DETERMINATION OF $f(\infty)$ FROM THE ASYMPTOTIC SERIES FOR $f(x)$ ABOUT $x = 0$

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ABSTRACT

A difficult and long-standing problem in mathematical physics concerns the determination of the value of $f(\infty)$ from the asymptotic series for $f(x)$ about $x = 0$. In the past the approach has been to convert the asymptotic series to a sequence of Padé approximants $\{P_n(x)\}$ and then to evaluate these approximants at $x = \infty$. Unfortunately, for most physical applications the sequence $\{P_n(\infty)\}$ is slowly converging and does not usually give very accurate results. In this paper we report the results of extensive numerical studies for a large class of functions $f(x)$ associated with strong-coupling lattice approximations. We conjecture that for large $n$, $P_n(\infty) \sim f(\infty) + B/\ln n$. A numerical fit to this asymptotic behavior gives an accurate extrapolation to the value of $f(\infty)$.

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PACS numbers: 02.60.+y, 11.15.Me, 02.90.+p

hep-lat/9312031
There are many examples in mathematical physics where it is necessary to calculate the value of a function $f(x)$ at $x = \infty$ but where $f(x)$ can only be determined perturbatively for small $x$.\textsuperscript{1,2,3} The result of such a perturbative calculation yields the first few terms of the asymptotic series for $f(x)$:

$$f(x) = x^\alpha \sum_{n=0}^{\infty} b_n x^n.$$  \hspace{1cm} (1)

The problem is then to use this series to determine $f(\infty)$ assuming, of course, that $f(\infty)$ exists.

A natural approach\textsuperscript{4,5,6,7,8} to solving this problem is to raise both sides of (1) to the power $1/\alpha$,

$$f(x)^{1/\alpha} = x \sum_{n=0}^{\infty} c_n x^n,$$  \hspace{1cm} (2)

and then to convert the right side of (2) to a finite sequence of Padé approximants, $P_n^n(x)$, $n = 1, 2, 3, \ldots, N$, where $2N - 1$ is the highest order of the perturbative calculation used to obtain (1). Since $P_n^n(\infty)$ exists, we compute the sequence of Padé extrapolants $[P_n^n(\infty)]^\alpha$ with the hope that as $n$ increases, this sequence rapidly approaches $f(\infty)$.

While this extrapolation procedure works well in some cases one encounters an important class of functions for which this procedure is rather ineffective. For this class of functions the coefficients $b_n$ in (1) have two characteristic properties:

(i) $b_n \sim n!$ as $n \to \infty$;
(ii) the $b_n$ exhibit a doubly-alternating sign pattern $+, +, -, -, +, +, -, -, \ldots$.

Asymptotic series whose coefficients exhibit properties (i) and (ii) arise in strong-coupling lattice expansions in quantum field theory.\textsuperscript{4,5,6,7,8} The problem of determining the value of $f(\infty)$ corresponds to extrapolating to the continuum limit of the lattice theory. For such functions, experience shows that while $[P_n^n(\infty)]^\alpha$ often comes close to $f(\infty)$, the sequence of Padé extrapolants appears to level off at some value that differs from $f(\infty)$ by several percent. This raises the question of whether the sequence actually converges to $f(\infty)$ or to some other limit near $f(\infty)$.

Here is a simple example that illustrates this problem: Consider the series

$$f(x) = \sum_{n=0}^{\infty} a_n x^n,$$  \hspace{1cm} (3)

where

$$a_{2n} = (-1)^n (2n)!,$$ $$a_{2n+1} = (-1)^n 2 (2n)!.$$  \hspace{1cm} (4)

We can evaluate this series exactly using Borel summation. The result is the integral representation

$$f(x) = (1 + 2x) \int_0^{\infty} \frac{e^{-t}}{1 + x^2 t^2} dt.$$  \hspace{1cm} (5)
from which we determine that
\[ f(\infty) = \pi . \]  

Let us try to obtain this result numerically by converting the series in (3) to a sequence of Padé extrapolants. On Fig. 1 we plot the value of \( P_n(\infty) \) as a function of \( 1/n \) for \( n = 1, 2, 3, \ldots, 20 \). Observe that the Padé approximants form a zigzag sequence that seems to tend to a limiting value on the y-axis (corresponding to \( n = \infty \)). If we extrapolate the sequence to \( n = \infty \) using a straight line, the sequence appears to have a limit that is too small (roughly 10% smaller than \( \pi \)). However, if we include many more terms \( (n = 1, 2, 3, \ldots, 300) \) in the sequence (see Fig. 2), we can see that the sequence actually lies on a curve that becomes steeper as \( n \to \infty \). Figure 2 indicates that the asymptotic behavior of \( P_n(\infty) \) for large \( n \) cannot have a straight-line form \( \pi + B/n \).

Because the sequence in Fig. 2 lies on a curve and not on a straight line it is difficult to predict its limiting value. A detailed numerical fit of the form
\[ P_n(\infty) \sim \pi + \frac{B}{n^C} \]
does not work for any value of \( C \). However, a more general numerical fit of the form
\[ P_n(\infty) \sim \pi + \frac{B}{n^C(\ln n)^D} \]
gives \( C = 0 \pm 0.1 \) and \( D = 1 \pm 0.1 \). Thus, we believe that
\[ P_n(\infty) \sim f(\infty) + \frac{B}{\ln n} . \]  

In fact, a fit of the form \( P_n(\infty) = A + B/\ln n \) gives \( A = \pi \) with a relative error of less than 1%, which is an order-of-magnitude improvement over the result of extrapolating the curve in Fig. 1. In Fig. 3 we plot the Padé extrapolants shown on Fig. 2 as a function of \( 1/\ln(20n) \). Observe that the zigzag curve now lies along a straight line that appears to approach the value \( \pi \).

Next, we consider the more complicated case of the Stirling series expansion for the factorial function:
\[ f(x) \sim x^{1/2} \left[ 1 + \frac{1}{12} x + \frac{1}{288} x^2 - \frac{139}{51,840} x^3 - \frac{571}{2,488,320} x^4 + \frac{163,879}{209,018,880} x^5 + \frac{5,246,819}{75,246,796,800} x^6 - \ldots \right] \quad (x \to 0) , \]  
where
\[ f(x) = \frac{1}{\sqrt{2\pi}} \ e^{\frac{1}{2} x} \ x^\frac{1}{2} \ (\frac{1}{x})! . \]

Note that the series in (8) exhibits properties \((i)\) and \((ii)\). Since \( 0! = 1 \) we see that
\[ f(\infty) = \frac{1}{\sqrt{2\pi}} = 0.398942 \ldots . \]
We attempt to calculate \( f(\infty) \) by raising (8) to the power \(-2\), computing \( P_n^2(x) \), and forming the sequence of extrapolants \( [P_n^2(\infty)]^{-1/2} \). As in the previous example if we plot these extrapolants as a function of \( 1/n \) for \( n = 1, 2, 3, \ldots, 90 \) (see Fig. 4) we see that the extrapolants do not lie along a straight line. From just the first 20 extrapolants we would predict the value of \( f(\infty) \) to be about 0.42, which is 5% high. However, it is clear that the extrapolants follow a curve which becomes increasingly steep as \( n \to \infty \). If we replot the data as a function of \( 1/\ln(20n) \) (see Fig. 5) we see that the same extrapolants lie on a straight line that appears to intersect the y-axis at precisely the correct result in (10).\(^{10}\) A numerical fit of the form in (7) gives \( f(\infty) \) correct to about 1%.

Our third example is taken from a quantum field theory calculation. Consider a \( g\phi^2K \) self-interacting scalar quantum field theory in \( D \)-dimensional Euclidean space. In recent papers\(^{12,13}\) we showed how to express the free energy for such a theory as a series in powers of \( D \) in the limit of strong bare coupling, \( g \to \infty \). The coefficient of \( D \) in this dimensional expansion can be expressed as the logarithm of an infinite series in powers of \( x \) like that in (1); we denote this infinite series \( f(x) \).\(^{14}\) For all \( K \) the coefficients of the series \( f(x) \) grow like \( n! \) and have a doubly-alternating sign pattern. The expansion parameter, \( x = [ga^{2K-D(K-1)}]^{-1/K} \), is a dimensionless combination of the coupling constant \( g \) and the lattice spacing \( a \), which is small for fixed \( a \) and large \( g \). But in the continuum limit for which \( a \to 0 \), we have \( x \to \infty \). Thus, we are confronted with the problem addressed in this paper, namely that of computing \( f(\infty) \).

As a special case, we consider the free theory corresponding to \( K = 1 \). For this case there is a closed-form expression for \( f(x) \):

\[
f(x) = x \exp\left\{ 2\int_0^\infty dt \: e^{-t} \ln[e^{-xt}I_0(zt)] \right\},
\]

where \( I_0 \) is the modified Bessel function of order 0. In the continuum limit, \( x \to \infty \), we have

\[
f(\infty) = \frac{e^\gamma}{2\pi} = 0.28347 \ldots
\]

The first few terms of the asymptotic series representation for \( f(x) \) in powers of \( x \) are

\[
f(x) = x \left( 1 - 2x + 3x^2 - \frac{10}{3}x^3 + \frac{29}{12}x^4 - \frac{11}{10}x^5 + \frac{391}{180}x^6 - \frac{2389}{630}x^7 - \frac{5303}{448}x^8 \\
+ \frac{2602051}{90720}x^9 + \frac{159662191}{907200}x^{10} - \frac{651255947}{1663200}x^{11} - \frac{435388434359}{119750400}x^{12} + \ldots \right).
\]

If we convert the first 250 terms in this series to a sequence of Padé extrapolants, we obtain results similar to those of the two examples above. On Fig. 6 we plot this sequence of extrapolants as a function of \( 1/n \) and observe that the extrapolants lie along a curve that is difficult to extrapolate to its value at \( n=\infty \). However, on Fig. 7 we plot these same extrapolants versus \( 1/\ln(4n) \) and obtain a straight line whose limit is clearly very close to the exact answer given in (12).\(^{15}\)

On the basis of our numerical studies of these examples we conjecture that the asymptotic behavior in (7) of the \( n \)th Padé extrapolant is generic if the coefficients exhibit properties \((i)\) and \((ii)\). We may express the Padé extrapolant \( P_n^2(\infty) \) constructed from the
asymptotic series \( x \sum_{n=0}^{\infty} c_n x^n \) as a ratio of two determinants, an \((n + 1) \times (n + 1)\) determinant divided by an \(n \times n\) determinant.\(^{16}\) Thus, a simple way to state this conjecture is in terms of determinants of large-dimensional matrices:

\[
P_n(\infty) = \frac{|c_{n-1} \cdots c_{2n-1}|}{|c_1 c_2 c_3 \cdots c_n|} \sim f(\infty) + \frac{B}{\ln n}.
\]  

We are indebted to L. N. Lipatov, G. McCartor, and M. VanDyke for useful discussions. We thank the U. S. Department of Energy for funding this research and one of us, SB, thanks the U. S. Department of Education for financial support in the form of a National Need Fellowship.
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2 In the field of fluid mechanics, M. VanDyke [J. Fluid Mech. 44, 813 (1970)] used a 24-term series in powers of the Reynolds number \( R \) to obtain the drag coefficient of a sphere in the Oseen linearization. Using an Euler transformation he was able to extrapolate the series to its value at \( R = \infty \). The accuracy of his result was about 5%. VanDyke applied similar techniques to a 24-term series in powers of Dean number \( K \) for laminar flow through a loosely coiled pipe [J. Fluid Mech. 86, 129 (1978)]. Extrapolating the series to its value at \( K = \infty \), VanDyke obtained the controversial result that there is a 1/20-power growth of the friction factor. VanDyke’s series differ from the series considered in this paper in that his series have a finite (nonzero) radii of convergence.

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15 For \( K > 1 \) the form of the series and its extrapolants are similar to the \( K = 1 \) case. However, when \( K > 1 \) the quantum field theory is not free and it is difficult to calculate more than half a dozen extrapolants.

16 See Ref. 11, pp. 383-384.
FIGURE CAPTIONS

Figure 1. The first twenty Padé extrapolants $P_n^m(\infty)$ for the series whose coefficients are given in (4). The approximants are plotted as a function of $1/n$ such that the vertical axis corresponds to $n = \infty$. Successive Padé extrapolants are connected by line segments to form a zigzag line. The vertices of the zigzag line are the values of the approximants. One would think that it is easy to extrapolate by eye to the limit of the sequence (the point where it intersects the vertical axis). However, the zigzag line of extrapolants appears destined to intersect the vertical axis well below the exact answer, $\pi$, which is indicated by the horizontal line.

Figure 2. Same as in Fig. 1 except that we have plotted the first 300 approximants. Having plotted many more approximants than in Fig. 1, we believe that the zigzag line of approximants is curving upward; it could well intersect the vertical axis at $\pi$. It is difficult to guess where such a curve might cross the vertical axis.

Figure 3. The same approximants as in Fig. 2 now plotted versus $1/\ln(20n)$. The zigzag line of approximants seems to be tending to $\pi$, the correct value of $f(\infty)$.

Figure 4. The first 90 Padé extrapolants constructed from the Stirling series (8) for the factorial function. As in Fig. 2, the zigzag line of extrapolants, when plotted versus $1/n$, begins to curve as $n$ gets large. For small values of $n$ the zigzag line appears to be headed for an intersection with the vertical axis that is too large compared with the correct answer $1/\sqrt{2\pi} = 0.398942\ldots$. For larger values of $n$, the curvature of the zigzag line makes it too difficult to predict where the line will cross the vertical axis.

Figure 5. The same approximants as in Fig. 4 now plotted versus $1/\ln(20n)$. As in Fig. 3, the zigzag line of approximants seems to be tending to the correct value of $f(\infty)$, which in this case is $1/\sqrt{2\pi} = 0.398942$. Apparently, one can use the Stirling series for $(1/x)!$, which is valid as $x \to 0$, to calculate $0! = 1$.

Figure 6. The first 125 Padé extrapolants constructed from the asymptotic series (13) taken from a field-theoretic calculation. As in Figs. 2 and 4, the zigzag line of extrapolants, when plotted versus $1/n$, begins to curve as $n$ gets large. For small values of $n$ the zigzag line appears to be headed for an intersection with the vertical axis that is too large compared with the correct answer $e^{\gamma}/(2\pi) = 0.28347\ldots$. For larger values of $n$, the curvature of the zigzag line makes it too difficult to predict where the line crosses the vertical axis.

Figure 7. The same approximants as in Fig. 6 now plotted versus $1/\ln(4n)$. As in Figs. 3 and 5, the zigzag line of approximants seems to be tending to the correct value of $f(\infty)$, which in this case is $3.52775\ldots$. 
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