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Asymptotic Fourier Coefficients for a C^∞ Bell (Smoothed-"Top-Hat") & the Fourier Extension Problem

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In constructing local Fourier bases and in solving differential equations with nonperiodic solutions through Fourier spectral algorithms, it is necessary to solve the Fourier Extension Problem. This is the task of extending a nonperiodic function, defined on an interval $x \in [-\chi, \chi]$, to a function $\tilde{f}$ which is periodic on the larger interval $x \in [-\Theta, \Theta]$. We derive the asymptotic Fourier coefficients for an infinitely differentiable function which is one on an interval $x \in [-\chi, \chi]$, identically zero for $|x| > \Theta$, and varies smoothly in between. Such smoothed "top-hat" functions are "bells" in wavelet theory. Our bell is (for $x \geq 0$) $\mathcal{T}(x; L, \chi, \Theta) = (1 + \mathrm{erf}(z))/2$ where $z = L\xi/\sqrt{1-\xi^2}$ where $\xi \equiv -1 + 2(\Theta - x)/(\Theta - \chi)$. By applying steepest descents to approximate the coefficient integrals in the limit of large degree j, we show that when the width L is fixed, the Fourier cosine coefficients a_j of $\mathcal{T}$ on $x \in [-\Theta, \Theta]$ are proportional to $a_j \sim (1/j) \exp(-L\pi^{1/2} 2^{-1/2} (1 - \chi/\Theta)^{1/2} j^{1/2}) \Lambda(j)$ where $\Lambda(j)$ is an oscillatory factor of degree given in the text. We also show that to minimize error in a Fourier series truncated after the Nth term, the width should be chosen to *increase* with N as $L = 0.91\sqrt{1 - \chi/\Theta}\, N^{1/2}$. We derive similar asymptotics for the function $f(x) = x$ as extended by a more sophisticated scheme with overlapping bells; this gives an even faster rate of Fourier convergence.

KEY WORDS: Fourier series; a symptotic Fourier coefficients; spectral methods; local Fourier basis; Fourier Extension.

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1. INTRODUCTION: LOCAL FOURIER BASES AND FOURIER EXTENSION

For some applications, it is very helpful to have smoothed approximations to the usual step-function and top-hat function, which are respectively

$$H(x) \equiv \begin{cases} 0, & x \le 0 \\ 1, & x > 0 \end{cases} \qquad T(x;\chi) \equiv \begin{cases} 0, & x < -\chi \\ 1, & x \in [-\chi, \chi] \\ 0, & x > \chi \end{cases} \tag{1}$$

(Note that the "top-hat" is just the superposition of two step-functions; this piecewise-constant function is known variously as the "box" function or as the "characteristic" or "indicator" function of the interval $[-\chi, \chi]$.) In wavelet and local Fourier basis theory, functions similar to H and T are called "ramps" and "bells", respectively. The smoothing replaces these discontinuous functions by other functions that are similar, but infinitely differentiable. Smoothed ramps and bells are useful to construct local Fourier bases (Averbuch *et al.* [1–5], Israeli *et al.* [32, 33], Vozovoi *et al.* [42, 43], Coifman and Meyer [21], Jawerth and Sweldens [34], Bittner and Chui [6], Matviyenko [35]). Ramps and bells are also useful to solve the Fourier extension problem, in which a non-periodic $f(x)$ defined on a certain interval is transformed into a function $\tilde{f}$ which is periodic on a larger interval (Boyd [17–19], Elghaoui and Pasquetti [23, 22], Nordström *et al.* [38], Högberg and Henningson [31], Garbey and Tromeur Dervout [29], Garbey [28], Haugen and Machenhauer [30]). In particular, [17] gives an example of how, using Fourier Extension, one can solve an ordinary differential equation with non-periodic boundary conditions using a Fourier basis with an exponential rate of convergence. Lastly, such functions are also useful to blend different local approximations into a global approximation as in Boyd [15].

Ramps and bells fall into two broad classes. The "C^{Ω}" class consists of functions that are analytic for all real x, but have flat portions that are only *approximately* equal to one. The "non-analytic" class sacrifices analyticity at the boundaries of the flat portion, $x = \pm\chi$, so that the top-hat is *identically equal to one* for all $x \in [-\chi, \chi]$.

There is much freedom to choose smoothed functions within each class; Matviyenko [35] has created a family of bells, later used widely in wavelets and local Fourier methods, which have discontinuous $(k+1)$st order derivatives at $x = \pm\chi$ and thus belong to C^k. Two different bells, themselves entire functions, but creating extended functions $\tilde{f}$ whose Fourier series have only a finite algebraic rate of convergence, are compared by Israeli *et al.* [32].

We prefer instead to choose a bell which is non-analytic, but nevertheless is such that the Fourier series of the extended function $\tilde{f}$ will converge *exponentially* fast with the truncation N of the Fourier series. Our bell has the advantage that it is identically one, and not merely approximately one, in the central region. Furthermore, our choice has no singularities except at the points where it is absolutely necessary to have singularities: at infinity and at the "breakpoints" $x = \pm\chi, \pm\Theta$. Lastly, our bell is very simple, being constructed of nothing more exotic than an error function and a square root. In the absence of a theory for optimizing non-analytic bells, our choice is a good combination of simplicity and smoothness.

Our bell, non-analytic but C^{∞}, is based on the erf-like function

$$\mathcal{E}(x; L) = \begin{cases} -1, & x < -1 \\ \operatorname{erf}\left(L \frac{x}{\sqrt{1-x^2}}\right), & x \in [-1, 1] \\ 1, & x > 1 \end{cases} \tag{2}$$

Note that the argument of the error function varies from $-\infty$ to ∞ as x varies from -1 to 1. L is a user-choosable width parameter; the central question of this article is: What choice of L is best?

From the erf-like function comes the ramp [smoothed step-function]

$$\mathcal{H}(x; L) \equiv (1/2)\,\{1 + \mathcal{E}\} \tag{3}$$

and, defining,

$$\Omega \equiv (\Psi - \chi)/2, \tag{4}$$

the bell [smoothed top-hat]

$$\mathcal{T}(x; L, \chi, \Psi) \equiv \begin{cases} \mathcal{H}([x + \chi + \Omega]/\Omega; L), & x \in [-\Psi, -\chi] \\ 1, & x \in [-\chi, \chi] \\ \mathcal{H}(-[x - \chi - \Omega]/\Omega; L), & x \in [\chi, \Psi] \end{cases} \tag{5}$$

At the "breakpoints" where $x = \pm\chi$ and $x = \pm\Psi$, $\mathcal{T}$ is infinitely differentiable, but all derivatives are zero and the function has essential singularities. In the Fourier extension problem, the flat portion of $\mathcal{T}$ is the physical region where the extended function $\tilde{f} \equiv f$ as marked in Fig. 1.

One might suppose that the singularities at the ends of each smoothing interval would poison the convergence of the Fourier series of $\mathcal{T}$ so that

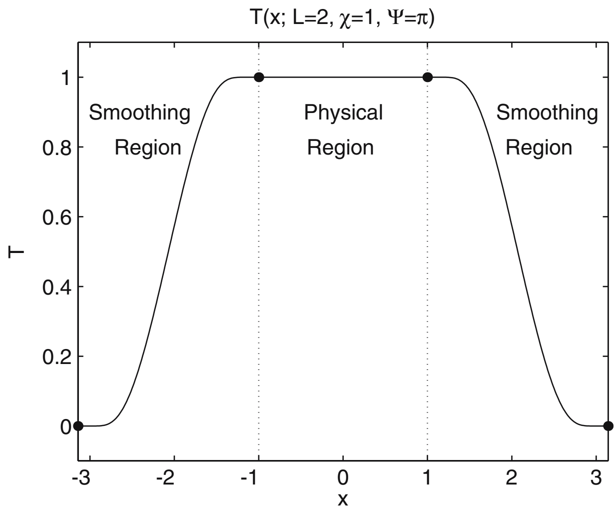

Fig. 1. Erf-smoothed top-hat function or bell, $\mathcal{T}$. The function $\mathcal{T} \equiv 1$ for all $x \in [-\chi, \chi]$ where here χ has been chosen to be one. This central interval is the "physical region" in applications. The function smoothly varies from to 1 to 0 on the intervals $x \in [-\Psi, -\chi]$ and $x \in [\chi, \Psi]$. The function is singular at both boundaries of each smoothing region as marked by the black disks. Derivatives of $\mathcal{T}$ to all orders exist (and are zero) at each essential singularity.

the coefficients would decrease very slowly. However, because the function is infinitely differentiable, its Fourier coefficients in fact fall off *exponentially* fast with N as illustrated in Fig. 2. Because $\mathcal{T}$ is symmetric with respect to $x = 0$, that is, $\mathcal{T}(x; L, \chi, \Psi) = \mathcal{T}(-x; L, \chi, \Psi)$, the Fourier series for the top-hat function is a *cosine* series. The figure also shows that the rate of convergence is strongly dependent upon L: our task is to assess how rapidly.

In the Fourier extension problem, the extended periodic function $\tilde{f}$ is constructed by multiplying the original, nonperiodic function f by $\mathcal{T}$. The true goal is to optimize the convergence of the Fourier series of $\tilde{f}$ by varying both the ratio of the width of the physical region to the extension region and also by independently varying L. Unfortunately, it is not possible to do this in an $f(x)$-independent way. As explained in Sec. 10, the best choice of the relative width of the extension interval is highly dependent on $f(x)$ with a narrow extension interval being best for $f(x)$ which are highly structured while a broad extension is preferred when $f(x)$ is very smooth. Therefore, we shall take the width of the physical region to be a fixed parameter χ.

Similarly, since $f(x)$ is not known *a priori*, the best we can hope to do is to choose the width parameter L so that the bell $\mathcal{T}$ is as smooth as

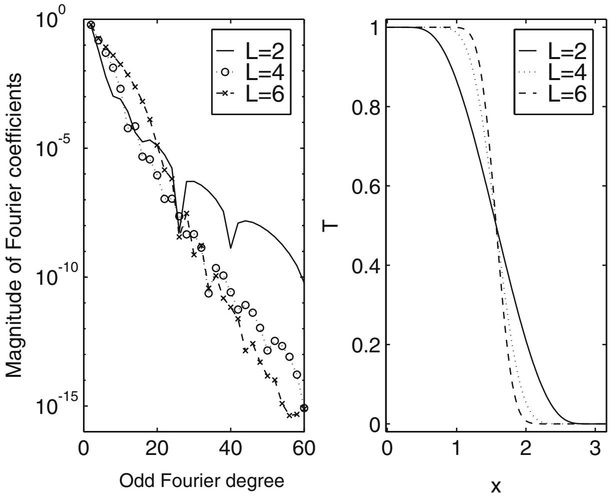

Fig. 2. Right: Top-hat function $\mathcal{T}(x; L, \chi, \Psi)$ for three different values of the width parameter, $L = 2, 4, 6$ where the gradient steepens as L increases. Left: Fourier cosine coefficients for each choice of L. $\chi = 0, \Psi = \pi$ (Note that the coefficients depend only on the ratio of χ/Ψ.)

possible in the sense of having the smallest error in a Fourier series truncated at the Nth term for $L = L_{\text{optimum}}(N)$. We assume, but cannot prove except for specific $f(x)$, that this will also optimize convergence for the extended function $\tilde{f}$, too.

As explained in the next section, there are several ways to perform the extension. For the "naive" or "non-overlapping" extension, it is sufficient to examine the Fourier series for $\mathcal{T}$, which is a problem of some interest in its own right. (There have been only limited analyses of Fourier series for functions which are C^{∞}.) The improved or "overlapping" extension has the property that the extension of $f(x) = 1$ is $\tilde{f} = 1$, which is completely trivial. Thus, in this case, we must look at the Fourier series for the simplest function with a nontrivial extension, which is that of $f(x) = x$. (In the limit $L \to \infty$, $\tilde{f}$ is the piecewise linear "sawtooth" function (Boyd [16]), so we shall refer to $\tilde{f}$ for finite L as a smoothed sawtooth.) Very conveniently, it turns out that the Fourier coefficients for the overlapping-smoothed sawtooth are proportional to the same integral, dubbed I^{+} below, as yields the Fourier coefficients for $\mathcal{T}$ itself. Thus, it is sensible to analyze both cases in a single article since both hinge on an asymptotic analysis of the same integral.

2. THE FOURIER EXTENSION PROBLEM

Definition 1 (Fourier Extension Problem).

Given a (generally) nonperiodic function $f(x)$ which is of interest on $x \in [-\chi, \chi]$, the Fourier Extension Problem is to define a function $\tilde{f}$ on a larger interval $x \in [-\Theta, \Theta]$ such that (i)

$$\tilde{f} \equiv f \qquad \forall x \in [-\chi, \chi] \tag{6}$$

and (ii) $\tilde{f}$ is periodic with period 2Θ and (iii) $\tilde{f}$ has a rapidly convergent Fourier series or meets similar criteria of smoothness. The extension is of the First Kind when $f(x)$ is known and analytical everywhere on the extended interval $x \in [-\Theta, \Theta]$; of the Second Kind when $f(x)$ is known but has singularities on either or both of the "extension intervals" $x \in [-\Theta, -\chi]$ and $x \in [\chi, \Theta]$ and of the Third Kind when $f(x)$ is not known outside the "physical" interval $x \in [-\chi, \chi]$. Boyd [17].

In this article, we shall focus only on the simplest case of Fourier Extension of the First Kind, and thus assume that $f(x)$ is known and analytical everywhere on the extended interval $[-\Theta, \Theta]$.

There are many strategies for an extension of the First Kind. We shall briefly list three. The first two are most easily explained through the method of imbricate series.

2.1. Imbricate Series

Let $G(x)$ be a function defined on $x \in [-\infty, \infty]$ with the property that it decays as fast as $1/|x|^{\alpha}$, $\alpha > 1$, or faster as $|x| \to \infty$. If we replicate an infinite number of copies of $G(x)$ and then superpose these copies with one copy centered at each point of an infinite lattice with even spacing 2Θ, then the sum converges and is by construction a function periodic with period 2Θ:

$$\tilde{f}(x) \equiv \sum_{m=-\infty}^{\infty} G(x - m2\Theta) \tag{7}$$

The sum is the "imbricate series" of $\tilde{f}$ and $G(x)$ is the "pattern" function (Boyd [11, 14]).

2.2. Naive or Non-Overlapping Extension

In this case, the pattern function is

$$G(x) \equiv \tilde{f} = f(x)\mathcal{T}(x; L; \chi, \Theta), \qquad x \in [-\Theta, \Theta] \tag{8}$$

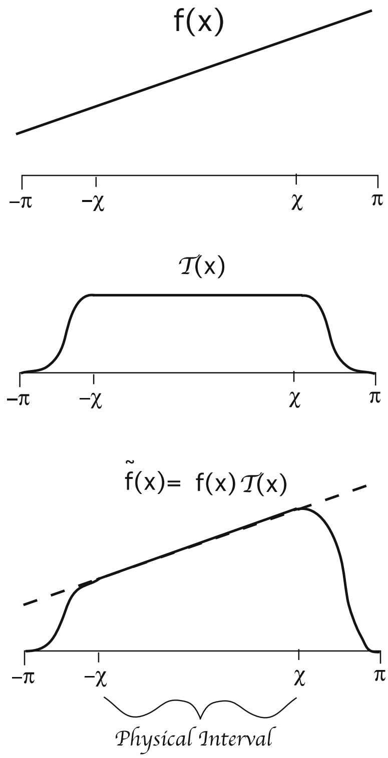

Fig. 3. Fourier Extension of the First Kind: $f(x)$ is known in analytical (or other computable) form outside the physical interval, $x \in [-\chi, \chi]$. The periodic function $\tilde{f}(x) \equiv f(x)$ for all x on the physical interval, but differs from $f(x)$ (dashed curve) in the "smoothing regions" $x \in [-\Theta, -\chi], x \in [\chi, \Theta]$ where here $\Theta = \pi$.

(Outside this interval, $G \equiv 0$ whereas $\tilde{f}$ is defined outside $x \in [-\Theta, \Theta]$ by its periodicity of period 2Θ.) Because $\mathcal{T} \equiv 0 \, \forall |x| > \Theta$, the pattern function is "infinitely flat" at $x = \pm\Theta$ in the sense that $\tilde{f}$ and all its derivatives are zero at these points. We may dub this the "non-overlapping extension" because the copies of the pattern function have zero overlap; if x is restricted to the fundamental period interval, $x \in [-\Theta, \Theta]$, then the imbricate series is truncated to the single term $f(x)\mathcal{T}$.

The extension is illustrated in Fig. 3. It can be shown by integration-by-parts that a function $\tilde{f}$ cannot have a Fourier series whose coefficients a_j decrease exponentially fast with j unless the values of $\tilde{f}$ and all its derivatives have the same values at $x = \Theta$ as at $x = -\Theta$ (Boyd [16]). For the non-overlapped extension, all the derivatives are *zero* at both ends of the period interval, and therefore the derivative matching condition is trivially satisfied.

The simplest $f(x)$ that can be extended this way is $f(x) \equiv 1$; its extension is simply $\mathcal{T}$. Thus, to find the Fourier coefficients of the simplest non-overlapped extension is to find the coefficients of $\mathcal{T}$ itself. As we shall prove through our asymptotics, however, this extension is not as efficient as the overlapped procedure described next.

2.3. Overlapped Extension

The deficiency of the the non-overlapped extension is that the "relaxation zone" where $\mathcal{T}$ varies from one to zero is crammed into the interval $x \in [\chi, \Theta]$. If we double the width of the extension zone by choosing the imbricate pattern function to be

$$G(x) = f(x)\mathcal{T}(x; L; \chi, \Theta + 2\Xi) \tag{9}$$

where

$$\Xi \equiv (\Theta - \chi)/2, \tag{10}$$

the copy of G centered on the origin and that centered on $x = 2\Theta$ will overlap on the interval $x \in [\chi, \Theta + 2\,\Xi]$. But so what? The leftward relaxation zone of $\mathcal{T}(x - 2\Theta; L; \chi, \Theta + 2\Xi)$ decreases from one at $x = \Theta + 2\Xi$ to zero at $x = \Theta - 2\Xi = \chi$, but it does not overlap with the "physical" interval $x \in [-\chi, \chi]$ where we demand that the extended function $\tilde{f}$ exactly equal $f(x)$. Because the relaxation zone has been doubled, the bell $\mathcal{T}$ is smoother than in the non-overlapped method, and the convergence of the Fourier series of $\tilde{f}$ is improved. The two species of extension are compared in Fig. 4.

There is also a second, more subtle advantage: If $f(x)$ is a periodic function of period 2Θ so that it does not need to be extended, then the overlapped extension has the virtue that $\tilde{f} \equiv f\ \forall x \in [-\Theta, \Theta]$ as proved in Boyd [17]. In other words, the extension modifies only those parts of $f(x)$, if it is a mixture of periodic and nonperiodic components, which actually need to be modified so that $\tilde{f}$ is periodic.

To optimize the width parameter L inside the bell function $\mathcal{T}$, it is not possible to examine the coefficients of the extension of $f(x) \equiv 1$ because for the overlapping extension, the extension is the constant $\tilde{f} \equiv 1$! The simplest nontrivial extended function is

$$Sw(x; L, \chi, \Theta) \equiv \sum_{m=-\infty}^{\infty} (x - 2m\Theta)\mathcal{T}(x - 2m\Theta; L, \chi, \Theta + 2\Xi) \quad \text{[Sawtooth Function]} \tag{11}$$

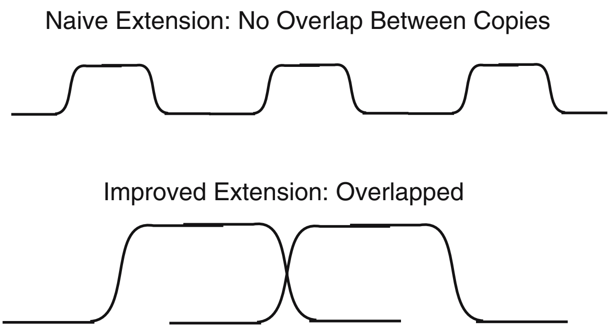

Fig. 4. Comparison of the non-overlapping ("naive") and overlapping extensions. Both graphs show three copies of the imbricate pattern function G for each case. In the overlapping method, copies of the pattern function are allowed to overlap in pairs. However, only the central copy is nonzero on the physical interval $x \in [-\chi, \chi]$ where $\mathcal{T} \equiv 1$ and $\tilde{f} = f$ so that the extension is faithful to the function being extended, $f(x)$, on this interval.

We shall dub this the "sawtooth" function because in the limit $L \to \infty$, it reduces to the piecewise constant linear function of that name Boyd [16]. In the rest of the article, we shall derive asymptotic approximations to the Fourier coefficients of the sawtooth function as well as for $\mathcal{T}((x; L, \chi, \Psi = \Theta)$, which is the extension of $f(x) = 1$ via the non-overlapped scheme.

3. ASYMPTOTICS, ENVELOPES AND GOALS

3.1. Horizontal and Uniform Limits

Before we dive into a rather complicated derivation of asymptotic approximations, it is important to be clear about our goals. The truncation error of a function $f(x; L)$ will be defined to be the L_∞ norm of the error when the Fourier series is truncated at the Nth term:

$$E_N(L) \equiv \max_{x \in \mathbb{R}} \left| f(x; L) - \sum_{j=0}^{N} a_j \cos(jx) \right| \tag{12}$$

It is a function of two parameters: the map parameter L and the truncation N. Fig. 5 shows the contours of E_N in the $N - L^2$ plane for a particular choice of the top-hat parameters χ, Ψ.

The usual Fourier theory corresponds to taking a "horizontal" limit: $N \to \infty$ for fixed L. We shall derive and discuss the asymptotics of the a_j in this limit in Secs. 7 and 9.

However, one may also ask what happens in the limit that N and L *simultaneously* tend to infinity. This calculation is harder because the

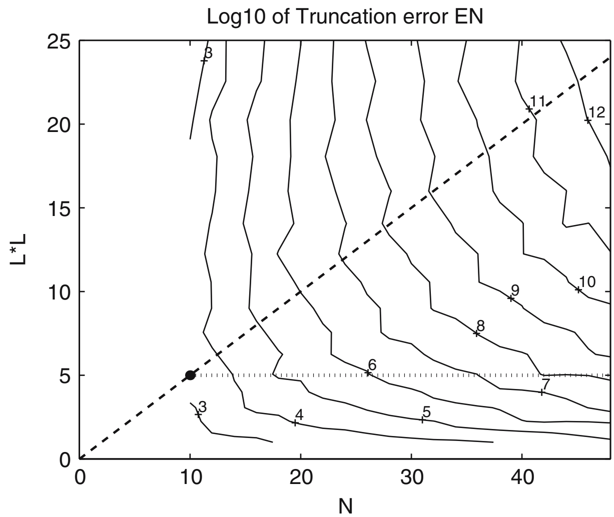

Fig. 5. Contours of $-\log_{10}(E_N)$ in the $N-L^2$ plane. The function f is defined by imbricating the top-hat function $\mathcal{T}(x; L, \chi, \Psi)$ for $\chi = 0$, $\Psi = \pi$ (the "naive" extension), but the truncation error is qualitatively similar for other choices of χ, Ψ, and other ways of extending the smoothed top-hat function into a periodic function. The fixed-L asymptotics corresponds to taking the limit $N \to \infty$ along a horizontal line in this plane. However, the axis of the "valley" is *diagonal* as marked by the thick dashed line. If we move horizontally from the black dot at $L^2 = 5, N = 10$ (along the thin dotted line) , the error falls to $O(10^{-9})$ by $N = 50$. However, moving along the diagonal from this same starting point, the errors falls to $O(10^{-12})$ by $N = 50$, an error reduction of an additional factor of a thousand. The diagonal limit in which N and L^2 increase simultaneously requires the "uniform" asymptotics.

asymptotic approximation must be "uniform" in the sense of accuracy when both parameters are large.

For many numerical applications of Fourier and other spectral expansions, these uniform limits are very important because the optimum choice of map parameter L *varies* with N (Boyd [7, 10, 9, 12], Cloot and Weideman [20], Tang [41], Schumer and Holloway [39], Shen [40]). In other words, the path of steepest descent with increasing N is not the "horizontal limit" (L fixed, $N \to \infty$), but rather the "diagonal limit" in which L^2 increases proportionally to N.

3.2. Oscillations and Envelopes

For many functions $f(x)$ (and for almost all C^∞-but-not-C^Ω functions), the spectral coefficients *oscillate with degree* as illustrated schematically in Fig. 6. One may always bound the coefficients rather tightly by

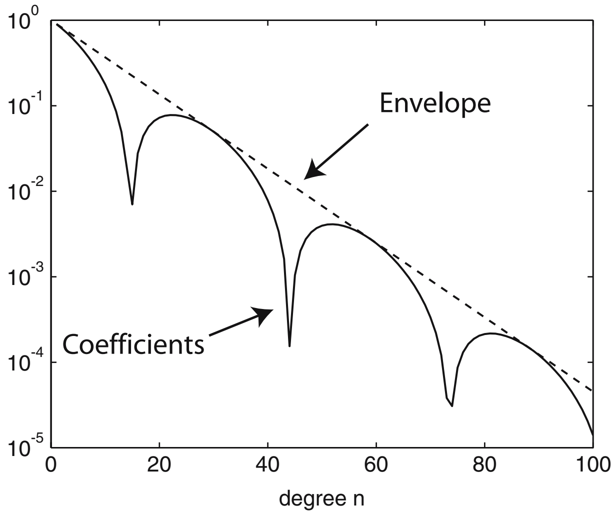

Fig. 6. Solid: logarithm of the absolute value of the spectral coefficients of a geometrically-converging series whose coefficients *oscillate* with degree n. Dashed: the "envelope" of the spectral coefficients.

a monontically-decaying function which is the "envelope" of the spectral series.

Fortunately, the asymptotic approximations to the coefficients a_j, derived below, are the product of the monotonically-decaying "envelope" with an oscillatory factor. It is possible to minimize a particular coefficient by choosing L so this coefficient is located at the dip of the curve. However, it is much more useful to *minimize* the *envelope* instead.

3.3. Goals: What Should be Minimized?

In the literature of spectral methods, error is estimated through several quantities including:

$$(i) \qquad E_N \equiv \left\| \sum_{j=N+1}^{\infty} a_j \cos(jx) \right\|_\infty \tag{13}$$

$$(ii) \qquad \Sigma_N \equiv \sum_{j=N+1}^{\infty} |a_j| \tag{14}$$

$$(iii) \qquad \text{Envelope of } a_N \tag{15}$$

Minimizing the truncation error is the obvious and also the most desirable goal. Σ_N, which is the sum of the absolute value of all the coefficients neglected by truncation, is provably an upper bound on the truncation error, but it is a tight bound only when all the coefficients are the same sign. The envelope of the last retained coefficient is at the farthest remove.

Unfortunately, we know only how to *analytically* calculate the asymptotic behavior of the spectral coefficients a_j, and therefore of the envelope of these coefficients. *Numerically*, it is straightforward to calculate the truncation error $|E_N|$, but such numerical estimates have two faults. First, they oscillate because it is impossible to disentangle the envelope factor from the factor that oscillates with degree, as displayed in the analytical asymptotics. Second, numerical results are much less efficient in predicting a good choice of L than a simple analytical formula.

Therefore, as in earlier articles, we shall unrepentantly concentrate on asymptotics for spectral coefficients. It is obvious that when the envelope of a_N is small, the truncation error will be small, too, even if we lack a precise qunatification of the proportionality. Asymptotic approximations to the spectral coefficients for fixed L are uncontroversial in any event.

However, in informal presentations of this work, we have been bombarded with criticism for deriving the envelope of the coefficients in the diagonal limit. The complaint is that $a_N(L(N))$ is not the Nth coefficient of a Fourier series; rather, the coefficients $a_j(L)$ are defined only for fixed map parameter. This complaint is correct but terribly misguided. First, in the diagonal limit, we are primarily interested in the envelope, not the complete coefficient, and that only as a proxy for the truncation error. Second, Fig. 5 shows clearly that for optimum performance, we *must* vary L with the truncation N. This in turn requires asymptotics in the *simultaneous* limit L and N go to infinity *together*. And so, as done in many earlier articles dating back over twenty years(Boyd [7, 9, 10, 12], Cloot and Weideman [20], Tang [41], Schumer and Holloway [39], Shen [40]), we shall derive asymptotics for the envelope of $a_N(L(N))$ without further apology.

With these concepts explained, we can turn to asymptotic evaluation of the Fourier coefficients integrals. In the next section, we describe some simple exact transformations (integration-by-parts, etc.) which allow the Fourier integrals for $\mathcal{T}(x)$ and $\mathrm{Sw}(x)$ to be expressed in terms of a single integral, I^+. After we have derived both the fixed-L and L-varying ("uniform") asymptotics for I^+ in Secs. 5–7, the envelope of the Fourier coefficients is simply the monotonic, exponentially-decaying factor of the asymptotics of I^+, multiplied by constants, as exploited in Sec. 8.

4. EXACT TRANSFORMATIONS

Because $\mathcal{T}$ is symmetric with respect to zero, all its sine coefficients are zero and the cosine coefficients can be computed by integrating over half the interval and doubling the result:

$$a_j = \frac{2}{\Theta} \int_0^{\Theta} \cos(j(\pi/\Theta)x)\mathcal{T}(x; L, \chi, \Theta)\, dx \qquad j > 0, \qquad [\mathcal{T}] \tag{16}$$

where

$$\mathcal{T}(x; L, \chi, \Theta) = \frac{a_0}{2} + \sum_{j=1}^{\infty} a_j \cos(j[\pi/\Theta]x), \quad x \in [-\Theta, \Theta] \tag{17}$$

Note that we have specialized the width parameter of $\mathcal{T}$ by setting $\Psi = \Theta$, and thus slaving the width of the "bell" to the spatial period; the methods described here can be easily extended to the general case where Ψ and Θ are independent parameters, but since the general case has no interesting applications, we have specialized Ψ in all the formulas below.

Similarly, all the cosine coefficients of the sawtooth function are zero. Noting that only two copies of the pattern function are nonzero at a given point, the sine coefficients of the smoothed sawtooth function are

$$b_j \equiv \frac{1}{\Theta} \int_0^{2\Theta} \sin(j(\pi/\Theta)x)\, \{x\mathcal{T}(x) + \{x - 2\Theta\}\mathcal{T}(x - 2\Theta)\}\, dx \quad [\mathrm{Sw}] \tag{18}$$

where

$$\mathrm{Sw}(x; L, \chi, \Theta) = \sum_{j=1}^{\infty} b_j \sin(j[\pi/\Theta]x), \qquad x \in [-\Theta, \Theta] \tag{19}$$

To put these integrals into a form suitable for the steepest descent method, it is helpful to

1. Integrate-by-parts with differentiation of the bell $\mathcal{T}$; the boundary terms are zero.
2. Shorten the interval of integration to exclude the portions where $d\mathcal{T}/dx$ (and therefore the integrand) is zero.
3. Invoke the differentiation identity $\frac{d}{dv}\{\mathrm{erf}(v)\} = \frac{2}{\sqrt{\pi}} \exp(-v^2)$.
4. Change coordinates to a new variable $\xi \in [-1, 1]$ which spans the smoothing regions. (For the coefficients of $\mathcal{T}$, ξ is the image of $x \in [\chi, \Theta]$; for the sawtooth, it is the image of $[\chi, \Theta + (\Theta - \chi)]$.

The coefficient integrals are transformed without approximation to

$$a_j = \frac{4L}{j\,\pi^{1/2}\,\Theta} \sin\left(j\frac{\pi}{2}\left\{1+\frac{\chi}{\Theta}\right\}\right) \Re\left\{I^{+}\left(j\frac{\pi}{2}\left(1-\frac{\chi}{\Theta}\right); L\right)\right\}$$

$$[\mathcal{T};\ \text{Non-overlapped Extension of } f=1] \tag{20}$$

$$b_j = \frac{(-1)^{j+1}4L\Theta}{\pi^{3/2}}\,\frac{1}{j}\,\Re\left\{I^{+}(j\,\pi\left(1-\frac{\chi}{\Theta}\right); L)\right\}$$

$$[\text{Sawtooth; Overlapping Extension of } f=x] \tag{21}$$

where $I^{+}(n; L)$ is the integral defined (and approximated) in the next three sections.

5. THE METHOD OF STEEPEST DESCENTS

$$I^{+}(n; L) \equiv \int_0^1 d\xi\ \exp(in\xi)\ \exp\left(-L^2\frac{\xi^2}{1-\xi^2}\right)\frac{1}{(1-\xi^2)^{3/2}} \tag{22}$$

To apply the method of steepest descent, it is convenient to rewrite the rapidly-varying part of the integrand as an exponential:

$$I^{+}(n; L) = \int_0^1 \exp(\Phi(\xi))\,h(\xi)\,d\xi \tag{23}$$

where

$$\Phi(\xi; n, L) \equiv in\xi - L^2\frac{\xi^2}{1-\xi^2} \tag{24}$$

and the slowly-varying, n-independent algebraic factor is

$$h(\xi) \equiv (1-\xi^2)^{-3/2} \tag{25}$$

Both in the uniform limit that L increases with n and in the non-uniform limit that L is fixed, the "phase function" Φ varies more and more rapidly as $n \to \infty$. This allows us to profit by deforming the contour of integration in the complex plane so that it passes through one or more "stationary points" of Φ as illustrated in Fig. 7. These are *local maxima* of the integrand along the integration contour. As n increases, the integrand becomes more and more steeply peaked about the stationary point, and the value of the integral is dominated by the contribution from that small

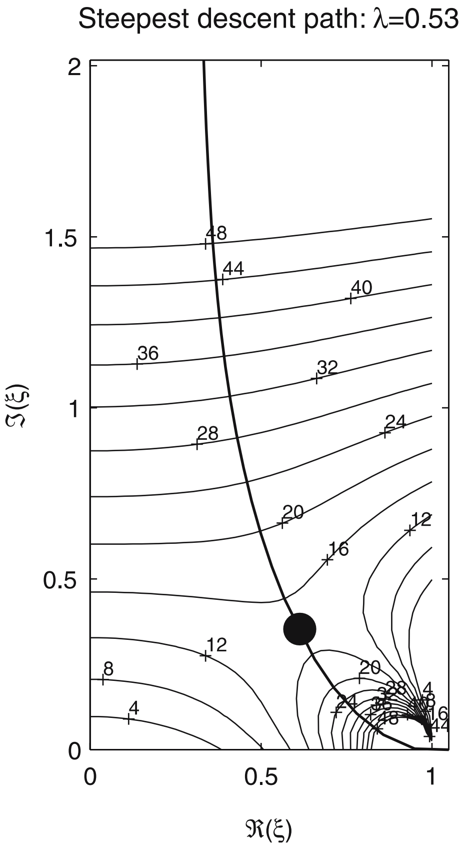

Fig. 7. The thick line shows the steepest descent path; the disk is the relevant stationary point. The thin lines are the contours of the rescaled phase function $\tilde{\Phi}$, defined in Sec. 4. The contour labels show (-100) times the isoline value (to avoid cluttering the figure with minus signs and decimal points).

portion of the integration path which is close to the stationary point. This allows us to approximate the integral by making a local approximation of the integrand by a Gaussian function which can then be integrated analytically.

The result is

$$\text{integral} \sim \sum \sqrt{2\pi} \sqrt{\frac{1}{-\Phi_{\xi\xi}(\xi_s)}}\, h(\xi_s)\, \exp(\Phi(\xi_s)) \tag{26}$$

where $\Phi_{\xi\xi}$ denotes the second derivative of Φ with respect to ξ and the sum is over all stationary points on the deformed contour of integration.

(Note that the integration path does not explicitly appear in the answer: although most texts lavish much attention on determining the precise steepest descent contour, the path is irrelevant to the asymptotic approximation except for the all-important issue of what stationary points lie upon the integration curve.)

In our application, the deformed path is from the origin to $i\infty$ along the imaginary axis, and then back to $\xi = 1$ in a curving arc that passes through a single stationary point. There is one minor technical complication: the integral along the imaginary axis is not zero and must be evaluated by a different asymptotic method. However, it is easy to show that this integral is purely imaginary, and therefore makes no contribution to $\Re(I^{+})$. Another way to see the same thing is to note that the real part of I^{+} is symmetric with respect to $\xi = 0$. Therefore, the real part is just half the result of integrating from $\xi = -1$ to $\xi = 1$. The integral over the doubled interval can be performed by two curving arcs from the endpoints to $i\infty$, and an integral along the path from the origin to infinity along the imaginary axis is unnecessary.

For both the uniform and non-uniform asymptotics, the equation $d\Phi/d\xi = 0$ is a quartic polynomial in ξ. By the fundamental theorem of algebra, there are four stationary points. However, only the two that are on the path of integration, each making an identical contribution, are relevant when integrating from $\xi = -1$ to $\xi = 1$, and only a single stationary point when the integration interval is restricted to $\xi \in [0, 1]$.

The method of steepest descent is ancient; its application to Fourier and Chebyshev series coefficient integrals began with the pioneering work of D. Elliott and his students: Elliott [24, 25], Elliott and Szekeres [26], Elliott and Tuan [27], Nemeth [37] and Miller [36] in the mid-60's. Boyd has used the method to optimize a variety of spectral algorithms [7–10, 12, 13].

6. UNIFORM ASYMPTOTICS: DEGREE j AND WIDTH L SIMULTANEOUSLY INCREASING

The non-uniform asymptotics of the next section will approximate $I^{+}(n; L)$, and thus a_j, in the limit that L is fixed while j, n increase without limit. To obtain the fastest convergence for a Fourier series truncated with the Nth term, it is better to instead allow the width parameter L to increase *simultaneously* with the scaled degree n so that

$$L^2 \equiv \lambda n \tag{27}$$

for some constant λ. Note that throughout this paper, the parameters χ and θ are taken as *fixed*, independent of n and λ. The phase is then

$$\Phi(\xi) \equiv n \left\{ i\,\xi - \lambda\, \frac{\xi^2}{1-\xi^2} \right\} \tag{28}$$

Because the Fourier degree n appears only as a multiplicative factor, the stationary points are independent of n, and vary only with λ. It is convenient to define the scaled phase function

$$\tilde{\Phi}(\xi) \equiv \frac{\Phi(\xi)}{n} = i\,\xi - \lambda\, \frac{\xi^2}{1-\xi^2} \tag{29}$$

The stationary points are the roots of

$$\frac{d\tilde{\Phi}}{d\xi} \equiv i - \lambda\, \frac{2\xi}{(1-\xi^2)^2} \tag{30}$$

which can be written by clearing denominators as the quartic

$$\xi^4 - 2\xi^2 + 2i\xi\,\lambda + 1 = 0 \tag{31}$$

By numerically solving this quartic for many values of λ and then evaluating the real part of $\tilde{\Phi}$ for each, one finds that $\tilde{\Phi}$ has the largest negative real part (and therefore, the jth Fourier coefficient is minimized) when

$$\lambda = 0.53033 \qquad L_{\text{optimum}} = 0.7282\sqrt{n} \tag{32}$$

$$\Re(I^{+}(n; \lambda = 0.53033) \sim \frac{1}{\sqrt{n}} \exp(-0.35355\,n) \times \left\{-0.336\cos(0.306n) + 1.017\sin(0.306n)\right\} \tag{33}$$

7. ASYMPTOTIC COEFFICIENTS FOR FIXED WIDTH L

When L is fixed, the condition that $d\Phi/d\xi = 0$ becomes

$$i\,\nu = \frac{2\xi}{(1-\xi^2)^2} \tag{34}$$

where it is convenient to introduce the parameter

$$\nu \equiv \frac{n}{L^2} \tag{35}$$

because the stationary point equation is a function only of the *ratio* of n to L^2, and not upon these parameters independently of each other. For fixed L and $n \to \infty$, $\nu \to \infty$. This makes it possible to solve the quartic equation for the stationary point perturbatively in inverse powers of $\nu^{-1/2}$ to obtain

$$\xi_s \equiv 1 - \exp(-i\pi/4)/\sqrt{2}\,\frac{1}{\nu^{1/2}} + O(\nu^{-3/2}) \tag{36}$$

where the stationary point on the integration contour is again that in the first quadrant of the complex ξ plane. Evaluating $\Phi(\xi_s)$ through a similar expansion gives

$$\begin{aligned}\Re\left\{I^+(n;L)\right\} \approx \frac{\pi^{1/2}}{2L}\ &\exp([3/4]L^2)\exp(-L\sqrt{n})\\ &\times\left\{\cos(n)\cos\left(L\sqrt{n}\right)+\sin(n)\sin\left(L\sqrt{n}\right)\right\}\end{aligned} \tag{37}$$

8. OPTIMIZATION OF THE WIDTH L FOR FOURIER EXTENSION

The L-varying asymptotics of I^+ implies that if the Fourier series is truncated after degree $j = N$, the optimum width parameter is

$$L_{\text{optimum}} = \begin{cases} 0.911\sqrt{1-\chi/\Theta}\,\sqrt{N} & [\mathcal{T};\ \text{Nonoverlapped Extension}] \\ 1.29\sqrt{1-\chi/\Theta}\,\sqrt{N} & [\text{Sw; Overlapped Extension}] \end{cases} \tag{38}$$

Note that these come from minimizing the “envelope” of the Fourier coefficients, as defined in Sec. (3); that is, the monotonically-decaying-with-degree factor is minimized while the oscillatory-with-degree factor in the asymptotic approximation is ignored.

Strictly speaking, we have shown only that these choices of L are optimal when $f(x) \equiv 1$ [for the non-overlapped method of extension, or equivalently for the Fourier coefficients of the bell $\mathcal{T}$] and for $f(x) = x$ when extended into the sawtooth function through the overlapping scheme. We conjecture that these choices are also optimal or near-optimal for the extensions of general $f(x)$.

Then

$$\log|a_N(L_{\text{opt}}(N))| \sim \begin{cases} -0.555\,(1-\chi/\Theta)\,N + \text{lower order terms} & [\mathcal{T}] \\ -1.110\,(1-\chi/\Theta)\,N + \text{lower order terms} & [\text{Sw}] \end{cases} \tag{39}$$

Figure 8 shows that the uniform asymptotic approximation is quite good.

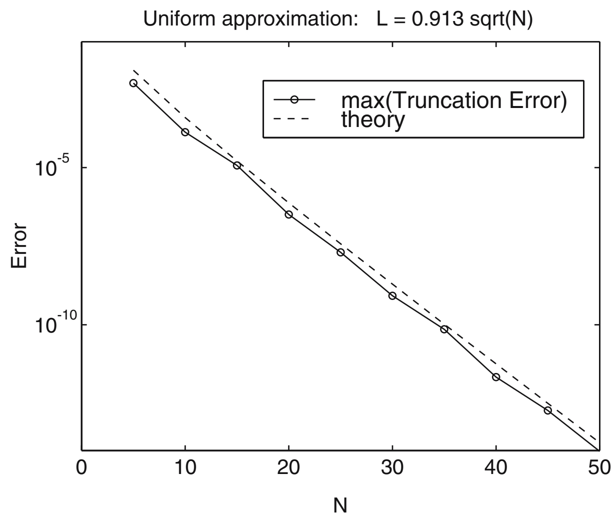

Fig. 8. The solid line with disks is the maximum error (L_∞ error) in the Fourier approximation of $\mathcal{T}(x; L, \chi = 0, \Theta = \pi)$ where $L = 0.913\sqrt{N}$. The dashed line is $\exp(-0.555N)/N$.

9. FIXED L ASYMPTOTICS: COMPARISON WITH ACTUAL COEFFICIENTS

In the limit degree $j \to \infty$ with L, χ, Θ all *fixed*, the Fourier coefficients of the top-hat function are

$$a_j \sim \frac{2}{\Theta}\,\frac{1}{j}\,\exp([3/4]L^2)\,\exp\left(-L\sqrt{\pi(1-\chi/\Theta)/2}\sqrt{j}\,\right)\sin\left(j\frac{\pi}{2}\left\{1+\frac{\chi}{\Theta}\right\}\right)$$
$$\times\left\{\cos(j\,\pi(1-\chi/\Theta)/2)\,\cos\left(L\sqrt{j\,\pi(1-\chi/\Theta)/2}\right)\right.$$
$$\left.+\sin(j\,\pi(1-\chi/\Theta)/2)\,\sin\left(L\sqrt{j\,\pi(1-\chi/\Theta)/2}\right)\right\} \qquad (40)$$

Figure 9 shows that the asymptotic approximation is indeed accurate even for rather small degree j.

The crucial point is that when the width parameter L is fixed, the coefficients (and truncation error) do still decrease exponentially with degree. However, the exponential is now of the *square root* of degree rather than degree itself. In the usual terminology Boyd [16], the "geometric" rate of convergence of the uniform, L-varies-as-$N^{1/2}$, asymptotics has been replaced by a "subgeometric" rate of convergence. Although the proportionality constant inside the exponential is larger (by a factor of two) for the overlapped extension, i. e., the sawtooth, the rate is again subgeometric with coefficients proportional to the square root of degree.

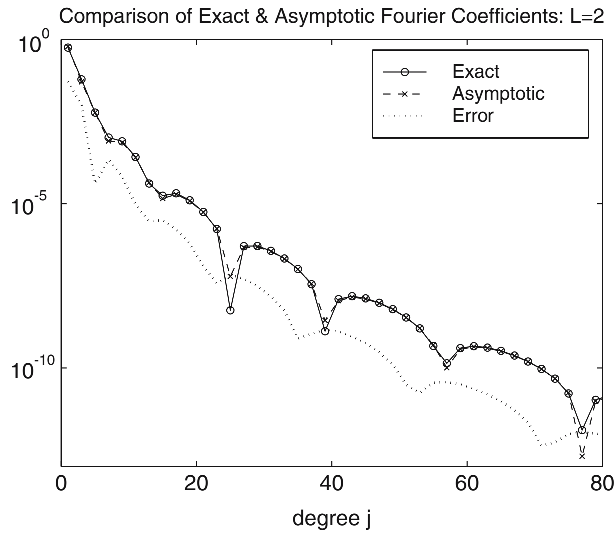

Fig. 9. The solid and dashed lines, labeled by disks and x's, respectively, are the exact and asymptotic Fourier coefficients for $\mathcal{T}(x; L = 2, \chi = 0, \Theta = \pi)$. These two curves are almost indistinguishable except at the dips of their mutual oscillations; the dotted curve, well below the others, is the absolute error.

10. OPTIMIZATION OF THE RATIO OF EXTENSION INTERVAL TO PHYSICAL INTERVAL

The Fourier coefficients of $\mathcal{T}$ and the sawtooth function Sw both converge most rapidly when the half-width of the physical interval χ is shrunk to *zero* as shown by our asymptotic approximations. The mathematics agrees with intuition: when the flat plateau where $\mathcal{T} \equiv 1$ is zero, the smoothing regions fill the entire extended interval and therefore are as wide and as smooth as possible. Conversely, narrowing the smoothing regions slows the rate of convergence of the Fourier series.

However, a "physical" interval of zero width defeats the whole purpose of Fourier Extension! And how should χ be chosen when more complicated $f(x)$ are extended?

The answer depends both on $f(x)$, which is the function being extended, and also on the purpose of the extension. For example, Israeli *et al.* [32] solve $u_{xx} - u = f(x)$ subject to Dirichlet boundary conditions by extending $f(x)$ to a function $\tilde{f}$ whose Fourier series is $\sum_j^N f_j \exp(ijx)$. A particular solution is then $u_P = \sum_j [f_j/(1 + j^2)] \exp(ijx)$. The general solution is $u = A\exp(x) + B\exp(-x) + u_P$ where A and B are chosen to satisfy the boundary conditions. Obviously, even if $f(x)$ is a constant or a very simple function, it is undesirable to choose an arbitrarily large extension interval $[-\Theta, \Theta]$. To evaluate u_P with M points within $x \in [-\chi, \chi]$ requires a Fast Fourier Transform on $M(\Theta/\chi)$ points, Thus, an arbitrarily large ratio of Θ/χ, as is best for optimizing Fourier convergence, is not optimum for Fourier summation.

When $f(x)$ is a function with a lot of internal structure, such as $f = \cos(Kx)$ where K is large, a large extension interval is a poor choice because this improves the resolution of the bell function at the expense of lowering resolution of $f(x)$. For particular classes of functions, one could in principle optimize Fourier extension by varying both L and χ and performing a steepest descent analysis. However, this would be restricted to $f(x)$ that are sufficiently simple that steepest descent is still possible.

For general $f(x)$, the only guidance is the commonsense precept: for smooth $f(x)$, a large extension interval is best whereas for rapidly-varying $f(x)$, a smaller extension interval (that is, χ/Θ close to one) would be better.

11. CONCLUSION

Even though the error-function-smoothed top-hat function is only C^{∞}, we have shown that the error in approximating it by a Fourier series, truncated at the Nth term, decreases as fast as $\exp(-0.55[1-\chi/\Theta]N)$ if the width parameter is varied with N as $L \approx 0.9\sqrt{1-\chi/\Theta}\sqrt{N}$. If L is fixed, then the error in the N-term truncated Fourier series decreases more slowly as $\sqrt{N}$.

If Fourier extension is performed in a more sophisticated way by overlapping the relaxation zones, then the rate of Fourier convergence for the extension $\tilde{f}$ of a smooth $f(x)$ can be greatly increased relative to the non-overlapped extension. We show this by deriving the asymptotic Fourier coefficients, both in the fixed and L-varying-with-N limits, for the extension of $f(x) \equiv x$, the "sawtooth" function.

The mathematics is clear, but why is it good to increase L with the truncation? As this width parameter increases, the derivative of $\mathcal{T}$ at the center of each smoothing region becomes larger. We seem almost to have gone round in a circle: choosing a functional form to smooth away the discontinuity of the top-hat function, and then increasing L so as to return closer and closer to the original discontinuous function as N increases.

The reason for this apparent paradox is that the smoothed top-hat function is *nearly* discontinuous at the center of each smoothing region and *weakly* singular at the boundaries of each smoothing region for all L. As L increases, the effects of the essential singularities at $x \pm \chi, \pm\chi$

are *weakened* because $\mathcal{T}$ becomes flatter and flatter in the neighborhood of these singularities. However, the derivative is steepening in the center of each smoothing interval.

As N increases, the N-term Fourier series is able to resolve steeper and steeper gradients in the center of each smoothing region. It then becomes a good "trade-off" to weaken the effects of the essential singularities by increasing L.

The major defect of our attempt to optimize Fourier extension methods is the fixing of the size of the "physical" interval (where $\tilde{f} \equiv f(x)$) at a predetermined width χ. For arbitrary $f(x)$, the convergence of the N-term Fourier series of the extended function $\tilde{f}$ is best for some pair of values (L, χ). However, as explained above, the choice of optimal physical interval width χ (relative to the size of the extended, periodic interval Θ) is highly dependent on the particular $f(x)$ which is being extended to a periodic function. The only general advice that can be given is: broad extension interval is best for smooth $f(x)$ [as displayed explicitly in our asymptotic Fourier coefficients for constant or linear f] whereas a narrow extension is best when $f(x)$ is a rapidly-varying or nearly singular function.

The steepest descent approach can be extended directly to other forms of Fourier extension such as the "odd-sine" scheme popular in wavelets. Steepest descent can also in principle be applied to more general classes of functions-to-be-extended $f(x)$. The practical difficulty is that it is hard to find f that are sufficiently general to be interesting and yet simultaneously so simple that steepest descent is analytically successful.

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