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The Optimization of Convergence for Chebyshev Polynomial Methods in an Unbounded Domain

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By using the method of steepest descent, I have compared the suitability of three different methods for solving problems in a semi-infinite or infinite domain using Chebyshev polynomials. Exponential mappings are uniformly bad. Domain truncation and algebraic mapping both work well, but each is superior for a different category of problems. When the solution is an entire function, then domain truncation is best. It is always simpler to apply than algebraic mapping and always at least as accurate—much more accurate for functions which decay very rapidly. For singular functions, on the other hand, algebraic mapping is better because it is less sensitive to the mapping scale factor L, permitting a better compromise in resolving both the singularity and the exponential decay. For both types of problems, I give simple, explicit estimates of both the optimum choice of domain size or mapping factor and of the attainable accuracy. For the model entire function $\exp[-Az^k]$ on a semi-infinite interval $[0, \infty]$, the optimum domain size is $L = 0.896(n/A)^{1/k}$ and the smallest attainable error is roughly $e^{-n(0.896)^k}$ where n is the number of Chebyshev polynomials used. Similar formulas for singular functions handled via algebraic mapping are given in (3.41) to (3.45) below.

1. INTRODUCTION

In a recent paper, Grosch and Orszag [1] have performed a numerical analysis of the problem of solving differential equations in a semi-infinite or infinite domain using Chebyshev polynomials. Since the polynomials are defined only on a finite interval, it is necessary to use one of three procedures. First, impose artificial boundaries at a large but finite distance (a procedure that will henceforth be called "domain truncation") and solve the problem on the interval $[0, L]$ instead of $[0, \infty]$. Second, one can employ an algebraic mapping of the form

$$Z = 2\left(\frac{z}{L + z}\right) - 1, \tag{1.1}$$

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where L is a constant to transform $z \in [0, \infty]$ into the finite interval $Z \in [-1, 1]$. Third, one can use an exponential mapping of the form

$$Z = 1 - 2e^{-z/L} \tag{1.2}$$

for the same purpose. Other types of mappings are possible, but (1.1) and (1.2) are representative of the range of options available.

Grosch and Orszag [1] found that if the exact solution to the original problem decayed exponentially fast as $|x| \to \infty$, then all three would work, but algebraic mapping gave the best results with domain truncation second and exponential mapping a very poor third.

The principal limitation of their study was that it was entirely empirical: they solved various differential equations in different ways and compared the numbers. The purpose of this present work is to extend theirs by deriving asymptotic approximations to the Chebyshev coefficients of simple model functions. Through them, it will be possible to make more systematic comparisons of different methods, extend the range of comparisons, and perhaps most important, give simple analytic formulas for choosing the optimum domain size or mapping parameter L for various situations.

In turn, this analytic simplicity imposes two limitations. First, the most common use of Chebyshev series is to solve differential or integral equations by the Lanczos tau-method (described in Gottlieb and Orszag [2]) or something similar. The resulting approximate solution has two sources of error. First, because only a finite number of polynomials N can be retained in the expansion, there is a series truncation error due to chopping off higher terms in the series. In addition, the N retained coefficients as generated by the tau-method usually differ slightly from the corresponding coefficients of the exact solution, a difference that may be denoted the "tau error." Unfortunately, there is no simple, general way of analyzing the tau error, so this work will concentrate strictly on the series truncation error and also, for domain truncation, on the error in using an interval of finite size.

This would seem quite restrictive, but Gottlieb and Orszag [2] have pointed out that empirically, the series truncation error and the tau error are almost always the same order of magnitude, regardless of the particular algorithm, the smoothness of the solution, or the finiteness of the domain. The property of exponential or "infinite order" convergence, which will be explained in Section 2, provides a strong theoretical justification for this conclusion: that optimizing the convergence of the first N coefficients of the *exact* solution will minimize the error in the approximate solution of the differential equation with the series truncation error and "tau-error" being roughly the same order of magnitude.

In consequence, in the rest of this work, "optimizing convergence" will refer to obtaining the best possible Chebyshev series approximation to a known, explicit model function. No differential equations will be solved.

The second restriction is the use of model functions of the form

$$f(z) = e^{-z^k} \tag{1.3}$$

or

$$f(z)=\frac{e^{-z^k}}{z+s}, \tag{1.4}$$

where k and s are constants. Similar but greater restrictions were implicit in Grosch and Orszag [1], who presented only specific case studies, and in any numerical analysis, one must impose some conditions on the class of problems studied. The obvious question is whether the set of functions given by (1.3) is sufficiently general to be useful.

The first part of the answer to this question is that Grosch and Orszag found—as common sense would suggest— that domain truncation and mapping work well only when the solution decays exponentially fast at infinity. By varying k in (1.3), we can here go beyond that to explore how the effectiveness of different methods varies with the *rate* of exponential decay. Although the numerical tables we will present are limited to integral k, the analytic formulas we derive are applicable to any k. Thus, the results of this paper are relevant to the Airy function $A_i(x)$, whose asymptotic form is proportional to $f(z)$ in (1.3) with $k=3/2$.

The second part of the answer is that we will show that the asymptotic convergence of the Chebyshev series for a function is dominated by a combination of (i) the factor causing strongest exponential decay and (ii) the location—but not the type—of the singularity nearest the computational interval. This means that if we must deal with a function such as

$$f(z)=e^{-z^4+z^2}, \tag{1.5}$$

the optimum choice of the domain size or mapping parameter L for (1.5) will be approximately the same as for (1.3) with $k=4$. Furthermore, it will be shown that the methods derived here can be almost trivially extended to (1.5) itself if need be, albeit at the expense of more complicated results.

Since the convergence depends only on the *location* of the singularity, with but a weak dependence on the type of the singularity, it follows that if we choose s to be the (possibly complex) location of the convergence-limiting singularity, we will obtain good predictions for the optimum L and for the number of polynomials N we need to achieve the desired degree of accuracy even if this singularity is actually a branch point or a higher order pole.

Thus, the model functions (1.3) and (1.4) will be sufficient to cover most cases which arise in practice. Little is sacrificed, and much simplicity gained, by concentrating on these simple functions.

The plan of the paper is as follows: Section 2 defines several useful measures of convergence and error. Section 3 explains how the method of the steepest descent can be used to derive simple asymptotic approximations to the Chebyshev coefficients and how in turn these approximations can be used to pick the best domain size or mapping parameter. The fine details of the steepest descent method are banished to Appendix A. Section 4 shows via numerical experiments that the asymptotic analysis does indeed work. The next section explains how the analysis presented here for a semi-infinite interval can be extended—sometimes trivially—to a fully infinite domain. Section 6 deals briefly with exponential mappings and the final section is a summary and prospectus.

2. Orders of Convergence

The parameter k which appears in (1.3) is the "order" of the entire function as usually defined in complex variable theory, and this definition will be here extended to the parameter k that appears in (1.4) although the latter functions are not entire because of the pole at $z = -s$. For purposes of discussion, it will be helpful to also define "orders" of convergence for Chebyshev series as well, and one must be careful to keep the distinction between "orders" of a *function* and "orders of convergence" for a *series* in mind.

The rate of convergence of a Chebyshev series is conventionally defined in terms of an "algebraic index of convergence" as follows:

Definition. A Chebyshev series whose coefficients are $\{b_n\}$ is said to have an "algebraic index of convergence j" if j is the largest number for which

$$\lim_{n\to\infty} n^j \, |b_n| < \infty. \tag{2.1}$$

If (2.1) is satisfied for any finite j, no matter how large, then the series is said to have "infinite order" or "exponential" convergence.

The weakness of this conventional definition is that *all* Chebyshev series for any function have "infinite order" convergence unless the function has an unbounded derivative of some order on the expansion interval itself—which is not true of any of the model functions used here. Consequently, more precise terminology is needed.

The coefficients of the geometric series $b_n = q^n$ satisfy

$$\lim_{n\to\infty} \log \frac{(|b_n|)}{n} = \log q, \tag{2.2}$$

where $\log q$ is a constant independent of n. This motivates the following.

Definition. A Chebyshev series whose coefficients are $\{b_n\}$ is said to have "supergeometric," "geometric," or "subgeometric" convergence if

$$\begin{aligned} \lim_{n\to\infty} \log(|b_n|)/n &= \infty && \text{(supergeometric)} \\ &= \text{constant} && \text{(geometric)} \\ &= 0 && \text{(subgeometric).} \end{aligned} \tag{2.3}$$

It has been shown (and will be demonstrated in Section 3) that the Chebyshev coefficients of an entire function on a finite interval satisfy

$$\log(|b_n|) \sim O[(n/k)\log(n)], \tag{2.4}$$

where k is the order of the entire function (Gottlieb and Orszag [2]). Since this is the only case of "supergeometric" convergence that will arise here, no further distinctions are necessary. The definition of "geometric" convergence is restrictive enough so that no additional qualifiers are needed. It can be shown (Gottlieb and Orszag [2]) that the coefficients of the expansion of a function with a simple pole on a finite interval must have "geometric" convergence with q in (2.2) being related to the location of the convergence-limiting singularity through a simple formula that will be given and exploited later.

When we begin to consider infinite intervals mapped into finite intervals, however, "subgeometric" convergence will be the rule, and here we must be more precise. A series such as

$$b_n = e^{-qn^{\beta}} \tag{2.5}$$

technically possesses "subgeometric," "infinite order" convergence for any positive q and β such that $\beta < 1$, so a more precise measure of convergence is desirable. This is given by the following.

DEFINITION. A sequence with coefficients $\{b_n\}$ is said to be subgeometrically convergent with exponential convergence order r if

$$\lim_{n\to\infty} \frac{\log|\log(|b_n|)|}{\log(n)} = r \tag{2.6}$$

with $r < 1$.

Thus, the series (2.5) has exponential convergence order $r = \beta$. We must refer to r as the "exponential" order of convergence to distinguish it from the more conventional definition of "algebraic" convergence given by (2.1) above.

The conventional measures of error are also inadequate for our purposes. The most obvious measure of error is simply to take the absolute value of the largest dfference between the exact $f(x)$ and its truncated expansion, the so-called L_∞ norm, but it is difficult or impossible to compute this analytically for the model dunctions considered here. If we are to make explicit suggestions for choosing a near-optimum domain size or map parameter L, we must have measures of error which are simple and analytic, even at the cost of some precision. We shall therefore define three such.

DEFINITION. The "domain error" $E_D(L)$ in applying the method of domain truncation to a function $f(z)$ is defined to be

$$E_D(L) = |f(L)|, \tag{2.7}$$

where the computational domain is $z \in [0, L]$. (It is implicitly assumed that

$$|f(z)| < |f(L)| \tag{2.8}$$

for all $z > L$ as is true of the model functions (1.3) and (1.4) used here.)

The motivation for this definition is fairly obvious. With domain truncation, we are in effect approximating the function $f(z)$ by a truncated Chebyshev expansion on $[0, L]$ and by $f(z) = 0$ on $[L, \infty]$. If the function is decaying outside the computational domain, as it must be for the method to work well, then the L_∞ error on $[L, \infty]$ will simply be the right-hand side of (2.7)—outside the computational domain, $f(z)$ differs most from 0 at $z = L$ itself.

It can be rigorously proven (Fox and Parker [3]) that the L_∞ error in truncating a Chebyshev expansion after N terms is bounded by the sum of the absolute values of all the higher order neglected terms, i.e.,

$$\left| f(Z) - \sum_{n=0}^{N} b_n T_n(Z) \right| \leqslant \sum_{n=N+1}^{\infty} |b_n|. \tag{2.9}$$

(This bound is the best possible since the equality holds whenever the coefficients are alternating or are all of the same sign.) Regrettably, it is usually impossible to sum these higher order coefficients exactly, so one must again define something cruder. Fortunately, it is normally the case that the Chebyshev coefficients converge so rapidly for a function which is infinitely differentiable everywhere on the expansion interval that

$$\sum_{n=N+1}^{\infty} |b_n| \sim O(|b_N|). \tag{2.10}$$

For a geometrically convergent series, one can prove (2.10) holds rigorously. This motivates the following.

DEFINITION. The series truncation error $E_S(L, N)$ is defined to be the absolute value of the largest coefficient *retained* in the truncation:

$$E_S(L, N) = |b_N|. \tag{2.11}$$

In later sections, we shall show that for entire functions, the optimized expansions do converge geometrically so that (2.11), although unorthodox, really is a reliable measure of error. For the subgeometrically convergent expansions which we shall encounter for the singular model functions (1.4), (2.11) can be a bit misleading. For

$$b_n = e^{-qn^r}, \tag{2.12}$$

where q and r are positive constants, one can show by bounding the sum by an integral which is the incomplete gamma function and then using the known asymptotic expansion for the latter that

$$|b_N| < \frac{1}{q} N^{1-r} \sum_{n=N+1}^{\infty} |b_n|. \tag{2.13}$$

Thus, for a subgeometrically convergent series ($r < 1$), $E_S(L, N)$ becomes smaller and smaller in comparison to be true error as N increases. However, the proportionality factor in (2.13) is increasing *algebraically* with N whereas the error in Chebyshev expansion is decreasing *exponentially* as more terms are added in the expansion. Therefore, $E_S(L, N)$ will give only a small relative error in the logarithm of the error in truncating the Chebyshev series even though the absolute error may be a factor of 10 or more larger than $E_S(L, N)$ when N is very large. It will turn out that a good estimate of the logarithm of the error is sufficient to obtain a simple, analytic prediction for the map parameter which differs by only a few percent from the true optimum L.

The steepest descent method, which is the basis for our analysis in later sections, gives asymptotic approximations to the Chebyshev coefficients which are the product of an algebraic factor of n (varying more slowly than linear) with an exponential function of n. Just as we have ignored the algebraic factor of N in (2.13) in defining the series truncation error $E_S(L, N)$, so we shall ignore the algebraic factors of n that fall out of the steepest descent method, and choose our best value for L by manipulating only that part of the asymptotic approximation which varies exponentially with n. When we do this and substitute the steepest descent formula, sans algebraic factor, into (2.12), the errors in neglecting algebraic factors will in fact largely cancel each other since the steepest descent factor always decreases with increasing n.

Thus, using (2.13) to define the error in truncating the series after N terms with the implicit assumption that the algebraic factor from the steepest descent result will be dropped before substitution into (2.13), is in fact a reasonable estimate for our purposes. The purist can always put the algebraic factors back in, but the tables given below will show that this is rarely worth the effort.

For singular functions, it is helpful to define a third error term. When the model function $f(z)$ has a pole, it may be necessary to deform the original contour into a steepest descent path in such a way that the pole lies between the steepest descent contour and the original path of integration. In this case, the asymptotic approximation to b_n consists of one or more stationary point contributions plus the residue at the pole. For singular functions, as for entire functions, we will take the error due to truncating the Chebyshev series as being roughly the order of magnitude of the highest retained coefficient, but we will reserve $E_S(L, N)$ for the stationary point contibutions and use the following for the residue term.

DEFINITION. The "pole error" $E_P(L, N)$ is defined to be

$$E_P \equiv \left[\frac{1}{S + (S^2 - 1)^{1/2}}\right]^n, \tag{2.14}$$

where S is the location of the pole in the transformed variable Z, and where the sign of the square root is that which maximizes the absolute value of the denominator.

A factor independent of n has been omitted from (2.14), consistent with the philosphy of considering only factors that vary exponentially with n; the exact contribution of the pole to the Chebyshev coefficients, obtained through the calculus of residues, is given in (3.32) below.

3. The Method of Steepest Descent

The Chebyshev coefficients b_n of a function can be asymptotically evaluated for large n by applying the method of steepest descent to an integral representation of the coefficients as first done by Elliot and Szekeres [4] and Miller [5]. The virtue of our model functions is that the asymptotic forms of their coefficients are sufficiently simple that one can easily determine what values of L, the domain size or mapping parameter, give the most rapid Chebyshev series convergence for a given function.

The method of steepest descents is applied to integrals of the form

$$I(n) = \int_C h(z)\, e^{\phi(z,n)}\, dz, \tag{3.1}$$

where C is some contour in the complex plane. The basic idea is to deform the contour of integration into new "steepest descent" path such that the integral is dominated, as $n \to \infty$, by the contributions from the neighborhoods of the stationary points $z_s(n)$, where

$$\frac{d\phi(z_s, n)}{dz} = 0. \tag{3.2}$$

Then as $n \to \infty$, the integral is approximately given by

$$I(n) = \sum \sqrt{\frac{2\pi}{-\phi''(z_s, n)}}\, e^{\phi(z_s,n)}\, h(z_s), \tag{3.3}$$

where the sum is over all stationary points on the new contour of integration and where the double prime denotes the second derivative with respect to z.

There are two additional terms that must sometimes be added to the sum of stationary point contributions in (3.3): (i) endpoint contributions (if the contour is open) and (ii) residues at singularities (if the integrand has a pole within the region between the old and new contours of integration). It will turn out that the only endpoint terms which arise here will cancel out and not affect the asymptotic approximations. For our singular model functions, however, the residues at the pole $z = -s$ must be added to the stationary point contributions and represent the principle difference between the entire functions and those with a simple pole. The stationary point contributions are essentially the same for either case except that the latter have $1/(z_s + s)$ in the factor $h(z_s)$ in (3.3).

The details of actually choosing the steepest descent path and computing the stationary points are not trivial and are given in the Appendix. Here, we will simply give a broad outline of the procedure.

The starting points for our work are the two equivalent integral representations

$$b_n = \frac{1}{\pi i} \int \frac{1}{(1-Z^2)^{1/2}} f(Z)\, e^{-n \log[Z+(Z^2-1)^{1/2}]} \tag{3.4}$$

due to Elliot [6] where the path of integration is any closed contour enclosing the interval $[-1, 1]$ and where the branch is chosen so that $(Z^2-1)^{1/2} \sim |Z|$ for large Z and second

$$b_n = \frac{1}{\pi} \int_0^{\pi} f(\cos t)\, e^{\text{int}}\, dt + \text{complex conjugate}, \tag{3.5}$$

which follows from the usual integral form of the Chebyshev coefficients by making the change of variable $Z = \cos t$, exploiting the well-known identity $T_n(\cos t) = \cos(nt)$ and then writing the $\cos(nt)$ as a sum of complex exponentials. The first integral representation is the most convenient for Chebyshev series with domain truncation because the contour is closed and we need not worry about endpoint contributions. With algebraic mapping, however, our transformed function $f(t)$ is singular at one endpoint, so (3.4) is not suitable. The integral which is written explicitly in (3.5) does have an endpoint contribution, but this is cancelled when the integral is added to its complex conjugate to give b_n itself.

Our model entire function is

$$f(z) = e^{-Az^k}. \tag{3.6}$$

In order to convert this to standard form, we must employ the transformations

$$\left.\begin{aligned} Z &= \frac{2z}{L} - 1 && (3.7) \\ z &= \frac{L}{2}(Z+1) && (3.8) \end{aligned}\right\} \text{ domain truncation}$$

and

$$\left.\begin{aligned} Z &= 2\frac{z}{L+z} - 1 && (3.9) \\ z &= L\frac{(1+Z)}{(1-Z)} && (3.10) \end{aligned}\right\} \text{ algebraic mapping}$$

Then the integrals which we must asymptotically evaluate are

$$b_n = \frac{1}{\pi i} \int \frac{1}{(1-Z^2)^{1/2}}\, e^{\phi(Z)}\, dZ \qquad \text{domain truncation} \tag{3.11}$$

with

$$\phi(Z) = -[A(L/2)^k](Z+1)^k - n\log[Z + (Z^2-1)^{1/2}] \tag{3.12}$$

and

$$I_n = \frac{1}{\pi}\int_0^{\pi} e^{\phi(t)}\, dt \qquad \text{algebraic mapping} \tag{3.13}$$

$$\phi(t) = -[AL^k]\,\mathrm{cotan}^{2k}(t/2) + int, \tag{3.14}$$

where the coefficients are given by $b_n = I_n + I_n^*$, where the asterisk denotes the complex conjugate.

There are actually two distinct asymptotic approximations that can be derived for each integral. The "regular" asymptotics are obtained by allowing $n \to \infty$ with L *fixed.* The "uniform" asymptotics are obtained by allowing both n and L to *simultaneously* tend to ∞ in such a way that $L \propto n^{1/k}$.

With L fixed, the stationary points of (3.11) all are such that $|Z_s| \to \infty$ as $n \to \infty$ while the stationary points $|t_s| \to 0$ in this same limit for (3.13). Because of this, ϕ in (3.12) [3.14] can be approximated by its large [small] limit so that both the stationary points and the value of ϕ at the stationary points can be obtained in simple analytic form as given in the Appendix. One finds

$$b_n \simeq [\ \ ]\, e^{(n/k - n\log[(Ak)^{1/k}L] - n/k\log(n))}, \qquad n \to \infty,\ L \text{ fixed [domain truncation]}, \tag{3.15}$$

$$b_n \simeq [\ \ ]\, e^{-pn^{2k/(2k+1)}} \cos[qn^{2k/(2k+1)} + \pi/(2k+2)], \qquad n \to \infty,\ L \text{ fixed [algebraic mapping]}, \tag{3.16}$$

where

$$p = (2 + 1/k)\, A^{1/(2k+1)} L^{k/(2k+1)} \cos\left[\frac{\pi k}{2k+1}\right], \tag{3.17}$$

$$q = (2 + 1/k)\, A^{1/(2k+1)} L^{k/(2k+1)} \sin\left[\frac{\pi k}{2k+1}\right]. \tag{3.18}$$

The empty square brackets in (3.15) and (3.16) denote the algebraic factors $[\{2\pi/(-\phi'')\}^{1/2} h$ in (3.3)] which, as described earlier, will be ignored in estimating the optimum values of L.

Equation (3.15) is dominated by the last term in the exponential which shows that one obtains "super-geometric" convergence in the sense defined in Section 2. This is actually a general property of the Chebyshev series for any entire function expanded on a finite interval as shown by Gottlieb and Orszag [2], but here it is misleading because we are interested in an approximation over a semi-infinite interval. With L fixed, the domain error E_D is fixed and does not converge at all unless L is somehow increasing with n. We need the "uniform" asymptotic approximations to obtain the best possible results for an entire function.

A similar remark is true for algebraic mapping. Although the Chebyshev series will converge even if the mapping parameter L is fixed, (3.16) shows that the convergence is "sub-geometric" with exponential convergence order $r = 2k/(2k+1)$, which is not impressive.

If we allow L to vary as $n^{1/k}$, however, we find that for both domain truncation and mapping, the total error decreases geometrically and that this is the best possible for a transcendental function. To evaluate the Chebyshev coefficients and choose the best proportionality factor for L, we must use the "uniform" asymptotics.

To obtain them, let

$$AL^k = \lambda n, \tag{3.19}$$

where λ is a constant independent of n, which implies

$$L = \left\{\frac{\lambda}{A}\right\}^{1/k} n^{1/k}, \tag{3.20}$$

where L is either the domain size or the mapping parameter. The functions can then be factored as

$$\phi(Z) = -n\left\{\frac{\lambda}{2^k}(Z+1)^k + \log[Z + (Z^2-1)^{1/2}]\right\} \qquad \text{[domain truncation]}, \tag{3.21}$$

$$\phi(t) = -n\{\lambda \cot\text{an}^{2k}(t/2) + it\} \qquad \text{[algebraic mapping]}. \tag{3.22}$$

Since n is a common factor, it can simply be divided out of the equation that determines the stationary points, (3.2), so that the stationary points are *independent* of n and functions only of the constants λ and k for the "uniform" asymptotics. Because the stationary points have fixed, finite values independent of n, however, instead of tending to zero or infinity for n large, one must use the full forms of (3.21) and (3.22) in (3.3) to obtain the stationary points.

It is, however, a trivial task to compute the stationary points for various λ and k and then determine which values of λ, $\lambda_{\text{opt}}(k)$, gives (ignoring algebraic factors and examining $\phi(Z_s)$ alone) the smallest total error. For domain truncation, the total error is the sum of the domain (E_{D}) and series (E_{S}) errors defined in Section 2; for algebraic mapping, the total error is simply the series truncation error.

The results for integral k are given in Tables I and II along with the parameter $\delta(k)$ for which the total error is

$$E_{\text{total}} \sim O\left[\left(\frac{1}{\delta}\right)^n\right] \tag{3.23}$$

when the optimum value of λ is employed. Note that λ and δ are *independent* of A in (3.6) and depend only on k, the *order* of the entire function.

TABLE I

Optimum Scaling and Accuracy for Domain Truncation

k	λ	δ
1	0.896	2.45
2	0.803	2.23
3	0.719	2.05
4	0.645	1.90
5	0.577	1.78

Note. λ defined by (3.19). The error is approximately $E_S = (1/\delta)^n$ when this optimum value of λ is used.

As k increases, $f(z)$ tends to the step function

$$\begin{aligned} f(z) &= 1, \qquad |z| \leqslant 1, \\ &= 0, \qquad |z| \geqslant 1, \end{aligned} \tag{3.24}$$

which is discontinuous and has a Chebyshev series whose coefficients decrease algebraically (rather than exponentially) with n, so it is obvious that increasing k is associated with less and less smoothness for $f(z)$. Hence, δ decreases with k, implying that one is forced to settle for less accuracy (for a given n) for an entire function of large order k than for one of lower order.

The results for domain truncation can be described analytically via

$$\begin{aligned} \lambda &= (0.896)^k \\ \delta &= e^{(0.896)^k} \end{aligned} \qquad \text{[domain truncation, entire function of order } k\text{]}, \tag{3.25}$$

TABLE II

Optimum Scaling and Accuracy for Algebraic Mapping

k	λ	δ
1	0.707	2.414
2	0.271	1.497
3	0.173	1.303
4	0.128	1.218
5	0.101	1.171

and those for algebraic mapping are

$$\lambda = \frac{1}{2k \cos\left[\frac{\pi}{4k}\right]}$$

$$\delta = \rho + \{\rho^2 + 1\}^{1/2} \qquad \text{[algebraic mapping, entire function of order } k], \qquad (3.26)$$

$$\rho = \tan\left[\frac{\pi}{4k}\right].$$

The simplicity of (3.25) and (3.26) clearly shows the tremendous dividend obtained by neglecting the algebraic factors of n represented by the empty brackets in (3.15) and (3.16). In the next section, explicit numerical experiments will show that these predictions are more than adequate for a numerical modeller, who after all is not interested in L and δ for their own sake, but only for the purposes of solving his problem efficiently. Here it will suffice to recall that (3.25) and (3.26) can be formally regarded as the lowest order terms in asymptotic expansions of λ and δ which becomes increasingly accurate as $n \to \infty$.

For $k = 1$, $\delta \sim 2.4$ for both domain truncation and algebraic mapping, but as k increases, domain truncation can give much higher accuracy than algebraic mapping for a given number of Chebyshev polynomials. The reason appears to be that with mapping, $f(Z)$ is so small that it is indistinguishable from 0 on a finite precision computer over a large part of the transformed interval $[-1, 1]$. In effect, a large part of $[-1, 1]$ is mapped from that portion of the original semi-infinite interval *outside* where one would put the domain boundary when using the other method, especially for large k. This is wasteful as reflected by lower values of δ for $k > 1$ with mapping. The choice of an explicit domain size, in contrast, is a very efficient way of ensuring that the Chebyshev polynomials do their work on that region of the original semi-infinite interval where $f(z)$ is larger than the preset tolerance E_D, and not on the region corresponding to larger z where the function is computationally indistinguishable from 0.

Why then did Grosch and Orszag [1] conclude that algebraic mapping was generally superior to domain truncation even for finding the eigenvalues of the quantum mechanical harmonic oscillator whose eigenfunctions (the Hermite functions) are entire functions of order $k = 2$? Part of the answer is that they employed the change of variable $z = x^2$ (by exploiting the symmetry of their problem) which effectively reduced the order of the solution to $k = 1$, for which optimized algebraic mapping and domain truncation give similar accuracy. The other and more important part of the answer is that they observed empirically that algebraic mapping was much less *sensitive* than domain truncation to the precise value of L.

The reason is that the optimum mapping parameter L is the minimum of a single curve (the series error E_S). It follows that the graph of E_S versus L must be flat and therefore relatively insensitive to the precise choice of L in the neighborhood of the minimum. In contrast, the domain size L for the other method is determined as the V-

necked intersection of two separate curves—one giving the domain error E_D as an exponentially decreasing function of L and the other displaying the series truncation error E_S as an exponentially increasing function of L. Figure 1 compares the δ, i.e., the logarithm of the total error divided by n, for both domain truncation and algebraic mapping as a function of λ divided by its optimum value. The graph shows clearly that if it were necessary to determine L by trial-and-error, as done by Grosch and Orszag, then algebraic mapping would be preferable, at least for $k = 1$, because the accuracy is relatively insensitive to one's choice of L. The purpose of this paper, however, is to make such trial-and-error unnecessary if one knows the asymptotic behavior of the solution $f(z)$ so that (for $k > 1$) one can exploit the greater accuracy of domain truncation for entire functions.

For singular $f(z)$, however, which we shall consider next, this insensitivity of algebraic mapping is crucially important as shall be shown below.

The Chebyshev coefficients d_n for the singular model function

$$f(z) = \frac{e^{-Az^k}}{z+s} \tag{3.27}$$

are asymptotically of the form

$$d_n = b_n + c_n, \tag{3.28}$$

where b_n are the stationary point contributions to the asymptotic evaluation of the integral representations for the coefficients and the c_n are the residues of the pole of

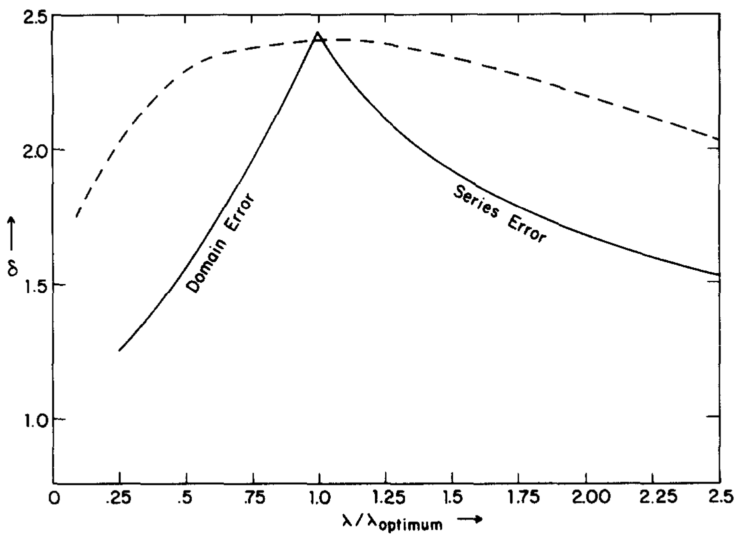

FIG. 1. δ versus $(\lambda/\lambda_{\text{optimum}})$ for domain truncation (solid) and algebraic mapping (dashed) where the total error is $O(1/\delta)^n$.

the integrand. As mentioned earlier, the presence of the denominator in (3.27) merely alters the function $h(z_s)$ in (3.3) and in our lowest order approximation, we are ignoring such factors which vary at most algebraically with n. Thus, the stationary point contributions b_n in (3.28) are identical with (3.15) and (3.16).

The pole contributions are given by the exact Chebyshev coefficients of the simple function

$$p(z) = \frac{R}{Z+S}, \tag{3.29}$$

where S, the location of the pole in the transformed coordinate $Z \in [-1, 1]$, is given by

$$S = -\frac{2s}{L} - 1 \qquad \text{[domain truncation]}, \tag{3.30}$$

$$S = -\frac{2s}{L-s} - 1 \qquad \text{[algebraic mapping]}. \tag{3.31}$$

The pole contributions are [6]

$$c_n = \frac{-2R}{(S^2-1)^{1/2}} \quad \left(\frac{1}{\Delta}\right)^n, \tag{3.32}$$

where

$$\Delta = S \pm (S^2-1)^{1/2} \tag{3.33}$$

with that sign in (3.33) which makes $|\Delta| > 1$ with

$$R = e^{-A(-s)^k}. \tag{3.34}$$

The reason that the pole contributions are given by the Chebyshev coefficients of $p(z)$ is that if we subtract $p(z)$ from $f(z)$, the difference is an entire function and the asymptotic form of the coefficients of $[f(z) - p(z)]$ must therefore be a sum of stationary point terms alone. One can of course verify (3.32) directly from the integral representations of d_n.

Although we shall explicitly examine only the case when the nearest singularity is a first order pole, Elliot [6] has shown that the coefficients for a logarithmic singularity or a second order pole are identical with (3.32), at least for large n, except for division by n for the logarithm (due to integrating the pole) or multiplication by n (due to differentiating to obtain a second order pole). Elliot [6] finds similar results for algebraic branch points. Such factors, although varying only algebraically with n, may be significant: the factor of n^3 for a fourth order pole with $n = 100$, for example, may be a great embarrassment if ignored, although this is a rather extreme example. Nonetheless, consistent with the philosophy of neglecting algebraic factors of n

which is adopted here, we can still state that the asymptotic Chebyshev coefficients are only weakly dependent on the *type* of the singularity—it is primarily its *location* relative to the interval $[-1, 1]$ in Z that is important. Consequently, considering only a simple pole in our model function is not a very serious restriction on the generality of our results.

It is clear from (3.30) through (3.34) that as L increases for either domain truncation or mapping, the singularity is moved closer to the expansion interval $[-1, 1]$ in Z and therefore the convergence of (3.32) is decreased. We have already seen, however, that it is necessary to *increase* L with n in order to obtain a geometric decrease in the stationary point and domain error. Thus, what is good for entire functions (L large) is the opposite of what is good for the pole contributions (L small) and the best choice of L will necessarily be a compromise.

Because of this, the best we can hope for is "subgeometric" convergence in the sense defined in Section 2: the stationary point contributions decrease geometrically only when L increases with n as rapidly as $n^{1/k}$ while the pole contributions decrease geometrically with n only when L is fixed. The fact that the best compromise will clearly involve increasing L with n, but more slowly than $n^{1/k}$, does have two virtues. First, the stationary points are no longer independent of n as they are when $L \propto n^{1/k}$ but instead tend to either zero or infinity so that we can use the simpler "regular" asymptotic approximations (3.15) and (3.16) instead of the more complicated "uniform" approximations involving the full forms of (3.21) and (3.22). Since the stationary point term decreases "supergeometrically" for domain truncation in this limit, we can ignore it because the dominant error term is the "subgeometrically" decreasing domain error $E_{\mathrm{D}} = \exp[-AL^k]$.

Second, since

$$L \gg s \tag{3.35}$$

for n large, we can approximate (3.30) through (3.33) to obtain

$$\Delta \sim -e^{2(s/L)^{1/2}} \tag{3.36}$$

for both algebraic mapping and domain truncation.

Our goal as before is to minimize the total error and in each case, the optimum L will be determined as the V-necked intersection of two curves, one giving c_n, which exponentially increases with L, and the other either E_{D} (domain truncation) or E_{S} (as given by (3.16); algebraic mapping) which decreases exponentially with L. One finds

$$\left.\begin{aligned} L &= qn^{2/(2k+1)} && (3.37)\\ q &\equiv \frac{2^{2/(2k+1)}}{A^{2/(2k+1)}}\, s^{1/(2k+1)} && (3.38)\\ \log E_{\mathrm{total}} &\sim -Qn^{2k/(2k+1)} && (3.39)\\ Q &= 2^{(2k)/(2k+1)} A^{1/(2k+1)} s^{k/(2k+1)} && (3.40)\end{aligned}\right\}\ \text{domain truncation,}$$

and for mapping

$$L = qn^{2/(4k+1)} \tag{3.41}$$

$$q = \left\{\frac{2s^{1/2}}{P}\right\}^{(4k+2)/(4k+1)} \tag{3.42}$$

$$P = \cos\left[\frac{\pi k}{2k+1}\right](2 + 1/k)[kA]^{1/(2k+1)} \quad \text{algebraic mapping.} \tag{3.43}$$

$$\log E_{\text{total}} \sim -Qn^{4k/(4k+1)} \tag{3.44}$$

$$Q = [2s^{1/2}]^{2k/(4k+1)} P^{(2k+1)/(4k+1)} \tag{3.45}$$

We see explicitly from (3.39) and (3.34) that we obtain subgeometric convergence in both cases, but the order is $r = 2k/(2k+1)$ for domain truncation and $r = 4k/(4k+1)$ for algebraic mapping. The reason for the more rapid convergence with mapping is, as explained earlier, that the stationary point contribution for mapping has a true minimum in L at that value which would be optimum for an entire function. In consequence, one can drastically decrease L from what would be its optimum value for an entire function without changing the logarithm of E_S very much. The domain error $E_D = \exp[-AL^k]$, in contrast, is always exponentially increasing as L is made smaller, so even modest changes in L from what would be optimum for an entire function will drastically increase the error.

Thus, with algebraic mapping, we can make a better compromise in balancing the conflicting demands of the exponential decay of $f(z)$ [as measured by the stationary point term] and of the singularity [as measured by (3.36)]. Hence, algebraic mapping is recommended for functions which have a singularity sufficiently close to the expansion interval to be important for the values of total error that is one is striving for while domain truncation is recommended for functions that are either entire or have singularities too remote from $z \in [0, \infty]$ to matter.

In the next section, we shall discuss some simple numerical experiments that demonstrate the accuracy of the formulas derived above.

4. Numerical Tests of the Theory

To verify the asymptotic analysis for the Chebyshev coefficients of the model functions, a numerical search procedure was used in which the domain size-mapping parameter L was varied to determine which value of L, L_{best}, gave the smallest error (in the L_∞ norm) when the Chebyshev series for a given function was truncated by discarding b_{n+1} and all higher coefficients. Results along with the values of L (L_{pred}) and absolute error (E_{pred}) calculated from the asymptotic theory are given in Tables III through VI. Clearly, the closer the ratio of L_{best} to L_{pred} is to 1.0, the better the prediction of the asymptotic Chebyshev coefficients. The last column of the tables provides a more precise measure: It is the ratio of the error computed numerically, not asymptotically, at $L = L_{\text{pred}}$ with the error at $L = L_{\text{best}}$. It thus shows by what ratio we increase the error by using the predictions of the asymptotic theory instead of finding the optimum L by numerical experimentation.

[redacted] converging to 1.0 from above, and for all tabulated values of n, $E(L_{\text{pred}})/E_{\text{best}}$ is roughly 2.0 to 4.0. This is impressive because the error generally decreases by roughly this same factor when we increase n by 1. Thus, one can obtain the same improvement in accuracy by adding one more Chebyshev polynomial as by keeping n fixed and carrying out careful (and possibly expensive) numerical experiments to refine L. Clearly, although one would not normally consider a 200% overestimate of the error as a function of n to be particularly praiseworthy, the proper test of the asymptotic analysis here is that it should give L and the order-of-magnitude of error E closely enough to make numerical experimentation to determine L and E both wasteful and unnecessary. In this sense and for the model functions used here, the asymptotic Chebyshev coefficient analysis is clearly successful.

The results for Table IV (algebraic mapping, entire functions) are similar to those for domain mapping for $k = 1$, but for larger k, one can see that algebraic mapping is poor in comparison to domain truncation for entire functions as the asymptotic analysis of Section 3 predicted. Again, however, for all values of the order k one sacrifices little by using the theoretical prediction for L; the best value of L for a given n reduces the error by a factor too small to be worth the bother.

One also notes that although the ratio of $L_{\text{best}}/L_{\text{pred}}$ is usually close to 1.0, convergence to 1.0 is not monotonic. In point of fact, this ratio is jumping all over the place as n is increased. Although the relatively unsophisticated search procedure employed to find L_{best} is a bit to blame, more careful searches showed that (i) the fact that the Chebyshev coefficients are discrete rather continuous functions of n and (ii) the insensitivity of algebraic mapping to L for entire functions are the primary culprits. For both domain truncation and mapping, the Chebyshev coefficients b_n are damped oscillations as functions of n. The asymptotic theory above considered only the "amplitude" of the $\{b_n\}$, but small shifts in L which move the "phase" of b_{n+1}, the first neglected coefficient, closer to a node in (n, L) parameter space may reduce the error a little. In all the tables, this phase shifting causes L to occasionally show non-monotonic convergence to its asymptotic value as L increases; the "amplitude" of the Chebyshev coefficients is so insensitive to L for entire functions treated with algebraic mapping that this phase shift effect is greatly exaggerated.

In spite of this, the most serious defect of the asymptotic theory for algebraic mapping is that the attainable accuracy is underestimated by roughly a factor of 10 for the tabulated n for $k = 1$. The abstract remedy is to carry the asymptotic analysis to higher order retaining the constants and factors which vary algebraically with n that were neglected earlier. The pragmatic remedy is to simply divide the predicted error by a factor of 10 on the authority of Table IV.

Tables V and VI give results for $k = 1$ and three different locations of the pole for domain truncation and algebraic mapping, respectively. To facilitate comparison with

TABLE III

(Domain Truncation) Comparison of Actual and Predicted Errors and Domain sizes for Entire Functions of Order k

n	L_{best}	L_{best}/L_{pred}	E_{best}	E_{best}/E_{pred}	$E(L_{pred})/E_{best}$
			$k=1$		
3	4.40	1.64	$3.38E-2$	0.497	2.18
6	7.19	1.34	$2.00E-3$	0.431	2.48
10	10.88	1.21	$4.93E-5$	0.384	2.76
13	13.57	1.16	$3.14E-6$	0.360	2.92
16	16.35	1.14	$2.03E-7$	0.342	3.07
20	20.02	1.12	$5.34E-9$	0.324	3.23
24	23.53	1.09	$1.42E-10$	0.309	3.37
28	27.26	1.09	$3.86E-12$	0.304	3.44
			$k=2$		
3	2.11	1.36	$4.32E-2$	0.480	2.32
6	2.63	1.20	$3.34E-3$	0.412	2.66
10	3.21	1.13	$8.77E-5$	0.269	3.85
13	3.58	1.11	$7.47E-6$	0.255	4.02
16	3.92	1.09	$6.32E-7$	0.240	4.29
20	4.35	1.09	$1.36E-8$	0.128	8.19
24	5.01	1.14	$7.47E-10$	0.174	6.01
28	5.01	1.06	$3.27E-11$	0.189	5.44
32	5.36	1.06	$1.04E-12$	0.150	6.89
			$k=5$		
3	1.41	1.27	$9.64E-2$	0.545	2.20
6	1.55	1.21	$1.09E-2$	0.345	3.41
10	1.56	1.10	$1.27E-3$	0.410	2.77
13	1.65	1.10	$1.46E-4$	0.265	4.29
16	1.63	1.04	$2.57E-5$	0.265	4.13
20	1.74	1.06	$2.19E-6$	0.227	4.90
24	1.76	1.04	$2.81E-7$	0.293	3.72
28	1.79	1.03	$2.53E-8$	0.266	3.95
32	1.84	1.03	$1.63E-9$	0.173	6.21
36	1.89	1.03	$2.11E-10$	0.225	4.81
40	1.91	1.02	$2.35E-11$	0.253	4.16

Note. L_{best} and E_{best} are determined by numerically computing the Chebyshev coefficients for various L and then picking that value of L, L_{best}, which gives the smallest error E_{best}, when the Chebyshev series is truncated by discarding b_{n+1} and all higher coefficients. L_{pred} and E_{pred} are those predicted by the asymptotic analysis (given in the text). $E(L_{pred})/E_{best}$ is the ratio of the error we would make by using $L = L_{pred}$ in comparison to the smallest error possible for a given value of n.

TABLE IV

(Algebraic Mapping) Comparison of Actual and Predicted Errors and Mapping Parameters for Entire Functions of Order k

n	L_{best}	L_{best}/L_{pred}	E_{best}	E_{best}/E_{pred}	$E(L_{pred})/E_{best}$
			$k=1$		
3	3.77	1.78	$8.87E-3$	0.125	2.83
.6	5.26	1.24	$4.95E-4$	0.098	2.52
10	8.41	1.19	$1.16E-5$	0.078	2.55
13	9.99	1.09	$7.72E-7$	0.073	2.30
16	14.93	1.32	$5.57E-8$	0.074	1.36
20	14.74	1.04	$1.41E-9$	0.064	1.91
24	14.88	0.88	$4.24E-11$	0.065	1.99
28	24.38	1.23	$1.20E-12$	0.063	2.09
			$k=2$		
3	0.85	0.95	$1.01E-1$	0.338	1.04
6	1.53	1.20	$2.09E-2$	0.235	1.64
10	1.53	0.93	$3.85E-3$	0.217	1.27
13	1.97	1.05	$9.34E-4$	0.177	1.42
16	2.34	1.13	$2.55E-4$	0.162	1.67
20	2.34	1.01	$4.77E-5$	0.152	1.02
24	2.36	0.93	$9.32E-6$	0.149	1.58
28	2.93	1.06	$1.55E-6$	0.124	1.72
32	2.94	1.00	$3.10E-7$	0.125	1.00
			$k=5$		
3	0.92	1.17	$3.29E-1$	0.529	1.25
6	1.44	1.59	$1.99E-1$	0.512	1.13
10	1.21	1.21	$8.32E-2$	0.403	1.18
13	0.99	0.93	$4.76E-2$	0.370	1.21
16	1.19	1.08	$2.45E-2$	0.305	1.42
20	0.88	0.76	$1.47E-2$	0.345	1.04
24	1.19	0.99	$6.17E-3$	0.272	1.02
28	1.31	1.06	$3.49E-3$	0.289	1.08
32	1.43	1.13	$1.53E-3$	0.238	1.33
36	1.22	0.94	$7.17E-4$	0.210	1.30
40	1.41	1.06	$2.45E-4$	0.135	1.84

the results for entire functions, the singular functions were taken in the normalized form $f(x) = s\exp(-x)/(x+s)$. The domain truncation error is defined as the value of $f(L)$ for purposes of numerically finding L_{best} even though the factor $1/(L+s)$ was omitted from the asymptotic theory of Section 3 for simplicity.

For domain truncation, the theory consistently overestimates the optimum value of L although there is clear convergence of L_{best}/L_{pred} to 1.0 from below as $n \to \infty$ for

TABLE V

(Domain Truncation) Comparison of Actual and Predicted Errors and Domain Sizes for Singular Functions with $k = 1$ and Various Locations of the Pole at $x = -s$

n	L_{best}	L_{best}/L_{pred}	E_{best}	E_{best}/E_{pred}	$E(L_{pred})/E_{best}$
		$S = 0.1$			
3	.72	0.47	0.140	0.658	1.40
6	1.21	0.50	$4.94E-2$	0.562	1.67
10	1.90	0.55	$1.66E-2$	0.506	1.90
13	2.39	0.59	$8.17E-3$	0.480	2.03
16	2.88	0.62	$4.29E-3$	0.491	2.13
20	3.51	0.65	$1.94E-3$	0.442	2.24
24	4.10	0.67	$9.30E-4$	0.427	2.33
28	4.67	0.69	$4.64E-4$	0.414	2.40
32	5.25	0.71	$2.39E-4$	0.401	2.43
36	5.80	0.72	$1.24E-4$	0.383	2.39
40	6.44	0.75	$6.25E-5$	0.346	2.23
		$S = 1.0$			
3	2.57	0.78	$5.73E-2$	1.56	1.14
6	4.14	0.79	$8.26E-3$	1.56	1.32
10	6.03	0.82	$9.48E-4$	1.50	1.47
13	7.28	0.83	$2.26E-4$	1.46	1.55
16	8.48	0.84	$6.00E-5$	1.43	1.62
20	9.97	0.85	$1.16E-5$	1.39	1.71
24	11.42	0.86	$2.49E-6$	1.36	1.78
28	12.74	0.87	$5.85E-7$	1.33	1.84
32	14.03	0.88	$1.47E-7$	1.31	1.90
36	15.28	0.88	$3.90E-8$	1.28	1.95
40	16.50	0.89	$1.08E-8$	1.25	1.97
		$s = 10.0$			
3	4.03	0.57	$3.48E-2$	42.8	2.2
6	6.58	0.58	$2.19E-3$	$1.76E2$	4.8
10	9.91	0.62	$6.21E-5$	$4.87E2$	10.4
13	12.39	0.66	$4.62E-6$	$7.51E2$	15.5
16	14.83	0.68	$3.64E-7$	$9.83E2$	20.8
20	18.07	0.72	$1.37E-8$	$1.20E3$	27.0
24	21.12	0.74	$5.79E-10$	$1.32E2$	31.3
28	24.07	0.76	$2.80E-11$	$1.39E3$	33.9

Note. The function is $f(x) = s\exp(-x)/(x+s)$ with the domain error $E_D = s\exp(-L)/(L+s)$.

TABLE VI

(Algebraic Mapping) Comparison of Actual and Predicted Errors and Mapping Parameters for Singular Functions with $k = 1$ and Various Locations of the Pole at $x = -s$

n	L_{best}	L_{best}/L_{pred}	E_{best}	E_{best}/E_{pred}	$E(L_{pred})/E_{best}$
			$s = 0.1$		
3	0.26	0.47	$1.18E-2$	1.52	4.30
6	0.35	0.48	$1.04E-3$	0.89	7.24
10	0.49	0.55	$3.88E-5$	0.32	$2.01E1$
13	0.56	0.57	$9.75E-6$	0.38	$1.65E1$
16	0.60	0.55	$2.49E-7$	0.43	$1.42E1$
20	0.72	0.61	$2.03E-7$	0.24	$2.56E1$
24	0.80	0.63	$4.78E-8$	0.35	$1.70E1$
28	0.92	0.68	$5.03E-9$	0.22	$2.72E1$
32	1.00	0.70	$1.28E-9$	0.31	$1.88E1$
36	1.10	0.74	$1.51E-10$	0.19	$2.93E1$
40	1.17	0.75	$4.66E-11$	0.31	$1.78E1$
			$s = 1.0$		
3	1.82	0.83	$2.37E-3$	0.1366	4.48
6	1.91	0.66	$2.47E-4$	0.287	3.10
10	2.76	0.78	$6.43E-6$	0.263	2.75
13	2.81	0.71	$8.78E-7$	0.429	1.61
16	4.16	0.97	$8.95E-8$	0.466	1.02
20	3.75	0.80	$4.20E-9$	0.450	1.39
24	4.57	0.91	$1.49E-10$	0.290	1.92
28	5.28	0.99	$5.88E-12$	0.190	1.38
32	5.69	1.01	$6.28E-13$	0.311	1.04
36	5.80	0.98	$1.24E-13$	0.875	1.02
40	6.90	1.12	$5.31E-14$	0.507	1.12
			$s = 10.0$		
3	4.07	0.47	$2.03E-2$	1.25	5.52
6	8.66	0.75	$7.47E-4$	5.38	8.27
10	7.72	0.55	$9.36E-6$	$1.91E1$	7.47
13	9.20	0.59	$5.51E-7$	$5.72E1$	4.04
16	13.84	0.81	$3.39E-8$	$1.50E2$	2.45
20	13.74	0.74	$7.61E-10$	$4.05E2$	2.99
24	19.91	0.99	$1.81E-11$	$9.57E2$	1.23
28	19.89	0.93	$5.55E-13$	$2.51E3$	2.03
32	25.83	1.15	$1.04E-13$	$3.54E4$	1.16

all three locations of the singularity. The theory is quite successful for both $s = 0.1$ and $s = 1.0$ in the sense that using L_{pred} instead of L_{best} increases the error by at worst a factor of 1.5 to 2.5. The large overestimates of L for $s = 0.1$ are rather deceiving in this sense because L is so small that the total error is not very sensitive to L. We could probably eliminate most of this overshoot by including the multiplicative factor of $2R$ (R is the residue at the pole) which was dropped for simplicity in Section 3 in estimating the error due to the pole contribution. For $n = 3$, this doubling of the pole error would force us to roughly halve L at the expense of increasing E_{D} by $\exp(-0.7)$, which is roughly also factor of 2. For $s = 1.0$, the pole error is much smaller for a given L so we can employ a much larger L than when the singularity is very close to the origin. The total error is much smaller for a given n than for $s = 0.1$ and so is much less sensitive to the factor of $2R$, giving us a much better ratio of $L_{\text{best}}/L_{\text{pred}}$.

For $s = 10.0$, the singularity is so far from the expansion interval of $z \in [0, L]$ that the pole has only a small impact on the Chebyshev coefficients. In consequence, we should ignore the pole (except for very, very large n) and use the theory for entire functions. The entries for this part of Table V for L and E_{best} are almost identical with those for the $k = 1$ section of Table III. The ratio of $L_{\text{best}}/L_{\text{pred}}$ is poor because the series error E_{S}—neglected in the two way balance between the pole contribution and the domain error E_{D} that was the basis of the analysis for singular functions in Section 3—is more important than the pole contribution for a distant singularity and moderate n.

Similar remarks apply with algebraic mapping; for $s = 10.0$, we should ignore the pole entirely except for very large s.

When the pole is important, however, comparison between Tables V and VI shows strikingly what was concluded in Section 3: algebraic mapping is far superior to domain truncation when $f(z)$ has a singularity close enough to the origin to significantly affect the Chebyshev series. When $n = 28$, for example, algebraic mapping gives an error only $5.3E-9$ versus $4.6E-4$ for domain truncation—a difference of a factor of 100,000. As explained in Section 3 (but worth reiterating here), the reason for this difference is shown in Fig. 1. Algebraic mapping for an entire function is insensitive to L because it has a true minimum at the optimum value of L. In consequence, we can take $L \ll L_{\text{optimum}}$, where L_{optimum} is the value of L that would be best for an entire function, with only a modest increase in the stationary point contribution to the asymptotic Chebyshev coefficients.

With domain truncation in contrast, the value of L that is optimum for an entire function is the cusp-shaped intersection found by minimizing the sum of the series error E_{S} (increasing with L) and the domain error E_{D} (which decreases with L). In order to accurately resolve the singularity, we must again take L as small as possible, but whereas algebraic mapping is insensitive to L, decreasing L causes the domain error E_{D} to increase exponentially.

If we arbitrarily set $L = 0.1L_{\text{optimum}}$—ignoring the pole for the moment—one could obtain the same accuracy for an entire function of order $k = 1$ by increasing n by 1.5, but one would need to increase n by 10 to do the same with domain truncation. This difference—one would need six times as many Chebyshev polynomials with domain truncation as algebraic mapping for an entire function with $L = 0.1L_{\text{optimum}}$—shows clearly that with algebraic mapping, one can take a smaller ratio of L/L_{optimum} and thus make a better compromise between the conflicting demands of the pole and the exponential decay.

5. Expansions on $[-\infty, \infty]$

When the computational domain is infinite, instead of merely semi-infinite, it is usually difficult to make a simple statement about the optimum choice of scale factor because $f(z)$ will usually exhibit different asymptotic behavior as $z \to -\infty$ than as $z \to \infty$. The most efficient L for an entire function will then be a compromise between what is best for large positive z and what is most effective for large negative z. For a singular function, the optimum L will emerge from a three way tug-of-war between two stationary point contributions and a pole term in the asymptotic evaluation of the Chebyshev coefficient a_n. The analysis for an infinite interval involves no new principles beyond those explained above for a semi-infinite interval, but the details do become complicated.

When $f(z)$ does exhibit the same asymptotic behavior as $|z| \to \infty$, however—a function symmetric about $z = 0$, for example—then the situation is very different because one can apply the results for a semi-infinite interval directly. There are, however, two good and one bad way to do this.

One good technique if $f(z)$ is symmetric about $z = 0$ was employed by Grosch and Orszag: change variable to $y = z^2$ and then solve the problem $y \in [0, \infty]$ by either algebraic mapping or domain truncation. The virtue of this change of variable is that it effectively halves the order k: $\exp(-z^2)$ $[k = 2] \to \exp(-y)$ $[k = 1]$, for example. Because of this Grosch and Orszag found that for the quantum harmonic oscillator ($k = 2$, entire function), algebraic mapping was superior to domain truncation because it gave as high an obtainable accuracy and was much less sensitive to the parameter L. This seems contrary to our earlier finding that one could obtain higher accuracy for $k = 2$ with domain truncation; the resolution of the paradox is that their change of variable reduced the order to $k = 1$ for which the highest accuracy attainable with domain truncation is no better than for mapping.

We can justify this halving-of-order argument and also the second way of dealing with an infinite domain by using the Chebyshev polynomial identity

$$T_{2n}(w) = T_n(2w^2 - 1). \tag{5.1}$$

In consequence, if in domain truncation we have the expansion

$$\frac{e^{-A(L/2)^k(Z+1)^k}}{[(L/2)(Z+1)+s]} = \sum_{j=0}^{n} b_j(k, L, A, s)\, T_j(Z), \tag{5.2}$$

making the replacement

$$Z \to 2Z^2 - 1$$

gives us

$$\frac{e^{-AL^k Z^{2k}}}{[LZ^2+s]}=\sum_{j=0}^{n} b_j(k, L, A, s)\, T_{2j}(Z). \tag{5.3}$$

Equation (5.3) is indeed an expansion of our model function on a truncated infinite interval, but the notation is that for a semi-infinite interval. If we attacked an infinite interval directly, it would be natural to define

$$Z=\frac{z}{L'} \tag{5.4}$$

where the computational domain is $z \in [-L', L']$, to take N to be the degree of the highest Chebyshev polynomial in (5.3), K the order of $f(z)$, and Λ the K-dependent constant in the analogue of (3.19), which is

$$AL'^K=\Lambda(K)N \tag{5.5}$$

and to write (5.3) as

$$\frac{e^{-AL'^K Z^K}}{[L'^2Z^2+s'^2]}=\sum_{\substack{j=0\\ [\text{even } j]}}^{N} B_j T_j \tag{5.6}$$

with $s'^2=s$. Comparison with (5.3) itself shows that

$$B_j(K, L', A, s')=b_{j/2}(K/2, L'^2, A, s'^2) \tag{5.7}$$

for all values of K, L', and A, and this is an exact relationship quite independent of the steepest descent approximations.

It is now trivial to obtain the optimized parameter values. For entire functions of order K, one finds

$$\Lambda(K)=\tfrac{1}{2}\lambda(K/2), \tag{5.8}$$

$$E_{\text{total}} \simeq O\left[\left(\frac{1}{\Delta}\right)^N\right], \tag{5.9}$$

where

$$\Delta(K)=\sqrt{\delta(K/2)}. \tag{5.10}$$

Thus, for domain truncation for a function which is asymptotically similar for both large positive and negative z, the optimum scalings for an infinite domain follow trivially from those for a semi-infinite interval.

Strictly speaking, the derivation above applies only to a symmetric function; however, it is essentially trivial to obtain similar results for an antisymmetric function merely by differentiating (5.3) with respect to x. Any function can be written as the sum of a symmetric function plus an antisymmetric function through the identity $f(z) = [f(z) + f(-z)]/2 + [f(z) - f(-z]/2$, so these are the only two cases we need to consider.

For a function $f(z)$ which is neither symmetric nor antisymmetric, the Chebyshev series will need both the even and odd degree polynomials. The square root in (5.10) shows that, logically enough, we need twice as many polynomials to obtain a given degree of accuracy for a given function on an infinite interval than on one which is only semi-infinite. If, however, $f(z)$ is either symmetric or antisymmetric about $z = 0$, we can obtain the same accuracy with half the numberof degrees of freedom by using only the Chebyshev polynomials of the same symmetry—the even degree polynomials for an even function as in (5.3) and the odd polynomials for an antisymmetric $f(z)$. In either event, the total error is proportional to

$$E_S \sim O[\delta(K/2)^{-n}] \qquad \text{(symmetric or antisymmetric } f(z)), \tag{5.11}$$

where $n = N/2$ is the number of degrees of freedom.

Equation (5.12) shows that a third alternative for a function of definite symmetry—solving the problem on the semi-infinite interval $z \in [0, \infty]$ with the boundary condition $f'(0) = 0$ (symmetric function) or $f(0) = 0$ (antisymmetric)—is inferior to the two strategies given earlier because

$$E_S \sim O[\delta(K)^{-n}] \qquad \text{(semi-infinite interval).} \tag{5.12}$$

Since $\delta(K) < \delta(K/2)$, it is always preferable to either change variable to $y = z^2$, as done by Grosch and Orszag, or to solve it on the full interval $[-\infty, \infty]$ using only the Chebyshev polynomials of the appropriate symmetry.

The reason for this difference is that for $f(z) = \exp(-z^2)$, for example, the function varies more and more rapidly as $|z| \to \infty$. Consequently, we need little resolution for small z and high resolution for large z. The Grosch–Orszag change of variable is also a variable stretching which equalizes the resolution requirements over the whole interval and thus improves the convergence of the Chebyshev series.

Solving the problem on the full interval $[-\infty, \infty]$ is equally effective for a different reason: as discussed at length in Boyd [7], the Chebyshev polynomials have in effect a built-in quadratic variable stretching that gives particularly high resolution at the ends of the interval. When the problem is solved on $z \in [0, \infty]$, one of these high resolution areas in Z is wasted because Z near -1 then corresponds to z near 0. When we use the full interval and keep only the even or odd polynomials, the two high resolution areas in Z correspond with large positive and negative z where this resolution is needed.

Similar remarks apply to algebraic mapping except that the form of the mapping must be changed to

$$Z = \frac{z}{L'^2 + z^2} \tag{5.13}$$

with the explicit inverse

$$z = \frac{L'Z}{(1 - Z^2)^{1/2}}. \tag{5.14}$$

For the model function on $z \in [-\infty, \infty]$

$$f(z) = \frac{e^{-Az^K}}{(z^2 + s'^2)} \tag{5.15}$$

the same substitution

$$Z \to 2Z^2 - 1, \tag{5.16}$$

which generates (5.3) from (5.2) also generates the Chebyshev expansion of (5.15) from that for the corresponding model function (3.27) with the algebraic mapping for the semi-infinite interval, (3.10). Therefore, (5.7) to (5.10), which give the relationships between the coefficients and parameters of expansions on infinite versus semi-infinite intervals, are exact for algebraic mapping as well as for domain truncation.

6. Exponential Mapping

Consider the mapping

$$Z = 1 - 2e^{-z/L} \tag{6.1}$$

with the inverse transformation

$$z = -L \log[(1 - Z)/2]. \tag{6.2}$$

The model function

$$f(z) = e^{-Az^k} \tag{6.3}$$

becomes

$$f(z) = e^{-a(-1)^k \log^k[(1-Z)/2]}, \tag{6.4}$$

where

$$a \equiv AL^k \tag{6.5}$$

For the special case $k = 1$, (9.4) simplifies to

$$f(z) = \frac{(1 - Z)^a}{2^a}. \tag{6.6}$$

This tells us immediately that exponential mappings are of doubtful value because unless a is an integer, (9.6) will be strongly singular at $Z = 1$. Elliot [6] has shown that the resulting Chebyshev coefficients are $O(n^{-2a-1})$, i.e., finite order convergence.

When $k \geqslant 2$, the convergence is again exponential, but very poor. By performing an analysis identical to that in Section 5, one can derive

$$b_n \sim e^{-2^k \log^k(n)} [\ ], \tag{6.7}$$

where the [ ] stands for algebraic and other factors of n which decrease more slowly than the factor written out explicitly. Since one can show

[illegible]

for any fixed j by rewriting n^j as an exponential, it follows that the Chebyshev series technically possesses the property of exponential or "infinite [algebraic] order" convergence. However, it is equally trivial to show that

$$\operatorname*{limit}_{n \to \infty} e^{n^r} b_n = \infty \tag{6.9}$$

for any $r > 0$ which means that the exponential convergence order r, as defined in Section 2, is 0 even though the usual algebraic convergence order is infinite. This strongly suggests that exponential mappings are highly inferior tools for attacking a problem on a semi-infinite domain because the transformed function is too strongly singular.

As noted earlier, the poorness of exponential mappings has already been found empirically by Grosch and Orszag [1]. The results of this section are first, to confirm their conclusions theoretically, and second, to show that the steepest descent method can be applied to assess the usefulness of almost any type of mapping.

7. Summary

Steepest descent methods can give simple predictions for the optimum choice of a domain size or mapping parameter L in applying Chebyshev polynomial techniques on infinite or semi-infinite intervals. For simplicity, attention has been largely confined to either (i) entire functions or (ii) exponentially decaying functions with a single singularity.

For entire functions, domain truncation is the surprise winner, particularly for higher values of k where k is the order of the entire function. The optimum value of L varies with n—this is true for singular functions as well—and the convergence is "geometric" in the sense defined in Section 2. The specific formulas are given both in Section 3 and the abstract.

When the function has a pole, the asymptotic Chebyshev coefficients are given by the sum of two terms: a stationary point term, identical with that for an entire function, plus a residue evaluated at the pole. The optimum choice of L for this—and more generally, for any function $f(z)$ with two distinct length scales— is necessarily a compromise between those values of L which would separately minimize the two terms. Here, algebraic mapping is far superior to domain truncation because its stationary point contribution is much less sensitive to L than its counterpart for domain truncation. One finds

$$L = qn^{2/(4k+1)} \tag{7.1}$$

$$E_{\text{total}} \sim O[e^{-Qn^{4k/(4k+1)}}], \tag{7.2}$$

where q, Q are constants defined in (3.41) through (3.45). The convergence is still "subgeometric" as defined in Section 2, but the numerical tables of Section 4 show that very good results are possible even when the singularity is close to the expansion interval.

TABLE VII

Summary of Results, Semi-Infinite Domain

Domain truncation		Algebraic mapping
	$k = 1$	
$L = 0.896\, n/A$; $\delta = 2.45$	entire functions, optimum	$L = 0.707\, n/A$; $\delta = 2.414$
$L = 1.59A^{-2/3}s^{1/3}n^{2/3}$; $\log E \simeq -1.59A^{1/3}s^{1/3}n^{2/3}$	singular functions, optimum	$L = 1.41s^{3/5}A^{-2/5}n^{2/5}$; $\log E \simeq -1.68s^{1/5}A^{1/5}n^{4/5}$
	$k = 2$	
$L = 0.896\, (n/A)^{1/2}$; $\delta = 2.23$	entire functions, optimum	$L = 0.521\, (n/A)^{1/2}$; $\delta = 1.50$
$L = 1.32A^{-2/5}s^{1/5}n^{2/5}$; $\log E \simeq -1.74A^{-1/5}s^{2/5}n^{4/5}$	singular functions, optimum	$L = 2.47s^{5/9}A^{-2/9}n^{2/9}$; $\log E \simeq -1.27s^{2/9}A^{1/9}n^{8/9}$

Note. The model functions are the entire function $f(z) = \exp[-Az^k]$ and the singular function $f(z) = \exp[-Az^k]/(z+s)$, where k is the "order" of the function and s is a constant. For "domain truncation," L is the size of the truncated computational domain $z \in [0, L]$ which is used to approximate the semi-infinite domain $z \in [0, \infty]$. For "algebraic mapping," L is the mapping parameter in the transformation $Z = 2z/(L+z) - 1$ from $z \in [0, \infty]$ to $Z \in [-1, 1]$. For both methods, the total error is $E_{\text{total}} \simeq O(\delta^{-n})$, where n is the number of Chebyshev polynomials in the approximation and δ is the "error constant" tabulated above.

The striking simplicity of formulas like (7.1) and (7.2) has been bought at the price of a number of simplifications: (i) use of model functions; (ii) neglect of factors varying algebraically with n; (iii) a semi-infinite interval and (iv) consideration of functions with only one or two characteristic length scales. All these simplifications can in principle be relaxed. Miller [5] and Tuan and Elliott [8] have attacked more complicated functions than the models used here. The methods of steepest descent and residues easily give the neglected algebraic factors. Section 5 discusses an infinite interval, and clearly, one can certainly juggle several distinct contributions to the asymptotic Chebyshev coefficients, instead of the limit of two arbitrarily imposed here, to find the best compromise between the conflicting demands of the nearest singularity, the scale of oscillation, the scales of exponential decay for large positive x and for large negative x and so on.

It is precisely because the possible refinements are endless, that ruthless simplicity has been practiced here even at the risk of offending the mathematical purist. Such refinements obscure the fact that the underlying ideas are simple and they work.

Further advances in the understanding of the asymptotic vehavior of Chebyshev series will be welcome, but the simple expressions derived here should be sufficient for most physics and engineering problems. If not, the methodology has been explained in enough detail so that one should be able to relax one or more of the simplifications made above so as to improve upon what is given here in a manner tailored to the problem at hand. Tables VII and VIII give a final summary of our results for selected parameter values.

TABLE VIII

Summary of Results, Infinite Domain

Domain truncation		Algebraic mapping
	$K=2$	
$L'=\sqrt{\dfrac{0.448N}{A}}$ $\Delta=1.55$	entire functions, optimum	$L'=\sqrt{\dfrac{0.354N}{A}}$ $\Delta=1.55$
$L'=1.00A^{-1/3}s'^{1/3}N^{1/3}$ $\log E \simeq -1.00A^{1/3}s'^{2/3}N^{2/3}$	singular functions, optimum	$L'=1.03A^{-1/5}s'^{3/5}N^{1/5}$ $\log E \simeq -0.96A^{1/5}s'^{2/5}N^{4/5}$

Note. The model functions are the entire function $f(z)=\exp[-Az^K]$ and the singular function $f(z)=\exp[-Az^K]/(z^2+s'^2)$, where K is the order and s' is a constant. For domain truncation, L' is the size of the finite domain $z\in[-L',L']$ which is used to approximate the infinite interval $z\in[-\infty,\infty]$. For algebraic mapping, L' is the parameter in the transformation $Z=z/(L'^2+z^2)$, from $z\in[-\infty,\infty]$ to $Z\in[-1,1]$. Only results for $K=2$ are given because the Chebyshev series coefficients on the infinite interval are isomorphic with those of the semi-infinite interval given in Table 7. The isomorphism is expressed by Eqs. (5.7) to (5.10) in the text and also the definition, $s'^2\equiv s$. N is the degree of the highest polynomial kept in the approximation. The total error is $O[\Delta^{-N}]$.

APPENDIX A: Details of Steepest Descent

In this brief addendum, we will examine some of the details of the application of steepest descent to asymptotically evaluate Chebyshev coefficients which were omitted in the main body of the paper. The general method of steepest descent is lucidly discussed in Bender and Orszag [9].

The phase function $\Phi(Z)$ of the integral representation we use with domain truncation is

$$\Phi = -[A(L/2)^k](Z+1)^k - n\log[Z + (Z^2-1)^{1/2}]. \tag{3.12}$$

The stationary points Z_s of the integral are the roots of

$$\frac{d\Phi}{dZ} = -[A(L/2)^k]\, k(Z+1)^{k-1} - \frac{n}{Z+(Z^2-1)^{1/2}}\left(1+\frac{Z}{(Z^2-1)^{1/2}}\right). \tag{A.1}$$

In general, these roots must be computed numerically, but when $|Z| \gg 1$, (A1) simplified to

$$Z^k = -\frac{n}{A(L/2)^k k}, \tag{A2}$$

which has the k solutions

$$Z_s = \frac{2n^{1/k}}{A^{1/k}Lk^{1/k}}\, e^{i\pi[1+2(j-1)]/k}, \qquad j = 1,\ldots, k. \tag{A3}$$

In the limit that $n \to \infty$ with L and k fixed, $|Z_s| \to \infty$ according to (A3), so this approximation for the stationary points is consistent and gives the "regular" asymptotics.

If the integral is deformed via Cauchy's theorem into a steepest descent path, then the integral is approximately given by the sum of the separate contributions from each stationary point on the path. Figure 2 shows some sample contours for various k. In the present case, all k stationary points lie on the path and $\mathrm{Re}[\phi(Z_s)]$ is the same for each, so we must add all k terms together. We need not worry about endpoint contributions because our contours are closed and thus have no endpoints.

For the "uniform" asymptotics in which $L \propto n^{1/k}$, the approximation (A3) is not justified and the roots of (3.12) were obtained numerically. The formulas (3.25) for λ and δ were found empirically rather than deductively. They agree with the numerical results to all places calculated and are probably exact, but I have not verified this.

Similarly, the phase function ϕ for the integral representation used with algebraic mapping is

$$\phi = -[AL^k]\cot\!an^{2k}(t/2) + \mathrm{int} \tag{3.14}$$

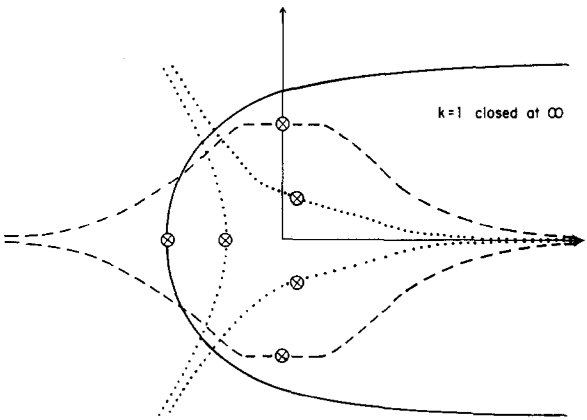

FIG. 2. Schematic steepest descent contours for (3.11) based on numerically tracing the exact contours, for $k = 1$ (solid line), $k = 2$ (dashed), and $k = 3$ (dotted). The stationary points are marked by a cross within a circle.

and thus the stationary points t_s are the roots of

$$\frac{d\phi}{dt} = \frac{\cos^{2k-1}(t/2)}{\sin^{2k+1}(t/2)} + \frac{in}{kAL^k}. \tag{A4}$$

In the limit $n \to \infty$ with L fixed, $|t_s| \to 0$ and (A4) can be approximated by

$$\left(\frac{t}{2}\right)^{2k+1} = \frac{ikAL^k}{n}. \tag{A5}$$

This also has multiple solutions like (A2), but unlike it, the only stationary point of (A5) which lies on the steepest descent path is the one nearest the positive real axis which is

$$t_s = 2\left(\frac{ikAL^k}{n}\right)^{1/(2k+1)}. \tag{A6}$$

The steepest descent path is shown in Fig. 3. The asymptotic form of I_n (defined by 3.13) is the sum of the contribution from the stationary point given by (A6) plus a (much larger!) end point contribution from near $t = \pi$. (There is no endpoint contribution from near $t = 0$ because the integrand is exponentially small there). However, $b_n = I_n + I_n^*$ and the endpoint contributions cancel out so that b_n is purely the sum of the stationary point term.

For the "uniform" asymptotics for which n and L jointly tend to infinity with

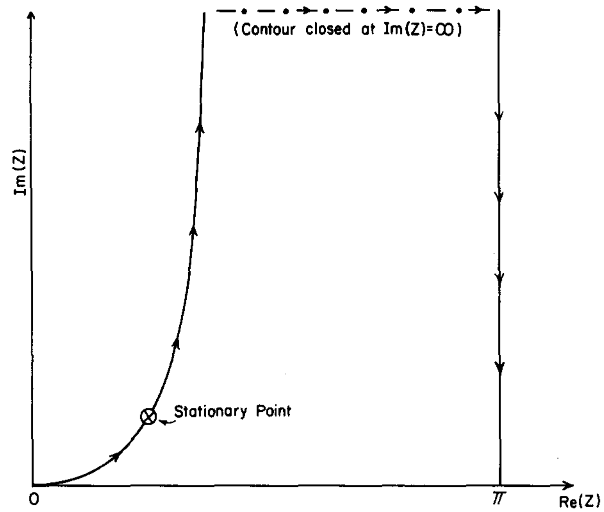

FIG. 3. Schematic steepest contour for evaluating the integral I_n, defined by (3.13), for $k=1$. The contours for higher k are similar.

$L \propto n^{1/k}$, (A4) must in general be solved numerically. However, for the special case of the optimum L, we can obtain an analytic solution for all the quantities of interest.

As before, let

$$AL^k = \lambda n, \tag{3.19}$$

where λ is a constant. The optimum λ is that which minimizes $\mathrm{Re}[\phi(t_s)]$ as a function

into it). This means that we want $\mathrm{Re}[d\phi/d\lambda]=0$ with t_s defined as an implicit function of λ through (A4). However,

$$\frac{d\phi}{d\lambda}=\frac{\partial\phi}{\partial\lambda}+\frac{\partial\phi}{\partial t}\frac{\partial t}{\partial\lambda} \tag{A7}$$

$$=\frac{\partial\phi}{\partial\lambda} \tag{A8}$$

$$=-\mathrm{cotan}^{2k}(t/2), \tag{A9}$$

where (A8) follows from the fact that $\partial\phi/\partial t=0$ is the condition for a stationary point and (A9) from direct differentiation of (3.14).

If we define the new variable

$$y=\mathrm{cotan}(t/2) \tag{A10}$$

then the condition that the real part of (A9) vanish gives

$$\arg(y) = \frac{-\pi}{4k}. \tag{A11}$$

The imaginary part of (A9) need not vanish, but the stationary point condition (A4) must be satisfied. By using the trigonometric identity

$$\frac{1}{\sin^2(t/2)} = 1 + \operatorname{cotan}^2(t/2) \tag{A12}$$

we can rewrite the stationary point condition (A4) as

$$y^{2k-1}(1 + y^2) = \frac{-i}{k\lambda}. \tag{A13}$$

Since $\arg(y)$ is already known, (A13) is (separating real and imaginary parts) equivalent to two equations in two unknowns ($|y|$ and λ) which may be trivially solved to give

$$\lambda = \frac{1}{2k \cos[\pi/4k]}, \tag{3.26a}$$

$$t_s = 2 \operatorname{cotan}^{-1}[e^{-i\pi/(4k)}]. \tag{A14}$$

Since $\operatorname{cotan}^{2k}(t_s/2)$ is imaginary when λ is equal to its optimum value given by (3.26a), (3.14) [or equivalently (3.22)] simplifies to

$$R_e[\phi(t_s)] = -nI_m[t_s]. \tag{A15}$$

To obtain the imaginary part of t_s, we can rewrite (A15) as

$$\tan\frac{(t_s)}{2} = e^{i\pi/4k}, \tag{A16}$$

define

$$t_s = X + iY, \tag{A17}$$

and then exploit two trigonometric identities from Abramowitz and Stegun [10]

$$\left|\tan\frac{(t_s)}{2}\right|^2 = \frac{\cosh(Y) - \cos(X)}{\cosh(Y) + \cos(X)} = 1, \tag{A18}$$

$$\arg\left[\tan\frac{(t_s)}{2}\right] = \tan^{-1}\frac{\sinh(Y)}{\sin(X)} = \frac{\pi}{4k}, \tag{A19}$$

where the right-hand sides follow from (A16). A moment's thought will show the first identity (A18) can only be satisfied if

$$X = \frac{\pi}{2}. \tag{A20}$$

Substituting this into (A19), taking the tangent of both sides and defining

$$\rho \equiv \tan\left(\frac{\pi}{4k}\right) \tag{3.26c}$$

gives

$$\rho = \sinh(Y) \tag{A21}$$

or equivalently

$$Y = \sinh^{-1}(\rho) \tag{A22}$$

$$= \ln[\rho + \{\rho^2 + 1\}^{1/2}], \tag{A23}$$

where we have used the logarithmic form of $\sinh^{-1}$in (A23). Equating

$$\delta^n = e^{-n\,\mathrm{Im}(t_s)} \tag{A24}$$

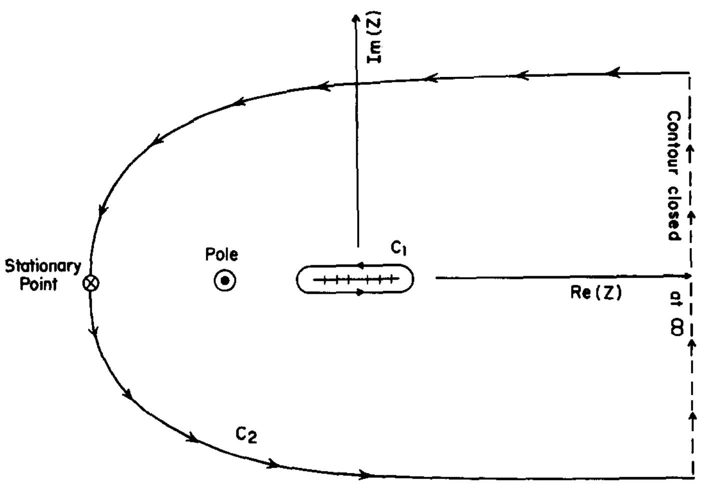

FIG. 4. The steepest descent contour C_2 and an allowable contour C_1 for the coefficient integral for the exponential-with-a-pole defined by (3.27) for $k = 1$. The stationary point is marked by an x enclosed in a circle. The cross-hatched line is the branch cut between -1 and 1 which both C_1 and C_2 enclose. It is assumed in the graph and the text that n is large enough so that C_2 encloses the pole. For smaller n for which C_2 does not enclose the pole, b_n is not affected by the pole to within the limits of the steepest descent approximation and the integrals around C_1 and C_2 are equal.

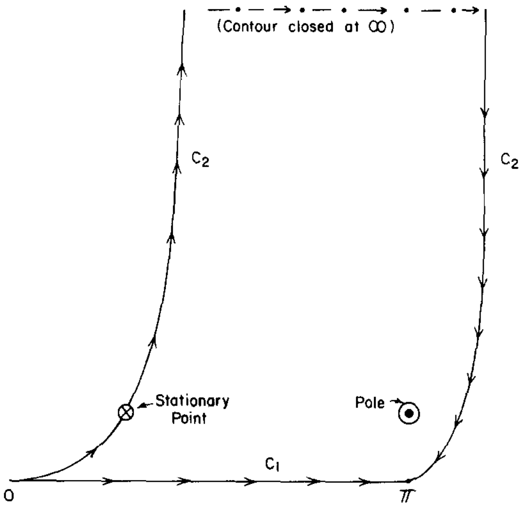

FIG. 5. Similar to Fig. 4 but for algebraic mapping. C_1 is the original contour of integration along the real axis and C_2 is the steepest descent path. The stationary point and pole are marked by circles enclosing × and a dot, respectively. The original pole in the variable Z is mapped by the trigonometric change of variable $Z = \cos t$ into a pair of complex conjugate poles, one in the upper half t-plane for I_n, the other below the real axis for I_n^*. For convenience, the pole has been taken to lie on the negative Z axis in both Fig. 4 and (implicitly) here, but its location may be complex.

and using (A17) and (A23) gives

$$\delta = \rho + \{\rho^2 + 1\}^{1/2}. \tag{3.26b}$$

Applying the method of steepest descent to a model function with a singularity is straight forward. The only complication is that in both cases as shown in Figs. 4 and 5, the integrals around original contours of integration C_1 differ from the integrals on the steepest descent paths C_2 by the residue at the pole.

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REFERENCES

1. C. E. GROSCH AND S. A. ORSZAG, *J. Comp. Phys.* **25** (1977), 273.
2. D. GOTTLIEB AND S. A. ORSZAG, "Numerical Analysis of Spectral Methods: Theory and Applications," Soc. Ind. and Appl. Math., Philadelphia, 1977.

3. D. Fox and L. Parker, "Chebyshev Polynomials in Numerical Analysis," Oxford Univ. Press, London, 1968.
4. D. Elliot and G.Szekeres, *Math. Comp.* **18** (1965), 25.
5. G. F. Miller, *J. SIAM Numer. Anal.* **3** (1966), 390.
6. D. Elliot, *Math. Comp.* **18** (1964), 274.
7. J. P. Boyd, *Mon. Wea. Rev.* **106** (1978), 1192.
8. P. D. Tuan and D. Elliott, *Math. Comp.* **26** (1972), 213.
9. C. E. Bender and S. A. Orszag, "Mathematical Methods for Scientists and Engineers," McGraw–Hill, New York, 1978.
10. M. Abramowitz and I. Stegun, "Handbook of Mathematical Functions," Dover, New York, 1965.