MATH 590: Meshfree Methods

Generalized Sobolev Spaces

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Outline

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- $f \in H^k(\Omega) = W_2^k(\Omega)$, Sobolev spaces
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The last example is not "standard", and so we would like to relate it to one or both of the others.

We will refine the concept of Sobolev spaces by adding a notion of scale.
Our spaces will not only emphasize sets of functions (i.e., with the same smoothness properties), but different structure (i.e., with different inner products/norms).

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- In the next chapter we will show that the kernel interpolant minimizes the native space norm.
- In Chapter 2 we said that it is difficult to understand the native space norm (sometimes Fourier transforms can be used).
- Now we will show that we can design this norm via the inner product (which in turn comes from the differential operator that defines a Green's kernel).

Weighted Sobolev spaces

[NW08, Appendix A.2.1] discusses three different examples of weighted Sobolev spaces:

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The first example is due to [TA96], the other two follow from [Hic98].

Example (First weighted Sobolev space)

The norm for the first example is induced by the inner product

$$\langle f, g \rangle_{H^{1,\varepsilon}([0,1])} = \int_0^1 f'(x)g'(x)\mathrm{d}x + \varepsilon^2 \int_0^1 f(x)g(x)\mathrm{d}x.$$

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The reproducing kernel for this example is given by

$$K(x,z) = \frac{\cosh(\varepsilon \min(x,z))\cosh(\varepsilon(1-\max(x,z)))}{\varepsilon \sinh(\varepsilon)}$$

and the eigenvalues and eigenfunctions are

$$\lambda_n = \frac{1}{\varepsilon^2 + ((n-1)\pi)^2}, \quad n = 1, 2, \ldots$$

$$\varphi_n(x) = \sqrt{2}\cos\left((n-1)\pi x\right).$$

Note $\lambda_1 = 1/\varepsilon^2$ and $\varphi_1(x) = 1$.

Remark

This example is different from the generalized Brownian bridge kernel $K_{1,\varepsilon}$.

While the inner products are the same for the two cases, the boundary conditions are different (just look at the eigenfunctions; sines vs. cosines).

For the Brownian bridge kernel the RKHS is the homogeneous space $H_0^{1,\varepsilon}([0,1])$, while here we have $H^{1,\varepsilon}([0,1])$.

Example (Second weighted Sobolev space)

Now the inner product is

$$\langle f, g \rangle_{H^{1,\varepsilon}([0,1])} = \int_0^1 f'(x)g'(x)\mathrm{d}x + \varepsilon^2 f(a)g(a),$$

where $a \in [0, 1]$ is referred to as an anchor.
The reproducing kernel is given by

$$K(x,z) = 1 + \frac{\varepsilon^2}{2}\left(|x-a| + |z-a| - |x-z|\right),$$

with special cases

$a = 0$: $K(x,z) = 1 + \varepsilon^2 \min(x,z)$

$a = 1$: $K(x,z) = 1 + \varepsilon^2 \min(1-x, 1-z)$

Remark

These kernels will always be piecewise linear, for any choice of ε and anchor a.

However, for values of $0 < a < 1$ this kernel appears to be less useful since multivariate integration based on a tensor product of this kernel was proven to be intractable in [NW01].

Example (Third weighted Sobolev space)

This time we use the inner product

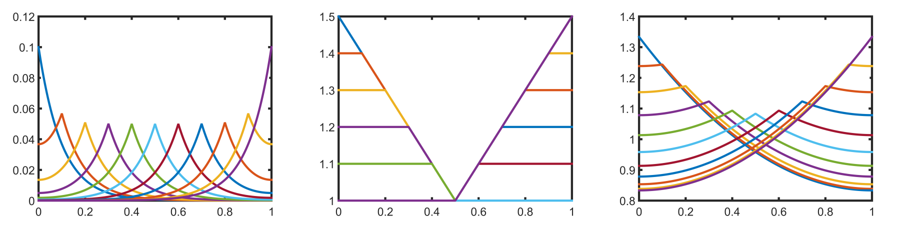
$$\langle f, g\rangle_{H^{1,\varepsilon}([0,1])} = \int_0^1 f'(x)g'(x)\mathrm{d}x + \varepsilon^2 \int_0^1 f(x)\mathrm{d}x \int_0^1 g(x)\mathrm{d}x,$$

which uses the product of the averages of f and g over $[0, 1]$ instead of their L_2 inner product as for the first example.
The reproducing kernel is given by

$$K(x, z) = 1 + \frac{\varepsilon^2}{2}\left(B_2(|x - z|) + 2(x - \frac{1}{2})(z - \frac{1}{2})\right),$$

where B_2 is the Bernoulli polynomial of degree 2, i.e., $B_2(x) = x^2 - x + \frac{1}{6}$.

Copies of reproducing kernels for the three weighted Sobolev spaces $H^{1,\varepsilon}([0,1])$



The first weighted kernel (left) uses $\varepsilon = 10$, the other two use $\varepsilon = 1$, and the second weighted kernel (middle) uses $a = \frac{1}{2}$.

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Our approach depends on the ability to identify a linear self-adjoint differential operator $\mathcal{L}$ that corresponds to a given Green's kernel K or vice versa.

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This means that we try to understand the generalized Sobolev space by either

- starting with a known kernel and then identifying its differential operator (and subsequently the inner product and norm in the associated Sobolev space as described below)
- starting with a differential operator (which again defines an inner product and a norm in the generalized Sobolev space) and then getting the reproducing kernel as the corresponding Green's kernel.

The latter approach is most likely the easier one, and we follow that here.

Given a linear self-adjoint differential operator $\mathcal{L}$, we decompose it into

$$\mathcal{L} = \mathcal{P}^*\mathcal{P},$$

with an appropriate differential operator $\mathcal{P}$ and its formal adjoint $\mathcal{P}^*$.

Example (Brownian bridge kernel)

Start with $\mathcal{L} = -\mathcal{D}^2$, so that $\mathcal{P} = \mathcal{D}$ and $\mathcal{P}^* = -\mathcal{D}$.
The inner product will turn out to be

$$\langle f, g \rangle_{\mathcal{H}_K} = \int_0^1 \mathcal{P}f(x)\mathcal{P}g(x)\mathrm{d}x = \int_0^1 f'(x)g'(x)\mathrm{d}x.$$

Remark

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Example

Consider $\mathcal{L} = \left(-\mathcal{D}^2 + \varepsilon^2\mathcal{I}\right)^3$ (for $\varepsilon = 0 \to$ quintic splines).

This operator can be decomposed in two different ways as

$$\begin{aligned}\mathcal{L} &= \left(-\mathcal{D}^3 + 3\varepsilon\mathcal{D}^2 - 3\varepsilon^2\mathcal{D} + \varepsilon^3\mathcal{I}\right)\left(\mathcal{D}^3 + 3\varepsilon\mathcal{D}^2 + 3\varepsilon^2\mathcal{D} + \varepsilon^3\mathcal{I}\right) \\ &= \left(-\mathcal{D}^3 - \varepsilon\mathcal{D}^2 + \varepsilon^2\mathcal{D} + \varepsilon^3\mathcal{I}\right)\left(\mathcal{D}^3 - \varepsilon\mathcal{D}^2 - \varepsilon^2\mathcal{D} + \varepsilon^3\mathcal{I}\right).\end{aligned}$$

The resulting norms will be different:

$$\|f\|^2_{\mathcal{H}_{K_{3,\varepsilon}}} = \int_0^1 \left(f'''(x) + 3\varepsilon f''(x) + 3\varepsilon^2 f'(x) + \varepsilon^3 f(x)\right)^2 \mathrm{d}x$$

$$\|f\|^2_{\mathcal{H}_{K_{3,\varepsilon}}} = \int_0^1 \left(f'''(x) - \varepsilon f''(x) - \varepsilon^2 f'(x) + \varepsilon^3 f(x)\right)^2 \mathrm{d}x.$$

We now present a rigorous framework for 1D bounded domains.

A theoretical framework supporting for more general vector distributional operators is provided in [FY11, FY13].

- The paper [FY11] contains the theory for generalized Sobolev spaces on the unbounded domain $\mathbb{R}^d$.
- The more complicated setting with bounded domains is the subject of [FY13].

We will not bother with this distributional setting.

Remark

Similar to the weighted Sobolev spaces, our generalized Sobolev spaces will in some cases be equivalent to a common classical Sobolev space $H^\beta(\Omega)$, i.e., they all consist of the same sets of functions, but are all equipped with their own individual norms.

Given a bounded domain Ω and the nonhomogeneous differential equation

$$\begin{aligned} \mathcal{L}u &= f, \quad \text{in } \Omega, \\ \boldsymbol{\mathcal{B}}u &= \boldsymbol{g}, \quad \text{on } \partial\Omega, \end{aligned}$$

we want to find the reproducing kernel K of the associated generalized Sobolev space $\mathcal{H}_{\mathcal{P},\boldsymbol{\mathcal{B}}}$.

Here

$\mathcal{L} = \mathcal{P}^*\mathcal{P}$: self-adjoint linear (partial) differential operator of order 2β,

$\mathcal{P}$: scalar linear (partial) differential operator of order β,

$\mathcal{P}^*$: formal adjoint of $\mathcal{P}$,

$\boldsymbol{\mathcal{B}} = (\mathcal{B}_1, \ldots, \mathcal{B}_{n_b})^T$: vector boundary operator of length n_b,

$\mathcal{B}_j$: boundary operators of order β (or lower) chosen so that the differential equation problem is well-posed.

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Assuming that the boundary conditions are specified such that

$$\text{null}(\boldsymbol{\mathcal{B}}) \cap \text{null}(\mathcal{P}) = \{0\},$$

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the desired direct sum decomposition of $\mathcal{H}_K$ is provided by these two spaces.

We therefore need to find the reproducing kernels of

- $\mathcal{H}_G = \text{null}(\boldsymbol{\mathcal{B}})$
- $\mathcal{H}_R = \text{null}(\mathcal{P})$

along with their corresponding inner products.

Reproducing kernel for the null space of $\mathcal{B}$

Consider the Green's kernel G for the problem with homogeneous BCs, i.e., for a fixed $\boldsymbol{z} \in \Omega$,

$$\begin{aligned} \mathcal{L}G(\boldsymbol{x},\boldsymbol{z}) &= \delta(\boldsymbol{x}-\boldsymbol{z}), \quad && \boldsymbol{x} \in \Omega, \\ \mathcal{B}G(\boldsymbol{x},\boldsymbol{z}) &= \mathbf{0}, && \boldsymbol{x} \in \partial\Omega. \end{aligned}$$

For functions $f, g \in \mathcal{H}_G(\Omega) = \text{null}(\mathcal{B})$ we define the inner product as

$$\langle f, g \rangle_{\mathcal{H}_G(\Omega)} = \int_\Omega \mathcal{P}f(\boldsymbol{x})\mathcal{P}g(\boldsymbol{x})\mathrm{d}\boldsymbol{x}.$$

G is the reproducing kernel for $\mathcal{H}_G(\Omega)$ since for any $f \in \mathcal{H}_G(\Omega)$

$$\langle G(\cdot, \boldsymbol{z}), f \rangle_{\mathcal{H}_G(\Omega)} = \int_\Omega \mathcal{P}G(\boldsymbol{x}, \boldsymbol{z}) \mathcal{P}f(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}$$

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&= \int_\Omega \mathcal{P}^*\mathcal{P}G(\boldsymbol{x},\boldsymbol{z})f(\boldsymbol{x})\mathrm{d}\boldsymbol{x} = \int_\Omega \mathcal{L}G(\boldsymbol{x},\boldsymbol{z})f(\boldsymbol{x})\mathrm{d}\boldsymbol{x}
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&= B(\mathcal{P}G(\cdot, \boldsymbol{z}), f)(\boldsymbol{x})|_{\boldsymbol{x} \in \partial\Omega} + \int_\Omega \mathcal{P}^*\mathcal{P}G(\boldsymbol{x}, \boldsymbol{z}) f(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} \\
&= \int_\Omega \mathcal{P}^*\mathcal{P}G(\boldsymbol{x}, \boldsymbol{z}) f(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} = \int_\Omega \mathcal{L}G(\boldsymbol{x}, \boldsymbol{z}) f(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} \\
&= \int_\Omega \delta(\boldsymbol{x} - \boldsymbol{z}) f(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} = f(\boldsymbol{z}).
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Here we have used something akin to Green's formula, i.e.,

$$\int_\Omega \left(f(\boldsymbol{x})\mathcal{P}g(\boldsymbol{x}) - g(\boldsymbol{x})\mathcal{P}^*f(\boldsymbol{x})\right)\mathrm{d}\boldsymbol{x} = B(f,g)(\boldsymbol{x})|_{\boldsymbol{x}\in\partial\Omega},$$

where B is called the bilinear concomitant which is coupled to the boundary operator $\mathcal{B}$ (see, e.g., [SV67] for the 1D setting of L-splines). Since $f \in \mathrm{null}(\mathcal{B})$ we have that $B(\mathcal{P}G(\cdot,\boldsymbol{z}), f)(\boldsymbol{x})|_{\boldsymbol{x}\in\partial\Omega} = 0$.

Reproducing kernel for the null space of $\mathcal{P}$

We now consider $\mathcal{H}_R = \text{null}(\mathcal{P})$ and note that this space has finite dimension n_a (since the order of $\mathcal{P}$ is β).

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Let $\{\psi_1, \ldots, \psi_{n_a}\}$ be an orthonormal basis of null($\mathcal{P}$) with respect to the boundary inner product

$$\langle f, g \rangle_{\mathcal{H}_R(\partial\Omega)} = \sum_{j=1}^{n_b} \langle \mathcal{B}_j f, \mathcal{B}_j g \rangle_{\partial\Omega}.$$

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Remark

The inner product $\langle f, g \rangle_{\partial\Omega}$ must be defined by the user, and the choice of inner product will have an impact on the native space of K.

Then we define

$$R(\boldsymbol{x},\boldsymbol{z}) = \sum_{k=1}^{n_a} \psi_k(\boldsymbol{x})\psi_k(\boldsymbol{z})$$

and see that R is the reproducing kernel of null($\mathcal{P}$) since any $f \in \text{null}(\mathcal{P})$ can be expressed as $f(\cdot) = \sum_{\ell=1}^{n_a} a_\ell \psi_\ell(\cdot)$ so that we have

$$\langle R(\cdot,\boldsymbol{z}), f\rangle_{\mathcal{H}_R(\partial\Omega)} = \sum_{j=1}^{n_b} \left\langle \mathcal{B}_j \left(\sum_{k=1}^{n_a} \psi_k(\cdot)\psi_k(\boldsymbol{z})\right), \mathcal{B}_j \left(\sum_{\ell=1}^{n_a} a_\ell \psi_\ell(\cdot)\right)\right\rangle_{\partial\Omega}$$

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&= \sum_{k=1}^{n_a} \psi_k(\boldsymbol{z}) \sum_{\ell=1}^{n_a} a_\ell \sum_{j=1}^{n_b} \langle \mathcal{B}_j\psi_k(\cdot), \mathcal{B}_j\psi_\ell(\cdot)\rangle_{\partial\Omega}
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&= \sum_{k=1}^{n_a} a_k \psi_k(\boldsymbol{z}) = f(\boldsymbol{z}).
\end{aligned}$$

Reproducing kernel of the generalized Sobolev space $\mathcal{H}_{\mathcal{P},\boldsymbol{\mathcal{B}}}$

Altogether, we have

$$K(\boldsymbol{x},\boldsymbol{z}) = G(\boldsymbol{x},\boldsymbol{z}) + R(\boldsymbol{x},\boldsymbol{z}) = G(\boldsymbol{x},\boldsymbol{z}) + \sum_{k=1}^{n_a} \psi_k(\boldsymbol{x})\psi_k(\boldsymbol{z}),$$

where G is the Green's kernel of $\mathcal{L}$ with respect to the homogeneous boundary conditions given by $\boldsymbol{\mathcal{B}}$.

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where G is the Green's kernel of $\mathcal{L}$ with respect to the homogeneous boundary conditions given by $\boldsymbol{\mathcal{B}}$.

The inner product in $\mathcal{H}_{\mathcal{P},\boldsymbol{\mathcal{B}}}$ is also given by the sum of the inner products, i.e.,

$$\begin{aligned}\langle f,g\rangle_{\mathcal{H}_{\mathcal{P},\boldsymbol{\mathcal{B}}}(\Omega)} &= \langle f,g\rangle_{\mathcal{H}_G(\Omega)} + \langle f,g\rangle_{\mathcal{H}_R(\partial\Omega)} \\ &= \int_\Omega \mathcal{P}f(\boldsymbol{x})\mathcal{P}g(\boldsymbol{x})\mathrm{d}\boldsymbol{x} + \sum_{j=1}^{n_b}\langle \mathcal{B}_j f, \mathcal{B}_j g\rangle_{\partial\Omega}.\end{aligned}$$

Remark

- *The exposition in [RS05, Chapter 20] (see also [BTA04, Chapter 6, Section 1.6.2]) is for ordinary differential equations with appropriate initial conditions and reflects the treatment of splines in [Wah90].*
- *In [DR93] the constraints for the ODE are generalized to arbitrary "boundary" conditions specified by an operator $\mathcal{B}$ such that* $\text{null}(\mathcal{L}) \cap \text{null}(\mathcal{B}) = \{0\}$.

An Example — The Brownian bridge kernel, again

Consider $\mathcal{L} = -\mathcal{D}^2 = \mathcal{P}^*\mathcal{P}$ with $\mathcal{P} = \mathcal{D}$ and $\mathcal{P}^* = -\mathcal{D}$ on $\Omega = [0, 1]$.

As boundary operator we have $\boldsymbol{\mathcal{B}} = (\mathcal{I}|_{x=0}, \mathcal{I}|_{x=1})^T$, i.e., point evaluation at $x = 0$ and $x = 1$, respectively.

The inner products for the two reproducing kernel spaces are given by

$$\langle f, g \rangle_{\mathcal{H}_G(\Omega)} = \int_0^1 \mathcal{P}f(x)\mathcal{P}g(x)\mathrm{d}x = \int_0^1 f'(x)g'(x)\mathrm{d}x,$$

$$\langle f, g \rangle_{\mathcal{H}_R(\partial\Omega)} = \sum_{j=1}^{2} \langle \mathcal{B}_j f, \mathcal{B}_j g \rangle_{\partial\Omega} = f(0)g(0) + f(1)g(1).$$

From the definitions of $\mathcal{P}$ and $\mathcal{B}$ we have

$$\text{null}(\mathcal{P}) = \text{span}\{1\},$$
$$\text{null}(\mathcal{B}) = \{f \in L_2([0,1]),\ f(0) = f(1) = 0\}.$$

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- Green's kernel of null($\mathcal{B}$): $G(x,z) = \min(x,z) - xz$,
- kernel for null($\mathcal{P}$): $R(x,z) = \frac{1}{2}$ (since we need to normalize the basis of null($\mathcal{P}$) with respect to the $\langle\cdot,\cdot\rangle_{\mathcal{H}_R(\partial\Omega)}$ inner product).

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Together this implies that

$$K(x,z) = \min(x,z) - xz + \frac{1}{2}$$

is the reproducing kernel for the generalized Sobolev space $\mathcal{H}_{\mathcal{P},\mathcal{B}}([0,1])$.

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This space is isomorphic to the classical Sobolev space $H^1_{\text{per}}([0,1])$.

However, the inner product of $\mathcal{H}_{\mathcal{P},\boldsymbol{\mathcal{B}}}([0,1])$ is

$$\langle f, g\rangle_{\mathcal{H}_{\mathcal{P},\boldsymbol{\mathcal{B}}}(\Omega)} = \int_0^1 f'(x)g'(x)\mathrm{d}x + f(0)g(0) + f(1)g(1),$$

while the standard inner product for $H^1_{\mathrm{per}}([0,1])$ is (see, e.g., [BTA04, Chapter 7, Example 19])

$$\langle f, g\rangle_{H^1(\Omega)} = \int_0^1 f'(x)g'(x)\mathrm{d}x + \int_0^1 f(x)\mathrm{d}x \int_0^1 g(x)\mathrm{d}x.$$

The periodicity can be deduced, e.g., by inspection or by employing the reproducing property, i.e.,

$$\langle K(\cdot,z), f\rangle_{\mathcal{H}_{\mathcal{P},\boldsymbol{\mathcal{B}}}} = \int_0^1 \frac{\mathrm{d}}{\mathrm{d}x} K(x,z) f'(x) \mathrm{d}x + K(0,z)f(0) + K(1,z)f(1)$$

The periodicity can be deduced, e.g., by inspection or by employing the reproducing property, i.e.,

$$\begin{aligned}\langle K(\cdot,z),f\rangle_{\mathcal{H}_{\mathcal{P},\boldsymbol{\mathcal{B}}}} &= \int_0^1 \frac{\mathrm{d}}{\mathrm{d}x}K(x,z)f'(x)\mathrm{d}x + K(0,z)f(0) + K(1,z)f(1) \\ &= \int_0^z (1-z)f'(x)\mathrm{d}x + \int_z^1 (-z)f'(x)\mathrm{d}x + \frac{f(0)}{2} + \frac{f(1)}{2}\end{aligned}$$

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&= \int_0^z (1-z)f'(x)\mathrm{d}x + \int_z^1 (-z)f'(x)\mathrm{d}x + \frac{f(0)}{2} + \frac{f(1)}{2} \\
&= (1-z)\left(f(z)-f(0)\right) - z\left(f(1)-f(z)\right) + \frac{f(0)}{2} + \frac{f(1)}{2}
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&= f(z) + \left(z - \frac{1}{2}\right) f(0) + \left(\frac{1}{2} - z\right) f(1)
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&= f(z) + \left(z-\frac{1}{2}\right)f(0) + \left(\frac{1}{2}-z\right)f(1) \\
&= f(z),
\end{aligned}$$

provided $f(0) = f(1)$.

Remark

The space $\mathcal{H}_{\mathcal{P},\boldsymbol{\mathcal{B}}}(\Omega)$ can be embedded in the classical Sobolev space $H^{\beta}(\Omega)$, where β is the order of $\mathcal{P}$.

$\mathcal{H}_{\mathcal{P},\boldsymbol{\mathcal{B}}}(\Omega)$ is isomorphic to $H^{\beta}(\Omega)$ if we generate the kernel R using $\text{null}(\mathcal{L})$ instead of $\text{null}(\mathcal{P})$.

We look at this setting next.

Outline

Using a Basis of null($\mathcal{L}$) Instead of null($\mathcal{P}$)

Up until now we assumed that

$$K(\boldsymbol{x},\boldsymbol{z}) = G(\boldsymbol{x},\boldsymbol{z}) + R(\boldsymbol{x},\boldsymbol{z}) = G(\boldsymbol{x},\boldsymbol{z}) + \sum_{k=1}^{n_a} \psi_k(\boldsymbol{x})\psi_k(\boldsymbol{z}),$$

where

- $G(\cdot,\boldsymbol{z}) \in \text{null}(\boldsymbol{\mathcal{B}})$, and
- $\{\psi_k\}$ is an ON basis of null($\mathcal{P}$).

This meant that $\mathcal{H}_{\mathcal{P},\boldsymbol{\mathcal{B}}}(\Omega)$ is equipped with the inner product

$$\begin{aligned}\langle f,g\rangle_{\mathcal{H}_{\mathcal{P},\boldsymbol{\mathcal{B}}}(\Omega)} &= \langle f,g\rangle_{\mathcal{H}_G(\Omega)} + \langle f,g\rangle_{\mathcal{H}_R(\partial\Omega)} \\ &= \int_\Omega \mathcal{P}f(\boldsymbol{x})\mathcal{P}g(\boldsymbol{x})\mathrm{d}\boldsymbol{x} + \sum_{j=1}^{n_b}\langle \mathcal{B}_j f, \mathcal{B}_j g\rangle_{\partial\Omega}.\end{aligned}$$

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It is also possible to take $\{\psi_k\}$ as an ON basis of null($\mathcal{L}$).
We now discuss this case (for details see [FY13]).

First we mention that the inner product in the case of $\{\psi_k\} \in \text{null}(\mathcal{P})$ can also be written as

$$\langle f, g \rangle_{\mathcal{H}_{\mathcal{P},\mathcal{B}}(\Omega)} = \langle f, g \rangle_{\mathcal{H}_G(\Omega)} + \sum_{k=1}^{n_a} \hat{f}_k \hat{g}_k \frac{I_{a_k}}{a_k},$$

where

$$\hat{f}_k = \langle f, \psi_k \rangle_{\mathcal{H}_R(\partial\Omega)} \quad \text{and} \quad \hat{g}_k = \langle g, \psi_k \rangle_{\mathcal{H}_R(\partial\Omega)}$$

and the a_k are appropriate coefficients [FY13, Thm. 3.2 & Cor. 3.1]. Here

$$I_x = \begin{cases} 1 & \text{if } x > 0, \\ 0 & \text{otherwise,} \end{cases}$$

and $0/0 \equiv 0$ (this indicator ensures that ψ_k does not contribute to the inner product if $a_k = 0$).

Now, in the case $\{\psi_k\} \in \mathrm{null}(\mathcal{L})$ the inner product becomes

$$\langle f, g\rangle_{\mathcal{H}_{\mathcal{P},\mathcal{B}}(\Omega)} = \langle f, g\rangle_{\mathcal{H}_G(\Omega)} + \sum_{k=1}^{n_a} \hat{f}_k \hat{g}_k \frac{l_{a_k}}{a_k} - \sum_{k=1}^{n_a}\sum_{\ell=1}^{n_a} \hat{f}_k \hat{g}_k \langle \psi_k, \psi_\ell\rangle_{\mathcal{H}_G(\Omega)} l_{a_k a_\ell},$$

and the kernel is of the form

$$K(\boldsymbol{x}, \boldsymbol{z}) = G(\boldsymbol{x}, \boldsymbol{z}) + R(\boldsymbol{x}, \boldsymbol{z}) = G(\boldsymbol{x}, \boldsymbol{z}) + \sum_{k=1}^{n_a} a_k \psi_k(\boldsymbol{x})\psi_k(\boldsymbol{z}).$$

Remark

This form of the kernel is slightly more general than before since it allows for use of nonnegative coefficients a_k that can be selected by the user.

Another Example

We already know that the Green's kernel for $\mathcal{L} = -\mathcal{D}^2 + \varepsilon^2\mathcal{I}$ with homogeneous boundary conditions is given by

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

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Since we can take $\mathcal{P} = \mathcal{D} + \varepsilon\mathcal{I}$ — similarly to the $\varepsilon = 0$ case — the inner product in null($\mathcal{B}$) is

$$(f,g)_{\mathcal{H}_G(\Omega)} = \int_0^1 \left(f'(x)g'(x) + \varepsilon^2 f(x)g(x) \right) \mathrm{d}x.$$

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We now look at the effects of adding a specific ON basis for null($\mathcal{L}$).

We can consider null $\mathcal{L} = \text{span}\{\tilde{\psi}_1, \tilde{\psi}_2\}$ with

$$\tilde{\psi}_1(x) = e^{\varepsilon x} + e^{\varepsilon(1-x)},$$
$$\tilde{\psi}_2(x) = e^{\varepsilon x} - e^{\varepsilon(1-x)}.$$

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For the normalization we compute

$$\langle \tilde{\psi}_1, \tilde{\psi}_1 \rangle_{\mathcal{H}_R(\partial\Omega)} = \tilde{\psi}_1(0)^2 + \tilde{\psi}_1(1)^2 = 2(e^{\varepsilon} + 1)^2$$
$$\langle \tilde{\psi}_2, \tilde{\psi}_2 \rangle_{\mathcal{H}_R(\partial\Omega)} = \tilde{\psi}_2(0)^2 + \tilde{\psi}_2(1)^2 = 2(e^{\varepsilon} - 1)^2$$

so that

$$\psi_1(x) = \frac{e^{\varepsilon x} + e^{\varepsilon(1-x)}}{\sqrt{2}\,(e^{\varepsilon} + 1)},$$
$$\psi_2(x) = \frac{e^{\varepsilon x} - e^{\varepsilon(1-x)}}{\sqrt{2}\,(e^{\varepsilon} - 1)}.$$

If we choose the positive coefficients

$$a_1 = \frac{e^{\varepsilon} + 1}{2\varepsilon e^{\varepsilon}}, \quad a_2 = \frac{e^{\varepsilon} - 1}{2\varepsilon e^{\varepsilon}}$$

then

$$K(x, z) = G(x, z) + \sum_{k=1}^{2} a_k \psi_k(x) \psi_k(z) = \frac{1}{2\varepsilon} e^{-\varepsilon|x-z|},$$

a scaled version of the C^0 Matérn kernel.

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a scaled version of the C^0 Matérn kernel.

The RKHS turns out to be $H^1(\Omega)$ with inner-product

$$\langle f, g \rangle_{H^1(\Omega)} = \int_0^1 \left(f'(x)g'(x) + \varepsilon^2 f(x)g(x) \right) \mathrm{d}x + 2\varepsilon \left(f(0)g(0) + f(1)g(1) \right),$$

where we now allow non-homogeneous BCs.

Further Generalizations

- Everything done with distribution theory using things such as
  - distributional Fourier transforms,
  - distributional adjoints,
  - distributional operators (allows pseudo-differential operators instead of just differential operators).
- Using vector differential operators $\boldsymbol{\mathcal{P}}$ so that $\mathcal{L} = \boldsymbol{\mathcal{P}}^* \boldsymbol{\mathcal{P}}$, e.g.

$$\mathcal{L} = -\mathcal{D}^2 + \varepsilon^2 \mathcal{I} \quad \text{with} \quad \boldsymbol{\mathcal{P}} = (\mathcal{D}, \varepsilon\mathcal{I})^T, \ \boldsymbol{\mathcal{P}}^* = (-\mathcal{D}, \varepsilon\mathcal{I}).$$

- null($\mathcal{L}$) not necessarily finite-dimensional, e.g., $\mathcal{L} = \nabla^2$ on $\Omega \subseteq \mathbb{R}^d$, $d \geq 2$.
- Full space instead of bounded domains.

Multivariate Full-space Kernels

The general Matérn kernels are of the form

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

where $K_{\beta-d/2}$ are modified Bessel functions of the second kind.
The Matérn kernels can be obtained as Green's kernels of

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We contrast this with the (conditionally positive definite) 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

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

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