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Error saturation in Gaussian radial basis functions on a finite interval

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ABSTRACT

Radial basis function (RBF) interpolation is a "meshless" strategy with great promise for adaptive approximation. One restriction is "error saturation" which occurs for many types of RBFs including Gaussian RBFs of the form $\phi(x; \alpha, h) = \exp(-\alpha^2(x/h)^2)$: in the limit $h \to 0$ for fixed α, the error does not converge to zero, but rather to $\mathcal{E}_S(\alpha)$. Previous studies have theoretically determined the saturation error for Gaussian RBF on an infinite, uniform interval and for the same with a single point omitted. (The gap enormously increases $\mathcal{E}_S(\alpha)$.) We show experimentally that the saturation error on the unit interval, $x \in [-1, 1]$, is about $0.06 \exp(-0.47/\alpha^2)\|f\|_\infty$ — huge compared to the $O(2\pi/\alpha^2)\exp\left(-\pi^2/[4\alpha^2]\right)$ saturation error for a grid with one point omitted. We show that the reason the saturation is so large on a finite interval is that it is equivalent to an infinite grid which is uniform except for a gap of many points. The saturation error can be avoided by choosing $\alpha \ll 1$, the "flat limit", but the condition number of the interpolation matrix explodes as $O(\exp(\pi^2/[4\alpha^2]))$. The best strategy is to choose the largest α which yields an acceptably small saturation error: If the user chooses an error tolerance δ, then $\alpha_{optimum}(\delta) = 1/\sqrt{-2\log(\delta/0.06)}$.

1. Introduction

Radial basis functions have become an important weapon in computer graphics and adaptive numerical solutions to differential equations [1–9]. The RBF approximation to a function in any number of dimensions d is

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

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. In the rest of this article, we shall concentrate on the one-dimensional case, $d = 1$, and assume that the centers and interpolation points coincide, that is, $\vec{c}_j = \vec{x}_j$.

Although many types of $\phi(r)$ have been used [10], we prefer an in-depth examination of a single important case: Gaussian RBFs for which

$$\phi(x) \equiv \exp(-\alpha^2(x/h)^2) \tag{2}$$

where h is the average grid spacing and α is a constant. In other work [11–13], we have treated the one-dimensional domain without boundaries. Here, we focus on the great increase in error saturation when the domain is restricted to a finite interval. This domain can be standardized to $x \in [-1, 1]$ without loss of generality.

The saturation error is a function of the width of the RBFs *relative* to the grid spacing h. It is therefore convenient to examine what happens as N, the number of interpolation points, is varied while α is fixed. This is labeled the "stationary

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Table 1
Errors in approximating the constant $f(x) \equiv 1$ in the limit of large N.

α	Infinite interval error [uniform grid]	Infinite interval error [gap grid]	Finite interval error [uniform grid]
1	0.020	0.53	0.070
1/2	2.8×10^{-17}	0.0013	0.0097
1/4	6.7×10^{-67}	2.3×10^{-16}	0.000017
1/6	4.9×10^{-155}	5.4×10^{-40}	1.8×10^{-9}
1/8	4.7×10^{-275}	5.3×10^{-70}	9.3×10^{-15}
asympt./$\|f\|_\infty$	$4\exp(-\pi^2/\alpha^2)$	$(2\pi/\alpha^2)\exp\left(-\pi^2/[4\alpha^2]\right)$	$0.06\exp(-0.47/\alpha^2)$

approximation" in Fasshauer [14]. The reader should be aware that it is also common to write RBFs in terms of an "absolute width" ϵ as $\phi(x) \equiv \exp(-\epsilon^2 x^2)$. However, this is not helpful here.

One major limitation of the present work is that it is non-adaptive. Successful function-adaptive experiments are reported in [15,16]. However, it is hardly a secret that adaptive methods are a subject of intense research despite many successes. Adaptive methods need a solid foundation in non-adaptive strategies, and that is what we aim to provide here.

RBFs on a finite interval, like polynomials which are the $\alpha \to 0$ limit of RBFs, exhibit the Runge Phenomenon, by which we mean that the error will diverge as $N \to \infty$ on some parts of the approximation interval. The RBF Runge Phenomenon (and the reduction of endpoint effects in general) is analyzed in [16–18,9,19] and so will not be discussed further here except to note that for Gaussian RBFs, the stationary approximation (fixed α) never diverges [20,14].

Some types of RBFs such as inverse quadratics (IQ; $\phi(r) \equiv 1/(1 + (\alpha^2/h^2)x^2)$) and sech RBFs (SH; $\phi(r) \equiv \mathrm{sech}([\alpha/h]x)$) have similar saturation errors. However, Buhmann [1] has shown that multiquadrics and inverse multiquadrics can reproduce the constant exactly, so clearly a different analysis for them is required to understand the effects of truncating an infinite domain to a finite interval.

2. Error saturation: Experimental results

Definition 1 (*Error Saturation*). When an RBF interpolant for fixed α, the "stationary limit" [14], does not converge to zero error for a function $f(x)$, but only to a finite error $\mathcal{E}_{saturation}(\alpha)$, this lack of convergence to zero is called "error saturation".

"Error saturation" has been known for many years as reviewed in [14], going back to Buhmann's [21] doctoral thesis.

Boyd and Wang [13] and, by a different route, Maz'ya and Schmidt [22], have shown that on a uniform, unbounded grid, the saturation error for Gaussian RBFs on an infinite, uniform interval is

$$\mathcal{E}_{saturation}(\alpha) \equiv \lim_{N\to\infty} \|f(x) - f_{RBF}(x; \alpha, N)\|_\infty = 4\exp(-\pi^2/\alpha^2)\, \|f(x)\|_\infty. \tag{3}$$

Boyd and Bridge [23] show that on a *nonuniform* grid, the saturation error rises steeply to $O(\exp(-\pi^2/(4\alpha^2)))$; for example, on an otherwise uniform grid with one point missing,

$$\mathcal{E}_{saturation}(\alpha) \sim \frac{2\pi}{\alpha^2} \exp\left(-\frac{\pi^2}{4\alpha^2}\right) \|f(x)\|_\infty. \tag{4}$$

But what is the saturation on a finite interval?

To determine the error saturation, it is sufficient to calculate the error in approximating the smoothest possible function, the trivial function $f(x) \equiv 1$, since the error for more complicated functions will only be worse. (A fuller justification of this assertion is given in [13] where it is shown in the limit $h \to 0$, the RBF coefficients of a general $f(x)$ tend, for centers near $x = y$, to those of the constant function $f(x) \equiv f(y)$.)

Fig. 1 and Table 1 show that the saturation error on a finite interval is many orders of magnitude larger than the error given by the asymptotic formula for the infinite interval. Fig. 2 shows that a good approximation to the saturation error on the finite, uniform grid is

$$E_{saturation} \approx 0.058\exp(-0.467/\alpha^2). \tag{5}$$

This empirical fit has the same form as for the infinite interval, both proportional to $\exp(-c/\alpha^2)$ for some constant c, but $c = \pi^2 \approx 10$ for the unbounded domain whereas $c \approx 0.467$, roughly twenty times smaller, for the finite domain.

Saturation error can be prevented by decreasing α with N as illustrated in the right panel of Fig. 1. However, it has long been known that the interpolation matrix is very ill-conditioned for small α. Boyd and Gildersleeve show experimentally that the condition number $\kappa \sim (1/2)\exp(\pi^2/(4\alpha^2))$ for $N \gg 1$. Thus, the nonstationary limit replaces one problem by another. Strategies to fight ill-conditioning are reviewed in [14] and [24], but these add complexity and there are other drawbacks of small α listed in Section 4. Error saturation needs to be understood as well as possible because it is a difficulty that can only be removed by trading it for other difficulties.

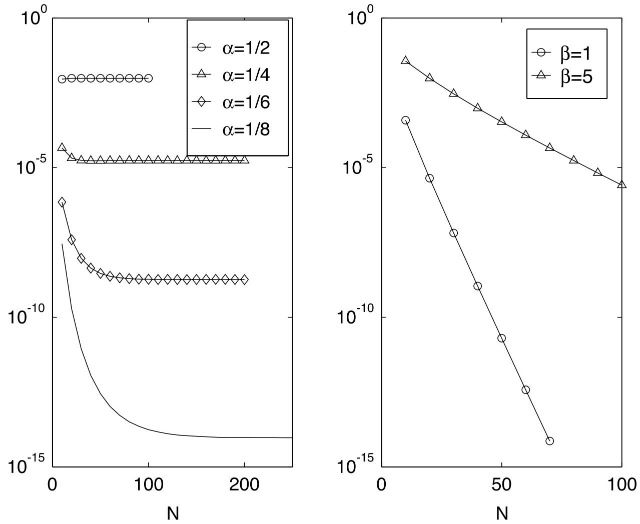

Fig. 1. Error in the L_∞ norm for the Gaussian RBF interpolant of $f(x) \equiv 1$. Left panel: fixed α and varying N where N is the number of RBFs and interpolation points. Right panel: Same but for the "nonstationary" limit with $\alpha = \sqrt{\beta/N}$ for fixed β; because the nonstationary error asymptotes to a straight line on a log-line plot, the rate of convergence is geometric, i.e., exponential with an argument which is linear in N. These are Maple computations with variable precision arithmetic, using 80 digits for $\alpha = 1/8$ to overcome the severe ill-conditioning of the interpolation matrix; the error in the L_∞ norm was computed by evaluating the pointwise error on a grid of 2000 evenly spaced points and taking the maximum.

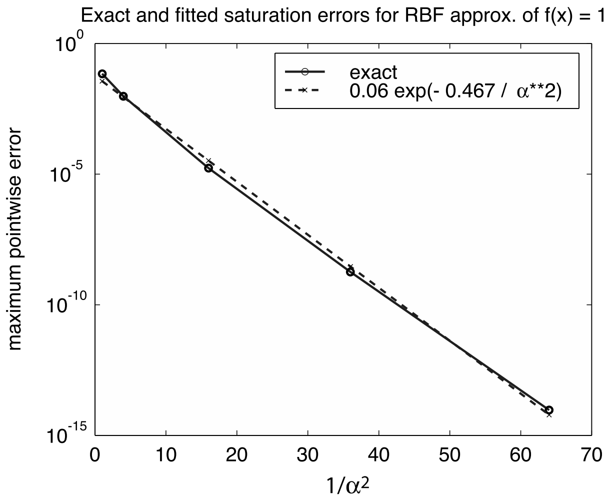

Fig. 2. The error in the L_∞ norm for the approximation of $f(x) \equiv 1$ on a finite interval by Gaussian radial basis functions. The thick curve with circles is computed in multiple precision arithmetic in Maple; the dashed curve is the analytic least-squares fit, $0.058\exp(-0.467/\alpha^2)$.

3. Analysis

We have been insufficiently clever to find a simple analytical solution for the effects of the finiteness of the interval on the RBF approximation of the trivial function, $f(x) \equiv 1$. However, analytical insight is possible.

First, let $f^{RBF,infinite}(x)$ denote the RBF approximation on the unbounded domain and let λ denote its coefficient, which is the same for all RBFs when the grid is uniform and $f(x) \equiv 1$. Let $f^{RBF}(x)$ denote the approximation using only RBFs with centers uniformly spaced on $x \in [-1, 1]$. Then without approximation, in a generalization of [23], we can write

$$f^{RBF}(x) = f^{RBF,infinite}(x; \alpha, h) - \Delta(x; \alpha, h). \qquad (6)$$

The function $\Delta(x; \alpha, h)$ can be expanded in the RBF cardinal function basis:

$$\sum_{j=-\infty}^{\infty} d_j C(x - jh; \alpha, h) \qquad (7)$$

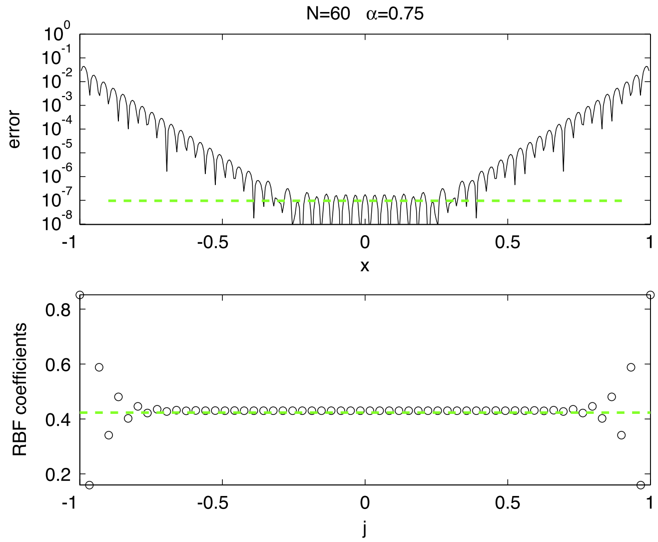

Fig. 3. Top: the pointwise error in the approximation of $f(x) \equiv 1$ by 60 Gaussian RBF with centers on $x \in [-1, 1]$ for an RBF width parameter of $\alpha = 3/4$. The horizontal dashed line is the asymptotic ($\alpha \to 0$) maximum pointwise error on the infinite interval. Bottom: same except that the RBF coefficients are the circles; the dashed line is the coefficient λ of all the RBFs in the infinite interval approximation.

where $C(x; \alpha, h)$ is the "master cardinal function" for the *infinite* interval, defined as that series of RBFs with the property that

$$C(x; \alpha, h) = \begin{cases} 1, & x = 0 \\ 0, & x = jh, \ j = \text{non-negative integer}. \end{cases} \tag{8}$$

(The cardinal basis, like the cardinal or "Lagrange" basis for polynomial interpolation, is just a set of linear combinations of the original basis that form a new, equivalent basis with the cardinal property.) However, $\Delta(x; \alpha, h)$ is zero at each of the interpolation points on $x \in [-1, 1]$ by construction and so the coefficients of the cardinal functions with peaks on those points must be zero, too. Thus, without approximation

$$f^{RBF}(x) = f^{RBF,infinite}(x; \alpha, h) - \sum_{j=1}^{\infty} a_j C(x - (-1 - jh); \alpha, h) - \sum_{j=1}^{\infty} b_j C(x - (1 + jh); \alpha, h). \tag{9}$$

The coefficients a_j and b_j are chosen so as to cancel all RBFs with centers outside the interval $x \in [-1, 1]$. This expansion applies to an arbitrary $f(x)$ and not merely to the trivial function.

Because two infinite series remain, (9) does not seem too promising. However, for $f(x) \equiv 1$, symmetry with respect to $x = 0$ implies that $a_j = b_j$. More important, because the RBF cardinal functions are spatially localized, the series decay exponentially fast with j. This assertion is justified by the very accurate cardinal function derived independently in [12,25]:

$$C(x; \alpha, h) \approx (\alpha^2/\pi) \frac{\sin(\pi x/h)}{\sinh(\alpha^2 x/h)} \left\{ 1 + O\left(4 \exp\left(-2\frac{\pi^2}{\alpha^2}\right)\right) \right\}. \tag{10}$$

This shows that the cardinal functions decay proportional to $\exp(-\alpha^2 x/h)$.

For any fixed α and sufficiently large N, the number of interpolation points, this implies that the infinite series represent *boundary layer corrections* to the infinite domain approximation. This is illustrated in Fig. 3. Away from the endpoints, the error oscillations are uniform, close to the theoretical prediction of the small-α asymptotic theory for the infinite grid given in [13]. It is only in layers near the endpoints, which have a fixed width in *grid points* and a decreasing-in-N width in x, that the finiteness of the interval matters. The width of the boundary layers in grid points unfortunately grows as $O(1/\alpha^2)$ and thus is rather wide for small α. This makes it difficult to obtain useful analytic approximations because it is only for small α that one has accurate approximations to λ and the RBF coefficients of the cardinal function.

Even so, the finite width of the boundary layers implies something else that is conceptually useful: the errors on $x \in [-1, 1]$ are the same whether we omit an *infinite* numbers of points $x_j = jh$ for $|x| \geq 1$, or simply make a gap of a *few* points in the infinite grid by dropping the points $x = 1 + jh$ for $j = 1, \ldots, M$ for some finite M, and similarly near $x = -1$. This is illustrated in Figs. 4 and 5.

The first figure shows that when one or more points is omitted from an otherwise uniform grid, a large error develops in the gap itself. This error decays exponentially fast away from the center of the gap, but to the left of the dividing dotted line at $x = 1$, the error is still quite noticeable, and much, much larger than on the interior of the domain: the approximation is

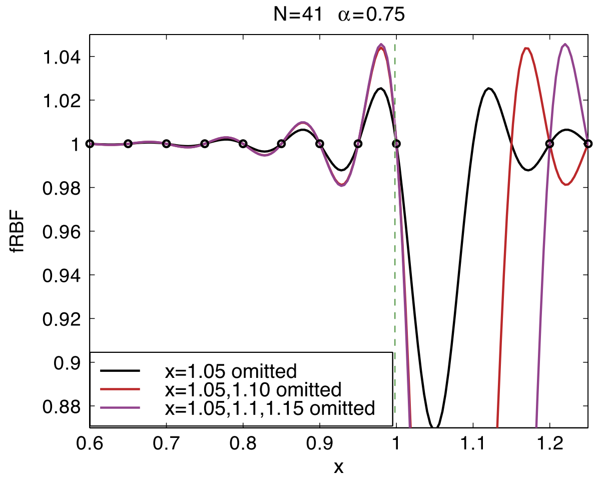

Fig. 4. Gaussian RBF approximation of the trivial function $f(x) \equiv 1$ using 41 grid points ($h = 1/20$) with $\alpha = 3/4$. The black curve is the approximation on an otherwise uniform grid with a single grid point omitted; the red curve is the same except that the centers and interpolation points at $x = 1.05$ and $x = 1.10$ are omitted and the magenta curve is the same with three points omitted. (Note that to the left of $x = 1$, the red and magenta curves are graphically indistinguishable.) For purposes of approximation on $x \in [-1, 1]$, only the error at and to the left of $x = 1$, which is marked by the vertical green dotted line, is relevant. Part of the domain to the right of $x = 1$ is shown to illustrate that a very large error develops in the gap which decays away from the gap — but nevertheless contaminates the neighborhood of $x = 1$ with much larger errors than for smaller $|x|$ where the error falls to the infinite grid saturation error. The disks denote the interpolation points, which are also the centers. (The three points deleted to make $M = 3$ (magenta) curve are not marked.) (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

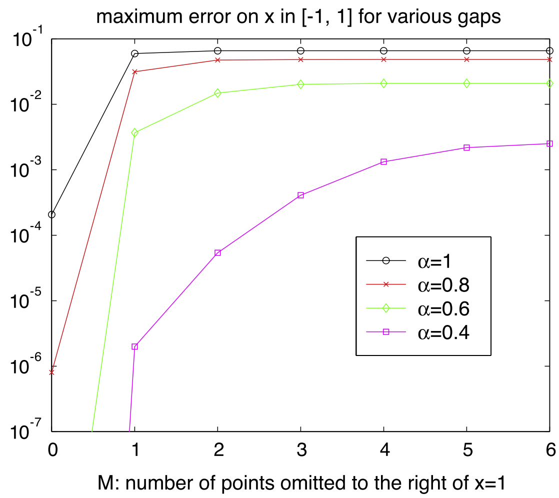

Fig. 5. Error on $x \in [-1, 1]$ when M points, just to the right of $x = 1$, are omitted from an otherwise uniform infinite grid, for Gaussian RBF approximation of the trivial function $f(x) \equiv 1$. $M = 0$ denotes the results on an infinite, uniform grid.

very flat and close to $f(x) \equiv 1$ at the left edge of the plot at $x = 0.6$ and becomes even flatter and more accurate for smaller x not shown. Although the curves with a two-point gap and a three-point gap are are quite different to the *right* of $x = 1$, they are almost indistinguishable to the *left* of $x = 1$. For this relatively large value of α, there is rapid convergence with M, the number of points omitted.

Qualitatively — the error induced by omitting M points resembles the RBF cardinal function. (For $\alpha \sim O(1)$, this resemblance is also quantitative.) This and (9) suggest that the width of the boundary layer of large error decays exponentially on the same scale as the cardinal function, $O(\exp(-\alpha^2||x| - 1|/h))$.

Fig. 5 shows that the behavior is similar for all RBF widths α. However, as the RBFs become wider (smaller α), convergence with M becomes slower and slower — a gap of half a dozen points to the right of $x = 1$ is necessary to approximate the omission of an infinite number of points for $\alpha = 0.4$, for example. Unfortunately, we also see a steep rise in the difference between the finite interval saturation error, which is the limit as $M \to \infty$, and the infinite interval result, which is $M = 0$. Indeed, the infinite interval saturation errors for $\alpha = 0.6$ and $\alpha = 0.4$, which are 5.0×10^{-12} and 6.5×10^{-27}, respectively, are too small to fit on the graph.

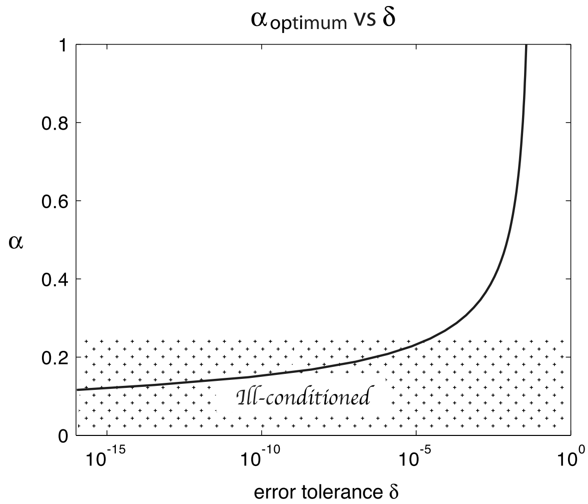

Fig. 6. $\alpha_{optimum}$ is plotted versus the error tolerance δ (on a logarithmic scale) for Gaussian RBFs on a uniform grid on a finite interval. The shaded area denotes where the condition number κ of the interpolation matrix is greater than the reciprocal of machine epsilon, $\epsilon_{machine} = 2.2 \times 10^{-16}$; when $\kappa\epsilon_{machine} \geq 1$, the solution of the interpolation problem may be inaccurate unless special tactics are employed.

4. Consequences of error saturation: An optimal choice of α

Small α (i.e., very wide RBFs) is undesirable because (i) the condition number of the interpolation matrix explodes as $(1/2)\exp(\pi^2/[4\alpha^2])$ [26] (ii) the RBF sum itself may be come very ill-conditioned [13] and (iii) the Runge Zone expands from the real interval $x \in [-1, 1]$ to the same rather large oval in the complex-plane as for polynomial interpolation [18]. On the other hand, saturation implies that the error will be disastrously huge when α is large or moderate.

A pragmatic strategy is to to choose the *largest* α compatible with the desired relative error tolerance δ where the word "relative" means that

$$\mathcal{E}/\|f\|_\infty \leq \delta \tag{11}$$

where $\mathcal{E}$ is the absolute error in the L_∞ norm. Solving $E_{saturation}(\alpha) = \delta$ gives

$$\alpha_{optimum}(\delta) = \sqrt{\frac{0.5}{-\log(\delta/0.06)}} \tag{12}$$

where we have slightly rounded the floating point numbers in view of the uncertainties in the empirical saturation formula. This curve is graphed in Fig. 6.

One difficulty, as noted earlier, is that when $\alpha < 1/4$, the interpolation matrix is very ill-conditioned. Some remedies are discussed in [24,27,28].

5. Summary

Our study has revealed that the change from an unbounded interval to a finite interval causes a huge increase in saturation error. Conceptually, the infinite-to-finite shift is equivalent to omitting the M points and centers just outside the interval $x \in [-1, 1]$ in the limit $M \to \infty$. Unfortunately, omitting even a single point creates a gap in the grid; the ensuing large error decays exponentially on a scale of h/α^2. Nevertheless, the result is a boundary layer to the left of $x = 1$ where the error is orders of magnitude larger than on an infinite grid without gaps.

The most interesting applications of RBFs are on *irregular* grids. However, the creation of a localized region of large error due to a gap in the grid is a very general principle. Although we have used a uniform grid to be precise, simple and quantitative, it is clear that the same principles apply on irregular grids. In particular, the transition from infinite grid to finite interval will always raise the saturation error.

We have emphasized the trivial function $f(x) \equiv 1$, but Maz'ya and Schmidt [25] and Boyd and Wang [13] show that the coefficients of general analytic $f(x)$ asymptote to those of the constant – and inherit the saturation error behavior – as the grid spacing $h \to 0$. Similarly, it is not much of a restriction to concentrate on one dimension: the arguments about gaps and omitted points qualitatively apply to multiple dimensions without modification. Lastly, we have specialized to Gaussian RBF, which are analytic and spatially localized, but Fornberg, Flyer, Hovde and Piret [29] show that many RBF species have *cardinal* functions that decaying exponentially away from their peaks even when $\phi(r)$ is not localized or even bounded. Much generalization remains for the future, but we have enumerated reasons why such generalizations are unlikely to produce many surprises.

In spite of the relatively large saturation error on the finite interval, it is nevertheless true that it is possible to obtain an approximation whose error falls exponentially fast with N until the saturation plateau is reached — even using a uniform grid where *polynomial* interpolation often *fails* because of the Runge Phenomenon. If an error tolerance δ is desired, our study gives a specific $\alpha_{optimum}(\delta)$ so that this tolerance can be achieved for a sufficiently large number of interpolation points N. In short, the saturation error does not prevent Gaussian radial basis functions from being useful on a finite interval. Efficient approximation, however, requires the saturation error and optimum RBF width formulas derived here.

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