MATH 590: Meshfree Methods

“Flat” Limits of Kernel Interpolants

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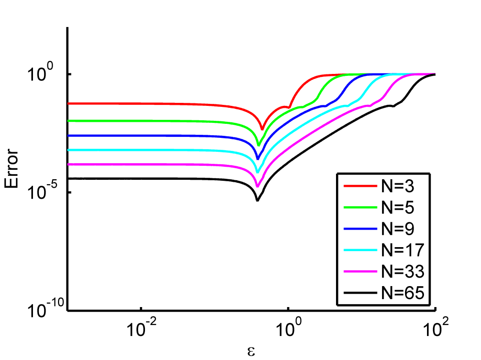
Fall 2014

Outline



- A "flat" limit seems to exist for interpolation with C^2 Wendland kernels on $[0, 1]$ based on N uniformly spaced points with ε varying from 10^{-3} to 100.
- Does this happen for other kernels?
- Does it happen for all kernels?
- What is this limit?

About 10 years ago an interesting connection was discovered between interpolants based on infinitely smooth RBFs such as Gaussians, generalized (inverse) multiquadrics and the oscillatory kernels[1]

$$K(\boldsymbol{x},\boldsymbol{z}) = \frac{J_{\beta/2-1}(\varepsilon\|\boldsymbol{x}-\boldsymbol{z}\|)}{\varepsilon\|\boldsymbol{x}-\boldsymbol{z}\|^{d\beta/2-1}}, \quad \beta \geq d$$

- In many cases the limiting (“flat”) RBF interpolants were identical to polynomial interpolants — especially in 1D experiments.

(see, e.g., [DF02, FF05, FW04, LF03, LF05])

[1] For fixed $\boldsymbol{z}$ these are fundamental solutions, bounded at the origin, of the d-dimensional Helmholtz operator in spherical coordinates (see [FLW06], where they are called Bessel kernels, see also [Fas07, Ch.4], where they are referred to as Poisson functions).

In [DF02] univariate ($d = 1$) interpolation with ε-scaled infinitely smooth radial kernels was studied.

Driscoll and Fornberg show that the RBF interpolant

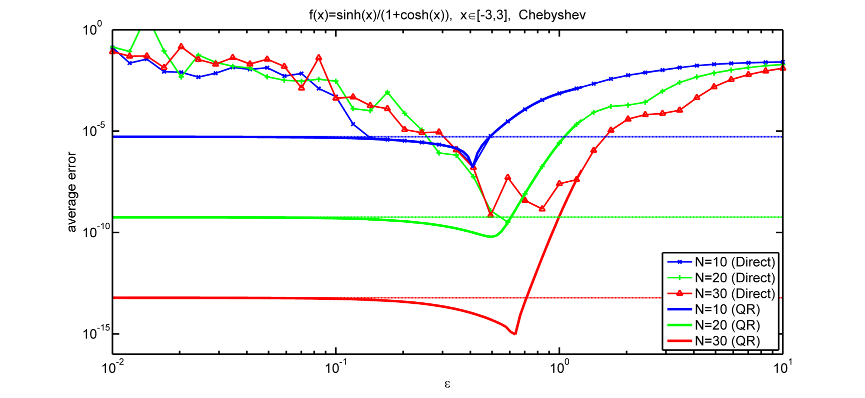
$$s^{\varepsilon}(x) = \sum_{j=1}^{N} c_j \kappa(\|\varepsilon(x - x_j)\|), \qquad x \in [a, b] \subset \mathbb{R},$$

to function values at N distinct data sites tends to the Lagrange interpolating polynomial of f as $\varepsilon \to 0$.

▸ Run `FlatGaussian.cdf`

Remark

In order to fully exploit this relationship it will be necessary to develop stable evaluation algorithms for "flat" kernels.



The “flat” polynomial limit for Gaussian interpolation, stably computed with the algorithm from [FM12].

The multivariate case is more complicated.

Remark

Note that most of the following results are limited to radial kernels, i.e., radial basis functions (RBFs).

- The limiting RBF interpolant is given by a low-degree multivariate polynomial (see [Boo06, LF05, LYY07, Sch05, Sch08]).
  - For example, if the data sites are located such that they guarantee a unique polynomial interpolant, then the limiting RBF interpolant is given by this polynomial.
  - If polynomial interpolation is not unique, then the RBF limit is still a polynomial whose form depends on the choice of basic function.
- Lee and Micchelli [LM13] recently showed that in the multivariate setting, when the interpolation points that are unisolvent for d-variate polynomials of total degree ℓ, there is also a unique polynomial limiting interpolant for a given (not necessarily radial) kernel, provided it is analytic.

Theorem (Driscoll, Fornberg, Larsson, Schaback, Yoon [2002-08])

Assume the strictly positive definite radial kernel κ has an expansion

$$\kappa(r) = \sum_{j=0}^{\infty} a_j r^{2j}$$

into even powers of r (i.e., κ is infinitely smooth), and that the data $\mathcal{X}$ are unisolvent with respect to any set of N linearly independent polynomials of degree at most m. Then

$$\lim_{\varepsilon \to 0} s^{\varepsilon}(\boldsymbol{x}) = p_m(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^s,$$

where p_m is determined as follows:

- *If interpolation with polynomials of degree at most m is unique, then p_m is that unique polynomial interpolant.*
- *If interpolation with polynomials of degree at most m is not unique, then p_m is a polynomial interpolant whose form depends on the choice of RBF.*

Some Examples

- Inverse quadratic

$$\kappa(\varepsilon r) = \frac{1}{1+\varepsilon^2 r^2} = 1 - (\varepsilon r)^2 + (\varepsilon r)^4 - (\varepsilon r)^6 + (\varepsilon r)^8 + \cdots$$

- Gaussian

$$\kappa(\varepsilon r) = e^{-\varepsilon^2 r^2} = 1 - (\varepsilon r)^2 + \frac{(\varepsilon r)^4}{2} - \frac{(\varepsilon r)^6}{6} + \frac{(\varepsilon r)^8}{24} + \cdots$$

- Inverse MQ

$$\kappa(\varepsilon r) = \frac{1}{\sqrt{1+\varepsilon^2 r^2}} = 1 - \frac{(\varepsilon r)^2}{2} + \frac{3(\varepsilon r)^4}{8} - \frac{5(\varepsilon r)^6}{16} + \frac{35(\varepsilon r)^8}{128} + \cdots$$

- Poisson, $\beta = d = 2$

$$\kappa(\varepsilon r) = J_0(\varepsilon r) = 1 - \frac{(\varepsilon r)^2}{4} + \frac{(\varepsilon r)^4}{64} - \frac{(\varepsilon r)^6}{2304} + \frac{(\varepsilon r)^8}{147456} + \cdots$$

Remark

- *The statements in the theorem require the RBFs to satisfy a condition on certain coefficient matrices $A_{p,J}$. This condition was left unproven in [LF05] and verified in [LYY07].*
- *For the special case of Gaussians [Sch05] shows that as $\varepsilon \to 0$ the RBF interpolant converges to the de Boor and Ron least polynomial interpolant (see [Boo92, BR90, BR92] and also [Boo06]).*
- *In [LF05] the authors use Taylor expansions to also provide an explanation for the error behavior for small values of the shape parameter, and for the existence of an optimal (positive) value of ε giving rise to a global minimum of the error function.*

Remark

- *The work by Narayan and Xiu [NX12] suggests that a connection may be found between other unique multivariate polynomial interpolants (determined by different families of orthogonal polynomials) and corresponding RBF interpolants.*
  - *In [NX12] it is shown that their orthogonal polynomial interpolant with Hermite polynomials corresponds to the de Boor and Ron least polynomial interpolant.*
  - *In [FM12] it was shown that the flat limit of Gaussians is given by Hermite polynomials.*

Remark

- *In [FW04] the authors describe a so-called Contour-Padé algorithm that makes it possible (for data sets of relatively modest size) to compute the RBF interpolant for all values of the shape parameter* ε *including the limiting case* $\varepsilon \to 0$.
- *Some numerical result obtained with Grady Wright's* MATLAB *toolbox are included in [Fas07, Ch. 17].*
- *Other recent work obtaining RBF interpolants close to the polynomial limit, i.e., for small* ε, *is [FM12, FLF11].*
- *We will discuss the Hilbert–Schmidt stable evaluation algorithm of [FM12] soon.*

Big Deal: “Flat” Limits, So What?

- One of the most intriguing aspects associated with the polynomial limit of RBF interpolants is the fact that RBF interpolants seem to be most accurate (for a fixed number N of given samples) for a positive value of the shape parameter ε.
  - The following figure clearly exhibits a minimum in the interpolation error distinctly away from zero.

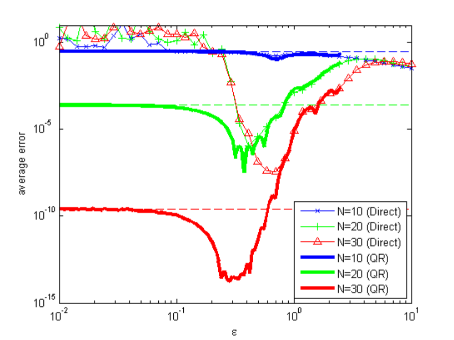


Figure: $f(x) = \sin(x/2) - 2\cos(x) + 4\sin(\pi x)$, $x \in [-4, 4]$

- The observations of this section imply that RBF interpolants are (more flexible) generalizations of polynomial interpolants, and therefore must be at least as accurate as (and often quite a bit more than) polynomial interpolants.
- However, polynomials are the basis of traditional algorithms (usually referred to a spectral methods) for the numerical solution of equations whose solution is known to be smooth.

Message from this section:

RBFs, using stable evaluation algorithms and good predictors of optimal shape parameters, should be able to do better than polynomials.

- The flat limit of RBFs with finite smoothness was not studied until the recent paper [SRFH12] in which interpolation on $\mathbb{R}^d$ was investigated.
    - The thesis [BS10] contains similar investigations done simultaneously and independently.
- Before we explain the results obtained in [SRFH12], we recall a few finitely smooth radial kernels and their interpretation as full space Green's functions.

Example (Radial kernels with finite smoothness)

- The univariate C^0 Matérn kernel $K(x,z) \doteq \mathrm{e}^{-\varepsilon|x-z|}$ is the full-space Green's function for the differential operator

$$\mathcal{L} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \varepsilon^2 \mathcal{I}.$$

  On the other hand, it is well-known that univariate C^0 piecewise linear splines may be expressed in terms of kernels of the form $K(x,z) \doteq |x-z|$. The corresponding differential operator is

$$\mathcal{L} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}.$$

  Note that the differential operator for the Matérn kernel "converges" to that of the piecewise linear splines as $\varepsilon \to 0$.

Example (cont.)

- The univariate C^2 tension spline kernel [Sch66, Ren87] $K(x,z) \doteq \mathrm{e}^{-\varepsilon|x-z|} + \varepsilon|x-z|$ is the Green's kernel of

$$\mathcal{L} = -\frac{\mathrm{d}^4}{\mathrm{d}x^4} + \varepsilon^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2},$$

while the univariate C^2 cubic spline kernel $K(x,z) \doteq |x-z|^3$ corresponds to

$$\mathcal{L} = -\frac{\mathrm{d}^4}{\mathrm{d}x^4}.$$

Again, the differential operator for the tension spline "converges" to that of the cubic spline as $\varepsilon \to 0$.

Example (cont.)

- In [BTA04] we find a so-called univariate *Sobolev kernel* of the form $K(x,z) \doteq \mathrm{e}^{-\varepsilon|x-z|} \sin\left(\varepsilon|x-z| + \frac{\pi}{4}\right)$ which is associated with

$$\mathcal{L} = -\frac{\mathrm{d}^4}{\mathrm{d}x^4} - \varepsilon^2 \mathcal{I}.$$

The operator for this kernel also “converges” to that of the cubic spline kernel, but the effect of the scale parameter is different than for the tension spline.

Remark

Note that this Sobolev kernel is different from the Sobolev splines (Matérn functions) discussed earlier — terminology . . .

Example (cont.)

- The general multivariate Matérn kernels are of the form

$$K(\boldsymbol{x},\boldsymbol{z}) \doteq K_{\beta-d/2}\left(\varepsilon\|\boldsymbol{x}-\boldsymbol{z}\|\right)\left(\varepsilon\|\boldsymbol{x}-\boldsymbol{z}\|\right)^{\beta-d/2}, \qquad \beta > \frac{d}{2},$$

and can be obtained as Green's kernels of (see [FY11])

$$\mathcal{L} = \left(\varepsilon^2\mathcal{I} - \Delta\right)^{\beta}, \qquad \beta > \frac{d}{2}.$$

We contrast this with the polyharmonic spline kernels

$$K(\boldsymbol{x},\boldsymbol{z}) \doteq \begin{cases} \|\boldsymbol{x}-\boldsymbol{z}\|^{2\beta-d}, & d \text{ odd},\\ \|\boldsymbol{x}-\boldsymbol{z}\|^{2\beta-d}\log\|\boldsymbol{x}-\boldsymbol{z}\|, & d \text{ even}, \end{cases}$$

and

$$\mathcal{L} = (-1)^{\beta}\Delta^{\beta}, \qquad \beta > \frac{d}{2}.$$

- All examples above show that the differential operators associated with finitely smooth RBF kernels "converge" to those of a piecewise polynomial or polyharmonic spline kernel as $\varepsilon \to 0$.
- We therefore ask if RBF interpolants based on finitely smooth kernels converge to (polyharmonic) spline interpolants for $\varepsilon \to 0$ as is the case for infinitely smooth radial kernels and polynomials.

- As mentioned above, infinitely smooth radial kernels can be expanded into an infinite series of even powers of r.
- Finitely smooth radial kernels can also be expanded into an infinite series of powers of r.
  - In this case there always exists some minimal odd power of r with nonzero coefficient indicating the smoothness of the kernel.

Example

For univariate C^0, C^2 and C^4 Matérn kernels, respectively, we have

$$
\begin{aligned}
\kappa(\varepsilon r) &\doteq e^{-\varepsilon r} \\
&= 1 - \varepsilon r + \frac{1}{2}(\varepsilon r)^2 - \frac{1}{6}(\varepsilon r)^3 + \cdots, \\
\kappa(\varepsilon r) &\doteq (1 + \varepsilon r)e^{-\varepsilon r} \\
&= 1 - \frac{1}{2}(\varepsilon r)^2 + \frac{1}{3}(\varepsilon r)^3 - \frac{1}{8}(\varepsilon r)^4 + \cdots, \\
\kappa(\varepsilon r) &\doteq \left(3 + 3\varepsilon r + (\varepsilon r)^2\right) e^{-\varepsilon r} \\
&= 3 - \frac{1}{2}(\varepsilon r)^2 + \frac{1}{8}(\varepsilon r)^4 - \frac{1}{15}(\varepsilon r)^5 + \frac{1}{48}(\varepsilon r)^6 + \cdots.
\end{aligned}
$$

Theorem ([SRFH12])

Suppose κ is radial and conditionally positive definite of order $m \leq n$ with an expansion of the form

$$\kappa(r) = a_0 + a_2 r^2 + \ldots + a_{2n} r^{2n} + a_{2n+1} r^{2n+1} + a_{2n+2} r^{2n+2} + \ldots,$$

where $2n+1$ denotes the smallest odd power of r present in the expansion (i.e., κ is finitely smooth). Also assume that the data $\mathcal{X}$ contain a unisolvent set with respect to the space Π_{2n}^d of d-variate polynomials of degree less than $2n$. Then

$$\lim_{\varepsilon \to 0} s^\varepsilon(\boldsymbol{x}) = \sum_{j=1}^{N} c_j \|\boldsymbol{x} - \boldsymbol{x}_j\|^{2n+1} + \sum_{k=1}^{M} d_k p_k(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^d,$$

where $\{p_k : k = 1, \ldots, M\}$ denotes a basis of Π_n^d.

Remark

The previous theorem does not cover Matérn kernels with odd-order smoothness. However, all other examples listed above are covered.

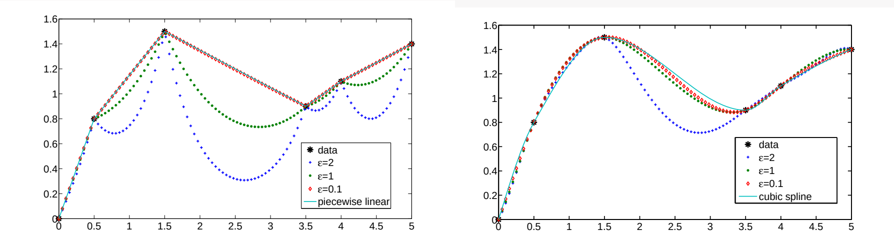


Figure: Convergence of C^0 (left) and C^2 (right) Matérn interpolants to piecewise linear (left) and cubic (right) spline interpolants.

On bounded intervals, interpolants with iterated Brownian bridge kernels (or tension splines) converge to piecewise polynomial spline interpolants as discussed earlier.
For $\beta = 1$ this means

$$K_{1,\varepsilon}(x,z) = \begin{cases} \frac{\sinh(\varepsilon x)\sinh(\varepsilon(1-z))}{\varepsilon\sinh(\varepsilon)}, & 0 \le x \le z \le 1, \\ \frac{\sinh(\varepsilon z)\sinh(\varepsilon(1-x))}{\varepsilon\sinh(\varepsilon)}, & 0 \le z \le x \le 1. \end{cases}$$

$$\stackrel{\varepsilon\to 0}{\longrightarrow} \quad K_1(x,z) = \min(x,z) - xz.$$

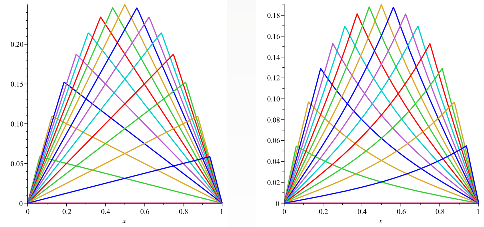


Figure: Brownian bridge (left) and tension spline (right) kernels for 15 equally spaced values of z in $[0,1]$.

The following “relaxation spline” kernel also converges to the Brownian bridge kernel:

$$K_{\text{relax}}(x,z) = \begin{cases} \dfrac{\sin(\varepsilon x)\sin(\varepsilon(1-z))}{\varepsilon\sin(\varepsilon)}, & 0 \le x \le z \le 1, \\ \dfrac{\sin(\varepsilon z)\sin(\varepsilon(1-x))}{\varepsilon\sin(\varepsilon)}, & 0 \le z \le x \le 1. \end{cases}$$

$$\longrightarrow \quad K_1(x,z) = \min(x,z) - xz.$$

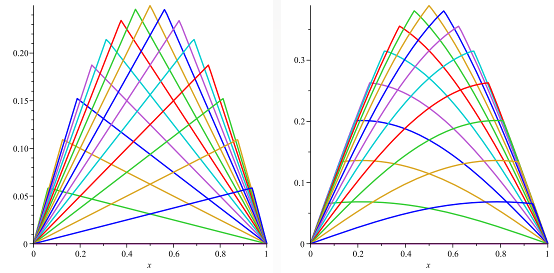


Figure: Brownian bridge (left) and relaxation spline (right) kernels for 15 equally spaced values of z in $[0,1]$.

Remark

Lee and Micchelli [LM13] show that in the univariate setting not only "flat" smooth RBF interpolants converge to polynomial interpolants, but that the same holds for interpolants based on "flat" smooth translation invariant kernels, and even for general smooth kernels.
In the multivariate setting the authors consider interpolation points that are unisolvent for d-variate polynomials of total degree ℓ. In this case they also obtain a unique polynomial limiting interpolant for a given (not necessarily radial) kernel, provided it is analytic.

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