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Transit sets of two-point crossover*

Manoj Changat

Department of Futures Studies, University of Kerala, Trivandrum, IN 695 581, India

Prasanth G. Narasimha-Shenoi

Department of Mathematics, Government College Chittur, Palakkad, IN 678 104, India

Ferdoos Hossein Nezhad

Department of Futures Studies, University of Kerala, Trivandrum, IN 695 581, India

Matjaž Kovše

School of Basic Sciences, IIT Bhubaneswar, Bhubaneswar, India

Shilpa Mohandas

Department of Futures Studies, University of Kerala, Trivandrum, IN 695 581, India

Abisha Ramachandran

Department of Mathematics, Sree Narayana College, Sivagiri, Varkala, IN 695145, India

Peter F. Stadler

Bioinformatics Group, Department of Computer Science & Interdisciplinary Center for Bioinformatics, Universität Leipzig, Härtelstraße 16-18, D-04107 Leipzig, Germany; German Centre for Integrative Biodiversity Research (iDiv) Halle-Jena-Leipzig, Competence Center for Scalable Data Services and Solutions Dresden-Leipzig, Leipzig Research Center for Civilization Diseases, and Centre for Biotechnology and Biomedicine at Leipzig University at Universität Leipzig; Max Planck Institute for Mathematics in the Sciences, Inselstraße 22, D-04103 Leipzig, Germany; Institute for Theoretical Chemistry, University of Vienna, Währingerstrasse 17, A-1090 Wien, Austria; Facultad de Ciencias at Universidad National de Colombia, Bogotá, Colombia; Santa Fe Insitute, 1399 Hyde Park Rd., Santa Fe NM 87501, USA

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Abstract

Genetic Algorithms typically invoke crossover operators to produce offsprings that are a "mixture" of two parents x and y. On strings, k-point crossover breaks parental genotypes at at most k corresponding positions and concatenates alternating fragments for the

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two parents. The transit set $R_k(x, y)$ comprises all offsprings of this form. It forms the tope set of an uniform oriented matroid with Vapnik-Chervonenkis dimension $k+1$. The Topological Representation Theorem for oriented matroids thus implies a representation in terms of pseudosphere arrangements. This makes it possible to study 2-point crossover in detail and to characterize the partial cubes defined by the transit sets of two-point crossover.

Keywords: Genetic algorithms, recombination, transit functions, oriented matroids, Vapnik-Chervonenkis dimension.

Math. Subj. Class.: 05C62, 05C75

1 Introduction

Genetic Algorithms, Evolutionary Algorithms, and Genetic Programming are heuristics commonly employed to solve complex optimization problems. A key component are crossover operators, which generate offsprings that are a mixture of two parents [16, 18, 22, 25]. Here we consider crossover operators on the set $X = \mathcal{A}^n$ strings with a fixed length n over some alphabet $\mathcal{A}$. A *k-mask* m is a binary string of length n with a most k break points between consecutive runs of 0s and 1s. That is, there are $0 \le h \le k < n$ "break points" $0 < i_1 < i_2 < \cdots < i_h < n$, such that (with $i_0 := 0$ and $i_{h+1} = n$) m satisfies $m_i = \mathtt{0}$ for $i_j < i \le i_{j+1}$ for even j and $m_i = \mathtt{1}$ for $i_j < i \le i_{j+1}$ for odd j. By definition, every k-mask starts with 0. For example, for $n = 15$ and $i_1 = 3$, $i_2 = 5$, $i_3 = 8$, $i_4 = 12$, we have the 4-mask

$$m = \mathtt{000110001111000}.$$

Note that m is also a k-mask for $4 \le k \le 15$. A k-mask thus is a binary string with *at most* $k+1$ alternating runs of 0s and 1.

Definition 1.1. A string $z \in X$ is a k-point crossover offspring of $x, y \in X$ if there is k-mask m such that either $z_i = x_i$ if $m_i = \mathtt{0}$ and $z_i = y_i$ if $m_i = \mathtt{1}$ for $1 \le i \le n$, or $z_i = y_i$ if $m_i = \mathtt{0}$ and $z_i = x_i$ if $m_i = \mathtt{1}$ for $1 \le i \le n$.

For instance, given two parents x and y, as well as the 4-mask m, we obtain the two offsprings z_1 and z_2 as follows:

$$\begin{aligned} x &= \mathtt{++-++-++-++-+++} \\ y &= \mathtt{-+--++--++--+--} \\ m &= \mathtt{000110001111000} \\ z_1 &= \mathtt{++--+-++++--+++} \end{aligned} \qquad \begin{aligned} x &= \mathtt{++-++-++-++-+++} \\ y &= \mathtt{-+--++--++--+--} \\ m &= \mathtt{000110001111000} \\ z_2 &= \mathtt{-+-+++---++-+--} \end{aligned}$$

Intuitively, k-point crossover subdivides the parents x and y into *at most* $k+1$ consecutive fragments that alternate in the offspring z. There is a rich literature on various aspects of k-point crossover operators. Algebraic properties are the focus of [7, 21, 24], disruption analysis is studied in [5], the relation between search spaces of crossover and mutation is discussed in [4, 23], coordinate transformation are explored in [8, 15]. The *recombination*

E-mail addresses: mchangat@gmail.com (Manoj Changat), prasanthgns@gmail.com (Prasanth G. Narasimha-Shenoi), ferdows.h.n@gmail.com (Ferdoos Hossein Nezhad), matjaz.kovse@gmail.com (Matjaž Kovše), rshilpam@gmail.com (Shilpa Mohandas), cyanabisha@gmail.com (Abisha Ramachandran), studla@bioinf.uni-leipzig.de (Peter F. Stadler)

sets $R_k(x, y)$ of possible crossover offsprings z of two parents x and y under k-point crossover. The function $R_k : X \times X \to 2^X$ satisfies, for all $x, y \in X$, (T1) $x, y \in R_k(x, y)$, (T2) $R_k(x, y) = R_k(y, x)$, and (T3) $R_k(x, x) = \{x\}$ [14]. These three axioms define *transit functions* [19], forming a common framework to describe intervals, convexities, and betweenness. In [3], we studied properties of the transit functions R_k deriving from k-point crossover. Convexity as a property of crossover operators is studied e.g. in [11, 12].

Here, we focus on the transit sets $R_k(x, y)$ themselves. Since $R_k(x, y)$ depends only on the positions in which x and y differ, it suffices to consider a two-letter alphabet $\mathcal{A} = \{+, -\}$ and thus $X = \{+, -\}^n$. We therefore interpret X as the vertex set of the n-dimensional Boolean Hypercube, and $R_k(x, y)$ as an induced subgraph of X. It is shown in [3, Cor. 4.2] that $R_k(x, y)$ is a *partial cube*, that is, an isometric subgraph of n-dimensional Boolean Hypercube [6].

The Hamming distance on X is the number $d(x, y)$ of positions in which x and y differ. Any two vertices x and y span a sub-hypercube $Q(x, y)$ of X with dimension $d(x, y)$, which coincides with the set of all crossover offsprings $R_k(x, y)$ whenever $d(x, y) \leq k$. Otherwise, $R_k(x, y)$ is an induced subgraph of $Q(x, y)$. Its cardinality

$$|R_k(x, y)| = \begin{cases} 2^t & \text{if} \quad t \leq k \\ 2\Phi_k(t-1) & \text{if} \quad t > k \end{cases} \tag{1.1}$$

depends only on the Hamming distance $t := d(x, y)$ and the parameter k [3, 14], where $\Phi_h(n) := \sum_{i=0}^{h} \binom{n}{i}$. In fact, the graphs $R_k(x, y)$ depend only on k and the Hamming distance $d(x, y)$:

Lemma 1.2. *Let $x, y \in \{+, -\}^n$ and $x', y' \in \{+, -\}^{n'}$. Then $R_k(x, y)$ and $R_k(x', y')$ are isomorphic if and only if $d(x, y) = d(x', y')$.*

Proof. Since every coordinate i for which $x_i = y_i$ is constant in $R_k(x, y)$ we know that $R_k(x, y)$ is an isometric subgraph of the subcube spanned by the $d := d(x, y)$ coordinates i with $x_i \neq y_i$. Relabeling the coordinates on $\{+, -\}^d$ is an isomorphism, hence $R_k(x, y)$ is isomorphic to $R_k(-^d, +^d)$, where $-^d$ and $+^d$ are the strings of length d with all coordinates being $-$ and $+$, respectively. Thus $R_k(x, y)$ and $R_k(x', y')$ are isomorphic if $d(x, y) = d(x', y')$. On the other hand, $R_k(-^d, +^d)$ and $R_k(-^{d'}, +^{d'})$ cannot be isomorphic if $d \neq d'$ since the diameter of the graphs differs. □

In this contribution, we show that the transit set of k-point forms the tope set of an uniform oriented matroid, which provides a means of gaining further insight into their structure and allows a characterization of the transit sets of two-point crossover.

2 VC-Dimension of Recombination Sets $R_k(x, y)$

The Vapnik-Chervonenkis dimension (VC-dimension) quantifies the complexity of set systems [26, 27]. Given some base set Y of cardinality $n := |Y|$, a family $\mathcal{H} \subseteq 2^Y$ forms an induced subgraph G of the Boolean hypercube $\{+, -\}^n$: for $A \in \mathcal{H}$, we identify $y \in A \subseteq Y$ with the y-coordinate of the corresponding point being $+$, while $y \notin A$ corresponds to $-$. A set $C \subseteq Y$ is said to be *shattered by* $\mathcal{H}$ if $\{Q \cap C | Q \in \mathcal{H}\} = 2^C$. The VC-dimension of $\mathcal{H}$ is the largest integer d_{VC} such that there is a set $C \subseteq Y$ of cardinality d_{VC} shattered by $\mathcal{H}$. By convention, $d_{VC} = -1$ for $\mathcal{H} = \emptyset$. Clearly, Y is always shattered by $\mathcal{H} = 2^Y$. Thus the VC-dimension of the Boolean hypercube $\{+, -\}^n$ itself is

n. Analogously, every subset $Y' \subseteq Y$ is shattered by $2^{Y'}$ and thus the VC-dimension of a sub-hypercube of dimensions $|Y| = n'$ is $d_{VC} = n'$.

As noted in [14], the 1-point crossover recombination set $R_1(x, y)$ is an isometrically embedded cycle C_{2t} for $t \geq 2$. It is not hard to check that $d_{VC} = 2$ in this case. For a partial cube G with d cuts the VC-dimension equals the dimension of the largest cube-minor in G, i.e., the largest cardinality of a set of coordinates shattered by the set of all d cuts of G. Here, a partial cube minor is either a contraction of cuts or the restriction to one of its sides, i.e., a specialization of the standard notion of graph minors [17]. Moreover, the cube-minor of a partial cube G is a graph isomorphic to a hypercube that can be obtained from G by a series of contractions and restrictions. Note that contractions can be seen as simply ignoring a coordinate.

Proposition 2.1. $d_{VC}(R_k(x, y)) = \begin{cases} k+1 & \text{if} \quad d(x,y) > k \\ d(x,y) & \text{if} \quad d(x,y) \leq k \end{cases}$

Proof. By Lemma 1.2 it suffices to consider $R_k(-^n, +^n)$. From the definition of k-point crossover it straightforwardly follows that $R_k(x, y) = \{+, -\}^n$, when $k = n - 1$, since there is a break point between any two coordinates. Now suppose $k < n - 1$. If the break points are consecutive, i.e., $i_j = j$ for $1 \leq j \leq k$, then $R_k(x, y)$ induces $\{+, -\}^{k+1}$ on the first $k + 1$ coordinates. The same holds if the break points are not consecutive and we contract consecutive coordinates j and $j + 1$ that do not have a break point between them. On the other hand, with k break points we can only "crossover" at most $k + 1$ coordinates, whence $d_{VC}(R_k(x, y)) \leq k + 1$. $\square$

3 Oriented matroids and 2-point recombination sets

Oriented matroids [1] are an axiomatic abstraction of geometric and topological structures including convex polytopes, vector configurations, (pseudo)hyperplane arrangements, point configurations in the Euclidean space, directed graphs, and linear programs. They reflect properties such as linear dependencies, facial relationship, convexity, duality, and have bearing on solutions of associated optimization problems. Among several equivalent axiomatizations of oriented matroids, the face or covector axioms best captures the geometric flavour and thus is the most convenient one for our purposes.

Let E be a finite set. A *sign vector* X on E is a vector $(X_e : e \in E)$ with coordinates $X_e \in \{+, 0, -\}$. The support of a sign vector X is the set $\underline{X} = \{e \in E \,|\, X_e \neq 0\}$. The *composition* $X \circ Y$ of two sign vectors X and Y is defined coordinate-wisely as $(X \circ Y)_e = X_e$, if $X_e \neq 0$, and $(X \circ Y)_e = Y_e$ otherwise. Their difference set is $D(X, Y) = \{e \in E \,|\, X_e = -Y_e\}$. We denote by $\leq$ the product (partial) order on $\{-, 0, +\}^E$ implied by the standard ordering $- < 0 < +$ of signs.

An *oriented matroid* M is ordered pair $(E, \mathcal{F})$ of a finite set E and a set of *covectors* $\mathcal{F} \subseteq \{+, -, 0\}^E$ satisfying, for all $X, Y \in \mathcal{F}$, the following (face or covector) axioms:

(F0) $0 = (0, 0, \ldots, 0) \in \mathcal{F}$.

(F1) $-X \in \mathcal{F}$.

(F2) $X \circ Y \in \mathcal{F}$.

(F3) There is $Z \in \mathcal{F}$ with $Z_e = 0$ for $e \in D(X, Y)$ and $Z_f = (X \circ Y)_f$ for $f \in E \setminus D(X, Y)$.

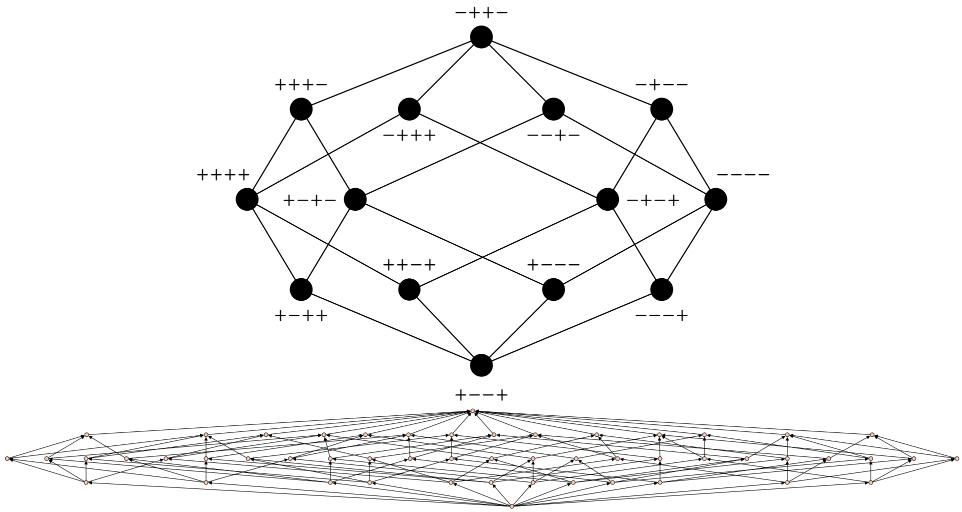

Figure 1: The rhombododecahedral graph $R_2(----, ++++)$ (top) with the binary labeling corresponding to the isometric embedding into 4-dimensional hypercube. Below we show its big face lattice generated using SageMath (`www.sagemath.org`).

Consider a subspace $V \subseteq \mathbb{R}^{|E|}$, define, for every $v \in V$, its sign vector $s(v)$ coordinate-wise by $s_e(v) = \mathrm{sgn}(v_e)$ for all $e \in E$, and denote by $\mathcal{F}$ the set of all sign vectors of V. Oriented matroids obtained from a vector space in this manner are called *representable* or *linear*.

The set $\mathcal{C} \subset \mathcal{F}$ of *cocircuits* or *vertices* of M consists of the non-zero covectors that are minimal with respect to the partial order $\leq$. The set $\mathcal{T} \subset \mathcal{F}$ of *topes* of M comprises the covectors that are maximal with respect to $\leq$. The cocircuits determine the set of covectors: every covector $X \in \mathcal{F} \setminus \{0\}$ has a representation of the form $X = V_1 \circ V_2 \circ \ldots \circ V_k$, where $V_1, V_2, \ldots V_k$ are cocircuits, and $V_1, V_2, \ldots V_k \leq X$. Similarly, the topes determine the oriented matroid: $\mathcal{F} = \{X \in \{+,-,0\}^E \mid \forall T \in \mathcal{T} : X \circ T \in \mathcal{T}\}$.

$M = (E, \mathcal{F})$ is *uniform* of rank r if $|\underline{X}| = r + 1$ for all cocircuits. The *big face lattice* $\widehat{\mathcal{F}}$ is a lattice obtained by adding the unique maximal element $\widehat{1}$ to the partial order $\leq$ on $\mathcal{F}$. The rank of a covector X is defined as its height in $\widehat{\mathcal{F}}$. The rank $\mathrm{rk}(M)$ of M is the maximal rank of its covectors. The corank of M is $|E| - \mathrm{rk}(M)$.

As an example consider $R_2(x, y)$ with $d(x, y) = 4$. It can be verified that the elements of $R_2(----, ++++)$ are exactly the topes of the oriented matroid corresponding to the Rhombododecahedron. It is shown together with its big face lattice in Figure 1. This observation can be generalized with the help of the following result:

Proposition 3.1 ([13]). *A set $T \subseteq \{+,-\}^X$ of VC-dimension d is the set of topes of a uniform oriented matroid M on X if and only if $T = -T$ and $|T| = 2\Phi_{d-1}(|X| - 1)$.*

By Proposition 2.1, Equ.(1.1), and Theorem 3.1, this immediately implies

Theorem 3.2. *For $x, y \in \{+,-\}^X$, with $d(x, y) = |X| = n$ the elements of $R_k(x, y)$ form the set of topes of a uniform oriented matroid M on X with VC-dimension $d_{VC} =$* $\mathrm{rk}(M) = k + 1$.

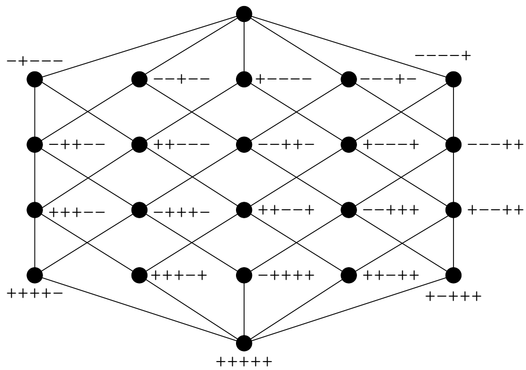

Figure 2: The transit graph $R_2(-----, +++++)$.

Since many of the known results on oriented matroids depend on the corank, we note that $R_k(x, y)$ has corank $n - k - 1$.

One of the cornerstones of the theory of oriented matroids is the Topological Representation Theorem, which connects oriented matroids with pseudosphere arrangements, see Appendix A for detailed definitions. Together with Theorem 3.2, it immediately implies the following topological characterization of the recombination sets of k-point crossover:

Theorem 3.3. *For $x, y \in \{+, -\}^X$, with $d(x, y) = |X| = n$, the recombination set $R_k(x, y)$ can be topologically represented by a pseudosphere arrangement of dimension k, where the minimal elements in the big face lattice correspond to the intersections of exactly k pseudospheres, and there are $2\binom{n}{k-1}$ such intersections.*

The significance of this result is that it provides a representation of crossover operators in terms of topological objects. As an illustration of the usefulness of Theorem 3.3, we now turn to a full characterization of the transit graphs of 2-point crossover operators. The smallest non-trivial examples are the graphs $R_2(----, ++++)$ in Figure 1 and $R_2(-----, +++++)$ in Figure 2.

Theorem 3.4. *$R_2(a, b)$ with $d(a, b) = t > 3$ induces antipodal planar quandrangulation, that is, a partial cube of diameter t with t^2-t+2 vertices, $2t^2-2t$ edges, t^2-t quadrangles, and all cuts of size $2t-2$.*

Proof. Let $|V|$, $|E|$, $|Q|$ and $|C|$ denote the number of vertices, edges, 4-faces, and edges of a cut, respectively. From the definition of crossover operator, we can arbitrarily permute coordinates, hence it follows that each cut has the same number of edges, this justifies that we study $|C|$. From Theorem 3.2 it follows that vertices of $R_2(a, b)$ form the set of topes of a uniform oriented matroid of rank 3 and corank $t - 3$. As shown by [10] and in the book by [1], rank 3 oriented matroids can be represented by pseudocircle arrangement on $\mathbb{S}^2$. The corresponding tope graph is therefore planar. Hence $R_2(a, b)$ induces in particular a planar antipodal partial cube. Corank $t-3$ implies that each intersection of pseudocurves is the intersection of exactly two of them. Hence all faces of the dual – the tope graph – are 4-cycles, therefore $R_2(a, b)$ induces planar quadrangulation. Moreover, each intersection

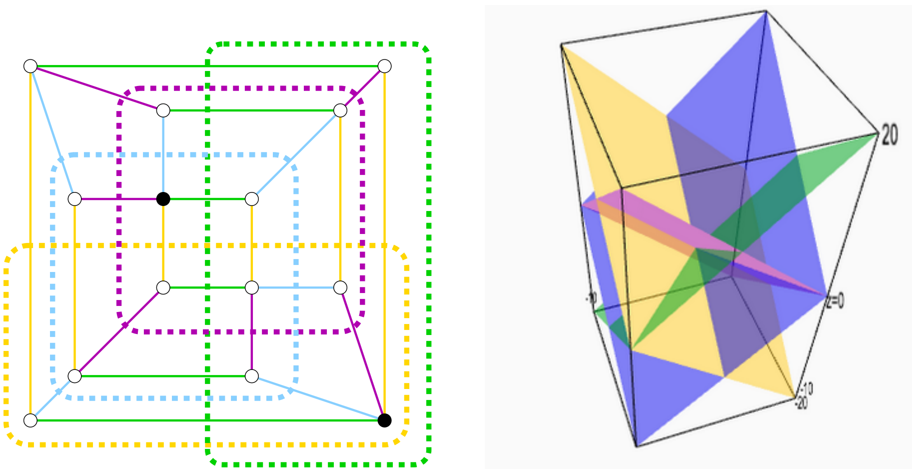

Figure 3: Topological representation of rhombododecahedron (l.h.s.) in terms of its pseudocircle arrangement (doted curves) and the corresponding hyperplane arrangement (r.h.s.).

of two pseudocircles corresponds to cocircuit. In uniform oriented matroid of corank $t-3$ there are exactly $2\binom{t}{t-2}$ cocircuits, which correspond to the 4-cycles in the dual graph.

Quadrangulations are maximal planar bipartite graphs – no edge can be added so that graph remains planar and bipartite. Using Euler formula for planar graphs [20], we obtain $|E| = 2|V| - 4$. Equ.(1.1) furthermore, implies $|E| = 2t^2 - 2t$ and thus $|C| = |E|/t = 2t - 2$. $\square$

As an example, Figure 3 shows the pseudocircle arrangement and the equivalent hyperplane arrangement of transit graph $R_2(----, ++++)$ of Figure 1.

In order to get a better intuition on the structure of the 2-point crossover graphs we derive their degree sequence.

Theorem 3.5. *The degree sequence of $R_2(a, b)$ with $t := d(a, b) > 3$ equals $(t, t, 4, \dots, 4, 3, \dots, 3)$ with $t^2 - 3t$ vertices of degree 4 and $2t$ vertices of degree 3.*

Proof. W.l.o.g., let $a = 0 \dots 0$ and $b = 1 \dots 1$. For any vertex $c = x \dots xyx \dots x$, $x, y \in \{0, 1\}$ we have that $c \in R_2(a, b)$, hence $deg(a) = deg(b) = t$. Let $c \in R_2(a, b) \setminus \{a, b\}$. Then we have two cases:

Case 1. $c = xx \dots xxyy \dots yy$ and $\{x, y\} = \{0, 1\}$. Then c has at most four neighbors in $R_2(a, b)$: $c_1 = yx \dots xxyy \dots yy$, $c_2 = xx \dots xxyy \dots yx$, $c_3 = xx \dots xyyy \dots yy$ and $c_4 = xx \dots xxxy \dots yy$. Since $t > 3$ it follows that c also has at least three neighbors in $R_2(a, b)$.

Case 2. $c = x \dots xxyy \dots yyxx \dots x$ and $\{x, y\} = \{0, 1\}$. Then c has at most four neighbors in $R_2(a, b)$: $c_1 = x \dots xxxy \dots yyxx \dots x$, $c_2 = x \dots xyyy \dots yyxx \dots x$, $c_3 = x \dots xxyy \dots yxxx \dots x$, and $c_4 = x \dots xxyy \dots yyyx \dots x$. Since $t > 3$ it follows that c also has at least three neighbors in $R_2(a, b)$.

Let x_3 and x_4 denote the number of vertices of degree 3 and 4 respectively. By the handshaking lemma $2|E| = \sum_{v \in V(G)} deg(v)$. Therefore, it follows from arguments above and Theorem 3.4 that

$$4t^2 - 4t = 2t + \sum_{v \in V(G) \setminus \{a,b\}} deg(v)$$
$$4t^2 - 6t = 3x_3 + 4x_4$$

Theorem 3.4 also implies that $t^2 - t = x_3 + x_4$. Solving this system of linear equations yields $x_3 = 2t$ and $x_4 = t^2 - 3t$. □

4 Concluding remarks

The recombination sets of 1-point crossover operators form isometric cycles in hypercube. The partial cubes corresponding to k-point crossover operators have a VC-dimension of $k+1$ unless they are smaller sub-hypercubes. We have considered here the uniform oriented matroids that correspond to the k-point crossover operators and used this connection to characterize the partial cubes of 2-point recombination sets. It remains an open question for future research whether the connection with oriented matroids and their topological representations can be utilized to better understand the structure of k-point recombination graphs.

ORCID iDs

Manoj Changat https://orcid.org/0000-0001-7257-6031
Prasanth G. Narasimha-Shenoi https://orcid.org/0000-0002-5850-5410
Matjaž Kovše https://orcid.org/0000-0001-9473-7545
Shilpa Mohandas https://orcid.org/0000-0003-3378-2339
Abisha Ramachandran https://orcid.org/0000-0003-2778-5584
Peter F. Stadler https://orcid.org/0000-0002-5016-5191

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Appendix A: Pseudosphere arrangements

Consider the d-dimensional sphere $\mathbb{S}^d$ in $\mathbb{R}^{d+1}$ and the corresponding $(d+1)$-dimensional ball $\mathbb{B}^{d+1} = \{(x_1, \ldots, x_{d+1}) \in \mathbb{R}^{d+1} \mid x_1^2 + \ldots + x_{d+1}^2 \leq 1\}$, whose boundary surface is $\mathbb{S}^d$.

A pseudosphere $S \subset \mathbb{S}^d$ is a tame embedded $(d-1)$-dimensional sphere. Its complement in B^d consist of exactly two regions, hence S can be oriented, by labeling one region by S_e^+ and the other by S_e^-. A pseudosphere arrangement $\mathcal{S} = \{S_e \mid e \in E\}$ in the Euclidean space $\mathbb{R}^d$ is a collection of $(d-1)$-dimensional pseudospheres on the d-dimensional unit sphere $\mathbb{S}^d$, where the intersection of any number of spheres is again a sphere and the intersection of an arbitrary collection of closed sides is either a sphere or a ball, i.e., for all $R \subset E$ holds

(i) $S_R = \mathbb{S}^d \cap_{i \in R} S_i$ is empty or homeomorphic to a sphere.

(ii) If $e \in E$ and $S_R \not\subset S_e$ then $S_R \cap S_e$ is a pseudosphere in S_R, $S_R \cap S_e^+ \neq \emptyset$ and $S_R \cap S_e^- \neq \emptyset$.

For a pseudosphere arrangement $\mathcal{S}$, the position vector $\sigma(x)$ of a point $x \in \mathbb{S}^d$ is defined as $\sigma(x)_e = 0$ for $x \in S_e$, $\sigma(x)_e = +$ for $x \in S_e^+$ and $\sigma(x)_e = -$ for $x \in S_e^-$. The set of all position vectors of $\mathcal{S}$ is denoted by $\sigma(\mathcal{S})$. A famous theorem due to [9] establishes an correspondence between oriented matroids and pseudosphere arrangement.

Topological Representation Theorem ([2, 9]). *Let $M = (E, \mathcal{F})$ be an oriented matroid of rank d. Then there exists a pseudosphere arrangement $\mathcal{S}$ in $\mathbb{S}^d$ such that $\sigma(\mathcal{S}) = \mathcal{F}$. Conversely, if $\mathcal{S}$ is a pseudosphere arrangement in $\mathbb{S}^d$, then $(E, \sigma(\mathcal{S}))$ is an oriented matroid of rank d.*

A pseudosphere arrangement naturally induces a cell complex on $\mathbb{S}^d$, whose partial order of faces corresponds precisely to the partial order $\leq$ on covectors of the corresponding oriented matroid. This fact served as motivation for the concept of covectors in the theory of oriented matroids.