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Approximation of Analytic Functions:
A Method of Enhanced Convergence

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Approximation of analytic functions: a method of enhanced convergence

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Abstract

We present a method of enhanced convergence for the approximation of analytic functions. This method introduces conformal transformations in the approximation problems in order to help extract the values of a given analytic function from its Taylor expansion. We show that conformal transformations can extend the radius of convergence of a power series far into infinity, enhance substantially its convergence rates inside the circle of convergence, and can produce a rather dramatic improvement in the conditioning of Padé approximation. This improvement, which we discuss theoretically for Stieltjes type functions, is most notorious in cases of very poorly conditioned Padé problems. In some instances, an application of enhanced convergence leads to results which are many orders of magnitude more accurate than those obtained by classical approximants.

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1 Introduction

Perturbation methods and series expansions lie at the heart of most mathematical discussions of problems in science and engineering. Linear partial and ordinary differential equations amount, in many cases, to first order perturbation theory applied to basic principles of physics. Perturbation theory of higher order, on the other hand, has lead to an understanding of phenomena that cannot be accounted for accurately by low order expansions [18, 12, 1, 13, 4, 17, 7]). Yet, high order perturbation series are often regarded critically. Convergence results for the classical approximation methods are not always available, and numerical ill-conditioning is always a concern. Thus, new summation methods and further understanding of classical methods is necessary.

In this paper we deal with a method of enhanced convergence for the approximation of analytic functions. This method, a version of which was presented recently in the context of a problem of wave scattering ([7], see also [6]), introduces conformal transformations in the approximation problems in order to help extract the values of a given analytic function from its Taylor expansion. The purpose of this paper is to study the numerical properties of the method of enhanced convergence from both a theoretical and an experimental point of view. In particular, we shall show that conformal transformations can extend the radius of convergence of a power series far into infinity, enhance substantially its convergence rates inside the circle of convergence, and can produce a rather dramatic improvement in the conditioning of Padé approximation.

Complex variable theory is the natural framework for studying approximation via perturbation series. The most straightforward approach to evaluating a given analytic function f from its series representation about a point is, simply, given by summation of the truncated series. However, the shortcomings of this type of approximation are evident: the series will diverge as soon as the point z , at which the value of the given function is sought, lies outside the circle of convergence. And, even inside the circle of convergence, bad approximations are to be expected unless z is close enough to the expansion point.

Clearly, poor convergence and lack of convergence are related to the relative arrangement of the singularities of f and the point z . The *method of enhanced*

convergence uses conformal maps to manipulate the complex z plane, so as to produce an arrangement of the singularities of f and the point z which is favorable for either the summation of the series or the calculation of its Padé approximants. (A Padé approximant to an analytic function f is simply a rational function whose Taylor series matches that of the function f up to a finite order). The beneficial effect of our method in the summation of a power series has already been mentioned above: it greatly enlarges the region of convergence. Even enhanced series of very low orders can produce results which are accurate up to and including $z = \infty$ (see section 2.2), and enhanced series of high orders can produce valuable results (section 4). In addition, Padé approximants of the enhanced function *with denominators of low degree* can be used at any point at which the conformal transformation has produced a convergent enhanced series, and can yield better approximations than the enhanced series itself with a negligible additional computational cost.

A different phenomenon occurs in connection with Padé approximation with denominators of high degree: the conditioning of the Padé problem of the function f in the new variables improves very substantially. In other words, enhanced convergence acts as a preconditioner for Padé approximation. Of the three methods proposed in this paper, summation of the truncated enhanced series, enhanced Padé with denominators of low degree and diagonal enhanced Padé, it is diagonal enhanced Padé the one that generally yields best results for high order approximations. For example, a Fortran double precision calculation of the function $f(z) = \log(1+z)$ via regular Padé approximation, of any order, will not yield, at $z = 20$, more than the first four correct digits of $\log(21)$. After composition with an appropriate conformal map 13 correct digits can be obtained. In fact, diagonal enhanced approximants of orders 50 already yield 9 correct digits, while the number of correct decimals is 13 for approximations of orders 120 to 180. For $z = 200$, an enhanced Padé approximation can produce up to 6 correct figures, while only one correct digit can be obtained through direct Padé calculation.

A comment is in order with regards to the calculation of the coefficients of the power series of a function f in the new variables. These coefficients can be produced either 1) by certain linear operations on the coefficients of the series of $f(z)$, or 2) by some alternative direct calculation of the coefficients of the composite function. The information contained in the enhanced coefficients calculated the first method will

be limited by that contained in the coefficients of the series of $f(z)$, even though the Taylor coefficients of the true enhanced series encode more information than those of the regular series. Therefore, the second approach is to be preferred, if the corresponding accurate calculation is possible.

2 Enhanced Series

Let Ω be a connected domain in the complex plane, $0 \in \Omega$, let $f(z)$ be an analytic function defined in Ω and let D denote the circle of convergence of f about $z = 0$. The divergence of the Taylor series of f at a point z_0 outside D is related to the presence of singularities of f on the boundary of D . We shall show that such singularities are also the cause of numerical ill-conditioning in Padé approximation; see section 3. We argue, then, that it should be useful to deform the domain Ω conformally, keeping $z = 0$ fixed, in such a way that the image of the point z_0 is closer to the origin than the image of any of the singularities. This simple observation is the basis of the method under investigation.

The implementation of this procedure relies on some a-priori knowledge of the domain of analyticity of the function f . In applications such information can usually be obtained from physical considerations, Padé approximation ([3, §2.2]) or even by studying the convergence of several enhanced series ([7]). Once this information is available, the rearrangement of the singularities can be performed in many ways; in the following section we discuss some natural choices of conformal transformations that have proved to perform well. A few simple examples follow in section 2.2. Further examples and applications, together with a discussion of the numerical aspects of the method in high order applications will be given in sections 3 and 4.

We begin our study by considering conformal maps which extend the radius of convergence of the Taylor series of an analytic function.

2.1 Geometrical considerations

Let f be an analytic function defined in Ω . We seek a conformal map $\xi = g(z)$ defined in Ω with $g(0) = 0$ and such that the image $\xi_0 = g(z_0)$ of a given point z_0 lies inside the circle of convergence of the Taylor series of $f \circ g^{-1}$ about $\xi = 0$. If such

a function g is available, the value $f(z_0)$ can then be approximated by summing the truncated power series of $f \circ g^{-1}(\xi)$ at $\xi = \xi_0$.

Motivated by their geometrical properties as well as by their simplicity, rational fractions of the form

$$g(z) = \sum_{i=1}^K \frac{A_i z}{z + B_i} \quad (1)$$

appear as natural choices. Powers of combinations of these transformations and translations can also be useful (see [7]). Our intuition here is that, if f is conformal, then clearly, an enhancer g that eliminates the singularities of f completely is the function f itself

$$g = f.$$

It therefore seems reasonable to allow for g to mimic part of the singular behavior of the function f . In this way, some of the singularities of f are mapped away to infinity.

The performance of the method depends in a critical way on the parameters A_i and B_i in (1). If we are interested in the computation of $f(z_0)$ by composition with g^{-1} , the optimal choice of parameters is the one for which the convergence of the series of $f \circ g^{-1}$ is fastest. In other words, the parameters A_i and B_i should be taken in such a way as to minimize the quotient

$$\left| \frac{g(z_0)}{R} \right| = \left| \frac{\xi_0}{R} \right|, \quad R = \text{radius of convergence of } f \circ g^{-1} \text{ about } \xi = 0, \quad (2)$$

since the error in a truncated expansion of degree n is of order $\left| \frac{\xi_0}{R} \right|^{n+1}$. Note that the parameters can be selected numerically by optimizing the convergence rates even if no information is known about the singularities of the function f .

To illustrate these ideas let f be an arbitrary function and assume we know its singularities lie in the interval $[-1/a, -1/b]$. For example, we can take f to be a

Stieltjes or Hamburger function of the form ([3, Chap. 5])

$$f(z) = \int_a^b \frac{\phi(u)}{1+uz} d\mathbf{E} = \sum_{n=0}^{\infty} c_n z^n \quad (3)$$

with $\langle f \rangle \geq 0$. For the conformal map we shall first use $g = \text{pi}$, where

$$g_1(z) = \frac{Az}{z+B} \quad (A, B \in \mathbb{R}). \quad (4)$$

The parameters A and B should be chosen so as to enhance the convergence in an optimal fashion. The singularities of $\log f^l$ are delimited by $g_1(-1/a)$ and $g_1(-1/b)$, and, therefore, the radius of convergence of the composite map is the smallest of the absolute values of these two numbers. It follows from (2) that an optimal choice of parameters minimizes

$$\max \left(\left| \frac{g_1(z_0)}{g_1(-1/a)} \right|, \left| \frac{g_1(z_0)}{g_1(-1/b)} \right| \right). \quad (5)$$

It is easily seen from (5) that the optimal B does not depend on z and that it is given by

$$B = \frac{2}{a+b}. \quad (6)$$

The parameter A cancels in formula (5) and can be normalized to 1.

The next simplest example of conformal maps of the type (1) is

$$g_2(z) = \frac{A_1 z}{z+B_1} + \frac{A_2 z}{z+B_2}. \quad (7)$$

Motivated by (3) and in order to ensure the invertibility of g -i we assume

$$A_1 A_2, B_1 B_2 > 0.$$

The (relevant branch of the) function g_2^{-1} is then given by

$$g_2^{-1}(\xi) = \frac{(B_1 + B_2)\xi - (A_1B_2 + A_2B_1) + \sqrt{\Delta}}{2(A_1 + A_2 - \xi)}$$

where

$$\Delta = (B_1 - B_2)^2\xi^2 + 2(B_1 - B_2)(A_1B_2 - A_2B_1)\xi + (A_1B_2 + A_2B_1)^2.$$

Again, the optimal choice of parameters minimizes the quotient

$$\left| \frac{\xi_0}{R} \right|, \quad R = \text{radius of convergence of } f \circ g_2^{-1} \text{ about } \xi = 0.$$

In this case it is not possible to derive a simple formula such as (6) for the parameters A_i and B_i . Here we need to deal not only with the singularities of f but also with those introduced by g_2^{-1} . It is not difficult to check however, that the optimal situation is the one in which the parameters minimize the expression

$$\max \left(\left| \frac{g_2(z_0)}{g_2(-1/\alpha)} \right|, \left| \frac{g_2(z_0)}{g_2(-1/\beta)} \right|, \left| \frac{g_2(z_0)}{r_\Delta} \right| \right), \quad (8)$$

where r_Δ denotes the absolute value of the (complex conjugate) roots of Δ as a function of ξ

$$r_\Delta = \frac{A_2B_1 + A_1B_2}{B_2 - B_1}.$$

As in (5), we can take one of the parameters A_i in (8), say A_1 , to equal 1.

It is reasonable in some cases to take $z_0 = \infty$ in (8) so as to optimize the performance of the approximator in the positive real axis (see section 2.2). With this provision (and taking $A_1 = 1$) the parameters A_2 , B_1 and B_2 must be chosen so as to minimize

$$\max \left(\left| \frac{1 + A_2}{g_2(-1/\alpha)} \right|, \left| \frac{1 + A_2}{g_2(-1/\beta)} \right|, \left| \frac{1 + A_2}{r_\Delta} \right| \right). \quad (9)$$

Geometrical insight can be gained by inspection of the effect of the conformal maps described above on circles in the ξ -plane. In Fig. 1(a) (resp. 1(b)) we have plotted the images C_r (resp. D_r) in the z -plane of the circles $|\xi| = r$ under the transformation $\xi = g_1(z)$ (resp. $\xi = g_2(z)$). We have chosen the singularity region to be the interval $[-2, -1/2]$, i.e. $a = 1/2, b = 2$, which corresponds to the function f in (10) below. From (6) it follows that the parameter B in g_1 is, in this case, equal to 0.8 while a numerical minimization of (9) yields the values $A_2 = 0.560$, $B_1 = 0.692$ and $B_2 = 1.234$ (cf. (12)) for the conformal map g_2 .

Take, for example, the curve $C_{1.25}$ in Fig. 1(a). This circle is the image under the map $\xi = g_1(z)$ of the circle $|\xi| = 1.25$. The region $|\xi| < 1.25$ is mapped onto the exterior of $C_{1.25}$, i.e. onto the connected component containing $z = 0$. Thus, since this region does not intersect the interval $[-2, -1/2]$, we see that, for *all* points z outside $C_{1.25}$, the value of $f(z)$ can be obtained by adding the Taylor series of $f \circ g_1^{-1}$ at $\xi = g_1(z)$. Similar considerations hold for all other curves in Figs. 1(a) and 1(b). The radius of convergence of $f \circ g_1^{-1}$ is $r = 5/3$ while that of $f \circ g_2^{-1}$ is $r = 3$. We see that the enhanced series will in fact converge to $f(z)$ for all z outside the critical curves $C_{5/3}$ and D_3 .

In the following section we illustrate the ideas above with a few low order approximation problems. Higher order approximation will be dealt with in sections 3 and 4.

2.2 Some simple examples

Let us first consider the function

$$f(z) = \sqrt{\frac{1+z/2}{1+2z}} = 1 - \frac{3}{4}z + \frac{39}{32}z^2 - \dots \quad (10)$$

A second order approximation problem for this function is used in [3] to demonstrate some of the outstanding properties of Padé approximants. (The $[L/M]$ -Padé approximant of a function

$$f(z) = \sum_{n=0}^{\infty} c_n z^n$$

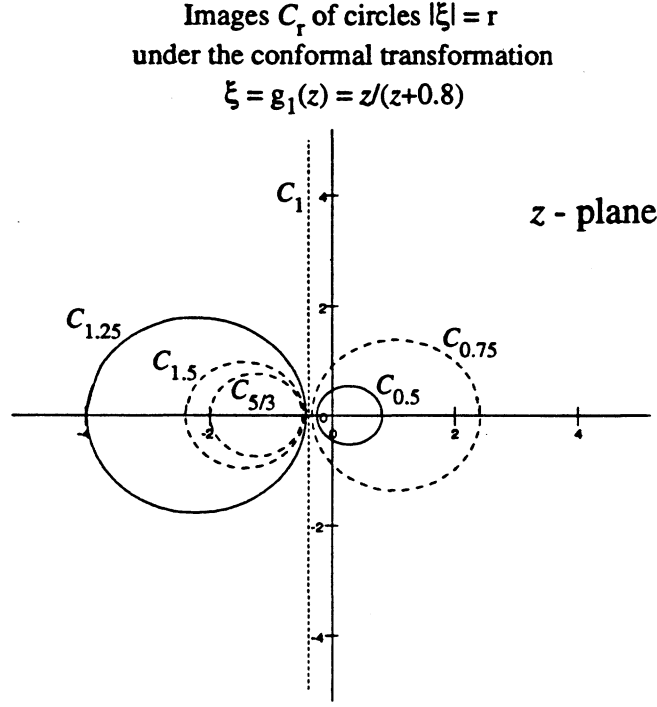


Figure 1(a).

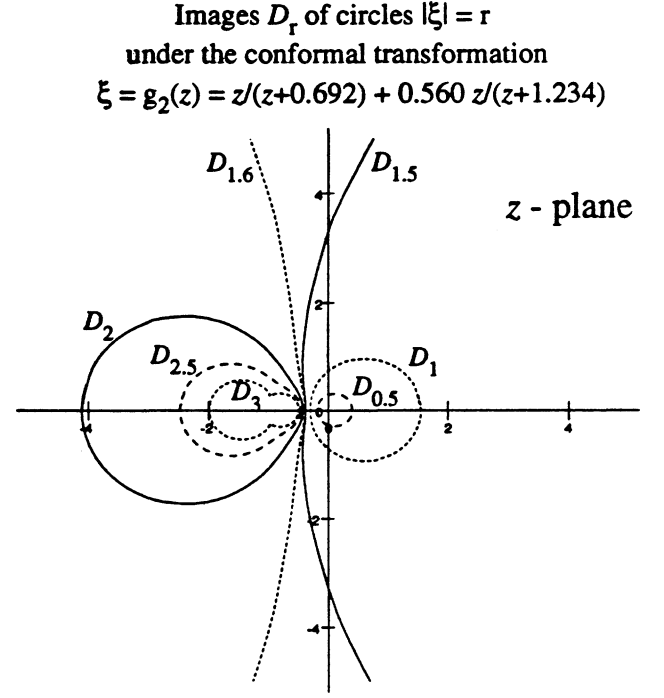


Figure 1(b).

is defined (see [3]) as a rational function

$$[L/M] = \frac{a_0 + a_1 z + \dots + a_L z^L}{1 + b_1 z + \dots + b_M z^M}$$

whose Taylor series agrees with that of f up to order $L + M$. A particular $[L/M]$ approximant may fail to exist but, generically, $[L/M]$ Padé approximants exist and are uniquely determined by L , M and the first $L + M + 1$ coefficients of the Taylor series of f . For convergence studies and numerical calculation of Padé approximants see [3, 5, 8, 11]).

The $[1/1]$ Padé approximant of the function f in (10) is given by

$$[1/1] = \frac{1 + \frac{7}{8}z}{1 + \frac{13}{8}z} \quad (11)$$

Certainly, the information we have used to construct (11) (namely the first three

terms in the Taylor series of f) would permit us to compute the $[2/0]$ and $[0/2]$ approximants also. The choice of the $[1/1]$ approximant may be seen as incorporating certain additional structural information one has about the function f .

Let us now find enhanced series of order 2 for (10). Consider first the conformal map g_1 defined in (4). In this case (6) yields

$$B = 0.8,$$

and taking $A = 1$, we obtain

$$g_1(z) = \frac{z}{z + 0.8}.$$

Therefore, our approximation reads

$$1 - \frac{0.6z}{z + 0.8} + \frac{0.18z^2}{(z + 0.8)^2} = \frac{29z^2 + 56z + 32}{2(5z + 4)^2}.$$

Another enhanced series can be obtained by using the conformal map g_2 in (7). The expression in (9) can be (numerically) minimized, and the optimal parameters turn out to be

$$A_2 = 0.560, \quad B_1 = 0.692, \quad B_2 = 1.234, \quad (12)$$

so that

$$g_2(z) = \frac{z}{z + 0.692} + \frac{0.560z}{z + 1.234}.$$

Our second enhanced series approximation is then given by

$$1 - \frac{0.395z}{z + 0.692} - \frac{0.221z}{z + 1.234} + 0.069 \left(\frac{z}{z + 0.692} + \frac{0.560z}{z + 1.234} \right)^2.$$

In Fig. 2 we show the graph of the function f together with those of its three approximations. The three of them lie close to the function f , with errors at $z = \infty$ of 8%, 16% and 10% for Padé, g_1 -enhanced and g_2 -enhanced, respectively. The Padé approximation is slightly more accurate than the other two; this need not be the case, however, as we illustrate with the following example.

Let

$$f(z) = \sqrt{\frac{z}{(z+2)(z+3)}} + 1.$$

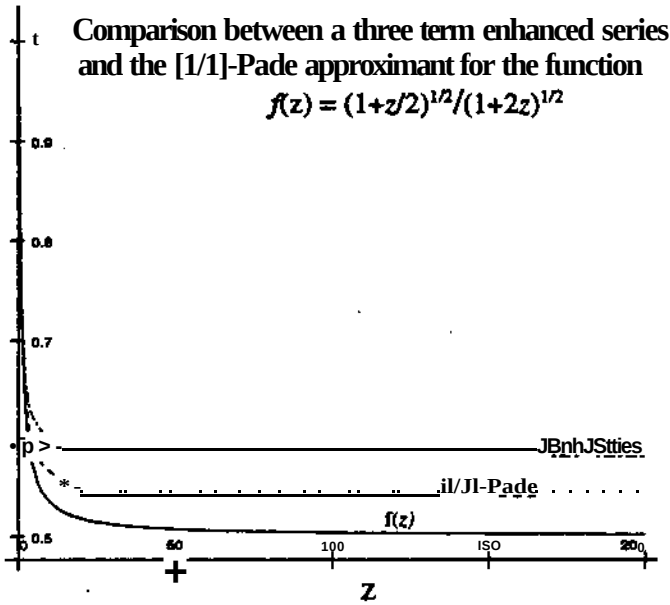


Figure 2(a). The conformal map for the enhanced series is $g_x(z) = z/(z+0.8)$.

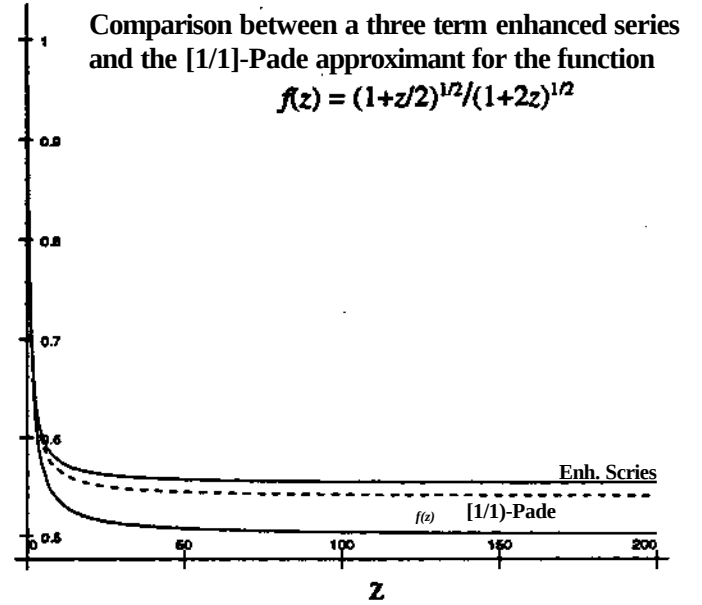


Figure 2(b). The conformal map for the enhanced series is $g_2(z) = z/(z+1.234)$.

The [1/1] Padé approximant to f is given by

$$[1/1] = \frac{1 + \frac{23}{24}z}{1 + \frac{7}{8}z}.$$

To compute the enhanced series corresponding to the map g_1 , we find from (6) that

$$B = 2$$

and we take $A = I$. Thus, the enhanced series is given by

$$1 + \frac{z}{6(z+2)} - \frac{z^2}{8(z+2)^2} = \frac{25z^2 + 104z + 96}{24(z+2)^2}$$

Analogously, it is found that the parameters corresponding to the conformal map g_2 are, in this case, given by

$$A_2 = 0.578, \quad E_1 = 1.732, \quad B_2 = 3.000,$$

so that the enhanced series is

$$1 + \frac{0.108z}{z + 1.732} + \frac{0.063z}{z + 3} - 0.051 \left(\frac{z}{z + 1.732} + \frac{0.578z}{z + 3} \right)^2.$$

Plots of the function and its three approximations are given in Fig. 3. Again we see that the three approximations are fairly accurate, taking into account the fact that they have been obtained by using only the first three coefficients of the Taylor expansion. In this case we do observe that either of the two enhanced series is a better approximation to the function f than the $[1/1]$ Padé approximant (the errors at $z = \infty$ are of 9.5%, 4.2% and 4.5% for Padé, g_1 -enhanced and g_2 -enhanced, respectively).

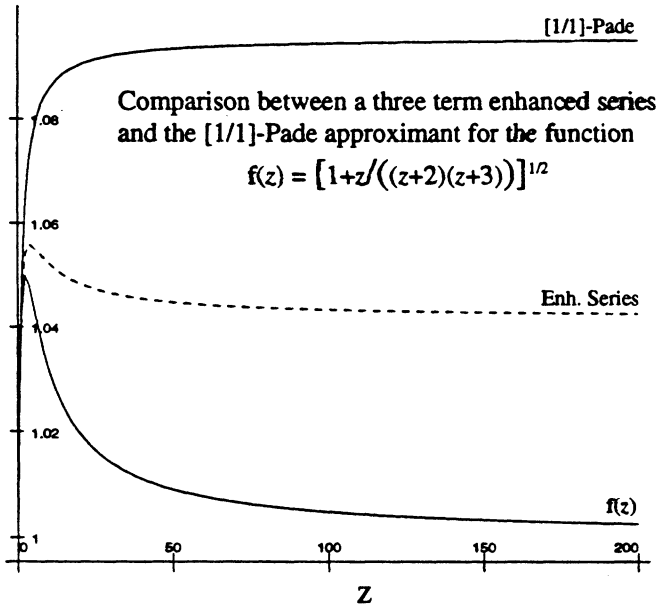


Figure 3(a). The conformal map for the enhanced series is $g_1(z) = z/(z+2)$.

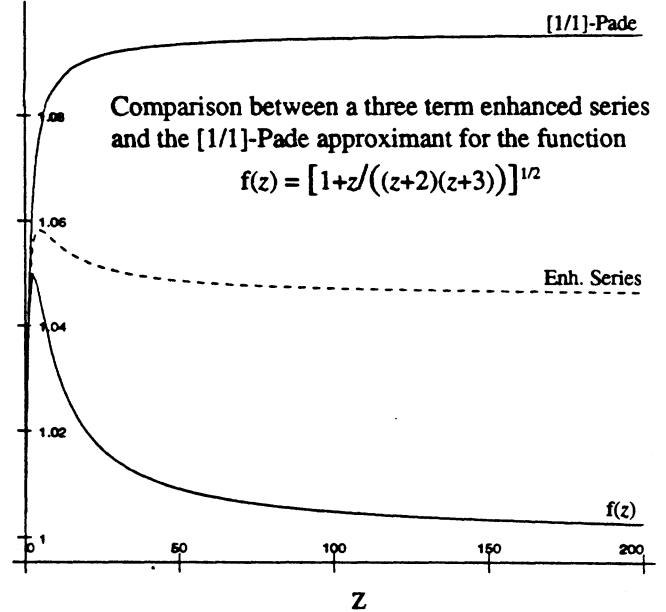


Figure 3(b). The conformal map for the enhanced series is $g_2(z) = z/(z+1.732) + 0.578 z/(z+3)$.

3 High order approximations

It is often the case in applications that a high number of terms in the power series representing the relevant physical quantities are required in order to reach a reasonable approximation (see e.g. [18, 12, 1, 13, 4, 17, 7]). In these cases, errors

in the computed Taylor coefficients play an important role in the approximation procedure. In this section we discuss the effect of these errors in the values of high order enhanced series and its Padé approximants, which we refer to as *enhanced Padé approximants*. To do this we introduce appropriate norms and corresponding condition numbers. In §3.1 we find the condition number for the calculation of the enhanced series via linear operations on the coefficients of the given series. We conclude that this approach leads to ill-conditioned numerics which should be avoided whenever a direct calculation of the coefficients of the enhanced series is possible.

In §3.2 we treat the conditioning of the value problem for the Padé *denominator* of both direct and enhanced series. The conditioning of the value problem for the full Padé approximants, on the other hand, is not well understood. Luke [16] has shown through some numerical experiments, that the relative error of a given $[L/M]$ Padé approximant evaluated at a given value of z is related to the corresponding errors of the numerator and denominator in a very subtle way. Luke's calculations show, and our own experiments confirm, that the relative error in the Padé fraction at a given value of z is always much smaller than the relative error in either the numerator or the denominator. Luke does not study the relative error in the denominator itself, and, indeed, our simple discussion in this regard appears to be the first one in the literature. Our estimation of the conditioning for the denominator problem together with numerous numerical examples such as those of §4 provide strong evidence for the generalized belief that better conditioning in the value problem for the Padé denominator is closely correlated to better conditioning for the value problem of the complete Padé fraction.

3.1 Enhanced series from direct series

As in the previous section, let $f : \Omega \rightarrow \mathbb{C}$ be an analytic function

$$f(z) = \sum_{n=0}^{\infty} c_n z^n, \quad (13)$$

and let g be a conformal map defined in Ω such that $g(0) = 0$. Denoting the Taylor series of g^{-1} by

$$g^{-1}(\xi) = \sum_{m=1}^{\infty} \beta_m \xi^m,$$

we have

$$\begin{aligned} f(\xi) = f(g^{-1}(\xi)) &= \sum_{n=0}^{\infty} c_n (g^{-1}(\xi))^n \\ &= \sum_{n=0}^{\infty} c_n \left(\sum_{m=1}^{\infty} \beta_m \xi^m \right)^n \\ &= c_0 + \sum_{m=1}^{\infty} \gamma_m \xi^m \end{aligned}$$

where γ_n is a linear combination of $c_1, \dots, c_n$ with coefficients depending on $\beta_1, \dots, \beta_n$.

If we write

$$(g^{-1}(\xi))^n = \sum_{m=n}^{\infty} a_{mn} \xi^m,$$

then the truncated power series expansion of order N for $f(\xi)$ (i.e. the enhanced series) takes the form

$$f(\xi) \simeq c_0 + \sum_{n=1}^N c_n \left(\sum_{m=n}^N a_{mn} \xi^m \right) = c_0 + \sum_{m=1}^N \left(\sum_{n=1}^m a_{mn} c_n \right) \xi^m$$

so that the coefficients γ_n of the composition satisfy

$$\begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \vdots \\ \gamma_N \end{bmatrix} = A_N \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{bmatrix} \quad (14)$$

where A_N is the lower triangular $N \times N$ matrix

$$(A_N)_{mn} = a_{mn} \quad n \leq m. \quad (15)$$

The numerical stability of the problem of computing the coefficients γ_n via (14) is governed by the (e.g. l^∞ -) condition number of the matrices A_N in (15), i.e by

$$\kappa(A_N) = \|A_N\|_\infty \|A_N^{-1}\|_\infty. \quad (16)$$

In other words, errors (δc_n) in the coefficients of (13) are amplified in the calculation of the product (14), and result in relative errors of the coefficients of γ_n which can be estimated by

$$\frac{\|(\delta \gamma_n)\|_\infty}{\|(\gamma_n)\|_\infty} \leq \kappa(A_N) \frac{\|(\delta c_n)\|_\infty}{\|(c_n)\|_\infty}.$$

Here, $\|(\alpha_n)\|_\infty$ denotes the l^∞ -norm of the vector (α_n)

$$\|(\alpha_n)\|_\infty = \max_{1 \leq n \leq N} |\alpha_n|.$$

Our main problem, however, is that of calculating the *values* of the enhanced series, and the condition number (16) does not provide a measure of the error in these values. In fact, the natural measure for this error is

$$\sum_{n=1}^N |\delta \gamma_n| |\xi|^n \quad (17)$$

For convenience we shall use a norm closely related to but different from (17), namely

$$\max_{1 \leq n \leq N} |\delta \gamma_n| |\xi|^n.$$

These two norms are related by

$$\max_{1 \leq n \leq N} |\delta \gamma_n| |\xi|^n \leq \sum_{n=1}^N |\delta \gamma_n| |\xi|^n \leq N \max_{1 \leq n \leq N} |\delta \gamma_n| |\xi|^n. \quad (18)$$

As we shall see below, the condition numbers for the value problem grow exponentially with N so that the constant N in (18) is not significant. Thus, a norm for a vector $\gamma = [\gamma_1, \dots, \gamma_N]$ in the range of the matrix A that is appropriate to deal with the value problem is

$$\|\gamma\|_\xi \equiv \max_{1 \leq n \leq N} |\gamma_n| |\xi|^n, \quad (19)$$

and we must consider the corresponding matrix norms

$$\|A_N\|_\xi \equiv \sup_{\|\alpha\|_\infty \leq 1} \frac{\|A_N \alpha\|_\xi}{\|\alpha\|_\infty} = \max_{1 \leq m \leq N} \left(\sum_{n=1}^N |a_{mn}| \right) |\xi|^m$$

and

$$\|A_N^{-1}\|_\xi \equiv \sup_{\|\gamma\|_\xi \leq 1} \frac{\|A_N^{-1} \gamma\|_\infty}{\|\gamma\|_\xi} = \max_{1 \leq m \leq N} \left(\sum_{n=1}^N |a_{mn}^{-1}| |\xi|^{-n} \right).$$

With these notations, we see that relative errors in the coefficients of (13) are amplified in the calculation of the values of the truncated series of $f \circ g^{-1}$ by a factor which can be roughly estimated by

$$\kappa_\xi(A_N) = \|A_N\|_\xi \|A_N^{-1}\|_\xi.$$

Notice that this condition number is unchanged if the problem is transformed via

$$\xi \rightarrow \lambda \xi \quad (A \in \mathbb{R}),$$

as expected from dimensional considerations. This is not true, however, of the condition number (16) for the coefficient problem, that is, the number $K(A\#)$ does change if the variable f is transformed homothetically.

Let us consider the example of the conformal map g in (4). In this case we can compute the conditions numbers $K(A\#)$ and $K(A_X)$ explicitly. Indeed, it is not hard to check that the transformation matrices A_N^I and $(A\#)^I$ are given by

$$(A_N^I)_{mn} = \frac{1}{N} \binom{m-1}{n-1} \quad (n \leq m), \quad (20)$$

and

$$(A_N^1)_{mn}^{-1} = (-1)^{n-m} \frac{A^n}{B^m} \binom{m-1}{n-1} \quad (n \leq m). \quad (21)$$

The condition numbers can be easily found from (20) and (21). For $\xi = \frac{Az}{z+B}$ we obtain

$$\kappa_\xi(A_N^1) = \max_{1 \leq m \leq N} \left((|B| + 1)^{m-1} \frac{|z|^{m-1}}{|z+B|^{m-1}} \right) \max_{1 \leq m \leq N} \left(\frac{1}{|B|^{m-1}} \left(1 + \frac{|z+B|}{|z|} \right)^{m-1} \right) \quad (22)$$

and

$$\kappa(A_N^1) = \max_{1 \leq m \leq N} \left(\frac{(1+B)^{m-1}}{A^{m-1}} \right) \max_{1 \leq m \leq N} \left(\frac{(1+A)^{m-1}}{B^{m-1}} \right).$$

The condition number κ measures the amplification of relative errors in the problem of determining the coefficients of the enhanced series from those of the direct series, while κ_ξ is the corresponding amplification factor for the *value* to be obtained for $f(z)$ via the enhanced series. These condition numbers depend on the constants that determine the conformal map g_1 . The constant B in (4) is to be chosen, as we pointed out in section 2.1, in such a way as to obtain optimal convergence rates. This determines the condition number $\kappa_\xi(A_N^1)$ which, as expected from dimensional considerations, is independent of the constant A . The condition number $\kappa(A_N^1)$ of the coefficient problem, however, does depend on A . It is easily seen that, for given B , a choice of A that minimizes the condition number κ is

$$A = B + 1; \quad (23)$$

with the parameters as in (6), (23), the condition number becomes

$$\kappa(A_N^1) = \frac{(2+B)^{N-1}}{B^{N-1}}.$$

This last remark is, however, not significant in the problem of calculating the values of the function f by summing its enhanced power series.

Having calculated the condition number of the value problem, we note from (22) that κ_ξ grows exponentially with N . Therefore, calculation of the coefficients of an enhanced series via (14) leads to approximations with relative errors that may be much larger than those present in the coefficients of the Taylor series of f . It is reasonable to expect, however, that, in a given problem, a direct and accurate calculation of the coefficients of the enhanced series is possible. If this is the case, as it is in the examples of section 4, the direct calculation is to be preferred. Nevertheless, enhanced series obtained by the methods of this section can still yield valuable results; see [7].

3.2 Conditioning of the denominator value problem of Padé and enhanced Padé approximants

The coefficients of the denominator of the $[L/M]$ Padé approximant of the function

$$f(z) = \sum_{n=0}^{\infty} c_n z^n$$

are given by the solution of the linear system of equations

$$\begin{bmatrix} c_{L-M+1} & c_{L-M+2} & \cdots & c_L \\ c_{L-M+2} & c_{L-M+3} & \cdots & c_{L+1} \\ \vdots & \vdots & \ddots & \vdots \\ c_L & c_{L+1} & \cdots & c_{L+M-1} \end{bmatrix} \begin{bmatrix} b_M \\ b_{M-1} \\ \vdots \\ b_1 \end{bmatrix} = - \begin{bmatrix} c_{L+1} \\ c_{L+2} \\ \vdots \\ c_{L+M} \end{bmatrix}. \quad (24)$$

To gain insight on the effect that a rearrangement of the singularities of the function f can have on the conditioning of the denominator problem, assume that the singularity of f that lies closest to the origin is a simple pole z_0 with $|z_0| = r$. Then, for large n we have $|c_n| = \text{const. } r^{-n} + o(r^{-n})$, and therefore, for large values of M , the dominating contribution in the last rows of (24) is the one related to the closest singularity z_0 . Thus, these rows are nearly linearly dependent which explains the ill conditioning of the matrix for large values of M . A conformal change of variables which equilibrates the influence of the closest singularities is therefore expected to

have a beneficial effect on the conditioning of the denominator problem. In this section we provide a quantitative measure of the improvement under the assumption that f is a Stieltjes function with a positive radius of convergence.

While theoretical studies of the conditioning of the value problem for Padé approximants are not available at present, the generalized belief is that the conditioning of the denominator problem determines the conditioning of the whole fraction (see [3]). It must not be understood, however, that the amplification of errors observed in the values of the Padé denominator is to be expected in the whole fraction. Indeed, and most remarkably, the conditioning of the Padé fraction is observed to be very substantially better than that of the Padé denominator. The numerical experiments of Luke [16] shed some light on this astonishing property of Padé approximants, which remains, otherwise, not understood. At any rate, our present study of the conditioning of the Padé denominator in both the direct and enhanced variables (which includes the introduction of appropriate condition numbers) together with the numerical experiments of §4 do demonstrate that there is a close correlation between the conditioning of the denominator problem and that of the whole fraction; or, in other words, that improvement in the denominator conditioning leads to improvement in the conditioning of the fraction, even though a quantitative measure of the former is not necessarily a good quantitative measure of the latter.

A typical example of a Padé problem which is very ill conditioned is that of the function

$$\log(1+z)/z.$$

The matrix corresponding to the denominator problem for the $[L/M]$ Padé approximant of this function is closely related to (and as poorly conditioned as) the Hilbert segment

$$\begin{bmatrix} \frac{1}{L-M+2} & \frac{1}{L-M+3} & \cdots & \frac{1}{L+1} \\ \frac{1}{L-M+3} & \frac{1}{L-M+4} & \cdots & \frac{1}{L+2} \\ \vdots & \vdots & & \vdots \\ \frac{1}{L+1} & \frac{1}{L+2} & \cdots & \frac{1}{L+M} \end{bmatrix} \quad (25)$$

which is a classical example of ill-conditioning in numerical linear algebra [10]. Tay-

lor [20] estimated the condition number of Gram matrices and, in particular, he showed that for the $(n + 1) \times (n + 1)$ Hilbert matrix

$$H^n = \begin{bmatrix} 1 & \frac{1}{2} & \cdots & \frac{1}{n+1} \\ \frac{1}{2} & \frac{1}{3} & \cdots & \frac{1}{n+2} \\ \vdots & \vdots & & \vdots \\ \frac{1}{n+1} & \frac{1}{n+2} & \cdots & \frac{1}{2n+1} \end{bmatrix} \quad (26)$$

the estimate

$$K_2(H^n) \geq 16^n / 7n$$

holds (κ_2 denotes the Z^2 -condition number). In this particular case one can in fact find an explicit formula for the inverse of the matrix (see e.g. [10]):

$$(H^n)^{-1}_{ij} = \frac{(-1)^{i+j} (n+i)! (n+j)!}{(n+1-j)! (n+1-i)! (j-1)!^2 (i-1)!^2 (i+j-1)!}; \quad (27)$$

replacing i by An and j by Xn in (27) and maximizing the expressions

$$\frac{(n+i)!}{(n-i)! i!^2} \Big|_{i=\lambda n} \quad \text{and} \quad \frac{(n+j)!}{(n-j)! j!^2} \Big|_{j=\lambda n}$$

for $0 < A < 1$ (which results in taking $A = 1/\sqrt{2}$) we find that the conditioning of this *coefficient* problem is even poorer:

$$\kappa(H^n) \text{ is } O(5.83^{2n}) = O(34^n).$$

We begin our discussion of the conditioning of the denominator *value* problem for Stieltjes functions with the following lemma, which follows readily from a change of variables.

Lemma 1 *Let*

$$f(z) = \int_a^b \frac{4\gamma(u)du}{1+zu}. \quad (28)$$

Then, for any A and B we have

$$f(z) = \frac{A}{z+B} \int_{\frac{Ba-1}{A}}^{\frac{Bb-1}{A}} \frac{\phi((Au+1)/B)du}{1+\xi u},$$

where

$$\xi = \frac{Az}{z+B}.$$

In other words, calling

$$e(\xi) = \int_{\frac{Ba-1}{A}}^{\frac{Bb-1}{A}} \frac{\phi((Au+1)/B)du}{1+\xi u}, \quad (29)$$

we have

$$zf(z) = \xi e(\xi) \quad \square$$

We continue with two lemmas about certain quadratic forms for the vector $x = (x_0, x_1, \dots, x_n) \in \mathbb{R}^{n+1}$. These quadratic forms are closely related to the Padé approximants of Stieltjes functions, and they are given by integrals such as

$$\begin{aligned} x^t A_\phi^{n,m} x &= \int_a^b (x_0 + x_1 u + \dots + x_n u^n)^2 u^m \phi(u) du \\ &= \sum_{i=0}^n \sum_{j=0}^n (-1)^{i+j+m} c_{i+j+m} x_i x_j, \end{aligned}$$

where a and b are real numbers, $a < b$ and c_k are the Taylor coefficients of f in (28), i.e.

$$c_k = (-1)^k \int_a^b u^k \phi(u) du.$$

Also, we shall denote

$$A^{n,m} = A_\phi^{n,m} \quad \text{if } \phi(u) \equiv 1.$$

We see that the matrices $A^{n,m}$ are positive definite provided either $0 < a < b$ or m is even; in the latter case we shall write

$$E^{n,l} = A^{n,m}, \quad \text{if } m = 2l. \quad (30)$$

Clearly, then

$$x^t E^{n,l} x = \int_a^b (x_0 u^l + x_1 u^{l+1} + \cdots + x_n u^{l+n})^2 du.$$

Lemma 2 *Let $m = 2l$. Then, we have*

$$x^t E^{n,l} x = (b-a) y^t H^{n+l} y$$

where y is related to x via

$$y = D T_a \mathcal{I} x. \quad (31)$$

Here, $D = D_{(b-a)}$ is the $(n+l+1) \times (n+l+1)$ diagonal matrix

$$D_{ii} = (b-a)^{i-1} \quad (1 \leq i \leq n+l+1), \quad (32)$$

T is the $(n+l+1) \times (n+l+1)$ matrix

$$(T_a)_{ij} = \binom{j-1}{i-1} a^{j-i} \quad (1 \leq i, j \leq n+l+1), \quad (33)$$

and $\mathcal{I}$ is the matrix of the inclusion of $\mathbb{R}^{n+1}$ into $\mathbb{R}^{l+n+1}$

$$\mathcal{I} x = (0, \dots, 0, x_0, \dots, x_n) \quad (34)$$

Proof: By a change of variables, we obtain

$$x^t E^{n,l} x = \int_0^{b-a} (x_0(v+a)^l + x_1(v+a)^{l+1} + \cdots + x_n(v+a)^{l+n})^2 dv =$$

$$\int_0^{b-a} (\bar{x}_0 + \bar{x}_1 v + \cdots + \bar{x}_{l+n} v^{l+n})^2 dv,$$

where $\bar{x} = (\bar{x}_0, \dots, \bar{x}_{l+n})$ is given by

$$\bar{x} = T_a \mathcal{I} x$$

with the matrices T_a and $\mathcal{I}$ defined by (33) and (34) respectively. A further change of variables yields

$$x^t E^{n,l} x = \int_0^1 (y_0 + y_1 u + \cdots + y_{l+n} u^{l+n})^2 (b-a) du = (b-a) y^t H^{n+l} y,$$

with $y = (y_0, \dots, y_{l+n}) = D \bar{x}$, and D given by (32) $\square$

Lemma 3 Assume the function ϕ is positive and bounded

$$0 < C_1 < \phi < C_2 < \infty. \quad (35)$$

Then, the following inequalities hold :

- $a > 0$ and m an arbitrary non-negative integer: then

$$K_1 y^t H^n y \leq x^t A_\phi^{n,m} x \leq K_2 y^t H^n y$$

for certain constants K_1 and K_2 . Here, x and y are related through the equation

$$y = D_{b-a} T_a x$$

where D_{b-a} and T_a are the $(n+1) \times (n+1)$ matrices whose entries are given by equations (32) and (33) (with $l = 0$) respectively.

- $a \in \mathbb{R}$ arbitrary and $m = 2l$ non-negative even integer: then

$$K_1 y^t H^{n+l} y \leq x^t A_\phi^{n,m} x \leq K_2 y^t H^{n+l} y.$$

Here, x and y are related through equation (31).

Proof: Follows easily from the previous lemma $\square$

To treat the value problem for the Padé denominator, we observe that its coefficients satisfy the following system of equations

$$\begin{bmatrix} c_{L-M+1} z^{L-M+1} & c_{L-M+2} z^{L-M+2} & \dots & c_L z^L \\ c_{L-M+2} z^{L-M+2} & c_{L-M+3} z^{L-M+3} & \dots & c_{L+1} z^{L+1} \\ \vdots & \vdots & \ddots & \vdots \\ c_L z^L & c_{L+1} z^{L+1} & \dots & c_{L+M-1} z^{L+M-1} \end{bmatrix} \begin{bmatrix} b_M z^M \\ b_{M-1} z^{M-1} \\ \vdots \\ b_1 z \end{bmatrix} = - \begin{bmatrix} c_{L+1} z^{L+1} \\ c_{L+2} z^{L+2} \\ \vdots \\ c_{L+M} z^{L+M} \end{bmatrix}, \quad (36)$$

as it follows from equations (24).

The condition number $\kappa_v(z)$ of the matrix

$$\begin{bmatrix} c_{L-M+1} z^{L-M+1} & c_{L-M+2} z^{L-M+2} & \dots & c_L z^L \\ c_{L-M+2} z^{L-M+2} & c_{L-M+3} z^{L-M+3} & \dots & c_{L+1} z^{L+1} \\ \vdots & \vdots & \ddots & \vdots \\ c_L z^L & c_{L+1} z^{L+1} & \dots & c_{L+M-1} z^{L+M-1} \end{bmatrix} \quad (37)$$

permits us to bound the error

$$\epsilon_{b,z} = \frac{\|\delta b\|_z}{\|b\|_z} \quad (38)$$

by the error

$$\epsilon_{e,z} = \frac{\|\llbracket c \rrbracket_z\|_z}{\|\llbracket c \rrbracket_z\|_z}, \quad (39)$$

(see (19)) i.e., roughly

$$\epsilon_{e,z}^* \leq K_v(z) \epsilon_{c,z}.$$

The estimation of the condition number for the value problem in Padé approximation is now a simple matter, which we present in the following theorem.

Theorem 1 *Let f and e be defined as in lemma 1. Let*

$$m = L-(M-l) = 2l \quad \text{and} \quad \mathbf{n} = M-l,$$

and define $\tilde{D}_z \in \mathbb{R}^{n+1 \times n+1}$ by

$$(\tilde{D}_z)_{ij} = z^{i+j-1}.$$

Then the condition numbers $K_v(Z)$ and $K_v(\xi)$ for the (denominator) value problem of the $[L/M]$ Padé approximants for the functions $f(z)$ and $e(\xi)$ satisfy

$$K_v(Z) \simeq K((D_{b-a} T_a I D_z \tilde{y} H^{n+l} (D_{b-a} T_a I D_{2j})) \quad (40)$$

and

$$\kappa_v(\xi) \simeq K((D_{72} r_{71} I^\wedge)' f^{n+l} (D_{72} T_{71} I^\wedge)) \quad (41)$$

where

$$\gamma_1 = \frac{Ba-l}{A} \quad \text{and} \quad \gamma_2 = \frac{B(b-a)}{A}.$$

If $a > 0$, then the estimate (40) sharpens to

$$K_v(Z) \simeq K((D_{b-a} T_a \tilde{D}_z)' H^n (D_{b-a} T_a \tilde{D}_z)).$$

Proof: We shall only show how to obtain (40) since, using lemma 1, (41) can be established in a similar way. Let S and $S(z)$ denote the matrices in (24) and (37) respectively, and let J be the $(n+1) \times (n+1)$ diagonal matrix with entries $J_{ii} = (-1)^{i+i-1}$. Since

$$\kappa(S(z)) = \kappa(JS(z)J)$$

it suffices to estimate the condition number of the matrix $R = JS(z)J$. Now, from the equation

$$R_{(i+1)(j+1)} = (JS(z)J)_{(i+1)(j+1)} = (-1)^{i+j+m} c_{i+j+m} z^{i+j+m} \quad (0 \leq i, j \leq n)$$

and (30) we deduce that

$$R = \tilde{D}_z A_\phi^{n,m} \tilde{D}_z.$$

Since for a positive definite and symmetric matrix F we have

$$\|F\| = \max_{\|x\|=1} x^t F x \quad \text{and} \quad \|F^{-1}\| = \frac{1}{\min_{\|x\|=1} x^t F x},$$

we conclude, from lemma 3, that

$$\kappa(R) = \kappa(\tilde{D}_z A_\phi^{n,m} \tilde{D}_z) \simeq \kappa((D_{b-a} T_a \mathcal{I} \tilde{D}_z)^t H^{n+l} (D_{b-a} T_a \mathcal{I} \tilde{D}_z)) \quad \square$$

The right hand sides of (40) and (41) can be evaluated using the equation (27) for the inverse of the Hilbert matrix and the fact that $T_s^{-1} = T_{-s}$. In Fig. 4 we show the dependence of the right hand side of (41) on the parameter B in (4) in the case $m = 0$, $a = 0$ and $b = 1$ (which yields, in particular, numbers that apply to the function $f(z) = \log(1+z)/z$). In the figure A was normalized to 1 so that

$$\xi = \frac{z}{z+B}$$

and we have plotted

$$(\kappa_{v,25}/\kappa_{v,20})^{1/5},$$

for $z = 20$.

In Fig. 5 we plot the errors in the [20/21] enhanced Padé approximants at $z = 20$ for $f(z) = \log(1+z)/z$ as a function of B . We observe that, as claimed at the

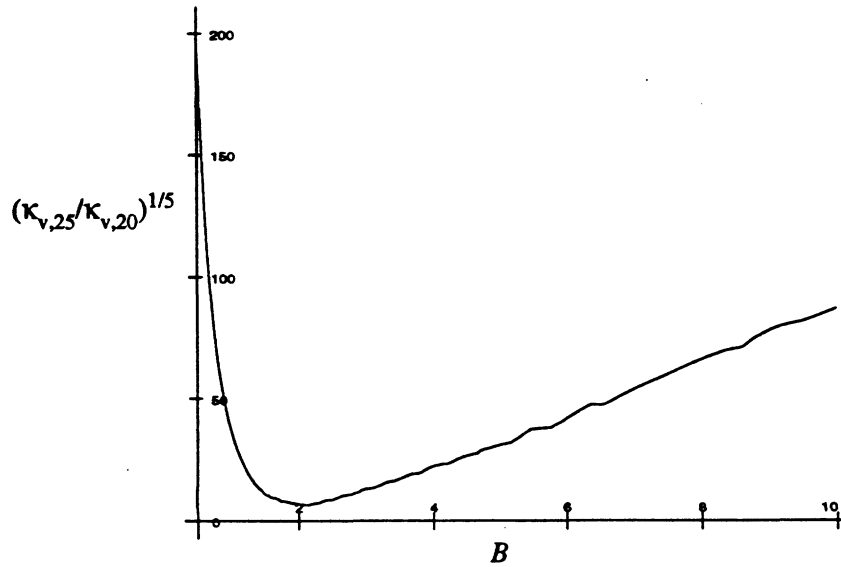


Figure 4. Condition number as a function of B ,
 $\xi=z/(z+B)$: $a=0$, $b=1$, $m=0$, $z=20$.

beginning of this section, the condition number in figure 4 as well as the errors in figure 5 are smallest for the value of B in (6).

Finally, in Fig. 6 we present a plot of the condition numbers for f ("z-variable") and e ("ξ-variable") (cf. (29)) again in the case $m = 0$, $a = 0$ and $b = 1$. Here the parameters for the conformal map are $A = 1$ and $B = 2$, and we see that the conditioning is in fact improved by the change of variables.

4 Examples

In this section we apply the methods and ideas presented in this paper to a number of elementary analytic functions. These functions have been chosen so as to illustrate the quality of the approximations that can be obtained –by means of a simple change of variables– in problems in which classical approximants have had limited success. As we have said, the key to the most successful approximations is an accurate calculation of the coefficients of the enhanced series. We noted in section 3.1 that calculation of these coefficients by direct composition of power series produces enhanced coefficients of poor quality. In most of the examples that follow, we

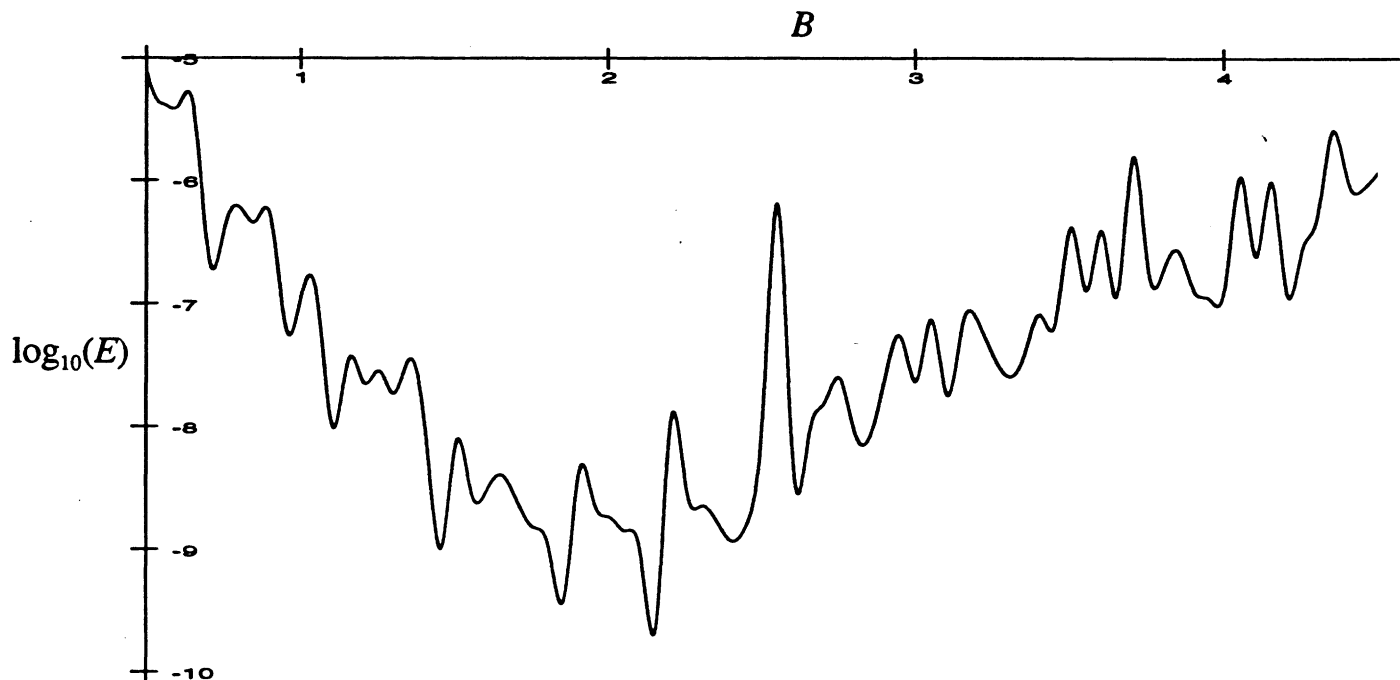


Figure 5. Error $E = |\log(1+z)/z - [n/n+1]_{\text{Enh. Padé}}|$ as a function of B ($\xi = z/(z+B)$; $z=20$, $n=20$).

will therefore obtain the enhanced coefficients by alternative means. Because of the simplicity of the elementary functions used below, such accurate calculations do not represent a challenge, and will be described in each case. In more complex applications, an accurate calculation of the enhanced coefficients may not be a simple matter and must be regarded as an integral part of the problem. These questions will, at any rate, be left for future work.

From numerous numerical experiments, among which the ones in this section were chosen, a clear picture emerges: diagonal or close to diagonal enhanced Padé fractions are probably never worse and can be very substantially better than classical Padé approximants or truncated enhanced series. The degree of improvement of the enhanced Padé method over regular Padé approximants is most notorious in cases of poorly conditioned Padé problems. Enhanced Padé fractions with denominators of low degree can be as accurate or, if the number of coefficients is large enough, slightly more accurate than enhanced diagonal Padé fractions. If a large

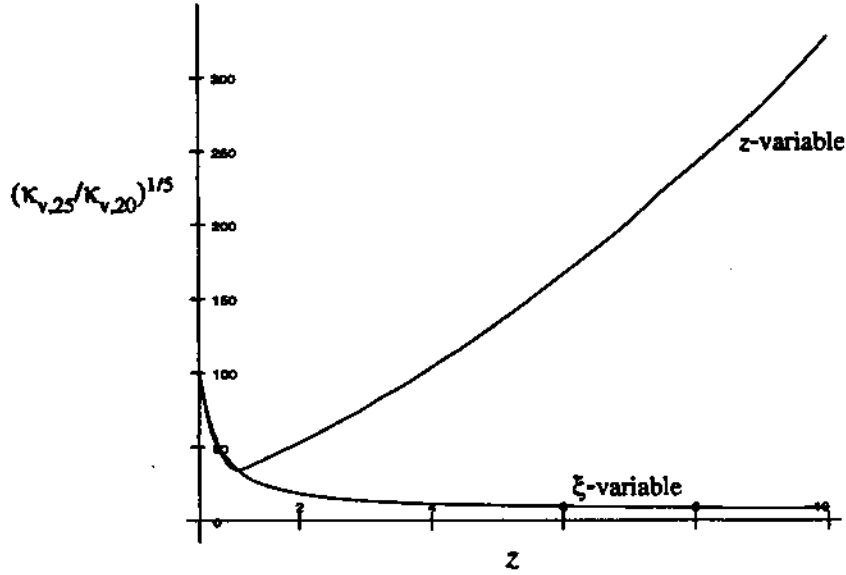


Figure 6. Condition numbers in the ξ and z variables: $a=0$, $b=1$, $m=0$.

number of coefficients are available, this option may be attractive since it reduces the ill-conditioning of the problem and, at the same time, it results in a lower computational cost. Summation of the truncated enhanced series, on the other hand, is an alternative to other approximants in low order problems (see section 2.2), but any of the other proposed methods performs better in problems of higher order.

The computations that follow have been performed in Fortran, and double precision arithmetic has been used in all cases. Padé approximants have been calculated by means of the approach recommended in [11, 3], that is, via solution of the denominator equations by Gaussian elimination with partial pivoting and iterative refinement [10]. Also, for simplicity, attention is restricted to conformal maps of the type (4). The accuracy of the enhanced approximants is independent of the parameter A in (4), and we have therefore taken $A = 1$. Other conformal maps can, of course, be useful in these and other circumstances.

Our first example is a classical one in approximation theory.

- $f(z) = \log(1 + z)$

In table 1 we show the values of the $[N/N]$ Padé and Enhanced Padé approximants for the function $f(z) = \log(1 + z)$. Since the singularities of $\log(1 + z)$ lie

on the interval $[-\infty, -1]$, we see from (6) that the optimal constant B is $B = 2$. The optimality of $B = 2$ is numerically illustrated in Fig. 7 where we have plotted the decimal logarithm $\log_{10}(E)$ of the error E in the computation of enhanced approximants as a function of the parameter B .

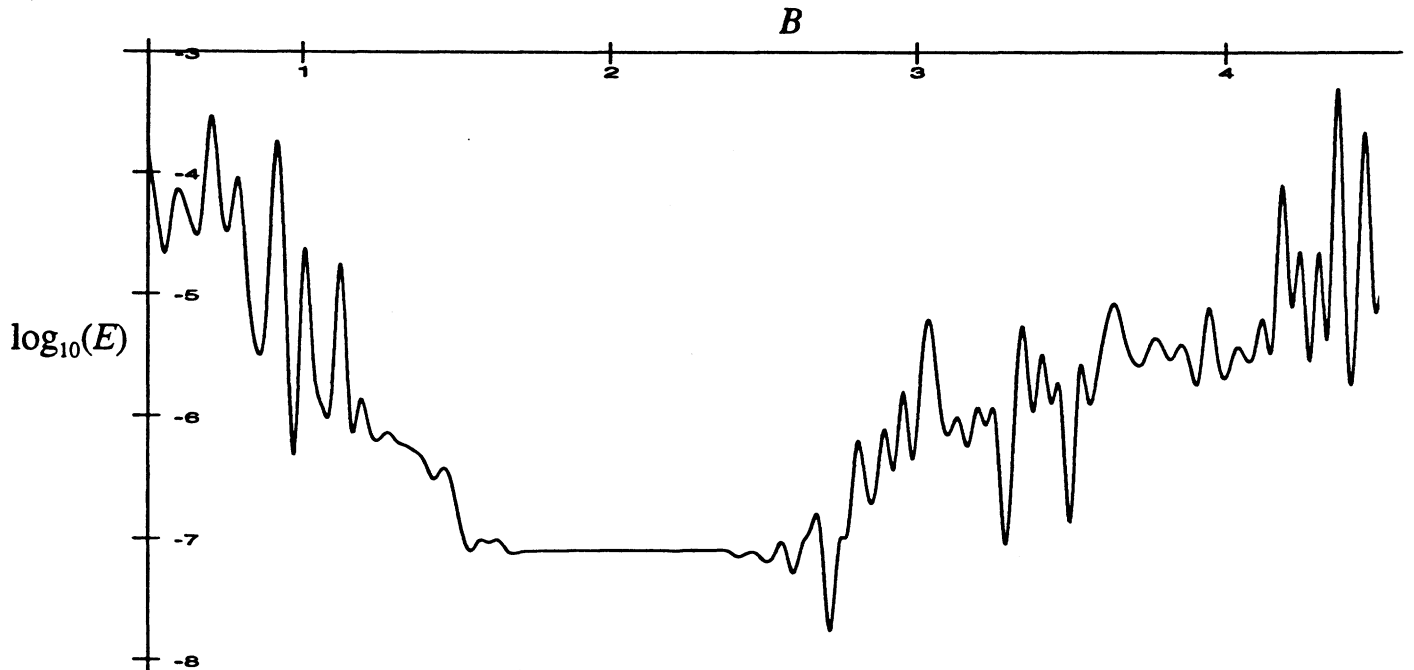


Figure 7. Error $E = |\log(1+z) - [n/n]_{\text{Enh. Padel}}|$ as a function of B ($\xi = z/(z+B)$; $z=20$, $n=20$).

Our last technical point here relates to the calculation of the coefficients of the enhanced series. Because the composite function $f \circ g_1^{-1}$ is given by

$$f \circ g_1^{-1} = \log\left(1 + \frac{2\xi}{1-\xi}\right) = \log(1+\xi) - \log(1-\xi)$$

the enhanced series can simply be obtained as the difference of the series of $\log(1+\xi)$ and $\log(1-\xi)$. A calculation of the enhanced coefficients by composition of the series of f and g_1 results in enhanced approximants of comparable or worse quality than the corresponding Padé fractions.

Table 1: $[\frac{N}{2}/\frac{N}{2}]$ approximants for $\log(1+z)$

N	z	$\log(1+z)$	Padé	Enh. Padé
20	20	3.044522437723	3.043989111079	3.043988784141
40			3.044612164211	3.044522360574
60			3.044477040660	3.044522437596
80			3.044175772366	3.044522437727
100			3.044463021924	3.044522437722
120			3.044489520809	3.044522437724
140			3.044496462919	3.044522437723
160			3.044619592662	3.044522437723
180			3.044362344599	3.044522437723
20	200	5.30330	5.03582	5.03577
40			5.32614	5.28588
60			5.17831	5.30093
80			5.08690	5.30276
100			5.16939	5.30305
120			5.18899	5.30324
140			5.19792	5.30328
160			5.70660	5.30329
180			5.13885	5.30330

Table 1 shows that, as noted in the introduction, close to diagonal enhanced Padé approximants produce up to 13 correct digits of $\log(21)$ while ordinary Padé fractions do not produce more than the first four digits. It is very remarkable, in any case, that the Padé approximation is so stable, and that it produces these four digits for N up to at least $N = 180$, in spite of the tremendous ill-conditioning of the denominator problem. A scaled version of this remark applies also to enhanced approximants. Also, table 1 shows the values of both approximants at $z = 200$; again an improvement is observed.

Another point of interest here relates to the fact that, for approximants with denominator and numerator of the same degree, *in exact arithmetic*, and for the conformal map (4) which is being used, the Padé and enhanced Padé calculations coincide. This is a well known and simple fact, sometimes called the theorem of Baker, Gammel and Wills [2], see also Edrei [9]. We conclude that the improvement in the approximation is solely due to a better conditioning for the value problem of

enhanced approximants. Indeed, Padé approximants for the function $\log(1+z)$ can be computed exactly (see e.g [14, 15]). One easy approach to doing this is to use the algorithm of Cabay and Choi [8] which has been implemented in the symbolic manipulator Maple. Because the Taylor coefficients of $\log(1+z)$ are quotients of small integers, Maple is able to produce (exact) high order approximants within a few seconds. This experiment reveals a residual ill-conditioning in enhanced Padé approximation which leads for example, when $N = 100$, to an agreement in the first 12 and 4 decimal places with the true approximants at $z = 20$ and $z = 200$, respectively. It should be mentioned, however, that if the coefficients of the series are first evaluated to floating point, the Maple computation of the approximants becomes impracticable due to the heavy computational cost of the exact arithmetic that is required in Cabay and Choi's algorithm.

- $f(z) = \sqrt{1 + 11z + 10z^2} = \sqrt{(1+z)(1+10z)}$

In table 2 we show some values of the $[\frac{N}{2} + 1/\frac{N}{2}]$ Padé and Enhanced Padé approximants. The particular choice of the degrees of numerator and denominator reflects the fact that f grows linearly at $z = \infty$. Other choices will not affect the enhanced approximants, since $z = \infty$ corresponds to the finite value $\xi = -0.2$, but they will substantially deteriorate the direct Padé approximants. With these choices of approximants, we observe a qualitative picture that is similar to those of the previous examples. In this case the set of singularities of the function consists of the interval $[-1, -1/10]$ and $z = \infty$, and therefore we must choose $B = 0.2$. The composite map $f \circ g_1^{-1}$ equals

$$f \circ g_1^{-1}(\xi) = \sqrt{(1 - 0.8\xi)(1 + \xi)}$$

Accurate values for the enhanced coefficients were obtained by multiplication of the series of the functions

$$f_1(\xi) = \sqrt{1 - 0.8\xi} \quad \text{and} \quad f_2(\xi) = \sqrt{1 + \xi}.$$

Table 2: $[\frac{N}{2} + 1/\frac{N}{2}]$ approximants for $\sqrt{(1+z)(1+10z)}$

N	z	$\sqrt{1+11z+10z^2}$	Padé	Enh. Padé
20	0.5	3.000000000000000	3.000000000191161	2.999999999840064
40			3.000000000054656	3.000000000000012
60			3.000000000082875	3.000000000000000
80			3.000000000091835	3.000000000000000
100			3.000000000035938	3.000000000000000
20	2.0	7.937253933193772	7.937254332064001	7.937252500684555
40			7.937254058190112	7.937253933190430
60			7.937254061840008	7.937253933193773
80			7.937254081724105	7.937253933193778
100			7.937254002610010	7.937253933193769
20	20.0	64.969223483123145	64.969274407050378	64.967419717272691
40			64.969241195626026	64.969223451000317
60			64.969240709896781	64.969223483029751
80			64.969242844255120	64.969223483120771
100			64.969233358919439	64.969223483123088
20	200.0	634.193188232103239	634.193864933881173	633.954302438057653
40			634.193426947070634	634.193182915836246
60			634.193419429349660	634.193188213653002
80			634.193447207852955	634.193188231637009
100			634.193321691795518	634.193188232415196

- $f(z) = \sqrt{\frac{1+z/2}{1+2z}}$

We include this function which, as mentioned in section 2.2, was used in [3] to illustrate some properties of the Padé approximants. The singularities here lie in the interval $[-2, -1/2]$, and, consequently, we set $B = 0.8$. In table 3 we show some values of the $[\frac{N}{2}/\frac{N}{2}]$ Padé and enhanced Padé approximants.

Table 3: $[f/f]$ approximants for $\sqrt{\frac{1+z/2}{1+2z}}$

N	z	$\sqrt{\frac{1+z/2}{1+2z}}$	Padé	Enh. Padé
20	1.0	0.707106781186547	0.707106781186552	0.707106781186548
60			0.707106781186522	0.707106781186547
100			0.707106781186551	0.707106781186547
20	2.0	0.632455532033676	0.632455532034468	0.632455532033708
60			0.632455532034382	0.632455532033676
100			0.632455532033877	0.632455532033676
20	20.0	0.517969770282812	0.517969770718025	0.517969770318570
60			0.517969770369511	0.517969770282812
100			0.517969770352077	0.517969770282812
20	200.0	0.501866839101296	0.501866840057933	0.501866839187716
60			0.501866839282608	0.501866839101296
100			0.501866839251020	0.501866839101294
20	2000.0	0.500187418011205	0.500187419048587	0.500187418105841
60			0.500187418207021	0.500187418011204
100			0.500187418173372	0.500187418011203

- Enhanced series and low degree denominator Enhanced Padé for $f(z) = \log(1 + z)/z$

Our first motivation to introduce conformal transformations in the approximation problems was the fact that they enlarge the convergence region for the series and can therefore be used to obtain the values of the functions. Since the series in the enhanced variables converges, its Padé approximants with denominators of low degree usually converge also. This high-order low-denominator-degree enhanced Padé approximants can produce very good results, as we illustrate in tables 4 and 5. This alternative may be of interest, since it results in a reduction in the computational costs. In any case, it is an interesting fact that a Padé with a denominator of degree as low as 5 can produce such a substantial improvement of the convergence rate of the enhanced series.

In table 4 we show the sum of the truncated enhanced series and the Padé approximants of order $N + 1$ with denominators of degree 5 for the function $f(z) = \log(1 + z)/z$ at $z = 20$ where

$$\log(21)/20 = 0.1522261218861712.$$

The left hand table was constructed by using enhanced coefficients obtained by composition of series (see section 3.1), the right hand one uses accurate enhanced coefficients obtained otherwise. The loss of significant digits in the left hand table is well explained by our analysis in section 3.1. Indeed, expression (22) predicts a loss of, 14 and 18 decimals of accuracy for $N = 30$ and $N = 40$ respectively, in the calculation of the enhanced series via composition, which is, roughly, observed. The right hand table does not suffer, of course, of this deficiency. We must not conclude, however, that the approach of § 3.1 is useless; see [7].

Table 4: Enhanced series and low denominator degree enhanced Padé approximants for $\log(1+z)/z$

N	Enh. Series	Enh. Padé	N	Enh. Series	Enh. Padé
10	0.14360068	0.15430450	10	0.14360068	0.15430450
20	0.15009266	0.15228496	20	0.15009265	0.15228495
30	0.15159762	0.15227847	30	0.15161534	0.15223062
40	0.06910705	0.15232884	40	0.15203828	0.15222664

Table 5 contains higher order approximations computed from accurate enhanced coefficients. Besides the regular Padé approximants and enhanced series we include enhanced Padé approximants with denominators of degree 5 (*low*) and of degree $N/2 + 1$ (*high*). Note that, for very large N , approximants of low denominator degree perform better than diagonal ones. In both tables 4 and 5 we observe a slow convergence of the enhanced series, and a greatly improved convergence as a result of incorporating enhanced approximants with denominators of low degree.

Table 5: High order approximants for $\log(1+z)/z$

N	Padé	Enh. Series	Enh. Padé (<i>low</i>)	Enh. Padé (<i>high</i>)
60	0.15222278964875	0.15224926415545	0.15222613236258	0.15222612189111
100	0.15222383792081	0.15222642286095	0.15222612190656	0.15222612188430
160	0.15222522532903	0.15222612249452	0.15222612188617	0.15222612188623
180	0.15220153083826	0.15222612196628	0.15222612188617	0.15222612188614

Finally, we present an example of a function whose singularities are not real. Even the simple conformal transformation (4) can provide excellent approximations in such cases.

$$\bullet f(z) = \sqrt{\frac{(1+(1+i)z)(1+(1-i)z)}{(1+10(1+i)z)(1+10(1-i)z)}}$$

In this case, as in our second and third examples, the coefficients of the enhanced series were calculated as products of series whose coefficients are given by simple formulae. It is easy to check that the optimal value for the parameter is $B = 0.1$. The computer produced NaN (“Not a Number”), an overflow indicator, in the case of the $[90/90]$ direct approximant for $z = 500$.

In table 6 we show some values of several $[\frac{N}{2}/\frac{N}{2}]$ Padé and enhanced Padé fractions. The qualitative picture remains unchanged.

Table 6: $[\frac{N}{2}/\frac{N}{2}]$ approximants for $\sqrt{\frac{(1+(1+i)z)(1+(1-i)z)}{(1+10(1+i)z)(1+10(1-i)z)}}$

N	z	$f(z)$	Padé	Enh. Padé
20	50	0.100903995976172	0.101690956502194	0.101690955078874
40			0.100851941698109	0.100907485427384
60			0.100829704353523	0.100904026370804
80			0.100862678889198	0.100903996274708
100			0.100859381474982	0.100903996124993
120			0.100978541936147	0.100903995972737
140			0.100961431193080	0.100903995978357
160			0.101015279273425	0.100903995976236
180			0.101038687309100	0.100903995976198
20	500	0.100090040445593	0.100925225656255	0.100925224160906
40			0.100032942757639	0.100093996177684
60			0.100008791942675	0.100090077056242
80			0.100044809049461	0.100090040827442
100			0.100041047921743	0.100090040634719
120			0.100170377177106	0.100090040440984
140			0.100152070923988	0.100090040448810
160			0.100209795827462	0.100090040445689
180			NaN	0.100090040445629

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References

- [1] Baker, G. A., *The theory and application of the Padé approximant method*, in Advances in theoretical physics, Vol I, K. A. Brueckner, Ed. Academic Press, (1965).
- [2] Baker, G. A., Gammel, J. L. and Wills, J. G., *An investigation of applicability of the Padé approximant method*, J. Math. Anal. Appl. **2**, 405–418 (1961)
- [3] Baker, G. A. and Graves–Morris, P., *Padé Approximants. Part I: Basic Theory*, Addison–Wesley, Massachusetts, (1981).
- [4] Baker, G. A. and Graves–Morris, P., *Padé Approximants. Part II: Extensions and Applications*, Addison–Wesley, Massachusetts, (1981).
- [5] Brezinski, C., *Procedures for estimating the error in Padé approximation*, Mathematics of Computation **53**, 639–648 (1965).
- [6] Bruno, O. P. and Reitich, F., *Solution of a boundary value problem for Helmholtz equation via variation of the boundary into the complex domain*, To appear in Proc. Royal Soc. Edinburgh.
- [7] Bruno, O. P. and Reitich, F., *Numerical solution of diffraction problems: a method of variation of boundaries*, Submitted
- [8] Cabay, S. and Choi, D., *Algebraic computations of scaled Padé fractions*, SIAM J. Comput. **15**, 243–270 (1986).
- [9] Edrei, A., *Sur les déterminants récurrents et les singularités d’une fonction données par son développement de Taylor*, Compositio Math. **7**, 20–88 (1939).
- [10] Forsythe, G. E. and Moler, C. B., *Computer solution of linear algebraic systems*, Prentice Hall, Inc. Englewood Cliffs, NJ
- [11] Graves–Morris, P., *The numerical calculation of Padé approximants*, Lecture Notes in Mathematics **765**, L. Wuytack Ed., 231–245 (1979).



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- [12] Isenberg, C., *Moment calculations in lattice dynamics. I. fcc lattice with nearest-neighbor interactions*, Phys. Rev. **132**, 2427–2433 (1963).
- [13] Isenberg, C., *Expansion of the vibrational spectrum at low frequencies*, Phys. Rev. **150**, 712–719 (1966).
- [14] Luke, Y. L., *Mathematical functions and their approximations*, Academic Press, New York (1977).
- [15] Luke, Y. L., *Algorithms for the computation of mathematical functions*, Academic Press, New York (1977).
- [16] Luke, Y. L., *Computations of coefficients in the polynomials of Padé approximations by solving systems of linear equations*, Journal of Computational and Applied Mathematics **6**, 213–218 (1980).
- [17] Mead, L. R. and Papanicolaou, N., *Maximum entropy in the problem of moments*, J. Math. Phys. **25**, 2404–2417 (1984).
- [18] Morse, P. M. and Feshbach, H., *Methods of theoretical physics*, vol. 2, McGraw-Hill, New York (1953).
- [19] Saff, E. B. and Varga, R. S., Eds. *Padé and rational approximation*, Academic Press, Inc. 323–398 (1977).
- [20] Taylor, J. M., *The condition of gram matrices and related problems*, Proc. Royal Soc. of Edinburgh **25**, 45–56 (1978).