Reproducing Kernels of Sobolev Spaces and Applications

Erich Novak

mit Mario Ullrich, Henryk Woźniakowski und Shun Zhang

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Two Sobolev Spaces of Continuous Functions

Let $C(D)$ be the space of cont. and bounded functions with $\|\cdot\|_\infty$, $D \subset \mathbb{R}^d$, mainly $D = \mathbb{R}^d$. Consider Sobolev spaces:

1) $W_2^s(\mathbb{R}^d)$ for $s \in \mathbb{N} \cup \{\infty\}$ with $s > d/2$ and the inner product

$$\langle f, g \rangle_{W_2^s(\mathbb{R}^d)} = \sum_{|\alpha|_1 \le s} \langle D^\alpha f, D^\alpha g \rangle_{L_2(\mathbb{R}^d)},$$

where $\langle f, g \rangle_{L_2(\mathbb{R}^d)} = \int_{\mathbb{R}^d} f(x)\, \overline{g(x)}\, \mathrm{d}x$.

2) $W_2^{s,\mathrm{mix}}(\mathbb{R}^d)$ with $\langle f, g \rangle = \sum_{|\alpha|_\infty \le s} \langle D^\alpha f, D^\alpha g \rangle_{L_2(\mathbb{R}^d)}$.

There will be more Sobolev spaces later.

Two Problems

- Given a Hilbert space $H(D) \subset C(D)$, what is the embedding constant $C = \|I\|, \ \ I : H(D) \to C(D)$?
- What is the error of optimal quadrature formulas

$$Q_n(f) = \sum_{i=1}^{n} a_i f(x_i)$$

for the approximation of integrals

$$\mathrm{INT}_\varrho(f) = \int_D f(x)\,\varrho(x)\,\mathrm{d}x \ ?$$

In particular: Is it enough, for obtaining an error $\|\mathrm{INT}_\varrho - Q_n\| \le \varepsilon$, to choose $n = n(\varepsilon)$ independently from d? Do we have the curse of dimension?

Reproducing Kernel Hilbert Spaces

These Sobolev spaces are RKHS, function evaluation is continuous,

$$f(x) = \langle f, \delta_x \rangle \quad \text{for all} \quad f \in H,$$

where $\delta_x \in H$. The function

$$K(x,y) = \langle \delta_x, \delta_y \rangle = \delta_y(x) \in \mathbb{R}$$

is the reproducing kernel of H.

Later we denote the kernel of $W_2^s(\mathbb{R}^d)$ by $K_{d,s}$.

Problem: Find an explicit formula for $K_{d,s}$.

We start with a tutorial on RKHS.

Tutorial on RKHS

Let $d \in \mathbb{N}$, $D \subset \mathbb{R}^d$, $\lambda^d(D) > 0$. Let H be a Hilbert space of real valued functions $f : D \to \mathbb{R}$, the functionals $x \mapsto f(x)$ are continuous, hence

$$f(x) = \langle f, \delta_x \rangle \quad \text{for a} \quad \delta_x \in H.$$

Let

$$K(x,t) = \langle \delta_x, \delta_t \rangle = \delta_t(x) = \delta_x(t).$$

Hence

$$\|\delta_x\|^2 = \delta_x(x) = K(x,x)$$

and the embedding constant is $C = \sup_{x \in D} K(x,x)^{1/2}$.

Tutorial on RKHS

Best linear estimation, optimal recovery, kriging, H-splines, interpolation:

Find $f \in H$ with minimal norm such that $f(x_i) = y_i$ for $i = 1, \dots, n$.

The solution is an "abstract spline" of the form

$$f^* = \sum_{i=1}^{n} \alpha_i \delta_{x_i}.$$

Optimal quadrature formulas are given by the spline algorithm

$$Q_n(f) = \mathrm{INT}_\varrho(f^*).$$

Tutorial on RKHS

Consider a quadrature formula $Q_n(f) = \sum_{i=1}^n a_i f(x_i)$ for a continuous functional

$$\mathrm{INT}_\varrho(f) = \int_D f(t)\,\varrho(t)\,\mathrm{d}t = \langle f, h\rangle\,.$$

The norm $\|\mathrm{INT}_\varrho\| = \|h\|$ is called initial error,

$$e(Q_n) = \|\mathrm{INT}_\varrho - Q_n\| = \sup_{\|f\|\le 1} |\mathrm{INT}_\varrho(f) - Q_n(f)|$$

is the worst case error of Q_n. Observe that

$$h(x) = \langle \delta_x, h\rangle = \mathrm{INT}_\varrho(\delta_x) = \int_D K(t,x)\varrho(t)\,\mathrm{d}t$$

and

$$\|h\|^2 = \mathrm{INT}_\varrho(h) = \int_D \int_D K(t,x)\varrho(t)\varrho(x)\,\mathrm{d}t\mathrm{d}x.$$

Tutorial on RKHS

The worst case error is $e(Q_n) = \| h - \sum_{i=1}^n a_i \delta_{x_i} \|$, hence

$$e(Q_n)^2 = \|h\|^2 - 2 \sum_{i=1}^n a_i h(x_i) + \sum_{i,j=1}^n a_i a_j K(x_i, x_j).$$

We want upper and lower bounds for

$$e(n) = \inf_{x_i, a_i} \| h - \sum_{i=1}^n a_i \delta_{x_i} \|,$$

also for "small" n, such as $n < 2^d$.

There is a simple lower bound if the kernel is positive and also the quadrature formula is positive, $a_i \geq 0$. Then

$$e(Q_n) \geq (1 - n\kappa^2)_+^{1/2} \cdot \|h\|,$$

where

$$\kappa = \frac{1}{\|h\|} \sup_x \frac{|h(x)|}{K(x,x)^{1/2}}.$$

For tensor product problems $\kappa = (\kappa_1)^d$, we obtain the curse of dimension for positive quadrature formulas and a normalized (by $\|h\|$) error.

More difficult: Lower bounds for $e(n)$, i.e., for all Q_n.

Results for the kernel

The kernel $K_{d,s}$ of $W^s(\mathbb{R}^d)$ (in the case $s > d/2$) is given by

$$K_{d,s}(x,t) = \int_{\mathbb{R}^d} \frac{\prod_{j=1}^d \cos\left(2\pi\,(x_j - t_j)u_j\right)}{1 + \sum_{0<|\alpha|_1\le s} \prod_{j=1}^d (2\pi\, u_j)^{2\alpha_j}}\,\mathrm{d}u$$

for all $x, t \in \mathbb{R}^d$, where $\alpha \in \mathbb{N}_0^d$ with $|\alpha|_1 = \sum_{j=1}^d \alpha_j$.

This is from Hegland and Marti (1986). Explicit formulas were known for $d = 1$ and $s \in \{1, 2\}$:

$$K_{1,1}(x,t) = \tfrac{1}{2}\exp\left(-|x-t|\right)$$

and

$$K_{1,2}(x,t) = \frac{\sqrt{3}}{3} e^{-|x-t|\sqrt{3}/2} \sin\left(\frac{|x-t|}{2} + \frac{\pi}{6}\right).$$

Results for the kernel

For $d = 1$ we show $\quad K_{1,s}(x,t) =$

$$-\sum_{j=1}^{s} \frac{e^{-|x-t|\,\sin(j\pi/(s+1))}}{s+1}\,\sin\left(\frac{j\pi}{s+1}\right)\,\cos\left(|x-t|\,\cos\left(\frac{j\pi}{s+1}\right) + \frac{2j\pi}{s+1}\right).$$

For the smoothness $s = \infty$ we obtain the kernel

$$K_{1,\infty}(x,t) = \frac{2}{\pi(x-t)^3}\,(\sin(x-t) - (x-t)\cos(x-t)).$$

The kernel of $W_2^{s,\mathrm{mix}}(\mathbb{R}^d)$ is given as a tensor product of $K_{1,s}$.

Infinite smoothness

We may take $s = \infty$ and obtain the kernel

$$K_{d,\infty}(x,t) = \prod_{j=1}^{d} \frac{2}{\pi(x_j - t_j)^3} \left(\sin(x_j - t_j) - (x_j - t_j)\cos(x_j - t_j)\right).$$

In particular

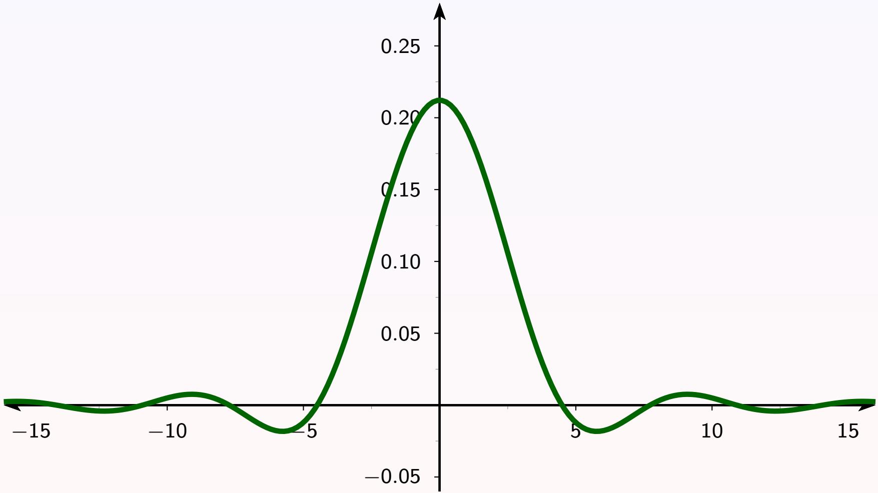
$$K_{d,\infty}(x,x) = \left(\frac{2}{3\pi}\right)^d \approx 0.2122^d.$$

The function $\delta_0(x) = K_{1,\infty}(x,0)$,

$$\delta_0(x) = \frac{2}{\pi x^3} \left(\sin x - x \cos x\right),$$

is the "simplest" function in the space $W_2^\infty(\mathbb{R})$, in particular, this is a C^∞ function with small derivatives.

δ_0 for $s = \infty$



Finite smoothness

We illustrate $K_{1,s}$ for $s = 1, 2, 3$. We have

$$K_{1,1}(x,t) = \frac{1}{2} e^{-|x-t|},$$
$$K_{1,2}(x,t) = \frac{\sqrt{3}}{3} e^{-|x-t|\sqrt{3}/2} \sin\left(\frac{|x-t|}{2} + \frac{\pi}{6}\right),$$
$$K_{1,3}(x,t) = \frac{1}{4}\left(e^{-|x-t|} + \sqrt{2} e^{-|x-t|/\sqrt{2}} \sin \frac{|x-t|}{\sqrt{2}}\right).$$

The function $K_{1,1}$ is positive on $\mathbb{R}$, while the other functions also take negative values.

Application 1: Embedding constants

The norm of $I_{d,s} : W_2^s(\mathbb{R}^d) \to C(\mathbb{R}^d)$ for $s > d/2$ (embedding constant) is given by

$$\|I_{d,s}\| = \frac{\delta_x(x)}{\|\delta_x\|_{W_2^s}} = K_{d,s}(0,0)^{1/2}.$$

We have explicit formulas for $d = 1$ or $s = \infty$ and upper and lower bounds in all cases.

For example: $\frac{2}{3\pi} = K_{1,\infty}(0,0) \le K_{1,s}(0,0) \le K_{1,1}(0,0) = \frac{1}{2}$.

$\left(\frac{2}{3\pi}\right)^d = K_{d,\infty}(0,0) \le K_{d,s}(0,0) \le \frac{2d^2}{2^d \pi^{d/2}} \quad (s > d/2 \text{ and } d \ge 2)$.

From the case $d = 1$ we get the values for the tensor product (mix) Sobolev spaces.

Application 2: Strong tractability of integration

Study the integration problem

$$\mathrm{INT}_\varrho(f) = \int_{\mathbb{R}^d} f(x)\varrho(x)\,\mathrm{d}x$$

for $f \in W_2^s(\mathbb{R}^d)$ and a probability density $\varrho : \mathbb{R}^d \to \mathbb{R}_0^+$. We assume $s > d/2$. Then

$$\|\mathrm{INT}_\varrho\|^2 = \int_{\mathbb{R}^{2d}} K_{d,s}(x,t)\varrho(x)\varrho(t)\,\mathrm{d}x\mathrm{d}t \le K_{d,s}(0,0).$$

The bound $\|\mathrm{INT}_\varrho\|^2 \le K_{d,s}(0,0)$ is optimal, it corresponds to the (normed) Dirac functional $K_{d,s}(0,0)^{-1/2} \cdot \delta_0$.

Let $x_1, x_2, \ldots, x_n \in \mathbb{R}^d$. For the worst case error of the respective QMC algorithm $Q_n(f) = \frac{1}{n}\sum_{j=1}^n f(x_j)$ we have

$$e^2(x_1, x_2, \ldots, x_n) = \sup_{\|f\|_{W_2^s(\mathbb{R}^d)} \le 1} \left| I_\varrho(f) - \frac{1}{n}\sum_{j=1}^n f(x_j) \right|^2 =$$

$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K(x,y)\varrho(x)\varrho(y)\,\mathrm{d}x\mathrm{d}y - \frac{2}{n}\sum_{i=1}^n \int_{\mathbb{R}^d} K(x_i,y)\varrho(y)\mathrm{d}y +$
$\frac{1}{n^2}\sum_{i=1}^n\sum_{j=1}^n K(x_i,x_j)$.

Average wrt $x_1, x_2, \ldots, x_n$ with densities ϱ, obtain

$$\int_{\mathbb{R}^{nd}} e^2(x_1, x_2, \ldots, x_n)\varrho(x_1)\ldots\varrho(x_n)\,\mathrm{d}x_1\ldots\mathrm{d}x_n$$
$$= \frac{1}{n}\left(\int_{\mathbb{R}^d} K_{d,s}(t,t)\varrho(t)\,\mathrm{d}t - \int_{\mathbb{R}^{2d}} K_{d,s}(t,x)\varrho(x)\varrho(t)\,\mathrm{d}x\mathrm{d}t\right).$$

We obtain the existence of $x_1^*, x_2^*, \dots, x_n^* \in \mathbb{R}^d$ such that

$$e(x_1^*, x_2^*, \dots, x_n^*) \le \frac{1}{\sqrt{n}} \left(\int_{\mathbb{R}^d} K_{d,s}(t,t) \varrho(t) \, \mathrm{d}t \right)^{1/2}.$$

The integral over ϱ is one, obtain

$$e(x_1^*, x_2^*, \dots, x_n^*) \le \frac{\|I_{d,s}\|}{\sqrt{n}}$$

or, for the spaces $W_2^s(\mathbb{R}^d)$,

$$e(x_1^*, x_2^*, \dots, x_n^*) \le \frac{1}{\sqrt{n}} \left(\int_{\mathbb{R}^d} \frac{\mathrm{d}u}{1 + \sum_{0<|\alpha|\le s} \prod_{j=1}^d (2\pi u_j)^{2\alpha_j}} \right)^{1/2}.$$

Application 2: Strong Polynomial Tractability of Integration

For an arbitrary integration problem $\int_{\mathbb{R}^d} f(x)\varrho(x)\,\mathrm{d}x$ with a probability density ϱ we obtain the worst case error bound

$$e(Q_n) \le \frac{\|I_{d,s}\|}{\sqrt{n}} \le \sqrt{\frac{2d^2}{2^d \pi^{d/2} n}}$$

for a deterministic quadrature formula Q_n for $W_2^s(\mathbb{R}^d)$ (with $s > d/2$ and $d \ge 2$) that uses n function values.

We can also consider tensor product Sobolev spaces for functions defined on $\mathbb{R}^d$ and obtain, for every natural smoothness s, the upper bound

$$e(Q_n) \le \frac{2^{-d/2}}{\sqrt{n}}$$

for a quadrature formula Q_n.

Equivalent norm on $W_2^s(\mathbb{R}^d)$

An equivalent (orthogonal invariant, isotropic) norm on $W_2^s(\mathbb{R}^d)$, again $s > d/2$:

$$\langle f, g \rangle = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \hat{f}(\omega) \, \overline{\hat{g}(\omega)} \, (1 + |\omega|_2^2)^s \, \mathrm{d}\omega.$$

For this norm, the kernel is known (see Wendland 2005) and always positive. In particular:

$$\widetilde{K}_{d,s}(x,x) = \frac{1}{2^{d/2}\Gamma(d/2+1)} \int_0^1 (t^{-1/s} - 1)^{d/2} \mathrm{d}t \le \frac{1}{2^{d/2}\Gamma(d/2+1)} \frac{2s}{2s-d}.$$

We obtain similar results as above if $s \in \mathbb{N}$. Observe, however, that we can take $s \in \mathbb{R}$ and then

$$\lim_{s \to d/2} \|\widetilde{I}_{d,s}\| = \infty.$$

Equivalent norm on $W_2^s(\mathbb{R}^d)$

For $s \in \mathbb{N}$, the scalar product can also be written as $\langle f, g\rangle_{H_2^s} =$

$$(2\pi)^{-d/2} \sum_{\ell=0}^{s} \frac{s!}{(s-\ell)!} \sum_{\substack{\beta\in\mathbb{N}_0^d \\ |\beta|_1=\ell}} \frac{1}{\prod_{j=1}^{d}(\beta_j!)} \left\langle D^\beta f, D^\beta g \right\rangle_{L_2(\mathbb{R}^d)} .$$

Since the kernel is always positive we can apply the lower bounds for positive quadrature formulas.

Another (larger) space for $s = \infty$

For $s = \infty$ we can consider the isotropic norm

$$\langle f, g \rangle = \int_{\mathbb{R}^d} \hat{f}(\omega)\, \overline{\hat{g}(\omega)}\, \exp(\|\omega\|^2/2)\, \mathrm{d}\omega.$$

This can be written as

$$\langle f, g \rangle = \sum_{\beta \in \mathbb{N}_0^d} \frac{1}{2^{|\beta|_1} \prod_{j=1}^d (\beta_j!)} \left\langle D^\beta f, D^\beta g \right\rangle_{L_2(\mathbb{R}^d)}.$$

One can show that the reproducing kernel for this space is the famous Gauss kernel,

$$K_\infty(x, y) = (2\pi)^{-d/2} \exp(-\|x - y\|_2^2/2).$$

Remark: Sobolev spaces on the cube

Same proof technique for Sobolev spaces on $[0,1]^d$. Embedding constant for $W_2^{1,\mathrm{mix}}([0,1]^d)$ is

$$\|\widetilde{I}_d\| = \sup_{x\in[0,1]^d} \widetilde{K}_d(x,x)^{1/2} = \left(\frac{e+e^{-1}}{e-e^{-1}}\right)^{d/2} \approx 1.15^d.$$

Hence the bound

$$e(Q_n) \le \frac{\|\widetilde{I}_d\|}{\sqrt{n}}$$

does not yield tractability.

We know the curse of dimension, but one needs a different proof.