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Extrapolation methods for first order ordinary differential equations.

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0. Abstract

Given a system of fist order differential equations, whose coefficient matrix has constant elements, with initial conditions specified, a family of extrapolating algorithms based on Pade approximants to the exponential function is developped.

An important application of such methods is seen to be the numerical solution of the diffusion equation.

1. Extrapolating algorithms

Given the system of N linear first order ordinary differential equations

(0) $$\underline{y}'(x) = A\underline{y}(x)$$

to be abbreviated as $\underline{y}' = A\underline{y}$, with initial conditions

(1) $$\underline{y}(0) = g ,$$

it is trivial to show that the solution is

(2) $$\underline{y}(x) = \exp(xA)\underline{y}(0) = \exp(xA)\underline{g}$$

The matrix A , which is of order NxN , will be assumed to have constant elements and any numerical solution of (2) will rely for its accuracy on the approximation to exp(xA) - Certain polynomial and rational approximations to exp(xA) , together with appropriate convergence criteria, were discussed in Legras [6] . In the present paper Pade approximants to exp(xA) will be used and it will be seen that, by a process of extrapolation, it is possible to improve an approximation by one or two powers of x .

The (m,k) Pade approximant to e^{θ} , where 6 is some scalar quantity, is of the form

$$R_{m,k}(\theta) = P_k(\theta)/Q_m(\theta)$$

where $P_k(\theta)$ and $Q_m(\theta)$ are polynomials in 6 of degrees k and m respectively, and $R_{m,k}(\theta)$ is such that

$$R_{m,k}(\theta) - e^{\theta} = 0(\theta^{m+k+1})$$

A table of *Padé* approximants to the exponential function may be found in a number of texts and an analysis and a review of computational methods appears in Chisolm [1]. If $Q_m\theta)$ is of the form $q_0+q_1\theta+q_2\theta^2 + \ldots + q_m\theta^m$ with $q_0 > 0$, then for convergence the condition

(3) $$|q_1\theta + q_2\theta^2 + \ldots + q_m\theta^m| < q_0$$

must be satisfied. The matrix analog of (3) is obvious and for each Pade approximant to exp(xA) yields a bound on some norm of A . Equation (2) may be written in step wise fashion as

(4) $$\underline{y}(x + h) = \exp(hA)\underline{y}(x) \quad ,$$

where h is the stepsize, and writing (4) over a double interval 2h with exp(2hA) replaced by its (1,0) Pade approximant gives

(5) $$\underline{y}(x+2h) = (I - 2hA)^{-1}\underline{y}(x)$$
$$= (I + 2hA + 4h^2A^2)\underline{y}(x) + 0(h^3) \quad .$$

Alternatively if equation (4) is applied twice, $\underline{y}(x+2h)$ is given by

(6) $$\underline{y}(x+2h) - (I - hA)^{-1}(I - hA)^{-1}\underline{y(x)}$$
$$= (I + 2hA + 3h^2A^2)\underline{y}(x) + 0(h^3)$$

The Maclaurin expansion of exp(2hA) produces

(7) $$y(x+2h)=(I+2hA+2h^2A^2+\frac{4}{3}h^3A^3+\frac{2}{3}h^4A^4+\frac{4}{15}h^5A^5+\ldots..)\,y(x) \quad ,$$

and defining the the values of $\underline{y}(x+2h)$ produced by (6) and (5) to be $\underline{y}^{(1)}$ *and* $\underline{y}^{(2)}$ respectively, it is seen that neither is $0(h^2)$ accurate. However, defining $\underline{y}$ by

(8) $$\underline{Y} = 2\underline{y}^{(1)} - \underline{y}^{(2)} \quad ,$$

gives

(9) $$\underline{Y} = (I + 2hA + 2h^2A^2)\underline{y}(x) + 0(h^3)$$

whose error is $0(h^3)$. The first order method based on the (1,0) Padé approximant has been extrapolated to give second order accuracy.

It is obvious that the method based on the (0,1) Padé approximant to exp(hA) , the Euler predictor formula, which is also first order accurate, can be extrapolated in the same way to give second order accuracy.

The (1,1) Padé approximants to exp(hA) and exp(2hA) yield

(10) $$\underline{y}^{(1)} = (I-\frac{1}{2}hA)^{-1}(I+\frac{1}{2}hA)(I-\frac{1}{2}hA)^{-1}(I+\frac{1}{2}hA)^{-1}(I+\frac{1}{2}hA)\underline{y}(x)$$
$$= (I+2hA+2h^2A^2+\frac{3}{2}h^3A^3+h^4A^4+\frac{5}{8}h^5A^5)y(x)+0(h^6)$$

and

(11) $$\underline{y}^{(2)} = (I-hA)^{-1}(I+hA)\underline{y}(x)$$
$$= (1+2hA+2h^2A^2+2h^3A^3+2h^4A^4+2h^5A^5)\underline{y}(x)+0(h^6)$$

Comparing (10) and (11) with (7) shows that $\underline{y}^{(1)}$ and $\underline{y}^{(2)}$ are both only second order accurate but that $\underline{y}$ defined by

(12) $$Y = \frac{4}{3}y^{(1)} - \frac{1}{3}y^{(2)}$$

is fourth order accurate. In this case the extrapolation proceedure has produced an extra order of accuracy, a phenomenon which is a useful feature of methods based on (m,m) Padé approximants to exp(hA) which is not evident in methods based on (m,k) approximants.

A table of fifteen extrapolation methods based on Padé approximants is given in Table I together with bounds for convergence on $h\,||A||_S$ as given in (3), where $||A||_S$ is the spectral norm of A The extrapolating formulas connecting $\underline{Y}$, $\underline{y}^{(1)}$ and $\underline{y}^{(2)}$ satisfy the relation

Table I: Extrapolation algorithms

Method	Pade approximant	Bound on $h\|\|A\|\|_s$	Order of error	Extrapolation algorithm	Order of error
1	(0,1)	-	h^2	$2\underline{y}^{(1)}-\underline{y}^{(2)}$	h^3
2	(1,0)	1	h^2	$2\underline{y}^{(1)}-\underline{y}^{(2)}$	h^3
3	(1,1)	2	h^3	$(4\underline{y}^{(1)}-\underline{y}^{(2)})/3$	h^5
4	(0,2)	-	h^3	$(4\underline{y}^{(1)}-y^{(2)})/3$	h^4
5	(1,2)	3	h^4	$(8\underline{y}^{(1)}-y^{(2)})/7$	h^5
6	(2,1)	1.16	h^4	$(8\underline{y}^{(1)}-y^{(2)})/7$	h^5
7	(2,0)	0.70	h^3	$(4\underline{y}^{(1)}-y^{(2)})/3$	h^4
8	(2,2)	1.58	h^5	$(16\underline{y}^{(1)}-y^{(2)})/15$	h^7
9	(0,3)	-	h^4	$(8\underline{y}^{(1)}-y^{(2)})/7$	h^5
10	(1,3)	4	h^5	$(16\underline{y}^{(1)}-y^{(2)})/15$	h^6
11	(2,3)	2	h^6	$(32\underline{y}^{(1)}-y^{(2)})/31$	h^7
12	(3,2)	1.23	h^6	$(32\underline{y}^{(1)}-y^{(2)})/31$	h^7
13	(3,1)	0.97	h^5	$(16\underline{y}^{(1)}-y^{(2)})/15$	h^6
14	(3,0)	0.70	h^4	$(8\underline{y}^{(1)}-y^{(2)})/7$	h^5
15	(3,3)	1.49	h^7	$(64\underline{y}^{(1)}-y^{(2)})/63$	h^9

(13) $$\underline{Y} = \frac{1}{2^{m+k} - 1}(2^{m+k}\underline{y}^{(1)} - \underline{y}^{(2)}) + O(h^{m+k+2})$$

when $m \neq k$, or, when $m = k$, the relation

(14) $$\underline{Y} = \frac{1}{2^{2m} - 1}(2^{2m}\underline{y}^{(1)} - \underline{y}^{(2)}) + O(h^{2m+3}) .$$

As will be seen in Section 3, Lawson and Morris [5] employed extrapolation methods which satisfy (13) or (14). Given that these methods are to be used, any strategy for solution will require the user to:

(i) determine $||A||_S$;

(ii) isolate the family of extrapolating algorithms which will converge for $h||A||_s$, where h is the known stepsize;

(iii) select that algorithm which will give the required accuracy, choosing, if possible, a method based on an (m,m) Pade approximant.

2. Numerical results

To demonstrate the behaviour of the extrapolation formulas of the previous section, the following four problems were solved by the fifteen methods of Table I using a FORTRAN program which calculated all fifteen results for each problem simultaneously, computing successive powers of the coefficient matrix as these were needed.

Pr*oblem 1* (Lawson [4])

$$y_1' = -y_1 + 23\,y_2 \;,$$
$$y_2' = -y_1 - 25\,y_2$$

with initial vector $Y(0) = [1,1]^T$. The eigenvalues of the coefficient matrix A are $\lambda_1 = -2$ and $\lambda_2 = -24$, and $\|A\|_s$ - 33.97 . The exact solution is

$$y_1 = \frac{23}{11}e^{-2x} - \frac{12}{11}e^{-24x} \;,$$
$$y_2 = \frac{12}{11}e^{-24x} - \frac{1}{11}e^{-2x} \;,$$

Problem 2

$$y_1' = 10y_1 - 9y_2 \;,$$
$$y_2' = -10y_1 + 11y_2 \;,$$

with initial vector $\underline{y}(0) = [10,-9]^T$. The eigenvalues of the coefficient matrix A are $\lambda_1 = 1$ and $\lambda_2 = 20$, and $\|A\|_s$ - 20.025 . The exact solution is

$$y_1 = e^x + 9e^{20x}$$
$$y_2 = e^x - 10e^{20x}$$

Problem 3 (Lambert [3])

$$y_1' = -21y_1 + 19y_2 - 20y_3 \;,$$
$$y_2' = 191 - 21y_2 + 20y_3 \;,$$
$$y_3' = 40y_1 - 40y_2 - 40y_3 \;,$$

with initial vector $\underline{y}(0) = [1,0,-1]^T$. The eigenvalues of the coefficient matrix A are $\lambda_1 = -2$, $\lambda_2 = 40+40i$, $\lambda_3 = -40-40\,i$ and $||A||_S = 75.0$. The exact solution is

$$y_1 = \tfrac{1}{2}e^{-2x} + \tfrac{1}{2}e^{-40x}(\cos 40x + \sin 40x) ,$$
$$y_2 = \tfrac{1}{2}^{-20x} - \tfrac{1}{2}e^{-40x}(\cos 40x + \sin 40x) ,$$
$$y_3 = -e^{-40x}(\cos 40x - \sin 40x)$$

Problem 4 (Henrici [2])

$$y_1' = y_2 ,$$
$$y_2' = -y_1 ,$$
$$y_3' = y_4 ,$$
$$y_4' = -y_3 ,$$

with initial vector $\underline{y}(0) = [1,0,0,1]^T$. The eigenvalues of the coefficient matrix A are $\lambda_1 = \lambda_2 = -\lambda_3 = -\lambda_4 = i$ and $||A||_s = 1$. The exact solution is

$$y_1 = \cos x ,$$
$$y_2 = -\sin x ,$$
$$y_3 = \sin x ,$$
$$y_4 = \cos x .$$

Each problem was tested on all fifteen methods of Table I with $h = 0.05, 0.1, 0.2$ for x in the interval $0 \le x \le 1$. It was noted that for Problems 1,3,4 the errors decreased as x increased and that for Problem 2, for which partial instability is experienced, the errors increased as x increased- A discussion of stability regions and difficulties encountered with stiff systems is given in Lambert [3]. The largest modulus component of the error vector for $x = 0.4, 0.8$ for all three values of h are given in Tables II(i), (ii), (iii), (iv). The theoretical solutions of the four problems for $x = 0.4$, 0,8 are given in Table III. The convergence bounds of Table I on $h||A||_s$ indicate that in the case of Problem 1 the results obtained for h - 0.1, 0.2 and in the case of Problem 3 the results obtained by most of the fifteen algorithms for h - 0.05, 0.1, 0.2 may be unreliable. Results obtained in the numerical experiments were largely in agreement with the convergence bounds of Table I and, when these were not violated, the errors were largely in keeping with the predicted values, that is, the indicated power of h in Table 1.

Table II(i) Largest error modulus for x = 0.4, 0.8 and h = 0.05, 0.1, 0.2 for Problem 1 using all fifteen methods of Table I .

x	0.4			0.8		
h	0.05	0.1	0.2	0.05	0.1	0.2
1	0.1(-2)	0.7(-l)	0.4(+2)	0.7(-3)	0.6(-2)	0.6(-1)
2	0.4(-1)	0.8	0.6(+3)	0.2(-1)	0.1	0.9
3	0.3(-2)	0.4	0.5(+3)	o.K-2)	0.1l(-1)	0.9(-1)
4	0.7 (-3)	0.1	0.1(+3)	0.3(-4)	0.6(-3)	0.8(-2)
5	0.4(-3)	0.1	0.3(+3)	o.1(-5)	0.4(-4)	0.2(-1)
6	0.4(-3)	0.1	0.3(+3)	0.1(-5)	0.4(-4)	0.2(-1)
7	0.7(-3)	0. 1	0.1(+3)	0.3 (-4)	0.6(-3)	0.8(-2)
8	0.6(-4)	0.6(-1)	0.7(+3)	0.4(-8)	0.4(-4)	0.5(-1)
9	0.4(-3)	0.1	0.3(+3)	0.1(-5)	0.4(-4)	0.2(-1)
10	0.2(-3)	0.9(-1)	0.5(+3)	0.3(-7)	0.6(-5)	0.3(-1)
11	0.6(-4)	0.6(-1)	0.7(+3)	0.3(-8)	0.4(-5)	0.5(-1)
12	0.6(-4)	0.6(-1)	0.7(+3)	0.3(-8)	0.4(-5)	0.5(-1)
13	0.2(-3)	0.9(-1)	0.5(+3)	0.3(-7)	0.6(-5)	0.3(-1)
14	0.4(-3)	0.1	0.3(+3)	0.1(-5)	0.4(-4)	0.2(-1)
15	0.5(-5)	0.2(-1)	0.1(+4)	0.3(-9)	0.2(-5)	0.7(-1)

Table II(ii) Largest error modulus for x = 0.4, 0.8 and h = 0.05, 0.1, 0.2 for Problem 2 using all fifteen methods of Table I .

x	0.4			0.8		
h	0.05	0.1	0.2	0.05	0.1	0.2
1	0.1(+5)	0.2(+5)	0.3(+5)	0.3(+8)	0.7(+8)	0.9(+9)
2	0.1(+5)	0.3(+5)	0.3(+5)	0.3(+8)	0.9(+8)	0.9(+9)
3	0.1(+5)	0.2 (+5)	0.3(+5)	0.3(+8)	0.6(+8)	0.8(+8)
4	0.4(+4)	0.2(+5)	0.3(+5)	0.1(+8)	0.5(+8)	0.9(+8)
5	0.2(+4)	0.1(+5)	0.3(+5)	0.5(+7)	0.3(+8)	0.8(+8)
6	0.2(+4)	0.1(+5)	0.3(+5)	0.5(+7)	0.3(+8)	0.8(+8)
7	0.4(+4)	0.2 (+5)	0.3(+5)	0.1(+8)	0.5(+8)	0.9(+8)
8	0.1(+3)	0.3(+4)	0.2(+5)	0.4(+6)	0.1(+8)	0.6(+8)
9	0.2(+4)	0.1(+5)	0.3(+5)	0.5(+7)	0.3 (+8)	0.8 (+8)
10	0.5(+3)	0.6(+4)	0.2(+5)	0.1(+7)	0.2(+8)	0.7(+8)
11	0.1(+2)	0.3(+4)	0.2(+5)	0.4(+6)	0.1(+8)	0.6(+8)
12	0.1(+3)	0.3(+4)	0.2(+5)	0.4(+6)	0.1(+8)	0.6(+8)
13	0.5(+3)	0.6(+4)	0.2(+5)	0.1(+7)	0.2(+8)	0.7(+8)
14	0.2(+ 4)	0.1(+5)	0.3(+5)	0.5(+7)	0.3(+8)	0.8(+8)
15	0.7(+1)	0.6(+3)	0.1(+5)	0.2(+5)	0.2(+7)	0.4(+8)

Table I I(iii) Largest error modulus for x = 0.4, 0.8 and h = 0.05, 0.1, 0.2 for Problem 3 using all fifteen methods of Table I .

x	0.4			0.8		
h	0.05	0.1	0.2	0.05	0.1	0.2
1	0.4(-3)	0.2(-l)	0.2(+3)	0.2(-3)	0.1(-2)	0.2(-l)
2	0.1(-1)	0.4	0.6(+4)	0.6(-2)	0.3(-l)	0.2
3	0.2(+l)	0.2(+3)	0.1(+5)	0.8(+l)	0.8(+2)	0.9(+3)
4	0.1(-3)	0.9(-l)	0.1(+4)	0.8(-5)	0.1(-3)	0.3(-2)
5	0.2(-3)	0.2	0.1(+5)	0.3(-6)	0.1(-4)	0.1(-2)
6	0.2(-3)	0.2	0.1(+5)	0.3(-6)	0.1(-4)	0.1(-2)
7	0.1(-3)	0.9(-1)	0.1(+4)	0.8(-5)	0.1(-3)	0.3(-2)
8	0.1(-3)	0.8	0.1(+6)	0.4(-9)	0.9(-7)	0.2(-l)
9	0.2(-3)	0.2	0.1(+5)	0.3(-6)	0.1(-4)	0.1(-2)
10	0.1(-3)	0.3	0.6(+5)	0.1(-7)	0.8{-6)	0.7(-2)
11	0.1(-3)	0.8	0.1(+6)	0.4(-9)	0.9(-7)	0.2(-l)
12	0.1(-3)	0.8	0.1(+6)	0.4(-9)	0.9(-7)	0.2(-l)
13	0.1(-3)	0.3	0.6(+5)	0.1(-7)	0.8(-6)	0.7(-2)
14	0.2(-3)	0.2	0.1(+5)	0.3(-6)	0.1(-4)	0.1(-2)
15	0.9(-4)	0.1(+l)	0.2(+7)	0.1(-9)	0.2(-6)	0.1

Table II (iv) Largest error modulus for x = 0.4, 0.8 and h = 0.05, 0.1, 0.2 for Problem 4 using all fifteen methods of Table I .

x	0.4			0,8		
h	0.05	0.1	0.2	0.05	0.1	0.2
1	0.2(-3)	0.1(-2)	0.l(-l)	0.1(-3)	0.1(-2)	0.9(-2)
2	0.1(-1)	0,4(-l)	0.2	0.8(-2)	0.2(-1)	0.2
3	0.2(-3)	0.2(-2)	0.3(-l)	0.2(-3)	0.2(-2)	0.1(-1)
4	0.4(-5)	0.6(-4)	0.1(-2)	0.3(-5)	0.5(-4)	0.9(-3)
5	0.8(-7)	0.3(-5)	0.9(-4)	0.6(-7)	0.2(-5)	0.8(-4)
6	0.8(-7)	0.3(-5)	0.9(-4)	0.6(-7)	0.2(-5)	0.8(-4)
7	0.4(-5)	0.6(-4)	0.1(-2)	0.3(-5)	0.5(-4)	0.9(-3)
8	0.2(-10)	0.2(-8)	0.3(-6)	0.2(-10)	0.2(-8)	0.3(-6)
9	0.8(-7)	0.3(-5)	0.9(-4)	0.6(-7)	0.2(-5)	0.8(-4)
10	0.1(-8)	0.9(-7)	0.6(-6)	0.1 (-8)	0.7(-7)	0.5(-5)
11	0.2(-10)	0.2(-8)	0.3(-6)	0.2 (-10)	0.2(-8)	0.3(-6)
12	0.2(-10)	0.2(-8)	0.3(-6)	0.2 (-10)	0.2(-8)	0.3(-6)
13	0.1(-8)	0.9(-7)	0.6(-5)	0.1(-8)	0.7(-7)	0.5(-5)
14	0.8(-7)	0.3 (-5)	0.9(-4)	0.6(-7)	0.2(-5)	0.8(-4)
15	0.7(-11)	0.4(-11)	0.7(-9)	0.3 (-10)	0.1(-10)	0.7(-9)

Table III Theoretical solutions of Problems 1,2,3,4 for $x = 0{,}4,\ 0{,}8$.

x	0.4	0.8
Problem 1		
y_1	0.939	0.422
y_2	-0.041	-0.018
Problem 2		
y_1	0.268(+5)	-0.298(+5)
Y_2	0.800 (+8)	-0.889(+8)
Problem 3		
y_1	0.225	0.101
y_2	0.225	0.101
y_3	-0.000	-0.000
Problem 4		
y_1	0.921	0.697
y_2	-0.389	-0.717
y_3	0.389	0.717
y_4	0.921	0.697

3. Application to parabolic partial differential equations

InsoIvind numerically the one-dimensional heat equation

(1.5)

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

over a region $R = \{[0 < x < 1] \times [t > 0]\}$, with boundary conditions

(16) $$u(0,t) = u(1,t) = 0 \quad , \quad t > 0$$

and initial conditions

(17) $$u(x,0) = g(x) \quad , \quad 0 \leq x \leq 1$$

one approach is to replace the second order space derivative with finite difference approximations at every time step and then to solve the resulting system of first order linear ordinary differential equations in time. If the space interval $0 \leq x \leq 1$ is divided into N-1 subintervals each of width h , and if $\underline{U} = (U_1, U_2 \ldots, U_N)^T$ is the vector of computed values of u at a given time level, this system of ordinary differential equations is given by

(18) $$\frac{dU}{dt} = A\underline{U} \quad ,$$

where the elements of the matrix operator A depend on the finite

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difference replacement of $\partial^2 u/\partial x^2$. As in Section 1, it is easy to show that the solution of (18) subject to (17) may be written in the stepwise form

(19) $$\underline{U}(t + \ell) = \exp(\ell A)\underline{U}(t)$$

where ℓ is the time step, and $\underline{U}(0) = g$ is the vector of initial conditions.

The accuracy in time of the vector U is dependent on the approximation to $\exp(\ell A)$ and the extrapolation techniques based on Padé approxiniants of Section 1 may thus be used. This approach was employed by Lawson and Morris [5] who extrapolated the low order (1,0), (0,1) and (1,1) Padé approximants to $\exp(\ell A)$. Clearly, the use of higher order approximants involves higher powers of the matrix A and thus more values of the computed function U at each time step.

An examination of how extrapolation techniques carry over to hyperbo1ic equations was given in Twizell [7].

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