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A proof that the discrete singular convolution (DSC)/Lagrange-distributed approximating function (LDAF) method is inferior to high order finite differences

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Abstract

Finite differences approximate the mth derivative of a function $u(x)$ by a series $\sum_{j=-N}^{N} d_j^{(m)} u(x_j)$, where the x_j are the grid points. The closely-related discrete singular convolution (DSC) and Lagrange-distributed approximating function (LDAF) methods, treated here as a single algorithm, approximate derivatives in the same way as finite differences but with different numerical weights that depend upon a free parameter a. By means of Fourier analysis and error theorems, we show that the DSC is worse than the standard finite differences in differentiating $\exp(ikx)$ for all k when $a \geqslant a_{\mathrm{FD}}$ where $a_{\mathrm{FD}} \equiv 1/\sqrt{N+1}$ with N as the stencil width is the value of the DSC parameter that makes its weights most closely resemble those of finite differences. For $a < a_{\mathrm{FD}}$, the DSC errors are *less* than finite differences for k near the aliasing limit, but much, much worse for smaller k. Except for the very unusual case of low-pass filtered functions, that is, functions with negligible amplitude in small wavenumbers k, the DSC/LDAF is less accurate than finite differences for all stencil widths N. So-called "spectrally-weighted" or "frequency-optimized" differences are superior for this special case. Consequently, DSC/LDAF methods are *never* the best way to approximate derivatives on a stencil of a given width.

Keywords: Pseudospectral; Lagrange-distributed approximating functional; Discrete singular convolution; High order finite difference; Nonstandard finite differences; Spectral differences

1. Introduction

A pseudospectral method is a finite difference method in which the stencil is the entire grid [10,15]. Boyd [5] showed that one could derive both standard finite differences and also a great variety of nonstandard difference schemes by applying "sum acceleration" or "summability" methods to the pseudospectral difference

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sums. Sum acceleration methods apply running averages or similar artifices to the slowly-converging pseudospectral series so that these can be truncated to stencils of finite width without a drastic loss of accuracy.

The linear distributed approximating functional (LDAF) method was invented in 1991 by Hoffman et al. [20]. By 1997, the original concept had been refined to use a basis in which each element is the product of a Lagrangian interpolating cardinal function (as in classic finite differences) but multiplied by a Gaussian tapering function. Wei replaced the polynomial by the sinc function and dubbed the result the discrete singular convolution (DSC) method [3,13,41,43]. It is impossible to review the work of this very prolific author in detail, but of the more than one hundred articles listed at http://www.math.msu.edu/wei/, most use the DSC or LDAF schemes. Since the sinc function is closely related to polynomial interpolation as lucidly explained in [14,15], the Gaussian-weighted LDAF and DSC are so closely related that it is sufficient for our purposes to treat them as one.

Although the LDAF/DSC literature justifies the method through a rather elaborate machinery of smoothed Delta functions, Schwarz distribution theory and so on, the end result is that derivatives are approximated by formulas of the same form as classical finite differences [4] except that the numerical weights of the grid point values are different. The LDAF/DSC is also a special case of Boyd's earlier theory of sum-accelerated pseudospectral methods: special in that the weighting function is a Gaussian. Is this a good weight?

In the remainder of this article, we answer a resounding: No! In Sections 2 and 3, we review two essential background technologies: Fourier analysis of derivative approximations and sum-accelerated sinc pseudospectral methods. In Section 4, we show that by using this formalism, one can derive standard finite differences by a non-standard route and prove a rigorous theorem for the error in differentiating $\exp(\mathrm{i}kx)$. In the following section, we derive a similar theorem for the error in the DSC method.

2. Fourier analysis

Fourier analysis has been widely used to analyze difference formulas ever since this was popularized by von Neuman. The reason is that the Fourier basis function, $\exp(\mathrm{i}kx)$, is an eigenfunction of both the differentiation operator and also of all possible difference formulas. This implies that the accuracy of difference formulas can be assessed – and improved – merely by comparing the eigenvalues.

Theorem 2.1. *Let h denote the spacing of a uniform grid:*

$$x_j \equiv jh. \tag{1}$$

Define a grid-scaled differentiation operator:

$$D_m \equiv \mathrm{i}^{-m} h^m \frac{\mathrm{d}^m}{\mathrm{d}x^m}, \tag{2}$$

where $\mathrm{i} = \sqrt{-1}$. Introduce the centered approximation

$$D_m^{\mathrm{app}} u(x) \equiv \sum_{j=-N}^{N} d_j^{(m)} u(x + jh), \tag{3}$$

where "centered" implies

$$d_j^m = (-1)^m d_{-j}^m. \tag{4}$$

The set of $(2N + 1)$ points $x_j \equiv jh$, $j = -N, \ldots, N$, is said to be the "stencil" of the difference formula. Define the scaled wavenumber

$$K \equiv kh. \tag{5}$$

Then the differentiation operator has the exact eigenrelation

$$D_m \exp(\mathrm{i}kx) \equiv K^m \exp(\mathrm{i}Kx/h) \tag{6}$$

and the difference operator has the exact eigenrelation

$$D_{2m+1}^{\text{app}} \exp(\mathrm{i}Kx/h) \equiv \kappa^{2m+1} \exp(\mathrm{i}Kx/h) \equiv \left\{ 2 \sum_{j=1}^{N} d_j^{(2m+1)} \sin(jK) \right\} \exp(\mathrm{i}Kx/h), \tag{7}$$

$$D_{2m}^{\text{app}} \exp(\mathrm{i}Kx/h) \equiv \kappa^{2m} \exp(\mathrm{i}Kx/h) \equiv \left\{ d_0^{(2m)} + 2 \sum_{j=1}^{N} d_j^{(2m+1)} \cos(jK) \right\} \exp(\mathrm{i}Kx/h). \tag{8}$$

The error in the differentiation eigenvalue is then

$$E^{(m)}(K; N, d_{-N}^{(m)}, d_{-N+1}^{(m)}, \ldots, d_N^m) \equiv K^m - \kappa^m. \tag{9}$$

The theorem reduces approximate differentiation to an exercise in Fourier approximation. The formulas have been scaled by the wavenumber h so that in this convention, the difference weights $d_j^{(m)}$ are independent of h; there is no loss of generality therefore in taking $h = 1$, i.e., *unit grid spacing*, in the rest of the article.

The reason that the approximate eigenvalue κ^m is a *periodic* function of scaled wavenumber K is because of aliasing: on a discrete grid, frequencies higher than the "aliasing limit"

$$K_{\text{alias}} \equiv \pi \leftrightarrow k_{\text{alias}} = \pi/h \tag{10}$$

are indistinguishable on the grid from lower frequencies in the range $K \in [-\pi, \pi]$, and therefore are differentiated as if they were the aliased frequency in this low frequency range instead of the true, higher frequency. Aliasing is an inevitable consequence of differentiation, and the choice of difference weights cannot alter it.

3. Sum-accelerated pseudospectral methods and the sinc basis

The sinc pseudospectral method is the ultimate difference scheme in the sense that it differentiates *exactly* all unaliased wavenumbers as proved by the Shannon–Whittaker sampling theorem [10,34]. The sinc difference weights are obtained by differentiating the infinite series

$$u(x) \approx u_{\text{sinc}}(x) = \sum_{j=-\infty}^{\infty} u(jh) \text{sinc}(x/h - j), \tag{11}$$

where

$$\text{sinc}(x) \equiv \frac{\sin(\pi x)}{\pi x}. \tag{12}$$

The basis functions are often called "Whittaker cardinal functions" because, defining the jth "cardinal function" as

$$C_j^{\text{sinc}}(x; h) \equiv \text{sinc}(x/h - j), \tag{13}$$

the basis functions have the property that

$$C_j^{\text{sinc}}(x_i; h) = \delta_{ij} \equiv \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases} \tag{14}$$

The differentiation weights are then

$$d_j^m = h^m \left. \frac{\mathrm{d}^m C_j^{\text{sinc}}(x)}{\mathrm{d}x^m} \right|_{x=0}. \tag{15}$$

The weights are independent of h (except for the explicit factor of h^m), and are conveniently evaluated for $h = 1$.

The great drawback of the sinc method is that its great accuracy is purchased at the price of an *infinite* stencil. In practice, the requirement that $u(x)$ decays exponentially for $|x| \to \infty$ implies that the grid can be truncated to some large-but-finite span; the derivative sums are then truncated to summations over the entire truncated grid. Although the sinc pseudospectral method and related Fourier and Chebyshev polynomial

pseudospectral algorithms have been enormously successful in all branches of science and engineering [9,10,15,28,34,35,38], it obviously would be desirable if one could somehow obtain (nearly) spectral accuracy from a difference formula with a small stencil instead of a summation over the entire grid.

For the first two derivatives in the sinc basis, the weights are

$$d_j^{(1),\mathrm{sinc}} = (-1)^{j+1}/j, \quad d_j^{(2),\mathrm{sinc}} = \begin{cases} (-1)^{|j|+1}(2/j^2), & |j| \geqslant 1, \\ -\pi^2/3, & j = 0 \end{cases} \tag{16}$$

and are given for the next four orders of derivatives in p. 569 of [10]. The sinc differentiation eigenvalue for the first derivative is the usual sine series for the piecewise linear or "sawtooth" function:

$$K = 2\sum_{j=1}^{\infty}(-1)^{j+1}\frac{1}{j}\sin(jK). \tag{17}$$

The first option to obtain a sparse stencil is to simply *truncate* the infinite series at some upper limit n. This is a really bad idea because the error in the series, truncated after n terms, is $O(1/n)$, and therefore unacceptably large.

However, the problem of summing slowly convergent series is an ancient one. A broad collection of schemes, known variously as "summability", "sequence acceleration" or "sum-acceleration" methods have been developed. Boyd [5] was the first to apply such ideas to pseudospectral series to invent the form of nonstandard differences called "sum-accelerated pseudospectral". Boyd's first effort used the "Euler" acceleration. Variants of the Euler summation are described in [7,8]. Nonlinear sequence accelerations, that is, sums which are nonlinear functions of the terms in the series, are applied to nonstandard differences in [6] ("Levin u-transform" and "Padé approximants").

Mazziotti and collaborators have successfully applied the Euler-sinc method to a variety of problems in quantum chemistry [12,23,29,30]. Boyd [6] showed that for a differential equation example, the Euler-sinc method is better than finite differences.

On the other hand, Lee and Seo [24] experimented with Euler acceleration and Chebyshev acceleration, but needed formulas of very small bandwidth for turbulence research, and opted for spectrum-fitted compact differences instead.

4. Finite differences as a sum-accelerated pseudospectral method

Finite differences are usually justified by Lagrangian interpolation, but Boyd [6] showed that the same standard formulas could be obtained by applying a sum acceleration method to the sinc derivative sums:

$$\frac{\mathrm{d}u}{\mathrm{d}x}(0) \approx \sum_{j=-N}^{N} u(x_j) w_{Nj}^{fd} d_j^{(1),\mathrm{sinc}}, \tag{18}$$

where the sinc derivative coefficients are defined by (16) and where the weights for the first two derivatives are

$$w_{Nj}^{fd} = \begin{cases} \frac{\Gamma(N+1)^2}{\Gamma(N+j+1)\Gamma(N-j+1)}, & j \geqslant 1, \\ \frac{6}{\pi^2}\sum_{k=1}^{N}\frac{1}{k^2}, & j = 0. \end{cases} \tag{19}$$

Amusingly, the finite difference weights are "self-truncating": the poles of the gamma function for negative real argument imply that $w_{Nj} = 0$ for all integer $|j| > N$.

Boyd [6] shows that the asymptotic approximation

$$\frac{\Gamma(N+1)^2}{\Gamma(N+j+1)\Gamma(N-j+1)} \sim \exp\left(-\frac{j^2}{N+1/2} - \frac{j^4}{6(N+1/2)^3}\right) \tag{20}$$

is very accurate. The fact the weight function is *nearly* a Gaussian will be very important to the connection between the LDAF and DSC methods discussed in the following section.

Theorem 4.1 (Finite difference error for the first derivative). *The error in the first derivative eigenvalue*

$$E^{(1)}(K) \equiv K - \sum_{j=1}^{\infty} (-1)^{j+1} w_{Nj}^{fd} \frac{2}{j} \sin(jK) \tag{21}$$

is given exactly by

$$E^{(1)}(K) = 2^{2N} \frac{(\Gamma(N+1))^2}{\Gamma(2N+1)} \int_{-\pi}^{-\pi+K} \cos^{2N}(y/2)\, \mathrm{d}y, \quad |K| \leqslant \pi \tag{22}$$

and is given asymptotically for large N by the uniform approximation

$$\begin{aligned} E^{(1)} &\sim \pi \left[\left\{ 1 + \frac{1}{8}\frac{1}{N} \right\} \right] \sin^{2N+1}\left(\frac{K}{2}\right) \exp\left(N \cos^2\left(\frac{K}{2}\right) \right) \operatorname{erfc}\left\{ \sqrt{N} \cos\left(\frac{K}{2}\right) \right\} \\ &\approx 2^{-(2N+1)} K^{2N} + \mathrm{O}(K^{2N+2}), \quad K \ll 1, \end{aligned} \tag{23}$$

where the maximum relative error in the approximation is about 0.15/N even for N as small as one and the maximum absolute error is about 0.4/N.

The proof of the theorem will be published separately because the argument is rather lengthy, employing ideas unrelated to the mean themes of this article. For present purposes, the important point is that the relative error for small K is about $2^{-2N+1}K^{2N}$, consistent with the usual definition of finite difference order. The fact that the error is proportional to $K^{2N} = k^{2N}h^{2N}$, has been known through different arguments for many decades: an error proportional to h^{2N} is the very definition of what it means for a classic finite difference formula to be of order "2N".

5. LDAF and DSC methods

In the DSC method, the sinc approximation is modified by multiplying each basis function by a Gaussian weighting function:

$$u(x) \approx \sum_{j=-N}^{N} u(x_j) \exp(-a^2[x - x_j]^2/h^2) C_j^{\mathrm{sinc}}(x; h). \tag{24}$$

Differentiation of this sum followed by evaluation at $x = 0$ and exploitation of the cardinal function property (14) gives

$$\frac{\mathrm{d}u}{\mathrm{d}x}(0) \approx \sum_{j=-N}^{N} u(x_j) w_{Nj}^{\mathrm{DSC/LDAF}} d_j^{(1),\mathrm{sinc}}, \tag{25}$$

where

$$w_{Nj}^{\mathrm{DSC/LDAF}} = \exp(-a^2 j^2). \tag{26}$$

This confirms the earlier assertion that the DSC derivative approximation is just the special case of a sum-accelerated sinc scheme where the weighting function is a Gaussian.

Since the finite difference weights are *nearly* Gaussian, one cannot escape the conclusion that the LDAF/DSC methods are really just high order finite difference methods in disguise! In reality, this is not true because the small but importance differences between the finite difference acceleration weights and the Gaussian weights make the LDAF/DSC significantly *worse*!

Fig. 1 shows the bad news: the error curve for 19th century differences is *always* below the error for the DSC/LDAF method when

$$a = a_{\mathrm{FD}} \equiv \sqrt{1/(N + 1/2)} \tag{27}$$

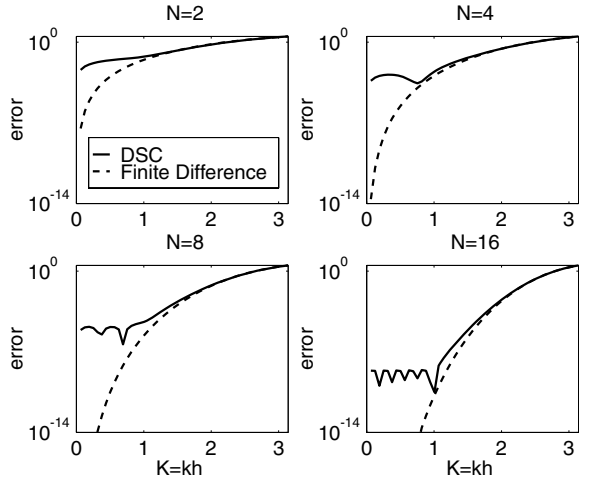

Fig. 1. Errors in the approximation of the piecewise linear (sawtooth) function using the DSC weighting (solid) with $a = a_{\mathrm{FD}} = \sqrt{1/(N+1/2)}$ and finite differences (dashed). The stencil width is $2N+1$; thus, $N=2$ in the upper left corner is equivalent to five-point, fourth order finite differences and the five-point DSC approximation. The free parameter a in the DSC method was chosen to match the asymptotic Gaussian form of the finite difference weights; experiments showed that larger or smaller a merely worsened the DSC errors.

to match the asymptotic form of the finite difference weights. For larger K, the error curves are almost indistinguishable, but as $K \to 0$, the finite difference error drops much rapidly than for the DSC method.

The reason is that the finite difference weights are such that the error for small K is $\mathrm{O}(K^{2N})$ which is also $\mathrm{O}(h^{2N})$; this is merely the usual definition of "order" for a finite difference method. In contrast, the pure Gaussian weight is a method of "order zero" in the sense that the DSC cannot exactly differentiate *any* polynomial in x, not even the constant polynomial.

The error for general scaling width a inside the weighting functions and for general stencil half-width N is given by the following.

Theorem 5.1 (Error in Gaussian-weighted/DSC). *The exact error for the Gaussian-weighted approximation to the first derivative eigenvalue*

$$E^{\mathrm{DSC}}(N;a) \equiv K - \sum_{j=1}^{\infty} (-1)^{j+1} \exp(-a^2 j^2) \frac{2}{j} \sin(jK) \tag{28}$$

is given by

$$E^{\mathrm{DSC}}(N;a) = E^{\mathrm{diff}} + E^{\mathrm{trunc}}, \tag{29}$$

where the "diffusion" error is

$$E^{\mathrm{diff}} \equiv \pi \sum_{m=-\infty}^{\infty} \left\{ \mathrm{erf}\left(\frac{[K - \pi(2m+1)]}{2a} \right) + \mathrm{erf}\left(\frac{\pi(2m+1)}{2a} \right) \right\} \tag{30}$$

and the "truncation" error is

$$E^{\mathrm{trunc}} \equiv \sum_{j=N+1}^{\infty} (-1)^{j+1} \exp(-a^2 j^2) \frac{2}{j} \sin(jK). \tag{31}$$

Proof. The first step is to recognize an analogy between Gaussian weighting and diffusion. When the diffusion equation is solved with boundary conditions of spatial periodicity, the general solution is a Fourier series in which $u(x,t)$ is just the initial condition with a Gaussian weight applied to each term. Thus, the Gaussian weighting can be conceptualized as a diffusion of the discontinuity of the sawtooth. Define

$$E^{\text{diff}} \equiv K - \sum_{j=1}^{\infty} (-1)^{j+1} \exp(-a^2 j^2) \frac{2}{j} \sin(jK). \tag{32}$$

Then the solution of the diffusion equation for the piecewise linear initial condition yields without approximation

$$E^{\text{diff}} = \pi \sum_{m=-\infty}^{\infty} \left\{ \text{erf}\left(\frac{[K - \pi(2m+1)]}{2a} \right) + \text{erf}\left(\frac{\pi(2m+1)}{2a} \right) \right\}. \tag{33}$$

E^{diff} is the error made by diffusing the *infinite* series, and DSC/LDAF differences are truncated after the Nth term, giving an additional error E^{trunc}. Subtracting the higher order sine terms gives the *exact* result quoted in the theorem. □

It is possible to derive useful asymptotic approximations to the error. When a is not too small, it is only necessary to keep the leading term in the truncation error, yielding

$$E^{\text{trunc}} \sim \frac{2}{N+1} \exp(-a^2(N+1)^2) \sin([N+1]K), \quad aN \gg 1, \ |K| \text{ small}. \tag{34}$$

Numerical experiments, not shown, indicate that even for $a \sim \text{O}(1)$, the approximation is correct to within a factor of two. Employing the large-argument asymptotics of the error function gives

$$E^{\text{diff}} \sim -\frac{2a\pi^{1/2}}{(K-\pi)} \exp\left\{ -\frac{1}{4} \frac{(K-\pi)^2}{a^2} \right\} - \frac{2a}{\pi^{1/2}} \exp\left\{ -\frac{1}{4} \frac{\pi^2}{a^2} \right\}, \quad a \ll 1, \ |K| < \pi. \tag{35}$$

The two errors, E^{diff} and E^{trunc}, behave very differently with respect to the width parameter a and K. The diffusion error goes to zero in the limit $a \to 0$ and is highly localized near $|K| = \pi$, decaying exponentially fast as $K \to 0$. In contrast, the truncation error decreases as a increases; when $a \gg 1$, the terms in the Fourier series are strongly damped and consequently the truncation error falls proportional to $\exp(-a^2(N+1)^2)$. However, the truncation error is not spatially localized in K but rather oscillates more or less uniformly over the whole domain.

Fig. 2 shows the errors for general a and K for a stencil width of 33, i.e., $N = 16$. The lower dashed line labeled FD where $a = a_{\text{FD}}(N)$ is the cross-section plotted in the lower right panel of the previous figure.

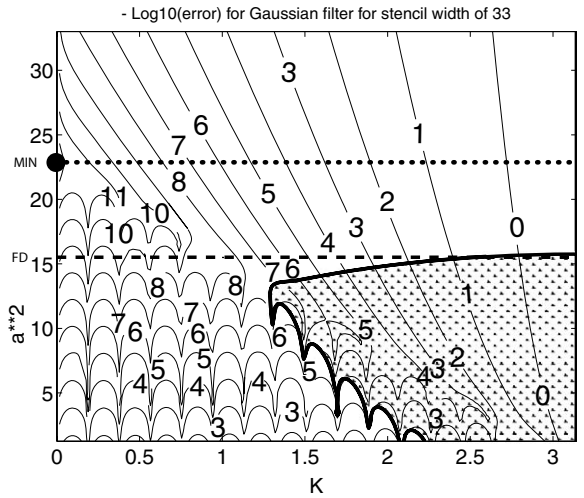

Fig. 2. The thin curves are the isolines of the negative of the base-10 logarithm of the error in approximating the eigenvalue of the first derivative for the DSC/Gaussian sum acceleration. The heavy dashed horizontal line, labeled "FD" to the left of the axis, marks the value of the scaling factor a^2 which matches that of the asymptotics of 32-d order finite differences. For small wavenumber K, the error is a minimum at the point marked by the black disk and horizontal dotted line. Most DSC calculations have chosen a weight close to this value of a^2. The shaded area shows where the error for the Gaussian weighting is smaller than for finite differences.

The shaded region shows that when $a < a_{\mathrm{FD}}$, the finite difference error is *worse* than that for the Gaussian weighting – but only for $K > \pi/2$. This implies that the DSC method could be superior in differentiating a function $u(x)$ that has a Fourier spectrum peaked near the aliasing limit. However, the shaded region does not extend much below $K = kh = \pi/2$, which means that *better* accuracy for *large* K has been purchased at the price of much *poorer* accuracy for Fourier components whose wavelengths are longer than $4h$.

The best accuracy for small K is obtained by choosing a to be slightly greater (typically 15%) than a_{FD}, yielding errors as small as $\mathrm{O}(10^{-11})$ near $K = 0$ instead of 10^{-7}. This is indeed the width of the Gaussian weights chosen in typical DSC papers such as [13,40] as marked on the figure by the black disk and dotted line. For this choice, the errors for the Gaussian-accelerated/DSC differences are *always* worse than finite differences of the same stencil width for *all wavenumbers* k.

Because of their relatively poor performance for small wavenumber K where most functions have their maximum Fourier amplitude, DSC papers use very wide stencils: never less than 17 points, and more often 65. The cost of a difference method is roughly $2(2N+1)N_{\mathrm{g}}$ operations (counting both multiplications and additions), where N_{g} is the total number of grid points. A Fourier method requires one forward and one reverse fast Fourier transform (FFT) to do the same job at a cost of about $(15/2)\log_2(N_{\mathrm{g}})N_{\mathrm{g}}$ operations. The pseudospectral method is faster for

$$N_{\mathrm{g}} < \exp(0.37N) \tag{36}$$

which implies that the Fourier method is more efficient for $N_{\mathrm{g}} < 20$ when $N = 8$, for $N_{\mathrm{g}} < 370$ when $N = 16$ and for $N_{\mathrm{g}} < 138{,}000$ when $N = 32$, the most popular half-stencil width in DSC applications. Clearly, one rapidly reaches a point of diminishing returns as the difference order increases, which is why very high order differences are rarely used in applications.

Why are finite differences so superior to DSC, given that both employ weights that are close-to-Gaussian? The answer is that the finite difference weights are tuned to give maximum accuracy in the limit $K \to 0$. In contrast, the truncation error E^{trunc} for the DSC does not decay as $K \to 0$. Given that the Fourier spectra of smooth functions fall off exponentially as $|K|$ increases, even small errors near $K = 0$ are intolerable.

6. Spectrally-weighted least squares differences

Since the DSC is more accurate than finite differences for $K > \pi/2$ when the width parameter a is chosen smaller than $1/\sqrt{N+1}$, one might suppose that the DSC would be useful for $f(x)$ that have Fourier spectra that are highly concentrated in $|K| \in [-\pi/2, \pi]$. Because there is another approach that is more targeted at such specialized functions, the answer is: Probably not.

The central idea of "spectrally-weighted" differences is to choose the differentiation weights in a difference formula so as to minimize error for a function whose Fourier spectrum is known, at least approximately.

Theorem 6.1 (Difference optimization). *Define the Fourier transform of a function $u(x)$ by*

$$U(k) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x) \exp(-\mathrm{i}kx)\, \mathrm{d}x. \tag{37}$$

Define the differentiation error as, repeating the earlier definition,

$$E^{(m)}(K; N, d_{-N}^{(m)}, d_{-N+1}^{(m)}, \ldots, d_N^m) \equiv K^m - \kappa^m, \tag{38}$$

where the $d_j^{(m)}$ are the weights for the approximation of the mth derivative. The mean square error is then

$$\Theta \equiv \int_{-\infty}^{\infty} \left(E^{(m)}(K)\right)^2 \mathrm{d}K = \frac{1}{h} \int_{-\infty}^{\infty} \left| U\left(\frac{K}{h}\right) \right|^2 \left| K^m - \sum_{j=-N}^{N} d_j^{(m)} \exp(\mathrm{i}jK) \right|^2 \mathrm{d}K. \tag{39}$$

Therefore, the least square error is minimized by choosing the differentiation weights to be the coefficients of a Fourier expansion of K^m with an integration weight that is the square of the Fourier transform of $u(x)$.

A proof is given in [6,42]. This theorem has been independently discovered several times, perhaps first by Wesseling [42]. The theorem motivates the following:

Definition 6.1 (*Spectrally-weighted differences*). A difference scheme is said to be "spectrally-weighted" if the weights for the mth order derivative with a centered stencil of $2N+1$ points are chosen to minimize

$$\int_{-\pi}^{\pi} \omega(K) \left| K^m - \sum_{j=-N}^{N} d_j^{(m)} \exp(\mathrm{i}jK) \right|^2 \mathrm{d}K, \tag{40}$$

where $x(K)$ is the user-chosen weight function. These are also known as "frequency-optimized", "wavenumber-optimized" and "dispersion-relation-preserving" differences, and also are labeled by the names of specific weight functions.

The limits of integration have been truncated to $[-\pi, \pi]$ since it is not possible to effectively approximate K^m outside the aliasing limit $|K| = \pi$.

The usual Fourier series, which gives the differentiation weights of the sinc pseudospectral method, corresponds to a weight of unity. In other words, the sinc weights are optimal for a function with a "white noise" spectrum that is everywhere equal to one over the entire unaliased range.

The finite difference weights correspond to the other extreme in which the L_2 norm of the error is minimized when weighted by the Dirac delta-function which concentrates all the weight at $K = 0$. Functions that are analytic in a strip of finite width about the real axis and decay exponentially for large x have Fourier tranforms that decay exponentially for large k. Thus, typical functions will lie between the sinc and finite difference extremes – and this is the fact that makes effective spectrally-weighted differences possible.

Because the literature is so large, we have tried to list a modest selection of articles in Table 1. There are undoubtably many omissions.

The weights can be calculated by solving a linear algebra problem. Define

$$\phi_j(K) \equiv \begin{cases} \sin(jK), & j = 1, 2, \ldots \quad [m \text{ odd}], \\ \cos(jK), & j = 0, 1, 2, \ldots \quad [m \text{ even}]. \end{cases} \tag{41}$$

Define the matrix and vector elements

$$G_{ij} \equiv \int_{-\pi}^{\pi} \phi_i(K)\phi_j(K)\omega(K)\,\mathrm{d}K, \quad \chi_i \equiv \int_{-\pi}^{\pi} \phi_i(K)K^m\omega(K)\,\mathrm{d}K. \tag{42}$$

Table 1
Spectrally-weighted differences: a partial bibliography

References	Comments
Adams and Shariff [2]	Upwind-biased dispersion-optimized
Adams [1]	Compact differences
Boyd [6]	Sech-weighted differences
Colonius [11]	Wave-optimized differences
Farnum and Mazziotti [12]	Gegenbauer-weighted differences
Gaitonde and Shang [16]	Optimized finite volume schemes
Gaitonde et al. [17]	Optimized finite volume schemes
Gray and Goldfield [18]	Dispersion-optimized differences
Haras and Taasan [19]	Space-and-time wave-optimized differences
Holberg [21,22]	Wave-optimized differences
Jordan and Mazziotti [23]	Gegenbauer-weighted differences
Lele [25]	Very high order compact finite differences
Liu [26]	Spectrally-weighted differences
Lockard et al. [27]	Wavenumber-range-optimized differences
Orlin et al. [31,33,32]	Dispersion-relation-optimized differences
Tam and Webb [37]	Dispersion-relation-preserving differences
Tam and Li [36]	Optimized for $K = 1.1$
Vanel and Baysal [39]	Dispersion-relation-optimized differences
Wesseling [42]	Frequency-optimized differences
Zingg et al. [45]	Wave-optimized differences
Zingg [44]	Comparisons of many schemes

Then the differentiation weights are obtained from solving the matrix problem

$$\vec{\vec{G}}\vec{d} = \vec{\chi}. \tag{43}$$

This matrix may be very ill-conditioned unless $\omega(K) = 1$, so Boyd [6] employed the singular value decomposition instead of the usual LU factorization.

Although we shall not perform detailed comparisons between DSC and spectrally-weighted differences, the good performance of DSC for high k and small a is an accident. It seems likely that for $f(x)$ which are known to have spectra concentrated between $K = \pi/2$ and $K = \pi$, one could obtain higher accuracy from spectrally-weighted differences than from DSC.

7. Summary

We have not shown that the DSC/LDAF method is inaccurate; on the contrary, by using stencils of 17–65 points, most published DSC calculations are extremely accurate. The point is rather that for the same very large stencil widths, finite difference approximations using the same number of points would be even more accurate.

We have not shown that the DSC is "spectrally-inferior" to finite differences (in the sense of giving a poorer approximation to the eigenvalue of the first derivative operator) for *all* wavenumbers k and *all* choices of the DSC width parameter a. For $a < 1/\sqrt{N+1}$, DSC errors are slightly *smaller* than finite differences for wavelengths between two and four times the grid spacing h. However, this high-k superiority is purchased at the price of much poorer accuracy than finite differences for *small* k where most functions have most of their Fourier amplitude. In the rare case of a function which is known to be "low-pass filtered" so that its Fourier transform is negligible for $k < (\pi/2)h$, one could obtain better accuracy than DSC by using "spectrally-weighted" or "frequency-optimized" differences as explained earlier.

Thus, the DSC/LDAF method is *never* the method of choice for approximating derivatives. It would, however, be premature to dismiss all the vast DSC/LDAF literature; the proliferation of papers has taken the concepts into wavelets, applications and a variety of other directions.

How can the DSC/LDAF algorithms be salvaged? One could of course try a different sum-acceleration weighting from the Gaussian. However, this is merely to explore various instances of the sum-acceleration methods of [5].

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Appendix A. Fourier analysis for nonperiodic functions

The partial sums of a Fourier series are always periodic, even if the function $f(x)$ they represent is not. Thus, the Fourier series of a nonperiodic function converges not to $f(x)$ itself but rather to a periodic function $\tilde{f}(x)$ which is equal to $f(x)$ on $x \in [-\pi, \pi]$ and then jumps discontinuously at the $x = \pm\pi$ so as to repeat the same shape periodically for all real x. Because of the discontinuities, the Fourier coefficients a_n and b_n decay as O(1/n); the Fourier coefficients of the first *derivative* do not decay at all.

This would seem to suggest that, except for the special case of applications to periodic functions, Fourier analysis of difference formulas would be a symptom of grave mental illness or mathematical imbecility. The reason that Fourier analysis is both very sensible and very general is that away from boundaries, a function $f(x)$ can *always* be represented by a rapidly convergent Fourier series. The trick is to multiply $f(x)$ by a "window" function so as to create a new function

$$\hat{f}(x) \equiv T(x) f(x), \tag{A.1}$$

where $T(x)$ is chosen to have the properties that (i) $T(x) \equiv 1$ over some finite interval and (ii) $T(x)$ decays smoothly to zero as $|x| \to \infty$. Many window functions are possible, but a suitable choice is

$$T(x) \equiv \begin{cases} 1, & x \in [-2,2], \\ \frac{1}{2}\left\{1 - \operatorname{erf}\left(L\,\operatorname{sign}(x)\,\frac{|x|-(1+\pi/2)}{\sqrt{(\pi/2-1)^2-[|x|-(1+\pi/2)]^2}}\right)\right\}, & 2 < |x| < \pi, \\ 0, & |x| \geqslant \pi, \end{cases} \tag{A.2}$$

where L is an arbitrary positive constant. The zones where $T = 1$ and $T = 0$ can be stretched by inserting additional scaling factors in the definition, but (A.2) demonstrates the basic idea.

Because the function $\hat{f}(x)$ agrees with $f(x)$ on a finite interval, here chosen as $[-2,2]$, the approximations and errors from applying difference formulas to $f(x)$ and $\hat{f}(x)$ will give identical results along as the span of the grid stencil is confined to this interval. At the same time, because $T(x)$ is "infinitely flat" at $x = \pm\pi$ in the sense that all its derivatives are zero, all derivatives of $\hat{f}$ at $x = \pi$ will match their counterparts at $x = -\pi$ – all in fact being zero. An elementary integration-by-parts argument then shows that the Fourier coefficients of $\hat{f}(x)$ will decay faster than any finite inverse power of degree n.

It follows that arguments based on Fourier analysis, as in the main body of this review, are completely general on the *interior* of the domain. Near the boundary, the windowing argument needs to be modified. However, near the endpoints, it is necessary to replace centered differences by partially or completely one-sided differences, and we have already agreed to exclude such regions from consideration.

In fact, it is possible at some cost in tedious detail to extend the principles of both windowing and the Fourier analysis of difference schemes to un-centered schemes near the endpoints, too. We shall not pursue such extensions here because our purpose is only to illustrate the general idea of nonstandard differences.

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