

MATH 590: Meshfree Methods

Iterated Brownian Bridge Kernels: A Green's Kernel Example

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Outline

- 1 Introduction
- 2 Iterated Brownian Bridge Kernels
- 3 Properties of Iterated Brownian Bridge Kernels



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Introduction

In this chapter we will **derive series representations** — and **where feasible** also **closed-form representations** — for the family of **iterated Brownian bridge kernels**.

We split the exposition into two parts:

- piecewise polynomial splines (corresponds to $\varepsilon = 0$)
- case with general ε

Then we look at various properties of these kernels, including MATLAB illustrations.



Iterated Kernels

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$$\mathcal{K}K_1(\mathbf{x}, \mathbf{z}) = \int_{\Omega} K_1(\mathbf{x}, \mathbf{t})K_1(\mathbf{t}, \mathbf{z})\rho(\mathbf{t})d\mathbf{t}$$



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Since φ_n are the eigenfunctions of \mathcal{K} corresponding to λ_n we have

$$\int_{\Omega} K_1(\mathbf{x}, \mathbf{t})\varphi_n(\mathbf{t})\rho(\mathbf{t})d\mathbf{t} = \lambda_n \varphi_n(\mathbf{x}).$$



Inserting

$$\int_{\Omega} K_1(\mathbf{x}, \mathbf{t}) \varphi_n(\mathbf{t}) \rho(\mathbf{t}) d\mathbf{t} = \lambda_n \varphi_n(\mathbf{x}).$$

into

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$$\begin{aligned} \mathcal{K}K_1(\mathbf{x}, \mathbf{z}) &= \sum_{n=1}^{\infty} \lambda_n^2 \varphi_n(\mathbf{x}) \varphi_n(\mathbf{z}) \\ &= K_2(\mathbf{x}, \mathbf{z}), \end{aligned}$$

a **new kernel** K_2 with the **same eigenfunctions** as K_1 , but whose **eigenvalues** are the squares of those of K_1 .



Remark

- *For a translation-invariant kernel* — and therefore also for a radial kernel — the operation described above is a *convolution*.
 - The *iterated kernel is smoother than the original one*.
 - The *process can be repeated*, leading to a family of kernels with increasing smoothness (determined by the decay of the eigenvalues) all built from a common set of eigenfunctions.
 - This *provides another way to design a custom family of kernels*.
- *Construction of smoother kernels via iteration is a classical idea* (see, e.g., [CH53, Section III.5.3], [Sta79, Section 6.3]).
- *We will construct our iterated kernels via an iterated differential operator*.
 - *I prefer this approach since here the boundary conditions are explicitly specified.*



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Basic Piecewise Polynomial Spline Kernels

In Chapter 5 we showed that the differential operator $\mathcal{L} = -\frac{d^2}{dx^2}$ coupled with the BCs $K(0, z) = K(1, z) = 0$ gives rise to the Brownian bridge kernel

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



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

The associated eigenvalue problem was

$$\mathcal{L}\varphi = \mu\varphi, \quad \varphi(0) = \varphi(1) = 0,$$

with eigenvalues and normalized eigenfunctions

$$\mu_n = (n\pi)^2, \quad \varphi_n(x) = \sqrt{2} \sin n\pi x, \quad n = 1, 2, \dots$$



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The generalized Fourier series (Mercer series) of the kernel is

$$K_1(x, z) = \min(x, z) - xz = \sum_{n=1}^{\infty} \frac{2}{n^2\pi^2} \sin n\pi x \sin n\pi z.$$



Now, the eigenvalue problem $\mathcal{L}^\beta \varphi = \eta \varphi$ has eigenvalues $\eta = \mu^\beta$ and the same eigenfunctions as before provided we use the BCs

$$\varphi(0) = \varphi(1) = \varphi''(0) = \varphi''(1) = \dots = \varphi^{(2\beta-2)}(0) = \varphi^{(2\beta-2)}(1) = 0.$$

Therefore, setting $\beta = 2$ we can derive the kernel (see HW)

$$K_2(x, z) = \begin{cases} \frac{1}{6}x(1-z)(1-x^2-(1-z)^2), & 0 \leq x \leq z \leq 1, \\ \frac{1}{6}z(1-x)(1-z^2-(1-x)^2), & 0 \leq z \leq x \leq 1. \end{cases}$$

Its eigenfunction expansion is given by

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For any fixed value of z this is a natural cubic spline that interpolates zero at $x = 0$ and $x = 1$.



Remark

- K_1 and K_2 satisfy zero boundary conditions.
- $K_1(0, z_j) = 0$ for *any* point z_j and so *an entire row of K will be zero* if $x = 0$ or $x = 1$ are included as data sites.



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- To prevent this from happening we must *exclude $x = 0$ and $x = 1$ from the sets of kernel centers and also from the data sites.*
- This imposes a *restriction on the problems we can accurately solve with K_1 or K_2 . These problems must satisfy the same homogeneous BCs as the kernel.*



Adding a kernel for null(\mathcal{L})

To be able to interpolate nonzero values at the endpoints $x = 0$ and $x = 1$ with K_1 or K_2 we could create a second (polynomial) kernel for the null space of the \mathcal{L} and \mathcal{L}^2 .



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This polynomial kernel can be added to $K_{1,0}$ or $K_{2,0}$ to yield a sum kernel which can handle arbitrary non-homogeneous boundary conditions (see, e.g., [RS05, Chapter 21]).



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Alternatively, we can add the linear interpolant $p(x) = (1 - x)y_1 + xy_N$, where y_1 and y_N are the data values at $x = 0$ and $x = 1$, respectively, to the (homogeneous) kernel interpolant.



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We could also subtract the linear interpolant from the data in a preprocessing step.



Higher-order Piecewise Polynomial Spline Kernels of Odd Degree

We now consider K_β , the Green's kernel of the differential operator

$$\mathcal{L}^\beta = (-1)^\beta \frac{d^{2\beta}}{dx^{2\beta}}, \quad \beta \in \mathbb{N},$$

with boundary conditions

$$\frac{d^{2\nu-2}}{dx^{2\nu-2}} K_\beta(x, z)|_{x=0} = \frac{d^{2\nu-2}}{dx^{2\nu-2}} K_\beta(x, z)|_{x=1} = 0, \quad \nu = 1, \dots, \beta,$$

where z is fixed.



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Our discussion of the two special cases, K_1 and K_2 above suggests that **the kernel K_β will be a piecewise polynomial spline.**

We now derive **closed form representations** for these piecewise polynomial spline kernels.



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*This idea is related to the more general concept of **L-splines** (see, e.g., [SV67, SV72, Var87]).*



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Our discussion of iterated kernels implies that the Mercer series for K_β , $\beta = 1, 2, \dots$, is given by

$$K_\beta(x, z) = \sum_{n=1}^{\infty} \frac{2}{(n\pi)^{2\beta}} \sin(n\pi x) \sin(n\pi z)$$

provided we use the boundary conditions from above, i.e.,

$$\frac{d^{2\nu-2}}{dx^{2\nu-2}} K_\beta(x, z)|_{x=0} = \frac{d^{2\nu-2}}{dx^{2\nu-2}} K_\beta(x, z)|_{x=1} = 0, \quad \nu = 1, \dots, \beta, \quad z \text{ fixed.}$$



Using the eigenvalues and eigenfunctions

$$\mu_n = (n\pi)^{2\beta}, \quad \varphi_n(x) = \sqrt{2} \sin(n\pi x), \quad n = 1, 2, \dots,$$

we now derive a **closed form for the Mercer series of K_β** which shows that it is indeed a **piecewise polynomial of degree $2\beta - 1$** .



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Main ingredients in the derivation:

- standard **trigonometric identity**

$$2 \sin(A) \sin(B) = \cos(A - B) - \cos(A + B)$$

with $A = n\pi x$ and $B = n\pi z$,



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- two applications of the **cosine series expansion of Bernoulli polynomials** (see, e.g., [DLMF12, Eq. 24.8.1] and [OLBC10])

$$B_{2\beta}(t) = (-1)^{\beta+1} \frac{2(2\beta)!}{(2\pi)^{2\beta}} \sum_{n=1}^{\infty} n^{-2\beta} \cos(2\pi nt), \quad 0 \leq t \leq 1, \quad \beta = 1, 2, \dots,$$

setting $t = \frac{x-z}{2}$ and $t = \frac{x+z}{2}$, respectively.



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However, it is possible to combine the two resulting formulas into the **desired symmetric closed form representation**

$$K_{\beta}(x, z) = (-1)^{\beta-1} \frac{2^{2\beta-1}}{(2\beta)!} \left[B_{2\beta} \left(\frac{|x-z|}{2} \right) - B_{2\beta} \left(\frac{x+z}{2} \right) \right],$$

which is valid for any $0 \leq x, z \leq 1$.



Bernoulli polynomials of degree n can be defined as (see, e.g., [DLMF12, Eq. 24.6.7] and [OLBC10])

$$B_n(x) = \sum_{k=0}^n \frac{1}{k+1} \sum_{j=0}^k (-1)^j \binom{k}{j} (x+j)^n.$$

The first few polynomials are given by

$$B_0(x) = 1,$$

$$B_1(x) = x - \frac{1}{2},$$

$$B_2(x) = x^2 - x + \frac{1}{6},$$

$$B_3(x) = x^3 - \frac{3}{2}x^2 + \frac{1}{2}x.$$



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If we want to use kernels based on these polynomials to solve PDEs we also need to know their **derivatives**:

$$B'_n(x) = nB_{n-1}(x)$$



With this knowledge about Bernoulli polynomials it is easy to verify that the closed form representation

$$K_{\beta}(x, z) = (-1)^{\beta-1} \frac{2^{2\beta-1}}{(2\beta)!} \left[B_{2\beta} \left(\frac{|x-z|}{2} \right) - B_{2\beta} \left(\frac{x+z}{2} \right) \right]$$

results (as we had earlier) in

$$K_1(x, z) = \min(x, z) - xz = \begin{cases} x - xz, & 0 \leq x \leq z, \\ z - xz, & z \leq x \leq 1, \end{cases}$$

(i.e., the Brownian bridge kernel) and

$$K_2(x, z) = \begin{cases} \frac{1}{6}x(1-z)(x^2 + z^2 - 2z), & 0 \leq x \leq z, \\ \frac{1}{6}(1-x)z(x^2 + z^2 - 2x), & z \leq x \leq 1. \end{cases}$$

For a fixed z , $K_3(x, z)$ gives piecewise quintic polynomials in x , and so on.



Plots of Piecewise Polynomial Spline Kernels

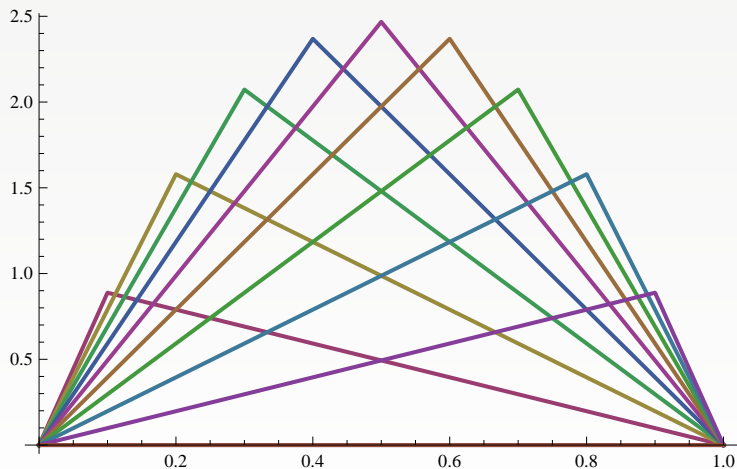


Figure: $\beta = 1$



Plots of Piecewise Polynomial Spline Kernels

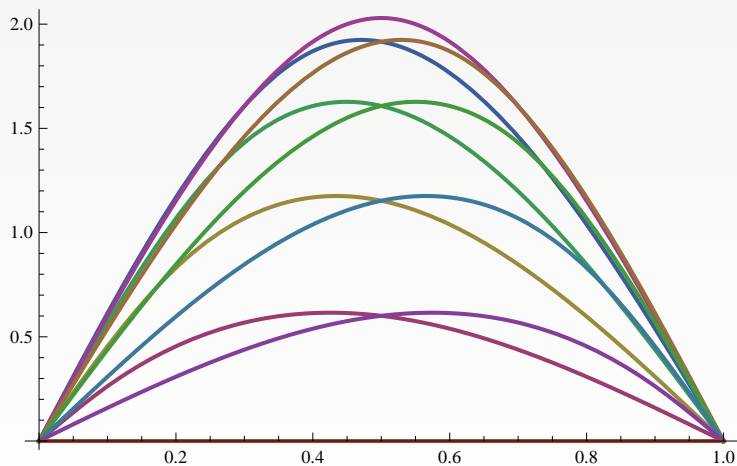


Figure: $\beta = 2$



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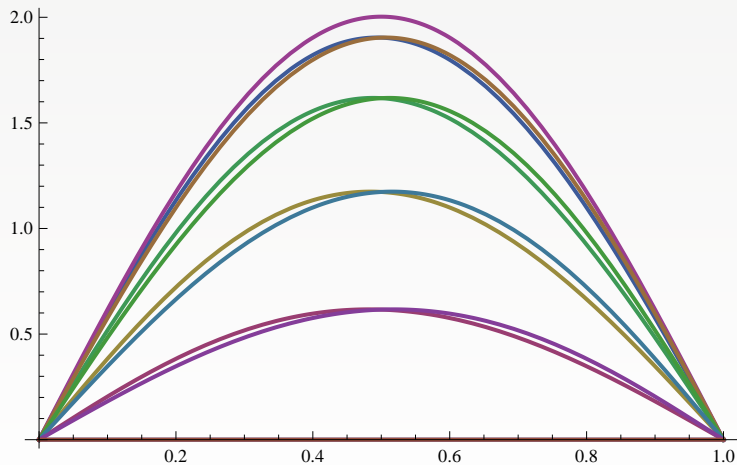


Figure: $\beta = 3$



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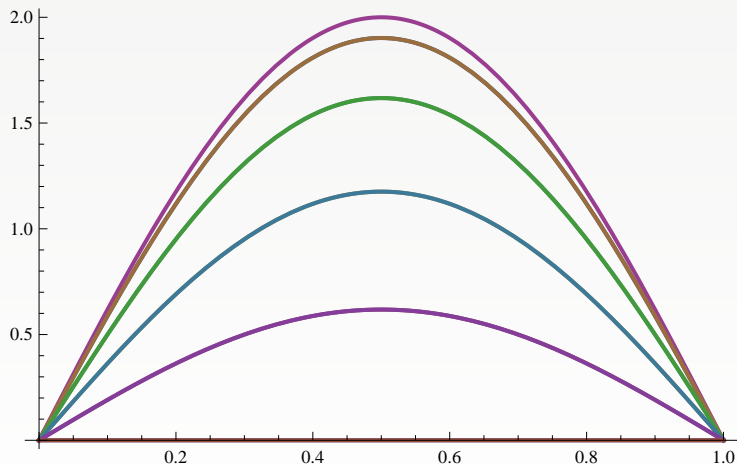


Figure: $\beta = 7$



Plots of Piecewise Polynomial Spline Kernels

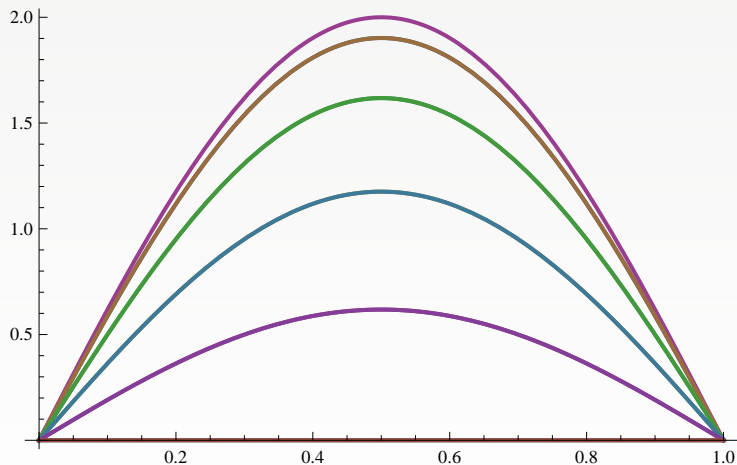


Figure: $\beta = 20$



Limitations of this representation are:

- Clearly, this is **not a good basis for practical implementations** since the set of translates of the kernel $K_\beta(\cdot, z)$ for different centers z becomes very nearly linearly dependent for larger β (the plots for $\beta = 7$ and $\beta = 20$ are virtually the same).



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Advantages of this representation are:

- We can represent natural splines of all orders simply by changing the eigenvalues in the series expansion.
- Once we understand **stable computation** we will be able to compute stably (although probably not as efficiently as with B-splines) with the eigenfunction basis.
- We will be able to move effortlessly to a related, iterated Brownian bridge, space which has a lot more added flexibility through the introduction of the shape parameter ε (next subsection).



General Iterated Brownian Bridge Kernels

If we change the differential operator to $\mathcal{L} = -\frac{d^2}{dx^2} + \varepsilon^2 \mathcal{I}$ then the eigenfunctions remain unchanged and the eigenvalues are shifted. Therefore, the SL eigenvalue problem

$$\mathcal{L}^\beta \varphi = \mu \varphi$$

with BCs

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results in the eigenpairs

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The generalized Fourier series of the iterated Brownian bridge kernels is

$$K_{\beta, \varepsilon}(x, z) = \sum_{n=1}^{\infty} 2 \left(n^2 \pi^2 + \varepsilon^2\right)^{-\beta} \sin(n\pi x) \sin(n\pi z).$$



Closed form representations for the iterated Brownian bridge kernels with $\varepsilon > 0$ are more complicated than those for piecewise polynomial splines ($\varepsilon = 0$).

- For $\beta = 1$ we can obtain (proceeding similarly to what we did for the $\varepsilon = 0$ case in Chapter 5)

$$\begin{aligned}
 K_{1,\varepsilon}(x, z) &= \begin{cases} \frac{\sinh(\varepsilon x) \sinh(\varepsilon(1-z))}{\varepsilon \sinh(\varepsilon)}, & 0 \leq x \leq z \leq 1, \\ \frac{\sinh(\varepsilon z) \sinh(\varepsilon(1-x))}{\varepsilon \sinh(\varepsilon)}, & 0 \leq z \leq x \leq 1, \end{cases} \\
 &= \frac{\sinh(\varepsilon \min(x, z)) \sinh(\varepsilon(1 - \max(x, z)))}{\varepsilon \sinh(\varepsilon)}, \quad x, z \in [0, 1]
 \end{aligned}$$



- The closed form expression for $K_{2,\varepsilon}$ is considerably more complex:

$$K_{2,\varepsilon}(x, z) = \frac{1}{2\varepsilon^3 \sinh(\varepsilon)} \left[\begin{aligned} &\varepsilon \min(x, z) \cosh(\varepsilon \min(x, z)) \sinh(\varepsilon(1 - \max(x, z))) \\ &+ \varepsilon(1 - \max(x, z)) \sinh(\varepsilon \min(x, z)) \cosh(\varepsilon(\max(x, z) - 1)) \\ &+ (\varepsilon \coth(\varepsilon) + 1) \sinh(\varepsilon \min(x, z)) \sinh(\varepsilon(\max(x, z) - 1)) \end{aligned} \right]$$

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- It was found by two REU students, Casey Bylund and Will Mayner.
- For larger β and $\varepsilon > 0$ closed form representations are unknown (to me).
- This is **not a drawback**. It might even be preferable to work with the series form of K . However, if we use an eigenexpansion directly we ignore the **special structure** of this series. The **Hilbert–Schmidt SVD will exploit this structure**.



Plots of Iterated Brownian bridge Kernels

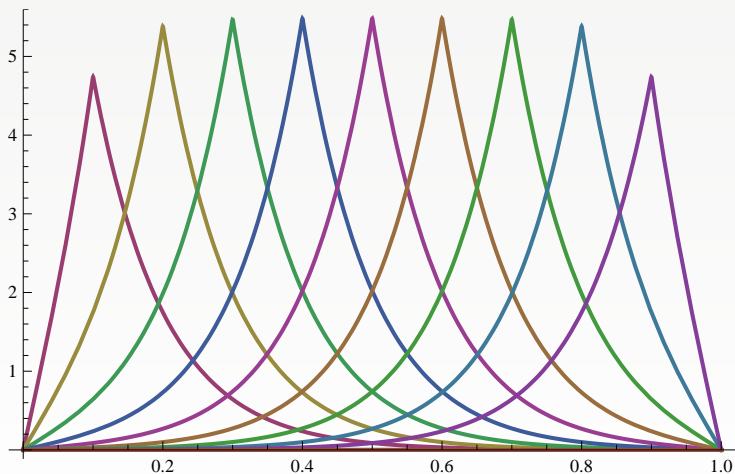


Figure: $\beta = 1, \varepsilon = 10$



Plots of Iterated Brownian bridge Kernels

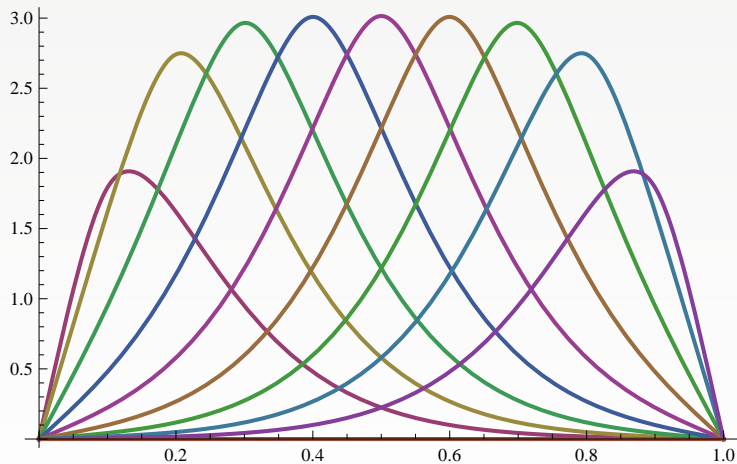


Figure: $\beta = 2, \varepsilon = 10$



Plots of Iterated Brownian bridge Kernels

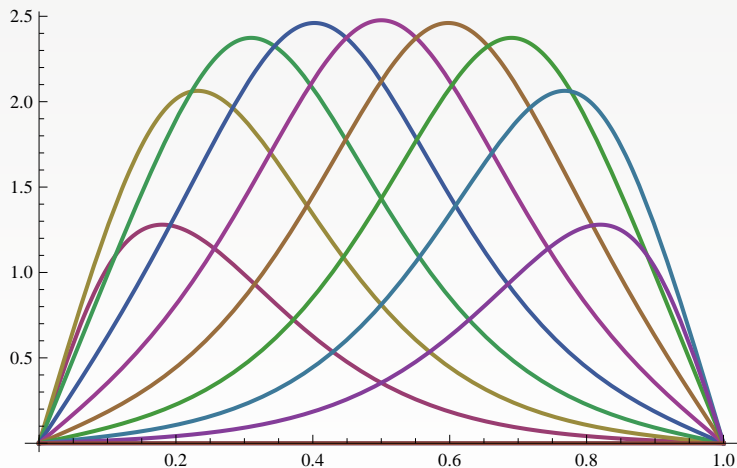


Figure: $\beta = 3, \varepsilon = 10$



Plots of Iterated Brownian bridge Kernels

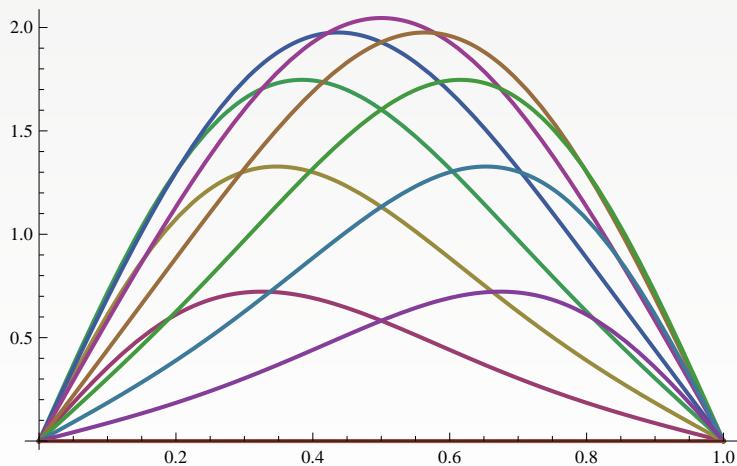


Figure: $\beta = 7, \varepsilon = 10$



Plots of Iterated Brownian bridge Kernels

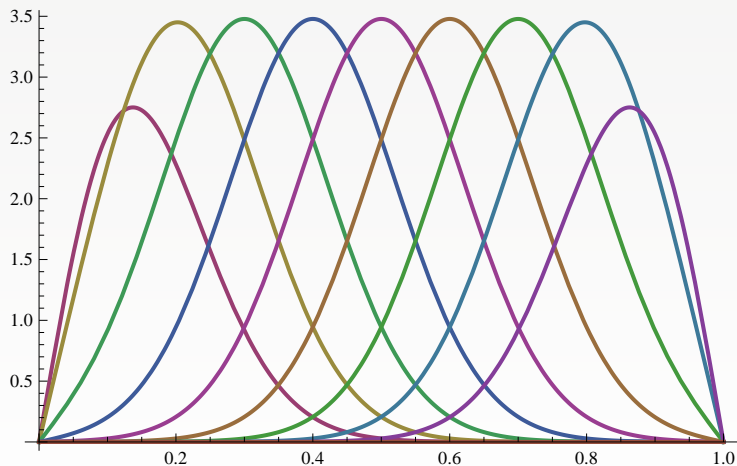


Figure: $\beta = 20, \varepsilon = 50$



Remark

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- Recall that the translates of the piecewise polynomial kernel $K_{\beta,0}$ become increasingly linearly dependent as β increases.
- Now we can increase ε to counter-balance this effect.
- For large values of ε the iterated Brownian bridge kernels more and more resemble translated Gaussian kernels as $\beta \rightarrow \infty$. However, by construction, these Gaussian-like iterated Brownian bridge kernels obey zero boundary conditions.
- It is known [UAE92] that B-splines tend to Gaussians as the smoothness index $\beta \rightarrow \infty$, so it is not surprising that we see similar “convergence” for iterated Brownian bridge kernels.



Outline

- 1 Introduction
- 2 Iterated Brownian Bridge Kernels
- 3 Properties of Iterated Brownian Bridge Kernels**



We now discuss

- truncation of the Mercer series of the iterated Brownian bridge kernel,
- numerical evidence for order of convergence for interpolation with these kernels as ε and β vary,
- effects of the boundary conditions in interpolation problems.

Some of the behavior observed in this section will be supported by theoretical analysis later on.



The Mercer series for iterated Brownian bridge kernels is of the form

$$K_{\beta,\varepsilon}(x, z) = \sum_{n=1}^{\infty} \frac{2}{(n^2\pi^2 + \varepsilon^2)^\beta} \sin(n\pi x) \sin(n\pi z),$$

with Hilbert-Schmidt eigenvalues and normalized eigenfunctions given by

$$\lambda_n = \frac{1}{(n^2\pi^2 + \varepsilon^2)^\beta}, \quad \varphi_n(x) = \sqrt{2} \sin(n\pi x). \quad (1)$$

Clearly,

- the eigenfunctions are bounded by $\sqrt{2}$,
- and, for a fixed value of ε , the eigenvalues decay as $n^{-2\beta}$.



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Remark

The boundedness of the eigenfunctions is not guaranteed for arbitrary positive definite kernels.

- The plots of the iterated Brownian bridge kernels above were obtained by **evaluating the Mercer series** (see code below).
- Of course, in practice we **cannot evaluate such an infinite series**.
- It needs to be truncated, and we need to **ensure that this truncation does not reduce accuracy**.
- This concern is valid for series in general, but the uniform convergence of the Mercer series allows us to guarantee a truncation value M_{TOL} exists, beyond which the remaining terms are less than some tolerance σ_{TOL} .



The truncation length M needed for accurate representation of the entries $K(\mathbf{x}_j, \mathbf{x}_j)$ of K can be easily determined as a function of β and ε :

In order to ensure that the $M + 1^{\text{st}}$ term contributes nothing of significance relative to the first term we want

$$\lambda_{M+1} < \sigma_{\text{TOL}} \lambda_1,$$

where σ_{TOL} denotes a (small) tolerance for the desired accuracy such as machine precision ϵ_{mach} .



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Using (1) and solving for M yields

$$M_{\text{TOL}}(\beta, \varepsilon; \sigma_{\text{TOL}}) = \left\lceil \frac{1}{\pi} \sqrt{\sigma_{\text{TOL}}^{-1/\beta} (\pi^2 + \varepsilon^2) - \varepsilon^2} \right\rceil,$$

where $\lceil x \rceil$ denotes the smallest integer greater than or equal to x (the *ceiling* of x).



Parameters		Precision		
β	ε	10^{-5}	10^{-10}	10^{-15}
1	.1	3×10^2	1×10^5	3×10^7
1	1	3×10^2	1×10^5	3×10^7
1	10	1×10^3	3×10^5	1×10^8
2	10	6×10^1	1×10^3	2×10^4
3	10	2×10^1	2×10^2	1×10^3
5	10	1×10^1	3×10^2	1×10^2
7	10	7×10^0	2×10^1	4×10^1

Table: Truncation values M_{TOL} required for series generated by various combinations of ε and β to reach certain precisions specified by σ_{TOL} . The precision column is the ratio of the last and first eigenvalues, λ_{M+1}/λ_1 . Increases in ε require a greater M_{TOL} , whereas increases in β require a smaller M_{TOL} .



Program (PlotKernelSeries.m)

```
% Evaluates iterated Brownian bridge kernels using Mercer series
1 x = linspace(0,1,11)'; xx = linspace(0,1,1201)';
  % iterated Brownian bridge kernel
2 x=x(2:end-1); N = length(x);
3 ep = 50; beta = 20;
4 phifunc = @(n,x) sqrt(2)*sin(pi*x*n);
5 lambdafunc = @(n) ((n*pi).^2+ep^2).^(-beta);
  % Mercer series
6 if beta < 3
7     M = 1000;
8 else
9     M = ceil(1/pi*sqrt(eps^(-1/beta)*(N^2*pi^2+ep^2)-ep^2));
10 end
11 Lambda = diag(lambdafunc(1:M));
12 Phi_interp = phifunc(1:M,x);
13 Phi_eval = phifunc(1:M,xx);
14 Kbasis = Phi_eval*Lambda*Phi_interp'/Lambda(1,1);
  % Plot kernel basis obtained via Mercer series
15 plot(xx,Kbasis)
```

Remark

- *PlotKernelSeries.m* provides a simple (but vectorized) MATLAB script that allows us to use the Mercer series for iterated Brownian bridge kernels with arbitrary β and ε .



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- *PlotKernelSeries.m* provides a simple (but vectorized) MATLAB script that allows us to use the Mercer series for iterated Brownian bridge kernels with arbitrary β and ε .
- Since the truncation values in the table show that M_{TOL} is very large for $\beta = 1, 2$ (and we should therefore use the closed-form representation), for simplicity we just fix $M = 1000$ in those two cases (see lines 6–10).



Effects of the boundary conditions

To see what the effect of the boundary conditions built into our kernels may be, we plot the **cardinal functions** for interpolation by iterated Brownian bridge kernels and by Gaussians (which are simply translated across the domain of interest).

We will explain cardinal functions in detail in Chapter 11, but they are formally the same as the optimal kriging weights, i.e.,

$$\hat{w}(x) = K^{-1} \mathbf{k}(x).$$



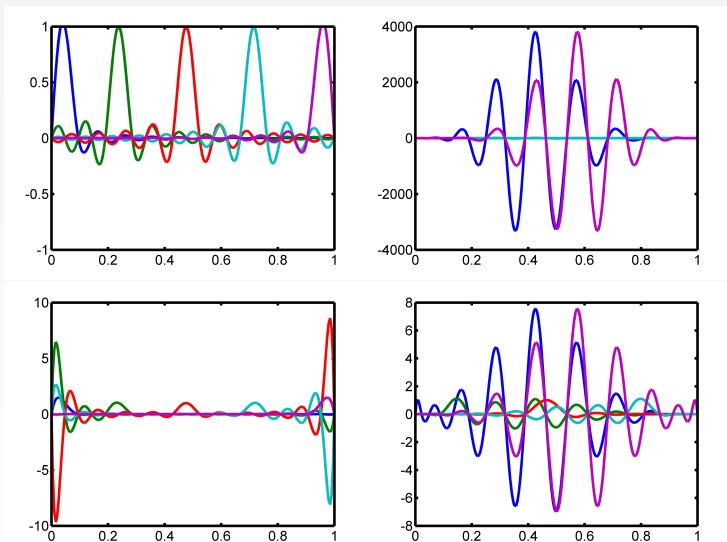


Figure: Cardinal functions for interpolation at 22 points in $(0, 1)$. Top: iterated Brownian bridge for equally spaced (left), Chebyshev (right) points; bottom: Gaussians for equally spaced (left), Chebyshev (right) points.



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- *However, It is known that interpolation with cubic splines also favors evenly distributed data [LS73, Mar74]. Also, optimal points for L_2 approximation with the Brownian bridge kernel are equally spaced [Rit00, Section II.3.7].*
- *For Gaussians the preference is not as clear. Chebyshev points will be favored as $\varepsilon \rightarrow 0$ (cf. our later discussion of the “flat” polynomial limit).*



Convergence Orders

- The differential operator $\mathcal{L} = \left(-\frac{d^2}{dx^2} + \varepsilon^2 \mathcal{I}\right)^\beta$ defining our piecewise polynomial splines falls into the class of operators defining ***L-splines*** [SV67, SV72].
- However, **we use different boundary conditions**.
- It is known that *L-spline* interpolation has an ***L₂ error of $\mathcal{O}(h^{2\beta})$*** for data sampled from $f \in H^{2\beta}([0, 1])$ and with BCs such that derivatives of f up to order β are interpolated at $\{0, 1\}$ ¹.
- Here h denotes the **meshsize**, i.e., $h = \max_j (x_{j+1} - x_j)$, $x_j \in [0, 1]$, $j = 1, \dots, N$.
- For **periodic boundary conditions** the **same order** can be achieved.
- We **expect similar convergence behavior for interpolation using iterated Brownian bridge kernels**.

¹Here $H^{2\beta}([0, 1])$ is the usual Sobolev space of functions with 2β derivatives in $L_2([0, 1])$.



This means

- piecewise linear splines will achieve $\mathcal{O}(h^2)$ convergence order provided the spline interpolates at all data points (including at the boundary),
- cubic splines will achieve $\mathcal{O}(h^4)$ provided the boundary conditions are matched, but otherwise only $\mathcal{O}(h^2)$.

We will specify convergence in terms of N .

For evenly spaced data we have $h = \frac{1}{N-1}$. So we should get

- $\mathcal{O}(N^{-2\beta})$ for data with homogeneous boundary conditions,
- $\mathcal{O}(N^{-\beta})$ otherwise.



Numerical Example

We consider the test function (similar to a function from [HM07])

$$G_n(x) = (1/2 - \gamma)^{-2n} (x - \gamma)_+^n (1 - \gamma - x)_+^n, \quad x \in [0, 1],$$

such that

- all derivatives at $x = 0$ and $x = 1$ are 0,
- G_n satisfies all BCs,
- the parameter $\gamma \in (0, 1/2)$ implies $G_n \equiv 0$ for $x \notin (\gamma, 1 - \gamma)$, with discontinuous n^{th} derivatives at $x = \{\gamma, 1 - \gamma\}$,
- manipulating n allows us to either satisfy or violate the required smoothness conditions of the underlying differential operator.

We fix $\gamma = .0567$ so that discontinuities do not coincide with data points.



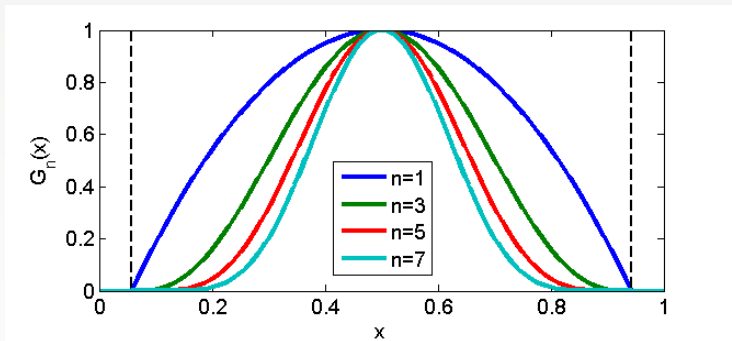


Figure: Sample plots of G_n with $n = 1, 3, 5, 7$, and $\gamma = .0567$. The vertical dashed lines are at $x = \gamma$ and $x = 1 - \gamma$, and indicate the point beyond which the function is 0.



We observe the order of convergence of iterated Brownian bridge kernel interpolation with

- a fixed $\varepsilon = 1$
- and $\beta = 1, \dots, 5$
- for G_6 .

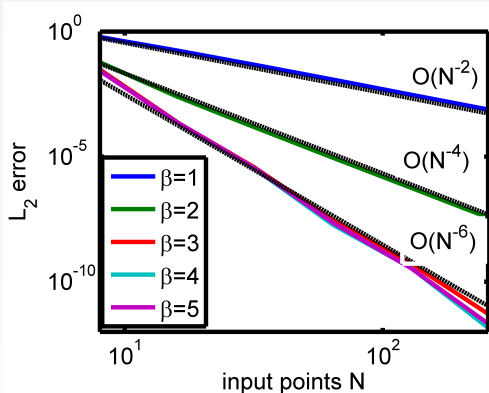


We observe the order of convergence of iterated Brownian bridge kernel interpolation with

- a fixed $\varepsilon = 1$
 - and $\beta = 1, \dots, 5$
 - for G_6 .
-
- For $\beta \leq 3$, the necessary smoothness conditions are satisfied.
 - For $\beta > 3$, the kernels are smoother than G_6 .

Note that there is little improvement in convergence for $\beta \geq 4$.





(a) Convergence order plot

β	exponent
1	-1.96
2	-4.01
3	-6.35
4	-6.75
5	-6.66

(b) Convergence order table

Figure: Errors for iterated Brownian bridge interpolation to samples from G_6 . As β increases, the order of convergence increases, until the kernels reach the smoothness of G_6 . Beyond that point (which occurs at $\beta = 3$) we encounter saturation, and there is no value in further increasing β . The N input points were evenly spaced in $(0, 1)$ as were the 400 evaluation points.



Remark

- *This supports our belief that functions which satisfy the homogeneous BCs of order 2β and have at least 2β smooth derivatives can be interpolated using $K_{\beta,\varepsilon}$ with $O(N^{-2\beta})$ convergence order.*



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- *We will later prove this for $\varepsilon = 0$.*



References I

- [CH53] R. Courant and D. Hilbert, *Methods of Mathematical Physics, Vol. 1*, Wiley, 1953, Reprinted 1989.
- [DLMF12] *NIST Digital Library of Mathematical Functions*, <http://dlmf.nist.gov/>, Release 1.0.5 of 2012-10-01, 2012, Online companion to [OLBC10].
- [HM07] S. Hubbert and S. Müller, *Thin plate spline interpolation on the unit interval*, Numerical Algorithms **45** (2007), 167–177.
- [LS73] Tom Lyche and Larry L. Schumaker, *On the convergence of cubic interpolating splines*, Spline functions and approximation theory (Proc. Sympos., Univ. Alberta, Edmonton, Alta., 1972), Internat. Ser. Numer. Math., vol. 21, Birkhäuser Verlag, Basel, 1973, pp. 169–189.
- [Mar74] Martin Marsden, *Cubic spline interpolation of continuous functions*, Journal of Approximation Theory **10** (1974), no. 2, 103–111.
- [OLBC10] F. W. J. Olver, D. W. Lozier, R. F. Boisvert, and C. W. Clark (eds.), *NIST Handbook of Mathematical Functions*, Cambridge University Press, New York, NY, 2010, Print companion to [DLMF12].



References II

- [Rit00] Klaus Ritter, *Average-Case Analysis of Numerical Problems*, Lecture Notes in Mathematics, vol. 1733, Springer, 2000.
- [RS05] James Ramsay and B. W. Silverman, *Functional Data Analysis*, 2nd ed., Springer, New York, 2005.
- [Sta79] I. Stakgold, *Green's Functions and Boundary Value Problems*, Wiley, 1979.
- [SV67] M. Schultz and R. Varga, *L-splines*, Numer. Math. **10** (1967), 319–345.
- [SV72] B. K. Swartz and R. S. Varga, *Error bounds for spline and I-spline interpolation*, Journal of Approximation Theory **6** (1972), no. 1, 6–49.
- [UAE92] M. Unser, A. Aldroubi, and M. Eden, *On the asymptotic convergence of B-spline wavelets to Gabor functions*, IEEE Transactions on Information Theory **38** (1992), no. 2, 864–872.
- [Var87] R. S. Varga, *Functional analysis and approximation theory in numerical analysis*, SIAM, 1987.

