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Truncated Gaussian RBF Differences are Always Inferior to Finite Differences of the Same Stencil Width

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Abstract. Radial basis functions (RBFs) can be used to approximate derivatives and solve differential equations in several ways. Here, we compare one important scheme to ordinary finite differences by a mixture of numerical experiments and theoretical Fourier analysis, that is, by deriving and discussing analytical formulas for the error in differentiating $\exp(ikx)$ for arbitrary k.'Truncated RBF differences" are derived from the same strategy as Fourier and Chebyshev pseudospectral methods: Differentiation of the Fourier, Chebyshev or RBF interpolant generates a differentiation matrix that maps the grid point values or samples of a function $u(x)$ into the values of its derivative on the grid. For Fourier and Chebyshev interpolants, the action of the differentiation matrix can be computed indirectly but efficiently by the Fast Fourier Transform (FFT). For RBF functions, alas, the FFT is inapplicable and direct use of the dense differentiation matrix on a grid of N points is prohibitively expensive ($\mathcal{O}(N^2)$) unless N is tiny. However, for Gaussian RBFs, which are exponentially localized, there is another option, which is to *truncate* the dense matrix to a banded matrix, yielding "truncated RBF differences". The resulting formulas are identical in form to finite differences except for the difference weights. On a grid of spacing h with the RBF as $\phi(x)=\exp(-\alpha^2(x/h)^2)$,

$$\frac{df}{dx}(0)\approx\sum_{m=1}^{\infty}w_m\{f(mh)-f(-mh)\},$$

where without approximation $w_m=(-1)^{m+1}2\alpha^2/\sinh(m\alpha^2)$. We derive explicit formula for the differentiation of the linear function, $f(X)\equiv X$, and the errors therein. We show that Gaussian radial basis functions (GARBF), when truncated to give differentiation formulas of stencil width $(2M+1)$, are significantly less accurate than $(2M)$-th order finite differences of the same stencil width. The error of the infinite series $(M=\infty)$ decreases exponentially as $\alpha\to 0$. However, truncated GARBF series have a second error (truncation error) that grows exponentially as $\alpha\to 0$. Even for $\alpha\sim\mathcal{O}(1)$

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where the sum of these two errors is minimized, it is shown that the finite difference formulas are always superior. We explain, less rigorously, why these arguments extend to more general species of RBFs and to an irregular grid. There are, however, a variety of alternative differentiation strategies which will be analyzed in future work, so it is far too soon to dismiss RBFs as a tool for solving differential equations.

AMS subject classifications: 65D05

Key words: Pseudospectral, radial basis function, high order finite difference, nonstandard finite differences, spectral differences.

1 Introduction

Radial basis functions (RBFs) are a popular method for multidimensional interpolation on irregular or scattered grids [7, 8, 35, 38]. RBFs are now widely applied for solving differential equations in many different branches of physics and engineering [1, 9, 11–15, 20, 22–27, 29, 31, 34, 36, 37, 39]. The form of the approximation is very simple: in any number of dimensions d,

$$f(\vec{x}) \approx \sum_{j=1}^{N} \lambda_j \phi\left(||\vec{x}-\vec{c}_j||_2\right) \qquad \vec{x} \in R^d \tag{1.1}$$

for some function $\phi(r)$ and some set of N points $\vec{c}_j$, which are called the "centers". The coefficients λ_j are usually found by interpolation at a set of points $\vec{x}_k$ that may or may not coincide with the centers. Under fairly mild conditions on ϕ, the interpolation problem is provably solvable even when the interpolation points and centers are scattered randomly over an irregularly-shaped domain.

To solve partial differential equations by RBFs, it is obviously necessary to have a strategy for differentiating the RBF series and evaluating the derivative sums at the grid points. There are at least seven distinct strategies for RBF differentiation. Curiously, there hasn't been a careful review comparing these different options; for the sake of brevity none is offered here. We shall only assert, as will be demonstrated in our future work, that all RBF differentiation methods have liabilities. The most common strategy is to apply RBFs as a global pseudospectral method which generates a *dense* matrix which is very expensive to manipulate; consequently, most applications even in multiple space dimensions have used a thousand basis functions or less. Our modest goal is to perform a detailed analysis of the merits and failings of one particular strategy, dubbed "truncated RBF differences", which is much less expensive than the global, dense matrix approach.

Although many types of $\phi(r)$ have been used in the literature as reviewed in [17], we prefer to forgo a catalogue of limited results in favor of an in-depth examination of a single important case: that of Gaussian RBFs for which

$$\phi(x) \equiv \exp(-\epsilon^2 x^2). \tag{1.2}$$

Furthermore, we shall ignore boundary effects by assuming that the spatial domain is unbounded and all $f(x)$ approximated by RBFs either decay as $|x|\to\infty$ or are otherwise sufficiently well-behaved that their RBF series converge rapidly. (However, many of the ideas and themes developed here can be extended to other RBFs.)

Part of the reason for this choice is that these RBFs are popular for solving differential equations as in [16]. Another reason is that Gaussian functions allow many theoretical simplifications as illustrated below. A third reason is that infinitely differentiable, analytic radial basis functions are more accurate than RBFs of finite smoothness, and are therefore a logical testbed for investigating RBF accuracy.

In the absence of boundaries, the *absolute* inverse width parameter ϵ is meaningless: what matters is only the inverse width parameter *relative* to the *grid spacing* where, denoting the average grid spacing by h,

$$\alpha\equiv\epsilon h \qquad \text{[Relative Width Parameter]} \tag{1.3}$$

so that the RBF basis is

$$\phi(x;\alpha,h)\equiv\exp(-[\alpha^2/h^2]x^2). \tag{1.4}$$

In most of this work, the grid spacing will be uniform and h will be a constant, but the primacy of the relative width parameter α remains unchanged if h is reinterpreted as the average grid spacing on a non-uniform grid.

The differentiation scheme that we analyze, which we dub "truncated RBF differences", has the advantage of low cost ($\mathcal{O}(4MN)$ were $2M+1$ is the stencil width and N is the number of points on the grid) compared to the dense matrix obtained by using the RBF differentiation matrix without truncation, which costs $\mathcal{O}(2N^2)$. Our strategy also does not require FFT-like transforms from grid point values to RBF coefficients λ_j or the reverse; as explained in our forthcoming work, it is difficult to perform such transforms efficiently in the parameter range where the RBF method is well-conditioned. Furthermore, our method does not require dividing the domain into subintervals and matching approximations across artificial interior walls.

A different strategy for obtaining small differentiation stencils is to fit an RBF interpolant with $(2M+1)$ basis functions through a point x and its $2M$ nearest neighbors. Such "local RBF differences" have been applied to differential equations by Wright and Fornberg [40], Chandhini and Sanyasiraju [10] and under a different name ("RPICM") by Liu *et al.* [30]. We briefly discuss these in the appendix.

Most of the applications of RBFs to PDEs have been demonstrations that the method *works* rather than convincing exercises to show that the method is actually *better* than more old-fashioned alternatives like finite differences. This article is the first of a series in which we hope to relentlessly address the question: what's best?

2 Truncated differences

In Section 4, we show that the GARBF difference formulas are, for a uniform grid with spacing h,

$$\frac{df}{dx}(x) \approx \sum_{m=1}^{M} (-1)^{m+1} \frac{\alpha^2}{\sinh(\alpha^2 m)} \{f(x+mh) - f(x-mh)\}. \tag{2.1}$$

Because the difference weights decay *exponentially* fast with m, truncating the infinite series at $m = M$ yields a differentiation matrix with bandwidth M, i. e., $2M+1$ nonzero elements in each row, and at the same time an error due to truncation no worse than roughly $\exp(-\alpha^2 M)$. Put another way, the truncation error can be kept smaller than a user-specified tolerance δ by choosing

$$M(\delta;\alpha) = -\frac{1}{\alpha^2}\log(\delta). \tag{2.2}$$

For *small* α, the bandwidth $M(\delta;\alpha)$ is huge, but for $\alpha \sim \mathcal{O}(1)$, it is indeed possible to obtain accurate derivatives from a differentiation matrix of modest bandwidth. (Note that this option is *not* available for Chebyshev and Fourier pseudospectral methods because the corresponding derivative series decay very slowly, proportional to $1/M$ [3].)

Unfortunately, there is a constraint on α. When the grid spacing $h \to 0$ with fixed α, the error in approximating a function $f(x)$, assumed analytic for all real x, does not asymptote to zero. Instead, we show in our companion paper [6] that the norm of the error asymptotes to the "α-plateau" or "error saturation":

$$\begin{aligned} E(f;\alpha) &\equiv \lim_{h\to 0} \max_x |f(x) - f_{RBF}(x;\alpha,h)| \\ &\sim 4\exp(-\pi^2/\alpha^2)||f||_\infty + \mathcal{O}(\exp(-2\pi^2/\alpha^2)). \end{aligned} \tag{2.3}$$

If we choose α to be as large as possible without raising this "alpha-plateau" error greater than the user-chosen tolerance δ, and assuming that $||f(x)||_\infty \sim \mathcal{O}(1)$, then

$$\alpha_{optimum}(\delta) = \frac{\pi}{\sqrt{-\log(\delta/4)}}. \tag{2.4}$$

With this optimum choice of α,

$$M(\delta;\alpha_{optimum}(\delta)) = \frac{1}{\pi^2}\log(\delta)\log(\delta/4). \tag{2.5}$$

Fornberg, Flyer, Hovde and Piret [18] have shown that RBFs of all flavors have differentiation weights w_m that decay exponentially with $|m|$[†]. Truncation of exponentially-decaying RBF differentiation series is therefore a serious option, analyzed with care in later sections.

[†]The cardinal functions of some RBFs of compact support decay exponentially as $|m|$ increases and then switch to a slower, algebraic decay. However, these tiny tails do not alter our theme that RBF cardinal functions are spatially localized and truncation of the cardinal function-based differentiation series is an intriguing option.

Alas, as we show in detail below, it turns out that for a given bandwidth M, ordinary centered finite differences are *always more accurate*. Truncated RBF differences are successful but never optimal.

3 Background

3.1 Specialization to unit gridspacing

In most of this article, we shall restrict attention to a uniform grid with a spacing of one. There is no loss of generality in so doing because what matters is not the grid spacing h nor the RBF width parameter ϵ, but rather only the product of width and gridspacing, $\alpha \equiv h\epsilon$ as before. More formally, we can always make the change of variable

$$X = x/h \tag{3.1}$$

and the RBF approximation with grid spacing h in x is converted into one with the same coefficients but unit grid spacing in X.

3.2 Poisson summation

Theorem 3.1 (Poisson Summation)**.** *If $g(X)$ and $G(K)$ are a function and its Fourier transform,*

$$G(K) \equiv \int_{-\infty}^{\infty} g(X)\exp(iKX)\,dX, \qquad g(x) = (1/2\pi)\int_{-\infty}^{\infty} G(K)\exp(-iKX)\,dK, \tag{3.2}$$

then for any positive constant q,

$$q\sum_{n=-\infty}^{\infty} g(qn)\exp(i\,nqx) = \sum_{m=-\infty}^{\infty} G\left(x - m\frac{2\pi}{q}\right). \tag{3.3}$$

Furthermore,

$$\sum_{n=-\infty}^{\infty} (-1)^n g(n) = \sum_{m=-\infty}^{\infty} G([2m+1]\pi). \tag{3.4}$$

In words, any periodic function can be alternatively represented as a series of identical but translated copies of the Fourier transform of the function $g(x)$ that gives the Fourier coefficients. Such "imbricate" series are valuable in the theory of solitary and cnoidal waves [2] and many other subdomains of science.

3.3 Cardinal functions

If the basis functions are linearly independent, then for any set of $(N+1)$ interpolation points X_j and an equal number of basis functions, new functions $C_j(X)$, dubbed the "cardinal functions" or "Lagrange basis", can be formed by taking linear combinations of the

basis functions such that

$$C_j(X_i)=\begin{cases} 1, & i=j \\ 0, & i\neq j \end{cases}. \tag{3.5}$$

The cardinal functions are very convenient because the interpolant to an arbitrary $f(X)$ can be written as

$$f(X)\approx f_N(X)\equiv\sum_{j=0}^{N} f(X_j)C_j(X). \tag{3.6}$$

In other words, the grid point values of $f(X)$ are its coefficients in the cardinal basis.

The cardinal basis is also useful because interpolation-based differentiation formulas are obtained by differentiating the interpolant. The weights of the differentiation formula are just the derivatives of the cardinal functions:

$$\frac{df}{dX}(X)\approx\sum_{m=-M}^{M} w_m f(x_m), \qquad w_m=\frac{dC_m}{dX}(X). \tag{3.7}$$

On an infinite, evenly spaced grid, the cardinal basis simplifies because all cardinal functions are simply the translates of a "master cardinal function" $C(X)$:

$$C_j(X)=C(X-j), \qquad j=-\infty,\cdots,\infty, \tag{3.8}$$

where $C(X)$ is just the cardinal function $C_0(X)$ which is equal to one at $X=0$. Unfortunately, no simple characterization of the cardinal function itself is known. However, although not needed here, a very accurate approximation to the cardinal function for Gaussian RBFs on an evenly spaced grid is derived in [6].

4 Fourier analysis of difference formulas

4.1 Eigenvalues of the differentiation and difference operators

One can learn much about the accuracy of RBF and finite difference formulas from a Fourier analysis, that is, from examining how well the formulas approximate the derivative of $\exp(iKX)$ for various K. (A discussion of the generality of Fourier analysis is given in the appendix of [5].) The reason is that $\exp(iKX)$ is not only an eigenfunction of the derivative operator with eigenvalue iK, but also an eigenfunction of all difference formulas with a slightly different eigenvalue $i\kappa$. It follows that $K-\kappa(K)$ is a measure of the accuracy of the difference formula. To be precise, let the difference formula approximate the derivative at $X=0$ by

$$\frac{df}{dX}(X=0)\approx\sum_{m=-M}^{M} w_m f(m). \tag{4.1}$$

Then the approximate eigenvalue of the difference formula when applied to $\exp(iKX)$ is, assuming $w_m = -w_{-m}$ as true of all RBF and centered finite difference approximations,

$$\kappa = \sum_{m=1}^{M} 2w_m \sin(mK). \tag{4.2}$$

Fornberg and Flyer [17] show that for Gaussian RBFs

$$\kappa_{GARBF}(K;\alpha) = \frac{\sum_{m=-\infty}^{\infty} (K - m2\pi)\exp\left\{-(K-m2\pi)^2/(4\alpha^2)\right\}}{\sum_{m=-\infty}^{\infty} \exp\left\{-(K-m2\pi)^2/(4\alpha^2)\right\}}. \tag{4.3}$$

Unfortunately, because this formula is the ratio of *two* series,there is no simple relationship between the coefficients of either the numerator or denominator series and the weights of the GARBF difference formula.

4.2 Exact differentiation weights via Theta function magic:

Comparing the series

$$\theta_3(K/2;q=\exp(-\alpha^2)) = \frac{\sqrt{\pi}}{\alpha} \sum_{m=-\infty}^{\infty} \exp\left(-\frac{(K-2\pi m)^2}{4\alpha^2}\right) \tag{4.4}$$

to κ_{GARBF} and using the known series for the logarithmic derivative of θ_3,

$$\frac{d}{dy}\log(\theta_3)(y;q) = 4\sum_{n=1}^{\infty} (-1)^n \frac{q^n}{1-q^{2n}} \sin(2ny) \tag{4.5}$$

shows

$$\begin{aligned}
\kappa_{GARBF}(K;\alpha) &= -2\alpha^2 \frac{\frac{d}{dK}\theta_3(K/2;q=\exp(-\alpha^2))}{\theta_3(K/2;q=\exp(-\alpha^2))} \\
&= -2\alpha^2 \frac{d}{dK}\left(\log\left(\theta_3(K/2;q=\exp(-\alpha^2))\right)\right) \\
&= 4\alpha^2 \sum_{n=1}^{\infty} (-1)^{n+1} \frac{\exp(-\alpha^2 n)}{1-\exp(-2\alpha^2 n)} \sin(nK) \\
&= \sum_{n=1}^{\infty} (-1)^{n+1} \frac{2\alpha^2}{\sinh(\alpha^2 n)} \sin(nK).
\end{aligned} \tag{4.6}$$

Because the coefficients of the Fourier series for κ are also twice the weights of the difference formula (4.1), we can truncate this series to M terms to obtain the eigenvalue

of the Gaussian RBF when the sum over all points on the grid is truncated to $(2M+1)$ terms:

$$\kappa_{GARBF}(K;\alpha,M)=\sum_{m=1}^{M}(-1)^{m+1}\frac{2\alpha^2}{\sinh(\alpha^2 m)}\sin(mK) \tag{4.7}$$

which implies that the differentiation weights are *without approximation*

$$w_m=(-1)^{m+1}\frac{\alpha^2}{\sinh(\alpha^2 m)}. \tag{4.8}$$

Note that these weights are *exact*. Thus, for integer X, i. e., a point on the unit-spaced grid, a truncated RBF formula is

$$\frac{df}{dX}(X)\approx\sum_{m=1}^{M}(-1)^{m+1}\frac{\alpha^2}{\sinh(\alpha^2 m)}\left\{f(X+m)-f(X-m)\right\}. \tag{4.9}$$

Fast Summation RBF formulas *indirectly* evaluate the infinite sum, $M=\infty$ while truncated differentiation formulas evaluate the sum directly with a finite truncation M.

4.3 Application: Errors in differentiation of the linear function $f(X)=X$

Theorem 4.1 (Derivative of $f(X)=X$)**.** *The error in approximating the derivative of the linear function without truncation of the Gaussian RBF series is*

$$\begin{aligned}
E_\infty(\alpha)\equiv&\frac{dX}{dX}-\sum_{m=1}^{\infty}w_m(m-(-m))\\
=&1+2\alpha^2\sum_{m=1}^{\infty}(-1)^m\frac{m}{\sinh(\alpha^2 m)}\\
=&\alpha^2\sum_{m=-\infty}^{\infty}(-1)^m\frac{m}{\sinh(\alpha^2 m)}\\
=&\frac{\pi^2}{2\alpha^2}\sum_{m=-\infty}^{\infty}\operatorname{sech}^2\left(\frac{\pi^2}{2\alpha^2}(2m+1)\right)\\
\approx&4\frac{\pi^2}{\alpha^2}\exp\left(-\pi^2/\alpha^2\right)\left\{1+\mathcal{O}\left(\exp\left(-2\pi^2/\alpha^2\right)\right)\right\}.
\end{aligned} \tag{4.10}$$

Proof. The first line of the theorem is simply a definition of the error in approximating the derivative of a function, in this instance $f(X)=X$, by a generalized difference approximation. The second line follows by substituting the weights obtained in the previous section.

The third line follows from rewriting the sum to run over both positive and negative m, a necessary precursor to applying the Poisson Summation Theorem to simplify the sum. There is a subtlety: There should be no term for $m=0$ because the weight $w_0=0$,

but the limit as $m\to 0$ of $-\alpha^2 m/\sinh(\alpha^2 m)$ is not zero, but rather -1. Therefore, we must add one outside the series to cancel the $m=0$ term in the sum.

For small α, the series in the first three lines of the theorem converge slowly. We can obtain an equivalent series by invoking the alternating series form of the Poisson Summation Theorem, Eq. (3.4),

$$\sum_{n=-\infty}^{\infty}(-1)^n g(n)=\sum_{m=-\infty}^{\infty}G([2m+1]\pi),$$

where $G(k)$ is the Fourier Transform of $g(x)$. Using the Fourier Transform

$$\int_{-\infty}^{\infty}\frac{x}{\sinh(\alpha^2 x)}\exp(ikx)\,dx=\frac{\pi^2}{2\alpha^2}\mathrm{sech}^2\left(\frac{\pi}{2\alpha^2}k\right)=\mathcal{FT}\left\{\frac{x}{\sinh(\alpha^2 x)}\right\}(k) \tag{4.11}$$

then gives the fourth line of the theorem.

For small α, only the $m=0$ and $m=-1$ terms contribute, and contribute equally. Invoking $\mathrm{sech}(z)\approx 2\exp(-z)$ for large z then gives the final line. □

The error of $4\exp(-\pi^2/\alpha^2)$ is the same as the error previously found for approximating the constant one in [6]. However, (4.10) does not follow trivially. The approximation of $f(X)\equiv 1$ is a Jacobian theta function, which undulates periodically and is a sum of Gaussians. In contrast, the approximation of dX/dX is a constant; the only error is that the magnitude of the constant is not quite right; that magnitude is given by a sum of squares of hyperbolic secant functions, and is in fact the value at the origin of the square of the elliptic cosine function.

4.4 Aliasing, dealiasing and restrictions on wavenumber K

Before making comparisons between GARBF and finite differences for various K, it is important to understand the range in K where accuracy is important and also the range in K where accuracy is unimportant or even irrelevant.

First, all Fourier components $\exp(ikx)$ with wavelengths shorter than twice the grid-spacing h will be *aliased* to lower wavenumbers [4]. Because of this, all differentiation formulas based on a uniform grid, whether finite difference, RBF or whatever, will yield an eigenvalue for differentiation κ which is a *periodic* function of wavenumber k with a period of $2\pi/h$, and can be expressed a truncated Fourier series in wavenumber. Consequently, there is no loss of generality in restricting attention to $k\in[-\pi/h,\pi/h]$ or equivalently, $K\in[-\pi,\pi]$.

Second, centered difference formulas have definite parity with respect to $K=0$, that is, the fact that weights for both finite difference and GARBF satisfy $w_{-m}=-w_m$ for the first derivative implies that $\kappa(K)$ is a *sine* series in wavenumber rather than a general Fourier series with both sines and cosines, as already noted. Furthermore, the error $|K-\kappa(K)|$ is a function only of the absolute value of K, and therefore we lose no generality by restricting attention to positive wavenumbers only.

Third, the Fourier transform $F(K)$ of smooth functions $f(x)$ are typically flat for small K, and then decay exponentially fast as $|K|\to\infty$ [4,28]. It is essential that $|F(K)|$ is negligible at the aliasing limit, $K_{alias}=\pi$ for a unit grid spacing, because if $|F(K)|$ is not negligible at the aliasing limit, then it will non-negligible for $|K|>K_{alias}$ and aliasing will destroy the accuracy of the computation irregardless of the choice of difference weights.

It follows that a good scheme must be "low-biased". That is, accuracy for small $|K|$ is exponentially more important (literally!) than accuracy in differentiating high wavenumbers near the aliasing limit.

Finite difference schemes are always "low-biased" because the approximate differentiation eigenvalue κ is not a function of k and h separately, but only of the product $K=kh$. This implies that when the $(2M+1)$ difference weights are chosen to given a relative accuracy of h^{2M} as $h\to 0$, this simultaneously guarantees that

$$|K-\kappa_{FD}(K;M)|\sim\mathcal{O}(K^{2M+1}) \qquad \text{as} K\to 0. \tag{4.12}$$

As reviewed in [5], the best weight for a function with Fourier transform $F(K)$ is to choose the weights to be the coefficients of a Fourier sine series approximation to K which is a weighted least-squares approximation with a weighting of $|F(K)|^2$. Of course, one never knows the exact transform of the unknown solution to a differential equation. However, the typical behavior of a transform — flat for small K, and exponentially decaying as $|K|\to\infty$ — again reinforces the idea that the best approximation is heavily weighted towards small $|K|$.

In the rare exceptions when $F(K)$ has a maximum for moderate K, instead of at or near zero, the best strategy is to use what are variously called "spectrally-weighted differences" or "frequency-optimized differences" in which the differentiation weights are tailored to the expected behavior of $F(K)$ [5]. The RBF weights, in contrast, are not in any sense tuned to the expected behavior of the Fourier transform.

Fourth, aliasing not only corrupts wavenumbers with $K>\pi$, but, in the solution of differential equations, also corrupts smaller K. A typical term in a differential equation such as $q(x)u(x)$ cannot be exactly represented as a trigonometric polynomial with $|K|<\pi$, even if this is true of the discrete approximations to $q(x)$ and $u(x)$ individually, because their *product* generates Fourier components as high as $K=2\pi$. These are aliased to lower wavenumbers so that the amplitude of the solution for wavenumbers $|K|<\pi$ is not quite correct.

In computational fluid mechanics, for example, it is common for energy to spuriously accumulate in wavenumber K near the aliasing limit ("spectral blocking"), triggering a catastrophic numerical failure known as "aliasing instability". Phillips and Orszag [32, 33] showed that this could be fixed by filtering the upper one-third of the wavespectrum. That is, at every timestep, the amplitudes of Fourier components with $|K|\in[-2\pi/3,\pi]$ are reset to zero. Orszag showed that aliasing is permitted with his Two-Thirds Rule, but this is irrelevant (in a quadratically nonlinear system such as the hydrodynamic equations) because the wavenumbers that are polluted are eliminated by the filter.

Such filtering is now very common in fluid dynamics. For such models, it is obviously pointless to accurately differentiate wavenumbers near the aliasing limit because these will have zero amplitude, and not merely an exponentially small amplitude, after the "Two-Thirds Rule" filter is applied. This reemphasizes the fact that it is very important to be accurate small for small $|K|$, and unimportant to be accurate for $|K|>2\pi/3$.

5 Numerical comparisons of derivative approximations between truncated Gaussian RBF differences and (standard) finite differences

5.1 First criterion: Minimal accuracy

A differentiation formula is quite useless if it gives a poor approximation to the differentiation eigenvalue. Somewhat arbitrarily, we have chosen an absolute error of 0.05 as a threshold of minimum acceptability, and graphed the performance of truncated Gaussian RBF differentiation formulas in the K-α plane for four different stencil widths in Fig. 1.

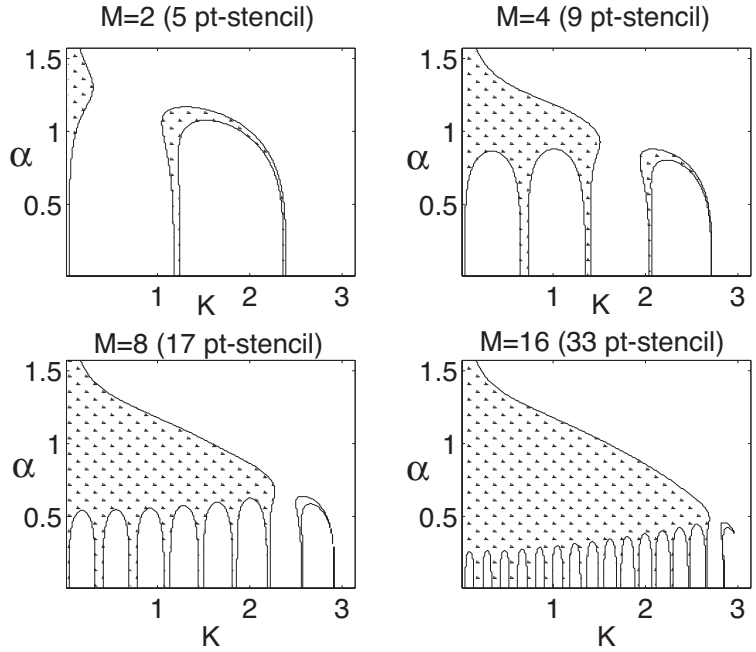

Figure 1: The shaded regions show where the absolute error in the eigenvalue of the first derivative, $|K-\kappa_{GARBF}(K;\alpha,M)|$, is smaller than 0.05 for four different values of M.

The upper left plot shows that there are only two tiny regions of acceptability for a five-point stencil, equivalent in work to a fourth order difference formula. The $M=2$ case is a disaster for $\alpha>1$ because even the $M=\infty$ limit is inaccurate, and the RBF differentiation formula is a disaster for smaller α because the error in truncating the infinite series is

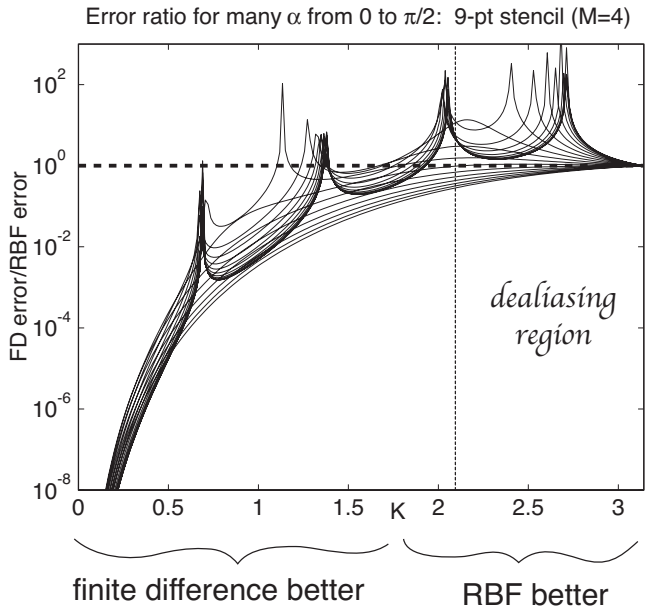

Figure 2: Finite difference error divided by Gaussian RBF error in the eigenvalue of the first derivative versus K for $M=4$, which is a stencil of nine points. The thick dashed horizontal line is where the ratio is one: the radial basis function method is better whenever the ratio is above this line, and the finite difference is better whenever the curve is below this dashed line. The thin dotted line marks the right one-third of the spectrum which would be removed by a dealiasing filter in a hydrodynamics computation.

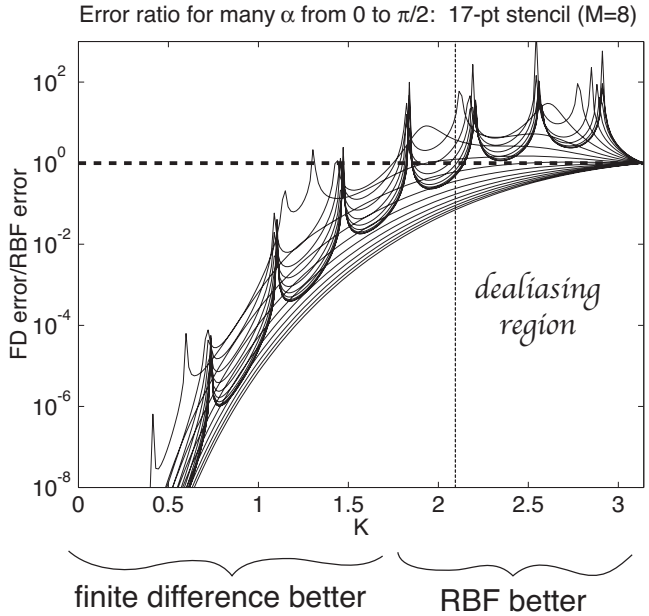

Figure 3: Same as previous figure but with M increased to 8. Finite difference error divided by Gaussian RBF error in the eigenvalue of the first derivative versus K for $M=8$, which is a stencil of seventeen points.

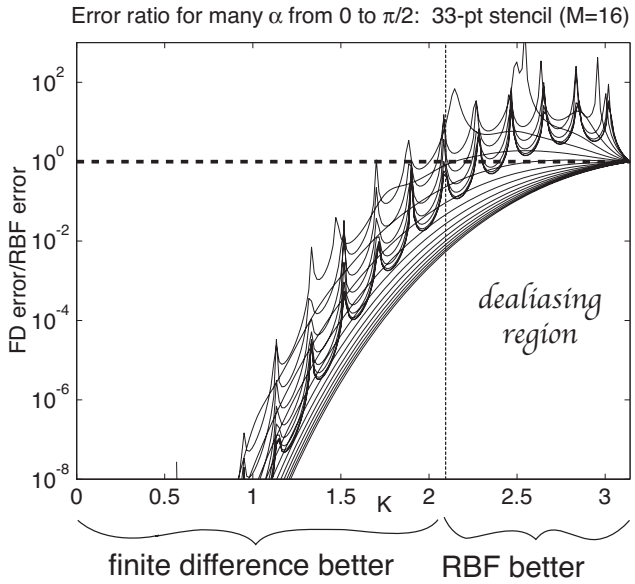

Figure 4: Same as previous figure but with the stencil width increased to thirty-three points (i. e., $M=16$). Finite difference error divided by Gaussian RBF error in the eigenvalue of the first derivative, plotted on a logarithmic scale versus K.

too severe. The $M=1$ three-point formula (not illustrated) is even worse. Consequently, we shall restrict attention to $M=4$ and larger in the remainder of this section.

5.2 Ratios of finite difference errors to truncated Gaussian RBF errors

Figs. 2, 3 and 4 plot the ratio of finite difference errors in the eigenvalue of the first derivative $\kappa(K)$ versus K for nine-point, seventeen-point, and thirty-three point stencils. The pattern is quite consistent between different orders M: the RBF method is *better* for K near the aliasing limit, but much worse by a huge factor for small K. For the thirty-three point wide stencil, the region of RBF superiority lies wholly in the right one-third of the wavenumber range. In realistic calculations, these Fourier components would likely be corrupted by aliasing error and in fact are completely eliminated by a dealiasing filter of the sort common in fluid mechanics. The range of RBF superiority is slightly larger for smaller M.

Still, there is no doubt that plain old nineteenth century finite differences are vastly superior to Gaussian radial basis differentiation formulas of the same order for the small wavenumbers K where accuracy really matters.

6 Summary

Other types of infinitely-differentiable RBFs are possible, of course. However, Fornberg and Flyer and their collaborators [17,18] have thoroughly analyzed the cardinal functions

for

$$\phi(X;\alpha)=\text{sech}(\alpha X)\ [\text{“sech” RBF}]$$

and

$$\phi(X;\alpha)=1/(1+\alpha^2X^2)\ [\text{“Inverse Quadratic”}].$$

Like Gaussian RBFs, these other species of cardinal functions decay no faster than exponentially as $|X|$, which does not encourage optimism that these alternatives are any better than Gaussians. It is an open problem to confirm this conjecture.

Thus, only a blockhead would employ truncated differences generated by Gaussian radial basis functions on an equispaced, unbounded grid. (Because of their very high cost, un-truncated differences are even less efficient.)

Some popular species of RBFs are practical only when combined with a linear or quadratic polynomial. This suggests that perhaps some of the flaws of Gaussian RBFs could be fixed by using a combined RBF-polynomial basis. Our analysis is based on truncation of a global RBF basis, and generalizing this to a global mixed polynomial/RBF basis would be a very bad idea on a supercomputer because a global polynomial part would couple all processors on a massively parallel machine. However, in the spirit of local RBF differences [10, 30, 40], one could compute a differentiation formula at a grid point x_j by fitting a mixed polynomial/RBF interpolant through a small number of the point's nearest neighbors. However, one would anticipate an accuracy intermediate between pure RBF and pure polynomial with the optimum strategy being to delete the RBF basis functions entirely! Further discussion of either global or local mixed RBF/polynomial interpolants is unprofitable.

It must be noted, however, that radial basis functions were originally invented for *multidimensional*, *scattered grid* approximation; the Central Dogma of RBF enthusiasts is that radial basis functions are better than any other alternative for irregular grids. Franke's masterful empirical study [21], which is the condensation of a very thorough five hundred page technical report that compared multiple methods for many real-world scattered grid interpolation problems, was very influential in promoting enthusiasm for RBFs. To criticize the failings of RBFs for a *one-dimensional*, *equispaced* grid is perhaps like criticizing a camel for being a really bad horse. Our investigation, restricted to one dimension and a uniform grid, is therefore necessarily incomplete, and making RBF/finite difference comparisons on a multidimensional, irregular grid is an important future problem.

However, it must be noted that because of the great difficulties of devising quantitative theories for multidimensional, scattered grids, almost all radial basis function theorists have written at least one paper and sometimes a whole series of papers using uniform one-dimensional grids, just like us. If this be folly or sin, then dunce caps and hairshirts will have to be distributed very broadly indeed within the RBF community.

More important, the germ of our argument transcends the simple framework used here. From a Fourier viewpoint, finite differences are optimized to differentiate $\exp(ikx)$ (and its multidimensional generalizations) for *small wavenumber*. For most functions $u(x)$,

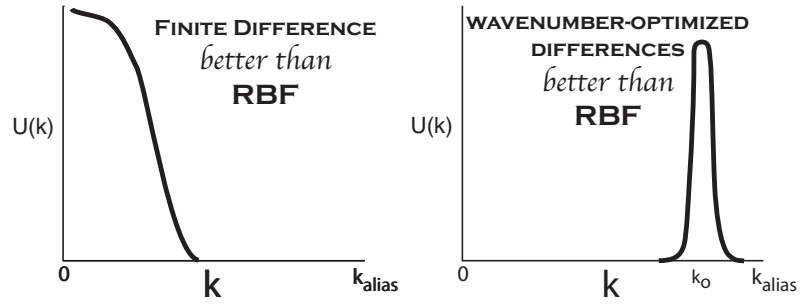

Figure 5: Left panel: schematic of $|U(k)|$, the Fourier transform of a typical function $u(x)$. The transform decays as k increases. In more than one dimension, k should be interpreted as the magnitude of the wavenumber vector $\vec{k}$. Unless the grid is very coarse, it is best to use a difference scheme with weights optimized for SMALL WAVENUMBER. For wavepackets of the form $\exp(ik_0x)A(x)$ where $A(x)$ is a slowly-varying envelope, or more generally for other functions with Fourier transforms concentrated about some wavenumber k_0 (right panel), it is best to use weights that are optimized for accuracy near $k=k_0$, a strategy known as "wavenumber-optimized" or "frequency-optimized" differences. For all classes of functions, RBF differences are not the best on a uniform or irregular grid in any number of dimensions because radial basis functions lack any strategy for optimizing accuracy for a specific range of wavenumber.

this is where the amplitude of the Fourier transform $U(k)$ is concentrated. The celebrated criminal Willie Sutton, when asked why he robbed banks, famously replied, "Because that's where the money is!" Finite differences, in one dimension or many, on a uniform grid or an irregular grid, are optimized in a way that Sutton would approve: they are best "where the money is". In contrast, Gaussian RBFs are not Fourier-optimized in any sense and have errors which are more uniform in k. This is bad because the amplitude of a typical Fourier transform $U(k)$ is *not uniform*, but is typically concentrated at *small* k. (This is always true for a well-behaved $u(x)$ for sufficiently small grid spacing h.)

For special classes of functions, of course, the Fourier transform may be peaked well away from $k=0$, and Gaussian RBFs may be better than finite differences for such functions. However, such instances of"accidental superiority" of RBFs over finite difference are little comfort to the RBF enthusiast. There is a rather large literature of "wavenumber-optimized" differences, as catalogued in [5], that systematically choose non-standard difference weights to improve accuracy when it is known *a priori* that the Fourier spectrum is peaked about a certain k_0. It goes without saying that when there is such *a priori* information, wavenumber-optimized differences, which are constructed specifically to exploit it, are superior to RBFs, which benefit only by accident. Fig. 5 shows the situation: for all classes of smooth functions, RBF truncated differences are inferior to either finite differences or wavenumber-optimized differences.

There is one exception: if the grid is so coarse that the error is large, and $U(k)$ has decayed only weakly by the time k is as large as the aliasing limit π/h, then optimizing for *small* k, as implicit in finite differences, is no longer optimum. Thus, functions that are so poorly resolved as to be "broad spectrum" all the way to the aliasing limit may indeed be better approximated by RBFs than finite differences.

The irregular grid problems in Franke [21] were almost always "broad spectrum" in

this sense because real-world observing networks are almost always coarse. Weather forecasting models use a million grid points per level, but the data to initialize the models comes from an irregular network of only 1700 weather balloon stations. Likewise, oil prospecting data is always poorly resolved because each data point requires seismometers and each measurement a charge of explosive. Weather balloons and seismometers must be placed where land and law allow.

Thus, there is no contradiction between our work and the "sacred scripture" of Franke. In solving differential equations, though, the modeler has the freedom to place grid points where he or she chooses, and the goal is to *not* underresolve the solution. For well-resolved solutions, Fourier analysis suggests that finite differences should be superior to RBFs even on irregular, multidimensional grids.

We intend to confirm this with future work now in progress. At present, no mechanism has been identified (except for poorly-resolved functions) that can somehow retrieve superiority for RBFs when the dimension is increased or when the grid becomes non-uniform.

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A Local RBF differences

Table 1: RBF weights.

Method	w_1	w_2
Trunc-RBF	$\frac{\alpha^2}{\sinh(\alpha^2)}$	$\frac{\alpha^2}{\sinh(2\alpha^2)}$
Local-3pt	$2\alpha^2\frac{\exp(3\alpha^2)}{\exp(4\alpha^2)-1}$	—
Local-5pt	$2\alpha^2\frac{\exp(3\alpha^2)(1+\exp(2\alpha^2))}{\exp(6\alpha^2)-1}$	$-2\alpha^2\frac{\exp(10\alpha^2)}{\exp(12\alpha^2)+\exp(10\alpha^2)+\exp(8\alpha^2)-\exp(4\alpha^2)-\exp(2\alpha^2)-1}$

Truncation of the infinite series for RBFs, as employed here, is not the only strategy for obtaining small differentiation stencils from an RBF approximation. "Local RBF differences" fit an RBF interpolant with $(2M+1)$ basis functions through a point x and its $2M$ nearest neighbors and then differentiate the interpolant to define the differentiation weights [10, 30, 40]. In contrast to the simple, explicit formula for the truncated-RBF weights, $w_m = (-1)^{m+1}\alpha^2/\sinh(\alpha^2 m)$, independent of M, one must solve a matrix problem of dimension $(2M+1)$. It is possible to obtain analytical expressions for small M, but these rapidly escalate in complexity with M as illustrated in Table 1. Furthermore, the

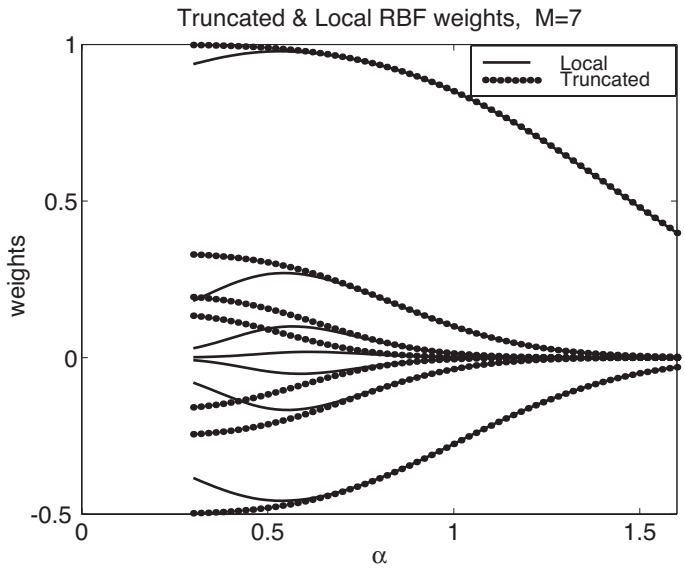

Figure 6: Comparison of the weights for local RBF differences, as the work of Fornberg and Wright (solid) and truncated RBFs (dotted) for $M=7$, which implies a 15-point stencil.

matrix problem is severely ill-conditioned for small α, this difficulty worsening with M, so that one must resort to the much more expensive "contour-Pade" algorithm [19].

We shall not discuss the local-RBF alternative at any length because the local-RBF weights asymptote to the usual finite difference weights for small α and asymptote to the truncated-RBF weights for moderate and large α as illustrated in Fig. 6. As M increases, the local-RBF weights become graphically indistinguishable from the truncated-RBF weights at smaller and smaller α. There is thus a rather narrow window of smallish α where the local RBFs are significantly different from either finite differences or truncated-RBF differences. In this window, local-RBF formulas will be more accurate than the truncated-RBF differences, but only because the numerical weights more closely resemble the finite difference weights to which they asymptote as $\alpha \to 0$. Thus, consideration of local-RBFs does not alter the conclusions of the main text.

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