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Chebyshev Domain Truncation Is Inferior to Fourier Domain Truncation for Solving Problems on an Infinite Interval

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"Domain truncation" is the simple strategy of solving problems on $y \in [-\infty, \infty]$ by using a large but finite computational interval, $[-L, L]$. Since $u(y)$ is not a periodic function, spectral methods have usually employed a basis of Chebyshev polynomials, $T_n(y/L)$. In this note, we show that because $u(\pm L)$ must be very, very small if domain truncation is to succeed, it is always more efficient to apply a Fourier expansion instead. Roughly speaking, it requires about 100 Chebyshev polynomials to achieve the same accuracy as 64 Fourier terms. The Fourier expansion of a rapidly decaying but nonperiodic function on a large interval is also a dramatic illustration of the care that is necessary in applying asymptotic coefficient analysis. The behavior of the Fourier coefficients in the limit $n \to \infty$ for fixed interval L is *never* relevant or significant in this application.

KEY WORDS: Spectral methods; Fourier series; Chebyshev polynomials.

1. INTRODUCTION

The method of "domain truncation" for solving differential equations on an unbounded interval has been discussed by many authors including Grosch and Orszag (1977) and Boyd (1982). If the solution $u(y)$ decays exponentially fast as $|y| \to \infty$, then only an exponentially small error is made by truncating the computational interval to $[-L, L]$. After this truncation has been made, one may then apply finite difference or spectral methods in the same way as for any problem on a bounded interval.

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There are two sources of error (Boyd, 1982): (1) the "domain" error caused by reducing the infinite interval to a bounded one

$$E_D \equiv \max |u(y)| \qquad \text{for all} \quad |y| \geqslant L \tag{1.1}$$

and (2) a "series" error

$$E_S \equiv \max \left| \sum_{n=0}^{N} a_n \phi_n(y) - u(y) \right| \qquad \text{for all} \quad |y| \leqslant L \tag{1.2}$$

where the $\{\phi_n(y)\}$ are the basis functions and N is the series truncation. In general, the most efficient procedure is to choose L as a function of N such that the domain error and series error are of the same magnitude. When L is too large (for a given N), the domain error will be tiny, but the series error will be huge because a small number of basis functions are trying (futilely) to approximate $u(y)$ over a huge interval. When L is too small, the series error will be tiny, but the domain error relatively large.

Because $u(y)$ is not periodic, the normal choice of spectral basis functions has been Chebyshev polynomials (Grosch and Orszag, 1977; Boyd, 1982). As stressed by Gottlieb *et al.* (1984), when a nonperiodic function is expanded in a Fourier series, the coefficients decrease as *algebraic* rather than *exponential* functions of the degree n. The purpose of this note is to show that this fact, although true, is *irrelevant* for domain truncation.

This conclusion is based on a blending of three key ideas. The first is that a function $u(y)$ that decays sufficiently fast as $|y| \to \infty$ may always be decomposed into a periodic part $P(y)$ and a nonperiodic part $\bar{P}(y)$. Because $u(y)$ is very small at the edges of the periodicity interval $y \in [-L, L]$—it *must* be small if the domain error is to be small—the nonperiodic part of $u(y)$ is very small in comparison to the periodic part. In particular, if $u(y)$ decays monotonically with $|y|$ for $|y| > L$, then

$$\bar{P}(y) \leqslant |u(L)| \leqslant E_D(L) \tag{1.3}$$

The second key idea is the "integration-by-parts" theorem, which shows that the smallest coefficient in the N-term Fourier series approximation of a nonperiodic function like $\bar{P}(y)$ is asymptotically $O([P(L) - P(-L)]/N)$—that is to say, is an order of magnitude *smaller* than the domain error, $E_D(L)$, in view of (1.3). This in turn implies that the lack of periodicity of $u(y)$ is *irrelevant* insofar as domain truncation is concerned.

The third key idea is to quantify the superiority of Fourier series over Chebyshev polynomials in this application by comparing the asymptotic coefficients of $P(y)$ with those of the Chebyshev series for $u(y)$. It is difficult to state a rigorous result that covers all cases, but we offer a theorem that suggests that the ratio quoted in the abstract—N Fourier terms give roughly the same accuracy as $(\pi/2)\ N$ Chebyshev polynomials—is a good rule of thumb.

2. THE DECOMPOSITION OF A FUNCTION INTO ITS PERIODIC AND NONPERIODIC PARTS: THE METHOD OF IMBRICATE SERIES

Theorem 1. If a function $u(y)$ decays as $|y| \to \infty$ as fast as $1/y^2$, then for any chosen period $2L$,

$$u(y) = P(y) + \bar{P}(y) \tag{2.1}$$

where

$$P(y) \equiv \sum_{m=-\infty}^{\infty} u(y - 2nL) \qquad [\text{"imbrication of } u(y)\text{"}] \tag{2.2}$$

is periodic with period $2L$ and

$$\bar{P}(y) = -\sum_{\substack{m=-\infty \\ m \neq 0}}^{\infty} u(y - 2mL) \qquad [\text{"nonperiodic part of } u(y)\text{"}] \tag{2.3}$$

Proof. $P(y)$ is periodic by construction; the restriction on the decay of $u(y)$ guarantees that the sums converge. Figure 1 is a schematic of the decomposition.

The periodic function $P(y)$ is the sum of an infinite number of evenly spaced, overlapping copies of $u(y)$. $P(y)$ is said to be the "imbrication" of the "pattern function" $u(y)$, and the sum (2.2) is said to be an "imbricate series" (Boyd, 1986). The theorem is true for any L, but is useful only when L is large. In this case, then on the interval $y \in [-L, L]$, the periodic function $P(y)$ is a very good approximation to the nonperiodic function $u(y)$, and $\bar{P}(y)$ is very tiny. If $u(y)$ decays exponentially fast as $|y| \to \infty$, then both $\|\bar{P}(y)\|_\infty$ and the error in approximating $u(y)$ by $P(y)$ decrease exponentially fast as L increases.

The reason that this decomposition is useful to understand domain truncation-cum-Fourier series is that the Fourier coefficients of $u(y)$ on $y \in [-L, L]$ are the sum of the coefficients of $P(y)$ and $\bar{P}(y)$, which have very different behavior. Because $P(y)$ is periodic, its coefficients will decrease exponentially fast with n. Because $\bar{P}(y)$ is not periodic, its coef-

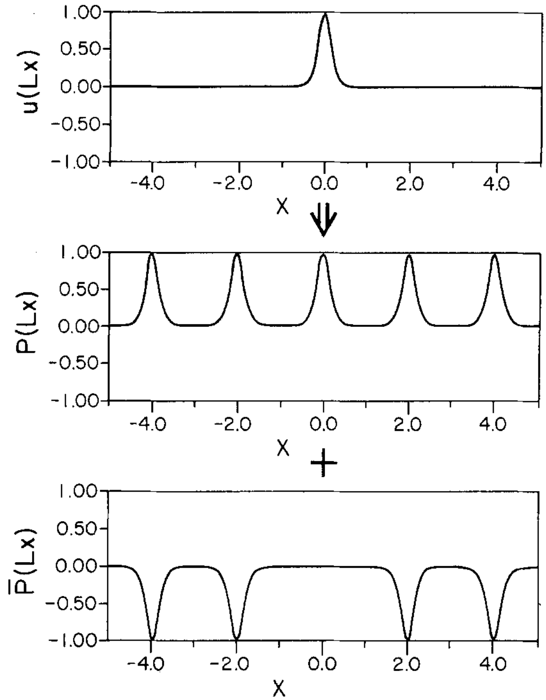

Fig. 1. Schematic showing how a function $u(y)$ which decays as $|y| \to \infty$ (top graph) may be decomposed into its periodic part (middle graph) and nonperiodic part (bottom). Note that the nonperiodic part of $u(y)$ is extremely small over the whole interval, $(y/L) \in [-1, 1]$.

ficients decrease only algebraically with n, typically as $O(1/n)$ or $O(1/n^2)$. *Asymptotically*, the coefficients of $u(y)$ will be dominated by the slowly converging coefficients of its nonperiodic part, and therefore decrease algebraically.

In domain truncation, however, one is *never* interested in the asymptotic limit $n \to \infty$ for fixed L. The reason is that the total error in approximating $u(y)$ is constrained by the domain error, E_D. For a given L, it is not sensible to add hundreds or thousands of terms to the Fourier series, but only to keep enough terms to reduce the series error $E_S(N; L)$ to the magnitude of $|u(\pm L)|$. If more accuracy is needed, one must increase the size of the truncated interval L to reduce the domain error $E_D(L)$ and then calculate a new Fourier series on the new interval. The relevant asymptotic limit is not $n \to \infty$ for *fixed* L but rather n and L *simultaneously* tending to infinity.

In this double limit, it is necessary to split $u(y)$ into two parts and calculate the large-n coefficients of each separately. In the next section, it is shown that it is the periodic part $P(y)$, not the tiny, nonperiodic function $\bar{P}(y)$, that determines the true asymptotic behavior of the Fourier coefficients of $u(y)$ in this simultaneous limit.

3. THE INTEGRATION-BY-PARTS AND GEOMETRIC CONVERGENCE THEOREMS

Theorem 2 (Integration-by-Parts). If a nonperiodic but analytic function $u(y)$ is expanded as a Fourier series on $y \in [-L, L]$, i.e.,

$$u(y) = a_0 + \sum_{n=1}^{\infty} a_n \cos(n\pi y/L) + \sum_{n=1}^{\infty} b_n \sin(n\pi y/L) \tag{3.1}$$

then asymptotically

$$a_n \sim [u'(L) - u'(-L)]\{(-1)^n L/(n^2\pi^2)\} + O(1/n^4), \qquad n \to \infty \tag{3.2}$$

$$b_n \sim [u(L) - u(-L)]\{(-1)^{n+1}/(n\pi)\} + O(1/n^3), \qquad n \to \infty \tag{3.3}$$

where $u'(y) \equiv du/dy$.

Proof. The proof is by repeated integration by parts, hence the name of the theorem. Details are given in Boyd (1989), but the theorem is classical.

Since the boundary differences of $u(y)$ and its nonperiodic part are identical, it follows that the theorem predicts identical asymptotic behavior for the coefficients of both functions as $n \to \infty$. However, because the boundary differences for $\bar{P}(y)$ are the same order of magnitude as max $|\bar{P}(y)|$, its Fourier coefficients are closely approximated by the asymptotic limits given in the theorem even for rather small n. In contrast, $u(y)$ contains a huge periodic part. The coefficients of $u(y)$ will not approach the limiting values (3.2) or (3.3) until n is sufficiently large that the coefficients of the large function $P(y)$ have decayed to smaller values than those of the small function $\bar{P}(y)$.

The rate of decay of the Fourier coefficients of the periodic part of $u(y)$ is given by the following.

Theorem 3 (Geometric Convergence). Let $u(y)$ be a periodic function whose singularities nearest the real axis are a pair of complex conjugate poles on the imaginary axis at

$$y = \pm iL\delta \tag{3.4}$$

with residues $\mp i(L\delta/2)$; then on the interval $y \in [-L, L]$, its Fourier sine coefficients are asymptotically negligible in comparison to the cosine coefficients, which asymptotically are

$$a_n \sim \pi\delta e^{-n\pi\delta}, \qquad n \gg 1 \tag{3.5}$$

The Chebyshev coefficients of a function with the same convergence-limiting singularities and residues, whether the function is periodic or not, are asymptotically

$$c_{2n} \sim 2[\delta^4/(\delta^4+\delta^2)]^{1/2}\,(-1)^n\,e^{-n\rho(\delta)}, \qquad n \gg 1 \tag{3.6}$$

$$e^{-\rho(\delta)} \equiv 2\delta^2 + 1 - 2(\delta^4+\delta^2)^{1/2} \tag{3.7a}$$

$$\approx 1 - 2\delta, \qquad \delta \ll 1 \tag{3.7b}$$

and where the odd degree coefficients are asymptotically negligible in comparison to the even degree coefficients:

$$u(y) = \sum_{n=0}^{\infty} c_n T_n(y/L) \tag{3.8}$$

Proof. The proof is given in Boyd (1988b), but again, both parts of the theorem have been known for decades.

The assumptions of the theorem seem rather restrictive—simple poles forming a complex conjugate pair on the imaginary axis. In reality, the asymptotic coefficient behavior described by (3.5) and (3.7) is *generic*. The assumptions were imposed merely to expose the heart of the theorem without a lot of irrelevant qualifiers.

A Fourier series converges within the largest strip, bounded by a pair of straight lines parallel to the real axis and disposed symmetrically above and below the axis, which contains no singularities of $u(y)$. It follows that if the poles are moved anywhere along the lines $\mathrm{Im}(y) = \pm\delta$, the limit of the supremum of the coefficients will be *unaltered*. The sole effect will be to multiply the asymptotic coefficients by an n-dependent phase factor without changing the exponential decay of the amplitude.

Similarly, a Chebyshev series converges within the largest singularity-free region bounded by an ellipse in the complex y plane with foci at $y = \pm L$. If the singularity is moved anywhere along the ellipse of convergence, the $\exp[-n\rho(\delta)]$ factor is not altered.

Replacing the simple poles by second-order poles would merely multiply the asymptotic Fourier and Chebyshev coefficients by a factor of n, while making the singularities simple logarithms would divide the asymptotic coefficients by n. The *type* of the convergence-limiting singularity merely multiplies the coefficients by an *algebraic* factor of n.

For large n, the behavior of the coefficients is always dominated by the *exponential* factor of n, which is determined solely by the *location* of the singularity. For this reason, the type of the singularity is *irrelevant* to the size of the region of convergence and it is also irrelevant to comparing the merits of Chebyshev and Fourier expansions.

Comparing (3.5) with (3.7b), we see that both series converge geometrically, that is, each term is smaller than its predecessor by a factor of $\exp(-\pi\delta)$ and (for small δ) $\exp(-2\delta)$, respectively. However, the Fourier series converges *faster* and achieves the same error with roughly $(2/\pi)$ as many terms as the Chebyshev series.

4. NUMERICAL EXAMPLES

Figure 2 compares the Fourier coefficients for the periodic and nonperiodic parts of two representative functions:

$$u(y) \equiv \Lambda(y; \delta) \equiv \delta^2/(\delta^2 + y^2/L^2) \tag{4.1}$$

which we shall call the "Lorentzian" function, also known as the "witch of Agnesi," and

$$u(y) \equiv \operatorname{sech}([\pi/2]\ y/[L\delta]) \tag{4.2}$$

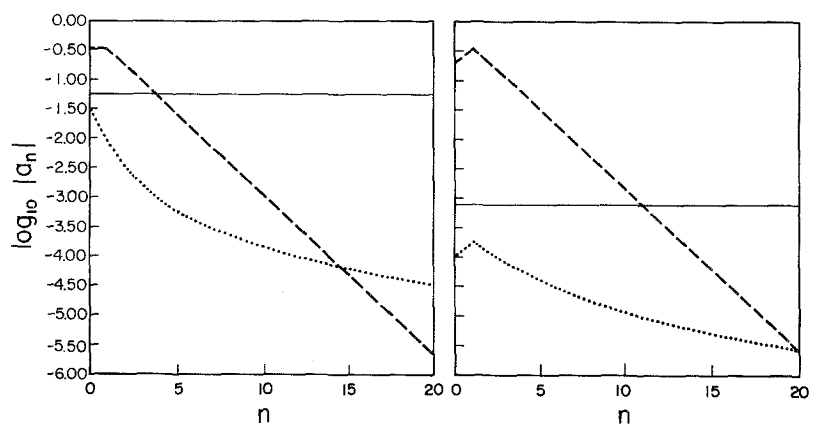

Fig. 2. Graph of the base-10 logarithm of the absolute values of the Fourier coefficients a_n for the periodic part (upper curve; solid) and nonperiodic part (lower curve; dashed) for (a) Lorentzian function, $\delta = 1/5$ and (b) the hyperbolic secant function, $\delta = 1/5$. The horizontal lines mark the boundary values of each function, $u(L)$. Note that since both functions have poles at $\pm i\delta$, the coefficients of their periodic parts asymptote to the same straight line.

Both functions are normalized so that $u(0)=1$ and both have convergence-limiting singularities at $y=\pm i\delta L$.

On these log-linear graphs, the Fourier coefficients for the large, nonperiodic parts of the Lorentzian and the sech both asymptote to straight lines in accord with the geometric convergence predicted by the theorem. The lower, dashed curves in each graph show that the coefficients for the nonperiodic parts flatten out and asymptote to horizontal lines from above, consistent with the $O(1/n^2)$ decrease predicted by Theorem 2. The dashed curves also show that the coefficients of the nonperiodic part of $u(y)$ for both cases are extremely small—orders of magnitude smaller—than those of the periodic part until a "cross-over" point for sufficiently large n. Only for $n>15$ (Lorentzian) and $n>20$ (sech) does $O(1/n^2)$ correctly describe the decay rate of the coefficients of $u(y)$.

In applications to domain truncation, however, one must always remember the other source of error: the domain error E_D. The solid horizontal lines in Fig. 2 mark E_D for each case. It is foolish to keep terms in the Fourier series that are smaller than the domain error because the total error cannot be smaller than the domain error. If we are unhappy with the size of E_D, the only rational recourse is to choose a larger domain size L and repeat the whole calculation. Consequently, everything *below* the horizontal lines in Fig. 2 is irrelevant to practical applications of domain truncation.

The graphs show clearly that the "cross-over" point only occurs where both parts of the coefficients of $u(y)$ are a hundred times smaller than the domain error. This is a vivid illustration of the fact that asymptotic formulas for Fourier coefficients must be applied asymptotically, i.e., only for large n. When $u(y)$ is decomposed into its periodic and nonperiodic parts, Theorems 2 and 3, applied to the appropriate part, accurately describe the asymptotic behavior of each part even for n as small as 5. However, blindly applying the "integration-by-parts" theorem to the sum of the two parts, i.e., to $u(y)$ itself, gives a prediction that is not even of the right order of magnitude until n is very large. Figure 3 shows the coefficients of the parts of the Lorentzian when δ is four times smaller than in Fig. 2: in this case, the "cross-over" point is off the graph at around $n=95$!

5. LITTLE WHITE LIES

The arguments given above, while fundamentally sound, have glossed over a couple of technical points that do not modify the conclusions, but do require comment, if only for the sake of mathematical completeness. First, in applying domain truncation, one is really interested in total error rather than the size of individual coefficients. In the worst case, which is a

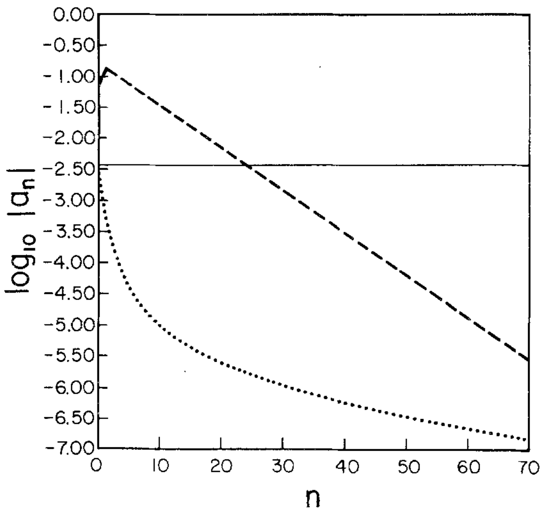

Fig. 3. Identical to 2(a) except for $\delta = 1/20$. Lorentzian function. Solid curve: coefficients of the periodic part, $P(y)$. Dashed curve: coefficients of the nonperiodic portion of $u(y)$. Horizontal solid line: $u(L)$, the boundary value of the function.

function that is unsymmetric about the origin, the coefficients decrease as $O(u(L) - u(-L)/n)$ as predicted by Theorem 2. However, because of the "Gibbs phenomenon" (Gottlieb and Orszag, 1978), the maximum pointwise error is $0.0895[u(L) - u(-L)]$, which is $O(n)$ larger than the smallest retained coefficient. Unfortunately, this error is independent of n, and therefore cannot be made smaller even if thousands of terms are retained.

Even in this worst case, however, this part of the series error, which is due to the lack of periodicity, is still less than a fifth of the domain error. It follows that even though $u(y)$ is not periodic and its Fourier series displays the Gibbs phenomenon, the greatest source of error in approximating $u(y)$ via domain truncation is not the lack of periodicity, but rather the magnitude of $u(y)$ for $|y| \geqslant L$.

The other slippery point is that the asymptotic rate of convergence for Chebyshev series may be *greater* than of the corresponding Fourier series if the convergence-limiting singularity is sufficiently near the ends of the interval $y \in [-L, L]$. The reason is that because the Fourier convergence region is bounded by a strip, a singularity a distance δ from the real axis is equally damaging to the Fourier series regardless of the real part of its location. However, the ellipse that bounds a Chebyshev expansion's domain of convergence curves close to and eventually cuts the real y axis at points outside the real interval $[-L, L]$. In consequence, a singularity at

$y = L(1 + i\delta)$ will yield a Chebyshev series whose terms are decreasing as $O(\exp[-n2\delta^{1/2}])$ for small δ and large n, in contrast to the $\exp(-n\pi\delta)$ convergence of the Fourier series.

The rub is that the contribution of a pole of $u(y)$ to the asymptotic coefficients of the function must always be weighted by its residue. If the pole is very near the end of the truncated interval $[-L, L]$, then this residue will be very, very small. Singularities close to the center of the interval will dominate the Chebyshev and Fourier coefficients for *moderate n* even when they are smaller than the contributions of end-point singularities in the asymptotic limit $n \to \infty$. For poles and branch points, as for discontinuities created by a lack of periodicity, asymptotic contributions that are always smaller than the domain error E_D are irrelevant to domain truncation.

Thus, it is singularities close to the center of the interval where $u(y)$ is large, not exponentially tiny, that matter. Because the ratio of Fourier-to-Chebyshev superiority varies with the location of the singularity, we must take the $(\pi/2)$ ratio quoted in the abstract as a rule of thumb. However, since the ratio does not vary much until one is *very* close to the ends of the interval, the rule of thumb is very useful.

6. SUMMARY

Because the notion of *always* applying Chebyshev polynomials to *nonperiodic* functions has become so firmly entrenched, we have tried to explain very carefully—perhaps for some readers, *too* carefully—why this principle fails when applied to domain truncation. However, the details of this patient, step-by-step presentation should not obscure the simplicity of the two key arguments.

First, if domain truncation is applied to compute the solution to a differential equation to, let us say, six decimal places, then both $u(L)$ and the error in chopping off the series after N terms are $O(10^{-6})$. The integration-by-parts theorem shows that the "Fourier penalty" for applying a trigonometric series to $u(y)$ is $O(u[L]/N)$, which is $O(10^{-8})$ for a reasonable N. [In narrow boundary layers of $O(1/N)$ width near the end points, the "Fourier penalty" is larger because of the Gibbs phenomenon, but still small in comparison to $u(L)$.] It is clearly foolish to worry that $u(y)$ is not periodic when the "Fourier penalty" is at least two orders of magnitude smaller than both the "domain" error and the "series" error defined in the Introduction.

Second, the Fourier pseudospectral grid has a nearest neighbor separation that is $(\pi/2)$ smaller than the maximum spacing on the

Chebyshev grid for the same N. One can show, as is done through Theorem 3 above, that this translates into a factor of 1.57 advantage for Fourier series over Chebyshev—one can achieve the same accuracy with 64% of the number of trigonometric functions as would be needed with Chebyshev polynomials. The wider the grid spacing, the poorer the accuracy—what could be simpler? The Chebyshev grid, which concentrates grid points near $y = \pm L$—precisely where $u(y) \ll 1$—is ludicrously inefficient.

F. Oliveira-Pinto (1973) has given a dramatic proof by example of the superiority of Fourier series for the Lorentzian function. He shows that one may obtain more rapid convergence by combining the Fourier series with a change of coordinate that creates a higher density of points near the origin—the opposite of the Chebyshev grid, which is densest near the boundaries. His mapping actually *worsens* the effects of the lack of periodicity because the Lorentzian function falls off more steeply—and therefore has a larger difference, $u'(L) - u'(-L)$—*after* the change of coordinate. The residue at the poles of the Lorentzian is decreased, however, because the poles are moved farther from the real axis in the new coordinate, so the net effect is to *improve* the rate of convergence.

As one who has sinned by using Chebyshev domain truncation himself, the author must admit that *mapping* methods (Grosch and Orszag, 1977; Boyd, 1982, 1987a, b) are usually superior to domain truncation if minimizing *execution* time is the primary goal. In that sense, the whole discussion of the article is irrelevant!

However, domain truncation is still superior to Chebyshev-with-change-of-coordinate algorithms in the sense of being easier to program and to understand. In this respect, Chebyshev domain truncation must be doubly damned. If accuracy is the goal, it is inferior to Fourier domain truncation. If simplicity is the chief criterion, Chebyshev polynomials are still inferior because they are more complex and harder to program than trigonometric series.

Because of its simplicity, domain truncation will undoubtably continue to be used in the real world, even if numerical analysts frown. It is hoped that this article will ensure that this simple approach to infinite intervals will be implemented simply—with Fourier series.

The second usefulness of this note is that it gives a very explicit illustration of how asymptotic spectral coefficients may be the sum of different types of contributions with wildly different strengths and different rates of decay. For the Fourier series of a function that falls off rapidly towards the ends of the interval, one must use two different asymptotic approximations—a geometrically decreasing formula for moderate n and an algebraically decreasing asymptotic approximation when n is very large.

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