

Abstract

A survey is given of possible applications of Padé approximation in several fields of numerical analysis : solving nonlinear equations, acceleration of convergence, numerical solution of ordinary and partial differential equations, numerical quadrature. Special attention is given to the convergence behavior of the corresponding numerical techniques.

1. Definition and properties of Padé approximants

Let P_n be the set of polynomials with degree at most n for all $n \geq 0$. The set of ordinary rational functions $r = \frac{p}{q}$ with $p \in P_m$, $q \in P_n$ and $\frac{p}{q}$ irreducible be denoted by $R_{m,n}$ for all $m, n \geq 0$. Consider the following formal power series

$$f(x) = c_0 + c_1 \cdot x + c_2 \cdot x^2 + c_3 \cdot x^3 + \dots \quad (1)$$

Definition of Padé approximant

The Padé approximant of order (m, n) for f is the unique element $r_{m,n} = \frac{p}{q}$ in $R_{m,n}$ such that

$$f(x) \cdot q(x) - p(x) = O(x^{m+n+1+k}) \quad (2)$$

for some integer k , which is as high as possible.

Since $r_{m,n}$ is defined for every $m, n \geq 0$ the following table can be constructed:

$r_{0,0}$	$r_{0,1}$	$r_{0,2}$	$r_{0,3}$...
$r_{1,0}$	$r_{1,1}$	$r_{1,2}$	$r_{1,3}$...
$r_{2,0}$	$r_{2,1}$	$r_{2,2}$	$r_{2,3}$...
$r_{3,0}$	$r_{3,1}$	$r_{3,2}$	$r_{3,3}$...
\vdots	\vdots	\vdots	\vdots	

This table is called the Padé table for f . The elements of the first column of this table are the partial sums of (1). An element $r_{m,n}$ is called normal if it

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appears only once in the Padé table or equivalently $r_{m,n} = \frac{p}{q}$ is normal if p and q have degree exactly m and n respectively and $k=0$ in (2).

Convergence of Padé approximants

The important topic of the convergence properties of certain sequences of Padé approximants has been treated in several books and papers, e.g. O.Perron (1929), H.S.Wall (1948), G.A.Baker (1965,1975). A survey of these properties has been given by C.K.Chui (1976) at the Austin Conference on Approximation Theory. From this theory it follows that the convergence domain of certain sequences of Padé approximants can be larger than this of the given power series (1). In a lot of cases this convergence can also be faster. Moreover Padé approximants can be used to approximate meromorphic functions successfully. These are some of the most important features which make Padé approximants suitable for practical work.

Connection with Chebyshev approximation

Padé approximants can be considered as uniform limits of certain sequences of Chebyshev approximants. This connection was pointed out by J.L.Walsh in a number of papers. Recently C.K.Chui, O.Shisha and P.W.Smith (1974) proved the following result :

Let f be an element of $C^{m+n+1} [0, \delta]$ with $\delta > 0$, and r_ϵ be the Chebyshev approximant from $R_{m,n}$ for f on $[0, \epsilon]$ for every ϵ in $[0, \delta]$. Then the sequence $\{r_\epsilon\}$ converges uniformly to $r_{m,n}$ on some closed interval $[0, \epsilon_0]$ with $\epsilon_0 \leq \delta$ as ϵ goes to zero. This property is called the locally best property of Padé approximants.

Algorithms for computing Padé approximants

Several algorithms exist for computing the elements in the Padé table. Some of them e.g. Baker's algorithm (1970) and Longman's algorithm (1971) make use of certain recurrence relations which do exist between neighboring elements in the Padé table. It is also possible to construct certain continued fractions whose convergents form certain sequences in the Padé table. Algorithms of this type are given by H.Rutishauser (1956), F.L.Bauer (1959), H.C.Thacher (1961), W.B.Gragg (1972), P.J.S.Watson (1973), G.Claessens (1975). To compute the value of a Padé approximant in a given point the ϵ -algorithm of P.Wynn (1956) or the η -algorithm of F.L.Bauer (1959) can be used. We refer to the paper of G.Claessens (1975) for more information concerning these algorithms.

Literature on Padé approximation

The topic of Padé approximation has been treated in a large number of books and papers. References to them will be found in the following books : O.Perron (1929), H.S.Wall (1948), G.A.Baker (1975) survey papers : J.Zinn-Justin (1971), J.L.Basdevant (1972), W.B.Gragg (1972), P.Wynn (1974), G.Claessens (1975), C.K.Chui (1976). bibliography : C.Brezinski (1976). proceedings of conferences and collection of papers : G.A.Baker and J.L.Gammel (1970), W.B.Jones and W.J.Thron (1974), P.R.Graves-Morris (1973), H.Cabannes (1975), D.Bessis, J.Gilewicz, P.Mery (1975).

The present paper is intended to be complementary to the survey papers mentioned above. We only will consider the applications of one-point Padé approximants in several fields of Numerical Analysis. A similar theory could also be given for the case of multipoint Padé approximation (where information of f at several points is used). We will mention applications of multi-point Padé approximation (also called rational Hermite interpolation) only briefly at the end of each section.

2. The use of Padé approximation in solving nonlinear equations

Consider a real-valued function f , defined in the interval $[a,b]$. The problem is to find an element x in $[a,b]$ such that $f(x) = 0$. To solve this problem the following method can be used.

Let x_i be an approximation for x and r_i be the Padé approximant of order (m,n) for f at the point x_i . The element x_{i+1} is now defined as being a zero of r_i or, if $r_i = \frac{p_i}{q_i}$, $p_i(x_{i+1}) = 0$.

If the sequence $\{x_i\}$ is convergent to a simple zero of f and if r_i is normal for every i then the following relation can be proved (L.Tornheim, 1964) :

$$\lim_{i \rightarrow \infty} \frac{|x_{i+1} - x|}{|x_i - x|^{m+n+1}} = c < \infty \quad (3)$$

This means that the order of convergence is at least $m+n+1$. Moreover it can be shown (L.Tornheim, 1964) that $\{x_0, x_1, x_2, \dots\}$ will converge as soon as x_0 is chosen close enough to x . A similar convergence result is also given by G.Merz (1968) and J.S.Frame (1953) for modified versions of the above technique.

It is important to remark that the order of convergence is only dependent on the sum of m and n , which means that the order remains unchanged if elements on an ascending diagonal in the Padé table are used. The use of $n > 0$ can be interesting since in this case the asymptotic error constant c can be much lower (G.Merz, 1968). Moreover it is important to note that the numerator p_i of r_i can be computed without having to compute q_i (e.g. using Baker's algorithm). This makes the case $m=1$, $n > 0$ particularly interesting.

Remark that the case $m=1$, $n=0$ reduces to the classical Newton's method. It is also possible to compute all the zeros or poles of f simultaneously by using Rutishauser's qd-algorithm. See e.g. P.Henrici (1963), A.S. Householder (1970) and [13] for more details.

Applications of the use of multipoint Padé approximants to the above problem are given by P.Jarratt (1966,1970), J.F.Traub (1964), G.R. Garside, P.Jarratt and C.Mack (1968), D.K. Dunaway (1974), J.C.P. Bus and T.J.Dekker (1975).

3. The acceleration of convergence using Padé approximation

Let $\{a_i\}$ be a given sequence with limit A or $\lim_{i \rightarrow \infty} a_i = A$. The problem is to find A . Since the convergence of $\{a_i\}$ can be slow it is interesting in some cases to construct a sequence $\{b_i\}$ satisfying the following properties:

$$\lim_{i \rightarrow \infty} b_i = A \quad \text{and} \quad \lim_{i \rightarrow \infty} \frac{|b_i - A|}{|a_i - A|^\alpha} = 0 \quad \text{with } \alpha > 1.$$

In order to construct $\{b_i\}$ the following technique can be used. Consider

$$f(x) = a_0 + \sum_{i=1}^{\infty} (a_i - a_{i-1}) \cdot x^i \quad (4)$$

Then $f_n(x) = a_0 + \sum_{i=1}^n (a_i - a_{i-1}) \cdot x^i$ satisfies $f_n(1) = a_n$ for $n \geq 0$. Let $r_{m,m}$ be the Padé approximant of order (m,m) for f . The sequence $\{b_i\}$ can now be defined as follows :

$$b_i = r_{i,i}(1) \quad \text{for } i \geq 0. \quad (5)$$

The elements b_i satisfying (5) can be computed easily by using the ϵ -algorithm of P.Wynn (1956). This algorithm works as follows :

Put $\epsilon_{i,-1} = 0$ and $\epsilon_{i,0} = a_i$ for $i \geq 0$

Compute $\epsilon_{k,1} = \epsilon_{k-1,1-2} + \frac{1}{\epsilon_{k,1-1} - \epsilon_{k-1,1-1}}$ for $k = 1, 2, 3, \dots$ and $1 = 1, 2, 3, \dots, k$.

Then $b_i = r_{i,i}(1) = \epsilon_{2i,2i}$ for $i \geq 0$.

The convergence of $\{b_i\}$ depends highly on the properties of $\{a_i\}$. This relation has been investigated e.g. by P.Wynn (1966), C.Brezinski (1972), A.Genz (1973). The ϵ -algorithm can also be used if the elements a_i are vectors or matrices. See P.Wynn (1962), E.Gekeler (1972), C.Brezinski (1974,1975).

Padé approximation has also been successfully applied for summing divergent series. See R.Wilson (1930), P.Wynn (1967). Applications of the use of multipoint Padé approximants for accelerating the convergence of a given sequence are given by R.Bulirsch and J.Stoer (1964), J.Oliver (1971), A.Genz (1973), L.Wuytack (1971).

4. The numerical solution of ordinary differential equations using Padé approximation.

Consider the problem of finding a solution for the following initial value problem $y' = f(x,y)$, $y(a) = y_0$ with x in $[a,b]$. Let $h = \frac{b-a}{k}$ for some integer k and $x_i = a + i \cdot h$, for $i = 0, 1, \dots, k$. In order to find approximations y_i for $y(x_i)$ the following idea could be used : Let r_i^* be the Padé approximant of a certain order for $y(x)$ at the point x_i and take $y_{i+1} = r_i^*(x_{i+1})$, for $i = 0, 1, \dots, k-1$. A power series expansion for the solution $y(x)$ at x_i however is not known. But it is possible to consider the following power series in h :

$$y_i + h \cdot f(x_i, y_i) + \frac{h^2}{2!} \cdot f'(x_i, y_i) + \frac{h^3}{3!} \cdot f''(x_i, y_i) + \dots \quad (6)$$

Starting with y_0 it is now possible to construct the sequence $\{y_1, y_2, \dots, y_k\}$ as follows : Let r_i be the Padé approximant of order (m,n) for (6), then define

$$y_{i+1} = r_i(x_{i+1}) \quad \text{for } i = 0, 1, \dots, k-1 \quad .$$

It is not hard to see that this relation can also be written in the following form

$$y_{i+1} = y_i + h \cdot g(x_i, y_i, h) \quad \text{for } i = 0, 1, \dots, k-1. \quad (7)$$

The above technique can now be considered as a one-step method for solving the given initial value problem.

Applying a convergence result for one-step methods [56, p.116] we get : if $g(x, y, h)$ is continuous and satisfies a Lipschitz condition in y , then

$\lim_{h \rightarrow 0} y_i = y(x_i)$. Moreover, using a similar argument as in [68, p.269], it is possible to prove that in the case of normal Padé approximants we have

$$y(x_i) - y_i = O(h^{m+n+1}) \quad (8)$$

In order to compute y_{i+1} as defined in (7) several techniques can be used. It is possible to construct explicit formulas for $g(x, y, h)$. See e.g. Z.Kopal (1959), J.D.Lambert and B.Shaw (1965). These formulas become fairly complicated for higher values of m and n . Another possibility is to use the ϵ -algorithm with $\epsilon_{n,0}$ equal to the n -th partial sum of (6). See [49] and A.Wambecq [63].

Remark that the choice of $n=0$ in the above technique corresponds to the Taylor series method in solving the given initial value problem.

Methods of the form (7) have the disadvantage that the derivatives of f must be known or computed. It is however possible to replace the derivations by linear combinations of values of f at different points, keeping a method with the same order of convergence. This replacement gives raise to nonlinear Runge-Kutta type methods. Some of the properties of these techniques are considered by A.Wambecq (1976). It is important to note that it is e.g. possible to derive nonlinear Runge-Kutta methods of order 5 using 5 evaluations of f , which is not possible in the linear case.

Formulas of the form (7) can also be used for solving systems of ordinary differential equations, see J.D.Lambert (1973) and [64].

Also multipoint Padé approximants can be used to solve initial value problems, giving raise to nonlinear multipoint methods. See e.g. J.D.Lambert and B.Shaw (1965, 1966), G.Opitz (1968), Y.L.Luke, W.Fair and J.Wimp (1975). Padé approximants for the exponential function play a very important rule to derive A-stable methods for solving initial value problems, see e.g. B.L.Ehle (1968, 1971), E.B.Saff and R.S.Varga (1975).

5. Numerical quadrature using Padé approximation.

The problem is to find the value of the definite integral $I = \int_a^b f(t) dt$. A first approach to this problem is as follows : approximate f by some rational function, e.g. a Padé approximant, and compute $\int_a^b r(t) dt$. The value of this last integral might not be easy to find and several difficulties can be encountered (see J.S.R. Chisholm, 1974). A second approach is based on the transformation of the given problem to the problem of finding the value $y(b)$ where $y(x)$ is the solution of the initial value problem $y'(x) = f(x)$, $y(a) = 0$, with $x \in [a, b]$. Since $y(x) = \int_a^x f(t) dt$ it is clear that $I = y(b)$.

Let h, x_i and y_i be defined as in the preceding section, then the following technique can be used to find the value of $y(b)$. Let r_i be the Padé approximant of order (m, n) for

$$y_i + h \cdot f(x_i) + \frac{h^2}{2!} \cdot f'(x_i) + \frac{h^3}{3!} \cdot f''(x_i) + \dots$$

then y_{i+1} can be defined as follows

$$y_{i+1} = r_i(x_{i+1})$$

$$\text{or } y_{i+1} = y_i + h \cdot s(x_i, h) \quad \text{for } i = 0, 1, \dots, k-1 \quad (9)$$

for some function $s(x, h)$. The formula (9) can be interpreted as a formula for approximate integration between x_i and x_{i+1} or

$$\int_{x_i}^{x_{i+1}} f(t) dt \approx h \cdot s(x_i, h) .$$

The convergence properties of the above technique follow immediately from the results in the previous section. We get : if $s(x, h)$ is continuous then $\lim_{h \rightarrow 0} y_k = I$ and $I - y_k = O(h^{m+n+1})$, in the case of normal Padé approximants. Again the ϵ -algorithm can be used to compute y_{i+1} in (9) or explicit formulas can be derived, e.g. in the case $m=n=1$ we get

$$s(x, h) = \frac{2 \cdot [f(x)]^2}{2 \cdot f(x) - h \cdot f'(x)} .$$

Remark that the derivatives of f can be replaced by linear combinations of values of f at different points, keeping a method with the same order of convergence (see [68] for more details and some numerical examples).

Padé approximants can also be used for evaluating integrals having a singular integrand, see [69].

6. The numerical solution of partial differential equations using Padé approximation.

Consider the problem of finding a solution $u(x,t)$ for the following boundary value problem :

$$\left. \begin{array}{l} \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \text{ for } a < x < b \text{ and } t > 0 \\ u(x,0) = g(x) ; u(a,t) = \alpha ; u(b,t) = \beta \end{array} \right\} \quad (10)$$

To find approximate values for $u(x_i, t_j)$ in certain points the following technique can be used (R.S. Varga, 1961). First spatial discretization of (10) is performed, with $h = \frac{b-a}{n+1}$ and $x_i = a + i.h$ for $i = 0, 1, \dots, n+1$. Put $u_i(t) = u(x_i, t)$ for $t \geq 0$ and $i = 1, \dots, n$, then (10) becomes :

$$\left. \begin{array}{l} \frac{du_i(t)}{dt} = -A \cdot u_i(t) \quad \text{for } t > 0 \text{ and } i = 1, 2, \dots, n \\ u_i(0) = g(x_i) \end{array} \right\}$$

where A is a real symmetric positive-definite $n \times n$ matrix.

The exact solution of this initial value problem is given by

$$U(t) = e^{-t \cdot A} \cdot G, \quad (11)$$

with $U(t) = [u_1(t), u_2(t), \dots, u_n(t)]^T$ and $G = [g(x_1), g(x_2), \dots, g(x_n)]^T$.

Let Δt be the stepsize in the t -direction then (11) can also be written as

$$U(t + \Delta t) = e^{-\Delta t \cdot A} \cdot U(t). \quad (12)$$

Let $r_{m,n} = \frac{p}{q}$ be the Padé approximant of order (m,n) for e^{-x} then (12) can be approximated by

$$U(t + \Delta t) = [q(\Delta t \cdot A)]^{-1} \cdot [p(\Delta t \cdot A)] \cdot U(t) \quad (13)$$

It can be proved that (13) is an unconditionally stable method if $n \geq m$. This property is based on the fact that $|r_{m,n}(x)| \leq 1$ for all $x \geq 0$ if and only if $n \geq m$ (see R.S.Varga, 1961). The case $m=0$, $n=1$ reduces (13) to a classical explicit method for solving (10). The case $m=1$, $n=1$ reduces to the Crank-Nicolson technique for solving (10).

The application of Padé approximation to solve more general parabolic partial differential equations can be found in R.S.Varga (1962).

7. Other applications.

In this section we only mention some other applications of the use of Padé approximation in numerical analysis :

- computation of Laplace Transform inversion, see I.M.Longman (1973)
- numerical differentiation, see [55], [67].
- solution of integral equations, see M.F.Barnsley and P.D.Robinson (1974), W.Fair (1974).
- analytic continuation, see [5], J.L.Gammel (1974), J.Devooght (1976).

Of course Padé approximations can also be used to approximate a given function, see E.G.Kogbetliantz (1960), Y.L.Luke (1969), A.Edrei (1975).

Several other applications to related fields can be found in the literature given in section 1.

8. Conclusion.

It has been shown that Padé approximation can be applied to derive nonlinear techniques in several fields of numerical analysis. These techniques have interesting convergence properties, similar to these for linear methods. Numerical examples show that nonlinear techniques can be more interesting than linear ones in the neighbourhood of singular points. Care must be taken in applying nonlinear techniques, due to the possibility of numerical instability during the computations.

Our experience shows that the use of Padé approximation is not better than the use of a linear technique in all situations. In those cases however where linear techniques give poor results or fail to converge it might be interesting to try a nonlinear technique.

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