choose to present three state-of-the-art local search-based MIP solution methods in detail: local branching [104], variable neighbourhood branching [169] and relaxation induced neighbourhood search [75]. These specific methods are selected for a detailed description because they are used later in this thesis for the comparison with the newly proposed heuristics.

2.4.1 Local Branching

Local branching (LB) was introduced in [104]. It is, in fact, the first local search method for 0-1 MIPs, as described above, which employs the linearisation (2.6) of the distance in the 0-1 MIP solution space defined by (2.5), and uses the general purpose CPLEX MIP solver as a black-box local search tool. For the current incumbent solution x', the search process begins by exploring the neighbourhood of x' of a predefined size $k = k^*$ (defined as a subproblem $P(k, x')$). A generic MIP solver is used as a black-box for exactly solving problems $P(k, x')$ for different values of k. The current neighbourhood size is updated (increased or decreased) in an iterative process, depending on the solution status obtained from the MIP solver, until the improvement of the objective function is reached or the other stopping criteria are fulfilled. After the new incumbent is found, the whole process is iterated. The LB pseudo-code can be represented in a general form given in Figure 2.22, with the special form of procedure `UpdateNeighbourhood`(&*proceed*, &k, k^*, `status`) as given in Figure 2.23. In the original implementation of LB, the stopping criteria (represented by the variable *proceed* in the pseudo-codes from Figures 2.22 and 2.23) include the maximum total running time, the time limit for subproblems, and the maximum number of diversifications (diversification, i.e. the increase of neighbourhood size, occurs whenever line 5 in pseudo-code from Figure 2.23 is reached). In addition, if the computed neighbourhood size is not valid anymore, the algorithm should stop (see line 9 in the pseudo-code in Figure 2.23).

```
UpdateNeighbourhood(&proceed, &k, k*, status)
1  if (status == ``optimalSolFound'' || status == ``feasibleSolFound'') then
2      $k = k^*$;
3  else
4      if (status == ``provenInfeasible'') then
5          $k = k + \lceil k^*/2 \rceil$;
6      else $k = k - \lceil k^*/2 \rceil$;
7      endif
8  endif
9  if ($k < 1$ || $k > |\mathcal{B}|$) then proceed=false; endif
```

Figure 2.23: Updating the neighbourhood size in LB.

2.4.2 Variable Neighbourhood Branching

In [169], it has been shown that a more effective local search heuristic for 0-1 MIPs than LB can be obtained if the neighbourhood change in the general local search framework from Figure 2.22 is performed in a variable neighbourhood search (VNS) manner [237]. As in the case of local branching, a generic MIP solver is used as a black-box for solving subproblems $P(k, x')$, i.e. neighbourhood exploration. Since neighbourhoods are explored completely, the resulting search method is a deterministic variant of VNS, so called variable neighbourhood descent (VND) (see [162] and Section 2.3 in Chapter 2). The pseudo-code of VND for MIPs, called VND-MIP, can also be represented in a general form given in Figure 2.22, but with the special form of procedure `UpdateNeighbourhood`($\&proceed, \&k, k^*,$ `status`) as given in Figure 2.24.

```
UpdateNeighbourhood($\&proceed, \&k, k^*$, status)
1  if (status == ``optimalSolFound'' || status == ``feasibleSolFound'') then
2     $k = 1$;
3  else
4     if (status == ``provenInfeasible'') then
5         $k = k + 1$;
6     else $proceed$ = false;
7     endif
8  endif
9  if ($k > k^*$) then $proceed$=false; endif
```

Figure 2.24: Neighbourhood update in VND-MIP.

Note that parameter k^* in VND-MIP represents the maximum allowed neighbourhood size, whereas in LB it represents the initial neighbourhood size for a given incumbent solution vector.

VND-MIP can be extended to a general VNS scheme for 0-1 MIPs if a diversification mechanism (shaking step in general VNS, see [237] and Section 2.3 in Chapter 2) is added. This GVNS scheme for 0-1 MIPs, called *variable neighbourhood branching* (VNB) was proposed in [169]. The diversification (shaking) in VNB implies choosing a new incumbent solution each time VND-MIP fails to improve the current incumbent and reiterating the whole search process starting from that new point. This can be performed by choosing the first feasible solution from the disk of radii k and $k + k_{step}$, where k is the current neighbourhood size, and k_{step} is a given input parameter. The disk size can then be increased as long as the feasible solution is not found. The pseudo-code of the shaking procedure is given in Figure 2.25.

```
Procedure Shake($P, x^*, \&k, k_{step}, k_{max}$)
1   Choose stopping criterion (set $proceed$ = true);
2   Set solutionLimit = 1; Set $x' = x^*$;
3   while ($proceed$ && $k \le k_{max}$) do
4      $Q = (P \mid k \le \delta(\mathcal{B}, x^*, x) \le k + k_{step})$;
5      $x'$ = MIPSolve($Q$, $x^*$, solutionLimit);
6      if (solutionStatus == proven_infeasible ||
          solutionStatus == no_feasible_found) then
7        $k = k + k_{step}$; // Next neighbourhood.
8        Update $proceed$;
9      else $proceed$ = false;
10  endwhile
11  Reset solutionLimit = $\infty$; return $x'$;
```

Figure 2.25: VNB shaking pseudo-code.

The complete pseudo-code of the VNB procedure is given in Figure 2.26. The input parameters of VNB are the minimum neighbourhood size k_{min}, the neighbourhood size increment step

k_{step}, the maximum neighbourhood size k_{max} and the maximum neighbourhood size k_{vnd} within VND-MIP. In all pseudo-codes the statement $y =$ `MIPSolve`$(P, t, x,$ `solutionLimit`$)$ denotes the call to a generic MIP solver, with input problem P, maximum running time t allowed for the solver, initial solution x, the maximum number of solutions to be explored set to `solutionLimit` and the solution found returned as y. If x is omitted, that means the initial solution is not supplied. If t and/or `solutionLimit` is omitted, that means the running time/number of solutions to be examined is not limited (we set `solutionLimit` to 1 if we are only interested in obtaining the first feasible solution).

```
Procedure VNB($P, k_{min}, k_{step}, k_{max}, k_{vnd}$)
 1   Choose stopping criterion (set proceed = true); Set solutionLimit = 1;
 2   $x' =$ MIPSolve($P$, solutionLimit);
 x   Set solutionLimit $= \infty$; Set $x^* = x'$;
 2   while (proceed) do
 x       $Q = P$; $x'' =$ VND-MIP($Q, k_{vnd}, x'$);
 4       if ($c^{\mathrm{T}}x'' < c^{\mathrm{T}}x^*$) then
 6           $x^* = x''$; $k = k_{min}$;
 8       else $k = k + k_{step}$;
 x       $x' =$ Shake($P, x^*, k, k_{step}, k_{max}$)
 x       if ($x' == x^*$) then break; //No feasible solutions found around $x^*$.
 7       Update proceed;
 9   endwhile
 10  return $x^*$;
```

Figure 2.26: Variable Neighbourhood Branching.

2.4.3 Relaxation Induced Neighbourhood Search

The *relaxation induced neighbourhoods search* (RINS for short), proposed by Danna et al. in 2005 (see [75]), solves reduced problems at some nodes of a branch-and-bound tree when performing a tree search. It is based on the observation that often an optimal solution of a 0-1 MIP problem and an optimal solution of its LP relaxation have some variables with the same values. Therefore, it is more likely that some variables in the incumbent integer feasible solution which have the same value as the corresponding variables in the LP relaxation solution, will have the same value in the optimal solution. Hence, it seems justifiable to fix the values of those variables and then solve the remaining subproblem, in order to obtain a 0-1 MIP feasible solution with a good objective value. On the basis of this idea, at a node of the branch-and-bound tree, the RINS heuristic performs the following procedure: (i) fix the values of the variables which are the same in the current continuous (i.e. LP) relaxation and the incumbent integral solution; (ii) set the objective cutoff to the value of the current incumbent solution; and (iii) solve the MIP subproblem on the remaining variables.

More precisely, let x^0 be the current incumbent feasible solution, $\bar{x}$ the solution of the continuous relaxation at the current node, $J = \{j \in \mathcal{B} \mid x^0_j = \bar{x}_j\}$, x^* the best known solution found and $\varepsilon > 0$ a small nonnegative real number. Then RINS solves the following reduced problem:

$$
(2.17) \qquad P(x^0,\, x^*,\, J) \quad \left[\begin{array}{lll}
\min & c^{\mathrm{T}}x & \\
\text{s.t.} & Ax \geq b & \\
& x_j = x_j^0 & \forall j \in J \\
& c^{\mathrm{T}}x \leq c^{\mathrm{T}}x^* - \varepsilon & \\
& x_j \in \{0,1\} & \forall j \in \mathcal{B} \neq \emptyset \\
& x_j \geq 0 & \forall j \in \mathcal{C}
\end{array}\right.
$$

2.5 Future Trends: the Hyper-reactive Optimisation

The future developments in metaheuristics are likely to evolve in some of the following directions: 1) hybridisation/cooperation, 2) parallelisation, 3) adaptive memory integration, 4) dynamic adjustment of components during the search, 5) different combinations of 1), 2), 3) and 4), etc.

In my view, automatic component tuning, together with adaptive memory integration, seems to be particularly auspicious in order to change the behaviour of the search process, which may depend on the search stage and search history. Note that the best performance is expected if not only the basic parameters of a particular method are considered, but also the different problem formulations and possible neighbourhood structures are included. This "all-inclusive" approach will be referred to as *hyper-reactive* search in the following text. The motivation for the name comes from the term "hyper-heuristics", which refers to methods which explore the search space comprised of heuristic methods for a particular optimisation problem (rather than the search space of the optimisation problem) and the term "reactive search", which refers to an automated tuning of parameters during the search process (see, for example, [13, 22, 23, 44, 227, 255]).

Indeed, any standard local search-based metaheuristic is defined by the search operator `Search` (a set of algorithmic rules for determining the next candidate solution, normally different in metaheuristic frameworks: simulated annealing, tabu search, variable neighbourhood search, etc.), the set of possible problem formulations $\mathcal{F}$ (most metahuristics operate on a single formulation), the set of possible initial solutions X, possible sets of neighbourhood structures $\mathbf{N}$, and the set Π of all possible method-specific parameters. Therefore, a standard local search-based metaheuristic can be viewed as a 5-tuple $(\texttt{Search}, \mathcal{F}, X, \mathbf{N}, \Pi)$, with a general pseudo-code as in Figure 2.27. By choosing particular values for each of the five components from $(\texttt{Search}, \mathcal{F}, X, \mathbf{N}, \Pi)$, a particular heuristic for a specific optimisation problem is obtained. More precisely, by choosing a specific search operator `Search`(defined by some local search metaheuristic), a specific problem formulation $\phi \in \mathcal{F}$, a specific initial solution $x \in X$, a set of neighbourhood structures $\{\mathcal{N}_k \mid 1 \leq k_{min} \leq k \leq k_{max}\} \subseteq \mathbf{N}$, and specific values $v_1, v_2, \ldots, v_\ell$ of parameters $\pi_1, \pi_2, \ldots, \pi_\ell$, $\ell \leq |\Pi|$, $\{\pi_1, \pi_2, \ldots, \pi_\ell\} \subseteq \Pi$, a problem-specific heuristic is obtained, for the optimisation problem P formulated by ϕ, with x as the initial solution. This way, one can observe that each metaheuristic generates a set of problem-specific heuristics. In a hyper-reactive approach, different heuristics from this set are chosen to tackle the input optimisation problem in the different stages of the search process. Therefore, the hyper-reactive search can be viewed as a special type of a hyper-heuristic method (and hence the first part of the word "hyper-reactive"). The general framework of the hyper-reactive search can be represented as in Figure 2.28, where S_ϕ is the solution space of the input problem P in formulation ϕ.

Obviously, a hyper-reactive approach can be integrated into any local search-based metaheuristic. An example of a hyper-reactive VNS, called HR-VNS, is provided in Figure 2.29. Usually,

```
Procedure LSMetaheuristic(Search, $\mathcal{F}, X, \mathbf{N}, \Pi$)
1   Select formulation $\phi \in \mathcal{F}$;
2   Select initial solution $x \in X$;
3   Select a set of neighbourhood structures $\mathcal{N}_{\cdot,\phi} : S_\phi \rightarrow \mathcal{P}(S_\phi)$ from $\mathbf{N}$;
4   Select the vector $\pi = (\pi_1, \pi_2, \ldots, \pi_\ell)$ of relevant parameters,
    $\{\pi_1, \pi_2, \ldots, \pi_\ell\} \subseteq \Pi$;
5   Define $\varphi_{stop} : \Pi^\ell \rightarrow \{$false, true$\}$;
6   Set $\pi = (v_1, v_2, \ldots, v_\ell)$; //Set parameter values.
7   repeat
8       $x' =$ Search($P, \phi, x, \mathcal{N}_{\cdot,\phi}, \pi$);
9       $x = x'$;
10      Update $\pi$;//Update parameter values.
11  until ($\varphi_{stop}(\pi) ==$ true);
12  return $x$.
```

Figure 2.27: A standard local search-based metaheuristic.

the set of relevant parameters is selected as $\pi = (k_{min}, k_{step}, k_{max}, t_{max})$, where $k_{min}, k_{step}, k_{max}$ are the neighbourhood size defining parameters and t_{max} is the maximum running time limitation. In that case, the stopping criterion function φ_{stop} is usually defined as

$$\varphi_{stop}(k_{min}, k_{step}, k_{max}, t_{max}) = (k \geq k_{max} \ ||; t \geq t_{max}),$$

where k is the current neighbourhood size, and t is the current amount of CPU time spent since the beginning of the search. Note that, in case that only parameters from π (including neighbourhood size defining parameters k_{min}, k_{step} and k_{max}) are kept fixed during the search, a variant of VNS-FSS is obtained.[4] If only the formulation ϕ is kept fixed, a general framework for reactive VNS is obtained. Finally, when parameters, together with the problem formulation ϕ, are all kept fixed during the search process, a standard BVNS scheme from Figure 2.16 is obtained.

Integrations of other local search-based metaheuristics with a hyper-reactive approach can be obtained in a similar way. Hyper-reactive GRASP can be constructed by applying a hyper-reactive local search in each restart.

[4]The VNS-FSS variant obtained in this way would be more flexible than the one presented in Figure 2.20, since it allows the update of neighbourhood structures in corresponding formulations in different iterations. In the VNS-FSS pseudo-code presented in Figure 2.20, neighbourhood structures for a specific formulation are defined as a part of the initialisation process and are not further updated during the search.

```
Procedure HRS(Search, $\mathcal{F}, X, \mathbf{N}, \Pi$)
 1    Select initial solution $x \in X$;
 2    Select the vector $\pi = (\pi_1, \pi_2, \ldots, \pi_\ell)$ of relevant parameters,
      $\{\pi_1, \pi_2, \ldots, \pi_\ell\} \subseteq \Pi$;
 3    repeat
 4        Select formulation $\phi \in \mathcal{F}$;
 5        Select a set of neighbourhood structures $\mathcal{N}_{\cdot,\phi} : S_\phi \to \mathcal{P}(S_\phi)$ from $\mathbf{N}$;
 6        Define $\varphi_{stop} : \Pi^\ell \to \{$false, true$\}$;
 7        Set $\pi = (v_1, v_2, \ldots, v_\ell)$; //Set parameter values.
 8        $x'$ = Search$(P, \phi, x, \mathcal{N}_{\cdot,\phi}, \pi)$;
 9        $x = x'$;
10        Update $\pi$; //Update parameter values.
11    until ($\varphi_{stop}(\pi)$ == true);
12    return $x$.
```

Figure 2.28: Hyper-reactive search.

```
Procedure HR-VNS($P, \mathcal{F}, X, \mathbf{N}, \Pi$)
 1    Select initial solution $x \in X$;
 2    Select the vector $\pi = (\pi_1, \pi_2, \ldots, \pi_\ell)$ of relevant parameters,
      $\{\pi_1, \pi_2, \ldots, \pi_\ell\} \subseteq \Pi$, where $\{k_{min}, k_{step}, k_{max}\} \subset \{\pi_1, \pi_2, \ldots, \pi_\ell\}$;
 3    repeat
 4        Define $\varphi_{stop} : \Pi^\ell \to \{$false, true$\}$;
 5        Set $\pi = (v_1, v_2, \ldots, v_\ell)$; //Set parameter values.
 6        Select formulation $\phi \in \mathcal{F}$;
 7        Select neighbourhood structures $\mathcal{N}_{k,\phi} : S_\phi \to \mathcal{P}(S_\phi)$, $k_{min} \le k \le k_{max}$, from $\mathbf{N}$;
 8        Set $k = k_{min}$;
 9        repeat
10            Select $x' \in \mathcal{N}_{k,\phi}(x)$ at random;
11            $x''$ = Improvement$(P, \phi, x', \mathcal{N}_{k,\phi}(x))$;
12            if $(f(x'', \phi) < f(x, \phi))$ then
13                $x = x''$; break; // Make a move.
14            else $k = k + k_{step}$; // Next neighbourhood.
15            endif
16            Update $\pi$; //Update parameter values.
17        until ($\varphi_{stop}(\phi)$ == true);
18    until ($\varphi_{stop}(\phi)$ == true);
19    return $x$.
```

Figure 2.29: The Hyper-reactive VNS.

Chapter 3

Variable Neighbourhood Search for Colour Image Quantisation

Colour image quantisation (or CIQ for short) is a data compression technique that reduces the total number of colours in an image's colour space, thus depicting the original image with a limited number of representative colours [170]. A true colour image is normally represented by a matrix of pixel colours, each consisting of 24 bits – one byte for red, one byte for green and one byte for blue component[1]. However, it is often the case that only 256 (of $2^{24} \approx 16.8$ million possible) colours can be displayed on a certain display device. Hence, it is necessary that images be quantised to 8 bits in order to be represented in these devices. In addition, the decrease of colour information implies a reduction of the image size and is therefore associated with data compression. This greatly reduces the task of transmitting images.

Given an original N-colour image, the quantiser first determines a set of M representative colours – a colourmap, then assigns to each colour in the original image its representative colour in the colourmap, and finally redraws the image by substituting the original colour in every pixel with the value previously assigned to it. It is not hard to see that the quantiser actually performs a clustering of the image's colour space into M desired clusters and maps each point of the colour space to its representative cluster colour (i.e. cluster centroid or median). The final objective of colour image quantisation is to minimize the difference between the reproduced M-colour image and the original N-colour image, i.e., to find an optimal solution to a colour space clustering problem. The difference is usually represented by the mean square error (MSE criterion); it will be formally defined later in the text.

Therefore CIQ problem may be modelled as a clustering problem. More formally, an image I can be considered as a function $I : S \to \mathbb{R}^3$, $S \subset \mathbb{Z} \times \mathbb{Z}$, with each dimension of the set $I(S) = \{I(x) \mid x \in S\}$ representing one of the red, green and blue components of the pixel's colour, respectively, and having an integer value between 0 and 255. The range $C = I(S)$, $C \subset \mathbb{R}^3$, of function I defines the colour space of I. Clearly, colour quantisation of I consists of solving the clustering problem for its colour space C and a given number of colours M, thus obtaining the clusters $C_1, C_2, \dots, C_M$, and then replacing the colour $I(x)$ of each pixel $x \in S$ with the centroid of it's associated cluster C_i.

[1]This representation of pixel colours in a true colour image is known as the RGB (red, green, blue) colour model. A number of other colour models exist in which colour image quantisation can be performed. Nevertheless, the method discussed here and the results reported later are all based on the RGB model. This method, however, could be easily implemented in any other colour model.

In order to find the desired set of M colours, we consider here two types of clustering problems:

(i) **The minimum sum-of-squares clustering problem** (MSSC for short), also known as M-Means problem. It is defined as follows: given a set $X = \{x_1, \ldots, x_N\}$, $x_j = (x_{1j}, \ldots, x_{qj})$, of N entities (or points) in Euclidean space $\mathbb{R}^q$, find a partition P_M of X into M subsets (or clusters) C_i, such that the sum of squared distances from each entity x_ℓ to the centroid $\overline{x}_i$ of its cluster C_i, $f(P_M) = \sum_{i=1}^{N} \sum_{x_\ell \in C_i} ||x_\ell - \overline{x}_i||^2$, is minimal, i.e., find a partition $P_M \in \mathcal{P}_M$ satisfying the following equation:

$$f(P_M) = \min_{P \in \mathcal{P}_M} \sum_{i=1}^{N} \sum_{x_\ell \in C_i} ||x_\ell - \overline{x}_i||^2 \tag{3.1}$$

where $\mathcal{P}_M$ denotes the set of all partitions P of set X, and

$$\overline{x}_i = \frac{1}{|C_i|} \sum_{\ell : x_\ell \in C_i} x_\ell$$

is the centroid of cluster C_i.

(ii) **The minimum sum-of-stars clustering problem**, also known as M-Median problem. Here the centroid $\overline{x}_i$ is replaced by an entity y from cluster (median) C_i, such that the sum of (squared) distances from y to all other entities in C_i, $f(P_M) = \sum_{i=1}^{N} \min_{y \in C_i} \sum_{x_\ell \in C_i} ||x_\ell - y||^2$, is minimal. More precisely, the M-Median problem is defined as finding a partition $P_M \in \mathcal{P}_M$ satisfying the following equation:

$$f(P_M) = \min_{P \in \mathcal{P}_M} \sum_{i=1}^{N} \min_{y_i \in C_i} \sum_{x_\ell \in C_i} ||x_\ell - y_i||^2 \tag{3.2}$$

where all notations are the same as in the definition of MSSC problem.

The distortion between the original image I and the quantised image is measured by the mean square error

$$MSE = \frac{f(P_M)}{n},$$

where n is the total number of pixels in S.

Usually CIQ is modelled as MSSC problem and then solved by using a well-known classical heuristic, k-Means (in our case M-Means). However, different models and techniques were also tried out, the best known being hierarchical methods, both top-down or divisive (see e.g. [170, 191, 322, 43]) and bottom-up or agglomerative methods (see [119, 332]), as well as clustering algorithms based on artificial neural networks and self-organising maps ([137, 83]).

Metaheuristcs, or frameworks for building heuristics usually outperform classical heuristic methods (for surveys of metaheuristic methods, see e.g. [128]). The same is the case in solving CIQ problem, as shown in two recent studies: genetic algorithm (GA) [288] and Particle swarm optimisation (PSO) ([250], [249]). Therefore, these two heuristics may be considered as the state-of-the-art heuristics. There are, however, many other approaches suggested in the literature [297], but they all prove to be outperformed by the metaheuristics (e.g., compare the results in [297] and [250]).

The purposes of this chapter are:

(i) to suggest new heuristic for solving CIQ problem based on the variable neighbourhood search metaheuristic [237, 160, 162, 164] that will outperform state-of-the art heuristics GA and PSO.

(ii) to suggest and test a decomposition variant of VNS for solving clustering problems. Previously only the basic VNS was designed for that purposes (e.g. see [160]).

(iii) to show that the M-Median clustering model may be successfully used for solving some CIQ problem instances instead of the usual M-Means model. For large values of M, the human eye is not able to distinguish solutions obtained by these two models, despite the fact that the error of the M-Means model is larger. However, the procedure for finding M medians is much faster than that for finding M means. At least, the M-median solution may be used as initial one for solving MSSC problem.

This chapter is organised as follows. In Section 2 we present an overview of two known heuristics for solving the CIQ problem. As mentioned earlier, these two heuristics may be considered as the state-of-the-art methods; to the best of our knowledge, they represent the only two metaheuristic approaches to solving the CIQ problem so far. In Section 3 we propose the variable neighbourhood decomposition search , an extension of the basic VNS method, for solving the MSSC problem and particularly the large instances corresponding to the CIQ problem. Finally, in Section 4 we present computational results obtained by applying VNDS to three digital images that are commonly used for testing within the image processing framework. We also compare these results with those of the two above mentioned heuristics. Brief conclusions are given in Section 5.

3.1 Related Work

In this section, two recent heuristics for solving the CIQ problem are described. They are based on two well-known metaheuristics, genetic search and particle swarm optimisation.

3.1.1 The Genetic C-Means Heuristic (GCMH)

The genetic search metaheuristic (GS for short) simulates the natural process of gene reproduction ([288]). Generally, GS takes the population of genetic strings (also called "chromosomes") as an input, performs a certain number of operations (cross-over, mutation, selection, ...) on that population, and returns one particular chromosome as a result. In the beginning, a fitness function is defined, assigning a value of fitness to each string in the population. Genetic operations favour strings with the highest fitness value, and the resulting solution is near-optimal (rather than just a local one, as in the K-Means alternate heuristic [218]).

A genetic approach can be used for data clustering. Let us denote the desired number of clusters with M. First, the initial population is generated, so that it consists of P random chromosomes, where each chromosome r is a set of M cluster centroids $\{v_1, \ldots, v_M\}$. If the clustering space is N-dimensional, then each chromosome is represented as a structure of N component strings, which are obtained by putting each coordinate into a separate string. Then all genetic operations on a certain chromosome are divided into N operations performed on each component string separately. The fitness function is defined as $1/MSE$. There are three different genetic operators:

1) *Regeneration*. Value of fitness is calculated for all chromosomes in the population. All chromosomes are pairwise compared and, for each pair, the chromosome with higher fitness value (i.e., lower MSE) is copied into the other.

2) *Crossover.* For each chromosome $\{v_1, \ldots, v_M\}$ a uniform random number r between 0 and 1 is generated and crossover is applied if $r < P_c$, $P_c = 0.8$. In other words, on each chromosome one-point crossover is applied with probability $P_c = 0.8$. The steps of the crossover operation are the following: first, a uniform integer random number i between 1 and P is generated and the ith chromosome $\{v'_1, \ldots, v'_M\}$ is chosen as a partner string for chromosome $\{v_1, \ldots, v_M\}$. Next, a random integer j between 1 and M is generated and both chromosomes are cut in two portions at position j. Finally, the portions thus obtained are mutually interchanged: $\{v_1, \ldots, v_M\} \rightarrow \{v_1, \ldots, v_j, v'_{j+1}, \ldots, v'_M\}$ and $\{v'_1, \ldots, v'_M\} \rightarrow \{v'_1, \ldots, v'_j, v_{j+1}, \ldots, v_M\}$.

3) *Mutation.* For each element v_j of each chromosome mutation is performed with a probability $P_m = 0.05$. Mutation consists of selecting one of the N components from v_j at random and adding a randomly generated value from the set $\{-1, 1\}$ to the selected component.

These three genetic operators together comprise a generation. In GS, generation is performed repeatedly in a loop. In each iteration, the chromosome with highest value of fitness is stored after a generation. The chromosome stored after G iterations (where G is the maximal number of iterations allowed) is returned as the output of the algorithm.

If the problem space is not one-dimensional, it may be necessary to define large populations and perform a large number of generations to increase the probability to obtain a near-optimal solution. Therefore, GS is combined with the K-Means heuristic in order to reduce the search space. In this new approach the K-Means heuristic is applied to all genetic strings before the regeneration step in each generation. The procedure thus obtained is called the genetic C-Means[2] heuristic (GCMH).

3.1.2 The Particle Swarm Optimisation (PSO) Heuristic

Particle swarm optimisation (PSO) metaheuristic is a population-based optimisation method which simulates the social behaviour of bird flocking ([250], [249]). The whole solution space in the PSO system is referred to as a "swarm", and each single solution in the swarm is referred to as a "particle". Like GS, the PSO heuristic searches the population of random solutions for an optimal one. However, instead of applying genetic operators, the swarm is updated by using the current information about the particles to update each individual particle in the swarm.

In the beginning, all particles are assigned fitness values according to the fitness function to be optimised. During the computation, particles fly through the search space directed by their velocities. Each particle in the swarm can be uniquely represented as a triple: current position, current velocity and personal best position (i.e., the best position visited during the computation, according to the resulting fitness values). The PSO heuristic takes a swarm of random particles as an input and then searches for a near-optimal solution by updating generations in a loop. In every iteration, the position of each particle is computed from its personal best position and the best position of any particle in its neighbourhood (a special case of the method is that one in which there is only one neighbourhood — the entire swarm). First, the velocity of the ith particle is updated by the following formula:

$$v_{i,j}(t+1) = v_{i,j}(t) + c_1 r_{1,j}(y_{i,j}(t) - x_{i,j}(t)) + c_2 r_{2,j}(\hat{y}_j(t) - x_{i,j}(t)),$$

where $v_i(t+1)$ and $v_i(t)$ are velocity vectors of the ith particle in time steps $t+1$ and t, respectively, c_1 and c_2 are learning factors (usually $c_1 = c_2 = 2$), r_1 and r_2 are vectors of random values between 0 and 1, x_i is the current position vector of the ith particle, y_i is the best position vector of the ith particle, $\hat{y}$ is the vector of the best position of any particle in the ith's particle neighbourhood, and

[2]The C-Means heuristic is another name for the K-Means heuristic.

index j denotes the current dimension. Then the following formula is used to update the position of the ith particle: $x_i(t+1) = x_i(t) + v_i(t+1)$. The loop is run until the maximum number of iterations allowed or minimum error criteria is attained.

The main difference between GS and PSO is in the information sharing mechanism. While in GS all chromosomes share information with each other, in PSO there is just one particle (the one with the best visited position) that sends the information to the rest of the swarm. Therefore all particles tend to converge to the optimal solution quickly, whereas in GS the whole population as a single group moves towards an optimal area, which results in slower performance compared to PSO.

3.2 VNS Methods for the CIQ Problem

In this section several new variants of variable neighbourhood search for the CIQ problem are proposed. Two different VNS schemes are exploited and combined: variable neighbourhood decomposition search (VNDS) [168] and reduced variable neighbourhood search (RVNS) [159]. Variable neighbourhood decomposition search is an extension of VNS that searches the problem space by decomposing it into smaller size subspaces. The improved solution found in a given subspace is then extended to a corresponding solution of the whole problem (see Chapter 2, Section 2.3 for more details). In this section, we describe a new VNDS-based technique for colour image quantisation. Moreover, this technique can also be viewed as a new approach to tackling the more general MSSC problem. It is particularly well-suited for solving very large problem instances. Reduced variable neighbourhood search is a stochastic variant of VNS, where new candidate solutions are chosen at random from appropriate neighbourhoods (see Chapter 2, Section 2.3). In this chapter some new CIQ techniques are developed based on the RVNS framework. The integration of RVNS within a general VNDS scheme is also studied.

The CIQ problem space is the set of all colour triplets present in the image to be quantised. Although our quantisation technique is not restricted to 8-bit quantisation, we assume that the RGB coordinates of each colour triplet are integers between 0 and 255 (it is possible to derive other implementations of our technique that do not satisfy this assumption). Since our problem space is a subset of $\mathbb{Z}^3$, we use the VNS methods adjusted for solving the M-Median problem. In other words, medians are always chosen to be some of the colour triplets from the original image. The points that coincide with centroids are referred to as "occupied" points, whereas all other points are referred to as "unoccupied" points. The MSE is used as the objective function. In the end, the solution obtained by VNDS is refined by applying the K-Means algorithm and rounding off the real components of the resulting triplets.

Let us denote with n the total number of pixels in the image to be quantised and with M the desired number of colours in the colourmap, i.e., the number of clusters of the colour space. The heuristic first initializes cluster centroids by randomly selecting M colour triplets from the colour space of the given image. All the remaining colour triplets are then assigned to their closest centroid (in terms of squared Euclidean distance) to form clusters of the image's colour space. The reduced VNS method (which will be explained in more details further in the text) is applied to this solution once and the resulting solution is used as the initial solution for the VNDS algorithm. The set of neighbourhood structures in the CIQ framework is defined so that any $k \leq M$ centroids from the current solution, together with their associated points, represent a point in the kth neighbourhood $\mathcal{N}_k$ of the current solution. After generating the initial solution, the VNDS algorithm repeatedly performs the following actions until the stopping criterion is met: selecting a point from $\mathcal{N}_k$ at random (starting with $k = 1$), solving the corresponding subproblem by some local search method (in our case the reduced VNS heuristic), extending the so-obtained solution to the corresponding solution in the whole problem space (i.e., adding the centroids outside $\mathcal{N}_k$ and their associated points) and either moving to the new solution if it is better than the incumbent and continuing the search in its first neighbourhood, or moving to the next neighbourhood of the current solution otherwise. The heuristic stops if a maximal number of iterations between two improvements or a maximal total number of iterations allowed is reached.

Since the subproblem solving method used in our implementation of VNDS heuristic is another VNS scheme — the so-called reduced VNS (RVNS) method, we will first provide the outline of the RVNS algorithm. It is based on the so-called *J-Means* (or *Jump Means*) heuristic for solving the MSSC problem [160, 26]: the neighbourhood of a current solution P_M is defined as all possible "centroid to entity re-locations" (not "entity to cluster re-allocations"), so that after the jump move, many entities (colours) change their cluster. Thus, the jump in re-allocation type of neighbourhood is performed.

Several variants of J-Means heuristic have been analysed in [160, 26]. After performing the jump move, the questions are: (i) whether and when the solution will be improved by alternate or K-Means heuristic? (ii) how many iterations of K-Means to perform? If K-Means is used always, and until the end, then the final procedure will be time consuming. Since CIQ problem instances are usually huge, we decide to apply the full K-Means only once, in the end of our VNDS. For the same reason, we use RVNS (instead of the basic VNS) within the decomposition. In that way, RVNS is used to create a set of M representative colours among the already existing colours of the image. In other words, we apply RVNS for solving M-Median problem (3.2), not M-Means problem (3.1). The steps of the RVNS algorithm are presented in Figure 3.1.

```
Initialisation. Set value $i_{\text{RVNS}}$ for the maximal number of iterations allowed between
two improvements. Set current iteration's counter: $i = 0$ and the indicator of iteration
in which optimal solution was found: $i_{best} = i$.
Main step.
Repeat the following sequence
(1) $k = 1$;
(2) Repeat the following steps
    (a) $i = i + 1$;
    (b) Shaking (J-Means moves).
        for $j = 1$ to $k$ do
            i)   Select one of the unoccupied points from the current solution $P_M$
                 at random; denote the selected point with $x_{add}$ and add it as a
                 new cluster centroid.
            ii)  Find index $del$ of the best centroid deletion.
            iii) Replace centroid $\overline{x}_{del}$ by $x_{add}$ and update assignments and ob-
                 jective function accordingly. Denote the so-obtained solution and
                 objective function value with $P'_M$ and $f'$, respectively.
        endfor
    (c) Neighbourhood change. If this solution is better than the incumbent ($f' <$
        $f_{opt}$), move there ($P_M = P'_M$, $f_{opt} = f'$ and $i_{best} = i$) and go to step (1);
        otherwise, continue the search in the next neighbourhood ($k = k + 1$) of the
        current solution;
    until $k = k_{max}$ or $i - i_{best} = i_{\text{RVNS}}$
until $i - i_{best} = i_{\text{RVNS}}$
```

Figure 3.1: RVNS for CIQ.

It is easy to see that the RVNS method is obtained from the basic VNS algorithm if we do not perform local search to randomly selected points from the corresponding neighbourhood. It depends on two parameters: k_{max} and i_{RVNS}. Therefore, we can write RVNS(k_{max}, i_{RVNS}). Usually k_{max} is set to 2, but i_{RVNS} is more problem dependent. For solving the CIQ problem we set the value for parameter i_{RVNS} to 5 in most cases, i.e., we use procedure RVNS(2,5). The steps of the VNDS heuristic are summarised in Figure 3.2.

```
Initialisation.
(1) Set value $i_{\text{VNDS}}$ for the maximal number of iterations allowed between two improve-
    ments.
(2) Find initial solution: select $M$ out of $n$ given points at random (taken from the colour
    space $S \subset \mathbb{R}^3$) to represent cluster centroids; assign all other points to their closest
    cluster centroid.
(3) Apply the RVNS algorithm to the current solution.
(4) Set the current iteration counter: $i = 0$ and the indicator of iteration in which the
    optimal solution was found: $i_{best} = i$.
Main step.
Repeat the following sequence
(1) $k = 2$;
(2) Repeat the following steps
    (a) $i = i + 1$;
    (b) Defining subproblem. Select one of the current centroids at random. Let
        $Y \subseteq X$ be the set of points comprised of the selected centroid, its $k - 1$ closest
        centroids and their associated points.
    (c) Solving subproblem. Find the local optimum in the space of $Y$ by applying
        the RVNS method; denote with $P'_k$ the best solution found, and with $P'_M$ and
        $f'$ the corresponding solution in the whole problem space and the new objective
        function, respectively ($P'_M = (P_M \backslash P_k) \cup P'_k$).
    (d) Neighbourhood change. If this local optimum is better than the incumbent
        ($f' < f_{opt}$), move there ($P_M = P'_M$, $f_{opt} = f'$ and $i_{best} = i$) and go to step (1);
        otherwise, continue the search in the next neighbourhood ($k = k + 1$) of the
        current solution.
    until $k = M$ or $i - i_{best} = i_{\text{VNDS}}$
until $i - i_{best} = i_{\text{VNDS}}$
```

Figure 3.2: VNDS for CIQ.

Using the above heuristics, we adapt our approach in two different ways when tackling the large instances of the CIQ problem: (*i*) we omit the time consuming local search step of the basic VNS by only generating solutions in the neighbourhoods of the incumbent at random; this reduction of the basic VNS scheme is called RVNS; (*ii*) we reduce the original search space by decomposition; then subproblems are solved by RVNS and inserted in the whole solution only if it is improved; this extension of the basic VNS scheme is a special case of VNDS.

3.3 Computational Results

In this section we present results for testing three variants of VNS-based heuristics on three different digital images: the above presented variable neighbourhood decomposition search method with running the reduced VNS to obtain the initial solution, which will in further text be referred to as RVNDS; the VNDS algorithm applied to randomly selected initial solution (i.e., without running the RVNS in step (3) of Initialisation), which will in further text be referred to as VNDS; and the RVNS heuristic alone, without performing the decomposition before running the K-Means algorithm.

The RVNDS, VNDS and RVNS heuristics are compared with the GCMH and PSO heuristics with respect to the MSE of the computation. We also compare the CPU times of RVNDS, VNDS and RVNS. In addition, we use two variants of RVNDS: one with the maximal number of iterations between two improvements i_{VNDS} set to 10 and maximal number of iterations in the local search step i_{RVNS} set to 20, and another with $i_{\text{VNDS}} = 5$ and $i_{\text{RVNS}} = 5$. The first variant will be denoted as RVNDS', whereas the latter will be denoted simply as RVNDS. The parametre k_{max} is set to 2 in all implementations. All variants of VNS were coded in FORTRAN 77 and run on a Pentium 4 computer with 3.2GHz processor and 1GB of RAM. The results for the GCMA and PSO heuristics were taken from [250] and [249]. The algorithms are tested on three 512×512 pixels digital images: Lenna, Baboon and Peppers, that are commonly used for testing in the image processing framework and can be found in the images' databases on the internet (for instance on `http://sipi.usc.edu/database/index.html`). The "Lenna" image is a digital photograph of a girl, consisting mainly of different nuances of orange (from light yellow to dark brown). "Baboon" is a digital image of a monkey, with a great number of different colours. Finally, "Peppers" is an image substantially comprised of a small number of pure colours: red, green, yellow and black, and therefore containing a lot of zero components in its representation matrix. The essential difference between these three images is in the number of different points in their colour spaces. There are 230 427 different colours in the "Baboon" image, 148 279 different colours in the "Lenna" image and 183 525 different colours in the "Peppers" image. In order to get precise results, each algorithm was run 10 times for each data set. The results are then presented in the form $average\_value \pm max\{maximal\_value - average\_value, average\_value - minimal\_value\}$.

Image	No. of clusters	RVNDS'	RVNDS	VNDS	RVNS	GCMH	PSO
Lenna	16	209.6±1.51	211.1±4.89	212.8±4.12	211.1±4.89	332	210.2±1.49
	32	117.4±0.16	117.7±1.04	117.7±0.45	117.7±1.01	179	119.2±0.45
	64	71.3±0.30	71.3±0.85	71.4±0.58	71.3±0.19	113	77.8±16.13
Baboon	16	629.0±4.62	629.2±3.36	629.2±3.37	628.9±2.32	606	631.0±2.06
	32	372.6±1.78	373.0±1.26	374.4±5.25	373.2±1.32	348	375.9±3.42
	64	233.8±1.45	234.1±0.51	234.4±1.44	233.9±0.82	213	237.3±2.02
Peppers	16	397.7±4.02	397.0±5.89	412.9±19.21	397.1±5.82	471	399.6±2.64
	32	227.6±2.39	228.5±2.57	228.3±2.53	228.5±2.56	263	232.0±2.30
	64	134.2±5.88	135.1±5.24	134.3±4.85	136.4±4.75	148	137.3±3.38

Table 3.1: The MSE of the VNS, GCMH and PSO heuristics, quantising images Lenna, Baboon and Peppers, to 16, 32, and 64 colours.

It is worth mentioning here that, since the basic VNS method was not originally designed for large instances of problems, having up to 262 144 entities, it has a very time consuming performance if applied to the above instances of the CIQ problem. Therefore we limit our discussion to VNDS and RVNS, the extended and the reduced version of the basic scheme. Regarding the MSE, we can see from Table 3.1 that VNS methods outperform GCMH in two of three images, whereas the results for the PSO are similar but systematically slightly worse than those obtained by VNS. Results from Table 3.2 suggest that increasing the maximal number of iterations allowed between two improvements (either in the outer or the inner loop) drastically increases the CPU time of the VNDS algorithm, but only slightly improves the MSE of the computation. By observing the time performances of the proposed VNS heuristics (Figure 3.3), we can see that RVNDS and

		RVNDS’		RVNDS		VNDS		RVNS	
Image	No. of col.	MSE	time (s)	MSE	time (s)	MSE	time (s)	MSE	time (s)
Lenna	16	209.6±1.51	318.23	211.1±4.89	36.50	212.8±4.12	69.67	211.1±4.89	17.03
	32	117.4±0.16	236.73	117.7±1.04	58.83	117.7±0.45	90.71	117.7±1.01	49.84
	64	71.3±0.30	245.98	71.3±0.85	115.08	71.4±0.58	202.60	71.3±0.19	118.18
	128	45.4±0.14	534.51	49.5±0.24	194.43	45.8±0.25	303.26	45.5±0.22	236.70
	256	29.6±0.08	900.80	29.7±0.11	310.24	29.9±0.17	598.36	29.7±0.10	383.18
Baboon	16	629.0±4.63	220.42	629.2±3.36	43.85	629.2±3.37	67.64	628.9±2.32	36.87
	32	372.6±1.78	170.21	373.0±1.26	68.43	374.4±5.25	87.97	373.2±1.32	64.80
	64	233.8±1.45	266.36	234.1±0.51	126.20	234.4±1.44	175.78	233.9±0.82	165.89
	128	149.5±0.36	317.36	149.5±0.56	291.87	149.7±0.76	415.18	149.5±0.38	339.09
	256	95.4±0.25	359.36	95.4±0.14	448.72	95.8±0.44	683.30	95.4±0.08	619.93
Peppers	16	397.7±4.02	215.39	397.0±5.89	34.41	412.9±19.21	52.62	397.1±5.82	16.61
	32	227.6±2.39	178.13	228.5±2.57	63.20	228.3±2.53	77.64	228.5±2.56	37.29
	64	134.2±5.88	284.85	135.1±5.24	124.15	134.3±4.85	162.12	136.4±4.75	72.90
	128	82.1±0.22	608.46	82.1±0.39	227.06	82.7±1.00	337.79	86.0±4.24	265.64
	256	52.8±0.31	956.45	53.0±0.34	399.45	53.5±0.47	882.58	53.0±0.27	535.88

Table 3.2: The MSE and the average CPU time of the RVNDS’, RVNDS, VNDS and RVNS algorithms, quantising images Lenna, Baboon and Peppers, to 16, 32, 64, 128 and 256 colours.

RVNS heuristics show the best results, whereas the RVNDS’ algorithm is generally the most time consuming. However, it is interesting to note that in the case of “Baboon” the time performance of RVNDS’ algorithm is improved by increasing the number of quantisation colours, so it is the least time consuming method for the quantisation to 256 colours.

In the remaining part of this section we will further analyse the M-Median solution vs. the M-Means solution obtained after running the K-Means algorithm in the RVNDS algorithm. The motivation for this kind of analysis is the long running time of K-Means within the proposed algorithms.

From the results shown in Table 3.3 and from Figure 3.4, it is clear that by increasing the number of quantisation colours the difference between the MSE of the M-Median solution and the M-Means solution decreases, whereas the time spent on performing the K-Means heuristic generally increases. So, in the case of quantisation to 256 colours, there is no visible difference between the M-Median and M-Means solution (Figures 3.7, 3.10 and 3.13), but more than 50% of the heuristic running time is spent on refining the solution by K-Means. Further analysis shows that for images “Lenna” and “Baboon” there is no significant difference even in the case of quantisation to 64 colours. For the “Peppers” image however M-Median quantisation to 64 colours gives sharper edges between the shaded and illuminated areas, so it appears that quantising to 128 colours is necessary in order to get a noticeable visual difference. We can therefore introduce the notion of *critical number of colours* which denotes the least number of quantisation colours such that both M-Median heuristic alone and with K-Means at the end give visually the same (or very similar) results. In this way, the critical number of colours for images “Lenna” and “Baboon” would be approximately 64, and for “Peppers” approximately 128. Yet, it is impossible to exactly determine this number for a particular image, since it is based on human eye perception, and can differ from person to person.

It is interesting to note that although the difference in MSE between the M-Median and the M-Means solution is the greatest in the case of “Baboon”, the visual difference between the solutions is the smallest. This could be explained by the fact that “Baboon” has the largest colour

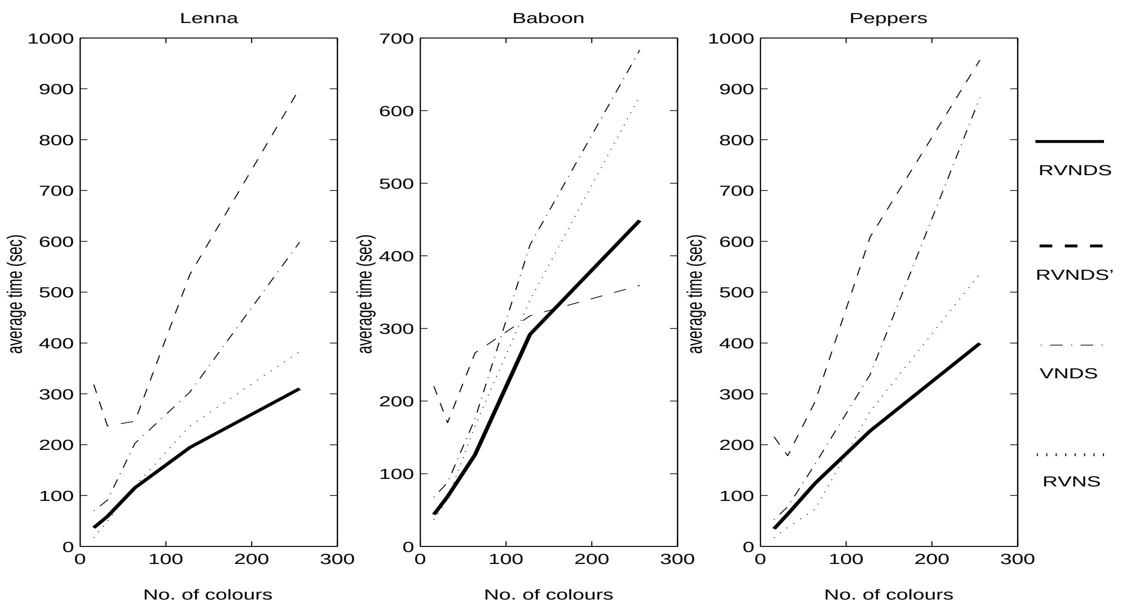


Figure 3.3: Time performance of VNS methods quantising images Lenna, Baboon and Peppers, to 16, 32, 64, 128 and 256 colours.

Image	No. of clusters	M-Median MSE	M-Means MSE	Average M-Median time (s)	Average M-Means time (s)	Average total time (s)
Lenna	16	253.2 ± 24.04	211.1 ± 4.89	26.65	9.85	36.50
	32	148.4 ± 14.26	117.7 ± 1.04	30.67	28.16	58.83
	64	90.4 ± 18.67	71.3 ± 0.85	50.74	64.34	115.08
	128	59.4 ± 13.82	45.5 ± 0.24	76.49	117.93	194.42
	256	37.2 ± 2.77	29.7 ± 0.11	127.36	182.88	310.24
Baboon	16	746.2 ± 50.40	629.2 ± 3.36	25.85	18.00	43.5
	32	449.9 ± 15.94	373.0 ± 1.26	30.10	38.33	68.43
	64	284.9 ± 41.95	234.1 ± 0.51	50.25	75.95	126.20
	128	184.8 ± 16.81	149.5 ± 0.56	77.51	214.36	291.87
	256	117.2 ± 7.55	95.4 ± 0.14	127.08	321.64	448.72
Peppers	16	474.3 ± 31.34	397.0 ± 5.89	25.57	8.84	34.41
	32	281.4 ± 15.03	228.5 ± 2.57	30.83	32.37	63.20
	64	168.9 ± 18.58	135.1 ± 5.24	50.54	73.61	124.15
	128	104.2 ± 11.31	82.1 ± 0.39	74.81	152.24	227.05
	256	66.6 ± 3.99	53.0 ± 0.34	133.35	266.10	399.45

Table 3.3: The comparison of MSE and time perfomance between the M-Median solution and the M-Means solution in the RVNDS algorithm.

space (i.e., that one with the greatest number of points), so that the selection of representative colours in the M-Median colourmap is more adequate than in other two cases. Also, the “Baboon” image is far more complex than in the other two cases, which makes it much harder for the human

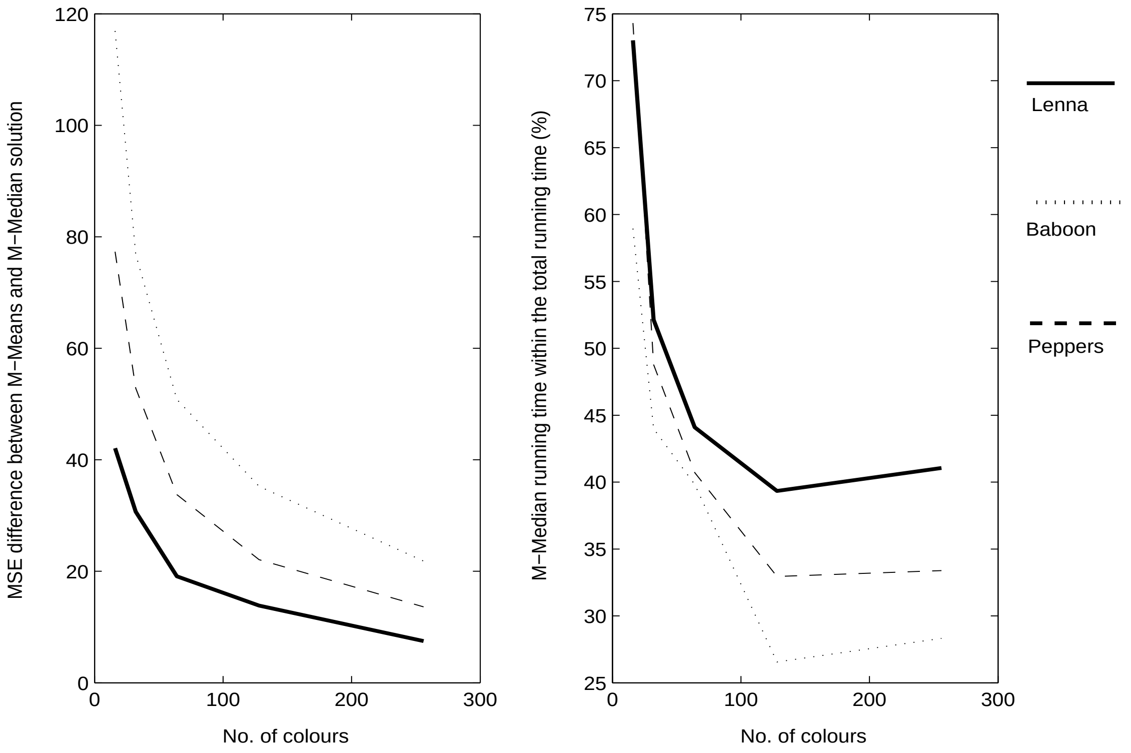


Figure 3.4: MSE and running time comparison between the M-Median and the M-Means solution.

eye to distinguish tiny details in difference between two similar solutions.

In summary, the results obtained show that the M-Median version of our proposed heuristic is much faster than the one including K-Means refining in the end, and yet provides solutions of fairly similar visual quality. Even more, since the quantisation to large number of colours (128 or 256) gives visually similar results in both cases, it appears that performing the full K-Means after VNDS might be redundant, especially taking into account its long running time in these cases.

3.4 Summary

In this chapter we show that the variable neighbourhood search (VNS) heuristic for data clustering can be successfully employed as a new colour image quantisation (CIQ) technique. In order to avoid long running time of the algorithm, we design the decomposed (VNDS) and the reduced (RVNS) versions of VNS heuristic. Results obtained show that the errors of the proposed heuristics can compare favourably to those of recently proposed heuristics from the literature, within a reasonable time.

In addition, the two different models for solving CIQ are compared. M-Median model and the usual M-means model. The results of that comparison show that VNS based heuristic for the M-Median is much faster, even in the case when the latter use M-Median solution as initial one. It is also shown that in the case of quantisation to large number of colours, solutions of the same visual quality are obtained with both models. Future research in this direction may include the use of a VNS technique for solving other similar problems such as colour image segmentation [54].

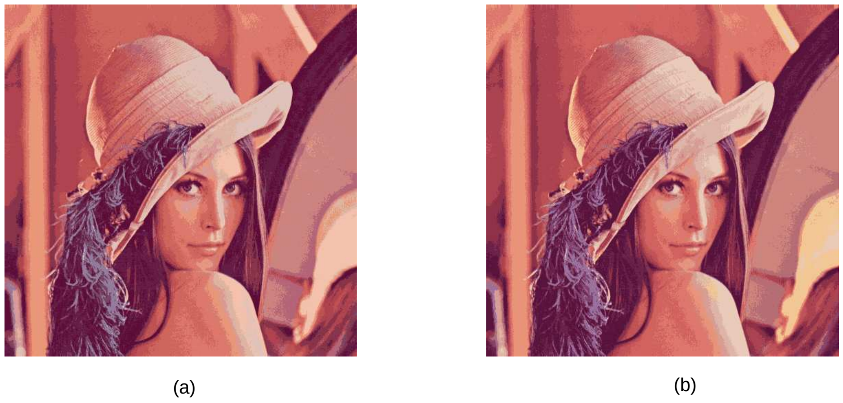


Figure 3.5: “Lenna” quantised to 16 colours: (a) M-Median solution, (b) M-Means solution.

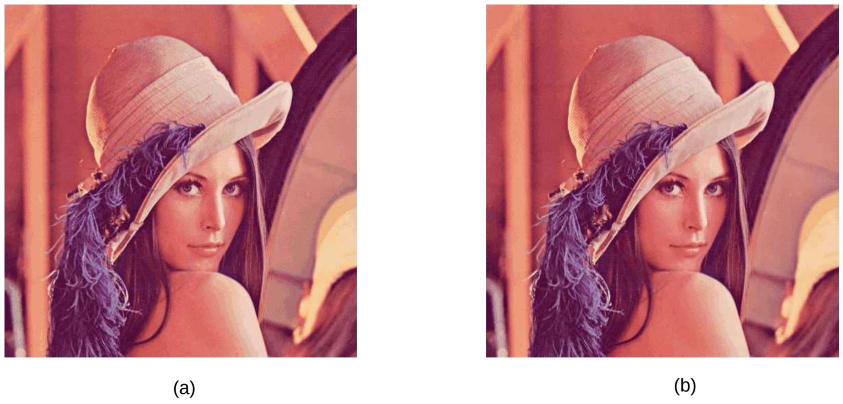


Figure 3.6: “Lenna” quantised to 64 colours: (a) M-Median solution, (b) M-Means solution.

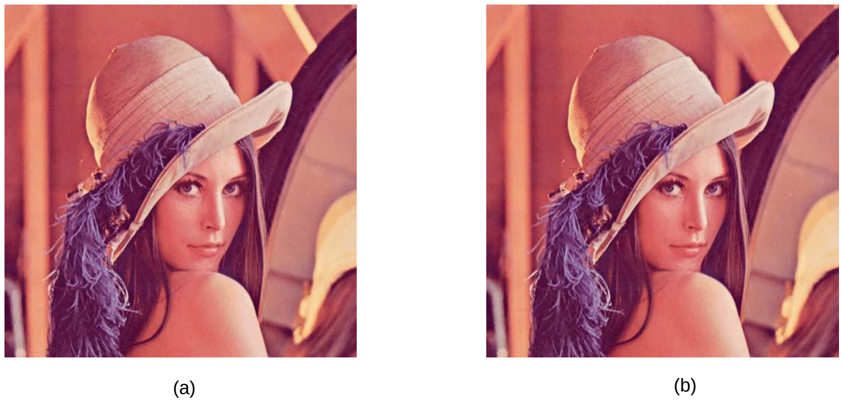
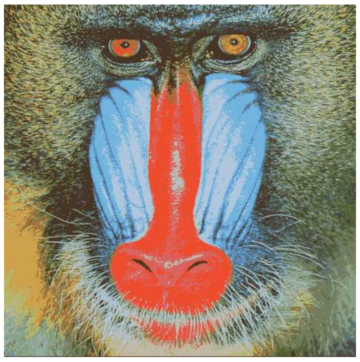


Figure 3.7: “Lenna” quantised to 256 colours: (a) M-Median solution, (b) M-Means solution.


(a)

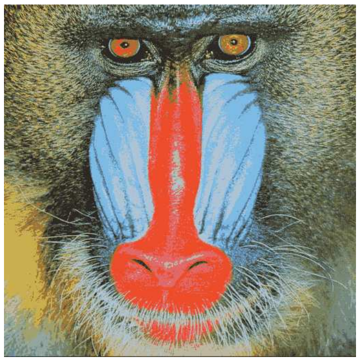
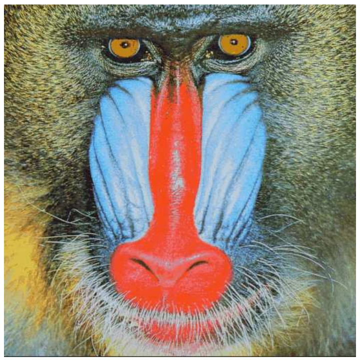

(b)

Figure 3.8: "Baboon" quantised to 16 colours: (a) M-Median solution, (b) M-Means solution.


(a)

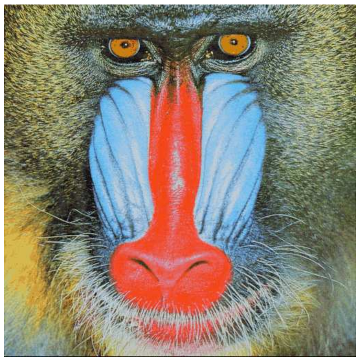
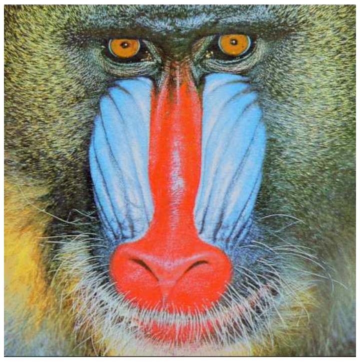

(b)

Figure 3.9: "Baboon" quantised to 64 colours: (a) M-Median solution, (b) M-Means solution.


(a)

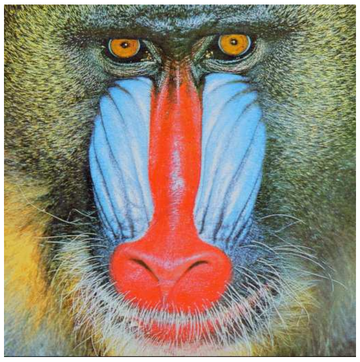
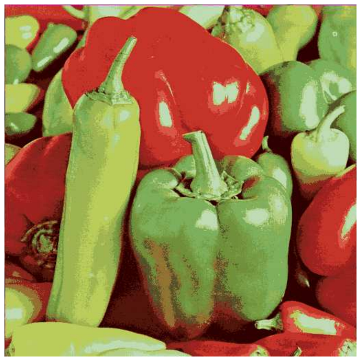

(b)

Figure 3.10: "Baboon" quantised to 256 colours: (a) M-Median solution, (b) M-Means solution.


(a)

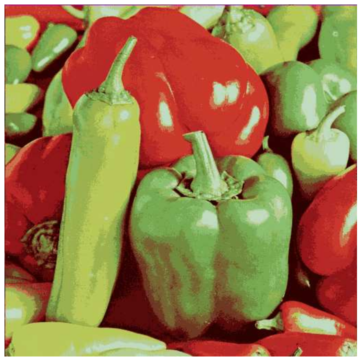
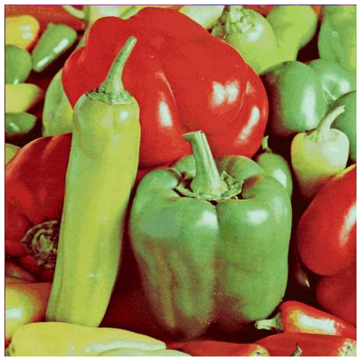

(b)

Figure 3.11: "Peppers" quantised to 16 colours: (a) M-Median solution, (b) M-Means solution.


(a)

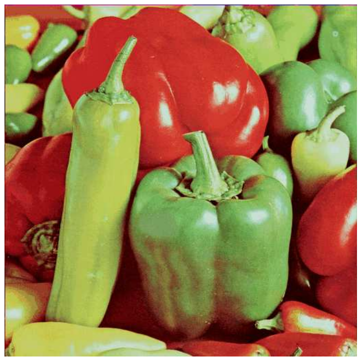
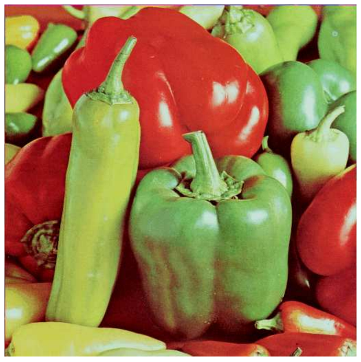

(b)

Figure 3.12: "Peppers" quantised to 64 colours: (a) M-Median solution, (b) M-Means solution.


(a)

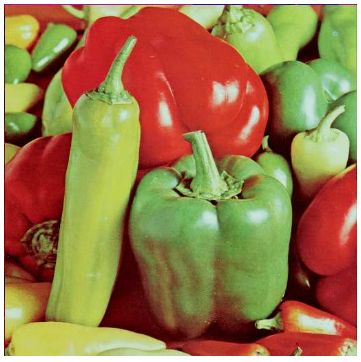

(b)

Figure 3.13: "Peppers" quantised to 256 colours: (a) M-Median solution, (b) M-Means solution.

Chapter 4

Variable Neighbourhood Decomposition Search for the 0-1 MIP Problem

The concept of variable fixing in order to find solutions to MIP problems was conceived in the late 1970s and early 1980s, when the first methods of this type for the pure 0-1 integer programming problems were proposed [21, 298]. This approach is sometimes referred to as a *core approach*, since the subproblems obtained by fixing a certain number of variables in a given MIP model are sometimes called *core problems*. The terms *hard variable fixing* or *diving* are also present in the literature [75]. The critical issue in this type of methods is the way in which the variables to be fixed are chosen. Depending on the selection strategy and the way of manipulating the obtained subproblems, different MIP solution methods are obtained. Successful extensions of the basic method from [21] were proposed in [259, 269]. Another iterative scheme for the 0-1 multidimensional knapsack problem, based on a dynamic fixation of the variables, was developed in [329]. This scheme also incorporates information about the search history, which is used to build up feasible solutions and to select variables for a permanent/temporary fixation. In [234, 235], variable neighbourhood search was combined with a very large scale neighbourhood search to select variables for fixing (so called *binding sets* in the original papers [234, 235]) and conduct the investigation of subproblems, for the general assignment problem. This approach was further extended for 0-1 mixed integer programming in general [233]. With the expansion of general-purpose MIP solvers over the last decade, different hybridisations of MIP heuristics with commercial solvers are becoming increasingly popular. A number of efficient heuristics, which perform some kind of variable fixing at each node of a B&B tree in the CPLEX MIP commercial solver, have been developed so far. Relaxation induced neighbourhood search (RINS) [75] fixes the values of the variables which are the same in the current continuous (i.e. LP) relaxation and in the incumbent integral solution. Distance induced neighbourhood search [120] performs a more intelligent fixation, by taking into account the values of variables in the root LP relaxation and memorising occurrences of different values during the search process, in addition to considering the values of the current LP relaxation solution. Relaxation enforced neighbourhood search [32] is an extension of RINS, which additionally performs a large-scale neighbourhood search over the set of general integer variables by an intelligent rebounding according to the current LP relaxation solution.

This chapter is organised as follows. In Section 4.1, a detailed description of the new VNDS heuristic for solving 0-1 MIP problems is described. Next, in Section 4.2, the performance of the

VNDS method is analysed, compared to the other three state-of-the-art 0-1 MIP solution methods and to the CPLEX MIP solver alone. Three methods used for comparison purposes are local branching [104], variable neighbourhood branching [169] and relaxation induced neighbourhood search [75]. They were described in detail in Chapter 2, Section 2.4. Last, in Section 4.3, some final remarks and conclusions are provided.

4.1 The VNDS-MIP Algorithm

In this section, a new variant of VNDS for solving 0-1 MIP problems, called VNDS-MIP, is proposed. This method combines a linear programming (LP) solver, MIP solver and VNS based MIP solving method VND-MIP in order to efficiently solve a given 0-1 MIP problem. A systematic hard variable fixing (or diving) is performed following the variable neighbourhood search rules. The variables to be fixed are chosen according to their distance from the corresponding linear relaxation solution values. If there is an improvement, variable neighbourhood descent branching is performed as the local search in the whole solution space.

The pseudo-code for VNDS-MIP is given in Figure 4.1. Input parameters for the VNDS-MIP algorithm are instance P of $0-1$ MIP problem, parameter d, which defines the value of variable k_{step}, i.e., defines the number of variables to be released (set free) in each iteration of the algorithm, the maximum running time allowed t_{max}, time t_{sub} allowed for solving subproblems, time t_{vnd} allowed for the VND-MIP procedure, time t_{mip} allowed for call to the MIP solver within the VND-MIP procedure and maximum size rhs_{max} of a neighbourhood to be explored within the VND-MIP procedure.

At the beginning of the algorithm, the LP relaxation of the original problem P is solved first, in order to obtain an optimal solution $\overline{x}$ (see line 1 in Figure 4.1). The value of the objective function $c^{\mathrm{T}}\overline{x}$ provides a lower bound on the optimal value $\nu(P)$ of P. Note that, if the optimal solution $\overline{x}$ is integer feasible for P, the algorithm stops and returns $\overline{x}$ as an optimal solution for P. Then, an initial feasible solution x of the input problem P is generated (see line 2 in Figure 4.1). Although solving 0-1 MIP problems to feasibility alone is not always an easy task, we will here assume that this step can be performed in a reasonable time. For more details on the 0-1 MIP feasibility issues the reader is referred to Chapter 6. At each iteration of the VNDS-MIP procedure, the distances $\delta_j =\mid x_j - \overline{x}_j \mid$ from the current incumbent solution values $(x_j)_{j\in\mathcal{B}}$ to their corresponding LP relaxation solution values $(\overline{x}_j)_{j\in\mathcal{B}}$ are computed and the variables $x_j, j \in \mathcal{B}$ are indexed so that $0 \leq \delta_1 \leq \delta_2 \leq \ldots \leq \delta_p$ (where $p =\mid \mathcal{B} \mid$). Then the subproblem $P(x, \{1, \ldots, k\})$, obtained from the original problem P, is solved, where the first k variables are fixed to their values in the current incumbent solution x. If an improvement occurs, the VND-MIP procedure (see Figure 4.2) is performed over the whole search space and the process is repeated. If not, the number of fixed variables in the current subproblem is decreased. Note that by fixing only the variables whose distance values are equal to zero, i.e., setting $k = \max\{j \in \mathcal{B} \mid \delta_j = 0\}$, RINS scheme is obtained.

The specific implementation of the VND-MIP procedure used as a local search method within the VNDS-MIP (see line 10 in Figure 4.1) is desribed next. Input parameters for the VND-MIP algorithm are instance P of the $0-1$ MIP problem, total running time allowed t_{vnd}, time t_{mip} allowed for the MIP solver, maximum size rhs_{max} of the neighbourhood to be explored, and starting solution x'. The output is new solution obtained. The VND-MIP pseudo-code is given in Figure 4.2.

```
VNDS-MIP($P, d, t_{max}, t_{sub}, t_{vnd}, t_{mip}, rhs_{max}$)
1  Find an optimal solution $\overline{x}$ of LP($P$); **if** $\overline{x}$ is integer feasible **then return** $\overline{x}$.
2  Find the first feasible 0-1 MIP solution $x$ of $P$.
3  Set $t_{start} = cpuTime(\,)$, $t = 0$.
4  **while** $(t < t_{max})$
5      Compute $\delta_j =\mid x_j - \overline{x}_j \mid$ for $j \in \mathcal{B}$, and index the variables $x_j, j \in \mathcal{B}$.
       so that $\delta_1 \leq \delta_2 \leq \ldots \leq \delta_p$, $p =\mid \mathcal{B} \mid$
6      Set $n_d =\mid \{j \in \mathcal{B} \mid \delta_j \neq 0\} \mid$, $k_{step} = [n_d/d]$, $k = p - k_{step}$;
7      **while** $(t < t_{max})$ **and** $(k > 0)$
8          $x' =$ MIPSolve($P(x, \{1, 2, \ldots, k\})$, $t_{sub}$, $x$);
9          **if** $(c^T x' < c^T x)$ **then**
10             $x =$ VND-MIP($P, t_{vnd}, t_{mip}, rhs_{max}, x'$); **break**;
11         **else**
12             **if** $(k - k_{step} > p - n_d)$ **then** $k_{step} = \max\{[k/2], 1\}$;
13             Set $k = k - k_{step}$;
14             Set $t_{end} = cpuTime(\,)$, $t = t_{end} - t_{start}$;
15         **endif**
16     **endwhile**
17 **endwhile**
18 **return** $x$.
```

Figure 4.1: VNDS for MIPs.

At each iteration of VND-MIP algorithm, the pseudo-cut $\delta(\mathcal{B}, x', x) \leq rhs$, with the current value of rhs is added to the current problem (line 4). Then the CPLEX solver is called to obtain the next solution x'' (line 5), starting from the solution x' and within a given time limit. Thus, the search space for the MIP solver is reduced, and a solution is expected to be found (or the problem is expected to be proven infeasible) in a much shorter time than the time needed for the original problem without the pseudo-cut, as has been experimentally shown in [104] and [169]. The following steps depend on the status of the CPLEX solver. If an optimal or feasible solution is found (lines 7 and 10), it becomes a new incumbent and the search continues from its first neighbourhood ($rhs = 1$, lines 9 and 12). If the subproblem is solved exactly, i.e., optimality (line 7) or infeasibility (line 13) is proven, we do not consider the current neighbourhood in further solution space exploration, so the current pseudo-cut is reversed into the complementary one ($\delta(\mathcal{B}, x', x) \geq rhs + 1$, lines 8 and 14). However, if a feasible solution is found but has not been proven optimal, the last pseudo-cut is replaced with $\delta(\mathcal{B}, x', x) \geq 1$ (line 11), in order to avoid returning to this same solution again during the search process. In case of infeasibility (line 13), neighbourhood size is increased by one ($rhs = rhs + 1$, line 15). Finally, if the solver fails to find a feasible solution and also to prove the infeasibility of the current problem (line 16), the VND-MIP algorithm is terminated (line 17). The VND-MIP algorithm also terminates whenever the stopping criteria are met, i.e., the running time limit is reached, the maximum size of the neighbourhood is exceeded, or the feasible solution is not found (but the infeasibility is not proven).

Hence, the VNDS-MIP algorithm combines two approaches: hard variable fixing in the main scheme and soft variable fixing in the local search. In this way, the state-of-the-art heuristics for difficult MIP models are outperformed, as will be shown in Section 4.2 which discusses the computational results.

```
VND-MIP($P, t_{vnd}, t_{mip}, rhs_{max}, x'$)
1  $rhs = 1$; $t_{start} = cpuTime(\,)$; $t = 0$;
2  while ($t < t_{vnd}$ and $rhs \leq rhs_{max}$) do
3      $TimeLimit = \min(t_{mip},\ t_{vnd} - t)$;
4      add the pseudo-cut $\delta(\mathcal{B}, x', x) \leq rhs$;
5      $x''$ = MIPSolve($P$, $TimeLimit$, $x'$);
6      switch solutionStatus do
7        case "optSolFound":
8            reverse last pseudo-cut into $\delta(\mathcal{B}, x', x) \geq rhs + 1$;
9            $x' = x''$; $rhs = 1$;
10       case "feasibleSolFound":
11           replace last pseudo-cut with $\delta(\mathcal{B}, x', x) \geq 1$;
12           $x' = x''$; $rhs = 1$;
13       case "provenInfeasible":
14           reverse last pseudo-cut into $\delta(\mathcal{B}, x', x) \geq rhs + 1$;
15           $rhs = rhs + 1$;
16       case "noFeasibleSolFound":
17           Go to 20;
18     end
19     $t_{end} = cpuTime(\,)$; $t = t_{end} - t_{start}$;
20 end
21 return $x''$.
```

Figure 4.2: VND for MIPs.

The maximum number of sub-problems solved by decomposition with respect to current incumbent solution x (lines 7 - 16 of the pseudo-code in Figure 4.1) is $d + \log_2(|\{j \mid \overline{x}_j \in \{0,1\}\}|) < d + \log_2 n$. In case of pure 0-1 integer programming problems, there are 2^n possible values for objective function value,[1] so there can be no more than $2^n - 1$ improvements of the objective value. As a consequence, the total number of steps performed by VNDS cannot exceed $2^n(d + \log_2 n)$. This proves that a worst-case complexity of VNDS-MIP in a pure 0-1 case is $\mathcal{O}(2^n)$. Furthermore, for any 0-1 MIP problem in general, if no improvement has occurred by fixing values of variables to those of the current incumbent solution x, then the last sub-problem the algorithm attempts to solve is the original problem P. Therefore, the basic algorithm does not guarantee better performance than the general-purpose MIP solver used as a black-box within the algorithm. This means that running the basic VNDS-MIP as an exact algorithm (i.e. without imposing any limitations regarding the total running time or the maximum number of iterations) does not have any theoretical significance. Nevertheless, when used as a heuristic with a time limit, VNDS-MIP has a very good performance (see Section 4.2).

4.2 Computational Results

In this section we present the computational results for our algorithm. All results reported in this section are obtained on a computer with a 2.4GHz Intel Core 2 Duo E6600 processor and 4GB RAM, using general purpose MIP solver CPLEX 10.1. Algorithms were implemented in C++ and

[1]Note that the number of possible values of the objective function is limited to 2^n only in case of pure $0-1$ programs. In case of 0-1 mixed integer programs, there could be infinitely many possible values if objective function contains continuous variables.

compiled within Microsoft Visual Studio 2005.

Methods compared. The VNDS-MIP is compared with the four other recent MIP solution methods: variable neighbourhood branching (VNB) [169], local branching (LB) [104], relaxation induced neighbourhood search (RINS) [75] and the CPLEX MIP solver (with all default options but without RINS heuristic). The VNB and the LB use CPLEX MIP solver as a black box. The RINS heuristic is directly incorporated within a CPLEX branch-and-cut tree search algorithm. It should be noted that the objective function values for LB, VNB and RINS reported here are sometimes different from those given in the original papers. The reasons for this are the use of a different version of CPLEX and the use of a different computer.

Test bed. The 29 test instances which are considered here for comparison purposes are the same as those previously used for testing performances of LB and VNB (see [104], [169]) and most of the instances used for testing RINS (see [75]). The characteristics of this test bed are given in Table 4.1: the number of constraints is given in column one, the total number of variables is given in column two, column three indicates the number of binary variables, and column four indicates the best known published objective value so far.

In order to clearly show the differences between all the techniques, the models are divided into four groups, according to the gap between the best and the worst solution obtained using the five methods. Problems are defined as *very small-spread*, *small-spread*, *medium-spread*, and *large-spread* if the gap mentioned is less than 1%, between 1% and 10%, between 10% and 100% and larger than 100%, respectively. A similar way of grouping the test instances was first presented in Danna et al. [75], where the problems were divided into three sets. We use this way of grouping the problems mainly for the graphical representation of our results.

CPLEX parameters. As mentioned earlier, the CPLEX MIP solver is used in each method compared. A more detailed explanation of the way in which its parameters are used is provided here. For LB, VNB and VNDS, the `CPX_PARAM_MIP_ EMPHASIS` is set to `FEASIBILITY` for the first feasible solution, and then changed to the default `BALANCED` option after the first feasible solution has been found. Furthermore, for all instances except for `van`, all heuristics for finding the first feasible solution are turned off, i.e., both parameters `CPX_PARAM_HEUR_FREQ` and `CPX_PARAM_RINS_HEUR` are set to -1. This is done because of the empirical observation that the use of heuristic within CPLEX slows down the search process, without improving the quality of the final solution.

After the first feasible solution has been found, the local heuristics frequency (parameter `CPX_PARAM_HEUR_FREQ`) is set to 100. For the instance `van`, the first feasible solution cannot be found in this way within the given time limit, due to its numerical instability. So, for this instance, both parameters `CPX_PARAM_HEUR_FREQ` and `CPX_PARAM_RINS_HEUR` are set to 100 in order to obtain the first feasible solution, and after this the RINS heuristic is turned off.

Termination. All methods were run for 5 hours ($t_{max} = 18,000$ seconds), the same length of time as in the papers about local branching ([104]) and VNB ([169]). An exception is the `NSR8K`, which is the largest instance in the test bed. Due to the long time required for the first feasible solution to be attained (more than 13,000 seconds), 15 hours are allowed for solving this problem ($t_{max} = 54,000$).

VNDS Implementation. In order to evaluate the performance of the algorithm and its sensitivity to the parameter values, different parameter settings were tried out. As the goal was to make the algorithm user-friendly, an effort has been made to reduce the number of parameters. In addition, it was aimed to use the same values of parameters for testing most of the test instances. As the result of preliminary testing, the two variants of VNDS for MIP were obtained, which differ

Instance	**Number of constraints**	**Total number of variables**	**Number of binary variables**	**Best published objective value**
mkc	3411	5325	5323	-563.85
swath	884	6805	6724	467.41
danoint	664	521	56	65.67
markshare1	6	62	50	7.00
markshare2	7	74	60	14.00
arki001	1048	1388	415	7580813.05
seymour	4944	1372	1372	423.00
NSR8K	6284	38356	32040	20780430.00
rail507	509	63019	63009	174.00
rail2536c	2539	15293	15284	690.00
rail2586c	2589	13226	13215	947.00
rail4284c	4287	21714	21705	1071.00
rail4872c	4875	24656	24645	1534.00
glass4	396	322	302	1400013666.50
van	27331	12481	192	4.84
biella1	14021	7328	6110	3065084.57
UMTS	4465	2947	2802	30122200.00
net12	14115	14115	1603	214.00
roll3000	2295	1166	246	12890.00
nsrand_ipx	735	6621	6620	51360.00
a1c1s1	3312	3648	192	11551.19
a2c1s1	3312	3648	192	10889.14
b1c1s1	3904	3872	288	24544.25
b2c1s1	3904	3872	288	25740.15
tr12-30	750	1080	360	130596.00
sp97ar	1761	14101	14101	662671913.92
sp97ic	1033	12497	12497	429562635.68
sp98ar	1435	15085	15085	529814784.70
sp98ic	825	10894	10894	449144758.40

Table 4.1: Test bed information.

only in the set of parameters used for the inner VND subroutine. Moreover, an automatic rule for switching between these two variants has been determined. The details are given below.

VNDS with the first VND version (VNDS1). In the first version, neither the size of the neighbourhoods, nor the time for the MIP solver was restricted (apart from the overall time limit for the whole VND procedure). In this version, the number of parameters is minimised (following the main idea of VNS that there should be as few parameters as possible). Namely, the settings $t_{mip} = \infty$ and $rhs_{max} = \infty$ were made, leaving the input problem P, the total time allowed t_{vnd} and the initial solution x' as the only input parameters. This allowed four input parameters for the whole VNDS algorithm (apart from the input problem P): d, t_{max}, t_{sub} and t_{vnd}. The setting $d = 10$ is made in all cases[2], total running time allowed t_{max} as stated above, $t_{sub} = 1200s$ and $t_{vnd} = 900s$ for all models except `NSR8K`, for which we put $t_{sub} = 3600s$ and $t_{vnd} = 2100s$.

VNDS with the second VND version (VNDS2). In the second version of the VND procedure, it is aimed to reduce the search space and thereby hasten the solution process. Therefore, the maximal size of neighbourhood that can be explored is limited, as well as the time allowed for the MIP solver. Values for the parameters d and t_{max} are the same as in the first variant, and the other settings are as follows: $rhs_{max} = 5$ for all instances, $t_{sub} = t_{vnd} = 1200s$ for all instances except `NSR8K`, $t_{sub} = t_{vnd} = 3600s$ for `NSR8K`, and $t_{mip} = t_{vnd}/d$ (i.e. $t_{mip} = 360s$ for `NSR8K` and

[2] d is the number of groups in which the variables (which differ in the incumbent integral and LP relaxation solution) are divided, in order to define the increase k_{step} of neighbourhood size within VNDS (see Figure 4.1).

$t_{mip} = 120s$ for all other instances). Thus, the number of parameters for this second variant of VNDS is again limited to four (not including the input problem P): d, t_{max}, t_{vnd} and rhs_{max}.

Problems classification. The local search step in VNDS1 is obviously more computationally extensive and usually more time-consuming, since there are no limitations regarding the neighbourhood size and time allowed for the call to CPLEX solver. Therefore VNDS2 is expected to be more successful with problems requiring more computational effort to be solved. For the less demanding problems, however, it seems more probable that the given time limit will allow the first variant of VND to achieve greater improvement.

To formally distinguish between these types of problems, we say that the MIP problem P is *computationally demanding with respect to time limit* T, if the time needed for the default CPLEX MIP optimiser to solve it is greater than $2T/3$, where T is the maximum time allowed for a call to the CPLEX MIP optimiser. The MIP model P is said to be *computationally non-demanding with respect to the time limit* T, if it is not computationally demanding with respect to T. Since the time limit for all problems in the test bed used is already given, the computationally demanding problems with respect to 5 hours (or 15 hours for the `NSR8K` instance) will be referred to as *demanding problems*. Similarly, the computationally non-demanding problems with respect to 5 hours will be referred to as *non-demanding problems*.

As the step of the final method, the following decision is made: to apply VNDS1 to non-demanding problems and VNDS2 to demanding problems. Since this selection method requires solving each instance by the CPLEX MIP solver first, it can be very time consuming. Therefore, it would be better to apply another method, based solely on the characteristics of the instances. However,the complexity of such a method would be beyond the scope of this thesis, so the results are presented as obtained with the criterion described above. In Figure 4.3 the average performance of the two variants VNDS1 and VNDS2 over the problems in the test bed is provided (large-spread instances are not included in this plot[3]). As predicted, it is clear that in the early stage of the solution process, heuristic VNDS2 improves faster. However, due to the longer time allowed for solving subproblems, VNDS1 improves its average performance later. This pattern of behaviour is even more evident in Figure 4.4, where we presented the average gap change over time for demanding problems. However, from Figure 4.5, it is clear that a local search in VNDS1 is more effective within a given time limit for non-demanding problems. Even more, Figure 4.5 suggests that the time limit for non-demanding problems can be reduced.

Table 4.2 provides the time needed until the finally best found solution is reached for each of the two variants VNDS1 and VNDS2. The better of the two values for each problem is in bold. As expected, the average time performance of VNDS2 is better, due to the less extensive local search. In Table 4.3, the objective values and the CPLEX running time for reaching the final solution for all instances in the test bed are presented, both for VNDS1 and VNDS2 . The results for demanding problems, i.e., rows where CPLEX time is greater than 12,000 seconds (36,000 seconds for `NSR8K` instance), are typewritten in italic font, and the better of the two objective values is further bolded. The value selected according to previously described automatic rule is marked with an asterisk. From the results shown in Table 4.3, one can see that by applying the automatic rule for selecting one of the two parameters settings, the better of the two variants is chosen in 24 out of 29 cases (i.e., in 83% of cases). This further justifies the previously described classification

[3]Problems `marshare1` and `markshare2` are specially designed hard small 0-1 instances, with a non-typical behaviour. Being large-spread instances, their behaviour significantly affects the form of the plot 4.3. The time allowed for instance `NSR8K` is 15 hours, as opposed to 5 hours allowed for all other instances. Furthermore, it takes a very long time (more than 13,000 seconds) to obtain the first feasible solution for this instance. For these reasons, we decided to exclude these three large-spread instances from Figure 4.3.

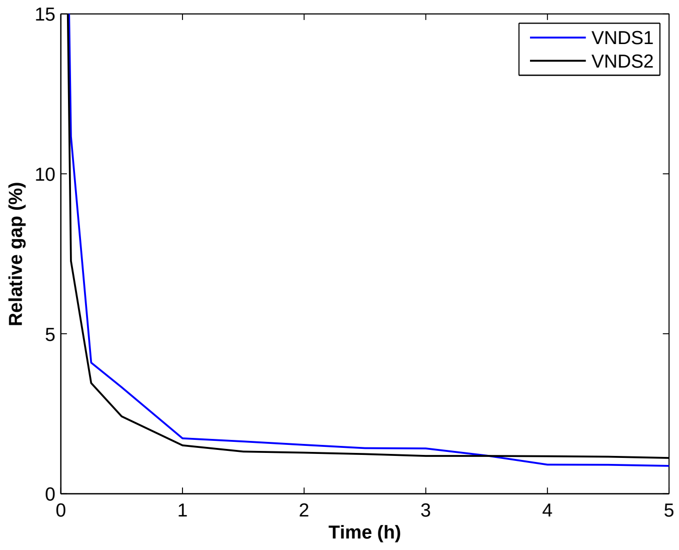


Figure 4.3: Relative gap average over all instances in test bed vs. computational time.

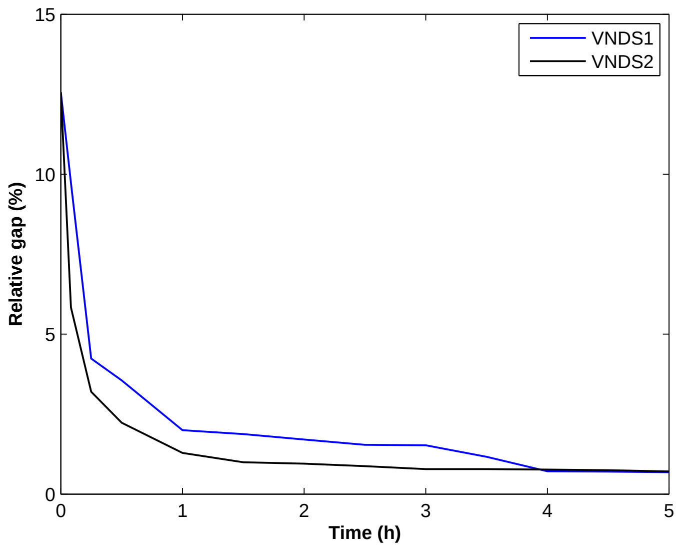


Figure 4.4: Relative gap average over demanding instances vs. computational time.

of problems and the automatic rule for selection between VNDS1 and VNDS2. With respect to running time, the better of the two variants is chosen in 15 out of 29 cases.

Comparison. In Table 4.4 the objective function values for the methods tested are presented. Here, the values are reported as obtained with one of the two parameters settings selected according to our automatic rule (see above explanation). For each instance, the best of the five values obtained in performed experiments is in bold, and the values which are better than the currently best known are marked with an asterisk.

It is worth mentioning here that most of the best known published results originate from the

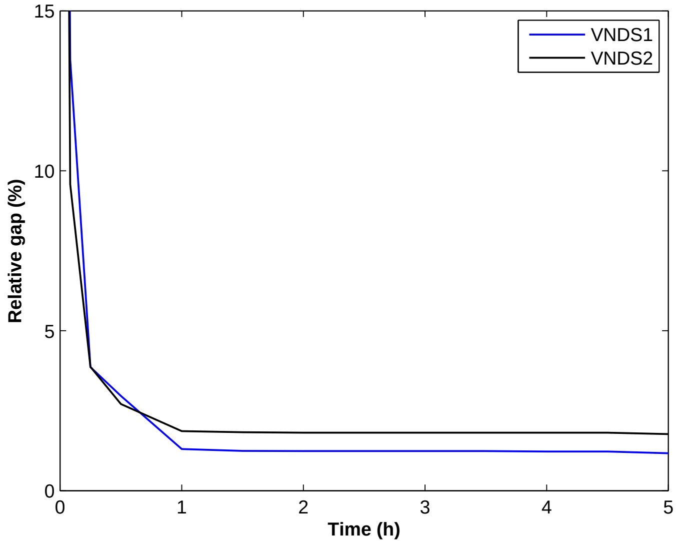


Figure 4.5: Relative gap average over non-demanding instances vs. computational time.

paper introducing the RINS heuristic [75]. However, these values were not obtained by pure RINS algorithm, but with hybrids which combine RINS with other heuristics (such as local branching, genetic algorithm, guided dives, etc.). In this thesis, however, the performance of the pure RINS algorithm, rather than different RINS hybrids is evaluated. It appears that:

(i) With VNDS-MIP heuristic, better objective values than the best published so far were obtained for as many as eight test instances out of 29 (`markshare1`, `markshare2`, `van`, `biella1`, `UMTS`, `nsrand_ipx`, `a1c1s1` and `sp97ar`). VNB improved the best known result in three cases (`markshare1`, `glass4` and `sp97ic`), and LB and RINS obtained it for one instance (`NSR8K` and `a1c1s1`, respectively); CPLEX alone did not improve any of the best known objective values.

(ii) With VNDS-MIP heuristic, the best result among all the five methods were reached in 16 out of 29 cases, whereas the RINS heuristic obtained the best result in 12 cases, VNB in 10 cases, CPLEX alone in 6 and LB in 2 cases.

In Table 4.5, the values of relative gap in % are provided. The gap is computed as

$$\frac{f - f_{best}}{|f_{best}|} \times 100,$$

where f_{best} is the better value of the following two: the best known published value, and the best among the five results we have obtained in our experiments. The table shows that the proposed VNDS-MIP algorithm outperforms on average all other methods; it has a percentage gap of only 0.654%, whereas the default CPLEX has a gap of 32.052%, pure RINS of 20.173%, local branching of 14.807%, and VNS branching of 3.120%.

Figure 4.6 shows how the relative gap changes with time for the instance `biella1`. The instance `biella1` was selected because it is a small spread instance, where the final gap values of different methods are very similar.

Figures 4.7-4.10 graphically displays the gaps for all the methods tested. Figures 4.7-4.10 show that the large relative gap values in most cases occur because the objective function value achieved by the VNDS algorithm is smaller than that of the other methods.

Instance	VNDS1 time (s)	VNDS2 time (s)
mkc	**6303**	9003
swath	**901**	3177
danoint	**2362**	3360
markshare1	12592	**371**
markshare2	**13572**	15448
arki001	**4595**	4685
seymour	**7149**	9151
NSR8K	54002	**53652**
rail507	2150	**1524**
rail2536c	13284	**6433**
rail2586c	**7897**	12822
rail4284c	**13066**	17875
rail4872c	10939	**8349**
glass4	3198	**625**
van	14706	**11535**
biella1	18000	**4452**
UMTS	11412	**6837**
net12	3971	**130**
roll3000	**935**	2585
nsrand_ipx	14827	**10595**
a1c1s1	1985	**1438**
a2c1s1	8403	**2357**
b1c1s1	**4595**	5347
b2c1s1	905	**133**
tr12-30	7617	**1581**
sp97ar	**16933**	18364
sp97ic	**2014**	3085
sp98ar	7173	**4368**
sp98ic	2724	**676**
average:	7650	**5939**

Table 4.2: VNDS1 and VNDS2 time performance.

Finally, Table 4.6 displays the computational time spent until the solution process is finished for all the methods. In computing the average time performance, instance `NSR8K` was not taken into account, since the time allowed for solving this model was 15 hours, as opposed to 5 hours for all other models. The results show that LB has the best time performance, with an average running time of nearly 6,000 seconds. VNDS-MIP is the second best method regarding the computational time, with an average running time of approximately 7,000 seconds. As regards the other methods, VNB takes more than 8,000 seconds on average, whereas both CPLEX and RINS take more than 11,000 seconds.

The values in Table 4.6 are averages obtained in 10 runs. All the actual values for a particular instance are within the $\pm 5\%$ of the value presented for that instance. Due to the consistency of the CPLEX solver, the objective value (if there is one) obtained starting from a given solution and within a given time limit is always the same. Therefore, the values in Table 4.4-4.5 are exact (standard deviation over the 10 runs is 0).

Statistical analysis. It is well known that average values are susceptible to outliers, i.e., it is possible that exceptional performance (either very good or very bad) in a few instances influences the overall performance of the algorithm observed. Therefore, comparison between the algorithms

Instance	VNDS1 objective value	VNDS2 objective value	CPLEX time (s)
mkc	***-563.85***	*-561.94**	*18000.47*
swath	**467.41***	480.12	1283.23
danoint	***65.67***	***65.67****	*18000.63*
markshare1	**3.00***	**3.00**	10018.84
markshare2	**8.00***	10.00	3108.12
arki001	**7580813.05***	7580814.51	338.56
seymour	***424.00***	*425.00**	*18000.59*
NSR8K	*20758020.00*	***20752809.00****	*54001.45*
rail507	**174.00***	**174.00**	662.26
rail2536c	**689.00***	**689.00**	190.194
rail2586c	*966.00*	***957.00****	*18048.787*
rail4284c	*1079.00*	***1075.00****	*18188.925*
rail4872c	*1556.00*	***1552.00****	*18000.623*
glass4	**1550009237.59***	1587513455.18	3732.31
van	*4.82*	***4.57****	*18001.10*
biella1	*3135810.98*	***3065005.78****	*18000.71*
UMTS	*30125601.00*	***30090469.00****	*18000.75*
net12	***214.00***	***214.00****	*18000.75*
roll3000	***12896.00***	*12930.00**	*18000.86*
nsrand_ipx	*51360.00*	***51200.00****	*13009.09*
a1c1s1	*11559.36*	***11503.44****	*18007.55*
a2c1s1	***10925.97***	*10958.42**	*18006.50*
b1c1s1	*25034.62*	***24646.77****	*18000.54*
b2c1s1	***25997.84***	***25997.84****	*18003.44*
tr12-30	**130596.00***	**130596.00**	7309.60
sp97ar	**662156718.08***	665917871.36	11841.78
sp97ic	431596203.84*	**429129747.04**	1244.91
sp98ar	**530232565.12***	531080972.48	1419.13
sp98ic	**449144758.40***	451020452.48	1278.13

Table 4.3: VNDS-MIP objective values for two different parameters settings. The CPLEX running time for each instance is also given to indicate the selection of the appropriate setting.

based only on the averages (either of the objective function values or of the running times) does not necessarily have to be valid. This is why the statistical tests were carried out, in order to confirm the significance of differences between the performances of the algorithms. Since no assumptions can be made about the distribution of the experimental results, a non-parametric (distribution-free) Friedman test [112] is applied, followed by the Bonferroni-Dunn [92] post hoc test, as suggested in [84](for more details on these statistical tests, see Appendix B).

Let $\mathcal{I}$ be a given set of problem instances and $\mathcal{A}$ a given set of algorithms. In order to perform the Friedman test, all the algorithms are ranked first, according to the objective function values (see Table 4.7) and running times (see Table 4.8). Average ranks by themselves provide a fair comparison of the algorithms. Regarding the solution quality, the average ranks of the algorithms over the $|\mathcal{I}| = 29$ data sets are 2.43 for VNDS-MIP, 2.67 for RINS, 3.02 for VNB, 3.43 for LB and 3.45 for CPLEX (Table 4.7). Regarding the running times, the average ranks are 2.28 for LB, 2.74 for VNDS-MIP, 2.78 for VNB, 3.52 for RINS, and 3.69 for CPLEX (Table 4.8). These results confirm the conclusions drawn from observing the average values: that VNDS-MIP is the best choice among the five methods regarding the solution quality and the second best choice, after LB, regarding the computational time. However, according to the average rankings, the second best method regarding the solution quality is RINS, followed by VNB, LB and CPLEX, in turn.

Instance	VNDS-MIP	VNB	LB	CPLEX	RINS
mkc	-561.94	**-563.85**	-560.43	**-563.85**	**-563.85**
swath	**467.41**	**467.41**	477.57	509.56	524.19
danoint	**65.67**	**65.67**	**65.67**	**65.67**	**65.67**
markshare1	**3.00***	**3.00***	12.00	5.00	7.00
markshare2	**8.00***	12.00	14.00	15.00	17.00
arki001	**7580813.05**	7580889.44	7581918.36	7581076.31	7581007.53
seymour	425.00	**423.00**	424.00	424.00	424.00
NSR8K	20752809.00	21157723.00	**20449043.00***	164818990.35	83340960.04
rail507	**174.00**	**174.00**	176.00	**174.00**	**174.00**
rail2536c	**689.00**	691.00	691.00	**689.00**	**689.00**
rail2586c	957.00	960.00	956.00	959.00	**954.00**
rail4284c	1075.00	1085.00	1075.00	1075.00	**1074.00**
rail4872c	1552.00	1561.00	**1546.00**	1551.00	1548.00
glass4	1550009237.59	**1400013000.00***	1600013800.00	1575013900.00	1460007793.59
van	**4.57***	4.84	5.09	5.35	5.09
biella1	**3065005.78***	3142409.08	3078768.45	3065729.05	3071693.28
UMTS	**30090469.00***	30127927.00	30128739.00	30133691.00	30122984.02
net12	**214.00**	255.00	255.00	255.00	**214.00**
roll3000	12930.00	**12890.00**	12899.00	**12890.00**	12899.00
nsrand_ipx	**51200.00***	51520.00	51360.00	51360.00	51360.00
a1c1s1	**11503.44***	11515.60	11554.66	11505.44	**11503.44***
a2c1s1	10958.42	10997.58	10891.75	**10889.14**	**10889.14**
b1c1s1	24646.77	25044.92	24762.71	24903.52	**24544.25**
b2c1s1	25997.84	25891.66	25857.17	25869.40	**25740.15**
tr12-30	**130596.00**	130985.00	130688.00	**130596.00**	**130596.00**
sp97ar	**662156718.08***	662221963.52	662824570.56	670484585.92	662892981.12
sp97ic	431596203.84	**427684487.68***	428035176.96	437946706.56	430623976.96
sp98ar	530232565.12	**529938532.16**	530056232.32	536738808.48	530806545.28
sp98ic	**449144758.40**	**449144758.40**	449226843.52	454532032.48	449468491.84

Table 4.4: Objective function values for all the 5 methods tested.

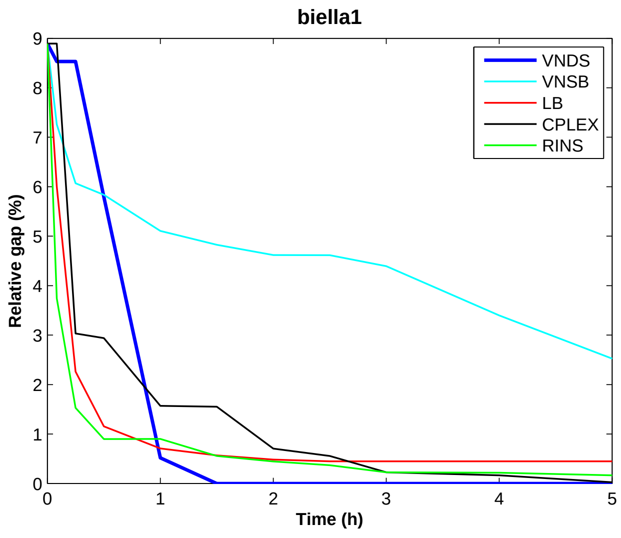


Figure 4.6: The change of relative gap with computational time for biella1 instance.

Regarding the computational time, the ordering of the methods by average ranks is the same as by average values.

In order to statistically analyse the difference between the ranks computed, the value of the F_F statistic is calculated for $|\mathcal{A}| = 5$ algorithms and $|\mathcal{I}| = 29$ data sets. This value is 2.49

Instance	VNDS-MIP	VNB	LB	CPLEX	RINS
mkc	0.337	**0.001**	0.607	**0.001**	**0.001**
swath	**0.000**	**0.000**	2.174	9.017	12.149
danoint	**0.000**	**0.000**	0.005	**0.000**	**0.000**
markshare1	**0.000**	**0.000**	300.000	66.667	133.333
markshare2	**0.000**	50.000	75.000	87.500	112.500
arki001	**0.000**	0.001	0.015	0.003	0.003
seymour	0.473	**0.000**	0.236	0.236	0.236
NSR8K	1.485	3.466	**0.000**	705.999	307.554
rail507	**0.000**	**0.000**	1.149	**0.000**	**0.000**
rail2536c	**0.000**	0.290	0.290	**0.000**	**0.000**
rail2586c	1.056	1.373	0.950	1.267	**0.739**
rail4284c	0.373	1.307	0.373	0.373	**0.280**
rail4872c	1.173	1.760	**0.782**	1.108	0.913
glass4	10.714	**0.000**	14.286	12.500	4.285
van	**0.000**	5.790	11.285	17.041	11.251
biella1	**0.000**	2.525	0.449	0.024	0.218
UMTS	**0.000**	0.124	0.127	0.144	0.108
net12	**0.000**	19.159	19.159	19.159	**0.000**
roll3000	0.310	**0.000**	0.070	**0.000**	0.070
nsrand_ipx	**0.000**	0.625	0.313	0.313	0.313
a1c1s1	**0.000**	0.106	0.445	0.017	**0.000**
a2c1s1	0.636	0.996	0.024	**0.000**	**0.000**
b1c1s1	0.418	2.040	0.890	1.464	**0.000**
b2c1s1	1.001	0.589	0.455	0.502	**0.000**
tr12-30	**0.000**	0.298	0.070	**0.000**	**0.000**
sp97ar	**0.000**	0.010	0.101	1.258	0.111
sp97ic	0.915	**0.000**	0.082	2.399	0.687
sp98ar	0.079	0.023	0.046	1.307	0.187
sp98ic	**0.000**	**0.000**	0.018	1.199	0.072
average gap:	**0.654**	3.120	14.807	32.052	20.173

Table 4.5: Relative gap values (in %) for all the 5 methods tested.

for the objective value rankings and 4.50 for the computational time rankings. Both values are greater than the critical value 2.45 of the F-distribution with $(|\mathcal{A}|-1, (|\mathcal{A}|-1)(|\mathcal{I}|-1)) = (4, 112)$ degrees of freedom at the probability level 0.05. Therefore, the null hypothesis that ranks do not significantly differ is rejected. This leads to a conclusion that there is a significant difference between the performances of the algorithms, both regarding solution quality and computational time.

Since the equivalence of the algorithms is rejected, the post hoc test is further performed. In the special case of comparing the control algorithm with all the others, the Bonferroni-Dunn test is more powerful than the Nemenyi test (see [84]), so the Bonferroni-Dunn test is chosen as the post-hoc test with VNDS-MIP as the control algorithm (see Appendix B). For $|\mathcal{A}| = 5$ algorithms, we get $q_{0.05} = 2.498$ and $q_{0.10} = 2.241$ (see [84]). According to the Bonferroni-Dunn test, the value of the critical difference is $CD = 1.037$ for $\alpha = 0.05$ and $CD = 0.931$ for $\alpha = 0.10$. Regarding the solution quality, from Table 4.9 we can see that, at the probability level 0.10, VNDS-MIP is significantly better than LB and CPLEX, since the corresponding average ranks differ by more than $CD = 0.931$. At the probability level 0.05, post hoc test is not powerful enough to detect any differences. Regarding the computational time, from Table 4.10, one can see that, at the probability level 0.10, VNDS-MIP is significantly better than CPLEX, since the corresponding

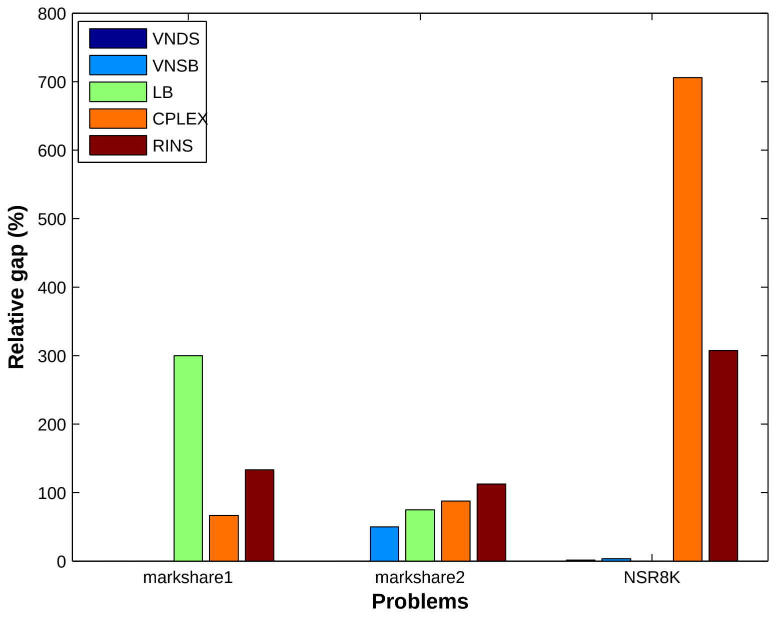


Figure 4.7: Relative gap values (in %) for large-spread instances.

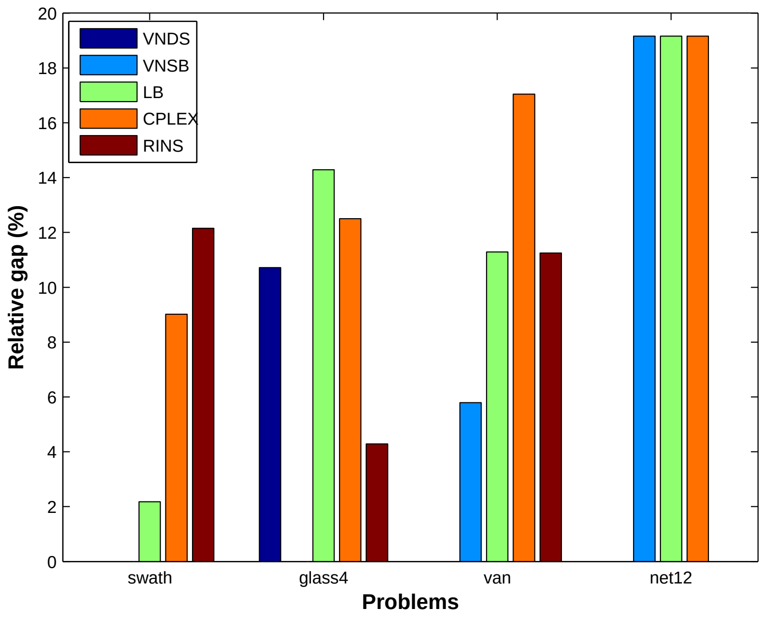


Figure 4.8: Relative gap values (in %) for medium-spread instances.

average ranks differ by more than $CD = 0.931$. Again, at the probability level 0.05, the post hoc test could not detect any differences. For the graphical display of average rank values in relation to the Bonferroni-Dunn critical difference from the average rank of VNDS-MIP as the control algorithm, see Figures 4.11-4.12.

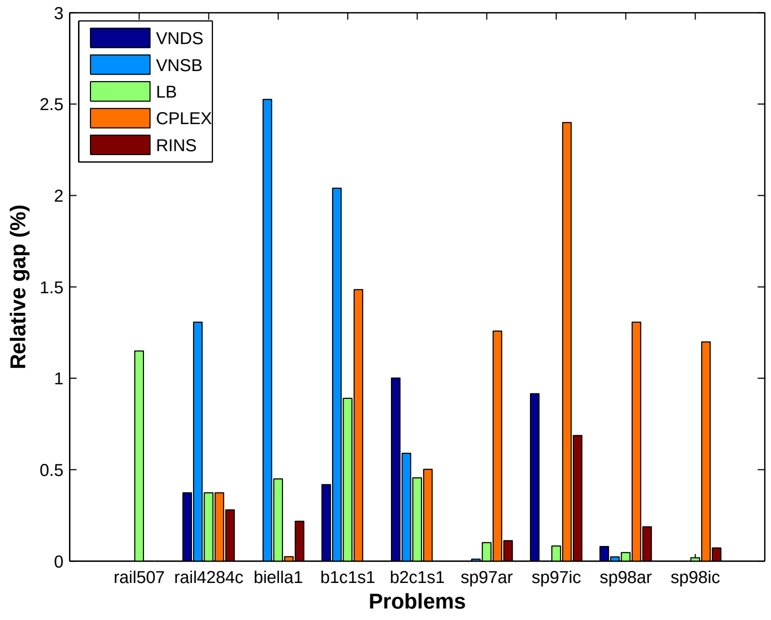


Figure 4.9: Relative gap values (in %) for small-spread instances.

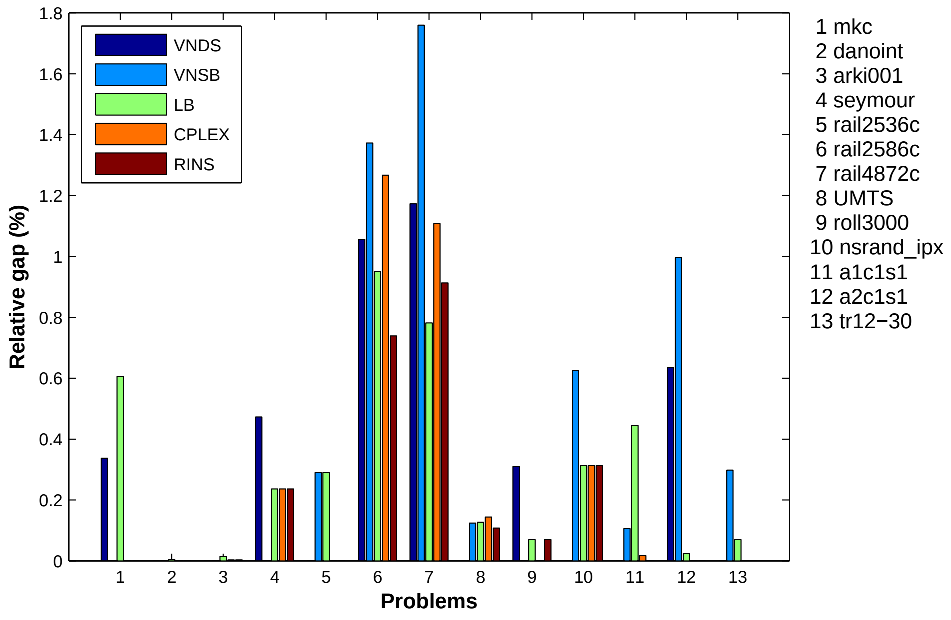


Figure 4.10: Relative gap values (in %) for very small-spread instances.

4.3 Summary

In this section a new approach for solving 0-1 MIP problems was proposed. The proposed method combines hard and soft variable fixing: hard fixing is based on the variable neighbourhood decomposition search framework, whereas soft fixing introduces pseudo-cuts as in local branching (LB)

Instance	VNDS-MIP	VNB	LB	CPLEX	RINS
mkc	9003	11440	**585**	18000	18000
swath	901	**25**	249	1283	558
danoint	3360	112	**23**	18001	18001
markshare1	12592	8989	**463**	10019	18001
markshare2	13572	14600	7178	**3108**	7294
arki001	4595	6142	10678	339	**27**
seymour	9151	15995	**260**	18001	18001
NSR8K	53651	53610	**37664**	54001	54002
rail507	2150	17015	**463**	662	525
rail2536c	13284	6543	3817	**190**	192
rail2586c	12822	15716	**923**	18049	18001
rail4284c	17875	**7406**	16729	18189	18001
rail4872c	8349	**4108**	10431	18001	18001
glass4	3198	10296	**1535**	3732	4258
van	11535	**5244**	15349.	18001	18959
biella1	**4452**	18057	9029	18001	18001
UMTS	6837	**2332**	10973	18001	18001
net12	**130**	3305	3359	18001	18001
roll3000	2585	**594**	10176	180001	14193
nsrand_ipx	10595	**6677**	16856	13009	11286
a1c1s1	**1438**	6263	15340	18008	18001
a2c1s1	2357	**690**	2102	18007	18002
b1c1s1	**5347**	9722	9016	18000	18001
b2c1s1	**133**	16757	1807	18003	18001
tr12-30	7617	18209	**2918**	7310	4341
sp97ar	16933	**5614**	7067	11842	8498
sp97ic	2014	7844	2478	1245	**735**
sp98ar	7173	6337	1647	1419	**1052**
sp98ic	2724	4993	2231	1278	**1031**
average time	6883	8103	**5846**	11632	11606

Table 4.6: Running times (in seconds) for all the 5 methods tested.

[104], according to the rules of the variable neighbourhood descent scheme [169]. Moreover, a new way to classify instances within a given test bed is proposed. We say that a particular instance is either computationally demanding or non-demanding, depending on the CPU time needed for the default CPLEX optimiser to solve it. Our selection of the particular set of parameters is based on this classification. However, it would be interesting to formulate another decision criterion, based solely on the mathematical formulation of the input problems, although deriving such criterion is beyond the scope of this thesis.

The VNDS-MIP proposed proves to perform well when compared with the state-of-the-art 0-1 MIP solution methods. More precisely, for the solution quality measures several criteria are considered: average percentage gap, average rank according to objective values and the number of times that the method managed to improve the best known published objective. The experiments show that VNDS-MIP proves to be the best in all the aspects stated. In addition, VNDS-MIP appears to be the second best method (after LB) regarding the computational time, according to both average computational time and average time performance rank. By performing a Friedman test on our experimental results, it is proven that a significant difference does indeed exist between the algorithms.

Instance	VNDS-MIP	VNB	LB	CPLEX	RINS
mkc	4.00	2.00	5.00	2.00	2.00
swath	1.50	1.50	3.00	4.00	5.00
danoint	2.50	2.50	5.00	2.50	2.50
markshare1	1.50	1.50	5.00	3.00	4.00
markshare2	1.00	2.00	3.00	4.00	5.00
arki001	1.00	2.00	5.00	4.00	3.00
seymour	5.00	1.00	3.00	3.00	3.00
NSR8K	2.00	3.00	1.00	5.00	4.00
rail507	2.50	2.50	5.00	2.50	2.50
rail2536c	2.00	4.50	4.50	2.00	2.00
rail2586c	3.00	5.00	2.00	4.00	1.00
rail4284c	3.00	5.00	3.00	3.00	1.00
rail4872c	4.00	5.00	1.00	3.00	2.00
glass4	3.00	1.00	5.00	4.00	2.00
van	1.00	2.00	3.50	5.00	3.50
biella1	1.00	5.00	4.00	2.00	3.00
UMTS	1.00	3.00	4.00	5.00	2.00
net12	1.50	4.00	4.00	4.00	1.50
roll3000	5.00	1.50	3.50	1.50	3.50
nsrand_ipx	1.00	5.00	3.00	3.00	3.00
a1c1s1	1.50	4.00	5.00	3.00	1.50
a2c1s1	4.00	5.00	3.00	1.50	1.50
b1c1s1	2.00	5.00	3.00	4.00	1.00
b2c1s1	5.00	4.00	2.00	3.00	1.00
tr12-30	2.00	5.00	4.00	2.00	2.00
sp97ar	1.00	2.00	3.00	5.00	4.00
sp97ic	4.00	1.00	2.00	5.00	3.00
sp98ar	3.00	1.00	2.00	5.00	4.00
sp98ic	1.50	1.50	3.00	5.00	4.00
average ranks	2.43	3.02	3.43	3.45	2.67

Table 4.7: Algorithm rankings by the objective function values for all instances.

Instance	VNDS-MIP	VNB	LB	CPLEX	RINS
mkc	2.00	3.00	1.00	4.50	4.50
swath	4.00	1.00	2.00	5.00	3.00
danoint	3.00	2.00	1.00	4.50	4.50
markshare1	4.00	2.00	1.00	3.00	5.00
markshare2	4.00	5.00	2.00	1.00	3.00
arki001	3.00	4.00	5.00	2.00	1.00
seymour	2.00	3.00	1.00	4.50	4.50
NSR8K	2.50	2.50	1.00	4.50	4.50
rail507	4.00	5.00	1.00	3.00	2.00
rail2536c	5.00	4.00	3.00	1.50	1.50
rail2586c	3.00	2.00	1.00	4.50	4.50
rail4284c	3.00	1.00	2.00	4.00	5.00
rail4872c	2.00	1.00	3.00	4.50	4.50
glass4	2.00	5.00	1.00	3.00	4.00
van	2.00	1.00	3.00	4.00	5.00
biella1	1.00	5.00	2.00	3.50	3.50
UMTS	2.00	1.00	3.00	4.50	4.50
net12	1.00	2.00	3.00	4.50	4.50
roll3000	2.00	1.00	3.00	5.00	4.00
nsrand_ipx	2.00	1.00	5.00	4.00	3.00
a1c1s1	1.00	2.00	3.00	4.50	4.50
a2c1s1	3.00	1.00	2.00	4.50	4.50
b1c1s1	1.00	3.00	2.00	4.50	4.50
b2c1s1	1.00	3.00	2.00	4.50	4.50
tr12-30	3.00	5.00	1.00	4.00	2.00
sp97ar	5.00	1.00	2.00	4.00	3.00
sp97ic	3.00	5.00	4.00	2.00	1.00
sp98ar	5.00	4.00	3.00	2.00	1.00
sp98ic	4.00	5.00	3.00	2.00	1.00
average ranks	2.74	2.78	2.28	3.69	3.52

Table 4.8: Algorithm rankings by the running time values for all instances.

ALGORITHM (average rank)	VNB (3.02)	LB (3.43)	CPLEX (3.45)	RINS (2.67)
Difference from VNDS-MIP rank (2.43)	0.59	1.00	1.02	0.24

Table 4.9: Objective value average rank differences from the average rank of the control algorithm VNDS-MIP.

ALGORITHM (average rank)	VNB (2.78)	LB (2.28)	CPLEX (3.69)	RINS (3.52)
Difference from VNDS-MIP rank (2.74)	0.03	-0.47	0.95	0.78

Table 4.10: Running time average rank differences from the average rank of the control algorithm VNDS-MIP.

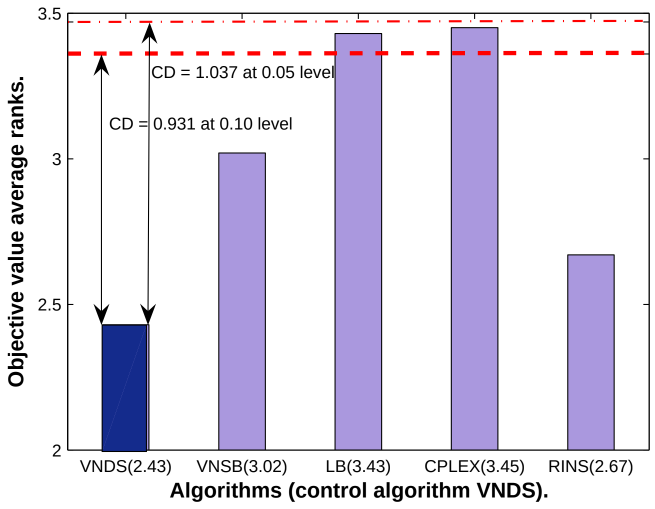


Figure 4.11: Average solution quality performance ranks with respect to Bonferroni-Dunn critical difference from the rank of VNDS-MIP as the control algorithm.

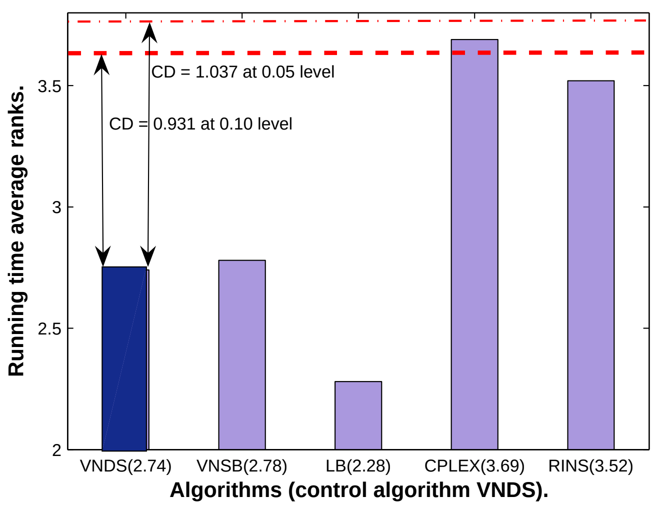


Figure 4.12: Average computational time performance ranks with respect to Bonferroni-Dunn critical difference from the rank of VNDS-MIP as the control algorithm.

Chapter 5

Applications of VNDS to Some Specific 0-1 MIP Problems

In Chapter 4, it has be shown that the proposed VNDS-MIP heuristic can be very effective in solving 0-1 MIP problems in general. In this chapter, attempts are made to further enhance the basic variant of VNDS-MIP and test the resulting heuristics on a few specific 0-1 MIP problems. The problems considered are the multidimensional knapsack problem in Section 5.1, the barge container ship routing problem in Section 5.2 and the two-stage stochastic mixed integer programming problem in Section 5.3.

5.1 The Multidimensional Knapsack Problem

In this section, new matheuristics for solving the multidimensional knapsack problem (MKP) are proposed. They are based on various decomposition strategies incorporated within the variable neighbourhood search, including both one-level and two-level decomposition. Basically, they can be viewed as enhancements of the basic VNDS-MIP scheme proposed in Chapter 4. In all proposed heuristics, pseudo-cuts are used in order to reduce the search space and to diversify the search process. Beside being competitive with the current state-of-the-art heuristics for MKP, this approach has led to 63 best known lower bound values and to 3 new lower bound values on two representative sets of MKP instances (for a total of 108 instances), studied for a long time. In addition, it is proven that two of the proposed methods converge to an optimal solution if no limitations regarding the execution time or the number of iterations are imposed.

The multidimensional knapsack problem (MKP) is a resource allocation problem which can be formulated as follows:

$$(5.1) \qquad (\text{MKP}) \left[\begin{array}{rll} \max & \sum\limits_{j=1}^{n} c_j x_j & \\ \text{subject to} & \sum\limits_{j=1}^{n} a_{ij} x_j \leq b_i & \forall i \in M = \{1,2,\ldots,m\} \\ & x_j \in \{0,1\} & \forall j \in N = \{1,2,\ldots,n\} \end{array} \right.$$

Here, n is the number of items and m is the number of knapsack constraints. The right hand side b_i ($i \in M$) represents the capacity of knapsack i. The matrix $A = [a_{ij}]$ is the weights matrix, whose element a_{ij} represents the resource consumption of the item $j \in N$ in the knapsack $i \in M$.

The profit income for the item $j \in N$ is denoted by c_j ($j \in N$). Being a special case of the 0-1 mixed integer programming problem (1.6), MKP is often used as a benchmark model for testing general purpose combinatorial optimisation methods.

A wide range of practical problems in business, engineering and science, can be modeled as MKP problems. They include the capital budgeting problem, cargo loading, allocating processors in a huge distributed computer system, cutting stock problem, delivery of groceries in vehicles with multiple compartments and many more. Since MKP is known to be NP-hard [115], there were numerous contributions over several decades to the development of both exact (mainly for the case $m = 1$, see, for instance, [222, 258, 261], and for $m > 1$, see, for instance [41, 111, 116]) and heuristic (for example [42, 58, 147, 326]) solution methods for MKP. For a complete review of these developments and applications of MKP, the reader is referred to [109, 328].

The mathematical programming formulation of MKP is especially convenient for the application of some general purpose solver. However, due to the complexity of the problem, sometimes it is not possible to obtain an optimal solution in this way. This is why a huge variety of problem specific heuristics has been tailored, their drawback being that they cannot be applied to a general class of problems. An approach for generating and exploiting small sub-problems was suggested in [121], based on the selection of consistent variables, depending on how frequently they attain particular values in good solutions and on how much disruption they would cause to these solutions if changed. More recently, a variety of neighbourhood search heuristics for solving optimisation problems have emerged, such as variable neighbourhood search (VNS) proposed in [237], large neighbourhood search (LNS) introduced in [294] and the large-scale neighbourhood search in [10]. In 2005, Glover proposed an adaptive memory projection (AMP) method for pure and mixed integer programming [124], which combines the principle of projection techniques with the adaptive memory processes of tabu search to set some explicit or implicit variables to some particular values. This philosophy gives a useful basis for unifying and extending a number of other procedures: LNS, local branching (LB) proposed in [104], the relaxation induced neighbourhood search (RINS) proposed in [75], variable neighbourhood branching (VNB) [169], or the global tabu search intensification using dynamic programming (TS-DP) [327] among others. LNS and RINS have been applied successfully to solve large-scale mixed integer programming problems. TS-DP is a hybrid method, combining adaptive memory and sparse dynamic programming to explore the search space, in which a move evaluation involves solving a reduced problem through dynamic programming at each iteration. Following the ideas of LB and RINS, another method for solving 0-1 MIP problems was proposed in [207](see also Chapter 4). It is based on the principles of variable neighbourhood decomposition search (VNDS) [168]. This method uses the solution of the linear programming relaxation of the initial problem to define sub-problems to be solved within the VNDS framework. In [298], a convergent algorithm for pure 0-1 integer programming was proposed. It solves a series of small sub-problems generated by exploiting information obtained through a series of relaxations. In further text, we refer to this basic algorithm as the linear programming-based algorithm (LPA). Hanafi and Wilbaut have proposed several enhanced versions of the Soyster's exact algorithm (see [154, 326]), by using a so called MIP relaxation of the problem. The first heuristic, which employs only the MIP relaxation, is referred to as the iterative relaxation based heuristic (IRH). The second one, in which MIP and LP relaxations are used in a parallel way, is referred to as the iterative independent relaxation based heuristic (IIRH).

This section is organised as follows. Subsection 5.1.1, provides an overview of the existing LPA, IRH and IIRH heuristics for MKP. In Subsection 5.1.2, the new heuristics are presented, based on the mixed integer and linear programming relaxations of the problem and the VNDS principle. Next, in Subsection 5.1.4, computational results are presented and discussed in an effort to assess and analyse the performance of the proposed algorithms. In Subsection 5.1.5, some outlines and conclusions are provided.

5.1.1 Related Work

An overview of the LPA [298], IRH and IIRH algorithms [154, 326] is provided here, since they are used later for the purpose of comparison with the new heuristics proposed in this section.

Linear Programming Based Algorithm

The LPA consists in generating two sequences of upper and lower bounds until justifying the completion of an optimal solution of the problem [298]. This is achieved by solving exactly a series of sub-problems obtained from a series of linear programming relaxations and adding a pseudo-cut in each iteration, which guarantees that sub-problems already explored are not revisited. For the sake of simplicity,the notation

$$P(x^0) = P(x^0, B(x^0)) \tag{5.2}$$

will be used in further text, to denote the reduced problem obtained by fixing the values of binary variables in P with binary values in a given vector x^0 (recall (2.4) and (2.9)) to the corresponding values in x^0.

At each iteration, LPA solves the reduced problem $P(\bar{x})$, obtained from an optimal solution $\bar{x}$ of the LP relaxation of the current problem. In practice, reduced problems within LPA can be very complex themselves, so LPA is normally used as a heuristic limited by a total number of iterations or a running time. Without the loss of generality, it can be assumed that $c_i > 0$, $i = 1, 2, \dots, n$. Let $c_{min} = \min\{c_i \mid i \in N\}$, $N = \{1, 2, \dots, n\}$. The outline of the LPA is given in Figure 5.1, where the input parameters are an instance P of the multidimensional knapsack problem and an initial feasible solution x^* of P.

```
LPA($P, x^*$)
 1  $Q = P$; $proceed$ = true;
 2  while ($proceed$) do
 3      $\overline{x}$ = LPSOLVE(LP($Q$));
 4      if $\overline{x} \in \{0,1\}^n$ then
 5          $x^* = argmax\{c^Tx^*, c^T\overline{x}\}$; break;
 6      endif
 7      $x^0$ = MIPSOLVE($P(\overline{x})$);
 8      if ($c^Tx^0 > c^Tx^*$) then $x^* = x^0$;
 9      $Q = (Q \mid \delta(B(\overline{x}), x, \overline{x}) \geq 1)$;
10      if ($B(\overline{x}) == \emptyset \;||\; c^T\overline{x} - c^Tx^* < c_{min}$) then $proceed$ = false;
11  endwhile
12  return $x^*$.
```

Figure 5.1: Linear programming based algorithm.

The LPA was originally proposed for solving pure 0-1 integer programming problems. In [154, 326], Hanafi and Wilbaut proposed several extensions for both pure 0-1 integer programming problems and 0-1 MIP problems in general. The validity of pseudo-cuts added within the LPA search process (line 9 in Figure 5.1) is guaranteed by Corollary 5.1 of Proposition 5.1. Corollary 5.1 is formulated as in [154] (where it was stated as a proposition on its own). Proposition 5.1 is a generalisation of the corresponding proposition in [154] and the proof provided below is based on the proof presented in [154]. A slightly different formulation of the Corollary 5.1 can also be found in [329].

Proposition 5.1 *Let P be a given $0-1$ mixed integer programming problem as defined in (1.6), $x^0 \in \{0,1\}^{|\mathcal{B}|} \times \mathbb{Z}_0^{+|\mathcal{G}|} \times \mathbb{R}_0^{+|\mathcal{C}|}$ and $J \subseteq \mathcal{B}$. An optimal solution of P is either an optimal solution of the reduced problem $P(x^0, J)$, or an optimal solution of the problem $(P \mid \delta(J, x^0, x) \geq 1)$.*

Proof. It is obvious that

$$\nu(P) = \min\{\nu((P \mid \delta(J, x^0, x) = 0)), \nu((P \mid \delta(J, x^0, x) \geq 1))\}$$

(recall that $\nu(P)$ denotes the optimal value of P). Since $P(x^0, J) = (P \mid \delta(J, x^0, x) = 0)$, if an optimal solution of P is not optimal for $P(x^0, J)$, it has to be optimal for $(P \mid \delta(J, x^0, x) \geq 1)$. ■

Corollary 5.1 *Let P be a given $0-1$ mixed integer programming problem, $\overline{x}$ a solution of* LP(P) *and x^0 an optimal solution of the reduced problem $P(\overline{x})$. An optimal solution of P is either the solution x^0 or an optimal solution of the problem $(P \mid \delta(B(\overline{x}), x, \overline{x}) \geq 1)$.*

Proof. Corollary 5.1 is obtained from Proposition 5.1 by substituting $x^0 = \overline{x}$ and $J = B(\overline{x})$. ■

Proposition 5.1 and Corollary 5.1 are formulated and proved for minimisation problems. Analogous results also hold for the case of maximisation. Therefore, the results of Proposition 5.1 and Corollary 5.1 (in their maximisation counterparts) are valid for the multidimensional knapsack problem. Corollary 5.1 implies Theorem 5.1, which states the finite convergence of the LPA [154, 325]. The proof of Theorem 5.1 is similar as in [325].

Theorem 5.1 *The LPA converges to an optimal solution of the input problem or indicates that the problem is infeasible in a finite number of iterations.*

Proof. There are $\binom{n}{k}2^k$ possible LP solution vectors $\overline{x}$ with exactly k integer components. Hence, there are $\sum_{k=0}^{n} \binom{n}{k}2^k = \sum_{k=0}^{n} \binom{n}{k}2^k 1^{n-k} = 3^n$ possible LP solution vectors $\overline{x}$ having integer components. However, if $\overline{x}$ is integer feasible, the algorithm stops. Therefore, the number of vectors whose all components are integer should be subtracted from the previously calculated total number of LP solutions to obtain the maximum number of LPA iterations. Thus, the total number of LPA iterations is limited by $3^n - 2^n$.

Let $F(Q)$ denote the feasible set of an optimisation problem Q. Let further P^k denote the problem considered in the kth iteration of LPA, P^{k+1} the problem obtained from P^k by adding the pseudo-cut in line 9 in Figure 5.1 to P^k and $\overline{x}^k$ the solution of LP(P^k). If

$$F^k = \bigcup_{i=1}^{k} F(P(\overline{x}^i, B(\overline{x}^i))),$$

then $F(P) = F^k \cup F(P^k)$ and $F^k \cap F(P^k) = \emptyset$. The incumbent best solution after k iterations of LPA is x^{*k}, such that

$$cx^{*k} = \max\{cx \mid x \in F^k\}.$$

According to Corollary 5.1, $\nu(P) = \max\{cx^{*k}, \max\{cx \mid x \in F(P^k)\}\}$. Since LPA finishes in a finite number of iterations k_{tot}, in the last iteration of LPA we have:

$$\nu(P) = \max\{cx^{*k_{tot}}, \max\{cx \mid x \in F(P^{k_{tot}})\}\}.$$

If $P^{k_{tot}}$ is infeasible, i.e. $F(P^{k_{tot}}) = \emptyset$, then $x^{*k_{tot}}$ is an optimal solution of P. Otherwise, $\nu(P) = \max\{cx^{*k_{tot}}, \nu(P^{k_{tot}})\}$ and LPA returns either $cx^{*k_{tot}}$ or an optimal solution of $P^{k_{tot}}$, whichever is better. ■

Iterative Relaxation Based Heuristics

Let P be a given 0-1 MIP problem as defined in (1.6) and $J \subseteq \mathcal{B}$. The *MIP relaxation* of P can be defined as:

$$\text{MIP}(P, J) = (\text{LP}(P) \mid x_j \in \{0, 1\}, j \in J). \tag{5.3}$$

The use of MIP relaxations for solving 0-1 MIP problems was independently proposed in [125] and [153]. In [326], it has been proved that MIP relaxation normally supplies tighter bounds than the LP relaxation. The corresponding proposition and proof are provided next, based on [326]. Although the following proposition was originally proposed for pure 0-1 integer programming problems, it should be emphasised that the same holds for 0-1 MIP problems in general, rather than only for the pure 0-1 case. The formulation of the proposition from [326] is amended accordingly.

Proposition 5.2 *Let P be a given 0-1 MIP problem as defined in (1.6). For any subsets $J, J' \subseteq \mathcal{B}$, such that $J' \subseteq J$, the following range of inequalities holds:*

$$\nu(P) \leq \nu(MIP(P, J)) \leq \nu(MIP(P, J')) \leq \nu(LP(P)).$$

Proof. Since $J' \subseteq J$, $\text{MIP}(P, J')$ is a relaxation of $\text{MIP}(P, J)$. Hence, $\nu(\text{MIP}(P, J)) \leq \nu(\text{MIP}(P, J'))$. Furthermore, $\nu(\text{MIP}(P, N)) = \nu(P)$, so $\nu(P) = \nu(\text{MIP}(P, N)) \leq \nu(\text{MIP}(P, J))$. Finally, $\nu(\text{MIP}(P, \emptyset)) = \nu(\text{LP}(P))$, so $\nu(\text{MIP}(P, J)) \leq \nu(\text{MIP}(P, \emptyset)) = \nu(\text{LP}(P))$, which completes the proof. ■

According to [326], empirical experience shows that combining both LP and MIP relaxations for solving 0-1 MIPs usually yields better lower bounds. In addition, this combination can lead to an efficient decrease and refinement of the upper bounds. Few 0-1 MIP solution heuristics which integrate LP and MIP relaxations were presented in [326]. Two of them are presented in this section: *iterative relaxation based heuristic* (IRH) and the *iterative independent relaxation based heuristic* (IIRH). The pseudo-code of the IRH heuristic is provided in Figure 5.2. In the following descriptions of IRH and IIRH, $\bar{x}$ and $\bar{x}^k$ denote optimal solutions of the LP relaxation of P and the current problem in the kth iteration, respectively, $\tilde{x}$ and $\tilde{x}^k$ denote optimal solutions of the MIP relaxations of P and the current problem in the kth iteration, respectively, $J^1(x) = \{j \in \mathcal{B} \mid x_j = 1\}$, and $J^*(x) = \{j \in \mathcal{B} \mid x_j \in (0, 1)\}$ for any $x \in \mathbb{R}^n$.

```
Procedure IRH($P$)
 2  Set $k = 1$; Set $P^1 = P$; Set $stop$ = false;
 3  repeat
 4      $\bar{x}^k$ = LPSolve(LP($P^k$));
 5      $\tilde{x}^k$ = MIPSolve(MIP($P^k$), $J^*(\bar{x}^k)$);
 6      $x^k$ = MIPSolve($P(\bar{x}^k)$);
 7      $y^k$ = MIPSolve($P(\tilde{x}^k)$);
 8      $\nu^* = \max(\nu^*, c^T x^k, c^T y^k)$; $\bar{\nu} = \min(c^T \bar{x}^k, c^T \tilde{x}^k)$;
 9      $P^{k+1} = (P^k \mid \{\delta(\bar{x}^k, x) \geq 1, \delta(\tilde{x}^k, x) \geq 1\})$;
10      $k = k + 1$;
12      Update $stop$;
13  until $stop$;
14  return $\nu^*, \bar{\nu}$;
```

Figure 5.2: An iterative relaxation based heuristic.

At each iteration, IRH solves both LP and MIP relaxations of the current problem to obtain relaxed solutions, $\bar{x}^k$ and $\tilde{x}^k$, respectively, used to generate two reduced problems $P(\bar{x}^k)$ and $P(\tilde{x}^k)$.

The feasible solutions x^k and y^k of these subproblems are then generated to update the current lower and upper bounds ν^* and $\bar{\nu}$. In addition, the current problem is updated by adding two different pseudo-cuts (see line 9 in Figure 5.2) and the whole process is iterated.

It is also possible to integrate MIP relaxations and LP relaxations into a MIP solution process in such a way that the MIP relaxation does not depend on the LP relaxation. The resulting heuristic, called iterative independent relaxation based heuristic (IIRH), is illustrated in Figure 5.3. More details about IRH and IIRH can be found in [326].

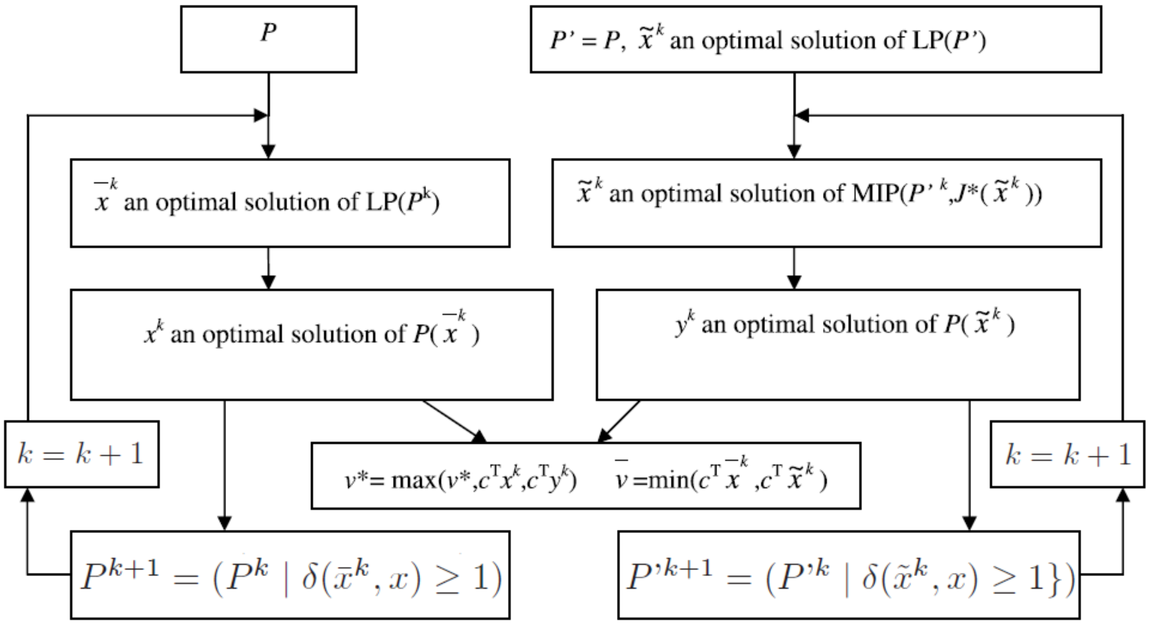

P
$P' = P$, $\tilde{x}^k$ an optimal solution of LP(P')
$\bar{x}^k$ an optimal solution of LP(P^k)
$\tilde{x}^k$ an optimal solution of MIP(P'^k,$J^*(\tilde{x}^k)$)
x^k an optimal solution of $P(\bar{x}^k)$
y^k an optimal solution of $P(\tilde{x}^k)$
$k = k + 1$
$\nu^* = \max(\nu^*, c^T x^k, c^T y^k)$ $\bar{\nu} = \min(c^T \bar{x}^k, c^T \tilde{x}^k)$
$k = k + 1$
$P^{k+1} = (P^k \mid \delta(\bar{x}^k, x) \geq 1)$
$P'^{k+1} = (P'^k \mid \delta(\tilde{x}^k, x) \geq 1\})$

Figure 5.3: An iterative independent relaxation based heuristic.

5.1.2 VNDS-MIP with Pseudo-cuts

The main drawback of the basic VNDS-MIP is the fact that the search space is not being reduced during the solution process (except for temporarily fixing the values of some variables). This means that the same solution vector may be examined many times, which may affect the efficiency of the solution process. This naturally leads to the idea of additionally restricting the search space by introducing pseudo-cuts, in order to avoid the multiple exploration of the same areas.

One obvious way to narrow the search space is to add the objective cut $c^T x > c^T x^*$, where x^* is the current incumbent solution, each time the objective function value is improved. This updates the current lower bound on the optimal objective value and reduces the new feasible region to only those solutions which are better (regarding the objective function value) than the current incumbent. In the basic VNDS-MIP version, decomposition is always performed with respect to the solution of the linear programming relaxation LP(P) of the original problem P. This way, the solution process ends as soon as all sub-problems $P(x, J_k)$ (recall (2.4)) are examined. In order to introduce further diversification into the search process, pseudo-cuts $\delta(J, \overline{x}, x) \geq k$ (recall (2.15) and (2.12)), for some subset $J \subseteq B(\overline{x})$ (recall (2.9)) and certain integer $k \geq 1$, are added whenever sub-problems $P(\overline{x}, J)$ are explored, completely or partially, by exact or heuristic approaches respectively. These pseudo-cuts guarantee the change of the LP solution $\overline{x}$ and also update the current upper bound on the optimal value of the original problem. This way, even if there is no improvement when decomposition is applied with respect to the current LP solution, the search process continues with the updated LP solution. Finally, further restrictions of the solution space can be obtained by keeping all the cuts added within the local search procedure VND-MIP.

The pseudo-code of the so obtained VNDS procedure for 0-1 MIPs, called `VNDS-MIP-PC1`, is presented in Figure 5.4. Input parameters for the `VNDS-MIP-PC1` algorithm are an instance P of the 0-1 MIP problem, parameter d which defines the number of variables to be released in each iteration, initial feasible solution x^* of P and the maximum size k_{vnd} of a neighbourhood explored within VND-MIP. The algorithm returns the best solution found within the stopping criteria defined by the variable *proceed*.

```
VNDS-MIP-PC1($P, d, x^*, k_{vnd}$)
 1  Choose stopping criteria (set $proceed1 = proceed2 =$ true);
 2  Add objective cut: $L = c^T x^*$; $P = (P \mid c^T x > L)$.
 3  while ($proceed1$) do
 4     Find an optimal solution $\overline{x}$ of LP($P$); set $U = \nu(\mathrm{LP}(P))$;
 5     if ($B(\overline{x}) = N$) break;
 6     $\delta_j = \mid x_j^* - \overline{x}_j \mid$; index $x_j$ so that $\delta_j \leq \delta_{j+1}$, $j = 1, \ldots, p-1$
 7     Set $n_d = \mid \{j \in N \mid \delta_j \neq 0\} \mid$, $k_{step} = [n_d/d]$, $k = p - k_{step}$;
 8     while ($proceed2$ and $k \geq 0$) do
 9        $J_k = \{1, \ldots, k\}$; $x' = \mathrm{MIPSOLVE}(P(x^*, J_k), x^*)$;
10        if ($c^T x' > c^T x^*$) then
11           Update objective cut: $L = c^T x'$; $P = (P \mid c^T x > L)$;
12           $x^* = \mathrm{VND\text{-}MIP}(P, k_{vnd}, x')$; $L = c^T x^*$; break;
13        else
14           if ($k - k_{step} > p - n_d$) then $k_{step} = \max\{[k/2], 1\}$;
15           Set $k = k - k_{step}$;
16        endif
17        Update $proceed2$;
18     endwhile
19     Add pseudo-cut to $P$ : $P = (P \mid \delta(B(\overline{x}), \overline{x}, x) \geq 1)$;
20     Update $proceed1$;
21  endwhile
22  return $L$, $U$, $x^*$.
```

Figure 5.4: VNDS-MIP with pseudo-cuts.

As opposed to the basic VNDS-MIP, the number of iterations in the outer loop of the `VNDS-MIP-PC1` heuristic is not limited by the number of possible objective function value improvements, but the number of all possible LP solutions which contain integer components. In case of a pure 0-1 integer programming problem, there are $\binom{n}{k}2^k$ possible solutions with k integer components, so there are $\sum_{k=1}^{n}\binom{n}{k}2^k = 3^n - 2^n$ possible LP solutions having integer components. Thus, the total number of iterations of `VNDS-MIP-PC1` is bounded by $(3^n - 2^n)(d + \log_2 n)$. The optimal objective function value $\nu(P)$ of current problem P is either the optimal value of

$(P \mid \delta(B(\overline{x}), \overline{x}, x) \geq 1)$, or the optimal value of $(P \mid \delta(B(\overline{x}), \overline{x}, x) = 0)$ i.e.

$$\nu(P) = \max\{\nu(P \mid \delta(B(\overline{x}), \overline{x}, x) \geq 1),\, \nu(P \mid \delta(B(\overline{x}), \overline{x}, x) = 0)\}.$$

If the improvement of the objective value is reached by solving subproblem $P(x^*, J_k)$, but the optimal value of P is $\nu(P \mid \delta(B(\overline{x}), \overline{x}, x) = 0)$, then the solution process continues by exploring the solution space of $(P \mid \delta(B(\overline{x}), \overline{x}, x) \geq 1)$ and fails to reach the optimum of P. Therefore, `VNDS-MIP-PC1` used as an exact method provides a feasible solution of the initial input problem P in a finite number of steps, but does not guarantee the optimality of that solution. One can observe that if sub-problem $P(\bar{x})$ is solved exactly before adding the pseudo-cut $\delta(B(\overline{x}), \overline{x}, x) \geq 1$ in P then the algorithm converges to an optimal solution. Again, in practice, when used as a heuristic with the time limit as a stopping criterion, `VNDS-MIP-PC1` has a very good performance (see Subsection 5.1.4).

Avoiding Redundancy in VNDS-MIP-PC1

To avoid redundancy in the search space exploration, two other variants are introduced, based on the following observation. The solution space of $P(x^*, J_\ell)$ is the subset of the solution space of $P(x^*, J_k)$ (with J_k as in line 9 of Figure 5.4), for $k < \ell, k, \ell \in \mathbb{N}$. This means that, in each iteration of `VNDS-MIP-PC1`, when exploring the search space of the current subproblem $P(x^*, J_k)$, the search space of the previous subproblem $P(x^*, J_{k+k_{step}})$ gets revisited. In order to avoid this repetition and possibly allow more time for exploration of those areas of the $P(x^*, J_k)$ search space which were not examined before, the search space of $P(x^*, J_{k+k_{step}})$ can be discarded by adding the cut $\delta(J_{k+k_{step}}, x^*, x) \geq 1$ to the current subproblem, i.e. solving $Q = (P(x^*, J_k) \mid \delta(J_{k+k_{step}}, x^*, x) \geq 1)$ instead of $P(x^*, J_k)$. The corresponding pseudo-code of this variant, called `VNDS-MIP-PC2`(P, d, x^*, k_{vnd}), is obtained from `VNDS-MIP-PC1`(P, d, x^*, k_{vnd}) (see Figure 5.4) by replacing line 9 with the following line $9'$:

$$9' : J_k = \{1, \ldots, k\}; x' = \text{MIPSOLVE}((P(x^*, J_k) \mid \delta(J_{k+k_{step}}, x^*, x) \geq 1), x^*);$$

Since the cut $\delta(J_{k+k_{step}}, x, x^*) \geq 1$ is only added to the current subproblem, but does not affect the original problem, the analysis regarding the number of iterations of VNDS-MIP-PC2 and the optimality/feasibility of the solution retrieved is the same as in the case of VNDS-MIP-PC1. Specifically, VNDS-MIP-PC2 as an exact method is guaranteed to finish in a finite number of iterations (bounded by $(3^n - 2^n)(d + \log_2 n)$) and returns a feasible solution of the original problem, but does not guarantee the optimality of the solution retrieved.

To further improve the version VNDS-MIP-PC2 in avoiding redundancy in the search space exploration, another version is considered, called `VNDS-MIP-PC3`(P, d, x^*, k_{vnd}), which is obtained from `VNDS-MIP-PC1`(P, d, x^*, k_{vnd}) by replacing the line 9 with the following line $9''$:

```
9'':  $J_k = \{1, \ldots, k\}; x' = \text{MIPSOLVE}(P(x^*, J_k), x^*);$
      $P = (P \mid \delta(J_k, x^*, x) \geq 1);$
```

and by dropping line 19 (the pseudo-cut $\delta(B(\overline{x}), \overline{x}, x) \geq 1$ is not used in this heuristic).

The following proposition states the convergence of the VNDS-MIP-PC3 algorithm for pure 0-1 integer programming problems.

Proposition 5.3 *The VNDS-MIP-PC3 algorithm finishes in a finite number of steps and either returns an optimal solution x^* of the original problem (if $L = U$), or proves the infeasibility of the original problem (if $L > U$).*

Proof. The number of outer loop iterations of `VNDS-MIP-PC3` is at most the number of all possible incumbent integer solutions, which is not greater than 2^n (because the cut $\delta(J_k, x^*, x) > 1$ enforces the change of incumbent integer solution in each iteration, except when $J_k = \emptyset$). When $J_k = \emptyset$, all possible integer solution vectors have been examined. The number of inner loop iterations is bounded by $d + \log_2 n$, so the total number of iterations is at most $2^n(d + \log_2 n)$.

The pseudo-cut $\delta(J_k, x^*, x) \geq 1$ does not necessarily change the optimal value of the LP relaxation of P at each iteration. However, we have that $P(x^*, J_k) = (P \mid \delta(J_k, x^*, x) = 0)$ and $\nu(P) = \max\{\nu((P \mid \delta(J_k, x^*, x) \geq 1)), \nu((P \mid \delta(J_k, x^*, x) = 0))\}$. So, if the optimal solution of the reduced problem $P(x^*, J_k)$ is not optimal for P, then the cut $\delta(J_k, x^*, x) \geq 1$ does not discard the optimal value of the original problem P. We have already proved that this algorithm finishes in a finite number of steps, so it follows that it either returns an optimal solution x^* of the original problem (if $L = U$), or proves the infeasibility of the original problem (if $L > U$). ■

Different Ordering Strategies.

In the VNDS-MIP variants discussed so far, variables in the incumbent integer solution were ordered according to the distances of their values to the values of the current linear programming relaxation solution. However, it is possible to employ different ordering strategies. For example, consider the following two problems:

$$(LP^-_{x^*})\left[\begin{array}{ll} & \min \delta(x^*, x) \\ \text{s.t.:} & Ax \leq b \\ & c^{\mathrm{T}}x \geq L + 1 \\ & x_j \in [0,1]\,,\ j \in N \end{array}\right. \qquad (LP^+_{x^*})\left[\begin{array}{ll} & \max \delta(x^*, x) \\ \text{s.t.:} & Ax \leq b \\ & c^{\mathrm{T}}x \geq L + 1 \\ & x_j \in [0,1]\,,\ j \in N \end{array}\right.$$

where x^* is the incumbent integer feasible solution and L is the best lower bound found so far (i.e., $L = c^{\mathrm{T}}x^*$). If $\overline{x}^-$ and $\overline{x}^+$ are optimal solutions of LP relaxation problems $LP^-_{x^*}$ and $LP^+_{x^*}$, respectively, then components of x^* could be ordered in ascending order of values $|\overline{x}^-_j - \overline{x}^+_j|$, $j \in N$. Since both solution vectors $\overline{x}^-$ and $\overline{x}^+$ are real-valued (i.e. from $\mathbb{R}^n$), this ordering technique is expected to be more sensitive than the standard one, i.e. the number of pairs (j, j'), $j, j' \in N, j \neq j'$ for which $|\overline{x}^-_j - \overline{x}^+_j| \neq |\overline{x}^-_{j'} - \overline{x}^+_{j'}|$ is expected to be greater than the number of pairs (h, h'), $h, h' \in N, h \neq h'$ for which $|x^*_h - \overline{x}_h| \neq |x^*_{h'} - \overline{x}_{h'}|$, where $\overline{x}$ is an optimal solution of the LP relaxation $LP(P)$. Also, according to the definition of $\overline{x}^-$ and $\overline{x}^+$, it is intuitively more likely that the variables x_j, $j \in N$, for which $\overline{x}^-_j = \overline{x}^+_j$, will have that same value $\overline{x}^-_j$ in the final solution, than it is for variables x_j, $j \in N$, for which $x^*_j = \overline{x}_j$ (and $\overline{x}^-_j \neq \overline{x}^+_j$), to have the final value x^*_j. In practice, if $\overline{x}^-_j = \overline{x}^+_j$, $j \in N$, then usually $x^*_j = \overline{x}^-_j$, which justifies the ordering of components of x^* in the described way. However, if we want to keep the number of iterations in one pass of VNDS-MIP approximately the same as in the standard ordering, i.e. if we want to use the same value for parameter d, then the subproblems examined will be larger than with the standard ordering, since the value of n_d will be smaller (see line 7 of Figure 5.4). The pseudo-code of this variant of VNDS-MIP, called `VNDS-MIP-PC4`, is provided in Figure 5.5. It is easy to prove that `VNDS-MIP-PC4` used as an exact method provides a feasible solution of the initial input problem P in a finite number of steps, but does not guarantee the optimality of that solution. As in the case of `VNDS-MIP-PC1`, one can observe that if subproblems $P(\bar{x}^+)$ and $P(\bar{x}^-)$ are solved exactly before adding pseudo-cuts $\delta(B(\overline{x}^+), \overline{x}^+, x) \geq 1$ and $\delta(B(\overline{x}^-), \overline{x}^-, x) \geq 1$ to P, then the algorithm converges to an optimal solution.

```
VNDS-MIP-PC4($P, d, x^*, k_{vnd}$)
1  Choose stopping criteria (set $proceed1$=$proceed2$=true);
2  Add objective cut: $L = c^{\mathrm{T}}x^*$; $P = (P \mid c^{\mathrm{T}}x > L)$.
3  while ($proceed1$) do
4      Find an optimal solution $\overline{x}$ of LP($P$); set $U = \nu(\mathrm{LP}(P))$;
5      if ($B(\overline{x}) = N$) break;
6      Find optimal solutions $\overline{x}^-$ of $LP^-_{x^*}$ and $\overline{x}^+$ of $LP^+_{x^*}$;
7      $\delta_j = \mid \overline{x}^-_j - \overline{x}^+_j \mid$; index $x_j$ so that $\delta_j \leq \delta_{j+1}$
8      Set $n_d = \mid \{j \in N \mid \delta_j \neq 0\} \mid$, $k_{step} = [n_d/d]$, $k = p - k_{step}$;
9      while ($proceed2$ and $k \geq 0$) do
10         $J_k = \{1, \ldots, k\}$; $x' = \mathrm{MIPSOLVE}(P(x^*, J_k), x^*)$;$P = (P \mid \delta(J_k, x^*, x) \geq 1)$;
11         if ($c^{\mathrm{T}}x' > c^{\mathrm{T}}x^*$) then
12             Update objective cut: $L = c^{\mathrm{T}}x'$; $P = (P \mid c^{\mathrm{T}}x > L)$;
13             $x^* = \mathrm{VND\text{-}MIP}(P, k_{vnd}, x')$; $L = c^{\mathrm{T}}x^*$; break;
14         else
15             if ($k - k_{step} > p - n_d$) then $k_{step} = \max\{[k/2], 1\}$;
16             Set $k = k - k_{step}$;
17         endif
18         Update $proceed2$;
19     endwhile
20     Add pseudo-cuts to $P$: $P = (P \mid \{\delta(B(\overline{x}^+), \overline{x}^+, x) \geq 1, \delta(B(\overline{x}^-), \overline{x}^-, x) \geq 1\})$;
21     Update $proceed1$;
22 endwhile
23 return $L$, $U$, $x^*$.
```

Figure 5.5: VNDS-MIP with upper and lower bounding and another ordering strategy.

5.1.3 A Second Level of Decomposition in VNDS

In this section we propose the use of a second level of decomposition in VNDS for the MKP. The MKP is tackled by decomposing the problem to several subproblems where the number of items to choose is fixed to a given integer value. Fixing the number of items in a knapsack to a given value $h \in \mathbb{N} \cup \{0\}$ can be achieved by adding the constraint $x_1 + x_2 + \ldots + x_n = h$, or, equivalently, $e^{\mathrm{T}}x = h$, where e is the vector of 1s.

Formally, let P_h be a subproblem obtained from the original problem by adding the hyperplane constraint $e^{\mathrm{T}}x = h$ for $h \in N$ and enriched by an objective cut, defined as follows:

$$(P_h) \left[\begin{array}{ll} \max & c^{\mathrm{T}}x \\ \text{s.t.:} & Ax \leq b \\ & c^{\mathrm{T}}x \geq L + 1 \\ & e^{\mathrm{T}}x = h \\ & x \in \{0,1\}^n \end{array} \right.$$

Solving the MKP by tackling separately each of the subproblems P_h for $h \in N$ appeared to be an interesting approach [41, 310, 311, 314] especially because the additional constraint ($e^{\mathrm{T}}x = h$) provides tighter upper bounds than the classical LP relaxation.

Let h_{min} and h_{max} denote lower and upper bounds of the number of variables with value 1 in an optimal solution of the problem. Then it is obvious that $\nu(P) = max\{\nu(P_h) \mid h_{min} \leq h \leq h_{max}\}$. Bounds $h_{min} = \lceil \nu(LP_0^-) \rceil$ and $h_{max} = \lfloor \nu(LP_0^+) \rfloor$ can be computed by solving the following two problems, where L is a lower bound on the objective value $\nu(P)$ of P:

$$(LP_0^-)\left[\begin{array}{ll} \min & e^{\mathrm{T}}x \\ \text{s.t.:} & Ax \leq b \\ & c^{\mathrm{T}}x \geq L+1 \\ & x \in [0,1]^n \end{array}\right. \qquad (LP_0^+)\left[\begin{array}{ll} \max & e^{\mathrm{T}}x \\ \text{s.t.:} & Ax \leq b \\ & c^{\mathrm{T}}x \geq L+1 \\ & x \in [0,1]^n \end{array}\right.$$

Exploring Hyperplanes in a Predefined Order

As we previously mentioned, the MKP problem P can be decomposed into several subproblems (P_h), such that $h_{min} \leq h \leq h_{max}$, corresponding to hyperplanes $e^{\mathrm{T}}x = h$. Based on this decomposition, we can derive several versions of the VNDS scheme. In the first variant considered, we define the order of the hyperplanes at the beginning of the algorithm, and then we explore them one by one, in that order. The ordering can be done according to the objective function values of linear programming relaxations LP(P_h), $h \in H = \{h_{min}, \dots, h_{max}\}$. In each hyperplane, `VNDS-MIP-PC2` is applied and if there is no improvement, the next hyperplane is explored. We refer to this method as `VNDS-HYP-FIX`. That corresponds to the pseudo-code in Figure 5.6. This idea is inspired by the approach proposed in [267], where the ordering of the neighbourhood structures in variable neighbourhood descent is determined dynamically, by solving relaxations of them.
It is important to note that the exact variant of `VNDS-HYP-FIX` (i.e. without any limitations regarding the running time or the number of iterations) converges to an optimal solution in a finite number of steps.

Proposition 5.4 *The VNDS-HYP-FIX algorithm finishes in a finite number of steps and either returns an optimal solution x^* of the original problem (if $L = U$), or proves the infeasibility of the original problem (if $L > U$).*

Proof. VNDS-HYP-FIX explores $h_{max} - h_{min}$ (a finite number) of hyperplanes and, in each hyperplane, the convergent `VNDS-MIP-PC3` is applied. Therefore, the best solution (with respect to the objective function value) among the optimal solutions found for all the hyperplanes is optimal for the original problem P. ■

```
VNDS-HYP-FIX($P, d, x^*, k_{vnd}$)
1  Solve the LP relaxation problems $LP_0^-$ and $LP_0^+$;
   Set $h_{min} = \lceil \nu(LP_0^-) \rceil$ and $h_{max} = \lfloor \nu(LP_0^+) \rfloor$;
2  Sort the set of subproblems $\{P_{h_{min}}, \dots, P_{h_{max}}\}$ so that
   $\nu(LP(P_h)) \leq \nu(LP(P_{h+1}))$, $h_{min} \leq h < h_{max}$;
3  Find initial integer feasible solution $x^*$;
4  for ($h = h_{min}; h \leq h_{max}; h++$)
5      $x' =$ VNDS-MIP-PC2($P_h, d, x^*, k_{vnd}$)
6      if ($c^{\mathrm{T}}x' > c^{\mathrm{T}}x^*$) then $x^* = x'$;
7  endfor
8  return $x^*$.
```

Figure 5.6: Two levels of decomposition with hyperplanes ordering.

Flexibility in Changing Hyperplanes

In the second variant we consider the hyperplanes in the same order as in the previous version. However, instead of changing the hyperplane only when the current one is completely explored, the change is allowed depending on other conditions (a given running time, a number of iterations without improving the current best solution, ...). Figure 5.7 provides a description of this algorithm, called `VNDS-HYP-FLE`, in which *proceed*3 corresponds to the condition for changing the hyperplane.

In this algorithm, we simply increase the value of h by one when the changing condition is satisfied; in case when $h = h_{max}$, h is fixed to the first possible value starting from h_{min}. When the best solution is improved, the values of h_{min} and h_{max} are also recomputed and the set H is updated if necessary (line 15 in Figure 5.7). In the same way, if a hyperplane is completely explored (or if it is proved not to contain an optimal solution) the set H is updated and the value of h is changed (line 8 in Figure 5.7). The condition *proceed*3 corresponds to a maximum running time fixed according to the size of the problem (see Subsection 5.1.4 for more details about parameters). It is easy to see that `VNDS-HYP-FLE` is not guaranteed to find an optimal solution of the input problem.

5.1.4 Computational Results

All values presented in this section are obtained using a Pentium 4 computer with 3.4GHz processor and 4GB RAM and general purpose MIP solver CPLEX 11.1 [183]. The C++ programming language was used to code the algorithms, which were compiled with g++ and the option -O2.

Test Bed

The proposed heuristics are validated on two sets of available and correlated instances of MKP. The first set is composed by 270 instances with $n = 100$, 250 and 500, and $m = 5$, 10, 30. These instances are grouped in the OR-Library, and the larger instances with $n = 500$ are known to be difficult. So we test our methods over the 90 instances with $n = 500$. In particular the optimal solutions of the instances with $m = 30$ are not known, whereas the running time needed to prove the optimality of the solutions for the instances with $m = 10$ is in general very important [41].

The second set of instances is composed by 18 MKP problems generated by [127], with number of items n between 100 and 2500, and number of knapsack constraints m between 15 and 100. We selected these problems because they are known to be very hard to solve by branch-and-bound technique.

Parameter Settings

As mentioned earlier, the CPLEX MIP solver is used in each method compared. We now give more detailed explanation how we use its parameters. We choose to set the `CPX_PARAM_MIP_ EMPHASIS` to `FEASIBILITY` for the first feasible solution, and then change to the default `BALANCED` option after the first feasible solution has been found.

Several variants of our heuristics use the same parameters. In all the cases we set the value of parameter d to 10, and we set $k_{vnd} = 5$. Furthermore, we allow running time $t_{sub} = t_{vnd} = 300s$

```
VNDS-HYP-FLE($P, d, x^*, k_{vnd}$)
 1  Solve the LP relaxation problems $LP_0^-$ and $LP_0^+$;
    set $h_{min} = \lceil \nu(LP_0^-) \rceil$ and $h_{max} = \lfloor \nu(LP_0^+) \rfloor$;
 2  Sort the set of subproblems $\{P_{h_{min}}, \ldots, P_{h_{max}}\}$ so that
    $\nu(LP(P_h)) \leq \nu(LP(P_{h+1}))$, $h_{min} \leq h < h_{max}$;
 3  Find an initial integer feasible solution $x^*$; $L = c^{\mathrm{T}} x^*$;
 4  Choose stopping criteria (set $proceed1$=$proceed2$=$proceed3$=true) ;
 5  Set $h = h_{min}$ and $P = P_h$;
 6  while ($proceed1$)
 7      Find an optimal solution $\overline{x}$ of LP($P$); $U = min\{U, \nu(\mathrm{LP}(P))\}$;
 8      if ($c^{\mathrm{T}} x^* \geq c^{\mathrm{T}} \overline{x}$ or $B(\overline{x}) = N$) then $H = H - \{h\}$ ;
        Choose the next value $h$ in $H$ and Set $P = P_h$;
 9      $\delta_j = | x_j^* - \overline{x}_j |$; index $x_j$ so that $\delta_j \leq \delta_{j+1}$
10      Set $n_d = | \{j \in N \mid \delta_j \neq 0\} |$, $k_{step} = [n_d/d]$, $k = p - k_{step}$;
11      while ($proceed2$ and $k \geq 0$)
12          $J_k = \{1, \ldots, k\}$; $x' = \mathrm{MIPSOLVE}(P(x^*, J_k), x^*)$;
13          if ($c^{\mathrm{T}} x' > c^{\mathrm{T}} x^*$) then
14              Update objective cut: $L = c^{\mathrm{T}} x'$; $P = (P \mid c^{\mathrm{T}} x > L)$;
15              Recompute $h_{min}$, $h_{max}$ and update $H$, $h$ and $P$ if necessary;
16              $x^* = \mathrm{VND\text{-}MIP}(P, k_{vnd}, x')$; $L = c^{\mathrm{T}} x^*$; break;
17          else
18              if ($k - k_{step} > p - n_d$) then $k_{step} = \max\{[k/2], 1\}$;
19              Set $k = k - k_{step}$;
20          endif
21          Update $proceed3$;
22          if ($proceed3$=false) then
                $proceed3$=true; goto 26;
23          Update $proceed2$;
24      endwhile
25      Add pseudo-cut to $P$ : $P = (P \mid \delta(B(\overline{x}), x, \overline{x}) \geq 1)$;
26      Update $proceed1$.
27  endwhile
28  return $L$, $U$, $x^*$.
```

Figure 5.7: Flexibility for changing the hyperplanes.

for calls to the CPLEX MIP solver for subproblems and calls to VND, respectively, for all instances in the test bed, unless otherwise specified. Finally, the running time limit is set to 1 hour (3,600 seconds) for each instance. VNDS-HYP-FLE has another parameter that corresponds to the running time before changing the value of σ (condition *proceed*3 in Figure 5.7). In our experiments this value is fixed at 900s (according to preliminary experiments).

Comparison

In Tables 5.1-5.3, the results obtained by all variants over the instances with $n = 500$ and $m = 5, 10, 30$ respectively, are provided. These values were obtained by several recent hybrid methods (see [41, 154, 311, 314, 326]). In these tables, in column "Best" the optimal value (or the best-known lower bound for $m = 30$) is reported. Then, for each variant, the difference between this best value and the value obtained by the observed heuristic is reported, as well as the CPU time to reach this value.

Table 5.1 shows that the proposed heuristics obtain good results over these instances, except for VNDS-HYP-FIX that visits only 3 optimal solutions. However, for $m = 5$ and $m = 10$ VNDS-HYP-FIX reaches good quality near-optimal solutions in much shorter time than other methods observed. The results for all variants are very similar, in particular for the average gap less than 0.001% (between 23 and 30 optimal solutions). One can also observe that VNDS-MIP slightly dominates the other variants in term of average running time needed to visit the optimal solutions, and that VNDS-HYP-FLE visits all the optimal solutions for these 30 instances. These results confirm the potential of VNDS for solving the MKP. Another encouraging point is the good behaviour of VNDS-HYP-FLE, which confirms the interest of using the hyperplane decomposition, even if the use of this decomposition seems to be sensitive (according to the results of VNDS-HYP-FIX). Finally, the VNDS-MIP-PC3 proves the optimality of the solution obtained for the instance 5.500.1 (the value is referred by a "*" in the table).

Table 5.2 shows that the behaviour of the heuristics is more different for larger instances. Globally the results confirm the efficiency of VNDS-MIP, even if it visits only 2 optimal solutions. VNDS-MIP-PC1 obtains interesting results with 6 optimal solutions and an average gap less than 0.01. That illustrates the positive impact of the upper and lower bounding in the VNDS scheme. That is also confirmed by the results of VNDS-MIP-PC2 with the visit of 5 optimal solutions and the same average gap. However the addition of the bouding method in these variants increases the average running time to reach the best solutions. The results obtained by VNDS-HYP-FIX confirm that this variant converges quickly to good solutions of MKP, but, in general, it soon gets stalled in the local optimum encountered during the search, due to the long computational time needed for exploration of particular hyperplanes. More precisely, since hyperplanes are explored successively, it is possible to explore only the first few hyperplanes within the CPU time allowed. Finally the VNDS-HYP-FLE is less efficient than for the previous instances. The increase of the CPU* can be easily explained by the fact that the hyperplane are explored iteratively. The quality of the lower bound can also be explained by the fact that the "good" hyperplanes can be explored insufficiently. However these results are still encouraging.

The results obtained for the largest instances with $m = 30$ are more difficult to analyse. Indeed, the values reported in Table 5.3 do not completely confirm the previous results. In particular we can observe that VNDS-MIP-PC3 is the "best" heuristic, if we consider only the average gap. In addition, the associated running time is not significantly greater than the running time of VNDS-MIP. It seems that, for these very difficult instances, the search space restrictions introduced in this heuristic have a positive effect over the VNDS scheme. The VNDS-MIP-PC4 is the most efficient heuristic if we consider only the number of best-known lower bounds visited. So, the other ordering strategy considered in this version, which can be considered as a diversification mechanism when compared to the other versions, conducts the search in promising regions for these instances. Finally, the methods based on the hyperplane decomposition are less efficient for these large instances, as expected. That confirms the previous conclusions for $m = 10$ that it is difficult to quickly explore all hyperplanes or perform a good selection of hyperplanes to be explored in an efficient way.

In Table 5.4, we provide the average results obtained by the proposed heuristics over the OR-Library instances. For each heuristic we report the average gap obtained for all objective values, and the number of optimal solutions (or best-known solutions) visited during the process.

The value $\alpha \in \{0.25, 0.5, 0.75\}$ was used to generate the instances according to the procedure in [110], and it corresponds to the correlation degree of the instances. There are 10 instances available for each (n, m, α) triplet. The main conclusions of this table can be listed as follows:

- According to the average gap, the VNDS-MIP-PC3 (very) slightly dominates the other variants based on VNDS-MIP. Globally, it is difficult to distinguish one version from the others.
- The VNDS-HYP-* are clearly dominated in average, but not clearly for $m = 10$ (in particular for VNDS-HYP-FLE and $\alpha > 0.5$).
- The VNDS-HYP-FLE obtains most optimal solutions, thanks to very good results for $m = 5$ and $m = 10, \alpha = 0.5$.
- All the variants have difficulties in tackling the largest instances with $m = 30$. However, if 1 hour of running time can be considered as an important value for heuristic approaches, it is necessary to observe that a large part of the optimal values and best-known values for the instances with $m = 10$ and $m = 30$, respectively, were obtained in a significantly short running time (see for instance [41, 314, 326].

According to the last remark, in Table 5.5 the average results obtained by the proposed heuristics with the running time limit set to 2 hours are reported. The results provided in this table are interesting since they show that if we increase the running time, then VNDS-MIP-PC1 dominates more clearly the VNDS-MIP heuristic, in particular for the instances with $m = 30$. That confirms the potential of the bounding approach. In addition, the results obtained by VNDS-MIP-PC4 are also really improved, confirming the interest in changing the ordering strategy for larger instances (with a larger running time). Globally the results of all the variants are clearly improved, in particular for $m = 30$ and $\alpha < 0.75$. Finally, a "*" is added for VNDS-MIP-PC1 and VNDS-MIP-PC4 when $m = 30$ and $\alpha = 0.25$ since these two variants visit one new best known solution for the instance 30.500-3 with an objective value equal to 115,370.

Tables 5.6-5.7 are devoted to the results obtained over the second data set of instances. Table 5.6 provides the overall results for all the heuristics compared to the best-known lower bounds reported in column "Best". These values were obtained by an efficient hybrid tabu search algorithm [310] and by the iterative heuristics proposed by Hanafi and Wilbaut [326]. Due to the large size of several instances and the long running time needed by the other approaches to obtain the best-known solutions, two different values for the running time of the proposed heuristics are used. The running time limit is set to 5 hours for the instances MK_GK04, MK_GK06 and MK_GK08-MK_GK11, and to 2 hours for all other MK_GK instances.

Table 5.6 demonstrates the global interesting behaviour of the proposed heuristics, which reach a significant number of best-known solutions and also two new best solutions. In general, the new versions derived from VNDS-MIP with some new modifications converge more quickly to the best solutions. That is particularly the case for the VNDS-MIP-PC1, VNDS-MIP-PC2 and VNDS-MIP-PC3. In average, we can observe that VNDS-MIP-PC1 obtains the best results. The previous conclusions about the hyperplane-based heuristics are still valid: the flexible scheme is more efficient for the medium size instances. However, for these instances the results obtained by VNDS-HYP-FIX are more encouraging, with the visit of a new best lower bound and the convergence to good lower bounds for the larger instances.

		VNDS-MIP		VNDS-MIP-PC1		VNDS-MIP-PC2		VNDS-MIP-PC3		VNDS-MIP-PC4		VNDS-HYP-FIX		VNDS-HYP-FLE	
inst.	Best	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*
5.500-0	120148	0	1524	3	794	0	2497	5	984	5	2859	38	120	0	1235
5.500-1	117879	0	138	0	475	0	525	0*	2663	16	2722	35	477	0	590
5.500-2	121131	0	2131	2	80	0	1999	0	2920	0	2524	47	167	0	484
5.500-3	120804	0	1703	5	3006	5	2807	5	2259	0	3138	17	373	0	3192
5.500-4	122319	0	93	0	7	0	203	0	303	0	240	0	35	0	323
5.500-5	122024	0	722	0	7	0	19	0	43	13	666	37	55	0	112
5.500-6	119127	0	580	0	2010	0	3195	0	2068	0	2567	20	538	0	322
5.500-7	120568	0	167	0	615	0	1067	0	1152	0	72	32	33	0	535
5.500-8	121586	0	1670	0	2820	11	1104	11	1109	11	209	18	222	0	901
5.500-9	120717	0	868	13	2943	6	3389	0	984	0	798	45	3458	0	3198
5.500-10	218428	0	170	0	316	0	648	0	12	3	1982	6	3211	0	1168
5.500-11	221202	0	704	0	356	0	435	0	1508	0	122	11	27	0	942
5.500-12	217542	0	1957	6	0	6	106	0	2341	0	389	0	2	0	1835
5.500-13	223560	0	89	0	10	0	236	0	133	0	738	26	16	0	301
5.500-14	218966	0	88	0	332	0	353	0	310	0	559	4	5	0	155
5.500-15	220530	0	1265	0	1562	0	953	0	1360	3	2417	44	3091	0	2075
5.500-16	219989	0	7	0	7	0	26	0	24	0	71	51	56	0	783
5.500-17	218215	0	1230	0	1875	0	1944	0	2391	0	91	35	812	0	774
5.500-18	216976	0	7	0	25	0	101	0	12	0	60	24	47	0	244
5.500-19	219719	0	457	0	437	0	648	0	833	0	1035	21	31	0	423
5.500-20	295828	0	5	0	5	0	47	0	71	0	28	40	135	0	1771
5.500-21	308086	0	2	0	235	0	268	0	162	3	855	20	226	0	28
5.500-22	299796	0	3	0	176	0	180	0	57	0	240	29	209	0	80
5.500-23	306480	0	2078	0	20	0	33	4	5	0	1041	11	81	0	35
5.500-24	300342	0	1	0	185	0	199	0	26	0	252	0	87	0	777
5.500-25	302571	0	1097	6	3076	0	1782	0	1625	0	909	22	40	0	133
5.500-26	301339	0	366	0	1355	0	1333	0	908	0	220	30	213	0	735
5.500-27	306454	0	366	0	1041	0	1183	0	524	0	759	32	11	0	212
5.500-28	302828	0	466	0	716	0	782	0	719	0	310	61	10	0	549
5.500-29	299910	4	0	4	16	6	28	4	67	0	281	29	51	0	2209
Avg. CPU*			665		817		936		919		938		461		871
Avg. Gap			<0.001		<0.001		<0.001		<0.001		<0.001		<0.001		0
#opt			29		23		25		25		23		3		30

Table 5.1: Results for the 5.500 instances.

		VNDS-MIP		VNDS-MIP-PC1		VNDS-MIP-PC2		VNDS-MIP-PC3		VNDS-MIP-PC4		VNDS-HYP-FIX		VNDS-HYP-FLE	
inst.	Best	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*
10.500-0	117821	12	326	21	1582	12	1580	12	419	42	1417	110	606	12	3044
10.500-1	119249	32	38	32	3547	32	847	32	348	49	2178	109	300	83	2711
10.500-2	119215	4	986	4	1163	4	2920	4	558	4	152	71	300	0	1847
10.500-3	118829	16	613	16	1867	16	2166	16	2006	16	611	54	399	16	1959
10.500-4	116530	21	27	21	1227	21	1527	50	1828	39	2992	89	917	37	2748
10.500-5	119504	14	852	25	1469	14	1170	14	1885	25	1364	91	300	43	364
10.500-6	119827	62	2411	14	911	37	606	55	1812	43	995	64	300	50	3494
10.500-7	118344	15	2409	21	2271	32	2870	32	1299	35	1728	98	919	11	3485
10.500-8	117815	39	3029	0	1233	34	2056	36	3338	39	378	27	454	39	600
10.500-9	119251	48	1231	33	1531	28	3332	44	3166	0	399	67	351	97	1825
10.500-10	217377	20	2315	0	1257	0	1557	0	1213	28	1111	43	2476	0	3399
10.500-11	219077	14	2721	16	2032	14	1999	11	3025	19	3060	57	901	14	1281
10.500-12	217847	50	1846	50	2447	0	2746	50	1404	0	211	92	26	0	1814
10.500-13	216868	0	63	0	93	0	393	0	363	17	904	0	69	0	1528
10.500-14	213873	14	1843	14	689	14	388	14	958	20	768	65	425	30	1225
10.500-15	215086	24	2579	24	1502	0	3002	50	1815	1	1944	11	430	0	1108
10.500-16	217940	33	2476	42	1042	9	3443	9	1496	9	3505	52	305	42	663
10.500-17	219990	6	2468	6	2154	6	1554	6	1475	21	2137	51	370	41	1954
10.500-18	214382	36	1932	27	3002	7	2402	30	3385	16	756	50	431	31	383
10.500-19	220899	27	877	17	1978	17	3191	27	1682	12	3188	63	334	27	3289
10.500-20	304387	37	1990	0	2218	24	3206	28	582	28	1665	49	302	34	1841
10.500-21	302379	32	2628	0	2000	23	3016	0	2113	21	1038	34	345	38	1650
10.500-22	302417	1	1824	1	2766	1	3041	8	1372	1	636	66	351	17	605
10.500-23	300784	27	2287	41	952	39	1226	41	1373	37	41	46	195	27	3072
10.500-24	304374	0	1258	0	1771	7	3577	8	2281	8	3575	33	182	17	3456
10.500-25	301836	40	1285	55	2174	40	1691	40	3112	40	3540	0	3509	40	2578
10.500-26	304952	3	663	3	1401	2	1391	1	393	0	411	3	1	7	1501
10.500-27	296478	12	717	12	2742	22	1234	12	3037	21	3349	68	335	22	2258
10.500-28	301359	2	2203	6	1044	2	1936	6	1601	15	489	44	358	6	1814
10.500-29	307089	17	1039	17	1044	0	1640	11	2475	0	724	51	102	17	1307
Avg. CPU*			1564		1703		2057		1727		1508		543		1960
Avg. Gap			0.013		0.009		0.009		0.013		0.012		0.034		0.016
#opt			2		6		5		3		4		2		5

Table 5.2: Results for the 10.500 instances.

		VNDS-MIP		VNDS-MIP-PC1		VNDS-MIP-PC2		VNDS-MIP-PC3		VNDS-MIP-PC4		VNDS-HYP-FIX		VNDS-HYP-FLE	
inst.	Best	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*
30.500-0	116056	124	3370	107	1628	132	2868	47	2543	78	2547	532	337	192	83
30.500-1	114810	30	2530	61	2945	30	2924	78	2534	78	3494	275	909	138	2510
30.500-2	116712	30	2993	51	2721	51	3093	27	2604	93	2910	208	912	279	15
30.500-3	115329	63	1796	64	3448	19	2505	19	2214	119	2831	135	307	153	7
30.500-4	116525	113	3410	91	3193	123	3240	70	1955	9	2885	291	637	119	2795
30.500-5	115741	7	3418	106	2381	15	1360	7	2864	7	2852	251	100	161	95
30.500-6	114181	33	542	168	991	162	2184	159	3240	125	3169	269	3526	137	1229
30.500-7	114348	98	1881	99	2108	53	1751	66	712	4	2219	315	1269	175	132
30.500-8	115419	0	2164	0	1008	0	1900	0	1652	161	1246	431	630	310	621
30.500-9	117116	93	3123	12	2448	93	1309	12	2317	0	3390	248	605	237	88
30.500-10	218104	71	2520	32	2052	36	839	36	3553	36	3211	175	3389	137	2727
30.500-11	214648	28	1319	57	2927	75	2241	27	2443	32	2329	300	3314	213	2423
30.500-12	215978	36	374	36	1808	36	1790	60	2076	77	1483	294	3473	122	14
30.500-13	217910	48	3251	48	1987	48	764	48	2171	109	3470	270	3306	218	3
30.500-14	215689	70	497	57	995	54	2486	57	2892	49	617	298	689	103	777
30.500-15	215890	21	2343	23	1346	21	1832	43	2782	23	1245	429	17	102	2693
30.500-16	215907	24	2211	24	2505	24	2181	24	2231	36	246	209	1513	129	5
30.500-17	216542	79	47	91	78	12	2804	97	952	76	3103	282	921	188	302
30.500-18	217340	3	1456	7	2063	3	547	3	660	28	2132	171	611	111	2768
30.500-19	214739	60	2656	88	2585	48	3516	52	3142	0	1280	205	3069	145	3006
30.500-20	301675	19	1468	19	1731	32	239	19	1177	32	400	224	3303	32	3016
30.500-21	300055	0	2022	7	3348	39	2148	7	1464	0	1959	190	304	95	3109
30.500-22	305087	25	1232	49	1661	11	2627	11	1254	11	2569	163	3310	148	4
30.500-23	302032	31	3166	17	2810	67	2166	28	1937	27	1017	166	932	79	3009
30.500-24	304462	35	3262	49	321	49	613	29	2687	37	2348	158	902	161	302
30.500-25	297012	53	1466	0	3307	53	1511	26	3044	29	3275	235	301	170	3309
30.500-26	303364	36	424	22	1825	22	2426	35	321	58	2001	285	3	131	2802
30.500-27	307007	8	2744	45	3044	70	2004	8	3352	74	2313	347	8	113	3
30.500-28	303199	37	2142	37	1363	41	435	37	1845	28	2105	288	912	135	9
30.500-29	300572	40	2189	56	1259	73	1432	40	2789	71	3449	309	305	137	617
Avg. CPU*			2067		2063		1925		2180		2270		1327		1282
Avg. Gap			0.027		0.032		0.030		0.023		0.031		0.152		0.091
# best			2		2		1		1		3		0		0

Table 5.3: Results for the 30.500 instances.

		5.500			10.500			30.500			
	α	0.25	0.5	0.75	0.25	0.5	0.75	0.25	0.5	0.75	Avg.
Avg. Gap	VNDS-MIP	0	0	<0.001	0.022	0.010	0.006	0.051	0.020	0.009	0.013
	VNDS-MIP-PC1	0.002	<0.001	<0.001	0.016	0.009	0.004	0.066	0.021	0.010	0.014
	VNDS-MIP-PC2	0.002	<0.001	<0.001	0.019	0.003	0.005	0.059	0.017	0.015	0.013
	VNDS-MIP-PC3	0.002	0	<0.001	0.025	0.009	0.005	0.042	0.021	0.008	0.012
	VNDS-MIP-PC4	0.004	<0.001	<0.001	0.025	0.007	0.006	0.058	0.022	0.012	0.015
	VNDS-HYP-FIX	0.002	0.01	0.001	0.066	0.022	0.013	0.256	0.122	0.078	0.067
	VNDS-HYP-FLE	0	<0.001	0	0.033	0.009	0.007	0.164	0.068	0.040	0.036
											Total
#opt	VNDS-MIP	10	10	9	0	1	1	1	0	1	33
	VNDS-MIP-PC1	6	9	8	1	2	3	1	0	1	31
	VNDS-MIP-PC2	7	9	9	0	4	1	1	0	0	31
	VNDS-MIP-PC3	7	10	8	0	2	1	1	0	0	29
	VNDS-MIP-PC4	6	8	9	1	1	2	1	1	1	30
	VNDS-HYP-FIX	1	1	1	0	1	1	0	0	0	5
	VNDS-HYP-FLE	10	10	10	1	4	0	0	0	0	35

Table 5.4: Average results on the OR-Library.

		10.500				30.500				Global
		0.25	0.5	0.75	Avg.	0.25	0.5	0.75	Avg.	Avg.
Avg. Gap	VNDS-MIP	0.015	0.004	**0.003**	**0.008**	0.029	0.015	0.009	0.018	0.013
	VNDS-MIP-PC1	**0.014**	0.007	**0.003**	**0.008**	0.020*	**0.012**	0.009	**0.014**	**0.011**
	VNDS-MIP-PC2	0.016	**0.003**	0.004	**0.008**	0.036	0.016	0.010	0.021	0.014
	VNDS-MIP-PC3	0.019	0.009	0.005	0.011	0.034	0.017	**0.006**	0.019	0.015
	VNDS-MIP-PC4	0.022	0.005	0.005	0.011	**0.016***	0.015	0.010	**0.014**	0.012
	VNDS-HYP-FIX	0.055	0.023	0.011	0.029	0.208	0.094	0.052	0.118	0.074
	VNDS-HYP-FLE	0.023	0.007	**0.003**	0.011	0.154	0.061	0.033	0.083	0.047
					Sub Total				Sub Total	Total
#opt	VNDS-MIP	1	3	3	7	1	1	2	4	11
	VNDS-MIP-PC1	2	2	4	**8**	3	2	1	**6**	**14**
	VNDS-MIP-PC2	0	5	2	7	2	0	0	2	9
	VNDS-MIP-PC3	0	2	2	4	1	0	1	2	6
	VNDS-MIP-PC4	1	3	2	6	3	2	1	**6**	12
	VNDS-HYP-FIX	0	1	1	2	0	0	0	0	2
	VNDS-HYP-FLE	1	4	3	**8**	0	0	0	0	8

Table 5.5: Extended results on the OR-Library.

				VNDS-MIP		VNDS-MIP-PC1		VNDS-MIP-PC2		VNDS-MIP-PC3		VNDS-MIP-PC4		VNDS-HYP-FIX		VNDS-HYP-FLE	
Inst.	n	m	Best	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*	Best-lb	CPU*
GK18	100	25	4528	0	1584	0	51	0	51	0	153	0	144	2	17	0	80
GK19	100	25	3869	0	22	0	321	0	299	0	296	0	65	2	2	0	613
GK20	100	25	5180	0	197	0	215	0	229	0	15	0	162	2	21	0	132
GK21	100	25	3200	0	302	0	63	0	63	0	742	0	181	2	358	0	713
GK22	100	25	2523	0	61	0	21	0	25	0	20	0	26	1	354	0	93
GK23	200	15	9235	0	172	0	1202	0	1583	0	729	0	1972	1	320	0	552
GK24	500	25	9070	0	2672	0	3021	2	614	1	342	0	1528	4	310	1	309
Mk_GK_01	100	15	3766	0	2	0	5	0	5	0	2	0	5	0	1	0	11
Mk_GK_02	100	25	3958	0	23	0	32	0	32	0	74	0	245	0	364	0	714
Mk_GK_03	150	25	5656	0	625	0	1380	0	1933	0	1307	0	524	1	770	0	3749
Mk_GK_04	150	50	5767	0	2458	**-1**	3673	0	7923	**-1**	6665	0	8677	0	1926	1	1837
Mk_GK_05	200	25	7560	0	3506	0	3191	0	1689	**-1**	882	1	204	**-1**	4913	0	306
Mk_GK_06	200	50	7678	1	9217	0	9641	1	15218	1	15688	0	14024	3	16006	0	8371
Mk_GK_07	500	25	19220	1	815	1	5169	0	6370	0	3533	2	3289	2	362	2	7186
Mk_GK_08	500	50	18806	2	5986	0	11658	0	4448	0	2287	2	5221	5	5605	7	14379
Mk_GK_09	1500	25	58091	4	3193	2	11148	3	7234	4	2535	2	3928	3	1893	5	10852
Mk_GK_10	1500	50	57295	4	13467	4	3787	3	6686	2	13275	5	17095	7	13395	8	2888
Mk_GK_11	2500	100	95237	9	11719	8	2581	9	8943	3	7461	11	6250	10	7996	14	1141
#best				12		13		13		11		12		3		11	
#imp				0		1		0		2		0		1		0	

Table 5.6: Average results on the GK instances.

To complete the analysis of these results, in Table 5.7 the results obtained by VNDS-MIP and VNDS-MIP-PC3 are compared with the current best algorithms for these instances. In this table, the values obtained by Vasquez and Hao [310] are reported in column "V&H", whereas the values for LPA, IIRH and IRH are reported as in [326]. These three algorithms were validated on the same computer, so the running time needed to reach the best solution by these methods is also reported. The hybrid tabu search algorithm of Vasquez and Hao was executed over several distributed computers, and it needs several hours to obtain the best solutions. This table confirms the efficiency of the heuristics proposed in this section, and in particular when combining some elements of the LPA with VNDS.

		LPA		IIRH		IRH		VNDS-MIP		VNDS-MIP-PC2	
Inst.	V&H	lb	CPU*	lb	CPU*	lb	CPU*	lb	CPU*	lb	CPU*
GK18	4528	4528	290	4528	**78**	4528	680	4528	1584	4528	153
GK19	3869	3869	65	3869	71	3869	25	3869	**22**	3869	296
GK20	5180	5180	239	5180	474	5180	365	5180	197	5180	**15**
GK21	3200	3200	**27**	3200	58	3200	245	3200	302	3200	742
GK22	2523	2523	60	2523	90	2523	117	2523	61	2523	**20**
GK23	9235	*9233*	5	9235	**44**	9235	184	9235	172	9235	729
GK24	9070	*9067*	1	*9069*	1168	9070	**2509**	9070	2672	*9069*	342
Mk_GK_01	3766	3766	**1**	3766	5	3766	**1**	3766	2	3766	2
Mk_GK_02	3958	3958	45	3958	50	3958	100	3958	**23**	3958	74
Mk_GK_03	5656	*5655*	457	5656	1924	5656	**32**	5656	625	5656	1307
Mk_GK_04	5767	5767	222	5767	282	5767	472	5767	2458	**5768**	6665
Mk_GK_05	7560	7560	458	7560	1261	7560	636	7560	3506	**7561**	882
Mk_GK_06	7677	7675	1727	**7678**	23993	**7678**	10042	7676	9217	7676	15688
Mk_GK_07	**19220**	19217	287	19219	8374	19219	15769	19219	815	**19220**	3533
Mk_GK_08	**18806**	18803	3998	18805	975	18805	11182	18804	5986	**18806**	2287
Mk_GK_09	58087	58082	396	**58091**	15064	58089	17732	58083	3193	58083	2535
Mk_GK_10	**57295**	57289	1999	57292	6598	57292	6355	57291	13467	57293	13275
Mk_GK_11	**95237**	95228	2260	95229	9463	95229	1921	95228	11719	95234	7461

Table 5.7: Comparison with other methods over the GK instances.

Statistical Analysis

As already mentioned in Chapter 4, the comparison between the algorithms based only on the averages does not necessarily have to be valid. By observing only the average gap values, one can only see that, in general, two-level decomposition methods are dominated by other VNDS-MIP based methods. However, due to the very small differences between the gap values, it is hard to say how significant this distinction in performance is. Also, it is difficult to single out any of the three proposed one-level decomposition methods. This is why statistical tests have been carried out to verify the significance of differences between the solution quality performances. Since no assumptions can be made about the distribution of the experimental results, a nonparametric (distribution-free) Friedman test [112] is applied, followed by the Nemenyi [245] post-hoc test (see Appendix B for more details about the statistical tests), as suggested in [84].

Let $\mathcal{I}$ denote the set of problem instances and $\mathcal{A}$ the set of algorithms. The Friedman test is carried out over the entire set of $|\mathcal{I}| = 108$ instances (90 instances from the OR library and 18 Glover & Kochenberger instances). Averages over solution quality ranks are provided in Table 5.8. According to the average ranks, VNDS-HYP-FIX has the worst performance with rank 4.74, followed by the VNDS-HYP-FLE with rank 3.46, whereas all other methods are very similar, with VNDS-MIP-PC3 being the best among the others. The value of the F_F statistic for $|\mathcal{A}| = 5$ algorithms and $|\mathcal{I}| = 108$ instances is 103.16, which is greater than the critical value 4.71 of the F-distribution with $(|\mathcal{A}| - 1, (|\mathcal{A}| - 1)(|\mathcal{I}| - 1)) = (4, 428)$ degrees of freedom at the probability level 0.001. Thus, we can conclude that there is a significant difference between the performances

Algorithm (Average Rank)	VNDS-MIP (2.25)	VNDS-MIP-PC1 (2.42)	VNDS-MIP-PC3 (2.12)	VNDS-HYP-FIX (4.74)	VNDS-HYP-FLE (3.46)
VNDS-MIP (2.25)	0.00	-	-	-	-
VNDS-MIP-PC1 (2.42)	0.17	0.00	-	-	-
VNDS-MIP-PC3 (2.12)	-0.13	-0.30	0.00	-	-
VNDS-HYP-FIX (4.74)	**2.49**	**2.32**	**2.62**	0.00	-
VNDS-HYP-FLE (3.46)	**1.21**	**1.04**	**1.34**	**-1.28**	0.00

Table 5.8: Differences between the average solution quality ranks for all five methods.

of the algorithms and proceed with the Nemenyi post-hoc test [245], for pairwise comparisons of all the algorithms.

For $|\mathcal{A}| = 5$ algorithms, the critical value q_α for the Nemenyi test at the probability level $\alpha = 0.05$ is $q_{0.05} = 2.728$ (see [84]), which yields the critical difference $CD = 0.587$. From Table 5.8, it is possible to see that VNDS-HYP-FIX is significantly worse than all the other methods, since its average rank differs more than 0.587 from all the other average ranks. Also, VNDS-HYP-FLE is significantly better than VNDS-HYP-FIX and significantly worse than all the other methods. Apart from that, there is no significant difference between any other two algorithms. Moreover, no more significant differences between the algorithms can be detected even at the probability level 0.1.

It is obvious that the result of the Friedman test above is largely affected by the very high ranks of the two-level decomposition methods, and it is still not clear whether there is any significant difference between the proposed one-level decomposition methods. In order to verify if any significant distinction between these three methods can be made, the Friedman test is further performed only on these methods, again over the entire set of 108 instances. According to the average ranks (see Table 5.9), the best choice is 1.85, followed by the basic VNDS-MIP with 2.01, whereas the variant VNDS-MIP-PC1 has the worst performance, having the highest rank 2.14. The value of the F_F statistic for $|\mathcal{A}| = 3$ one-level decomposition algorithms and $|\mathcal{I}| = 108$ data sets is 2.41. The test is able to detect the significant difference between the algorithms at the probability level 0.1, for which the critical value of the F-distribution with $(|\mathcal{A}|-1, (|\mathcal{A}|-1)(|\mathcal{I}|-1)) = (2, 214)$ degrees of freedom is equal to 2.33.

In order to further examine to which extent VNDS-MIP-PC3 is better than the other two methods, the Bonferroni-Dunn post-hoc test [92] is performed. The Bonferroni-Dunn test is normally used when one algorithm of interest (the control algorithm) is compared with all the other algorithms, since in that special case it is more powerful than the Nemenyi test (see [84]). The critical difference for the Bonferroni-Dunn test is calculated as for the Nemenyi test (see Appendix B), but with the different critical values q_α. For $|\mathcal{A}| = 3$ algorithms, the critical value is $q_{0.1} = 1.96$, which yields the critical difference $CD = 0.27$. Therefore, Table 5.9 shows that VNDS-MIP-PC3 is significantly better than VNDS-MIP-PC1 at the probability level $\alpha = 0.1$. The post-hoc test is not powerful enough to detect any significant difference between VNDS-MIP-PC3 and VNDS-MIP at this probability level.

Performance Profiles

Since small differences in running time can often occur due to the CPU load, the ranking procedure described above does not necessarily reflect the real observed runtime performance of the

Algorithm (Average Rank)	VNDS-MIP (2.01)	VNDS-MIP-PC1 (2.14)	VNDS-MIP-PC3 (1.85)
VNDS-MIP (2.01)	0.00	-	-
VNDS-MIP-PC1 (2.14)	0.13	0.00	-
VNDS-MIP-PC3 (1.85)	-0.16	**-0.30**	0.00

Table 5.9: Differences between the average solution quality ranks for the three one-level decomposition methods.

algorithms. This is why we use the performance profiling approach for comparing the effectiveness of the algorithms with respect to the computational time (see Appendix C and [87]).

Since different running time limits are set for the different groups of instances, performance profiling of the proposed algorithms is employed separately for the instances from the OR library (with the running time limit of 1 hour) and for those GK instances for which the running time limit is set to 2 hours. The plotting of the performance profiles of all seven algorithms for the 90 instances from the OR library is given in Figure 5.8. The logarithmic scale for τ is chosen in order to make a clearer distinction between the algorithms for the small values of τ. From Figure 5.8, it is clear that VNDS-HYP-FIX strongly dominates all other methods for most values of τ. In other words, for most values of τ, VNDS-HYP-FIX has the greatest probability of obtaining the final solution within a factor τ of the running time of the best algorithm. By examining the performance profile values for $\tau = 1$ (i.e. $\log_2(\tau) = 0$) in Figure 5.8, it can be concluded that VNDS-HYP-FIX is the fastest algorithm on approximately 41% of problems, basic VNDS-MIP is the fastest on approximately 19% of problems, VNDS-HYP-FLE is the fastest on approximately 18%, VNDS-MIP-PC4 on 9%, VNDS-MIP-PC1 and VNDS-MIP-PC2 on 5.5% and VNDS-MIP-PC3 on 2% of problems. Figure 5.8 also shows that the basic VNDS-MIP has the best runtime performance among all five one-level decomposition methods.

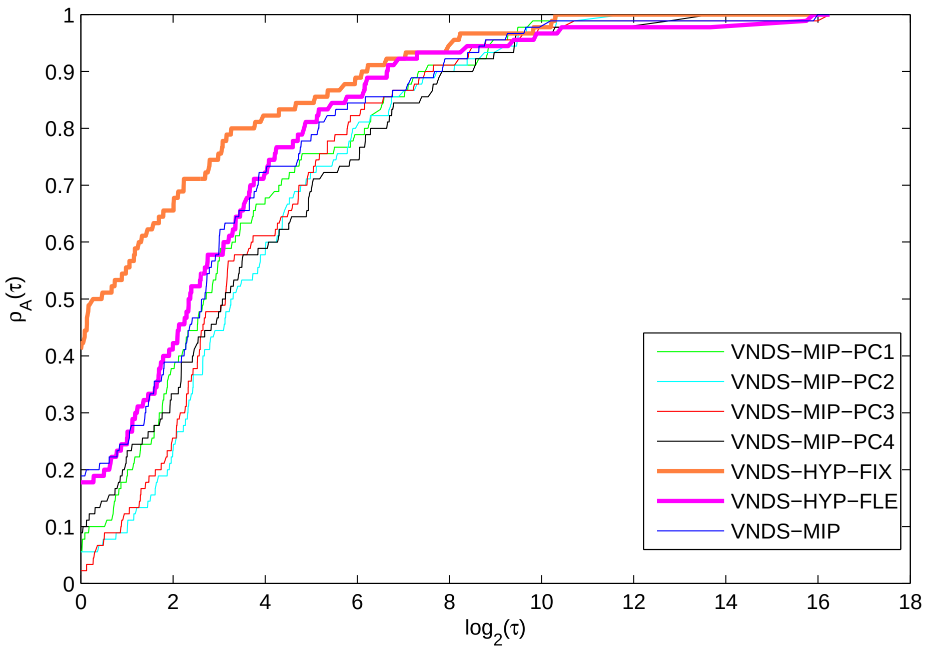


Figure 5.8: Performance profiles of all 7 algorithms over the OR library data set.

The performance profiles plot of all 7 methods for the 16 GK instances with running time limit set to 2 hours is given in Figure 5.9. Again, VNDS-HYP-FIX largely dominates all the other methods. However, VNDS-MIP-PC3 appears to be the best among the 5 one-level decomposition methods, since it dominates the others for most values of τ, and especially for small values of τ which are more directly related to the actual computational speed. By observing the performance profile values $\tau = 1$ in Figure 5.9, we can conclude that VNDS-HYP-FIX is the fastest algorithm on approximately 33% of problems, VNDS-MIP-PC3 is the fastest on 20% of problems, basic VNDS-MIP, VNDS-MIP-PC4 and VNDS-HYP-FLE all have the same number of wins and are fastest on approximately 13.3% of all instances observed, whereas VNDS-MIP-PC2 has the lowest number of wins and is fastest on only 7% of problems. It may be interesting to note that VNDS-HYP-FLE has much worse performance on the GK set: for small values of τ it is only better than VNDS-MIP-PC1 and VNDS-MIP-PC2, whereas for most larger values of τ it has the lowest probability of obtaining the final solution within the factor τ of the best algorithm.

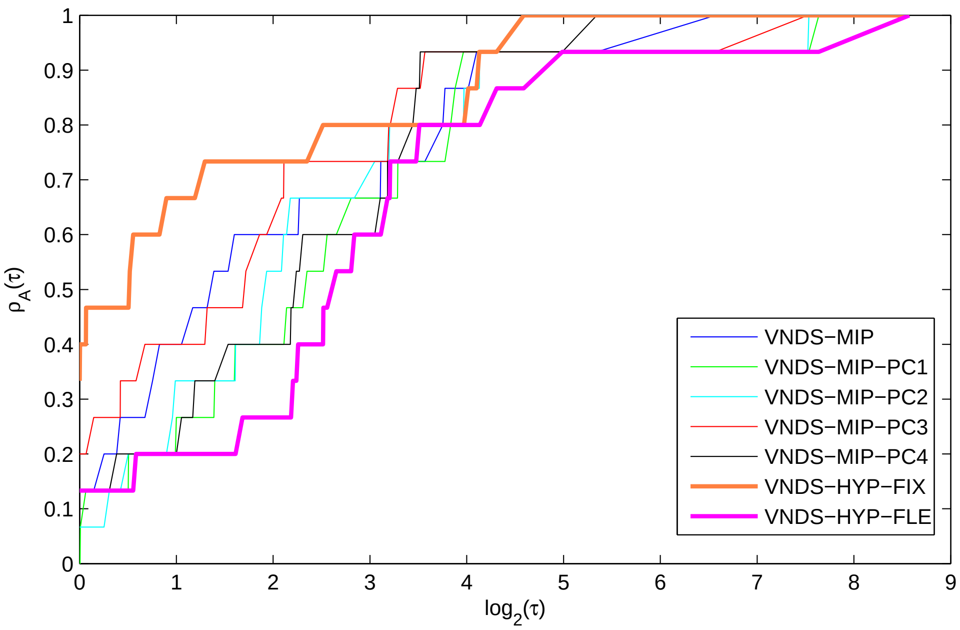


Figure 5.9: Performance profiles of all 7 algorithms over the GK data set.

5.1.5 Summary

In this section new heuristics for solving 0-1 MIP are proposed, which dynamically improve lower and upper bounds on the optimal value within VNDS-MIP. Different heuristics are derived by choosing a particular strategy of updating lower and upper bounds, and thus defining different schemes for generating a series of sub-problems. A two-level decomposition scheme is also proposed, in which sub-problems derived using one criterion are further divided into subproblems according to another criterion. The proposed heuristics have been tested and validated on the MKP.

Based on extensive computational analysis performed on benchmark instances from the literature and several statistical tests designed for the comparison purposes, we may conclude that VNDS based matheuristic has a lot of potential for solving MKP. One of the proposed variants, VNDS-MIP-PC3, which is theoretically shown to converge to an optimal solution, performs better than others in terms of solution quality. Furthermore, the proposed two-level decomposition methods are clearly the fastest in solving very large test instances, although not as effective as others in terms of solution quality. In fact VNDS-HYP-FIX, which is also proven to be convergent, is significantly faster than all the other methods. In summary, the results obtained show that this approach is efficient and effective:

- the proposed algorithms are comparable with the state-of-the-art heuristics,
- a few new best lower bound values are obtained.
- two of the proposed methods converge to an optimal solution if no limitations regarding the execution time or the number of iterations are imposed.

5.2 The Barge Container Ship Routing Problem

This section addresses the issue of barge container transport routes, connected to maritime container services. It means that this transport mode is considered as a hinterland transportation system. More precisely, we investigate the hinterland barge transport of containers arrived to or departing from a transshipment port (the sea port located at river mouth) by sea or mainline container ships. This clearly indicates that container barge transport acts, in this way, as a typical feeder service.

Determining transport routes of barge container ships has recently received a lot of attention [63, 197, 270]. One of the most important parts of this problem is adjusting the barge and sea container ships arrival times in the transshipment port. Optimality may be defined in accordance with various factors (total number of transported containers, satisfaction of customer demands, shipping company profit, etc.) [6, 273, 274, 295]. Obtaining an optimal solution by any factor is very important for doing successful transport business. Unfortunately, like in many other practical cases, the complexity of real life problems exceeds the capacity of the present computation systems.

In this section, alternative ways for solving this problem are discussed. The use of MIP solution heuristic methods is proposed to obtain good suboptimal solutions. Three state-of-the-art heuristics for 0-1 MIP problem are applied: local branching (LB) [104], variable neighbourhood branching (VNB) [169] and variable neighbourhood decomposition search for 0-1 MIP problems (VNDS-MIP) [207].

The rest of this section is organised as follows. In Subsection 5.2.1 we describe the considered problem: optimisation of transport routes of barge container ships. An intuitive description as well as the mathematical formulation is given and the problem complexity is discussed. Experimental evaluations are described in Subsection 5.2.2, while Subsection 5.2.3 contains concluding remarks.

5.2.1 Formulation of the Problem

The barge container ship routing problem addressed in this section corresponds to the problem of maximising the shipping company profit while picking up and delivering containers along the inland waterway. This form of problem was first studied in [220, 221]. The following assumptions impose the restrictions on the routing:

- the model assumes a weekly known cargo demand for all port pairs (origin–destination); this assumption is valid as the data regarding throughput from previous periods and future prediction allow obtaining reliable values of these demands;

- the barge shipping company has to deal with transshipment costs, port dues and empty container repositioning costs, in addition to the cost of container transport;
- maximum allowed route time, including sailing time and service time in ports, has to be set in accordance with the schedule of the mainline sea container ship calling at the transshipment port;
- the ship follows the same route during a pre-specified planning time horizon; as a common assumption, it may be assumed that this horizon is one year long;
- the demand for empty containers at a port is the difference between the total traffic originating from the port and the total loaded container traffic arriving at the port for the specified time period; the assumption is valid since this study addresses the problem of determining the optimal route of a barge container ship for only one ship operator (similar to the case studied by [295]);
- empty container transport [69, 82, 202] does not occur additional costs as it is performed using the excess capacity of barge company ships (this transport actually incurs some costs, but its value is negligible in comparison with empty container handling, storage and leasing costs);
- if a sufficient container quantity is not available at a port, the shortage is made up by leasing containers with the assumption that there are enough containers to be leased (for details see [295]).

Problem Overview

Routing is a fairly common problem in transport, but the barge container transport problem addressed here has certain intrinsic features that make the design of transport routes and corresponding models particularly difficult:

- the barge shipping company (or charterer) wants to hire a ship or tow for a period of one or several years ('period time charter') in order to establish container service on a certain inland waterway;
- all the container traffic emanating from a port may not be selected for transport even if that port is included in the route;
- the trade route is characterised by one sea or hub port located at a river mouth and several intermediate calling river ports;
- the barge container ship route corresponds to a feeder container service; the starting and ending point on the route should be the same, i.e. in this case it is the sea port where transshipment of containers from barge to sea container ships and vice versa takes place;
- the barge container ship travels upstream from the starting sea port to the final port located on the inland waterway, where from the ship sails in the downstream direction to the same sea port ending the route;
- it is not necessary for the barge container ship to visit all ports on the inland waterway; in some cases, calling at a particular port or loading all containers available at that port may not be profitable;
- the ship doesn't have to visit the same ports in upstream and downstream directions.

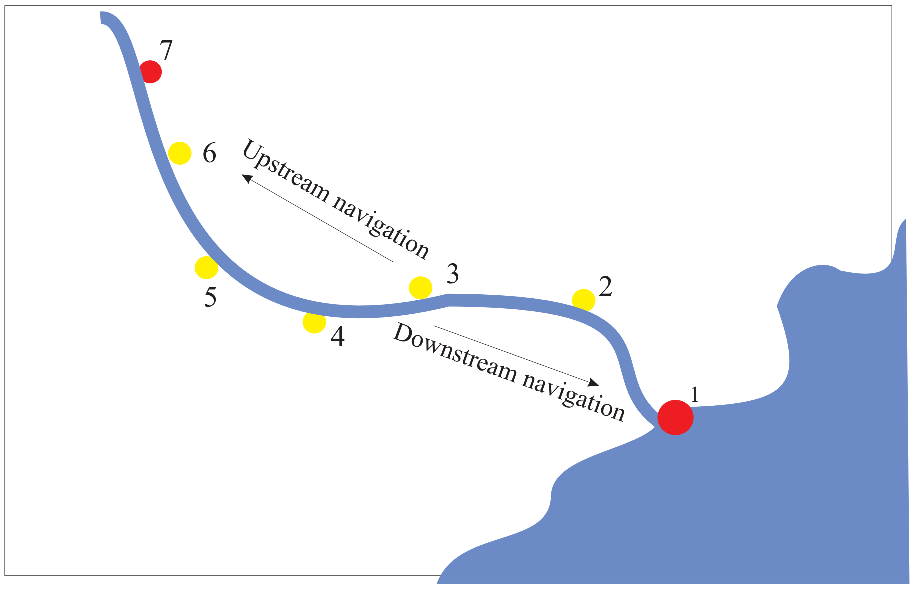


Figure 5.10: Example itinerary of a barge container ship

An example itinerary of a barge container ship is given in Fig. 5.10. Port 1 is the sea or hub port, while ports 2–7 represent river ports. The number associated to each port depends on its distance from port 1. The arrows indicate streams for the sequence of calling ports.

The objective when designing the transport route of a barge container ship is to maximise the shipping company profit, i.e. the difference between the revenue arising from the service of loaded containers (R) and the transport costs (costs related to shipping, TC and empty container related costs, EC). Therefore, the objective function has the form (see [295]):

$$Y = R - TC - EC. \tag{5.4}$$

It is necessary to generate results relating with the assumption that one ship or tow is performing all weekly realised transport. Total number of ships employed on the route might be determined as the ratio of barge container ship round-trip time and service frequency of mainline sea container ships. This model can be extended to a multi-ship problem in a straightforward way. It meets customer demands more closely, but requires modification of the presented one-ship problem. On the other hand, if the shipping company has an option to charter one among several ships at its disposal, then each ship can be evaluated separately using this model to determine the best option.

Mathematical Formulation

In this section the barge container ship routing, with an aim to maximise the shipping company profit, is formulated as a mixed integer programming (MIP) problem. The problem is characterised by the following input data (measurement units are given in square brackets when applied):

n:	number of ports on the inland waterway, including the sea port;
v_1 and v_2:	upstream and downstream barge container ship speed, respectively, [km/h];
scf and scl:	specific fuel and lubricant consumption, respectively [t/kWh];
fp and lp:	fuel and lubricant price, respectively [US$/t];
P_{out}:	engine output (propulsion) [kW];
dcc:	daily time charter cost of barge container ship [US$/day];
C:	carrying capacity of the barge container ship in Twenty feet Equivalent Units [TEU];
max_{tt} and min_{tt}:	maximum and minimum turnaround time on a route [days];
t_l:	total locking time at all locks between ports 1 and n [h];
t_b:	total time of border crossings at all borders between ports 1 and n [h];
zr_{ij}:	weekly expected number of loaded containers available to be transported between ports i and j [TEU];
r_{ij}:	freight rate per container from port i to port j [US$/TEU];
l:	distance between ending ports 1 and n [km];
ufc_i and lfc_i:	unloading and loading cost, respectively per loaded container at port i [US$/TEU];
uec_i and lec_i:	unloading and loading cost, respectively per empty container at port i [US$/TEU];
pec_i:	entry cost per call at port i [$];
uft_i and lft_i:	average unloading and loading time, respectively, per loaded container at port i [h/TEU];
uet_i and let_i:	average unloading and loading time, respectively, per empty container at port i [h/TEU];
pat_i and pdt_i:	standby time for arrival and departure, respectively, at port i [h];
sc_i:	storage cost at port i [US$/TEU];
lc_i:	short-term leasing cost at port i [$/TEU];

The optimal route of the barge container ship may be identified by solving the following mathematical model (linear program). Decision variables of the model are:

- binary variables x_{ij} defined as follows:

$$x_{ij} = \begin{cases} 1 & \text{if ports } i \text{ and } j \text{ are directly connected in the route,} \\ 0 & \text{otherwise;} \end{cases}$$

- z_{ij} and w_{ij}, integers representing the number of loaded and empty containers, respectively, transported from port i to port j [TEU].

The model formulation is as follows

$$\max Y \tag{5.5}$$

$$s.t.$$

$$z_{ij} \leqslant zr_{ij} \sum_{q=i+1}^{j} x_{iq},\ i=1,2,\ldots,n-1;\ j=i+1,\ldots,n \tag{5.6}$$

$$z_{ij} \leqslant zr_{ij} \sum_{q=j}^{i-1} x_{iq},\ i=2,\ldots,n;\ j=1,\ldots,i-1 \tag{5.7}$$

$$z_{ij} \leqslant zr_{ij} \sum_{q=i}^{j-1} x_{qj},\ i=1,2,\ldots,n-1;\ j=i+1,\ldots,n \tag{5.8}$$

$$z_{ij} \leqslant zr_{ij} \sum_{q=j+1}^{i} x_{qj},\ i=2,\ldots,n;\ j=1,\ldots,i-1 \tag{5.9}$$

$$\sum_{q=1}^{i}\sum_{s=j}^{n}(z_{qs}+w_{qs}) \leqslant C+M(1-x_{ij}), i=1,2,\ldots,n-1;\ j=i+1,\ldots,n \tag{5.10}$$

$$\sum_{q=i}^{n}\sum_{s=1}^{j}(z_{qs}+w_{qs}) \leqslant C+M\left(1-x_{ij}\right), i=2,\ldots,n;\ j=1,\ldots,i-1 \tag{5.11}$$

$$\sum_{j=2}^{n} x_{1j} = 1 \tag{5.12}$$

$$\sum_{i=2}^{n} x_{i1} = 1 \tag{5.13}$$

$$\sum_{i=1}^{q-1} x_{iq} - \sum_{j=q+1}^{n} x_{qj} = 0,\ q=2,\ldots,n-1 \tag{5.14}$$

$$\sum_{i=q+1}^{n} x_{iq} - \sum_{j=1}^{q-1} x_{qj} = 0,\ q=2,\ldots,n-1 \tag{5.15}$$

$$min_{tt} \leqslant \frac{t_{tot}}{24} \leqslant max_{tt} \tag{5.16}$$

where M represents large enough constant and

$$\begin{aligned} t_{tot} = {} & (l/v_1 + l/v_2 + t_l + t_b) \\ & + \sum_{i=1}^{n}\sum_{j=1}^{n}\left(z_{ij}\left(lft_i + uft_j\right) + w_{ij}\left(let_i + uet_j\right) + x_{ij}\left(pdt_i + pat_j\right)\right) \end{aligned} \tag{5.17}$$

Constraints (5.6) - (5.9) model the departure ((5.6) - (5.7)) and arrival ((5.8) - (5.9)) of ship and containers to and from each port on the route, respectively, in both upstream and downstream direction. Capacity constraints (5.10) and (5.11), guarantee that the total number of loaded and empty containers on-board will not exceed the ship carrying capacity at any voyage segment. Constraints (5.12) - (5.15) are network constraints ensuring that the ship visits the end ports making a connected trip. The barge container ship is left with a choice of calling or not calling at any port. Round trip time of the barge container ship, denoted by t_{tot} [h], can be calculated as the sum of total voyage time, handling time of full and empty containers in ports and time of entering and leaving ports (5.17). Constraint (5.16) prevents round trip ending and calling at port 1 long before or after arriving of the sea ship in this port.

According to the equation (5.4) and given input data, the profit value Y is calculated as follows:

$$\begin{aligned} Y = & \sum_{i=1}^{n}\sum_{j=1}^{n} z_{ij} r_{ij} \\ & -\Bigg(dcc \cdot max_{tt} + P_{out}\left(l/v_1 + l/v_2\right)\left(fp \cdot scf + lp \cdot scl\right) \\ & + \sum_{i=1}^{n}\sum_{j=1}^{n} x_{ij} \cdot pec_j + \sum_{i=1}^{n}\sum_{j=1}^{n} z_{ij}\left(ufc_i + lfc_j\right)\Bigg) \\ & - \left(\sum_{i=1}^{n}\left(sc_i \cdot sW_i + lc_i \cdot lW_i\right) + \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}\left(uec_i + lee_j\right)\right) \end{aligned} \tag{5.18}$$

The number of containers to be stored at each port i, sW_i, and the number of containers to be leased at each port i, lW_i, can be defined by using the expressions (5.19) - (5.22), [295].

$$S_i = \max\{P_i - D_i, 0\} \tag{5.19}$$

$$M_i = \max\{D_i - P_i, 0\} \tag{5.20}$$

$$lW_i = M_i - \sum_{j=1}^{n} w_{ji} \tag{5.21}$$

$$sW_i = S_i - \sum_{j=1}^{n} w_{ij} \tag{5.22}$$

where:

M_i:	the number of demanded containers at each port i [TEU];
S_i:	the number of excess containers at each port i [TEU];
P_i:	the number of containers destined for port i [TEU];
D_i:	the number of containers departing from port i [TEU].

Problem Complexity and Optimal Solution

The solution of this problem defines upstream and downstream calling sequence and number of loaded and empty containers transported between any two ports while achieving maximum profit of the shipping company. The calling sequence (in one direction) is defined by the upper right (and down left) triangle of the binary matrix X containing decision variables x_{ij}. At most $n-1$ elements (for each direction) are equal to one. Therefore, to determine the calling sequence we have to assign values to n^2 binary variables.

The container traffic between calling ports is defined by the elements of $n \times n$ matrices $Z = z_{ij}$ and $W = w_{ij}$. Again, only the elements corresponding to the non-zero x_{ij} are having positive integer values. In addition, we have to determine the total round trip time t_{tot} and number of leased and stored empty containers at each port. To summarise, we have to determine n^2 binary variables, $2(n^2+n)$ integer variables and two real (floating point) values.

In his previous works [220, 221] Maraš has used the Lingo programming language [289] to find the optimal solutions for small instances of the given problem. Optimal solutions in [220, 221] have been obtained for 7 and 10 possibly calling ports, respectively. Switching to CPLEX ([184]) and a more powerful computer under Linux, we were able to optimally solve instances with 15 ports within 10min to 1h of CPU time, and also some of the instances with 20 ports, but the required CPU time exceeded 29h. Obviously, like in many other combinatorial optimisation problems, real examples are too complex to be solved to optimality. Since the large instances cause the memory lack problems for the CPLEX MIP solver, we turn to heuristic approach in order to tackle the barge container ship routing problem.

5.2.2 Computational Results

In this section, computational results are presented and discussed in an effort to assess and analyze the efficiency of the presented model. We study the performance of different solution methods for our model from two points of view: mathematical programming and transportation usefulness.

Hardware and software. The applied MIP-based heuristics are all coded in the C++ programming language for Linux operating system and compiled with gcc (version 4.1.2) and the option -O2. The tests are performed on Intel Core 2 Duo CPU E6750 on 2.66GHz with RAM=8Gb under Linux Slackware 12, Kernel: 2.6.21.5. For exact solving we used CPLEX 11.2 ([184]) and AMPL ([108, 185]) running on the same machine. Moreover, CPLEX 11.2 is used as generic MIP solver in all tested MIP-based heuristics.

Test bed. Test examples were generated randomly, in such a way that the number of ports n is varied from 10 to 25 with increment 5. Moreover, for each value of n, 5 instances were produced with different ship characteristics (capacities, charter costs, speed, fuel and lubricant consumption). In such a way we produced hard and easy examples within each problem size. The set of instances with their basic properties is summarised in Table 5.10.

Instance	Number of variables			Number of
	Total	Binary	General integer	constraints
10ports_1 – 10ports_5	358	110	240	398
15ports_1 – 15ports_5	758	240	510	818
20ports_1 – 20ports_5	1308	420	880	1388
25ports_1 – 25ports_5	2008	650	1350	2108

Table 5.10: The barge container ship routing test bed.

Methods compared. Three state-of-the-art heuristics for 0-1 MIP problem are applied: local branching (LB) [104], variable neighbourhood branching (VNB) [169] and variable neighbourhood decomposition search for 0-1 MIP problems (VNDS-MIP) [207] (for more details on LB and VNB see Chapter 2; for more details on VNDS-MIP see Chapter 4). All heuristics are compared with the exact CPLEX 11.2 solver. After preliminary testing, it was decided to use the VNDS-MIP-PC1 version of VNDS (see Section 5.1).

Parameters. According to our preliminary experiments, we have decided to use different parameter settings for different instance sizes. Thus, different parameter settings were used for the four groups of instances generated for 10, 15, 20 and 25 ports, respectively. According to the preliminary experiments, the total running time limit for all methods (including CPLEX MIP solver alone) was set to 60, 900, 1800 and 3600 seconds for 10, 15, 20 and 25 ports, respectively. In all heuristic methods, the time limit for subproblems within the main method was set to 10% of the total running time limit. In VNB, parameters regarding initialization and change of neighbourhood size are set in the following way: the maximum neighbourhood size k_{max} is approximately 50% of the number of binary variables and minimum neighbourhood size k_{min} and neighbourhood size increase step k_{step} are set to 10% of the maximum neighbourhood size. Namely, $k_{min} = k_{step} = \lceil b/20 \rceil$ and $k_{max} = 10k_{min}$, where b is the number of binary variables for the particular instance. For example, for 10 ports this yields $k_{min} = k_{step} = 6$ and $k_{max} = 60$. In LB, the initial neighbourhood size k is set to approximately 20% of the number of binary variables for the particular instance: $k = \lceil b/5 \rceil$. All CPLEX parameters are set to their default values.

Instance	Optimal value	Time (s)
10ports_1	22339.01	21.30
10ports_2	24738.23	0.99
10ports_3	23294.74	19.79
10ports_4	20686.27	3.03
10ports_5	25315	8.83
15ports_1	12268.96	925.73
15ports_2	25340	212.76
15ports_3	13798.22	873.43
15ports_4	22372.58	3666.78
15ports_5	15799.96	426.72
20ports_1	out of memory	103455.45
20ports_2	33204.57	104990.05
20ports_3	out of memory	61288.61
20ports_4	out of memory	23174.40
20ports_5	out of memory	108130.25
25ports_1	out of memory	30175.02
25ports_2	out of memory	30938.14
25ports_3	out of memory	26762.03
25ports_4	out of memory	24725.92
25ports_5	out of memory	30587.42

Table 5.11: Optimal values obtained by CPLEX/AMPL and corresponding execution times.

Results. In Table 5.11, optimal values for the tested instances are presented, as obtained by the CPLEX MIP solver invoked by AMPL.It can be observed that for the largest instances CPLEX failed to provide the optimal solution. Objective values obtained by all four methods tested: CPLEX MIP solver with time limitations as above, LB, VNB and VNDS, are provided in Table 5.12. All methods were also ranked according to their solution quality performance (1 is assigned to the best method, 4 to the worst method, and methods with equal performance are assigned the average rank), to avoid drawing the false conclusions in case that extreme objective values for some instances affect the average values for some methods. The ranks and the rank averages are also provided in Table 5.12. According to average objective values and average ranks from Table 5.12, we can see that VNB has the best performance regarding the solution quality, whereas LB and VNDS are worse than CPLEX. However, regarding the running times presented in Table 5.13, the CPLEX MIP solver is the slowest, with 1518.34s average running time and average rank of 3.23, followed by VNB with 1369.42s average running time and the average rank of 3.08. LB and VNDS have the best running time performance with similar average running times of 517.03s and 508.77s, respectively. The average ranks for LB and VNDS (1.65 and 2.05, respectively) show that LB achieves better execution time for more instances than VNDS. The average running time values, however, show that the difference in the execution times of LB and VNDS is usually not that significant. The execution time values of the CPLEX MIP solver for the large instances (20 and 25 ports) in Table 5.13 indicate the memory consumption problem in the CPLEX solver.

Instance	Objective values				Objective value ranks			
	CPLEX	LB	VNB	VNDS	CPLEX	LB	VNB	VNDS
10ports_1	**22339.01**	22339.00	22339.00	22339.00	1	3	3	3
10ports_2	**24738.23**	24738.00	**24738.23**	24737.92	1.5	3	1.5	4
10ports_3	**23294.74**	**23294.74**	**23294.74**	23035.97	2	2	2	4
10ports_4	**20686.27**	20686.00	**20686.27**	20686.26	1.5	4	1.5	3
10ports_5	25315.00	25315.00	25315.00	25315.00	2.5	2.5	2.5	2.5
15ports_1	**12268.96**	**12268.96**	12268.54	11452.19	1.5	1.5	3	4
15ports_2	25340.00	25340.00	25340.00	25340.00	2.5	2.5	2.5	2.5
15ports_3	13798.22	12999.34	**13798.64**	**13798.64**	3	4	1.5	1.5
15ports_4	**22372.58**	**22372.58**	**22372.58**	22303.90	2	2	2	4
15ports_5	15799.96	**15800.00**	**15800.00**	**15800.00**	4	2	2	2
20ports_1	18296.19	16653.70	**19586.02**	17731.09	2	4	1	3
20ports_2	32789.55	32250.44	**33204.26**	31844.83	2	3	1	4
20ports_3	19626.28	19539.69	**21043.05**	19396.66	2	3	1	4
20ports_4	26996.03	25928.76	**27962.31**	25244.94	2	3	1	4
20ports_5	23781.17	23904.21	**24235.86**	23872.98	4	2	1	3
25ports_1	20539.88	**21619.18**	17708.32	19011.24	2	1	4	3
25ports_2	32422.19	**33528.22**	33342.05	29875.93	3	1	2	4
25ports_3	20008.23	17651.27	**23019.65**	20450.20	3	4	1	2
25ports_4	27364.50	**28388.23**	25334.19	25549.91	2	1	4	3
25ports_5	22897.03	22303.71	**24621.21**	23367.28	3	4	1	2
Average:	22533.70	22346.05	**22800.50**	22057.70	2.33	2.63	**1.93**	3.13

Table 5.12: Objective values (profit) and corresponding rankings for the four methods tested.

5.2.3 Summary

In summary, we may conclude that using the heuristic methods for tackling the presented ship routing problem is beneficial, both regarding the solution quality and (especially) the execution time. VNB heuristic proves to be better than the CPLEX MIP solver regarding both criteria (solution quality/execution time). LB and VNDS do not achieve as good solution quality as CPLEX, but have significantly better execution time (they are approximately 3 times faster than CPLEX). Soft variable fixing (VNB and LB) appears to be more effective (quality-wise) for this model than the hard variable fixing (VNDS). The solution quality performance of VNDS may be explained by the fact that the number of general integer variables in all instances is more than twice as large as the number of binary variables, and therefore the subproblems generated during the VNDS process by fixing only binary variables are still large and not so easy for the CPLEX MIP solver. Hence, the improvement in VNDS usually does not occur in the late stages of the search process.

5.3 The Two-Stage Stochastic Mixed Integer Programming Problem

In this section a variant of VNDS-MIP matheuristic is proposed for solving a two-stage stochastic mixed integer programming problem with binary variables in the first stage. A set of sub problems,

Instance	Running times (s)				Running time ranks			
	CPLEX	LB	VNB	VNDS	CPLEX	LB	VNB	VNDS
10ports_1	21.30	**11.20**	41.32	15.91	3	1	4	2
10ports_2	**0.99**	**0.10**	3.77	**0.25**	2	2	4	2
10ports_3	19.79	**5.90**	39.04	38.95	2	1	3.5	3.5
10ports_4	3.03	**1.00**	7.30	5.54	2	1	4	3
10ports_5	8.83	**3.40**	32.93	8.15	2.5	1	4	2.5
15ports_1	900.00	81.90	**16.73**	52.67	4	3	1	2
15ports_2	212.76	172.70	**27.50**	181.75	4	2	1	3
15ports_3	873.43	261.50	**7.36**	189.27	4	3	1	2
15ports_4	900.00	171.30	**54.61**	581.97	4	2	1	3
15ports_5	426.72	87.50	**3.25**	114.09	4	2	1	3
20ports_1	1800.00	**358.10**	1832.86	438.86	3	1	4	2
20ports_2	1800.00	521.70	1450.61	**246.74**	4	2	3	1
20ports_3	1800.00	894.30	1822.16	**635.93**	3	2	4	1
20ports_4	1800.00	529.90	1571.32	**274.28**	4	2	3	1
20ports_5	1800.00	**1067.00**	1858.44	1624.39	3	1	4	2
25ports_1	3600.00	1789.10	3838.32	**1575.40**	3	2	4	1
25ports_2	3600.00	1787.00	3645.61	**83.09**	3	2	4	1
25ports_3	3600.00	**1426.65**	3670.78	1600.20	3	1	4	2
25ports_4	3600.00	**812.24**	3586.98	1318.52	4	1	3	2
25ports_5	3600.00	**358.10**	3877.59	1189.42	3	1	4	2
Average:	1518.34	517.03	1369.42	**508.77**	3.23	**1.65**	3.08	2.05

Table 5.13: Running times and corresponding rankings for the four methods tested.

derived from the first-stage problem, is generated according to the variable neighbourhood decomposition search principle, by exploiting the information from the linear programming relaxation solution of the first-stage problem. Sub problems are examined using the general-purpose CPLEX MIP solver for a deterministic equivalent and new constraints are added to the original problem in case that a sub problem is solved exactly. The proposed heuristic was tested on a benchmark of 25 instances from an established SIPLIB library of stochastic integer programming problems, and compared with the CPLEX 12.1 MIP solver for a deterministic equivalent. The results show that VNDS required more time for the easiest problems, but performed much better than CPLEX applied to a deterministic equivalent for the three hardest instances. This is quite remarkable because these instances have hundreds of thousands of binary variables in the deterministic equivalent.

The two-stage stochastic programming model with recourse (2SSP) is probably the most important class of stochastic programming (SP) problems [24, 77, 324] and can be seen as a *decision* followed by possible *recourse* actions [291]. In this section, it is assumed that the random parameters have a discrete finite distribution, and only linear models are considered.

Let S be the number of *scenarios*, i.e. possible outcomes of the random event, the ith outcome occurring with probability p_i. If we denote by x the vector of the first decision variables, then the values of x are determined by solving the following *first-stage* problem:

$$(5.23)\qquad (P)\quad \left[\begin{array}{ll} \min & c^T x + \sum_{i=1}^{S} p_i\, q_i(x) \\ \text{s.t.} & Ax = b,\ x \geq 0, \\ & x \in K_i \ \ (i = 1, \ldots, S), \end{array}\right.$$

where c and b are given vectors and A is a given matrix, with compatible sizes, and $q_i : K_i \to \mathbb{R}$ is a *polyhedral* (i.e. piecewise linear) convex function. We assume that the feasible set $X = \{x \,|Ax = b,\, x \geq 0\}$ is a non-empty bounded polyhedron. The expectation in the objective, $Q(x) =$

$\sum_{i=1}^{S} p_i\, q_i(x)$, is called the *expected recourse function.* This is a polyhedral convex function with the domain $K = K_1 \cap \ldots \cap K_S$.

Once the first decision has been made with the result x and the ith scenario realised, the second decision concerns solving the following *second-stage problem* or *recourse problem*:

$$(R_i(x)) \quad \left[\begin{array}{ll} \min & q_i(x) = q_i^T y \\ \text{s.t.} & T_i x + W_i y = h_i, \\ & y \geq 0, \end{array} \right. \tag{5.24}$$

where q_i, h_i are given vectors, T_i, W_i are given matrices of compatible sizes and y denotes the decision variable. We assume that the optimal objective value $q_i(x)$, $x \in K_i$, of the recourse problem $R_i(x)$ satisfies $q_i(x) > -\infty$.[1]

The two-stage stochastic programming problem (5.23)-(5.24) can be formulated as a single linear programming (LP) problem called the *deterministic equivalent problem* (DEP for short):

$$\left[\begin{array}{lccccccccc} \min & c^T x & + & p_1 q_1^T y_1 & + & \ldots & + & p_S q_S^T y_S & & \\ \text{s.t.} & Ax & & & & & & & = & b, \\ & T_1 x & + & W_1 y_1 & & & & & = & h_1, \\ & \vdots & & & & \ddots & & & & \vdots \\ & T_S x & + & & & & & W_S y_S & = & h_S, \\ & \multicolumn{9}{l}{x \geq 0, y_1 \geq 0, \ldots, y_S \geq 0.} \end{array} \right. \tag{5.25}$$

In this section we deal with 0-1 mixed integer 2SSP models, where both the first-stage and the second-stage problem can contain variables with integrality constraints and the set of binary variables in the first-stage problem is non-empty. In other words, it is assumed that the feasible set X of the first-stage problem (5.23) is of the form

$$X = \{0,1\}^{n_1} \times \mathbb{Z}_0^{+\,n_2} \times \mathbb{R}_0^{+\,n_3}, n_1, n_2, n_3 \in \mathbb{Z}_0^+, n_1 > 0, \tag{5.26}$$

where $\mathbb{Z}_0^+ = \mathbb{N} \cup \{0\}, \mathbb{R}_0^+ = \{x \in \mathbb{R} \mid x \geq 0\}$, n_1 is the number of binary variables, n_2 is the number of general integer variables and n_3 is the number of continuous variables. In that case, the feasible set $\overline{X}$ of the first-stage problem of the linear programming relaxation of the problem (5.23)-(5.24) is given by $\overline{X} = [0,1]^{n_1} \times \mathbb{R}_0^{+\,n_2+n_3}$.

Since the first-stage problem (5.23) is a special case of the 0-1 MIP problem, the (partial) distance (see (2.5) and (2.13)) and neighbourhood structures (see (2.3)) can be defined in the feasible set X of (5.23) in the same way as for any 0-1 MIP problem in general. By introducing the neighbourhood structures into the feasible set X of problem (5.23), it becomes possible to apply some variable neighbourhood search [237] based heuristic for solving the first-stage problem (5.23). In this section, the variable neighbourhood decomposition search [168] is used to tackle the first-stage problem (5.23) and thus speed up the overall solution process for a given 2SSP problem (5.23)-(5.24).

The rest of this section is organised as follows. In Subsection 5.3.1, we provide a brief overview of the existing solution methods for 0-1 mixed integer 2SSP. In Subsection 5.3.2, we provide a detailed description of the proposed variable neighbourhood decomposition search heuristic for 0-1 mixed integer 2SSP. Next, in Subsection 5.3.3, we analyse the performance of the proposed method as compared to the commercial IBM ILOG CPLEX 12.1 MIP solver for the deterministic equivalent. In Subsection 5.3.4, we summarise our conclusions.

[1]Equivalently, we assume that the dual of the recourse problem $R_i(x)$ has a feasible solution. Solvability of the dual problem does not depend on x.

5.3.1 Existing Solution Methodology for the Mixed Integer 2SSP

A number of real-world problems can be modelled as stochastic programming problems [321]. Some of the many examples of mixed integer 2SSP which often occur in practice are set covering problem (SCP), vehicle routing problem with stochastic demands (VRPSD), travelling salesman problem with time windows (TSPTW), probabilistic travelling salesman problem (PTSP), stochastic shortest path (SSP) problem, stochastic discrete time cost problem (SDTCP) (see, for instance, [35]). Results from the complexity theory state that the two-stage stochastic integer programming (SIP) is as hard as the stochastic linear programming (SLP) [93]. However, in practice, SIP problems are usually much harder to solve than SLP problems, as in the case of deterministic optimisation.

Over the years, different solution approaches have emerged in an attempt to tackle mixed integer 2SSP. One possible approach is to convert a given 2SSP to its deterministic equivalent and then use some of the well-known methods for the deterministic mixed integer programming (MIP) problem. However, this approach has its drawbacks [338], one of them being that an obtained DEP is usually of very large dimensions and cannot be successfully solved by the best known deterministic MIP solution methods. This compares with our experience of processing SLPs by DEP formulation and the improvements gained by applying customised solution methods [338].

Another approach consists in designing exact methods for mixed integer 2SSP by combining existing methods and ideas for deterministic MIPs, such as branch-and-bound, branch-and-cut, Benders decomposition [28], Dantzig-Wolfe decomposition [78] etc., and existing methods for SLP. Some solution methods of this type can be found in [9, 99, 292]. Recently, many of the well-known metaheuristics, such as tabu search, iterated local search, ant colony optimisation or evolutionary algorithms, have been used as a framework for designing heuristics for mixed integer 2SSP (see [35] for a comprehensive survey). Some of the new metaheuristic methods were developed specifically for 2SSP, like progressive hedging algorithm or rollout algorithm [35]. Given the tremendous advance in deterministic solver algorithms, both MIP and LP, a new matheuristic approach, in which a generic solver (usually a deterministic solver applied to DEP) is used as a search component within some metaheuristic framework, appears to be very promising. It became even more evident now that many of the major software vendors, namely, XPRESS, AIMMS, MAXIMAL, and GAMS offer SP extensions to their optimisation suites. Furthermore, there is a very active ongoing research in further development of modelling support and scenario generation for a SP solver system [86, 232], implying even better performance of SP solver systems in the near future.

In this section, we propose a new heuristic for a mixed integer 2SSP, which exploits generic stochastic MIP and LP solvers as search components within the framework of variable neighbourhood decomposition search [168] metaheuristic.

5.3.2 VNDS Heuristic for the 0-1 Mixed Integer 2SSP

In this section, a similar idea as in the basic `VNDS-MIP` from Chapter 4 is exploited. An observation can be made that by fixing a great portion of variables in the first-stage problem of a given mixed integer 2SSP, a much easier problem is obtained, which can usually be solved much faster than the original problem. Ideally, if all the variables from the first-stage problem are fixed, then only solving the second-stage problems of a specific block-structure remains. The pseudo-code of the VNDS heuristic for mixed integer 2SSP, called `VNDS-SIP`, is given in Figure 5.11. Note that this variant of VNDS does not incorporate any pseudo-cuts, since this would destroy the specific block-structure of the second-stage problems, thus making them much harder to solve. Input parameters for the `VNDS-SIP` procedure are input problem SIP (with the first-stage problem P) and initial integer feasible solution x^*. A call to the generic stochastic integer programming solver is denoted with x'=SIPSOLVE(SIP, x^*), where SIP is a given input problem, x^* is a starting solution vector, and x' is the new returned solution vector (if SIP is infeasible, then $x' = x^*$).

```
VNDS-SIP($SIP, x^*$)
 1  Choose stopping criterion (set $proceed$=true);
 2  Set $U = c^T x^* + \sum_{i=1}^{S} p_i \, q_i(x^*)$;
 3  while ($proceed1$) do
 4      Solve the LP relaxation of $SIP$ to obtain LP solution $\overline{x}$;
 5      Set $L = c^T \overline{x} + \sum_{i=1}^{S} p_i \, q_i(\overline{x})$;
 6      if ($\overline{x} \in \{0,1\}^{n_1} \times \mathbb{Z}_0^{+n_2} \times \mathbb{R}_0^{+n_3}$)
 7          $x^* = \overline{x}$; $U = L$; break;
 8      endif
 9      $\delta_j =\mid x_j^* - \overline{x}_j \mid$; index $x_j$ so that $\delta_j \leq \delta_{j+1}$, $j = 1, \ldots, n_1 - 1$;
10      Set $k = n_1$;
11      while ($proceed$ and $k \geq 0$) do
12          $J_k = \{1, \ldots, k\}$; Add constraint $\delta(J_k, x^*, x) = 0$;
13          $x'$=SIPSOLVE($SIP, x^*$);
14          if (solutionStatus == OPTIMAL || solutionStatus == INFEASIBLE)
15              Reverse last added constraint into $\delta(J_k, x^*, x) > 0$;
16          else Delete last added constraint: $\delta(J_k, x^*, x) = 0$;
17          endif
18          if $\left(c^T x' + \sum_{i=1}^{S} p_i \, q_i(x') < c^T x^* + \sum_{i=1}^{S} p_i \, q_i(x^*)\right)$ then
19              $x^* = x'$; $U = c^T x^* + \sum_{i=1}^{S} p_i \, q_i(x^*)$; break;
20          else $k = k - 1$;
21          endif
22          Update $proceed$;
23      endwhile
24      Update $proceed$;
25  endwhile
26  return $U$, $L$, $x^*$.
```

Figure 5.11: VNDS-SIP pseudo-code.

We first solve the linear programming relaxation of a given input problem to obtain the LP relaxation solution $\overline{x}$. Values of $\overline{x}$ are then used to iteratively select the set of variables from the incumbent integer solution x^* to be fixed and solve the resulting smaller subproblem. If the subproblem is solved exactly (i.e. either solved to optimality or proven infeasible) the constraint $\delta(J_k, x^*, x) > 0$, so called *pseudo-cut*, is added, so that the examination of the same sub problem is avoided in future. The term "pseudo-cut" refers to an inequality which is not necessarily valid (see definition 1.1). Similar search space reductions by adding pseudo-cuts are used for the case of pure 0-1 MIPs in, for instance, [298, 326]. We use the general CPLEX MIP solver for the deterministic equivalent problems (DEP) as a black-box for solving the generated sub problems. After all sub problems are explored, the new linear programming relaxation of the first stage problem is solved, and the whole process is iterated. Note that the optimal objective value of the current problem SIP is either the optimal objective value of the problem obtained by adding the constraint $\delta(J_k, x^*, x) = 0$ to SIP, or the optimal objective value of the problem obtained by adding $\delta(J_k, x^*, x) > 0$ to SIP. Therefore, adding the pseudo-cut $\delta(J_k, x^*, x) > 0$ to the current problem, in case that the current sub problem is solved exactly, does not discard the original optimal solution from the reduced search space. In our experiments, the condition *proceed* corresponds to the maximum execution time allowed.

5.3.3 Computational Results

In this section we report the results of our computational experiments on two-stage stochastic integer programming problems. All the benchmark problems we used are available in the SMPS format from SIPLIB, a stochastic integer programming test problem library [7].

The experiments were carried out on a Windows XP SP2 machine with 3 GB of RAM and Intel Core2 660 CPU running at 2.40 GHz. CPLEX 12.1 barrier and MIP optimisers with default settings were used for solving deterministic equivalent problems. The VNDS algorithm for SIP was implemented in the FortSP stochastic programming solver system [98].

In our VNDS implementation we tried to use the same stopping conditions as in CPLEX. The relative mipgap stopping tolerance was set to 0.01% and it was computed using the formula $(U - L)/(|U| + 0.1)$, where U is the objective value of the best integer feasible solution and L is a lower bound on the objective value. A time limit was set to 1800 seconds. All problems that took less than this time were solved to optimality within the given tolerance. For runs where the time limit was reached the best objective value of an integer feasible solution found is reported.

In our experiments, we noticed that for problems with small dimensions, CPLEX for DEP appears to be much more effective than VNDS in terms of execution time. This is why we tried to combine the good features both of CPLEX for DEP and of VNDS, by running CPLEX for DEP until reaching a certain time limit and only triggering VNDS if the optimal solution has not been found by the DEP solver in that time. According to our preliminary experiments, we decide to set this time limit to 720 seconds. This hybrid algorithm is later denoted as "Hybrid" in all the tables. A more extensive computational analysis (performed on a greater number of instances) might be able to indicate another criteria for triggering VNDS, based solely on the mathematical formulation of the problem (probably the portion of binary variables in the first-stage problem, or the total number of scenarios).

The DCAP Test Set. The first collection is taken from [8], where the problem of dynamic capacity acquisition and assignment often arising in supply chain applications is addressed. It is formulated as a two-stage multiperiod SIP problem with mixed-integer first stage, pure binary second stage and a discrete distribution of random parameters. The dimensions of the DCAP problem instances are given in Table 5.14. The variable n_1 indicates the number of binary variables as in (5.26), and variable n_3 indicates the number of continuous variables. For all instances in the benchmark we used in this section, the number of general integer variables is 0 ($n_2 = 0$).

The test results shown in Table 5.15 indicate that VNDS performed worse than the plain deterministic equivalent solver (except for decap332 with 300 scenarios). However using the hybrid method gave the same results as the deterministic equivalent.

The SIZES Test Set. The second test set is from [190]. It consists of three instances of a two-stage multiperiod stochastic integer programming problem arising in product substitution applications. Tables 5.16 and 5.17 show the problem dimensions and test results respectively. The results are similar to the ones for the previous test set with deterministic equivalent and hybrid algorithms being equivalent and outperforming VNDS.

The SSLP Test Set. The final test suite consists of 12 instances of stochastic server location problems by [247] with up to a million binary variables in deterministic equivalents. These are two-

		Stage 1		Det. Eq.			
Name	Scen	n_1	n_3	Rows	Columns	Nonzeros	Binaries
dcap233	200	6	6	3006	5412	11412	5406
	300	6	6	4506	8112	17112	8106
	500	6	6	7506	13512	28512	13506
dcap243	200	6	6	3606	7212	14412	7206
	300	6	6	5406	10812	21612	10806
	500	6	6	9006	18012	36012	18006
dcap332	200	6	6	2406	4812	10212	4806
	300	6	6	3606	7212	15312	7206
	500	6	6	6006	12012	25512	12006
dcap342	200	6	6	2806	6412	13012	6406
	300	6	6	4206	9612	19512	9606
	500	6	6	7006	16012	32512	16006

Table 5.14: Dimensions of the DCAP problems

		Det. Eq.		VNDS		Hybrid	
Name	Scen	Time	Obj	Time	Obj	Time	Obj
dcap233	200	2.25	1834.60	13.67	1834.59	1.31	1834.60
	300	1800.86	1644.36	1800.25	1644.36	1800.16	1644.36
	500	3.88	1737.52	60.38	1737.52	3.59	1737.52
dcap243	200	4.22	2322.59	34.31	2322.50	4.06	2322.59
	300	12.03	2559.45	24.86	2559.45	11.88	2559.45
	500	34.64	2167.40	65.67	2167.40	34.53	2167.40
dcap332	200	1800.64	1060.70	1800.15	1060.70	1800.02	1060.70
	300	1800.65	1252.88	1423.54	1252.88	1800.01	1252.88
	500	1800.70	1588.81	1800.31	1588.82	1800.05	1588.82
dcap342	200	90.86	1619.59	144.74	1619.58	91.34	1619.59
	300	1800.62	2067.70	1800.25	2067.70	1800.02	2067.70
	500	1800.55	1904.66	1800.41	1904.73	1800.02	1904.66

Table 5.15: Test results for DCAP

		Stage 1		Det. Eq.			
Name	Scen	n_1	n_3	Rows	Columns	Nonzeros	Binaries
SIZES	3	10	65	124	300	795	40
	5	10	65	186	450	1225	60
	10	10	65	341	825	2300	110

Table 5.16: Dimensions of the SIZES problems

		Det. Eq.		VNDS		Hybrid	
Name	Scen	Time	Obj	Time	Obj	Time	Obj
SIZES	3	0.72	224433.73	1800.02	224433.73	0.69	224433.73
	5	2.64	224486.00	1800.16	224486.00	2.63	224486.00
	10	592.79	224564.30	1800.13	225008.52	586.51	224564.30

Table 5.17: Test results for SIZES

		Stage 1		Det. Eq.			
Name	Scen	n_1	n_3	Rows	Columns	Nonzeros	Binaries
sslp-5-25	50	5	0	1501	6505	12805	6255
	100	5	0	3001	13005	25605	12505
sslp-10-50	50	10	0	3001	25510	50460	25010
	100	10	0	6001	51010	100910	50010
	500	10	0	30001	255010	504510	250010
	1000	10	0	60001	510010	1009010	500010
	2000	10	0	120001	1020010	2018010	1000010
sslp-15-45	5	15	0	301	3465	6835	3390
	10	15	0	601	6915	13655	6765
	15	15	0	901	10365	20475	10140

Table 5.18: Dimensions of the SSLP problems

stage stochastic mixed-integer programming problems with pure binary first stage, mixed binary second stage and discrete distributions. For the three largest instances in the SSLP collection (sslp-10-50 with 500, 1000 and 2000 scenarios) the final objectives returned by VNDS were much closer to optimality than those obtained by solving deterministic equivalent problems.

By comparing results from the three different test sets, we can observe that `VNDS-SIP` is most effective when all the variables in the first-stage problem are binary. It can be explained by the fact that, when all the variables in the first-stage problem are fixed, the solution process continues with solving the second-stage problems, which are of a special-block structure and usually not too hard to solve. When only a small portion of variables in the first-stage problem is fixed, the remaining sub problem is still hard to solve and solving a number of these sub problems, as generated within the VNDS framework (see Figure 5.11), causes the long execution time of `VNDS-SIP`. Furthermore, by observing all the results from the SSLP collection (where all the variables from the first-stage problem are binary), we can see that the greater the number of scenarios is, the more effective is the `VNDS-SIP` algorithm. Therefore, for the last three instances with only 5 to 15 scenarios, VNDS has a poor time performance. This observation may be explained by the fact that, the greater the number of scenarios is, the greater the dimensions of the corresponding DEP are, and therefore the less effective is the DEP solver.

5.3.4 Summary

Although much work has been done in the field of the stochastic linear programming (SLP), stochastic integer programming (SIP) is still a rather unexplored research area. According to the

		Det. Eq.		VNDS		Hybrid	
Name	Scen	Time	Obj	Time	Obj	Time	Obj
sslp-5-25	50	3.34	-121.60	3.38	-121.60	3.17	-121.60
	100	11.83	-127.37	14.67	-127.37	11.42	-127.37
sslp-10-50	50	462.23	-364.62	1800.18	-364.62	463.71	-364.62
	100	1800.68	-354.15	1800.43	-354.18	1800.18	-354.18
	500	1804.24	-111.87	1803.27	-348.81	1800.45	-283.25
	1000	1808.39	-115.04	1803.46	-336.94	1801.04	-283.91
	2000	1819.39	-108.30	1809.30	-321.99	1580.33	-250.58
sslp-15-45	5	4.42	-262.40	82.69	-262.40	4.39	-262.40
	10	16.45	-260.50	1800.13	-260.50	16.38	-260.50
	15	99.33	-253.60	1800.11	-253.60	99.50	-253.60

Table 5.19: Test results for SSLP

theoretical complexity results, stochastic integer programming problems are not harder to solve than the continuous problems [93]. However, in practice, SIP problems are usually much harder than SLP problems, as in the case of deterministic optimisation. This calls for the development of new advanced techniques which can obtain high-quality solutions of SIP problems in reasonable time. In this section we propose a matheuristic method for solving a mixed integer two-stage stochastic programming (mixed integer 2SSP) problem. The heuristic proposed in this section uses the generic stochastic LP solver and generic stochastic MIP solver (which is employed as a MIP solver for the deterministic equivalent problem (DEP)) within a variable neighbourhood decomposition search framework [168].

Based on the computational analysis performed on an established benchmark of 25 SIP instances [7], we may conclude that VNDS based matheuristic has a lot of potential for solving mixed integer 2SSP problems. Computational results show that the proposed `VNDS-SIP` method is competitive with the CPLEX MIP solver for the DEP regarding the solution quality (it achieves the same objective value as the CPLEX MIP solver for DEP in 15 cases, has better performance in 7 cases and worse performance in 3 cases). `VNDS-SIP` usually requires much longer execution time than the DEP solver. However, it is remarkable that, for the three largest instances whose deterministic equivalents contain hundreds of thousands binary variables, `VNDS-SIP` obtains a significantly better objective value (about 200% better) than the DEP solver (see Table 5.19), within the allowed execution time of 1800 seconds reached by both methods. Furthermore, these objective values are very close to optimality [7].

In summary, we can conclude that the greater the percentage of binary variables (with respect to the total number of variables) and the greater the number of scenarios, the more effective is the `VNDS-SIP` method for solving the mixed integer 2SSP problem.

Chapter 6

Variable Neighbourhood Search and 0-1 MIP Feasibility

Various heuristic methods have been designed in an attempt to find good near-optimal solutions of hard 0-1 MIPs. Most of them start from a given feasible solution and try to improve it. Still, finding a feasible solution of 0-1 MIP is proven to be NP-complete [331] and for a number of instances remains hard in practice. This calls for the development of efficient constructive heuristics which can attain feasible solutions in short time. A number of heuristics which address the problem of MIP feasibility have been proposed in the literature, although the research in this area has only significantly intensified in the last decade. Whereas some of the proposed heuristics are based on the standard metaheuristic frameworks, such as tabu search [213], genetic algorithm [246], scatter search [134], the others are specific approaches intended solely for tackling the 0-1 MIP feasibility problem. Interior point based methods were proposed in [176]. Pivoting methods, in which special pivot moves are constructed and performed in order to decrease the integer infeasibility, were proposed in [19, 20, 94, 214]. Few heuristics proposed in [187] combine constraint programming and LP relaxations in order to locate feasible solutions by means of the specialised propagation algorithms. Relaxation enforced neighbourhood search (RENS), proposed in [32], performs a large neighbourhood search on the set of solutions obtained by intelligent fixing and rounding of variables, based on the values of the variables in the LP relaxation solution. In [103], feasibility pump (FP) heuristic was proposed for the special case of pure 0-1 MIPs. The basic idea of feasibility pump consists in generating a sequence of linear programming problems, whose objective function represents the infeasibility measure of the initial MIP problem. This approach was further extended for the case of general MIPs [31]. The FP heuristic is quite efficient in terms of computational time, but usually provides poor-quality solutions. The introduction of feasibility pump has triggered a number of recent research results regarding the MIP feasibility. In [5], objective FP was proposed, with the aim to improve the quality of feasible solutions obtained. However, the computational time was prolonged in average compared to the basic version of FP. Another approach, proposed in [105], applies the local branching heuristic [104] to near-feasible solutions obtained from FP in order to locate the feasible solutions. First, a given problem is modified so that the original objective function is replaced by an infeasibility measure which takes into account a weighted combination of the degrees of violation of the single linear constraints. Then, LB is applied to this modified problem, usually yielding a feasible solution in a short time, but the solution obtained is often of low-quality, since the original objective function is discarded. Some other heuristics which address the 0-1 MIP feasibility problem include [94, 129, 130, 287].

By analysing the approaches mentioned above, one can observe that fast heuristics for 0-1

MIP feasibility normally yield low-quality solutions, whereas heuristics which provide good initial solutions are often time consuming. In this chapter, two new variable neighbourhood search based heuristics for the 0-1 MIP feasibility are proposed, which aim to provide good-quality initial solutions within a short computational time. The first heuristic, called variable neighbourhood pump (VNP), combines the feasibility pump approach with variable neighbourhood descent. The second heuristic is based on the principle of variable neighbourhood decomposition search and represents a variant of VNDS-MIP which was proposed in Chapter 4, adjusted for 0-1 MIP feasibility. Both proposed heuristics exploit the fact that a generic MIP solver can be used as a black-box for solving MIP problems to feasibility, rather than only to optimality. In this chapter, only pure 0-1 MIP problems are considered, i.e. problems in which the set of general integer variables is empty.

In the descriptions of algorithms presented in the remainder of this chapter, the following definitions are used. The *rounding* $[x]$ of any vector x is defined as:

$$[x]_j = \begin{cases} \lfloor x_j + 0.5 \rfloor, & j \in \mathcal{B} \\ x_j, & j \in \mathcal{C}. \end{cases} \tag{6.1}$$

We say that a solution x is *integer* if x_j is integer for all $j \in \mathcal{B}$ (thus ignoring the continuous components), and *fractional* otherwise. The notation $\mathrm{LP}(P, \widetilde{x}, \delta)$ will be used to denote the linear programming relaxation of a modified problem, obtained from a given problem P by replacing the original objective function with $\delta(x, \widetilde{x})$:

$$\mathrm{LP}(P, \widetilde{x}, \delta) \quad \left[\begin{array}{lll} \min \delta(\widetilde{x}, x) & & \\ \text{s.t.} & \sum_{j=1}^{n} a_{ij} x_j \geq b_i & \forall i \in M = \{1, 2, \ldots, m\} \\ & x_j \in [0, 1] & \forall j \in \mathcal{B} \neq \emptyset \\ & x_j \geq 0 & \forall j \in \mathcal{C}, \end{array} \right. \tag{6.2}$$

where all notations are the same as in (1.6) and δ is a distance function in the 0-1 MIP solution space as defined in (2.6). Note that all definitions in this chapter are adapted for the case of pure 0-1 MIPs, i.e. they take into account that $\mathcal{G} = \emptyset$, where $\mathcal{G}$ denotes the set of indices of general integer variables in the definition of a 0-1 MIP problem (1.6).

This chapter is organised as follows. The feasibility pump (the basic version and some enhancements) is described in more details in Section 6.1, as it is closely related to the heuristics proposed later in this chapter. In Section 6.2, the variable neighbourhood pump heuristic is described in detail. Section 6.3 is devoted to the constructive VNDS heuristic for 0-1 MIP feasibility. In Section 6.4, experimental results are presented and analysed. Finally, in Section 6.5, concluding remarks are provided.

6.1 Related Work: Feasibility Pump

The feasibility pump heuristic was proposed in [103] for finding initial feasible solutions for 0-1 MIP problems. It generates a sequence of linear programming problems, whose objective function represents the infeasibility measure of the initial MIP problem. The solution of each subproblem is used to define the objective function of the next subproblem, so that the infeasibility measure is reduced in each iteration. In this section, a detailed algorithmic description of feasibility pump is provided. In addition, some recent enhancements of the basic scheme proposed in [103] are also described.

6.1.1 Basic Feasibility Pump

Feasibility pump (FP), introduced in [103], is a fast and simple heuristic for finding a feasible solution for the 0-1 MIP problem. Starting from an optimal solution of the LP relaxation, the FP heuristic generates two sequences of solutions $\overline{x}$ and $\widetilde{x}$, which satisfy LP feasibility and integrality feasibility, respectively. The two sequences of solutions are obtained as follows: at each iteration a new binary solution $\widetilde{x}$ is obtained from the fractional $\overline{x}$ by simply rounding its integer-constrained components to the nearest integer, while a new fractional solution $\overline{x}$ is defined as an optimal solution of LP$(P, \widetilde{x}, \delta)$. Each iteration thus described is referred to as a *pumping cycle*. However, it often appears that, after a certain number of iterations (pumping cycles), solution $[\overline{x}]$ obtained by rounding the LP solution $\overline{x}$ is the same as the current integer solution $\widetilde{x}$. In that case, the process gets stalled in solution $\widetilde{x}$. Moreover, it is possible that rounding the LP solution $\overline{x}$ yields an integer solution $\widetilde{x}$ which has already occurred in some of the previous iterations. In that case, the solution process can end up cycling through the same sequence of solution vectors over and over again. In practice, the cycles are usually detected heuristically, for example by counting the number of successive iterations without an improvement of feasibility measure $\delta(x, \widetilde{x})$, or by checking whether the current integer solution $\widetilde{x}$ has already occurred in the last n_{it} iterations, where n_{it} is some predefined value (see [31, 103]).

To avoid this kind of cycling, some random perturbations of the current solution $\widetilde{x}$ are performed. In the original implementation, $rand[T/2, 3T/2]$ entries x_j, $j \in \mathcal{B}$, with highest values of $|\widetilde{x}_j - \overline{x}_j|$ are flipped whenever cycling is detected, where T is an input parameter for the algorithm. Flipping a certain number k of variables in the current solution $\widetilde{x}$ can actually be viewed as replacing the current solution x with a solution from the kth neighbourhood $\mathcal{N}_k(\widetilde{x})$ of $\widetilde{x}$, where the neighbourhood structures $\mathcal{N}_k$ are defined as (note the difference from $\mathcal{N}_k$ in (2.3)):

$$\mathcal{N}_k(x) = \{y \in S \mid \delta(x, y) \ = \ k\}, \tag{6.3}$$

with S being the solution space of a 0-1 MIP problem (1.6) and $x, y \in S$. Thus, in the original implementation, the neighbourhood size k is selected randomly from the interval $rand[T/2, 3T/2]$, where T is a given parameter. Furthermore, flipping those k values $\widetilde{x}_j$, for which the values $|\widetilde{x}_j - \overline{x}_j|$ are the highest, means choosing the next solution $x' \in \mathcal{N}_k(\widetilde{x})$ as the closest one to $\overline{x}$, i.e. so that $\delta(\overline{x}, x') = \min\{\delta(\overline{x}, y) \mid y \in \mathcal{N}_k(\widetilde{x})\}$, where δ is a generalised distance function as defined in (2.10). The stopping criteria is usually set to a running time limit and/or the total number of iterations (in case that algorithm fails to detect any feasible solutions). The pseudo-code of the basic FP is given in figure 6.1.

Note that feasibility pump as presented above can be considered as an instance of the hyper-reactive VNS (see Chapter 2, Section 2.5), for the special case of $k_{min} = k_{max} = k$ (meaning that in each iteration only a single neighbourhood is explored[1]). Indeed, the size of a neighbourhood is determined at each iteration, rather than initiated at the beginning and fixed to that initial value throughout the search process. Furthermore, the formulation of the problem to be solved is also changed at each iteration, because the objective function changes.

6.1.2 General Feasibility Pump

The basic feasibility pump operates only on pure 0-1 MIP models. In [31], a more general scheme was proposed, which takes into account general integer variables, i.e. the case $\mathcal{G} \neq \emptyset$ (recall (1.6)). The basic feasibility pump employs the distance function (2.5) which is defined only on the set of

[1]The special case of VNS where only a single neighbourhood is explored in each iteration is sometimes referred to as a fixed neighbourhood search [45].

```
Procedure FP($P$)
1   Set $\overline{x}$ = LPSolve($P$); Set $proceed$ = true;
2   while ($proceed$) do
3       if ($\overline{x}$ is integer) then return $\overline{x}$;
4       Set $\widetilde{x} = [\overline{x}]$;
5       if (cycle detected) then
6           Select $k \in \{1, 2, \ldots, |\mathcal{B}|\}$;
7           Select $x' \in \mathcal{N}_k(\widetilde{x})$, such that $\delta(\overline{x}, x') = \min\{\delta(\overline{x}, y) \mid y \in \mathcal{N}_k(\widetilde{x})\}$;
8           Set $\widetilde{x} = x'$;
9       endif
10      $\overline{x}$ = LPSolve(LP($P, \widetilde{x}, \delta$));
11      Update $proceed$;
12  endwhile
```

Figure 6.1: The basic feasibility pump.

binary variables. The general feasibility pump proposed in [31] employs the distance function in which the general integer variables also contribute to the distance:

$$\Delta(x, y) = \sum_{j \in \mathcal{B} \cup \mathcal{G}} |x_j - y_j| \tag{6.4}$$

Unfortunately, the linearisation of the distance function $\Delta(x, y)$ as defined in (6.4) is not as simple as in the pure binary case (see (2.6)) and requires the introduction of additional variables. More precisely, for any integer feasible vector y, function $\Delta(x, y)$ as defined in (6.4) can be linearised as follows:

$$\Delta(x, y) = \sum_{j \in \mathcal{B} \cup \mathcal{G}: y_j = l_j} (x_j - l_j) + \sum_{j \in \mathcal{B} \cup \mathcal{G}: y_j = u_j} (u_j - x_j) + \sum_{j \in \mathcal{B} \cup \mathcal{G}: l_j < y_j < u_j} d_j, \tag{6.5}$$

where new variables $d_j = |x_j - y_j|$ need to satisfy the following constraints:

$$d_j \geq x_j - l_j, \ d_j \geq u_j - x_j, \quad \text{for all } j \in \{i \in \mathcal{B} \cup \mathcal{G} \mid l_i < y_i < u_i\}. \tag{6.6}$$

At each pumping cycle of the feasibility pump for the general MIP case, the fractional solution $\overline{x}$ can be obtained as the solution of the linear programming problem

$$(LP(P, \widetilde{x}, \Delta) \mid \{\{d_j \geq x_j - l_j, \ d_j \geq u_j - x_j\} \mid j \in \mathcal{B} \cup \mathcal{G} : l_j < y_j < u_j\}),$$

where $\widetilde{x}$ is the current integer solution. As in the case of pure 0-1 MIPs, the next integer feasible solution is again obtained by rounding the components of $\overline{x}$ to their nearest integer values.

Due to the different functionalities of binary and general integer variables in a MIP model, it is usually more effective to perform the basic feasibility pump on the set of the binary variables first (by releasing the integrality constraint on general integer variables), and only perform the general feasibility pump after the stopping criteria for the basic feasibility pump are fulfilled (see [31]). The stopping criteria for the basic feasibility pump may include encountering a feasible solution, cycle detection, maximum iteration count, maximum running time, etc.

6.1.3 Objective Feasibility Pump

According to the computational results reported in [31, 103], the feasibility pump is usually quite effective with respect to computational time needed to provide the first feasible solution, but the solution provided is often of a poor-quality. The reason is that original objective function is completely discarded after solving the LP relaxation of the original problem in order to construct the starting point for the search. In an attempt to provide good-quality initial solutions, a modification of the basic FP scheme, so called *objective feasibility pump*, was proposed in [5]. The idea of the objective FP is to include the original objective function as a part of the objective function of the problem considered at a certain pumping cycle of FP. At each pumping cycle, the actual objective function is computed as a linear combination of the feasibility measure and the original objective function:

$$\Delta_\alpha(x, \widetilde{x}) = (1-\alpha)\Delta(x, \widetilde{x}) + \alpha\frac{\sqrt{|\mathcal{B}\cup\mathcal{G}|}}{||c||}c^{\mathrm{T}}x,\ \alpha \in [0,1], \tag{6.7}$$

where $||\cdot||$ denotes the Euclidean norm and $\sqrt{|\mathcal{B}\cup\mathcal{G}|}$ is the Euclidean norm of the objective function vector (6.5). The fractional solution $\overline{x}$ at a certain iteration of the objective FP is then obtained by solving the LP problem $(\mathrm{LP}(P, \widetilde{x}, \Delta_\alpha) \mid C)$, for the current integer solution $\widetilde{x}$ and current value of α, where $C = \{\{d_j \geq x_j - l_j,\ d_j \geq u_j - x_j\} \mid j \in \mathcal{B}\cup\mathcal{G} : l_j < y_j < u_j\}$ is the set of constraints which newly introduced variables d_j need to satisfy. Furthermore, it has been observed in [5] that the best results are obtained if the value of α is geometrically decreased at each iteration, i.e. if in iteration t the value α_t is used, with $\alpha_0 \in [0,1]$ and $\alpha_{t+1} = q\alpha_t$, where $q \in (0,1)$ is a given geometric sequence ratio.

An important issue which arises with this approach is the detection of a cycle. Whereas in the basic version of FP (both for pure binary and general integer case) visiting an integer solution $\widetilde{x}$ which has already occurred in some previous iteration implies that the search process is caught in a cycle, in the objective FP it is not necessarily the case. Indeed, since different objective functions Δ_{α_t} are used in different iterations t, changing the value of α_t may force the algorithm to leave the cycle. Therefore, in the original implementation of the objective FP, a list L of pairs $(\widetilde{x}, \alpha_t)$ is kept for the purpose of cycle detection. Perturbation is performed at iteration t, with the current integer solution $\widetilde{x}$, if $(\widetilde{x}, \alpha_{t'}) \in L$, $t' < t$, and $\alpha_{t'} - \alpha_t < \varepsilon$, where $\varepsilon \geq 0$ is some predefined parameter value.

Results reported in [5] indicate that this approach usually yields considerably higher-quality solutions than the basic FP. However, it generally requires much longer computational time.

6.1.4 Feasibility Pump and Local Branching

In [105], the local branching heuristic [104] is applied to near-feasible solutions obtained from FP in order to locate the feasible solutions. The underlying idea is to start from an infeasible initial solution $\widetilde{x}$ and use local branching to gradually decrease the number of constraints which are violated by $\widetilde{x}$, until all constraints are finally satisfied.

In order to achieve this, some artificial variables are introduced. First, binary variables y_i are introduced to the 0-1 MIP model defined in (1.6), with the role to indicate the violated constraints. For each violated constraint $a_i^{\mathrm{T}}x \geq b_i$, $1 \leq i \leq m$, from the set of constraints $Ax \geq b$ in (1.6), variable y_i is set to 1. Otherwise, if the ith constraint from $Ax \geq b$ in (1.6) is not violated, variable y_i is set to 0. The new objective is to minimise the number of violated constraints $\sum_{i=1}^m y_i$. Furthermore, additional artificial non-negative continuous variables σ_i and δ_i are introduced in order to repair the infeasibility of $\widetilde{x}$. More precisely, each constraint $a_i^{\mathrm{T}}x \geq b_i$, $1 \leq i \leq m$, from (1.6) is modified as $a_i^{\mathrm{T}}x + \sigma_i \geq b_i$, while the additional constraints $\delta_i y_i \geq \sigma_i$ are introduced, for the large enough preselected values $\delta_i \geq 0$. In summary, the modified problem is formulated as follows:

$$(6.8)\quad \left[\begin{array}{ll} \min \sum_{i=1}^{m} y_i & \\ \text{s.t.}\quad \sum_{j=1}^{n} a_{ij}x_j + \sigma_i \geq b_i & \forall i \in M = \{1,2,\ldots,m\} \\ \qquad x_j \in \{0,1\} & \forall j \in \mathcal{B} \neq \emptyset \\ \qquad x_j \in \mathbb{Z}_0^+ & \forall j \in \mathcal{G}, \mathcal{G} \cap \mathcal{B} = \emptyset \\ \qquad x_j \geq 0 & \forall j \in \mathcal{C}, \mathcal{C} \cap \mathcal{G} = \emptyset, \mathcal{C} \cap \mathcal{B} = \emptyset \\ \qquad \delta_i y_i \geq \sigma_i & \forall i \in M = \{1,2,\ldots,m\} \\ \qquad \sigma_i \geq 0 & \forall i \in M = \{1,2,\ldots,m\} \\ \qquad y_i \in \{0,1\} & \forall i \in M = \{1,2,\ldots,m\} \end{array}\right.$$

Since variables y_i, which indicate the constraints violation, are binary, this reformulation of the original problem is especially convenient for the application of some 0-1 MIP local search heuristic, such as local branching [104] or variable neighbourhood branching [169]. In the original paper [105], local branching was applied in order to minimise the degree of violation. The results reported in [105] are encouraging, but the solutions obtained with this approach are often of a low-quality, since the original objective function is completely discarded. Potential ways to overcome this drawback may include the introduction of objective cuts $c^{\mathrm{T}}x \leq c^{\mathrm{T}}\widetilde{x}$ (in a minimisation case) into the modified problem, where $\widetilde{x}$ is the current integer solution, or possibly some formulation space search approach [239, 240] to alternate between the original and the modified formulation in order to achieve a better solution quality.

6.2 Variable Neighbourhood Pump

In this section a new heuristic for 0-1 MIP feasibility, called variable neighbourhood pump (VNP), is proposed. It combines two approaches: the feasibility pump [103] and the variable neighbourhood descent for 0-1 MIPs (VND-MIP) [169]. Although it is based on a similar idea as in [105], there are some major differences. First, a more systematic VND-MIP local search is applied to a near-feasible solution vector obtained from FP, instead of LB. More importantly, the original model is not changed during the search process. Namely, we just use the original objective function in all the subproblems generated during the VND-MIP search. In that way, high-quality feasible solutions are obtained in short time.

For the purpose of finding initial feasible solutions, the basic version of VND-MIP as presented in Figure 4.2 needs to be appropriately modified. The constructive variant of VND-MIP should start from any reference integer solution, not necessarily LP feasible, and should finish as soon as a feasible solution is encountered. The pseudo code for the constructive VND-MIP procedure, denoted as C-VND-MIP, is given in figure 6.2. Parameters k_{min}, k_{step} and k_{max} denote the minimum neighbourhood size, neighbourhood change step and the maximum neighbourhood size, respectively.

As mentioned previously, variable neighbourhood pump heuristic combines the FP [103] and the C-VND-MIP [169] approaches in order to detect a good quality initial feasible solution of a 0-1 MIP problem. In the beginning of the algorithm, the linear programmin relaxation solution $\overline{x}$ of the initial 0-1 MIP problem is obtained and pumping cycles of the feasibility pump is applied to the rounded vector $[\overline{x}]$ to obtain a near-feasible vector $\widetilde{x}$ as long as the process is not stalled in $\widetilde{x}$. We then apply the deterministic search procedure C-VND-MIP to $\widetilde{x}$, in an attempt to locate a feasible solution of the original problem. Our approach is based on the observation that $\widetilde{x}$ is

```
C-VND-MIP($P, x', k_{min}, k_{step}, k_{max}$)
$k = k_{min}$; status = ‘‘noFeasibleSolFound’’;
while ($k \leq k_{max}$ && (status == ‘‘noFeasibleSolFound’’) do
    $x'' =$ MIPSolve($P(k, x')$, $x'$);
    status = getSolutionStatus($P(k, x')$);
    if (status == ‘‘noFeasibleSolFound’’) then
        Add (reverse last) pseudo-cut (into) $\delta(x', x) \geq k + k_{step}$;
        $k = k + k_{step}$;
    else
        $x' = x''$;
    endif
end
return $x'$.
```

Figure 6.2: Constructive VND-MIP.

usually near-feasible and it is very likely that some feasible solution vectors can be found in some small neighbourhoods (with respect to Hamming distance) of $\widetilde{x}$. In addition, if C-VND-MIP fails to detect the feasible solution due to the time or neighbourhood size limitations, a pseudo-cut is added to the current subproblem in order to change the linear programming relaxation solution, and the process is iterated. If no feasible solution has been found, the algorithm reports failure and returns the last (infeasible) integer solution. The pseudo-code of the proposed VNP heuristic is given in figure 6.3.

```
Procedure VNP($P$)
Set $proceed1 =$ true;
while ($proceed1$) do
    Set $\overline{x} =$ LPSolve($P$); Set $\widetilde{x} = [\overline{x}]$; Set $proceed2 =$ true;
    while ($proceed2$) do
        if ($\overline{x}$ is integer) then return $\overline{x}$;
        $\overline{x} =$ LPSolve(LP($P, \widetilde{x}$));
        if ($\widetilde{x} \neq [\overline{x}]$) then $\widetilde{x} = [\overline{x}]$
        else Set $proceed2 =$ false;
        endif
    endwhile
    $k_{min} = \lfloor \delta(\widetilde{x}, \overline{x}) \rfloor$; $k_{max} = \lfloor (p - k_{min})/2 \rfloor$; $k_{step} = (k_{max} - k_{min})/5$;
    $x' =$ VNB($P, \widetilde{x}, k_{min}, k_{step}, k_{max}$);
    if ($x' = \widetilde{x}$) then //VNB failed to find the feasible solution.
        $P = (P \mid \delta(x, \widetilde{x}) \geq k_{min})$;
        Update $proceed1$;
    else return $x'$;
    endif
endwhile
Output message: "No feasible solution found"; return $\widetilde{x}$;
```

Figure 6.3: The variable neighbourhood pump pseudo-code.

6.3 Constructive Variable Neighbourhood Decomposition Search

Variable neighbourhood decomposition search for 0-1 MIPs, as described in Chapter 4, is a heuristic based on the systematic hard variable fixing (diving) process, according to the information obtained from the linear programming relaxation solution of the problem. The VNDS approach introduced in Chapter 4 can easily be adjusted to tackle the 0-1 MIP feasibility problem, by observing that a general-purpose MIP solver can be used not only for finding (near) optimal solutions of a given input problem, but also for finding an initial feasible solution. The resulting constructive VNDS-MIP procedure, called C-VNDS-MIP, can be described as follows.

The algorithm begins with obtaining the LP relaxation solution $\overline{x}$ of the original problem P, and generating an initial integer (not necessarily feasible) solution $\widetilde{x} = [\overline{x}]$, by rounding the LP solution $\overline{x}$. Note that, if the optimal solution $\overline{x}$ is integer feasible for P, we stop and return $\overline{x}$. At each iteration of the C-VNDS-MIP procedure, the distances $\delta_j =\mid \widetilde{x}_j - \overline{x}_j \mid$ from the current integer solution values $(\widetilde{x}_j)_{j\in\mathcal{B}}$ to the corresponding LP relaxation solution values $(\overline{x}_j)_{j\in\mathcal{B}}$ are computed and the variables $\widetilde{x}_j, j \in \mathcal{B}$ are indexed so that $\delta_1 \leq \delta_2 \leq \ldots \leq \delta_p$ (where $p =\mid \mathcal{B} \mid$). Then the subproblems $P(\widetilde{x}, \{1,\ldots,k\})$ obtained from the original problem P are successively solved, where the first k variables are fixed to their values in the current incumbent solution $\widetilde{x}$. If a feasible solution is found by solving $P(\widetilde{x}, \{1,\ldots,k\})$, it is returned as a feasible solution of the original problem P. Otherwise, a pseudo-cut $\delta(\{1,\ldots,k\}, \widetilde{x}, x) \geq 1$ is added in order to avoid exploring the search space of $P(\widetilde{x}, \{1,\ldots,k\})$ again and the next subproblem is examined. If no feasible solution is detected after solving all subproblems $P(\widetilde{x}, \{1,\ldots,k\})$, $k_{min} \leq k \leq k_{max}$, $k_{min} = k_{step}$, $k_{max} = |\mathcal{B}| - k_{step}$, the linear programming relaxation of the current problem P, which includes all the pseudo-cuts added during the search process, is solved and the process is iterated. If no feasible solution has been found due to the fulfilment of the stopping criteria, the algorithm reports failure and returns the last (infeasible) integer solution. The pseudo-code of the proposed C-VNDS-MIP heuristic is given in figure 6.4.

6.4 Computational Results

In this section we present the computational results for our algorithms. All results reported are obtained on a computer with a 2.4GHz Intel Core 2 Duo E6600 processor and 4GB RAM, using the general purpose MIP solver IBM ILOG CPLEX 11.1. Algorithms were implemented in C++ and compiled within Microsoft Visual Studio 2005. The 83 test instances which are considered here for comparison purposes are the same as those previously used for testing performances of the basic FP (see [103]). The detailed description of this benchmark can be found in Tables 6.1–6.2. The first column in Tables 6.1–6.2 presents the instance name, whereas the second, third and fourth column show the total number of variables, the number of binary variables and the number of constraints, respectively.

In both of the propsoed methods, the CPLEX MIP solver is used as a black-box for solving subproblems to feasibility. For this special purpose, the parameter `CPX_PARAM_MIP_ EMPHASIS` was set to `FEASIBILITY` and the parameter `CPX_PARAM_INTSOLLIM` was set to 1. Since we wanted to make an explicit comparison with FP, the FP heuristic in CPLEX as a black-box is switched off, i.e. the parameter `CPX_PARAM_FPHEUR` is set to -1. All other parameters are set to their default values. Furthermore, as we are only interested in the first feasible solution found by the CPLEX MIP solver alone, results for the CPLEX MIP solver were also generated with these parameter

Model	n	$\|\mathcal{B}\|$	m
10teams	2025	1800	230
A1C1S1	3648	192	3312
aflow30a	842	421	479
aflow40b	2728	1364	1442
air04	8904	8904	823
air05	7195	7195	426
cap6000	6000	6000	2176
dano3mip	13873	552	3202
danoint	521	56	664
ds	67732	67732	656
fast0507	63009	63009	507
fiber	1298	1254	363
fixnet6	878	378	478
glass4	322	302	396
harp2	2993	2993	112
liu	1156	1089	2178
markshare1	62	50	6
markshare2	74	60	7
mas74	151	150	13
mas76	151	150	12
misc07	260	259	212
mkc	5325	5323	3411
mod011	10958	96	4480
modglob	422	98	291
momentum1	5174	2349	42680
net12	14115	1603	14021
nsrand-ipx	6621	6620	735
nw04	87482	87482	36
opt1217	769	768	64
p2756	2756	2756	755
pk1	86	55	45
pp08a	240	64	136
pp08aCUTS	240	64	246
protfold	1835	1835	2112
qiu	840	48	1192
rd-rplusc-21	622	457	125899
set1ch	712	240	492
seymour	1372	1372	4944
sp97ar	14101	14101	1761
swath	6805	6724	884
t1717	73885	73885	551
tr12-30	1080	360	750
van	12481	192	27331
vpm2	378	168	234

Table 6.1: Benchmark group I: instances from the MIPLIB 2003 library.

Model	n	$\lvert\mathcal{B}\rvert$	m
biella1	7328	6110	1203
NSR8K	38356	32040	6284
dc1c	10039	8380	1649
dc1l	37297	35638	1653
dolom1	11612	9720	1803
siena1	13741	11775	2220
trento1	7687	6415	1265
rail507	63019	63009	509
rail2536c	15293	15284	2539
rail2586c	13226	13215	2589
rail4284c	21714	21705	4284
rail4872c	24656	24645	4875
A2C1S1	3648	192	3312
B1C1S1	3872	288	3904
B2C1S1	3872	288	3904
sp97ic	12497	12497	1033
sp98ar	15085	15085	1435
sp98ic	10894	10894	825
bg512142	792	240	1307
dg012142	2080	640	6310
blp-ar98	16021	15806	1128
blp-ic97	9845	9753	923
blp-ic98	13640	13550	717
blp-ir98	6097	6031	486
CMS750_4	11697	7196	16381
berlin_5_8_0	1083	794	1532
railway_8_1_0	1796	1177	2527
usAbbrv.8.25_70	2312	1681	3291
manpower1	10565	10564	25199
manpower2	10009	10008	23881
manpower3	10009	10008	23915
manpower3a	10009	10008	23865
manpower4	10009	10008	23914
manpower4a	10009	10008	23866
ljb2	771	681	1482
ljb7	4163	3920	8133
ljb9	4721	4460	9231
ljb10	5496	5196	10742
ljb12	4913	4633	9596

Table 6.2: Benchmark group II: the additional set of instances from [103].

```
C-VNDS-MIP($P, d$)
Set $proceed1 = proceed2 =$ true;
while ($proceed1$) do
    $\overline{x} =$ LPSolve($P$); $\widetilde{x} = [\overline{x}]$;
    if ($\overline{x} == \widetilde{x}$) return $\widetilde{x}$;
    $\delta_j = \mid \widetilde{x}_j - \overline{x}_j \mid$; index $x_j$ so that $\delta_j \leq \delta_{j+1}$, $j = 1, \ldots, p-1$
    Set $n_d = \mid \{j \in N \mid \delta_j \neq 0\} \mid$, $k_{step} = [n_d/d]$, $k = p - k_{step}$;
    while ($proceed2$ and $k \geq 0$) do
        $J_k = \{1, \ldots, k\}$; $x' =$ MIPSolve($P(\widetilde{x}, J_k), \widetilde{x}$);
        status = getSolutionStatus($P(\widetilde{x}, J_k)$);
        if (status == ``noFeasibleSolFound'') then
            $P = (P \mid \delta(J_k, \widetilde{x}, x) \geq 1)$;
        else return $x'$;
        if ($k - k_{step} > p - n_d$) then $k_{step} = \max\{[k/2], 1\}$;
        Set $k = k - k_{step}$;
        Update $proceed2$;
    endwhile
    Update $proceed1$;
endwhile
Output message: "No feasible solution found"; return $\widetilde{x}$;
```

Figure 6.4: Constructive VNDS for 0-1 MIP feasibility.

settings, except that the parameter which controls the usage of FP is set to CPX_PARAM_FPHEUR=2, meaning that FP is always applied.

All three methods (VNP, C-VNDS-MIP and CPLEX MIP) were allowed 1 hour (3600 seconds) total running time. In addition, the time limit for solving subproblems within VND-MIP was set to 180 seconds for all instances except van . Due to the numerical instability of this instance, a longer running time for subproblems is needed and was set to 1200 seconds. The time limit for subproblems within C-VNDS-MIP was set to 180 seconds for all instances.

Tables 6.3–6.4 provide the results regarding the solution quality of the three methods compared. The first three columns contain the objective values, whereas the following three columns contain the values of the gap from the best solution. For each instance, the gap from the best solution was computed according to the formula $\frac{f - f_{best}}{|f_{best}|} \times 100$, where f is the observed objective function value, and f_{best} is the best of the three objective values obtained by the CPLEX MIP solver, VNP and C-VNDS-MIP, respectively. For both objective values and computational time, all methods are ranked according to their performance: rank 1 is assigned to the best method and rank 3 to the worst method (in case of ties average ranks are assigned). The objective value ranks are reported in the last three columns of Tables 6.3–6.4.

Tables 6.5–6.6 provide the results regarding the computational time of the three methods compared. The first three columns contain the actual running times (in seconds), whereas the last three columns contain the running time value ranks. For the sake of robustness, the performances of two methods are considered equal, if the difference between their running time values is less then 1 second.

All experimental results are summarised in Table 6.7. Number of instances solved, average gap values and average computational time values are reported. Average rank values are also reported in Table 6.7 to avoid the misinterpretation of results in case that few exceptional values (either very good or very bad) influence the average scores.

From Table 6.7, we can see that the heuristics proposed in this chapter achieve a significantly

	Objective value			*Gap from best solution (%)*			*Objective value rank*		
Model	**CPLEX**	**VNP**	**VNDS**	**CPLEX**	**VNP**	**VNDS**	**CPLEX**	**VNP**	**VNDS**
10teams	1074.00	**924.00**	928.00	16.234	0.000	0.433	3	1	2
a1c1s1	20682.55	15618.14	**11746.63**	76.072	32.958	0.000	3	2	1
aflow30a	1387.00	1362.00	**1291.00**	7.436	5.500	0.000	3	2	1
aflow40b	1387.00	1362.00	**1291.00**	7.436	5.500	0.000	3	2	1
air04	60523.00	57648.00	**56301.00**	7.499	2.392	0.000	3	2	1
air05	29584.00	**26747.00**	26981.00	10.607	0.000	0.875	3	1	2
cap6000	-85207.00	**-2445700.00**	-2442801.00	96.516	0.000	0.119	3	1	2
dano3mip	768.38	768.38	768.38	0.001	0.000	0.000	2	2	2
danoint	80.00	69.50	**66.50**	20.301	4.511	0.000	3	2	1
ds	5418.56	1750.42	**630.74**	759.080	177.518	0.000	3	2	1
fast0507	733.00	185.00	**184.00**	298.370	0.543	0.000	3	2	1
fiber	418087.98	1010929.02	**414548.63**	0.854	143.863	0.000	2	3	1
fixnet6	97863.00	**4505.00**	7441.00	2072.320	0.000	65.172	3	1	2
glass4	4900040900.00	**3900031400.00**	4500033900.00	25.641	0.000	15.385	3	1	2
harp2	-72135642.00	-72021532.00	**-72920242.00**	1.076	1.232	0.000	2	3	1
liu	6450.00	6022.00	**4514.00**	42.889	33.407	0.000	3	2	1
markshare1	7286.00	**230.00**	**230.00**	3067.826	0.000	0.000	3	1.5	1.5
markshare2	10512.00	**338.00**	**338.00**	3010.059	0.000	0.000	3	1.5	1.5
mas74	157344.61	**14372.87**	19197.47	994.733	0.000	33.567	3	1	2
mas76	157344.61	**43774.26**	44877.42	259.446	0.000	2.520	3	1	2
misc07	4030.00	**3205.00**	3315.00	25.741	0.000	3.432	3	1	2
mkc	0.00	0.00	**-307.45**	100.000	100.000	0.000	2.5	2.5	1
mod011	0.00	0.00	0.00	0.000	0.000	0.000	2	2	2
modglob	36180511.32	35147088.88	**34539160.71**	4.752	1.760	0.000	3	2	1
momentum1	533874.74	315196.95	**109159.39**	389.078	188.749	0.000	3	2	1
net12	296.00	337.00	**214.00**	38.318	57.477	0.000	2	3	1
nsrand_ipx	**56160.00**	57440.00	185600.00	0.000	2.279	230.484	1	2	2
nw04	18606.00	19882.00	**16868.00**	10.304	17.868	0.000	3	2	1
opt1217	0.00	**-14.00**	**-14.00**	100.000	0.000	0.000	3	1.5	1.5
p2756	3584.00	3227.00	**3134.00**	14.359	2.967	0.000	3	2	1
pk1	731.00	**18.00**	**18.00**	3961.111	0.000	0.000	3	1.5	1.5
pp08a	27080.00	**8500.00**	8870.00	218.588	0.000	4.353	3	1	2
pp08aCUTS	12890.00	**8040.00**	8380.00	60.323	0.000	4.229	3	1	2
protfold	-9.00	**-17.00**	-14.00	47.059	0.000	17.647	3	1	2
qiu	1691.14	326.43	**-49.68**	3503.860	757.024	0.000	3	2	1
rd-rplusc-21	**174299.46**	185144.34	176147.03	0.000	6.222	1.060	1	3	2
set1ch	479735.75	378254.50	**56028.75**	756.231	575.108	0.000	3	2	1
seymour	666.00	479.00	436.00	52.752	9.862	0.000	3	2	1
sp97ar	**688614230.08**	695336779.52	721012280.96	0.000	0.976	4.705	1	2	3
swath	623.52	1512.12	**509.58**	22.359	196.736	0.000	2	3	1
t1717	**321052.00**	328093.00	341796.00	0.000	2.193	6.461	1	2	3
tr12-30	149687.00	235531.00	**134892.00**	10.968	74.607	0.000	2	3	1
vpm2	15.75	**15.25**	18.00	3.279	0.000	18.033	2	1	3

Table 6.3: Solution quality results for instances from group I.

	Objective value			*Gap from best solution (%)*			*Objective value rank*		
Model	**CPLEX**	**VNP**	**VNDS**	**CPLEX**	**VNP**	**VNDS**	**CPLEX**	**VNP**	**VNDS**
dc1c	1618738986.63	36152795.63	**4107014.47**	39314.007	780.269	**0.000**	3	2	1
dc1l	16673751825.80	17247576.53	**3012208.66**	553439.071	472.589	**0.000**	3	2	1
dolom1	2424470932.40	199413533.17	**194111743.99**	1149.008	2.731	**0.000**	3	2	1
siena1	560995341.87	**119249933.42**	195662038.65	370.437	0.000	64.077	3	1	2
trento1	5749161137.01	**35681229.00**	175605900.00	16012.565	0.000	392.152	3	1	2
bg512142	915353362.00	120738665.00	**96697404.00**	846.616	24.862	0.000	3	2	1
dg012142	1202822003.00	153406921.50	**78275846.67**	1436.645	95.982	0.000	3	2	1
blp-ar98	7243.24	**6851.27**	7070.51	5.721	0.000	3.200	3	1	2
blp-ic97	4813.25	4701.73	**4252.57**	13.185	10.562	0.000	3	2	1
blp-ic98	5208.83	5147.47	**5022.09**	3.718	2.496	0.000	3	2	1
blp-ir98	2722.02	2656.70	**2529.36**	7.617	5.035	0.000	3	2	1
CMS750_4	993.00	276.00	**260.00**	281.923	6.154	0.000	3	2	1
berlin_5_8_0	100.00	71.00	**62.00**	61.290	14.516	0.000	3	2	1
railway_8_1_0	500.00	421.00	**401.00**	24.688	4.988	0.000	3	2	1
van		6.62	**5.35**		23.633	0.000	3	2	1
biella1	45112270.55	3393472.21	**3374912.36**	1236.695	0.550	0.000	3	2	1
NSR8K	4933944064.89	6201012913.01	**60769054.15**	8019.172	10104.228	0.000	2	3	1
rail507	451.00	**180.00**	190.00	150.556	0.000	5.556	3	1	2
core2536-691	1698.00	719.00	**707.00**	140.170	1.697	0.000	3	2	1
core2586-950	2395.00	993.00	**986.00**	142.901	0.710	0.000	3	2	1
core4284-1064	2701.00	1142.00	**1101.00**	145.322	3.724	0.000	3	2	1
core4872-1529	3761.00	1636.00	**1584.00**	137.437	3.283	0.000	3	2	1
a2c1s1	20865.33	12907.27	**10920.87**	91.059	18.189	0.000	3	2	1
b1c1s1	69933.52	44983.15	**26215.81**	166.761	71.588	0.000	3	2	1
b2c1s1	70575.52	36465.72	**27108.67**	160.343	34.517	0.000	3	2	1
sp97ic	1464309330.88	575964341.60	**499112908.16**	193.382	15.398	0.000	3	2	1
sp98ar	2374928235.04	2349465005.92	**582657477.60**	307.603	303.233	0.000	3	2	1
sp98ic	1695655079.52	553276346.56	**506529902.72**	234.759	9.229	0.000	3	2	1
usAbbrv	200.00	142.00	**126.00**	58.730	12.698	0.000	3	2	1
manpower1	6.00	6.00	6.00	0.000	0.000	0.000	2	2	2
manpower2	6.00	6.00	6.00	0.000	0.000	0.000	2	2	2
manpower3	6.00	6.00	6.00	0.000	0.000	0.000	2	2	2
manpower3a	6.00	6.00	6.00	0.000	0.000	0.000	2	2	2
manpower4	6.00	6.00	6.00	0.000	0.000	0.000	2	2	2
manpower4a	6.00	6.00	6.00	0.000	0.000	0.000	2	2	2
ljb2	7.24	**7.24**	**7.24**	0.014	0.000	0.000	3	1.5	1.5
ljb7	8.62	**8.61**	**8.61**	0.105	0.000	0.000	3	1.5	1.5
ljb9	9.51	**9.48**	**9.48**	0.338	0.000	0.000	3	1.5	1.5
ljb10	7.37	7.31	7.30	0.931	0.123	0.000	3	2	1
ljb12	6.22	**6.20**	**6.20**	0.339	0.000	0.000	3	1.5	1.5

Table 6.4: Solution quality results for instances from group II.

	Running time (s)			*Running time rank*		
Model	**CPLEX**	**VNP**	**VNDS**	**CPLEX**	**VNP**	**VNDS**
10teams	**6.09**	18.90	20.64	1	2	3
a1c1s1	**0.53**	187.09	180.13	1	3	2
aflow30a	0.05	0.25	0.66	2	2	2
aflow40b	0.05	0.24	0.64	2	2	2
air04	**5.66**	12.06	**6.45**	1.5	3	1.5
air05	**1.88**	7.02	38.75	1	2	3
cap6000	0.09	0.11	0.08	2	2	2
dano3mip	17.17	19.15	14.91	2	3	1
danoint	1.30	0.58	0.45	2	2	2
ds	**0.89**	114.57	204.80	1	2	3
fast0507	**0.59**	27.71	13.75	1	3	2
fiber	0.03	0.052	0.14	2	2	2
fixnet6	0.00	0.03	0.03	2	2	2
glass4	0.05	0.16	0.38	2	2	2
harp2	0.03	0.11	0.41	2	2	2
liu	0.03	0.06	0.06	2	2	2
markshare1	0.00	0.00	0.01	2	2	2
markshare2	0.00	0.00	0.02	2	2	2
mas74	0.00	0.01	0.02	2	2	2
mas76	0.00	0.01	0.01	2	2	2
misc07	0.08	0.12	0.09	2	2	2
mkc	0.09	0.31	0.19	2	2	2
mod011	0.03	0.06	0.06	2	2	2
modglob	0.00	0.00	0.01	2	2	2
momentum1	**0.39**	22.49	87.94	1	2	3
net12	2116.08	**24.59**	550.50	3	1	2
nsrand_ipx	0.48	0.94	1.17	2	2	2
nw04	3.16	**0.72**	29.81	2	1	3
opt1217	0.00	0.01	0.00	2	2	2
p2756	0.08	0.13	0.58	2	2	2
pk1	0.00	0.00	0.00	2	2	2
pp08a	0.00	0.07	0.03	2	2	2
pp08aCUTS	0.00	0.06	0.03	2	2	2
protfold	486.28	**25.28**	182.08	3	1	2
qiu	**0.09**	14.11	5.63	1	3	2
rd-rplusc-21	**176.01**	94.45	1083.06	1	3	2
set1ch	0.00	0.03	0.28	2	2	2
seymour	**0.06**	1.63	1.41	1	2.5	2.5
sp97ar	**1.81**	4.21	**1.28**	1.5	3	1.5
swath	**0.59**	**0.62**	180.29	1.5	1.5	3
t1717	**47.95**	83.71	186.41	1	2	3
tr12-30	**1.47**	184.70	161.04	1	3	2
vpm2	0.00	0.01	0.02	2	2	2

Table 6.5: Computational time results for instances from group I.

	Running time (s)			*Running time rank*		
Model	**CPLEX**	**VNP**	**VNDS**	**CPLEX**	**VNP**	**VNDS**
dc1c	**0.16**	8.01	5.34	1	3	2
dc1l	**0.58**	173.44	31.92	1	3	2
dolom1	**0.23**	15.01	186.90	1	2	3
siena1	**16.80**	36.15	30.33	1	3	2
trento1	**0.11**	5.63	4.67	1	2.5	2.5
bg512142	0.00	0.14	0.11	2	2	2
dg012142	0.02	0.49	0.48	2	2	2
blp-ar98	**2.13**	6.90	181.35	1	2	3
blp-ic97	**0.44**	**0.88**	77.14	1.5	1.5	3
blp-ic98	**0.88**	**1.74**	181.41	1.5	1.5	3
blp-ir98	**1.16**	**1.65**	3.11	1.5	1.5	3
CMS750_4	**0.41**	219.07	189.40	1	3	2
berlin_5_8_0	**0.01**	**0.63**	182.30	1.5	1.5	3
railway_8_1_0	**0.05**	181.15	89.44	1	3	2
van	3600.29	1125.67	**193.92**	3	2	1
biella1	**0.09**	3.55	2.66	1	2.5	2.5
NSR8K	**351.18**	3105.12	545.05	2	3	1
rail507	**0.75**	33.88	7.95	1	3	2
core2536-691	**0.22**	59.17	7.80	1	3	2
core2586-950	**0.17**	30.73	204.13	1	2	3
core4284-1064	**0.31**	68.79	224.88	1	2	3
core4872-1529	**0.42**	78.53	236.30	1	2	3
a2c1s1	**0.05**	299.73	180.13	1	3	2
b1c1s1	**0.05**	142.01	180.15	1	2	3
b2c1s1	**0.06**	190.79	180.16	1	3	2
sp97ic	0.52	1.53	1.09	2	2	2
sp98ar	**0.81**	4.15	1.95	1	3	2
sp98ic	**0.58**	4.09	**1.14**	1.5	3	1.5
usAbbrv	**0.06**	192.99	181.35	1	3	2
manpower1	9.17	20.96	**6.73**	2	3	1
manpower2	32.98	57.05	**29.34**	2	3	1
manpower3	31.45	44.27	**24.52**	2	3	1
manpower3a	61.08	**55.76**	57.70	3	1	2
manpower4	524.24	**31.50**	70.69	3	1	2
manpower4a	**36.08**	65.93	38.25	1	3	2
ljb2	0.02	0.06	0.05	2	2	2
ljb7	0.08	0.96	0.33	2	2	2
ljb9	**0.08**	1.30	**0.30**	1.5	3	1.5
ljb10	**0.11**	2.01	**0.69**	1.5	3	1.5
ljb12	**0.08**	1.51	**0.39**	1.5	3	1.5

Table 6.6: Computational time results for instances from group II.

	CPLEX	VNP	VNDS
Solution quality			
Instances solved	82	83	83
Average gap (%)	7856.67	173.79	10.52
Average rank	2.72	1.85	1.42
Computational time			
Average (sec)	90.88	85.77	78.26
Average rank	1.62	2.27	2.11

Table 6.7: Summarised results.

better solution quality than CPLEX (with FP), according to both average gap and average rank values. Regarding the computational time, we can see that all three methods have a very similar performance. According to the average computational time values, VNDS slightly dominates the others, whereas the CPLEX MIP solver is moderately slower than the other two methods. According to the average ranks however, the CPLEX MIP solver solves the most instances first. Nevertheless, by observing the actual time differences, it is easy to see that for those instances differences are usually much smaller than in those cases where VNP and/or VNDS is faster than CPLEX. We can also note that the CPLEX solver fails to provide a feasible solution for one instance (`van`).

Results in Table 6.7 also show that the constructive VNDS is the better choice among the two proposed heuristics, both regarding the solution quality and the computational time. This outcome may be explained by the fact that subproblems generated by the hard variable fixing, which are examined in the VNDS search process, are smaller in size than those generated by soft variable fixing, as in the case of VNP. Therefore, they are much easier to explore and require less computational time. In addition, instances for which solving the linear programming relaxation is time consuming (such as `NSR8K`) are particularly inadequate for the VNP method, since a number of linear programming relaxation problems $\mathrm{LP}(P, \widetilde{x})$ needs to be solved in the feasibility pump stage of VNP.

6.5 Summary

In this chapter we propose two new heuristics for constructing initial feasible solutions of 0-1 mixed integer programming problems (0-1 MIPs), which are based on the variable neighbourhood search metaheuristic framework.

The first heuristic, called variable neighbourhood pump (VNP), combines ideas of feasibility pump (FP) [103] and variable neighbourhood branching (VNB) [169] heuristics. It uses FP to obtain a near-feasible solution vector to be passed as a starting vector to the VNB local search, which attempts to locate the feasible solution of the original problem. If VNB fails to detect the feasible solution due to the time or neighbourhood size limitations, a pseudo-cut is added to the current subproblem in order to change the linear programming relaxation solution, and the process is iterated.

The second heuristic, which is a constructive variant of VNDS-MIP presented in Chapter 4, performs systematic hard variable fixing according to the rules of variable neighbourhood decomposition search (VNDS) [168], in order to generate smaller subproblems whose feasible solution (if one exists) is also feasible for the original problem. Pseudo-cuts are added during the search process in order to prevent the exploration of already visited search space areas. Both methods use the generic CPLEX MIP solver as a black-box for finding feasible solutions.

The two proposed heuristics were tested on an established set of 83 benchmark problems (proven to be difficult to solve to feasibility) and compared with the IBM ILOG CPLEX 11.1 MIP solver (which already includes standard FP as a primal heuristic). Based on the average best solution gap and average rank values, we can conclude that both methods significantly outperform the CPLEX MIP solver regarding the solution quality. The constructive VNDS heuristic has the best performance, with the average gap of only 10.52% and average rank 1.43, followed by VNP with gap 173.79% and rank 1.84, whereas the CPLEX MIP solver has the worst performance, with average gap 7856.67% and rank 2.73. Regarding the computational time, the difference between the methods is not that remarkable. Still, VNDS has the smallest average computational time (78.26 seconds), VNP is the second best method with average running time 85.77 seconds and the CPLEX MIP solver is the slowest with 90.88 seconds average running time. However, by comparing the average computational time ranks, we can see that the CPLEX MIP solver solved most of the instances first. Finally, it is noteworthy that both proposed heuristics successfully solved all of the 83 instances from the benchmark, whereas CPLEX failed to find a feasible solution for one instance.

Chapter 7

Conclusions

The research reported in this thesis focuses on the development of novel variable neighbourhood search (VNS) [237] based heuristics for 0-1 mixed integer programming (MIP) problems and clustering. The major part of this thesis is devoted to designing matheuristics for 0-1 mixed integer programming problems derived from the variable neighbourhood search metaheuristic. Neighbourhood structures are implicitly defined and updated according to the set of parameters acquired from the mathematical formulation of the input problem. Normally, the general-purpose CPLEX MIP solver is used as a search component within VNS. However, the aim of this thesis is not solely to design specific heuristics for specific problems. Some new variants of the VNS metaheuristic itself are also proposed, in an endeavour to develop a more general framework, which is able to adapt to the specific features of a specific problem instance. Moreover, a new unifying perspective on modern advances in metaheuristics, called hyper-reactive optimisation, was proposed.

In Chapter 2, a thorough survey of the local search based metaheuristic methods was supplied. Most theoretical and practical aspects of neighbourhood search were covered, from the simplest local search to the highly modern techniques, involving large-scale neighbourhood search, reactive approaches and formulation space search. Local search techniques for 0-1 MIP problems were also studied. Apart from outlining the existing concepts and components of a neighbourhood search in combinatorial optimisation, the aim of Chapter 2 was also to point out the possible future trends in the developments of explorative methods. The prospects of incorporating automatic component tuning, together with adaptive memory, into the search process were discussed, especially for the case when not only the basic search parameters are considered, but also the different problem formulations and possible neighbourhood structures. As a result, a comprehensive approach to solving combinatorial optimization problems was proposed, called *hyper-reactive* optimisation, which integrates the philosophies of a reactive search and a hyper-heuristic search.

Chapter 3 shows that the variable neighbourhood search (VNS) heuristic for data clustering can be successfully employed as a new colour image quantisation (CIQ) technique. In order to avoid long running time of the algorithm, the decomposed (VNDS) and the reduced (RVNS) versions of the VNS heuristic were designed. Results obtained show that the errors of the proposed heuristics can compare favourably to those of recently proposed heuristics from the literature, within a reasonable time. In addition, the two different models for solving CIQ were compared: the M-Median model and the usual M-means model. The results of that comparison showed that the VNS based heuristic for the M-Median is much faster, even in the case when the latter use the M-Median solution as initial one. It is also shown that in the case of quantisation to large number of colours, solutions of the same visual quality are obtained with both models. Future research in this direction may include the use of a VNS technique for solving other similar problems such as colour image segmentation [54].

In Chapter 4 a new approach for solving 0-1 MIP problems was proposed. The proposed method, called VNDS-MIP, combines hard and soft variable fixing: hard fixing is based on the variable neighbourhood decomposition search framework, whereas soft fixing introduces pseudo-cuts as in local branching (LB) [104], according to the rules of the variable neighbourhood descent scheme [169]. The proposed VNDS-MIP proved to perform well when compared with the state-of-the-art 0-1 MIP solution methods and the exact CPLEX MIP solver. The current state of the art methods considered for the purpose of comparison with VNDS-MIP were local branching (LB) [104], variable neighbourhood branching (VNB) [169] and relaxation induced neighbourhood search (RINS) [75]. The experiments showed that VNDS-MIP was the best choice among all the solution methods compared, regarding all the aspects considered: average percentage gap, average objective value rank and the number of times that the method managed to improve the best known published objective. In addition, VNDS-MIP appeared to be the second best method (after LB) regarding the computational time, according to both average computational time and average time performance rank. The conclusions about the performance of the compared algorithms were reinforced by conducting a statistical analysis on the experimental results, which proved that a significant difference between the compared algorithms indeed exists.

Chapter 5 was dedicated to various applications of VNDS for some specific 0-1 MIP problems: the multidimensional knapsack problem (MKP), the problem of barge container ships routing and the two-stage stochastic mixed integer programming problem (2SSP). New heuristics for solving the MKP were proposed, which dynamically improve lower and upper bounds on the optimal value within VNDS-MIP. Different heuristics were derived by choosing a particular strategy of updating lower and upper bounds, and thus defining different schemes for generating a series of sub-problems. A two-level decomposition scheme for MKP was also proposed, in which sub-problems derived using one criterion are further divided into subproblems according to another criterion. Furthermore, for two of the proposed heuristics convergence to an optimal solution was proven if no limitations regarding the execution time or the number of iterations are imposed. Based on extensive computational analysis performed on benchmark instances from the literature and several statistical tests designed for the comparison purposes, it was concluded that VNDS based matheuristic has a lot of potential for solving MKP. In particular, the proposed algorithms are comparable with the current state-of-the-art heuristics for MKP and a few new best known lower bound values were obtained. For the case of the barge container ship routing problem, the use of MIP heuristics was also proved to be beneficial, both regarding the solution quality and (especially) the execution time. The same set of solution methods was used as in Chapter 4, which deals with 0-1 MIP problems in general. The VNB heuristic proved to be better than the CPLEX MIP solver regarding both criteria (solution quality/execution time). LB and VNDS did not achieve as good solution quality as CPLEX, but had significantly better execution time (they were approximately 3 times faster than CPLEX). Based on the computational analysis performed on an established benchmark of 25 stochastic integer programming (SIP) instances [7], it was concluded that the VNDS based matheuristic has a lot of potential for solving mixed integer two-stage stochastic (2SSP) problems as well. Computational results showed that the proposed `VNDS-SIP` method was competitive with the CPLEX MIP solver for the deterministic equivalent problem (DEP) regarding the solution quality: it achieved the same objective value as the CPLEX MIP solver for DEP in 15 cases, had better performance in 7 cases and worse performance in 3 cases. `VNDS-SIP` usually required longer execution time than the DEP solver. However, it is remarkable that, for the three largest instances whose deterministic equivalents contain hundreds of thousands binary variables, `VNDS-SIP` obtained a significantly better objective value (approximately 200% better) than the DEP solver, within the allowed execution time of 1800 seconds reached by both methods. Furthermore, these objective values were very close to optimality [7].

In Chapter 6, two new heuristics for constructing initial feasible solutions of 0-1 mixed integer programs (0-1 MIPs) were proposed, based on the variable neighbourhood search metaheuristic framework. The first heuristic, called variable neighbourhood pump (VNP), combines ideas of feasibility pump (FP) [103] and variable neighbourhood branching [169]. It uses FP to obtain a near-feasible solution vector to be passed as a starting vector to the VNB local search, which attempts to locate the feasible solution of the original problem. If VNB fails to detect the feasible solution due to the time or neighbourhood size limitations, a pseudo-cut is added to the current subproblem in order to change the linear programming relaxation solution, and the process is iterated. The second heuristic, which is a constructive variant of VNDS-MIP presented in Chapter 4, performs systematic hard variable fixing according to the rules of variable neighbourhood decomposition search (VNDS) [168], in order to generate smaller subproblems whose feasible solution (if one exists) is also feasible for the original problem. Pseudo-cuts are added during the search process in order to prevent the exploration of already visited search space areas. Both methods use the generic CPLEX MIP solver as a black-box for finding feasible solutions. The two proposed heuristics were tested on an established set of 83 benchmark problems (proven to be difficult to solve to feasibility) and compared with the IBM ILOG CPLEX 11.1 MIP solver (which already includes standard FP as a primal heuristic). Based on the average best solution gap and average rank values, it is concluded that both methods significantly outperform the CPLEX MIP solver regarding the solution quality. The constructive VNDS heuristic had the best performance, with the average gap of only 10.52% and average rank 1.43, followed by VNP with gap 173.79% and rank 1.84, whereas the CPLEX MIP solver had the worst performance, with average gap 7856.67% and rank 2.73. Regarding the computational time, the difference between the methods was not that remarkable. Still, VNDS had the smallest average computational time (78.26 seconds), VNP was the second best method with average running time 85.77 seconds and the CPLEX MIP solver was the slowest with 90.88 seconds average running time. However, by comparing the average computational time ranks, one could observe that the CPLEX MIP solver managed to solve most of the instances first. Finally, it is noteworthy that both proposed heuristics successfully solved all of the 83 instances from the benchmark, whereas CPLEX failed to find a feasible solution for one instance.

In summary, the research reported in this thesis and the results obtained may be of benefit to various scientific and industrial communities. On one hand, an up to date coverage of existing metaheuristic approaches and the new solution methodologies proposed in this thesis may help academic researchers attempting to develop computationally effective search heuristics for large-scale discrete optimisation problems. On the other hand, practitioners from variety of areas, such as different industries, public services, government sectors, may benefit from the applications of the proposed solution techniques to find solutions to problems arising in diverse real-world applications. In particular, the integration of some of the proposed solution methods into a general purpose MIP solver may enhance the overall performance of that solver, thus improving its overall potential for solving difficult real-world MIP models. For example, the integration of VNDS based heuristic for solving the 2SSP problem into the OptiRisk FortSP stochastic programming solver has led to promising results regarding the SP problems (see Chapter 5, Section 5.3). The theory and algorithms presented in this thesis indicate that hybridisation of the CPLEX MIP solver and the VNS metaheuristic can be very effective for solving large instances of mixed integer programming problems. More generally, the results presented in this thesis suggest that hybridisation of exact (commercial) integer programming solvers and some metaheuristic methods is of high interest and such combinations deserve further practical and theoretical investigation. The author hopes that this thesis may encourage a broader adoption of exploiting the mathematical formulations of problems within metaheuristic frameworks in the area of linear and mixed integer programming.

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Appendix A

Computational Complexity

The origins of the complexity theory date back to the 1930s, when a robust theory of computability was first conceived in the work of Turing [307], Church [59, 60, 61], Gödel and other mathematicians [136]. Although von Neumann was first to distinguish between the algorithms with a polynomial time performance and algorithms with a non-polynomial time performance back in the 1950s [315, 316], it is widely accepted that a notion of computability in polynomial time was introduced by Cobham [62] and Edmonds [95] in the 1960s. In the work of Edmonds [95], polynomial algorithms (i.e. algorithms "whose difficulty increases only algebraically with the size of the input instance") were referred to as *good algorithms*.

In 1971, Cook introduced the notion of NP-completeness, by means of the formal languages theory [65, 66]. Although the notion of NP-completeness had been present in the scientific world even before that, it was not clear whether NP-complete problems indeed exist. Cook managed to prove that a few real-world problems, including the satisfiability problem (SAT), are NP-complete. A year later, Karp used these findings to prove that 20 other real-world problems are NP-complete [192], thus illustrating the importance of Cook's results. Independently of Cook and Karp, Levin has introduced the notion of a *universal search problem*, which is very similar to an NP-complete problem, and provided 6 examples of such problems [210], including SAT. Since then, several hundreds of NP-complete problems have been identified [115].

The remainder of this chapter is organised as follows. Section A.1 is devoted to formal languages and decision problems. In Section A.2, the notion of a Turing machine as a computational model is introduced and some basic types of Turing machines are described. Section A.3 introduces the two most important time complexity classes P and NP. Finally, the notion of NP-completeness is defined in Section A.4 and the importance of the problem "P=NP" is explained.

A.1 Decision Problems and Formal Languages

There are two approaches in studying the theory of computability: one includes the theory of *formal languages*, and the other includes the theory of *decision problems*. All terms and statements can be analogously defined/formulated in each of these two approaches. The formal languages theory is more convenient for further development of the theory of NP-completeness, whereas the decision problems are more convenient for practical applications. Here we aim to clarify the relation between these two approaches.

We here provide a not so formal definition of a decision problem, according to [281]:

Definition A.1 *A* decision problem *is a yes-or-no question on a specified set of inputs.*

A decision problem is also known as an *Entscheidungsproblem*. More on the formal theory of decision problems can be found in, for example, [38, 59]. Note that a combinatorial optimisation problem as defined in (1.1), with an optimal value μ, can be formulated as a decision problem in the following way: "*Is it true that, for each $x \in X$, $f(x) \geq \mu$ and there exists $x_0 \in X$ such that $f(x_0) = \mu$?* ".

Definition A.2 *An* alphabet Σ *is a finite, non-empty set of symbols.*

Definition A.3 *A* word *(or a* string*) over an alphabet Σ is a finite sequence of symbols from Σ. The* length $|w|$ *of a string w from Σ is the number of symbols in w. The string of length 0 (i.e. with no symbols) is called an* empty string *and denoted as λ.*

Definition A.4 *Let Σ be an alphabet. The set Σ^* of all words (or strings) over Σ is defined as follows:*

- $\lambda \in \Sigma^*$
- *If $a \in \Sigma$ and $w \in \Sigma^*$, then $aw \in \Sigma^*$.*

Definition A.5 *Let Σ be an alphabet. Then a* language L *over Σ is a subset of Σ^*.*

More on the theory of the formal languages can be found in, for example, [320].

Definition A.6 *Let Σ be an alphabet and $L \subseteq \Sigma^*$ a language over Σ. The* decision problem D_L for a language L *is the following task:*

$$\text{For an arbitrary string } I \in \Sigma^*, \text{verify whether } I \in L.$$

The input string I is called an instance of the problem D_L. *I is a* positive *or a "yes" instance if $I \in L$. Otherwise, I is a* negative *or a "no" instance.*

Any decision problem in computer science can be represented as a decision problem for a certain formal language L. The corresponding language L ís the set of all instances of a given decision problem to which the answer is "yes". Conversely, every formal language L induces the decision problem D_L. Therefore, both approaches will be used concurrently in further text and no formal difference between them will be emphasised.

A.2 Turing Machines

A *Turing machine* is a hypothetical machine which comprises of the two basic compontents: a memory and a set of instructions. The memory is represented as an infinite sequence of cells arranged linearly on an infinite tape (unbounded from both ends). Each cell contains one piece of information: a symbol from a finite tape alphabet Γ. Each cell can be accessed using a read/write head which points to exactly one cell at a time. The head may move only one cell left or right from the current position. All computations on a Turing machine are performed with respect to a given set of instructions. Informally, each instruction may be interpreted in the following way: *when a machine is in the state p and its head points to a cell containing symbol a, then write symbol b into that cell, move the head left/right or leave it at the same position and change the current state p to another state q.* Formally, a Turing machine may be defined as follows.

Definition A.7 *A* Turing machine T *is a 8-tuple* $(Q, \Sigma, \Gamma, \delta, q_0, B, q_A, q_R)$*, where:*

- Q *is the finite set of states,* $Q \cap \Sigma = \emptyset$*;*
- Σ *is the finite set of symbols, called* input alphabet*,* $B \notin \Sigma$*;*
- Γ *is the finite set, called* tape alphabet*,* $\{B\} \cup \Sigma \subseteq \Gamma$*;*
- $q_0 \in Q$ *is the* initial state*;*
- B *is the* blank symbol*;*
- $q_A \in Q$ *is the* accepting state*;*
- $q_R \in Q$ *is the* rejecting state*;*
- δ *is the* transition function

$$\delta : Q \backslash \{q_A, q_R\} \times \Gamma \to Q \times \Gamma \times \{L, R, S\}$$

Function δ defines the set of instructions of a Turing machine. The expression $\delta(q, a) = (r, b, U)$ means that, when the machine is in the state q and the head points to a cell which contains symbol a, then a gets rewritten with symbol b, machine switches to a new state r, and the head moves depending on the element $U \in \{L, R, S\}$ (to the left if $U = L$, to the right if $U = R$ and does not move if $U = S$).

Definition A.8 *A* configuration *of a Turing machine T is a triplet* (w_1, q, w_2)*, where*

- $w_1 \in \Sigma^*$ *is the content of the tape left of the head pointing cell,*
- $q \in Q$ *is the current state,*
- $w_2 \in \Sigma^*$ *is the content of the tape right of the head pointing cell.*

A configuration of a Turing machine contains information necessary to proceed with a (possibly interrupted) computation. At the beginning and at the end of computation, the configuration needs to satisfy certain conditions:

- the *starting configuration* for a given input $w \in \Gamma^*$ has to be $q_0 w$
- the *accepting configuration* is any configuration of the form $uq_A v$, $u, v \in \Gamma^*$
- the *rejecting configuration* is any configuration of the form $uq_R v$, $u, v \in \Gamma^*$.

Accepting and rejecting configurations are the only *halting* configurations. A Turing machine performs computations as long as the accepting or the rejecting state is not reached. If none of these states is ever visited, then the computation continues infinitely.

Definition A.9 *Let* $T = (Q, \Sigma, \Gamma, \delta, q_0, B, q_A, q_R)$ *be a Turing machine with the transition function* $\delta : Q \backslash \{q_A, q_R\} \times \Gamma \to Q \times \Gamma \times \{L, R, S\}$ *and let* $u, v \in \Gamma^*$*,* $q_i, q_j \in Q$ *and* $a, b \in \Gamma$*. The* next move *relation, denoted as* $\vdash_{\mathrm{T}}$*, is defined so that:*

- $uaq_i bv \vdash_{\mathrm{T}} uacq_j v$ *if and only if* $\delta(q_i, b) = (q_j, c, R)$
- $uq_i av \vdash_{\mathrm{T}} uq_j bv$ *if and only if* $\delta(q_i, a) = (q_j, b, S)$
- $uaq_i bv \vdash_{\mathrm{T}} uq_j acv$ *if and only if* $\delta(q_i, b) = (q_j, c, L)$.

Definition A.10 *Let C and D be two configurations of a given Turing machine T. Then*

$$C \vdash_{\mathrm{T}}^{k} D$$

for $k \in \mathbb{N}$, $k \geq 1$, if and only if there exists a finite sequence of configurations $C_1, C_2, \ldots, C_k$, such that $C = C_1 \vdash_{\mathrm{T}} C_2 \vdash_{\mathrm{T}} \ldots \vdash_{\mathrm{T}} C_k = D$. Furthermore,

$$C \vdash_{\mathrm{T}}^{*} D$$

if and only if $C = D$, or there exists $k \in \mathbb{N}$, $k \geq 1$, such that $C \vdash_{\mathrm{T}}^{k} D$.

Definition A.11 *A Turing machine $T = (Q, \Sigma, \Gamma, \delta, q_0, B, q_A, q_R)$* accepts *an input word $w \in \Sigma^*$ if and only if $q_0 w \vdash_{\mathrm{T}}^{*} I$, where I is an accepting configuration. Turing machine T* rejects *an input word $w \in \Sigma^*$ if and only if $q_0 w \vdash_{\mathrm{T}}^{*} I$, where I is a rejecting configuration.*

Definition A.12 *Let $T = (Q, \Sigma, \Gamma, \delta, q_0, B, q_A, q_R)$ be a Turing machine, and $L(T)$ a language consisting of words accepted by T, i.e.*

$$L(T) = \{w \in \Sigma^* \mid T \textit{ accepts } w\}.$$

Then we say that Turing machine T accepts *language $L(T)$.*

Definition A.13 *Language L is* Turing-acceptable *(or* recursively enumerable*) if there exists a Turing machine T such that $L = L(T)$.*

Note that, if a language L is Turing-acceptable, then, for an input word $w \notin L$, machine T can either halt in a rejecting configuration or not halt at all.

Definition A.14 *Two Turing machines T and T' are* equivalent *if and only if $L(T) = L(T')$.*

Definition A.15 *Language $L \subseteq \Sigma^*$ is* Turing-decidable *(or* recursive*) if there exists a Turing machine $T = (Q, \Sigma, \Gamma, \delta, q_0, B, q_A, q_R)$ such that $L = L(T)$ and T halts for each input $w \in \Sigma^*$: T halts in an accepting configuration if $w \in L$ and T halts in a rejecting configuration if $w \notin L$. In that case we also say that T* decides *L.*

Turing machine as defined above can also be used for computing string functions.

Definition A.16 *Let $T = (Q, \Sigma, \Gamma, \delta, q_0, B, q_A, q_R)$ be a given Turing machine and $f : \Sigma^* \to \Sigma^*$. Turing machine T* computes *f if, for any input word $w \in \Sigma^*$, T halts in configuration $(f(x), q_R, \lambda)$, where $\lambda \in \Sigma^0$ is the empty word.*

We next provide some extended concepts of a basic one-tape Turing machine. These concepts are intended to provide more convincing arguments for the *Church's thesis*, which basically states that a Turing machine is as powerful as any other computer (see, for example, [178, 254]). However, there are not formal proofs for this statement up to date.

A k-tapes Turing machine has k different tapes, each with its own read/write head.

Definition A.17 *A* multi-tape Turing machine *T with k tapes, $k \in \mathbb{N}$, $k \geq 1$, is an 8-tuple $(Q, \Sigma, \Gamma, \delta, q_0, B, q_A, q_R)$, where:*

- *Q is the finite set of states, $Q \cap \Sigma = \emptyset$;*

- Σ *is the finite set of symbols, called* input alphabet*,* $B \notin \Sigma$*;*
- Γ *is the finite set, called* tape alphabet*,* $\{B\} \cup \Sigma \subseteq \Gamma$*;*
- $q_0 \in Q$ *is the* initial state*;*
- B *is the* blank symbol*;*
- $q_A \in Q$ *is the* accepting state*;*
- $q_R \in Q$ *is the* rejecting state*;*
- δ *is the* transition function

$$\delta : Q \backslash \{q_A, q_R\} \times \Gamma^k \rightarrow Q \times \Gamma^k \times \{L, R, S\}^k.$$

Given a state q, symbols $a_1, a_2, \ldots, a_k \in \Gamma$ on tapes $1, 2, \ldots, k$, respectively, and $\delta(q, a_1, a_2, \ldots, a_k) = (p, b_1, b_2, \ldots, b_k, D_1, D_2, \ldots, D_k)$, where $p \in Q$, $b_1, b_2, \ldots, b_k \in \Gamma$ and $D_1, D_2, \ldots, D_k \in \{L, R, S\}$, machine T switches to the new state p, writes new symbols $b_1, b_2, \ldots, b_k \in \Gamma$ on tapes $1, 2, \ldots, k$, respectively, and moves the ith head according to the direction D_i, $1 \leq i \leq k$. All definitions regarding Turing machines with one tape can be extended in an analogous way for Turing machines with k tapes, $k \in \mathbb{N}$, $k > 1$.

The following theorem holds, for which the proof can be found in [254].

Theorem A.1 *For any multi-tape Turing machine T there is an equivalent one-tape Turing machine T'.*

In both one-tape and multi-tape Turing machines defined so far, there was always only one next move possible from a given configuration. This why they are also called *deterministic* Turing machines. However, the concept of a Turing machine can be further extended, so that more than one move from a certain configuration is allowed. The resulting machine is called a *nondeterministic Turing machine* and is formally defined as follows.

Definition A.18 *A* nondeterministic Turing machine *T is an 8-tuple* $(Q, \Sigma, \Gamma, \delta, q_0, B, q_A, q_R)$*, where:*

- Q *is the finite set of states,* $Q \cap \Sigma = \emptyset$*;*
- Σ *is the finite set of symbols, called* input alphabet*,* $B \notin \Sigma$*;*
- Γ *is the finite set, called* tape alphabet*,* $\{B\} \cup \Sigma \subseteq \Gamma$*;*
- $q_0 \in Q$ *is the* initial state*;*
- B *is the* blank symbol*;*
- $q_A \in Q$ *is the* accepting state*;*
- $q_R \in Q$ *is the* rejecting state*;*
- δ *is the* transition function

$$\delta : Q \backslash \{q_A, q_R\} \times \Gamma \rightarrow \mathcal{P}(Q \times \Gamma \times \{L, R, S\}).$$

Similarly as in the case of multi-tape Turing machines, all definitions regarding deterministic Turing machines with one tape can be extended in an analogous way for nondeterministic Turing machines. The following theorem holds, for which the proof can be found in [254].

Theorem A.2 *For any nondeterministic Turing machine T there is an equivalent deterministic one-tape Turing machine T'.*

A.3 Time Complexity Classes P and NP

The computability theory deals with the following type of queries: "Is it (not) possible to solve a certain problem algorithmically, i.e. using a computer?". On the other hand, once it is determined that a certain problem can be solved, the question arises how hard it is to solve it. The answers to such questions can be sought in *computational complexity* theory.

Computational complexity can be studied from two aspects:

- time complexity: what is the minimum number of steps required for the computation?
- space complexity: what is the minimum number of memory bits required for the computation?

In case of Turing machines, memory bits are actually tape cells.

Definition A.19 *Let $T = (Q, \Sigma, \Gamma, \delta, q_0, B, q_A, q_R)$ be a Turing machine and $w \in \Sigma^*$. If $t \in \mathbb{N}$ is a number such that $q_0 w \vdash_{\mathrm{T}}^{t} I$, where I is a halting configuration, then* the time required by T on input w is t.

In other words, the time required by a Turing machine for a certain input is simply a number of steps to halting.

Definition A.20 *Let $T = (Q, \Sigma, \Gamma, \delta, q_0, B, q_A, q_R)$ be a Turing machine which halts for any input and $f : \mathbb{N} \to \mathbb{N}$. Then machine T* operates within time $f(n)$ *if, for any input string $w \in \Sigma^*$, the time required by T on w is not greater than $f(|w|)$. If T operates within time $f(n)$, then function $f(n)$ is the* time complexity *of T.*

The following extensions of theorems A.1 and A.2, respectively, hold (see [254]).

Theorem A.3 *For any multi-tape Turing machine T operating within time $f(n)$, there is an equivalent one-tape Turing machine T' operating within time $\mathcal{O}(f(n)^2)$.*

Theorem A.4 *For any nondeterministic Turing machine T operating within time $f(n)$, there is an equivalent deterministic one-tape Turing machine T' operating within time $\mathcal{O}(c^{f(n)})$, where $c > 1$ is some constant depending on T.*

There are no known proofs that for any nondeterministic machine operating within $f(n)$ a one-tape deterministic equivalent which operates within a polynomial function of $f(n)$ can be found. This is a crucial difference between a nondeterministic machine and any type of a deterministic machine.

Definition A.21 *For a function $f : \mathbb{N} \to \mathbb{N}$, the* time complexity class $\textsc{time}(f(n))$ *is the set of all languages L decided by a multi-tape Turing machine operating within time $\mathcal{O}(f(n))$.*

Definition A.22 *The class of languages decided by a deterministic one-tape Turing machine operating within polynomial time is denoted with* P *and defined as:*

$$\textsc{p} = \bigcup_{k \in \mathbb{N}} \textsc{time}(n^k).$$

Definition A.23 *For a function $f : \mathbb{N} \to \mathbb{N}$, the* time complexity class $\textsc{ntime}(f(n))$ *is the set of all languages L decided by a nondeterministic Turing machine operating within time $\mathcal{O}(f(n))$.*

Definition A.24 *The class of languages decided by a nondeterministic Turing machine operating within polynomial time is denoted with* NP *and defined as:*

$$\text{NP} = \bigcup_{k\in\mathbb{N}} \text{NTIME}(n^k).$$

Obviously, P $\subseteq$ NP, since the set of all deterministic one-tape machines is a subset of the set of all nondeterministic machines (see definitions A.7 and A.18).

A.4 NP-Completeness

Definition A.25 *Let Σ be a finite alphabet and let $f : \Sigma^* \to \Sigma^*$. We say that f is* computable in polynomial time *if there is a Turing machine with alphabet Σ which computes f and which is operating in $p(n)$, where p is a polynomial function.*

Definition A.26 *Let Σ be a finite alphabet. We say that a language $L_1 \subseteq \Sigma^*$ is* reducible *to a language $L_2 \subseteq \Sigma^*$ in polynomial time and write $L_1 \leq_p L_2$, if there is a function $f : \Sigma^* \to \Sigma^*$ computable in polynomial time, such that*

$$w \in A \Leftrightarrow f(w) \in B, \forall w \in \Sigma^*.$$

Function f is called a reduction *from L_1 to L_2.*

The following proposition can be found in [254].

Proposition A.1 *If f is a reduction from language L_1 to language L_2 and g is a reduction from language L_2 to language L_3, then $f \circ g$ is a reduction from L_1 to L_3.*

The notion of reducibility is essential for the introduction of *completeness*.

Definition A.27 *Let $\mathcal{C}$ be a complexity class. Language L is said to be $\mathcal{C}$-*complete *if*

1) $L \in \mathcal{C}$,

2) any language $L' \in \mathcal{C}$ can be reduced to L in polynomial time.

Definition A.28 *A complexity class $\mathcal{C}$ is* closed under reductions *if, for any two languages L_1 and L_2, $L_1 \leq_p L_2$ and $L_2 \in \mathcal{C}$ implies $L_1 \in \mathcal{C}$.*

The following proposition holds (see [254]).

Proposition A.2 *Complexity classes* P *and* NP *are closed under reductions.*

Definition A.29 *A language L_2 is* NP-hard, *if $L_1 \leq_p L_2$ for any language $L_1 \in$* NP.

The following definition can be derived from definitions A.27 and A.29.

Definition A.30 *A language L is* NP-complete *if:*

1) $L \in$ NP

2) L is NP*-hard.*

NP-complete problems are the hardest problems in NP (more about the NP-complete problems can be found in [178, 254, 320], for example). The following theorems can be proved.

Theorem A.5 *If there is an* NP*-complete language L_2, such that $L_2 \in$* P*, then $L_1 \in$* P *holds for all languages $L_1 \in$* NP.

Theorem A.6 *If L_2 is an* NP*-complete language, $L_1 \in$* NP *and $L_2 \leq_p L_1$, then language L_1 is also* NP*-complete.*

The previous two theorems imply that, if there is an NP-complete language $L_2 \in$ P, inclusion NP$\subseteq$P holds. Since it is trivial that P$\subseteq$NP, this would mean that P = NP. In addition, if there was a language $L_2 \in$ NP, such that $L_2 \notin$ P, it would imply that P$\subsetneq$NP.

The first problem proved to be NP-complete was the satisfiability problem.

Theorem A.7 (*Cook*, 1971.) *The SAT problem is* NP*-complete.*

Before the Cook's theorem was proved, it was not known whether NP-complete problems exist at all. The Cook's theorem provides the basis for proving the NP-completeness of other problems (according to theorem A.6). If SAT could be solved in polynomial time, that would mean that every other problem from NP could be solved in polynomial time (see theorem A.5), which would imply P=NP. Problem "P=NP?" is considered to be one of the most important problems of the modern mathematics and computer science.

Appendix B

Statistical Tests

When no assumptions about the distribution of the experimental results can be made, a non-parametric (distribution-free) test should be performed. One of the most common non-parametric tests is the Friedman test [112], which investigates the existence of significant differences between the multiple measures over different data sets. Specifically, it can be used for detecting differences between the performances of multiple algorithms.

If the equivalence of the measures (algorithms' performances) is rejected, the post hoc test can be further applied. The most common post hoc tests used after the Friedman test are the Nemenyi test [245], for pairwise comparisons of all algorithms, or the Bonferroni-Dunn test [92] when one algorithm of interest (the control algorithm) is compared with all the other algorithms (see [84]). In the special case of comparing the control algorithm with all the others, the Bonferroni-Dunn test is more powerful than the Nemenyi test (see [84]).

B.1 Friedman Test

Given ℓ algorithms and N data sets, the Friedman test ranks the performances of algorithms for each data set (in case of equal performance, average ranks are assigned) and tests if the measured average ranks $R_j = \frac{1}{N}\sum_{i=1}^{N} r_i^j$ (r_i^j as the rank of the jth algorithm on the ith data set) are significantly different from the mean rank. The statistic used is

$$\chi_F^2 = \frac{12N}{\ell(\ell+1)}\left[\sum_{j=1}^{\ell} R_j^2 - \frac{\ell(\ell+1)^2}{4}\right],$$

which follows a χ^2 distribution with $\ell - 1$ degrees of freedom. Since this statistic proved to be conservative [186], a more powerful version of the Friedman test was developed [186], with the following statistic:

$$F_F = \frac{(N-1)\chi_F^2}{N(\ell-1) - \chi_F^2},$$

which is distributed according to the Fischer's F-distribution with $\ell-1$ and $(\ell-1)(N-1)$ degrees of freedom. For more details, see [84].

B.2 Bonferroni-Dunn Test and Nemenyi Test

According to the Bonferroni-Dunn test [92] and the Nemenyi test [245], the performance of two algorithms is significantly different if the corresponding average ranks differ by at least the critical difference

$$CD = q_\alpha \sqrt{\frac{\ell(\ell+1)}{6N}},$$

where q_α is the critical value at the probability level α that can be obtained from the corresponding statistical table, ℓ is the number of algorithms and N is the number of data sets. Note that, although the formula for calculating the critical difference is the same for both tests, the critical values (i.e. the corresponding statistical tables) for these two tests are different.

Appendix C

Performance Profiles

Let $\mathcal{I}$ be a given set of problem instances and $\mathcal{A}$ a given set of algorithms. The *performance ratio* of running time of algorithm $\Lambda \in \mathcal{A}$ on instance $I \in \mathcal{I}$ and the best running time of any algorithm from $\mathcal{A}$ on I is defined as [87]:

$$r_{I,\Lambda} = \frac{t_{I,\Lambda}}{\min\{t_{I,\Lambda} | \Lambda \in \mathcal{A}\}},$$

where $t_{I,\Lambda}$ is the computing time required to solve problem instance I by algorithm Λ. The *performance profile* of an algorithm $\Lambda \in \mathcal{A}$ denotes the cumulative distribution of the performance ratio $r_{I,\Lambda}$:

$$\rho_\Lambda(\tau) = \frac{1}{|\mathcal{I}|}\{I \in \mathcal{I} \mid r_{I,\Lambda} \leq \tau\},\ \tau \in \mathbb{R}.$$

Obviously, $\rho_\Lambda(\tau)$ represents the probability that the performance ratio $r_{I,\Lambda}$ of algorithm Λ is within a factor $\tau \in \mathbb{R}$ of the best possible ratio. The performance profile $\rho_\Lambda : \mathbb{R} \to [0, 1]$ of algorithm $\Lambda \in \mathcal{A}$ is a nondecreasing, piecewise constant function. The value $\rho_\Lambda(1)$ is the probability that algorithm Λ solves the most problems in the shortest computational time (compared to all other algorithms). Thus, if we are only interested in the total number of instances which the observed algorithm solves the first, it is sufficient to compare the values $\rho_\Lambda(1)$ for all $\Lambda \in \mathcal{A}$.