Placement of cuts in Padé-like approximation (1)

R. T. Baumel (2), J. L. Gammel (3) and J. Nuttall (2)

ABSTRACT

We propose a method for continuing an analytic function from its power series expansion that enables us to choose the location of cuts joining the branch points. The method is superior to the Padé approximant method in this respect and also because point-wise convergence may be proved.

1. INTRODUCTION

It has been shown that in many instances the Padé approximants to the formal power series representing a function with branch points place the cuts on a set of minimum capacity joining the branch points [6]. Sometimes these cuts prevent calculation of the function at a point of interest. Consider the classic example

$$f(x) = \sqrt{\frac{1+2x}{1+x}} = 1 + \frac{1}{2}x - \frac{5}{8}x^2 + \ldots \tag{1}$$

The zeros and poles of the [N/N] Padé approximants all lie on the real axis in the interval (–1/2, –1), so that for large N the [N/N] approximant alternates rapidly between zero and infinity in the interval in such a way that it is impossible to calculate f(x) at x = - 3/4, for example. If one is interested in x = - 3/4, he would like to move this dense set of zero and poles, that is, this cut, to the semi-circle S shown in fig. 1. Of course, this choice means that one is continuing the function

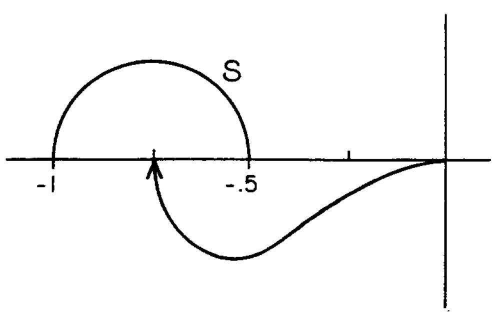

Fig. 1. A path of continuation of f(x) from x=0 to x = -.75 when f(x) is cut along the semi-circle S.

along some such path as shown by the curve marked with arrows in fig. 1. If he wants to continue along a path in the upper half plane, he will have to place the semi-circle in the lower half plane.

Perhaps the most remarkable feature of Padé approximants is that their calculation requires absolutely no information about the location of the singularities. The Padé approximant locates the singularities and when necessary places cuts on the set of minimum capacity (in the x^{-1} plane) joining the branch points. In the scheme we are going to describe one has to know the location of the singularities. These could be located by using Padé approximants or other techniques. But having located the branch points we place the cuts where we want them.

An alternative method of continuation has been proposed by Brezinski [3]

2. THE METHOD

Let f(x) be a function with a known power series expansion about x = 0 (we assume f to be analytic in a neighborhood of the origin). We may approximate f by rational functions

$$f(x) \approx \frac{P_N(x)}{Q_N(x)} \tag{2}$$

where P_N and Q_N are polynomials of degree N. The ordinary [N/N] Padé approximant is obtained by matching the power series of the right and left sides of (2), for all terms up to order 2N. As is well known [1], this approach leads to a set of linear equations for the coefficients of P_N and Q_N, but these equations split naturally into two subsets :

(i) There are N equations which determine the coef-

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(2) R. T. Baumel and J. Nuttall, Department of Physics, University of Western Ontario, London, Ontario, Canada. N6A 3K7.

(3) J. L. Gammel, Department of Physics, St. Louis University, St. Louis, Missouri, USA.

ficients of the denominator Q_N.

(ii) There are N + 1 additional equations which trivially determine the coefficients of P_N, once the coefficients of Q_N are known. In effect, once Q_N is known, one simply multiplies it by the powers series of f, and then truncates the resulting series to an Nth order polynomial to find P_N.

In the approach that we describe here, we ignore part (i) of the Padé procedure, and simply choose an appropriate denominator Q_N with zeros along the particular arc where we wish to place a cut. We then calculate the numerator P_N using part (ii) of the usual Padé procedure. This method can also be described by saying that we first choose Q_N, and then calculate P_N by matching power series in (2) using only the terms up to order N.

The major difficulty with this method is in choosing an appropriate denominator Q_N. The method does not work if, for example, we simply distribute the zeros of Q_N uniformly along the desired cut. As we explain below, the polynomials Q_N that we actually use are derived from an appropriate set of orthogonal polynomials.

The properties that Q_N must have, in order for the approximation to work, become apparent when we examine a formula for the error of the approximation. Walsh [7] has studied a class of rational approximations, which includes the type of approximation we consider here. In our case, Walsh's formula for the error reduces to

$$f(x) - \frac{P_N(x)}{Q_N(x)} = \frac{1}{2\pi i Q_N(x)} \int_{\gamma_x} \frac{f(x')Q_N(x')\left(\frac{x}{x'}\right)^{N+1} dx'}{x' - x} \tag{3}$$

where the integration path γ_x is a counterclockwise contour enclosing the origin and enclosing the point x, but not enclosing any singularities of f.

The content of (3) is more easily understood by transforming the integral to the $t = 1/x$ plane, and by defining the polynomial

$$q_N(t) = t^N Q_N(1/t) \tag{4}$$

With this substitution, (3) becomes

$$f(x) - \frac{P_N(x)}{Q_N(x)} = \frac{1}{2\pi i q_N(t)} \int_{\gamma_t} \frac{f\left(\frac{1}{t'}\right) q_N(t')\, dt'}{t - t'} \tag{5}$$

where the integration path γ_t is now a counterclockwise contour enclosing all the singularities of f, but not enclosing the point $t = 1/x$.

We remark that (5) is equivalent to the error formula for Padé approximants stated by Nuttall and Singh [5], but we emphasize that this formula depends only on part (ii) of the Padé procedure, and does not depend on whether or not Q_N is the correct Padé denominator found from part (i) of the Padé procedure.

Furthermore, as we prove in the appendix, the function Q_N in (3) and (5) need not even be a polynomial. To be specific, let S be a set in the extended complex plane which includes all the singularities of f(x) and is such that f(x) is single-valued outside S. In particular, if we wish to place cuts along certain arcs, then S would consist of those arcs, as well as any other singularities (i.e., poles or essential singularities) of f.

We let T denote the image of S in the $t = 1/x$ plane. Under these conditions, (3) holds provided only that Q_N is analytic and single-valued everywhere outside S (except possibly at $x = \infty$), and (5) holds provided only that q_N is analytic and single-valued everywhere outside T, except for a pole of at most order N at $t = \infty$.

We remark that if Q_N is not a polynomial, then the prescription for calculating the numerator (i.e., part (ii) of the Padé procedure) must be generalized as follows : Multiply the power series (in x) of Q_N by the power series of f; truncate the result to an Nth order polynomial to find P_N.

Examination of (5) shows that the error in approximating f(x) by $P_N(x)/Q_N(x)$ will be small if the modulus of q_N is much smaller along the contour γ_t than it is at the point $t = 1/x$. Since the contour γ_t may be shrunk down very close to the boundary ∂T of the singularity set T, we try to choose q_N to minimize the expression

$$M(t, T, q_N) = \frac{\sup_{t' \epsilon \partial T} |q_N(t')|}{|q_N(t)|} \tag{6}$$

If T is a connected set, then, as we show in the appendix, the expression (6) is easily minimized, and the result depends only on the set T (it does not depend on the particular point t where we wish to evaluate the function). The optimal choice for q_N is

$$q_N(t') = [\psi(t')]^N = e^{N\phi(t')} \tag{7}$$

where ψ is a function which conformally maps the exterior of T onto the exterior of the unit circle and maps ∞ to ∞ (or equivalently, ϕ is an analytic function whose real part is the two-dimensional electrostatic potential produced by charges distributed on T in such a way that the total charge on T is one, and the potential of T is zero). It is evident from (5) that if q_N is given by (7), then the error in approximating f(x) will be of order $\exp[-N\phi(t)]$, which decays exponentially as $N \to \infty$.

The optimal form for q_N, given by (7), is not a polynomial, and is usually not very easy to calculate (although, if T is bounded by a polygonal line, then ψ may be calculated using the Schwartz-Christoffel transformation). In general, the approach that we recommend for calculation is to let q_N be an Nth degree polynomial with the same asymptotic form (for large N) as (7).

Many polynomial sets with this asymptotic form are known to exist. For example, one can define such a sequence of polynomials by choosing an appropriate "norm" relating to the set T. Given such a norm, the Nth polynomial in the sequence is the minimum-norm polynomial of the form

$$q_N(t) = t^N + a_{N-1}t^{N-1} + \dots + a_0 \qquad (8)$$

If we choose to minimize the sup-norm (i.e., the supremum of the modulus of the polynomial on T), then we obtain the generalized Chebyshev polynomials corresponding to T [4]. Other polynomial sets with the desired asymptotic form are obtained by using L^p norms of the form

$$\|q_N\|_{p,\mu} = \left[\int |q_N(t')|^p \, d\mu(t') \right]^{1/p} \qquad (9)$$

where p is a positive number and μ is a positive measure concentrated on T [8].

It is intuitively clear that by minimizing either the sup-norm or an L^p norm, we force the zeros of q_N to lie on, or close to, the set T. It is easily proved that, in general, the zeros of q_N always lie within the convex hull of T. In the simple cases that arise with our cut-placement method, the zeros tend to be extremely close to T. We remark that the distribution of zeros along T, for large N, is of the same form as the charge distribution that makes T an equipotential (this is to be expected if q_N is to have the asymptotic form of (7) (see Widom [9]).

If, in (9), we let p = 2, then the resulting polynomials q_N are just the orthogonal polynomials corresponding to the measure μ. Orthogonal polynomials are particularly straightforward to calculate numerically. It is only necessary to calculate the matrix of inner products

$$\langle t^k, t^\ell \rangle = \int t^k (t^\ell)^* \, d\mu(t), \qquad (10)$$

and then apply the Gram-Schmidt orthogonalization procedure to the set of functions $\{t^k\}$.

The set T usually consists of a number of arcs (aside from isolated singularities, T is just the set of desired cuts, viewed in the t = 1/x plane). Since the asymptotic form of the orthogonal polynomials is largely independent of the precise measure μ, we have, in actual calculations, simply let μ denote arc length along the set T, so that (10) becomes

$$\langle t^k, t^\ell \rangle = \int_T t^k (t^\ell)^* |dt| \qquad (11)$$

The integral in (11) can, for reasonable choices of the cuts, be evaluated analytically.

Our complete algorithm for placement of cuts in a rational approximation can now be described as follows :

1) Assuming that the branch points of f are known (and assuming, for the moment, that f has no other singularities besides branch points), choose a set of possible cuts, preferably simple curves in the t plane, in such a way that f is analytic and single-valued outside the cuts.
2) Calculate the inner products in (11).
3) Use Gram-Schmidt orthogonalization to find the orthogonal polynomials q_N.
4) Trivially determine the Q_N from the q_N using equation (4).
5) Multiply Q_N by the power series of f to find the numerator P_N.

We remark that if f has other singularities besides branch points, then these must also be accounted for in the choice of denominator. For example if f has a simple pole, then a corresponding zero in the polynomial q_N (at the pole of f or at least as close to it as possible) must be inserted by hand.

We also remark that although our derivation of the optimal form of the denominator (theorem 2 in the appendix) is valid only when the set T is connected, the method just described (using orthogonal polynomials) works just as well even if T has several components. When T is not connected, the function

$$\psi(t) = e^{\phi(t)}$$

still exists, but is not single valued. Nevertheless, Widom [8] has shown that the orthogonal polynomials q_N are still of the form

$$|q_N(t)| \approx |e^{N\phi(t)}| \qquad (12)$$

so that from the error formula (5), we see that the approximation error will still be of order $|\exp[-N\phi(t)]|$.

3. NUMERICAL EXAMPLE

The application of our method to the example of (1) is illustrated by figs. 2 and 3 and by tables 1 and 2. Fig. 2 shows what happens when the denominator Q_N is chosen, not by the method of orthogonal polynomials, but by just placing zeros uniformly on the semi-circle S in the x plane. With ordinary Padé approximants, the zeros of the numerator interlace those of the denominator. This also happens with our method (when it

TABLE 1

Values of (N/N) approximants to f(−0.75) with f given by (1), and denominators chosen with zeros placed uniformly on semicircle S, as in figure 2. Actual value of f(−0.75) is $-i\sqrt{2}$

N	Re(N/N)(x=−.75)	Im(N/N)(x=−.75)
1	0.625000	−1.125000
2	0.062500	−1.826772
3	−0.260304	−2.087077
4	−0.190565	−2.008459
5	0.151636	−1.690821
6	0.469281	−1.214965
7	0.446288	−0.712419
8	−0.071127	−0.431324
9	−0.918809	−0.693459
10	−1.567500	−1.690881

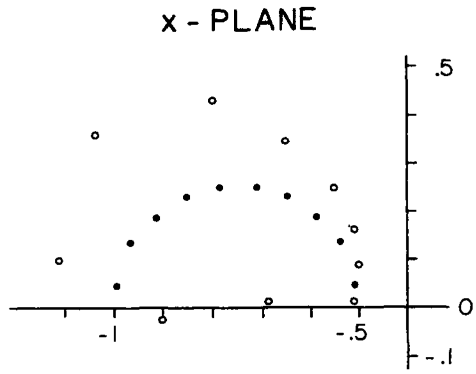

Fig. 2. Zeros of numerator (open circles) and denominator (solid circles) of the (10/10) approximant to $(1+2x)^{1/2}\ (1+x)^{-1/2}$ when the zeros of the denominator are distributed uniformly along the semicircle S of fig. 1.

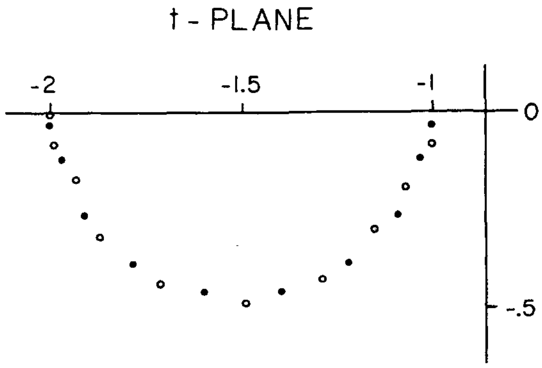

Fig. 3. Zeros of numerator (open circles) and denominator (solid circles) of the (10/10) approximant to $(1+2x)^{1/2}(1+x)^{-1/2}$, plotted in the $t = x^{-1}$ plane. The denominator is the orthogonal polynomial based on $T = S^{-1}$.

works). But in fig. 2, the zeros of the numerator do not follow the same curve as the zeros of the denominator. In fact, some zeros of the numerator lie almost on the real axis in the interval (-1, -1/2). Clearly this approach has not succeeded in moving the cut away from the interval [-1, -1/2]. We have tried evaluating the approximants at $x = -.75$, but they do not appear to converge (table 1).

Fig. 3 shows that the zeros of numerator and denominator *do* interlace when orthogonal polynomials are used as the denominators. Table 2 displays some of the approximants, computed for a number of real values of x. One feature of the function f in (1) is that its values are purely real for real x outside the interval [-1, -1/2]; but are purely imaginary for x inside this interval. The approximants in table 2 reproduce this behavior (as $N \to \infty$) even though the power series of f has all real coefficients (the non-zero imaginary parts arise entirely from the denominators Q_N that we have chosen).

TABLE 2

Values of (N/N) approximants to the function of (1), with denominators chosen as orthogonal polynomials, as in figure 3.

N	Re(N/N)(x=-.4)	Im(N/N)(x=-.4)	Re(N/N)(x=-.8)	Im(N/N)(x=-.8)
5	.57671921637	.4187E-03	-.120771	-2.020327
6	.57769992776	.5462E-04	-.164839	-1.862066
7	.57731068682	-.1503E-03	-.141036	-1.753480
8	.57730444777	.3096E-04	-.091403	-1.696116
9	.57736479161	.9027E-05	-.042526	-1.678596
10	.57735018646	-.5260E-05	-.007126	-1.684949
11	.57734880335	.1102E-05	.012158	-1.701058
12	.57735090868	.2468E-06	.018318	-1.717505
13	.57735023545	-.2488E-06	.016333	-1.729639
14	.57735019720	.5256E-07	.010854	-1.736342
15	.57735029745	.1306E-07	.005130	-1.738524
16	.57735026819	-.1078E-07	.000848	-1.737852
17	.57735026612	.2255E-08	-.001544	-1.735927
18	.57735027045	.5312E-09	-.002333	-1.733892
19	.57735026913	-.4924E-09	-.002097	-1.734355
20	.57735026905	.1054E-09	-.001405	-1.731489
21	.57735026925	.2537E-10	-.000669	-1.731200
22	.57735026919	-.2227E-10	-.000110	-1.731284
23	.57735026918	.4832E-11	.000206	-1.731536
24	.57735026919	.1143E-11	.000313	-1.731805
25	.57735026919	-.1031E-11	.000283	-1.732011
f(x)	.57735026919	0.	0.	-1.732051

The example of (1) is sufficiently trivial that the function is easily evaluated directly, enabling us to check convergence. The approximants in table 2 converge exponentially to the desired function, although, as one would expect, the convergence is slowest inside the interval [-1, -1/2]. If for a fixed x, the successive approximants to f(x) are plotted in the complex plane, it is seen that the approximants converge toward f(x) along a logarithmic spiral. For example, at $x = -0.8$, the errors of successive approximants tend to be in the ratio of about $0.62 - (0.36)i$, which has a modulus of about 0.72. According to the theory of the previous section, we expect that this figure corresponds to the convergence factor of $\exp[-\phi(t)]$.

We remark that in calculating the approximants described here, as in the case of ordinary Padé approximants, large cancellations take place, so that many digits must be carried to prevent loss of precision. All our calculations were performed in 4-fold precision on the Cyber 73 computer. Thus, we were working with an effective mantissa of 192 bits (roughly 58 decimal digits). In another calculation using this method, where we let the set T have the shape of a letter "H", we extended the calculation to considerably higher values of N than in the calculations described above. In that case, although we were using 4-fold precision, we discovered evidence of numerical breakdown in the calculation of the orthogonal polynomials when N reached about 90.

4. DISCUSSION

We have described a method of Padé-like approximation, which allows us to place a cut in a different position than the Padé approximant would place it, and thereby enables us to analytically continue a function farther than is possible by Padé approximants. In addition to the trivial example presented here, we have applied the method to a non-trivial hydrodynamics problem [2] with fairly good results (although we were able to obtain slightly better results by another method which used more of the available information about the function).

One obvious limitation of the method is that it requires knowledge of the locations of the singularities of the function. The accuracy with which these are known can limit the accuracy with which the function can be calculated.

Even when the singularities have been located very precisely, the method still does not always allow us to analytically continue too far. For example, for the function of equation (1), suppose that we wish to extend the cut to the curve T in fig. 4 (drawn in the t plane), and that we wish to evaluate the function at the point t. It is clear that if the set T is an equipotential, at potential zero, then the potential at point t will also be very close to zero. Thus, the convergence factor $\exp[-N\phi(t)]$ will not be small, even for very large N, so that convergence will be very poor.

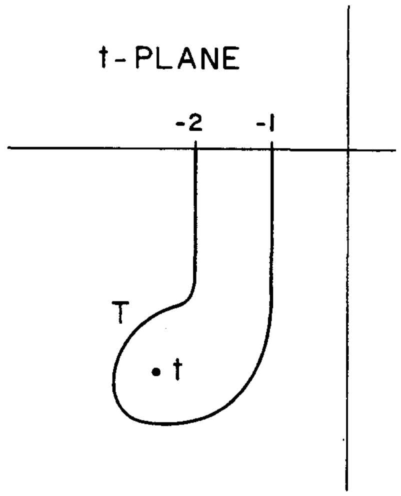

Fig. 4. A point t ($= x^{-1}$) at which convergence of the method would be slow if the cut is chosen along the arc T.

In spite of these limitations, we think that the method presented here can be useful for calculating functions in some cases where the ordinary Padé approximant fails.

APPENDIX

Error formula and optimal choice of denominator

Theorem 1

Let f(x) be a single-valued function on the extended complex plane, analytic everywhere except for a set S (which includes a desired set of cuts to make f single-valued, in the case where f has branch points). We assume that the complement of S includes a neighborhood of the origin. Let $Q_N(x)$ be any function which is analytic and single-valued everywhere on the complement of S (except, possibly, at $x = \infty$). Finally, let $P_N(x)$ be the Nth degree polynomial obtained by multiplying the power series of f by the power series of Q_N (both expanded about $x = 0$), and then truncating the result to an Nth degree polynomial. Then

$$f(x) - \frac{P_N(x)}{Q_N(x)} = \frac{1}{2\pi i Q_N(x)} \int_{\gamma_x} \frac{f(x')Q_N(x')(\frac{x}{x'})^{N+1}}{x' - x} dx' \tag{A1}$$

where γ_x is a counterclockwise contour, enclosing the origin, and enclosing the point x, but not enclosing any points of S.

Proof

Since f and Q_N are both analytic in a neighborhood of $x = 0$, the product of their power series is just the power series of the product $f(x)Q_N(x)$. We write the product series

$$f(x)Q_N(x) = \sum_{n=0}^{\infty} p_n x^n \tag{A2}$$

$$p_n = \frac{1}{2\pi i} \oint \frac{f(x')Q_N(x')}{(x')^{n+1}} dx' \tag{A3}$$

where the integral is taken counterclockwise around a contour enclosing the origin, but not enclosing any points of the set S. By definition, the polynomial P_N is formed by truncating the series (A2) :

$$P_N(x) = \sum_{n=0}^{N} p_n x^n = \frac{1}{2\pi i} \oint \frac{f(x')Q_N(x')}{x'} \sum_{n=0}^{N} (\frac{x}{x'})^n dx'$$

$$P_N(x) = \frac{1}{2\pi i} \oint \frac{f(x')Q_N(x')}{x' - x} [1 - (\frac{x}{x'})^{N+1}] dx' \tag{A4}$$

Equation (A4) holds whether or not the integration path encloses the point x. In the event that the path does enclose x, we have

$$P_N(x) = f(x)Q_N(x) - \frac{1}{2\pi i} \oint \frac{f(x')Q_N(x')}{x' - x} (\frac{x}{x'})^{N+1} dx'$$

which immediately implies equation (A1).

Theorem 2

Let T be a closed, bounded, connected subset of the complex plane (bounded by a finite number of Jordan arcs) and let t be a given point outside T. Let ψ be the function which conformally maps the exterior of T onto the exterior of the unit circle, with $\psi(\infty) = \infty$. Then the function q_N, analytic outside T except for a pole of at most Nth order at ∞, which minimizes the expression $M(t, T, q_N)$ from (6) is

$$q_N(z) = k[\psi(z)]^N \qquad \text{(A5)}$$

where k is any non-zero constant.

Proof

Let q_N be any function analytic outside T, except for a pole of at most Nth order at ∞. Define the function

$$h(z) = \frac{q_N(z)}{\psi(z)^N}, \qquad \text{(A6)}$$

which is analytic everywhere outside T (including $z = \infty$). Applying the maximum modulus principle to h(z) on the exterior of T,

$$\frac{|q_N(t)|}{|\psi(t)^N|} \leq \sup_{t' \in \partial T} \left| \frac{q_N(t')}{\psi(t')^N} \right| = \sup_{t' \in \partial T} |q_N(t')| \qquad \text{(A7)}$$

so that, combining (A7) and (6),

$$M(t, T, q_N) \geq \frac{1}{|\psi(t)^N|} \qquad \text{(A8)}$$

We minimize $M(t, T, q_N)$ by demanding equality in (A7) and (A8). By the maximum modulus principle, this equality holds if and only if h(z) is a constant. This completes the proof of theorem 2.

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