

# MATH 590: Meshfree Methods

## The Connection to Green's Kernels

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# Outline

- 1 Introduction
- 2 Green's Kernels
- 3 Sturm-Liouville Theory
- 4 Eigenfunction Expansions
- 5 Summary



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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**.



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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, FoI92, 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

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

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

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



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

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



## Remark

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

$$G(\mathbf{x}, \mathbf{z})|_{\mathbf{x} \in \partial\Omega} = 0 \quad \text{or} \quad \lim_{\|\mathbf{x}\| \rightarrow \infty} G(\mathbf{x}, \mathbf{z}) = 0.$$



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- 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

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

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

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The **integral operator**

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

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

$$\mathcal{L}u = f \quad \iff \quad u = \mathcal{G}f.$$



## 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

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

with eigenvalues  $\mu_n$ , eigenfunctions  $\varphi_n$ ,  $n = 1, 2, \dots$ , weight function  $\rho$ , and assume  $G$  is the Green's kernel of  $\mathcal{L}$ .



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

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

$$\lambda\varphi(\mathbf{x}) = \int_{\Omega} G(\mathbf{x}, \mathbf{z})\varphi(\mathbf{z})\rho(\mathbf{z})d\mathbf{z} \iff \mathcal{G}\varphi(\mathbf{x}) = \lambda\varphi(\mathbf{x}).$$





# 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.



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



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### 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  $\frac{dG}{dx}$  has a jump discontinuity at  $x = z$  of the form

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

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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

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



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Thus, so far

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



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Using the **jump condition** for the first derivative,

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

we get

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



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

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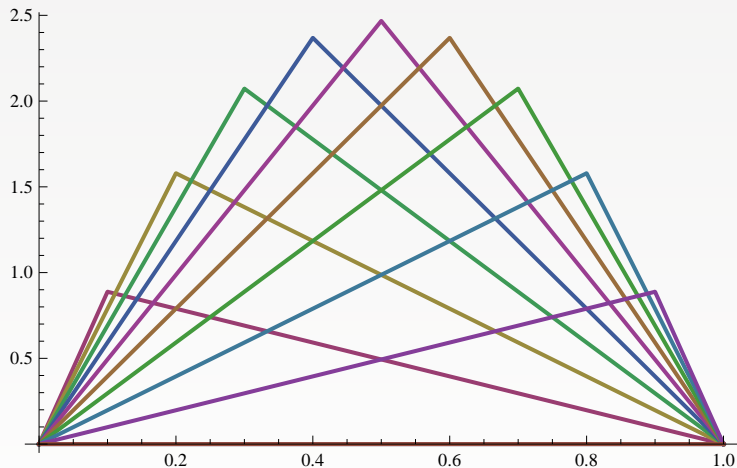
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### Remark

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  $z = \frac{j}{10}, j = 1, \dots, 9$ .





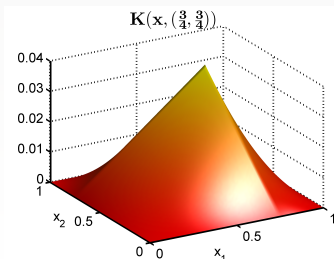
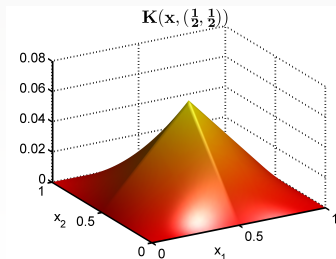
## Multivariate Brownian bridge kernel

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

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

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



# Iterated Brownian Bridge Kernels

Using the differential operator

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

and boundary conditions

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

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

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



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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.



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## Standard 1D SL-Theory [Fol92, Hab13]

Consider the ODE

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

with boundary conditions

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

where the  $\gamma_i$  are real numbers.



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If  $p$ ,  $q$ ,  $\sigma$  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**.



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### 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:  $\mu_1 < \mu_2 < \mu_3 < \dots$
- 3 Every eigenvalue  $\mu_n$  has an associated eigenfunction  $\varphi_n$  which is unique up to a constant factor. Moreover,  $\varphi_n$  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**

$$a_n = \frac{\int_a^b f(x) \varphi_n(x) \sigma(x) dx}{\int_a^b \varphi_n^2(x) \sigma(x) dx}, \quad n = 1, 2, 3, \dots$$





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

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

- 6 The Rayleigh quotient is given by

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

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

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



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# Green's kernels and eigenfunction expansions

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Starting from the ODE

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

with regular SL BCs we consider the SL ODE eigenvalue problem

$$(\mathcal{L}\varphi)(\mathbf{x}) = \mu\sigma(\mathbf{x})\varphi(\mathbf{x}) \quad (3)$$

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

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

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



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

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



In particular, if the eigenfunctions are orthonormal with respect to  $\sigma$  then

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

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



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### 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).*

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### 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

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

has eigenvalues and eigenfunctions

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

and we can verify

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

with

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

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# Summary

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

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

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

$$\mathcal{K}\varphi = \lambda\varphi, \quad \mathcal{K}f(\mathbf{x}) = \int_{\Omega} K(\mathbf{x}, \mathbf{z})f(\mathbf{z})\rho(\mathbf{z})d\mathbf{z},$$

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

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

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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