MATH 590: Meshfree Methods

The Connection to Green's Kernels

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Outline

Over the last few lectures you learned about native spaces (reproducing kernel Hilbert spaces associated with the kernel K). There are several issues with this standard theory:

- We often don't really understand what these spaces are. In particular, it would be nice to have a more "intuitive" definition for them. Can we say what kind of functions lie in these spaces?
  - What is their smoothness (like for classical Sobolev spaces)?
  - On what sort of length scale do these functions exist (not part of standard Sobolev space theory)?
- Standard error bounds are often sub-optimal, and proofs of improved results are not elegant (more later).
- The role and choice of the shape parameter is not fully understood.
- Ultimately: *Which kernel should I use to solve my problem?*

By establishing a connection between positive definite reproducing kernels and Green's kernels we can understand some of these issues better. Note that some of these issues are still ongoing research.

We now go over some classical material related to Green's functions.

There are many references for this material such as the books on

Applied/Functional Analysis [Che01, Fol92, HN01]

Mathematical Physics [CH53]

Boundary Value Problems [Duf01, Sta79]

and even Statistics [RS05, Chapters 20 and 21]

Green's kernels defined

Definition

A Green's kernel G of the linear (ordinary or partial) differential operator $\mathcal{L}$ on the domain $\Omega \subseteq \mathbb{R}^d$ is defined as the solution of

$$\mathcal{L}G(\boldsymbol{x}, \boldsymbol{z}) = \delta(\boldsymbol{x} - \boldsymbol{z}), \qquad \boldsymbol{z} \in \Omega \text{ fixed.}$$

Here $\delta(\boldsymbol{x} - \boldsymbol{z})$ is the *Dirac delta functional* evaluated at $\boldsymbol{x} - \boldsymbol{z}$, i.e.,

$$\delta(\boldsymbol{x} - \boldsymbol{z}) = 0 \text{ for } \boldsymbol{x} \neq \boldsymbol{z} \quad \text{and} \quad \int_\Omega \delta(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} = 1.$$

In particular, δ acts as a point evaluator for any $f \in L_2(\Omega)$, i.e.,

$$\int_\Omega f(\boldsymbol{z}) \delta(\boldsymbol{x} - \boldsymbol{z}) \mathrm{d}\boldsymbol{z} = f(\boldsymbol{x}).$$

Remark

- *Homogeneous boundary or decay conditions are usually added to make the Green's kernel unique, i.e.,*

$$G(\boldsymbol{x},\boldsymbol{z})|_{\boldsymbol{x}\in\partial\Omega} = 0 \quad \textit{or} \quad \lim_{\|\boldsymbol{x}\|\to\infty} G(\boldsymbol{x},\boldsymbol{z}) = 0.$$

- *The solution of $\mathcal{L}G(\boldsymbol{x},\boldsymbol{z}) = \delta(\boldsymbol{x}-\boldsymbol{z})$ without boundary conditions is called either a fundamental solution of $\mathcal{L}u = 0$ or a full-space Green's kernel of $\mathcal{L}$.*
- *In the engineering literature Green's kernels are also known as*
  - *impulse response (in signal processing),*
  - *influence function (in mechanical engineering).*

G is usually used to solve boundary value problems since

$$u(\boldsymbol{x}) = \int_\Omega G(\boldsymbol{x},\boldsymbol{z}) f(\boldsymbol{z}) \mathrm{d}\boldsymbol{z}$$

satisfies $\mathcal{L}u = f$ with the appropriate boundary or decay conditions:

$$\mathcal{L}u(\boldsymbol{x}) = \mathcal{L}\int_\Omega G(\boldsymbol{x},\boldsymbol{z}) f(\boldsymbol{z}) \mathrm{d}\boldsymbol{z} = \int_\Omega \underbrace{\mathcal{L}G(\boldsymbol{x},\boldsymbol{z})}_{=\delta(\boldsymbol{x}-\boldsymbol{z})} f(\boldsymbol{z}) \mathrm{d}\boldsymbol{z} = f(\boldsymbol{x}).$$

The integral operator

$$\mathcal{G}f(\boldsymbol{x}) = \int_\Omega G(\boldsymbol{x},\boldsymbol{z}) f(\boldsymbol{z}) \mathrm{d}\boldsymbol{z}$$

can be regarded as the inverse of the differential operator $\mathcal{L}$, i.e.,

$$\mathcal{L}u = f \qquad \Longleftrightarrow \qquad u = \mathcal{G}f.$$

Remark

- *The inverse is guaranteed to exist if and only if the homogeneous equation* $\mathcal{L}u = 0$ *has only the trivial solution* $u = 0$.
- *Our Hilbert–Schmidt integral operators are compact, but their inverse differential operators are unbounded whenever* $\mathcal{H}_G$ *has an infinite-dimensional orthonormal basis.*

Eigenvalue problems

Consider the differential eigenvalue problem

$$\mathcal{L}\varphi(\boldsymbol{x}) = \mu\rho(\boldsymbol{x})\varphi(\boldsymbol{x}), \qquad \rho(\boldsymbol{x}) > 0, \ \mu \neq 0,$$

with eigenvalues μ_n, eigenfunctions φ_n, $n = 1, 2, \ldots$, weight function ρ, and assume G is the Green's kernel of $\mathcal{L}$.

Now solve this equation in terms of G, i.e., solve $\mathcal{L}\varphi = f$ with $f(\boldsymbol{z}) = \mu\rho(\boldsymbol{z})\varphi(\boldsymbol{z})$:

$$\begin{aligned} \varphi(\boldsymbol{x}) &= \int_\Omega G(\boldsymbol{x}, \boldsymbol{z}) f(\boldsymbol{z}) \mathrm{d}\boldsymbol{z}, \\ &= \int_\Omega G(\boldsymbol{x}, \boldsymbol{z}) \mu\rho(\boldsymbol{z})\varphi(\boldsymbol{z}) \mathrm{d}\boldsymbol{z}. \end{aligned}$$

This looks just like our Hilbert–Schmidt eigenvalue problem but — as we saw in the min-kernel example — with eigenvalues $\lambda_n = \frac{1}{\mu_n}$:

$$\lambda\varphi(\boldsymbol{x}) = \int_\Omega G(\boldsymbol{x}, \boldsymbol{z})\varphi(\boldsymbol{z})\rho(\boldsymbol{z}) \mathrm{d}\boldsymbol{z} \quad \Longleftrightarrow \quad \mathcal{G}\varphi(\boldsymbol{x}) = \lambda\varphi(\boldsymbol{x}).$$

Computing Green's Kernels

We don't want to use Green's kernels to solve differential equations. We want to recognize them as positive definite reproducing kernels and use this connection

- to create new reproducing kernels,
- and to gain new insights about our work by drawing from known results from harmonic analysis.

Being able to compute a specific Green's kernel depends heavily on

- the differential operator $\mathcal{L}$,
- the space dimension d,
- the shape of the domain Ω,
- and the boundary conditions.

Example (1D ODE Boundary Value Problem)

Show that the Green's kernel of $-u''(x) = f(x)$ with $u(0) = u(1) = 0$ is the Brownian bridge kernel $G(x,z) = \min(x,z) - xz$.

Solution

From the definition of the Green's kernel one can derive that

- $\mathcal{L}G(x,z) = 0$ for $x \neq z$, z fixed,
- $G(x,z)|_{x\in\{0,1\}}$ satisfies homogeneous BCs,
- G is continuous at $x = z$,
- and $\frac{\mathrm{d}G}{\mathrm{d}x}$ has a jump discontinuity at $x = z$ of the form

$$\lim_{x\to z^-} \frac{\mathrm{d}}{\mathrm{d}x} G(x,z) = \lim_{x\to z^+} \frac{\mathrm{d}}{\mathrm{d}x} G(x,z) + 1.$$

Therefore G is a piecewise defined function, i.e.,

$$G(x,z) = \begin{cases} G_-(x,z), & x < z, \\ G_+(x,z), & x > z. \end{cases}$$

Since $\mathcal{L} = -\frac{d^2}{dx^2}$ it is clear that the kernel is a piecewise linear polynomial which we express as

$$G(x,z) = \begin{cases} a_0 + a_1 x, & x < z, \\ b_0 + b_1(x-1), & x > z. \end{cases}$$

Let's consider the section $x < z$ and the left BC:

$$0 \stackrel{BC}{=} G(0,z) = a_0 \quad \Longrightarrow \quad a_0 = 0.$$

Similarly, for $x > z$ the right BC yields $G(1,z) = b_0 = 0$.

Thus, so far

$$G(x,z) = \begin{cases} a_1 x, & x < z, \\ b_1(x-1), & x > z. \end{cases}$$

To determine the remaining coefficients a_1 and b_1 we use the interface conditions at $x = z$.
Continuity of G implies

$$\lim_{x\to z^-} G(x,z) = \lim_{x\to z^+} G(x,z)$$

so that

$$a_1 z = b_1(z-1) \quad \Longleftrightarrow \quad a_1 = b_1 \frac{z-1}{z}.$$

Using the jump condition for the first derivative,

$$\lim_{x\to z^-} \frac{\mathrm{d}}{\mathrm{d}x} G(x,z) = \lim_{x\to z^+} \frac{\mathrm{d}}{\mathrm{d}x} G(x,z) + 1,$$

we get

$$a_1 = b_1 + 1 \quad \Longleftrightarrow \quad b_1 \frac{z-1}{z} = b_1 + 1 \quad \Longleftrightarrow \quad b_1 = -z.$$

Putting everything together, we have $a_0 = b_0 = 0$, $b_1 = -z$ and $a_1 = 1 - z$ to that the Green's kernel

$$G(x,z) = \begin{cases} a_0 + a_1 x, & x < z, \\ b_0 + b_1(x-1), & x > z, \end{cases}$$

turns out to be

$$G(x,z) = \begin{cases} (1-z)x, & x < z, \\ -z(x-1), & x > z, \end{cases}$$

or

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

Remark

Note that G is symmetric. This will be true whenever $\mathcal{L}$ is a self-adjoint differential operator.

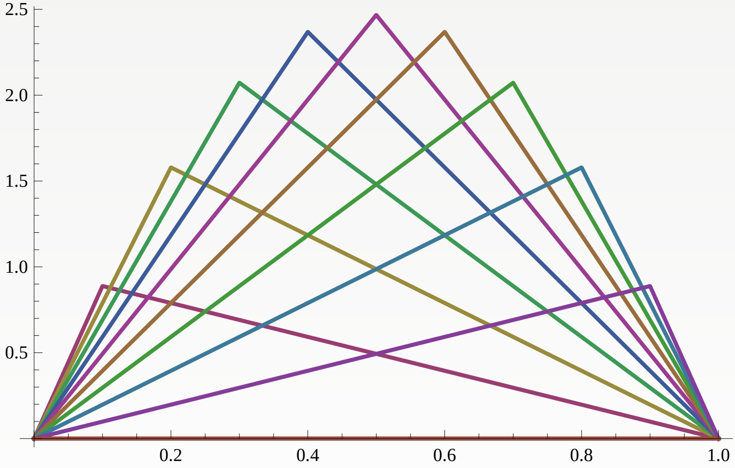


Figure: Plots of multiple copies of the Brownian bridge kernel, centered at $z = \frac{j}{10}$, $j = 1, \ldots, 9$.

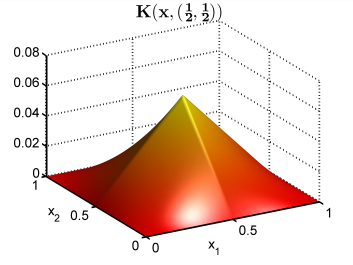
Multivariate Brownian bridge kernel

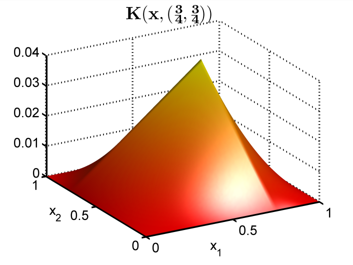
As we saw in Chapter 3, it is straightforward to extend the 1D kernel G to a kernel in higher dimensions using a tensor product approach. In this case, the domain will be the unit cube $[0,1]^d$.

The kernel is then given by

$$K(\boldsymbol{x},\boldsymbol{y}) = \prod_{\ell=1}^{d} G(x_\ell, y_\ell) = \prod_{\ell=1}^{d} \left(\min\{x_\ell, y_\ell\} - x_\ell y_\ell\right),$$

where $\boldsymbol{x} = (x_1, \ldots, x_d)$ and $\boldsymbol{y} = (y_1, \ldots, y_d)$.





Iterated Brownian Bridge Kernels

Using the differential operator

$$\mathcal{L} = \left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \varepsilon^2 \mathcal{I}\right)^\beta, \qquad \beta \in \mathbb{N},\ \varepsilon \geq 0$$

and boundary conditions

$$G(0,z) = G''(0,z) = \ldots = G^{(2\beta-2)}(0,z),$$
$$G(1,z) = G''(1,z) = \ldots = G^{(2\beta-2)}(1,z).$$

one obtains the so-called iterated Brownian bridge kernels as Green's kernels of $\mathcal{L}G(\boldsymbol{x},\boldsymbol{z}) = \delta(\boldsymbol{x}-\boldsymbol{z})$.

Above, we saw the example for $\beta = 1$ and $\varepsilon = 0$.

For $\beta = 2$, $\varepsilon = 0$ one obtains natural cubic interpolating splines. We will discuss this family of kernels in Chapter 6.

Standard 1D SL-Theory [Fol92, Hab13]

Consider the ODE

$$\frac{d}{dx}\left(p(x)\varphi'(x)\right) + q(x)\varphi(x) + \mu\sigma(x)\varphi(x) = 0, \qquad x \in (a, b) \tag{1}$$

with boundary conditions

$$\begin{aligned} \gamma_1\varphi(a) + \gamma_2\varphi'(a) &= 0 \\ \gamma_3\varphi(b) + \gamma_4\varphi'(b) &= 0 \end{aligned} \tag{2}$$

where the γ_i are real numbers.

Definition

If p, q, σ and p' in (1) are real-valued and continuous on $[a, b]$ and if $p(x)$ and $\sigma(x)$ are positive for all x in $[a, b]$, then (1) with (2) is called a regular Sturm-Liouville problem.

Remark

Note that the BCs don't capture those of the periodic or singular type.

Facts for regular 1D SL problems

1. All eigenvalues are real.
2. There are countably many eigenvalues which can be strictly ordered: $\mu_1 < \mu_2 < \mu_3 < \ldots$
3. Every eigenvalue μ_n has an associated eigenfunction φ_n which is unique up to a constant factor. Moreover, φ_n has exactly $n-1$ zeros in the open interval (a, b).
4. The set of eigenfunctions, $\{\varphi_n\}_{n=1}^{\infty}$, is complete, i.e., any piecewise smooth function f can be represented by a generalized Fourier series

$$f(x) \sim \sum_{n=1}^{\infty} a_n \varphi_n(x)$$

with generalized Fourier coefficients

$$a_n = \frac{\int_a^b f(x)\varphi_n(x)\sigma(x)\,\mathrm{d}x}{\int_a^b \varphi_n^2(x)\sigma(x)\,\mathrm{d}x}, \qquad n = 1, 2, 3, \ldots$$

5. The eigenfunctions associated with different eigenvalues are orthogonal on (a, b) with respect to the weight σ, i.e.,

$$\int_a^b \varphi_n(x)\varphi_m(x)\sigma(x)\,\mathrm{d}x = 0 \quad \text{provided } \lambda_n \neq \lambda_m.$$

6. The Rayleigh quotient is given by

$$\mu = \frac{-p(x)\varphi(x)\varphi'(x)|_a^b + \int_a^b \left(p(x)\left[\varphi'(x)\right]^2 - q(x)\varphi^2(x)\right)\,\mathrm{d}x}{\int_a^b \varphi^2(x)\sigma(x)\,\mathrm{d}x}$$

7. Truncating the Fourier series yields mean-squared best approximation:

$$a_n = \arg\min_{\alpha_n} \left\| f - \sum_{n=1}^{M} \alpha_n \varphi_n \right\|_2$$

Green's kernels and eigenfunction expansions

We now study how the eigenfunctions of linear self-adjoint differential operators, such as the SL operator, are related to Green's kernels.
Starting from the ODE

$$(\mathcal{L}G)(\boldsymbol{x},\boldsymbol{z}) = \delta(\boldsymbol{x}-\boldsymbol{z}), \quad \boldsymbol{z} \text{ fixed},$$

with regular SL BCs we consider the SL ODE eigenvalue problem

$$(\mathcal{L}\varphi)(\boldsymbol{x}) = \mu\sigma(\boldsymbol{x})\varphi(\boldsymbol{x}) \tag{3}$$

with the same BCs.
The choice of the weight σ is free. Once σ is chosen we have unique eigenvalues and eigenfunctions and we write

$$G(\boldsymbol{x},\boldsymbol{z}) = \sum_{n=1}^{\infty} a_n(\boldsymbol{z})\varphi_n(\boldsymbol{x}). \tag{4}$$

To find $a_n(\boldsymbol{z})$ we apply $\mathcal{L}$ and use linearity:

$$\delta(\boldsymbol{x}-\boldsymbol{z}) = (\mathcal{L}G)(\boldsymbol{x},\boldsymbol{z}) = \sum_{n=1}^{\infty} a_n(\boldsymbol{z})(\mathcal{L}\varphi_n)(\boldsymbol{x}) \stackrel{(3)}{=} \sum_{n=1}^{\infty} a_n(\boldsymbol{z})\mu_n\sigma(\boldsymbol{x})\varphi_n(\boldsymbol{x})$$

Next we multiply

$$\delta(\boldsymbol{x}-\boldsymbol{z}) = \sum_{n=1}^{\infty} a_n(\boldsymbol{z})\mu_n\sigma(\boldsymbol{x})\varphi_n(\boldsymbol{x})$$

by $\varphi_m(\boldsymbol{x})$ and integrate from a to b:

$$\int_a^b \delta(\boldsymbol{x}-\boldsymbol{z})\varphi_m(\boldsymbol{x})\mathrm{d}\boldsymbol{x} = \sum_{n=1}^{\infty} a_n(\boldsymbol{z})\mu_n \int_a^b \sigma(\boldsymbol{x})\varphi_n(\boldsymbol{x})\varphi_m(\boldsymbol{x})\mathrm{d}\boldsymbol{x}$$

$$\overset{\text{Def } \delta,\ \varphi \text{ orthog}}{\Longrightarrow} \qquad \varphi_m(\boldsymbol{z}) = a_m(\boldsymbol{z})\mu_m \int_a^b \sigma(\boldsymbol{x})\varphi_m^2(\boldsymbol{x})\mathrm{d}\boldsymbol{x}$$

and so

$$a_n(\boldsymbol{z}) = \frac{\varphi_n(\boldsymbol{z})}{\mu_n \int_a^b \varphi_n^2(\boldsymbol{x})\sigma(\boldsymbol{x})\mathrm{d}\boldsymbol{x}}$$

Putting this back into the eigenfunction expansion (4) for G we have

$$G(\boldsymbol{x},\boldsymbol{z}) = \sum_{n=1}^{\infty} \frac{\varphi_n(\boldsymbol{z})}{\mu_n \int_a^b \varphi_n^2(\boldsymbol{\xi})\sigma(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi}}\varphi_n(\boldsymbol{x}).$$

In particular, if the eigenfunctions are orthonormal with respect to σ then

$$G(\boldsymbol{x}, \boldsymbol{z}) = \sum_{n=1}^{\infty} \frac{1}{\mu_n} \varphi_n(\boldsymbol{x}) \varphi_n(\boldsymbol{z}),$$

which matches the Mercer series for G with $\lambda_n = \frac{1}{\mu_n}$ (as it should be).

Remark

- *This approach provides an alternative approach to finding Green's functions in infinite series form (as opposed to the closed form derivation we went through for the Brownian bridge kernel).*
- *As we will see later, it is not necessary to have a closed form representation of a kernel K in order to be able to use it to solve the approximation problems we are interested in. In fact, it may even be advantageous to work with its series representation, provided it is available.*

Example (More Brownian bridge)

A simple exercise in standard SL theory tells us that the BVP

$$-\varphi''(x) = \mu\varphi(x), \qquad \varphi(0) = \varphi(1) = 0,$$

has eigenvalues and eigenfunctions

$$\mu_n = (n\pi)^2, \quad \varphi_n(x) = \sin n\pi x, \qquad n = 1, 2, 3, \ldots,$$

and we can verify

$$G(x,z) = \min(x,z) - xz = \sum_{n=1}^{\infty} a_n(z) \sin n\pi x$$

with

$$a_n(z) = 2\int_0^1 (\min(x,z) - xz) \sin n\pi x dx = \frac{2}{(n\pi)^2} \sin n\pi z = \frac{1}{\mu_n} \frac{\varphi_n(z)}{\|\varphi_n\|^2}.$$

Summary

Chapters 2 and 5 tell us that we can get an eigenfunction series

$$K(\boldsymbol{x},\boldsymbol{z}) = \sum_{n=1}^{\infty} \lambda_n \varphi_n(\boldsymbol{x})\varphi_n(\boldsymbol{z})$$

for a given positive definite kernel K. This can be done

- via Mercer's theorem using the eigenvalues and $L_2(\Omega,\rho)$-normalized eigenfunctions of the Hilbert–Schmidt integral operator $\mathcal{K}$, i.e., as solutions of

$$\mathcal{K}\varphi = \lambda\varphi, \qquad \mathcal{K}f(\boldsymbol{x}) = \int_\Omega K(\boldsymbol{x},\boldsymbol{z})f(\boldsymbol{z})\rho(\boldsymbol{z})\mathrm{d}\boldsymbol{z},$$

- or via a generalized Fourier series based on the eigenvalues and eigenfunctions of the corresponding SL eigenvalue problem

$$\mathcal{L}\varphi = \frac{1}{\lambda}\rho\varphi, \qquad \mathcal{L}K(\boldsymbol{x},\boldsymbol{z}) = \delta(\boldsymbol{x}-\boldsymbol{z})$$

  with appropriate boundary conditions.

We will show later that such series expansions can be used to generate the Hilbert–Schmidt SVD which allows us to compute with kernels in a numerically stable and highly accurate way.

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