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Numerical Analytic Continuation Using Padé Approximants

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We present a new method of using Padé approximants to numerically continue a function for which the only obtainable representation consists of the first few terms of a series, as in the case where a curve is fitted to experimental data. The procedure yields good results, but no assessment has been made as to its stability under small perturbations in the values of the coefficients of the original series.

INTRODUCTION

In many areas of physics [1–4], mathematics [5–10], seismology [11], and engineering [12–14], the first few terms in the series representation of a quantity of interest are used to calculate its Padé approximants. These in turn are used to locate its poles and zeros which determine the characteristics of the function. All these applications share a common feature: the coefficients of the series representation have been derived from theoretical considerations. In this note we suggest that Padé approximants may be used to advantage to obtain a functional representation of a physical quantity which is known only by its experimentally determined values at a set of discrete points on a limited interval along the real axis.

It is customary in such cases to employ some sort of curve fitting procedure. However, the representation thus obtained can rarely be extrapolated with confidence. To be able to do so requires some knowledge of the poles and zeros of the function. One method of locating them is to calculate the Padé approximants directly from the fitted representation. We shall call these the direct approximants. An alternate method is to convert the fitted representation into a meromorphic function by forming its Laplace transform and then obtaining the Padé approximants to the Laplace transform. We shall call these the indirect approximants. We suggest that inverting the indirect approximants yields a representation which is more accurate than the direct approximants and can be extrapolated with greater confidence. The procedure is essentially that of approximating empirical data by a linear combination of exponentials [15, 16].

PROCEDURE

Let the fitted function be

$$f(x) = \sum_{k=0}^{N} a_k x^k. \tag{1}$$

A term by term Laplace transformation gives

$$F(s) = (1/s) \sum_{k=0}^{N} b_k/s^k, \qquad b_k = k!\, a_k\,. \tag{2}$$

For ease of computation, it is convenient to introduce the variable $\sigma = 1/s$, enabling the summation in the equation above to be written

$$\hat{F}(\sigma) = \sum_{k=0}^{N} b_k \sigma^k. \tag{3}$$

We recall that the $[M, N]$ Padé approximant $P_{MN}(x)$ to $\hat{F}(\sigma)$ is given by the ratio $A_M(x)/B_N(x)$, where $A_M(x)$ and $B_N(x)$ are polynomials of degree M and N, respectively. They are defined through the relationship

$$B_N(x) f(x) - A_M(x) = 0 + O(x^{M+N+1}). \tag{4}$$

The coefficients p_m and q_n of the two polynomials can be found by solving the system of equations

$$\sum_{r=0} q_r b_{s-r} = p_s\,, \qquad s = 0, 1, 2,..., M, \tag{5}$$

$$\sum_{r=0} q_r b_{s-r} = 0, \qquad s = M + 1, M + 2, M + 3,..., M + N. \tag{6}$$

There is no loss of generality in setting $B(0) = 1$.

The approximants $[M, N]_\sigma$ to $\hat{F}(\sigma)$ are then found. Transforming back to s gives the approximants

$$[M', N']_s = (1/s)[M, N]_\sigma\,. \tag{7}$$

Having obtained the Padé approximants it is a simple matter to invert them using partial fractions.

EXAMPLE. Suppose that somehow we have obtained only the first four terms in $I_0(x)$, the modified zero-order Bessel function of the first kind.

$$I_0(x) \approx f(x) = 1 + 0.25x^2 + 0.0156x^4 + 0.00043x^6. \tag{8}$$

Then

$$F(s) = (1/s)(1 + 0.5/s^2 + 0.37/s^4 + 0.31/s^6), \tag{9}$$

and

$$\hat{F}(\sigma) = 1 + 0.5\sigma^2 + 0.37\sigma^4 + 0.31\sigma^6. \tag{10}$$

The first two approximants to $\hat{F}(\sigma)$ are

$$[0, 2]_\sigma = 1/(1 - 0.5\sigma^2), \tag{11}$$

$$[2, 2]_\sigma = (1 - 0.25\sigma^2)/(1 - 0.75\sigma^2), \tag{12}$$

from which,

$$(1/s)[0, 2]_\sigma = s/(s^2 - 0.5) = [1, 2]_s, \tag{13}$$

$$(1/s)[2, 2]_\sigma = (s^2 - 0.25)/(s^3 - 0.75s) = [2, 3]_s. \tag{14}$$

These indirect approximants to $f(x)$ are readily inverted, yielding

$$f_{12}(x) = \cosh(x/2^{1/2}) \tag{15}$$

and

$$f_{23}(x) = [2\cosh(x3^{1/2}/2) + 1]/3. \tag{16}$$

In Fig. 1 are shown plots of $f_{12}(x)$, $f_{23}(x)$, and $f_{34}(x)$ versus a plot of $I_0(x)$. It is

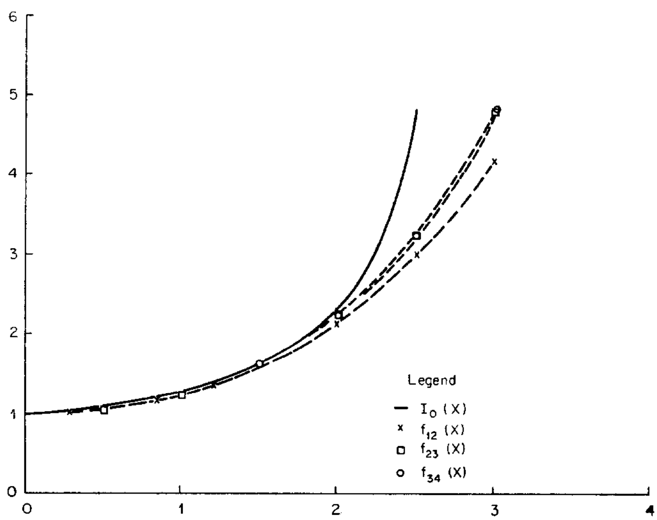

FIG. 1. Three indirect approximants to $I_0(x)$.

remarkable how good the approximations are, even though only four nonzero terms have been used. For comparison, a few direct approximants to $f(x)$ are given below.

$$[0, 2]_x = 1/(1 - 0.25x^2), \tag{17}$$

$$[2, 2]_x = (1 + 0.312x^2)/(1 - 0.0625x^2), \tag{18}$$

$$[2, 4]_x = (1 + 0.175x^2)/(1 - 0.074x^2 + 0.00289x^4). \tag{19}$$

The first two of these have poles at $x = 2$ and $x = 4$, respectively, and clearly do not provide a good representation. The third has four complex poles located at $\pm 3.9 \pm i1.7$. Evaluation of $[2, 4]_x$ shows a monotonic increase up to $x = 3.6$ at which point its value is 81.88 and then at $x = 3.7$ it has dropped steeply to -243 after which it increases slowly. Note that inversion of the indirect approximants provides a very much better representation than the direct approximants even though both derive from the same expression.

As a second example consider the first few terms in $J_0(x)$, the zero order Bessel function of the first kind.

$$J_0(x) \approx f(x) = 1 - 0.25x^2 + 0.156x^4 - 0.00043x^6. \tag{20}$$

As the right-hand side of Eq. (20) can be obtained from Eq. (8) by replacing x by ix, the results pertaining to the first example can be transferred to this example by substituting $i\sigma$ for σ, in the right-hand side of Eqs. (9)–(16). In particular, Eqs. (15) and (16) yield for the second example,

$$f_{12}(x) = \cos(x/2^{1/2}), \tag{21}$$

$$f_{23}(x) = [1 + 2\cos(x3^{1/2}/2)]/3. \tag{22}$$

Both these approximations show the general oscillatory behavior expected but not the damping. However a higher order indirect approximant, taking a few more terms from $f(x)$, is

$$[4, 4]_\sigma = (1 + 0.775\sigma^2 + 0.0687\sigma^4)/(1 + 0.127\sigma^2 + 0.3313\sigma^4), \tag{23}$$

i.e.,

$$[4, 5]_s = (s^4 + 0.775s^2 + 0.0687)/(s^5 + 0.127s^3 + 0.3313s). \tag{24}$$

Inverting this gives $f_{45}(x)$ which is plotted in Fig. 2 versus a plot of $J_0(x)$. The agreement is again good.

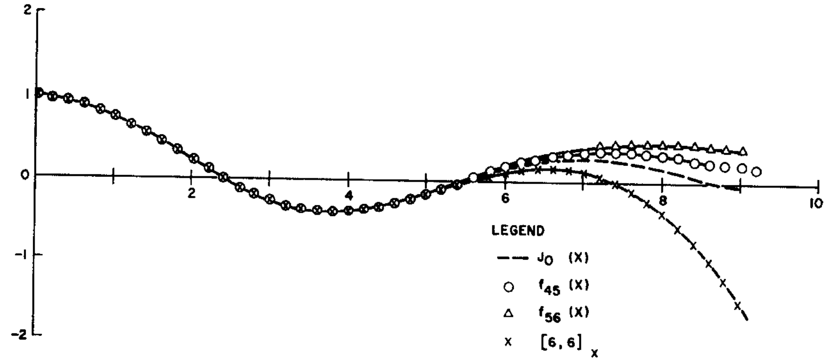

FIG. 2. One direct and two indirect approximants to $J_0(x)$.

For comparison, the direct approximants are,

$$[0, 2]_x = 1/(1 + 0.25x^2), \tag{25}$$

$$[2, 2]_x = (1 - 0.187x^2)/(1 + 0.063x^2), \tag{26}$$

$$[2, 4]_x = (1 - 0.176x^2)/(1 + 0.074x^2 + 0.00289x^4). \tag{27}$$

The first of these approximants decreases monotonically, asymptotically approaching zero. The next approximant keeps getting smaller, becomes negative and stays negative. The third approximant becomes zero at about $x = 2.3$ which is very close to the first zero of $J_0(x)$ but it keeps getting more negative for a long time before it turns over and asymptotically approaches zero from below. Inasmuch as it locates the first zero of $J_0(x)$ it is a good representation but it does not show any oscillation. It is necessary to go as high as $[6, 6]_x$ before the first reasonably good representation is obtained. This is shown in Fig. 2.

We see that for both these examples, inverting the indirect approximant to a truncated series representation provides a very good approximate way of numerically continuing a function and assessing its behavior.

DISCUSSION AND CONCLUSIONS

Although the procedure presented leads to good extrapolations for the examples shown, we have not yet examined the limitations on its applicability nor developed criteria to select which approximant or which diagonal of the Padé table will give the best results. For instance, in Fig. 2, $f_{5,6}$ provides a poorer fit than $f_{4,5}$. This may be related to the spurious poles which sometimes appear in certain approximants [1].

In the spirit of our approach, obtaining more terms in the original series is dependent on obtaining more experimental data points and we feel that this should lead to more accurate results. However, if the original coefficients a_k be perturbed slightly to $a_k + \delta_k$, then clearly the location of the poles and zeros s_n will be shifted to values $s_n + \Delta_n$. Bellman [17] has cautioned that arbitrary small changes in $F(s)$ can produce arbitrary large changes in $f(x)$. Thus the stability question as well as that of convergence needs to be resolved.

We are attempting to resolve these and other questions such as estimate of error, which arise in applying the method presented here to obtain a functional representation of a physical quantity, which is valid beyond the interval on the real axis along which it is known only by its experimentally determined values.

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