MATH 590: Meshfree Methods

Chapter 3: Examples of Kernels

Greg Fasshauer

Department of Applied Mathematics
Illinois Institute of Technology

Fall 2014

Outline

1. Radial Kernels
2. Translation Invariant Kernels
3. Series Kernels
4. General Anisotropic Kernels
5. Compactly Supported (Radial) Kernels
6. Multiscale Kernels
7. Space-Time Kernels
8. Learned Kernels
9. Designer Kernels

Outline

1. Radial Kernels
2. Translation Invariant Kernels
3. Series Kernels
4. General Anisotropic Kernels
5. Compactly Supported (Radial) Kernels
6. Multiscale Kernels
7. Space-Time Kernels
8. Learned Kernels
9. Designer Kernels

Isotropic Radial Kernels

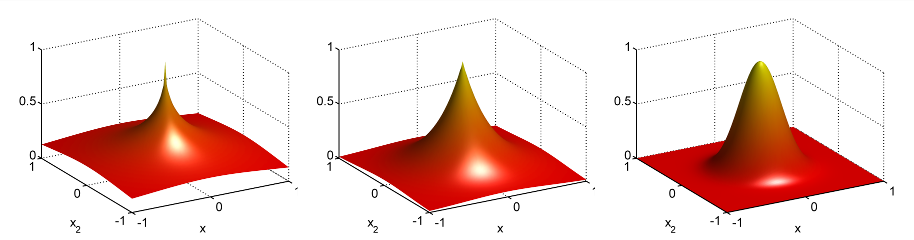
- Of the form

$$K(\boldsymbol{x},\boldsymbol{z}) = \kappa(\|\boldsymbol{x}-\boldsymbol{z}\|), \quad \boldsymbol{x},\boldsymbol{z} \in \mathbb{R}^d, \quad \kappa : \mathbb{R}_0^+ \to \mathbb{R},$$

Example

Powered exponential kernel (plotted with $\beta = 0.5, 1, 2$, $\varepsilon = 3$)

$$\kappa(r) = e^{-(\varepsilon r)^\beta}, \quad \beta \in (0,2]$$



- The family of powered exponential kernels is common in the statistics and machine learning literature since the two parameters ε and β provide flexibility with respect to scale and smoothness.
- However, the powered exponential kernel is smooth only for $\beta = 2$, i.e., the Gaussian.
- They are positive definite on $\mathbb{R}^d$ for all d.
- The case $\beta = 1$ is known as the Ornstein–Uhlenbeck kernel, and also corresponds to the Matérn kernel with $\beta = \frac{d+1}{2}$ (see next).
- The Gaussian is sometimes referred to as squared exponential in the machine learning or statistics literature.

Example

Matérn (or Sobolev) kernel (plotted with $d = 2$, $\varepsilon = 3$)

$$\kappa(\varepsilon r) = \frac{K_{d/2-\beta}(\varepsilon r)}{(\varepsilon r)^{d/2-\beta}}, \quad \beta > \frac{d}{2}$$

K_ν: modified Bessel functions of the second kind of order ν

Example

Matérn (or Sobolev) kernel (plotted with $d = 2$, $\varepsilon = 3$)

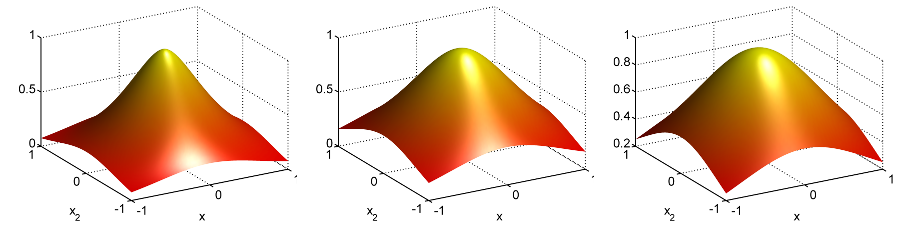
$$\kappa(\varepsilon r) = \frac{K_{d/2-\beta}(\varepsilon r)}{(\varepsilon r)^{d/2-\beta}}, \quad \beta > \frac{d}{2}$$

K_ν: modified Bessel functions of the second kind of order ν

$$\kappa(\varepsilon r) = (1+\varepsilon r)e^{-\varepsilon r}, \qquad \text{(when } \beta = (d+3)/2)$$

$$\kappa(\varepsilon r) = (1+\varepsilon r + \frac{1}{3}(\varepsilon r)^2)e^{-\varepsilon r}, \qquad \text{(when } \beta = (d+5)/2)$$

$$\kappa(\varepsilon r) = (1+\varepsilon r + \frac{2}{5}(\varepsilon r)^2 + \frac{1}{15}(\varepsilon r)^3)e^{-\varepsilon r}, \qquad \text{(when } \beta = (d+7)/2)$$



- Matérn kernels are popular in the statistics and approximation theory communities.
- They are fundamental solutions of the d-dimensional iterated modified Helmholtz operator in Euclidean coordinates, i.e.,

$$\mathcal{D} = \left(-\nabla^2 + \varepsilon^2 \mathcal{I}\right)^\beta,$$

  with $\mathcal{I}$ the identity operator.

- The parameters ε and β specify scale and smoothness of the kernel, respectively.
- Matérn kernels generate classical Sobolev spaces $H^\beta(\mathbb{R}^d)$ as their RKHSs.
- They are positive definite on $\mathbb{R}^d$, but only when $\beta > \frac{d}{2}$.

Example

(Inverse) Multiquadric kernels (plotted with $\varepsilon = 3$)

$$\kappa(\varepsilon r) = (1 + \varepsilon^2 r^2)^\beta, \quad \beta \in \mathbb{R} \setminus \mathbb{N}_0$$

$\beta < 0$: inverse MQs (positive definite)
$\beta > 0$: MQs (conditionally positive definite of different orders)

Example

(Inverse) Multiquadric kernels (plotted with $\varepsilon = 3$)

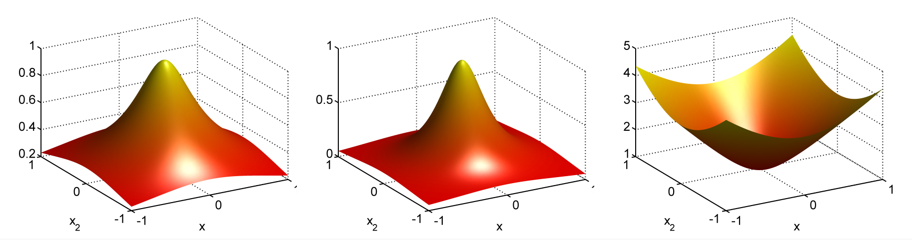
$$\kappa(\varepsilon r) = (1 + \varepsilon^2 r^2)^\beta, \quad \beta \in \mathbb{R} \setminus \mathbb{N}_0$$

$\beta < 0$: inverse MQs (positive definite)
$\beta > 0$: MQs (conditionally positive definite of different orders)

$$\kappa(\varepsilon r) = \frac{1}{\sqrt{1 + \varepsilon^2 r^2}}, \qquad \text{(IMQ)}$$

$$\kappa(\varepsilon r) = \frac{1}{1 + \varepsilon^2 r^2}, \qquad \text{(IQ or Cauchy)}$$

$$\kappa(\varepsilon r) = \sqrt{1 + \varepsilon^2 r^2}, \qquad \text{(MQ)}$$



- Popular mostly in approximation theory and engineering applications.
- The IQ kernel is equivalent to the rational quadratic kernel (see, e.g., [Gen02]) since

$$\frac{1}{1+\varepsilon^2 r^2} = 1 - \frac{r^2}{\theta + r^2}$$

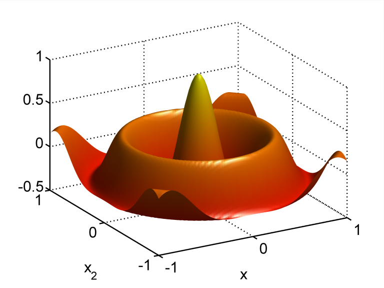
  with $\theta = 1/\varepsilon^2$. This kernel is sometimes recommended as a computationally cheaper alternative to the Gaussian kernel in the machine learning literature.
- (Inverse) MQ kernels are (conditionally) positive definite on $\mathbb{R}^d$ for all d.

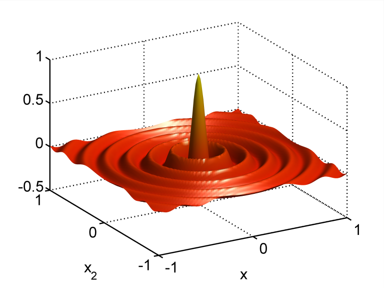
Oscillatory kernels (plotted with $\varepsilon = 10$, $d = 2$)

$$\kappa(\varepsilon r) = \frac{J_{d/2-1}(\varepsilon r)}{(\varepsilon r)^{d/2-1}}, \qquad \text{(Poisson or Bessel)}$$

$$\kappa(\varepsilon r) = \frac{\sin(\varepsilon r)}{\varepsilon r}, \qquad \text{(wave, Poisson with } d = 3\text{)}$$

J_ν: Bessel functions of the first kind of order ν





Bessel kernels were introduced in [FLW06]. The wave kernel sometimes appears in machine learning (see, e.g., [Gen02]).

They are positive definite only in dimension $\leq d$.

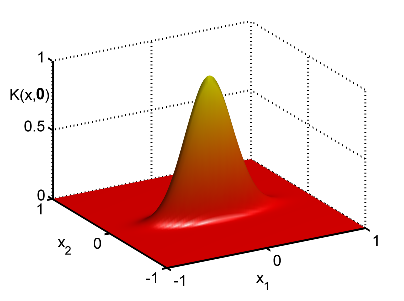
Anisotropic Radial Kernels

Any isotropic radial kernel can be turned into an anisotropic radial kernel by using a weighted 2-norm instead of an unweighted one.

Example (Anisotropic Gaussian)

$$K(\boldsymbol{x}, \boldsymbol{z}) = \mathrm{e}^{-(\boldsymbol{x}-\boldsymbol{z})^T \mathsf{E}(\boldsymbol{x}-\boldsymbol{z})},$$

with E a symmetric positive definite matrix.
If $\mathsf{E} = \varepsilon^2 \mathsf{I}_d$, with I_d a $d \times d$ identity matrix, then the kernel is isotropic.



- Anisotropic kernels are not common in the approximation theory literature. They have been
  - analyzed, e.g., in [Bax06, BDL10] and
  - applied, e.g., in [CBM+03, CLMM06].
- But they are very popular in the literature on information-based complexity, e.g., [NW08].
- [FHW12a, FHW12b] used $\mathsf{E} = \mathrm{diag}(\varepsilon_1^2, \ldots, \varepsilon_d^2)$, a diagonal matrix with dimension-dependent shape parameters, to avoid the curse of dimensionality and obtain dimension-independent error bounds.

Remark

Some authors have applied a different scale to each basis function in the RBF interpolation expansion resulting in, e.g.,

$$s(\boldsymbol{x}) = \sum_{j=1}^{N} c_j e^{-\varepsilon_j^2 \|\boldsymbol{x}-\boldsymbol{x}_j\|^2}, \qquad \boldsymbol{x} \in \mathbb{R}^d.$$

Now the interpolant is no longer generated by a single kernel and the theoretical foundation must be reconsidered.

The most promising paper to address this approach — especially on a theoretical level — is [BLRS14], where the problem is tackled by embedding a d-dimensional interpolation problem into $\mathbb{R}^{d+1}$ so that the additional dimension houses the locally varying shape parameter. In $\mathbb{R}^{d+1}$ one then works with a "standard" kernel with fixed global shape.

Outline

1 Radial Kernels

2 Translation Invariant Kernels

3 Series Kernels

4 General Anisotropic Kernels

5 Compactly Supported (Radial) Kernels

6 Multiscale Kernels

7 Space-Time Kernels

8 Learned Kernels

9 Designer Kernels

Translation Invariant Kernels

- A kernel is called translation invariant (or stationary in the statistics literature) if $K(\boldsymbol{x}+\boldsymbol{h}, \boldsymbol{z}+\boldsymbol{h}) = K(\boldsymbol{x}, \boldsymbol{z})$ for any $\boldsymbol{h} \in \mathbb{R}^d$. This means that K is a function of the difference of $\boldsymbol{x}$ and $\boldsymbol{z}$, i.e., it's of the form

$$K(\boldsymbol{x}, \boldsymbol{z}) = \widetilde{K}(\boldsymbol{x} - \boldsymbol{z}).$$

Translation Invariant Kernels

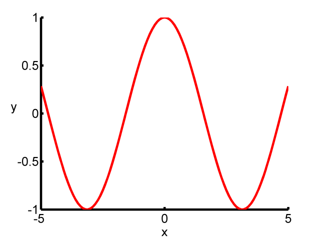
- A kernel is called translation invariant (or stationary in the statistics literature) if $K(\boldsymbol{x}+\boldsymbol{h}, \boldsymbol{z}+\boldsymbol{h}) = K(\boldsymbol{x}, \boldsymbol{z})$ for any $\boldsymbol{h} \in \mathbb{R}^d$. This means that K is a function of the difference of $\boldsymbol{x}$ and $\boldsymbol{z}$, i.e., it's of the form

$$K(\boldsymbol{x}, \boldsymbol{z}) = \widetilde{K}(\boldsymbol{x} - \boldsymbol{z}).$$

Example

Cosine kernel

$$K(x, z) = \cos(x - z)$$



- In the literature on integral equations, translation invariant kernels are often called convolution kernels.

- In the literature on integral equations, translation invariant kernels are often called convolution kernels.
- Discretized convolution kernels (i.e., matrices) find applications in image processing.

- In the literature on integral equations, translation invariant kernels are often called convolution kernels.
- Discretized convolution kernels (i.e., matrices) find applications in image processing.
- The Fourier transform is the ideal tool to analyze translation invariant kernels. This results in, e.g., Bochner's theorem.

- In the literature on integral equations, translation invariant kernels are often called convolution kernels.
- Discretized convolution kernels (i.e., matrices) find applications in image processing.
- The Fourier transform is the ideal tool to analyze translation invariant kernels. This results in, e.g., Bochner's theorem.
- Any nonnegative (infinite) linear combination of kernels of the form $K_n(x,z) = \cos(n(x-z))$ is positive definite and translation invariant on $\mathbb{R}$.

- In the literature on integral equations, translation invariant kernels are often called convolution kernels.
- Discretized convolution kernels (i.e., matrices) find applications in image processing.
- The Fourier transform is the ideal tool to analyze translation invariant kernels. This results in, e.g., Bochner's theorem.
- Any nonnegative (infinite) linear combination of kernels of the form $K_n(x,z) = \cos(n(x-z))$ is positive definite and translation invariant on $\mathbb{R}$.
  - E.g., periodic univariate splines can be represented with the kernel

$$K(x,z) = \sum_{n=1}^{\infty} \frac{2}{(2n\pi)^{2\beta}} \cos\left(2n\pi(x-z)\right)$$

whose RKHS is $H^{\beta}_{\text{per}}(0,1)$ (see [Wah90, Chapter 2]).

- In the literature on integral equations, translation invariant kernels are often called convolution kernels.
- Discretized convolution kernels (i.e., matrices) find applications in image processing.
- The Fourier transform is the ideal tool to analyze translation invariant kernels. This results in, e.g., Bochner's theorem.
- Any nonnegative (infinite) linear combination of kernels of the form $K_n(x, z) = \cos(n(x - z))$ is positive definite and translation invariant on $\mathbb{R}$.
  - E.g., periodic univariate splines can be represented with the kernel

$$K(x, z) = \sum_{n=1}^{\infty} \frac{2}{(2n\pi)^{2\beta}} \cos\left(2n\pi(x - z)\right)$$

    whose RKHS is $H^{\beta}_{\text{per}}(0, 1)$ (see [Wah90, Chapter 2]).
- To get a kernel in higher dimensions we can take a tensor product of one-dimensional translation invariant kernels, e.g.,

$$K(\boldsymbol{x}, \boldsymbol{z}) = \prod_{\ell=1}^{d} \sum_{n=0}^{\infty} \alpha_{n,\ell} K_n(x_\ell, z_\ell), \qquad \alpha_{n,\ell} \geq 0.$$

Outline

1. Radial Kernels
2. Translation Invariant Kernels
3. Series Kernels
4. General Anisotropic Kernels
5. Compactly Supported (Radial) Kernels
6. Multiscale Kernels
7. Space-Time Kernels
8. Learned Kernels
9. Designer Kernels

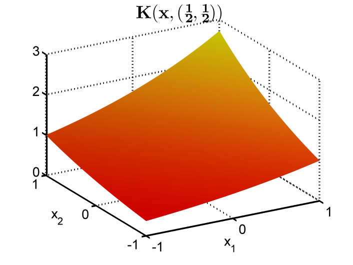
Power Series Kernels

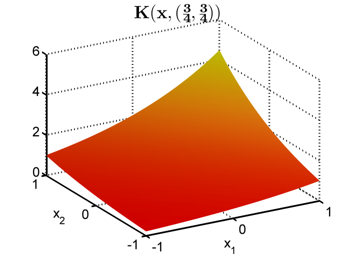
- Of the form [Zwi08]:

$$K(\boldsymbol{x},\boldsymbol{z}) = \sum_{\boldsymbol{\alpha}\in\mathbb{N}_0^d} w_{\boldsymbol{\alpha}} \frac{\boldsymbol{x}^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!}\frac{\boldsymbol{z}^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!}, \qquad \sum_{\boldsymbol{\alpha}\in\mathbb{N}_0^d} \frac{w_{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!^2} < \infty,$$

Example (Exponential kernel)

$$K(\boldsymbol{x},\boldsymbol{z}) = e^{\boldsymbol{x}\cdot\boldsymbol{z}} = \sum_{n=0}^{\infty} \frac{1}{n!}(\boldsymbol{x}\cdot\boldsymbol{z})^n = \sum_{\boldsymbol{\alpha}\in\mathbb{Z}^d} \frac{1}{|\boldsymbol{\alpha}|!}\binom{|\boldsymbol{\alpha}|}{\boldsymbol{\alpha}} \boldsymbol{x}^{\boldsymbol{\alpha}}\boldsymbol{z}^{\boldsymbol{\alpha}}$$





Example (Taylor series kernels [ZS13])

$$K(x,z) = \frac{1}{(1-z\overline{x})^2} = \sum_{n=0}^{\infty}(n+1)z^n\overline{x}^n, \qquad \text{(Bergman kernel)}$$

$$K(x,z) = \frac{1}{1-z\overline{x}} = \sum_{n=0}^{\infty} z^n\overline{x}^n, \qquad \text{(Hardy or Szegő kernel)}$$

$$K(x,z) = -\frac{\ln(1-z\overline{x})}{z\overline{x}} = \sum_{n=0}^{\infty}\frac{1}{n+1}z^n\overline{x}^n, \qquad \text{(Dirichlet kernel)}$$

Here $x, z \in \mathbb{D}$, the open complex unit disk, i.e., $\mathbb{D} = \{x \in \mathbb{C} : |x| < 1\}$.

- Native spaces:
  - Bergman space $B^2 = L^2(\mathbb{D})$, the space of analytic functions in $\mathbb{D}$ that are square summable with respect to planar Lebesgue measure.
  - Hardy space H^2, the space of analytic functions in $\mathbb{D}$ with square summable Taylor coefficients. $H^2 \subset B^2$.
  - Dirichlet space $\mathcal{D}$, the space of analytic functions in D whose derivatives are in B^2.

- Other examples of series kernels are
  - Fourier-type series such as the periodic spline kernels,

$$K(x,z) = \sum_{n=1}^{\infty} \frac{2}{(2n\pi)^{2\beta}} \cos\left(2n\pi(x-z)\right).$$

  - Kernels specified via their Mercer/Hilbert–Schmidt series such as

$$\begin{aligned} K(x,z) &= \sum_{n=1}^{\infty} \frac{8}{(2n-1)^2\pi^2} \sin\left((2n-1)\frac{\pi x}{2}\right) \sin\left((2n-1)\frac{\pi z}{2}\right) \\ &= \min(x,z). \end{aligned}$$

Outline

1. Radial Kernels
2. Translation Invariant Kernels
3. Series Kernels
4. General Anisotropic Kernels
5. Compactly Supported (Radial) Kernels
6. Multiscale Kernels
7. Space-Time Kernels
8. Learned Kernels
9. Designer Kernels

Dot Product Kernels

These kernels depend on $\boldsymbol{x}$ and $\boldsymbol{z}$ only through their dot product. They are also known as ridge functions (or zonal kernels if $\boldsymbol{x}, \boldsymbol{z} \in \mathbb{S}^2$).

Dot Product Kernels

These kernels depend on $\boldsymbol{x}$ and $\boldsymbol{z}$ only through their dot product. They are also known as ridge functions (or zonal kernels if $\boldsymbol{x}, \boldsymbol{z} \in \mathbb{S}^2$).

- Zonal kernels are of the form

$$K(\boldsymbol{x}, \boldsymbol{z}) = \tilde{\kappa}(\boldsymbol{x} \cdot \boldsymbol{z}), \quad \boldsymbol{x}, \boldsymbol{z} \in \mathbb{S}^2, \quad \tilde{\kappa} : [-1, 1] \to \mathbb{R}$$

Dot Product Kernels

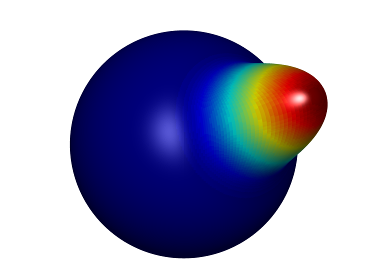
These kernels depend on $\boldsymbol{x}$ and $\boldsymbol{z}$ only through their dot product. They are also known as ridge functions (or zonal kernels if $\boldsymbol{x}, \boldsymbol{z} \in \mathbb{S}^2$).

- Zonal kernels are of the form

$$K(\boldsymbol{x}, \boldsymbol{z}) = \tilde{\kappa}(\boldsymbol{x} \cdot \boldsymbol{z}), \quad \boldsymbol{x}, \boldsymbol{z} \in \mathbb{S}^2, \quad \tilde{\kappa} : [-1, 1] \to \mathbb{R}$$

Example (Spherical Gaussian kernel)

$$K(\boldsymbol{x}, \boldsymbol{z}) = \tilde{\kappa}(\boldsymbol{x} \cdot \boldsymbol{z}) = \mathrm{e}^{-2\varepsilon(1-\boldsymbol{x}\cdot\boldsymbol{z})}, \quad \tilde{\kappa}(t) = \mathrm{e}^{-2\varepsilon(1-t)}$$



Example (Polynomial kernel)

$$K(\boldsymbol{x},\boldsymbol{z}) = \left(\varepsilon + \boldsymbol{x}^T\boldsymbol{z}\right)^{\beta}, \qquad \boldsymbol{x},\boldsymbol{z} \in \mathbb{R}^d$$

- Plays an important role in machine learning.
- It is positive definite for all $\varepsilon \geq 0$ and $\beta \in \mathbb{N}_0$.
- The special case $\varepsilon = 0$ and $\beta = 1$ is known as the linear kernel.

Example (Sigmoid kernel)

$$K(\boldsymbol{x},\boldsymbol{z}) = \tanh(1 + \varepsilon\boldsymbol{x}^T\boldsymbol{z}), \qquad \boldsymbol{x},\boldsymbol{z} \in \mathbb{R}^d$$

- Also popular in machine learning.
- But this kernel is **not** positive definite for any choice of ε.

Remark

- *Ridge functions are discussed, e.g., in [CL99, Chapter 22] or [Pin13].*
- *They first arose in the context of computerized tomography [LS75].*
- *Zonal functions on spheres $\mathbb{S}^d$ in $\mathbb{R}^{d+1}$ can be analyzed using Mercer series.*
    - *The expansion can be written in terms of Legendre or Gegenbauer polynomials (and ultimately spherical harmonics).*
    - *This was done in, e.g., [Men99, RS96, XC92] (see also [SS02, Section 4.6]).*

Tensor Product Kernels

Weighted tensor products of various univariate kernels also produce general anisotropic kernels.

Example (Product of the Brownian motion kernel)

$$K(\boldsymbol{x}, \boldsymbol{z}) = \prod_{\ell=1}^{d} \left(1 + \varepsilon_\ell \min(x_\ell, z_\ell)\right), \qquad \varepsilon_1 \geq \varepsilon_2 \geq \ldots \geq \varepsilon_d \geq 0,$$

where $\boldsymbol{x} = (x_1, \ldots, x_d)^T \in \mathbb{R}^d$.

- Neither radially nor translation invariant.
- Positive definite in $[0, 1]^d$.

Tensor Product Kernels

Weighted tensor products of various univariate kernels also produce general anisotropic kernels.

Example (Product of the Brownian motion kernel)

$$K(\boldsymbol{x}, \boldsymbol{z}) = \prod_{\ell=1}^{d} (1 + \varepsilon_\ell \min(x_\ell, z_\ell)), \qquad \varepsilon_1 \geq \varepsilon_2 \geq \ldots \geq \varepsilon_d \geq 0,$$

where $\boldsymbol{x} = (x_1, \ldots, x_d)^T \in \mathbb{R}^d$.

- Neither radially nor translation invariant.
- Positive definite in $[0, 1]^d$.

Remark

Such kernels play an important role in the theory of Monte-Carlo and quasi Monte-Carlo methods, where they are used to avoid the curse of dimensionality.

Remark

A related kernel is the kernel for fractional Brownian motion (see, e.g., [BTA04])

$$K(\boldsymbol{x},\boldsymbol{z}) = \frac{1}{2}\left(\|\boldsymbol{x}\|^{2\beta} + \|\boldsymbol{z}\|^{2\beta} - \|\boldsymbol{x}-\boldsymbol{z}\|^{2\beta}\right), \qquad \boldsymbol{x},\boldsymbol{z} \in \mathbb{R}^d.$$

However, this kernel is not a tensor product kernel.
For $\beta = \frac{1}{2}$ and $d = 1$ this simplifies to the standard Brownian motion kernel.

Remark

A related kernel is the kernel for fractional Brownian motion (see, e.g., [BTA04])

$$K(\boldsymbol{x},\boldsymbol{z}) = \frac{1}{2}\left(\|\boldsymbol{x}\|^{2\beta} + \|\boldsymbol{z}\|^{2\beta} - \|\boldsymbol{x}-\boldsymbol{z}\|^{2\beta}\right), \qquad \boldsymbol{x},\boldsymbol{z} \in \mathbb{R}^d.$$

However, this kernel is not a tensor product kernel.
For $\beta = \frac{1}{2}$ and $d = 1$ this simplifies to the standard Brownian motion kernel.

Remark

The linear covariance kernel is actually a radial kernel even though it is obtained by adding the kernels of two independent Brownian motions:

$$\begin{aligned} K(x,z) &= \min(x,z) + \min(1-x, 1-z) \\ &= \min(x,z) + 1 - \max(x,z) \\ &= 1 - |x-z|. \end{aligned}$$

Remark

A related kernel is the kernel for fractional Brownian motion (see, e.g., [BTA04])

$$K(\boldsymbol{x},\boldsymbol{z}) = \frac{1}{2}\left(\|\boldsymbol{x}\|^{2\beta} + \|\boldsymbol{z}\|^{2\beta} - \|\boldsymbol{x}-\boldsymbol{z}\|^{2\beta}\right), \qquad \boldsymbol{x},\boldsymbol{z} \in \mathbb{R}^d.$$

However, this kernel is not a tensor product kernel.
For $\beta = \frac{1}{2}$ and $d = 1$ this simplifies to the standard Brownian motion kernel.

Remark

The linear covariance kernel is actually a radial kernel even though it is obtained by adding the kernels of two independent Brownian motions:

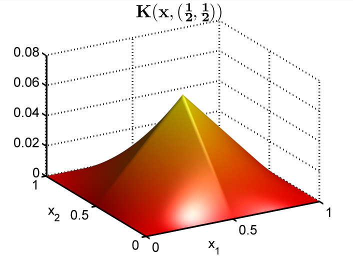
$$\begin{aligned} K(x,z) &= \min(x,z) + \min(1-x, 1-z) \\ &= \min(x,z) + 1 - \max(x,z) \\ &= 1 - |x-z|. \end{aligned}$$

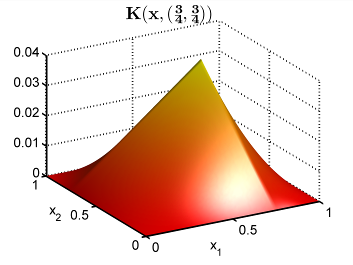
We can also view this as a positive definite modification of the (conditionally negative definite) norm kernel.

Example

Brownian bridge product kernel

$$K(\boldsymbol{x}, \boldsymbol{z}) = \prod_{\ell=1}^{d} (\min(x_\ell, z_\ell) - x_\ell z_\ell)$$





- Neither radially nor translation invariant.
- Positive definite in $[0, 1]^d$.

Outline

1. Radial Kernels
2. Translation Invariant Kernels
3. Series Kernels
4. General Anisotropic Kernels
5. Compactly Supported (Radial) Kernels
6. Multiscale Kernels
7. Space-Time Kernels
8. Learned Kernels
9. Designer Kernels

Compactly Supported (Radial) Kernels

- One of the benefits of using compactly supported kernels is that — with an appropriate scaling — they lead to sparse kernel matrices.
- We concentrate on the Wendland family.
- Other families have been introduced by Buhmann, Gneiting or Wu (see [Fas07, Chapter 11]), as well as Johnson [Joh12].
- We will not do much with compactly supported kernels in this class.
- These kernels are discussed in detail in [Fas07, Wen05].
- Notation:
  - We use $r = \|\boldsymbol{x} - \boldsymbol{z}\|$ to indicate we are working with radial kernels, i.e., $K(\boldsymbol{x}, \boldsymbol{z}) = \kappa(\|\boldsymbol{x} - \boldsymbol{z}\|)$.
  - Below, $\doteq$ denotes equality up to a constant factor.

Original Wendland kernels [Wen95]

The family of kernels $\kappa_{d,k}$ includes

$$\kappa_{d,0} \doteq (1-r)_+^{\ell}$$
$$\kappa_{d,1} \doteq (1-r)_+^{\ell+1}\left((\ell+1)r+1\right)$$
$$\kappa_{d,2} \doteq (1-r)_+^{\ell+2}\left(\frac{\ell^2+4\ell+3}{3}r^2+(\ell+2)r+1\right)$$
$$\kappa_{d,3} \doteq (1-r)_+^{\ell+3}\left(\frac{\ell^3+9\ell^2+23\ell+15}{15}r^3+\frac{6\ell^2+36\ell+45}{15}r^2+(\ell+3)r+1\right)$$

- d: $K_{d,k}$ strictly positive definite on $\mathbb{R}^d \times \mathbb{R}^d$
- k: smoothness index, i.e., $\kappa_{d,k} \in C^{2k}(\mathbb{R})$
- ℓ: auxiliary variable with value $\ell = \lfloor \frac{d}{2} + k + 1 \rfloor$

Original Wendland kernels [Wen95]

The family of kernels $\kappa_{d,k}$ includes

$$\kappa_{d,0} \doteq (1-r)_+^{\ell}$$

$$\kappa_{d,1} \doteq (1-r)_+^{\ell+1}\left((\ell+1)r+1\right)$$

$$\kappa_{d,2} \doteq (1-r)_+^{\ell+2}\left(\frac{\ell^2+4\ell+3}{3}r^2+(\ell+2)r+1\right)$$

$$\kappa_{d,3} \doteq (1-r)_+^{\ell+3}\left(\frac{\ell^3+9\ell^2+23\ell+15}{15}r^3+\frac{6\ell^2+36\ell+45}{15}r^2+(\ell+3)r+1\right)$$

- d: $K_{d,k}$ strictly positive definite on $\mathbb{R}^d \times \mathbb{R}^d$
- k: smoothness index, i.e., $\kappa_{d,k} \in C^{2k}(\mathbb{R})$
- ℓ: auxiliary variable with value $\ell = \lfloor \frac{d}{2} + k + 1 \rfloor$

Associated reproducing kernel Hilbert space:

$$\mathcal{H}_{K_{d,k}}(\Omega) = H^{k+(d+1)/2}(\mathbb{R}^d) \quad \text{(classical Sobolev space)}$$

Remark

- *The construction of [Wen95] with RKHS $H^{k+(d+1)/2}(\mathbb{R}^d)$ does not allow for Sobolev spaces of integer order when d is even.*
- *This, it appears that some functions are missing.*

Remark

- *The construction of [Wen95] with RKHS $H^{k+(d+1)/2}(\mathbb{R}^d)$ does not allow for Sobolev spaces of integer order when d is even.*
- *This, it appears that some functions are missing.*
- *This gap was filled when Schaback [Sch11] derived the so-called "missing" Wendland functions (see also [Hub12, CH14]).*

"Missing" Wendland kernels

Typical examples of the family $\kappa_{\ell,k}$ are (see [CSW14, Hub12, Sch11])

$$\kappa_{2,\frac{1}{2}}(r) \doteq (1+2r^2)\sqrt{1-r^2} + 3r^2 \log\left(\frac{r}{1+\sqrt{1-r^2}}\right)$$

$$\kappa_{3,\frac{3}{2}}(r) \doteq \left(1 - 7r^2 - \frac{81}{4}r^4\right)\sqrt{1-r^2} - \frac{15}{4}r^4(6+r^2)\log\left(\frac{r}{1+\sqrt{1-r^2}}\right)$$

These formulas hold for $r \in [0,1]$ and the functions are zero otherwise.

- ℓ: Sobolev smoothness, as before $\ell = \lfloor \frac{d}{2} + k + 1 \rfloor$
- k: half-integer, connected to smoothness of $\kappa_{\ell,k}$
- d: space dimension, but $K_{2,\frac{1}{2}}$ and $K_{3,\frac{3}{2}}$ both strictly positive definite on $\mathbb{R}^2 \times \mathbb{R}^2$

"Missing" Wendland kernels

Typical examples of the family $\kappa_{\ell,k}$ are (see [CSW14, Hub12, Sch11])

$$\kappa_{2,\frac{1}{2}}(r) \doteq (1+2r^2)\sqrt{1-r^2} + 3r^2 \log\left(\frac{r}{1+\sqrt{1-r^2}}\right)$$

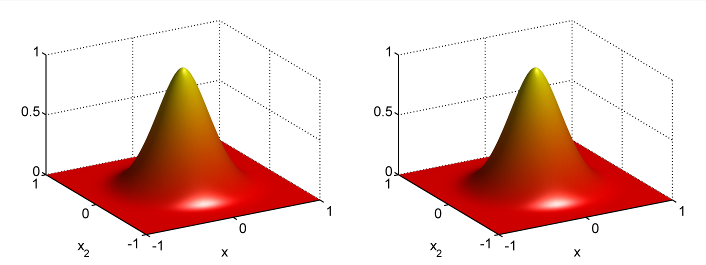
$$\kappa_{3,\frac{3}{2}}(r) \doteq \left(1-7r^2-\frac{81}{4}r^4\right)\sqrt{1-r^2} - \frac{15}{4}r^4(6+r^2)\log\left(\frac{r}{1+\sqrt{1-r^2}}\right)$$

These formulas hold for $r \in [0,1]$ and the functions are zero otherwise.

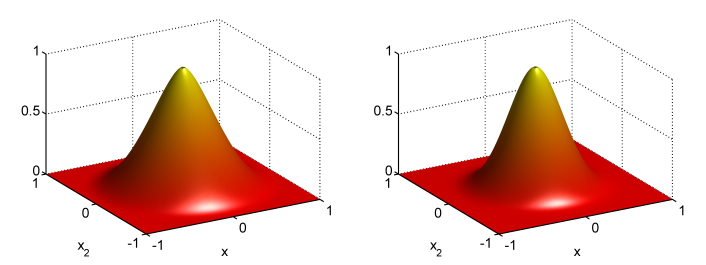
- ℓ: Sobolev smoothness, as before $\ell = \lfloor \frac{d}{2} + k + 1 \rfloor$
- k: half-integer, connected to smoothness of $\kappa_{\ell,k}$
- d: space dimension, but $K_{2,\frac{1}{2}}$ and $K_{3,\frac{3}{2}}$ both strictly positive definite on $\mathbb{R}^2 \times \mathbb{R}^2$

Associated reproducing kernel Hilbert space:

$$\mathcal{H}_{K_{2,\frac{1}{2}}}(\Omega) = H^2(\mathbb{R}^2), \quad \mathcal{H}_{K_{3,\frac{3}{2}}}(\Omega) = H^3(\mathbb{R}^2)$$



"Original" Wendland kernels: $\kappa_{3,1}$ (left, C^2) and $\kappa_{3,2}$ (right, C^4)



"Missing" Wendland kernels: $\kappa_{2,1/2}$ (left, C^1) and $\kappa_{3,3/2}$ (right, C^3)

Remark

- *Schaback [Sch11] derived the "missing" Wendland functions using fractional derivatives.*
- *In contrast to the "original" Wendland functions, these new functions are no longer polynomials on their support.*
- *Hubbert [Hub12] gives closed form representations of both the "original" and the "missing" Wendland functions in terms of associated Legendre functions (of the first and second kinds).*
- *Chernih [CSW14] showed that, as their smoothness increases, all (appropriately normalized) Wendland functions converge to Gaussians.*

Outline

1 Radial Kernels

2 Translation Invariant Kernels

3 Series Kernels

4 General Anisotropic Kernels

5 Compactly Supported (Radial) Kernels

6 Multiscale Kernels

7 Space-Time Kernels

8 Learned Kernels

9 Designer Kernels

General multiscale kernels [Opf06] are of the form

$$K(\boldsymbol{x},\boldsymbol{z}) = \sum_{j\geq 0} w_j K_j(\boldsymbol{x},\boldsymbol{z}) = \sum_{j\geq 0} w_j \sum_{\boldsymbol{k}\in\mathbb{Z}^d} \phi(2^j\boldsymbol{x}-\boldsymbol{k})\phi(2^j\boldsymbol{z}-\boldsymbol{k}),$$

with $w_j > 0$ and ϕ a compactly supported (possibly refinable) function whose shifts (at level j) produces the single-scale kernel K_j.

General multiscale kernels [Opf06] are of the form

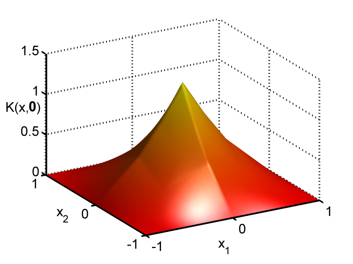
$$K(\boldsymbol{x},\boldsymbol{z}) = \sum_{j\geq 0} w_j K_j(\boldsymbol{x},\boldsymbol{z}) = \sum_{j\geq 0} w_j \sum_{\boldsymbol{k}\in\mathbb{Z}^d} \phi(2^j\boldsymbol{x}-\boldsymbol{k})\phi(2^j\boldsymbol{z}-\boldsymbol{k}),$$

with $w_j > 0$ and ϕ a compactly supported (possibly refinable) function whose shifts (at level j) produces the single-scale kernel K_j.

Example (Multiscale piecewise linear kernel)

$$K(\boldsymbol{x},\boldsymbol{z}) = \sum_{j=0}^{3} 2^{-2j} \sum_{\boldsymbol{k}\in\mathbb{Z}^2} \phi(2^j\boldsymbol{x}-\boldsymbol{k})\varphi(2^j\boldsymbol{z}-\boldsymbol{k})$$

with $\phi(\boldsymbol{x}) = \prod_{\ell=1}^{d}(1-x_\ell)_+$



- [Opf06] described the RKHSs of these kernels.
- He used them in wavelet-like applications such as image compression.
- Very little work has been performed otherwise with these kernels.

Outline

1. Radial Kernels
2. Translation Invariant Kernels
3. Series Kernels
4. General Anisotropic Kernels
5. Compactly Supported (Radial) Kernels
6. Multiscale Kernels
7. **Space-Time Kernels**
8. Learned Kernels
9. Designer Kernels

Space-Time Kernels

- Many problems have both a spatial as well as a temporal component, so the idea to construct and use space-time kernel is natural.

Space-Time Kernels

- Many problems have both a spatial as well as a temporal component, so the idea to construct and use space-time kernel is natural.
- The most common approach is to use a tensor product kernel that factors into a spatial and a temporal component.

Space-Time Kernels

- Many problems have both a spatial as well as a temporal component, so the idea to construct and use space-time kernel is natural.
- The most common approach is to use a tensor product kernel that factors into a spatial and a temporal component.
- But sometimes the data does not seem to allow such separability since it contains spatio-temporal interactions which a separable model would not be able to pick up on (see, e.g., [CH99, GGG07]).

In the RBF literature these kernels are rare.

Li & Mao [LM11] solved an ill-posed inverse heat conduction problem using an anisotropic IMQ kernel

$$K((\boldsymbol{x},s),(\boldsymbol{z},t)) = \frac{1}{\sqrt{1+\varepsilon^2\|\boldsymbol{x}-\boldsymbol{z}\|^2+\gamma^2(s-t)^2}}, \ \boldsymbol{x},\boldsymbol{z}\in\mathbb{R}^d, \ s,t\in\mathbb{R},$$

where $d = 1, 2$.

The spatial coordinates are augmented by an additional time coordinate, but note the use of two different scale parameters.

In the statistics literature space-time kernels are more common.

- Stein uses kernels that are translation invariant in both space and time, i.e., of the form $K((\boldsymbol{x}, s), (\boldsymbol{z}, t)) = \widetilde{K}(\boldsymbol{x} - \boldsymbol{z}, s - t)$. He derives
  - generalizations of Matérn kernels [Ste05], and
  - power law covariance functions (which generalize polyharmonic splines) [Ste13].

In the statistics literature space-time kernels are more common.

- Stein uses kernels that are translation invariant in both space and time, i.e., of the form $K((\boldsymbol{x},s),(\boldsymbol{z},t)) = \widetilde{K}(\boldsymbol{x}-\boldsymbol{z}, s-t)$. He derives
  - generalizations of Matérn kernels [Ste05], and
  - power law covariance functions (which generalize polyharmonic splines) [Ste13].
- Porcu [PMB07] allows for spatial anisotropy with temporal translation invariance leading to kernels such as, e.g.,

$$K((\boldsymbol{x},s),(\boldsymbol{z},t)) = \frac{\exp\left(-\frac{|s-t|^2}{K_{\text{space}}(\boldsymbol{x},\boldsymbol{z})}\right)}{\sqrt{K_{\text{space}}(\boldsymbol{x},\boldsymbol{z})}}, \qquad \boldsymbol{x},\boldsymbol{z} \in \mathbb{R}^d,\ s,t \in \mathbb{R},$$

where $K_{\text{space}}(\boldsymbol{x},\boldsymbol{z}) = \log\left(2 + \frac{1}{2}\left(2\varepsilon(\boldsymbol{x}+\boldsymbol{z}) - \frac{1+\varepsilon(\boldsymbol{x}+\boldsymbol{z})}{1+\varepsilon(\boldsymbol{x}-\boldsymbol{z})}\right)\right)$.

Outline

1 Radial Kernels
2 Translation Invariant Kernels
3 Series Kernels
4 General Anisotropic Kernels
5 Compactly Supported (Radial) Kernels
6 Multiscale Kernels
7 Space-Time Kernels
8 Learned Kernels
9 Designer Kernels

Learned Kernels

In the machine learning literature one finds kernels that are learned directly from the data.

- Micchelli and Pontil [MP05] suggest learning the kernel via regularization techniques.
  - They start with a — possibly uncountable — set $\mathbb{K}$ of kernels and then determine the optimal kernel for a given set of N pieces of data $\{(\boldsymbol{x}_i, y_i) : i = 1, \ldots, N\}$ as a finite convex combination of kernels from $\mathbb{K}$.
  - The set $\mathbb{K}$ is assumed to be compact and convex, and then the optimal learned kernel is obtained by solving a convex optimization problem.
  - Once the kernel K has been found, the kernel approximation is obtained by solving a finite-dimensional convex optimization problem.

Learned Kernels

In the machine learning literature one finds kernels that are learned directly from the data.

- Micchelli and Pontil [MP05] suggest learning the kernel via regularization techniques.
  - They start with a — possibly uncountable — set $\mathbb{K}$ of kernels and then determine the optimal kernel for a given set of N pieces of data $\{(\boldsymbol{x}_i, y_i) : i = 1, \ldots, N\}$ as a finite convex combination of kernels from $\mathbb{K}$.
  - The set $\mathbb{K}$ is assumed to be compact and convex, and then the optimal learned kernel is obtained by solving a convex optimization problem.
  - Once the kernel K has been found, the kernel approximation is obtained by solving a finite-dimensional convex optimization problem.
- Lanckriet [LCB$^+$04] suggests that the kernel matrix (instead of the actual kernel) can be learned from the given data by employing semi-definite programming techniques.

Outline

1. Radial Kernels
2. Translation Invariant Kernels
3. Series Kernels
4. General Anisotropic Kernels
5. Compactly Supported (Radial) Kernels
6. Multiscale Kernels
7. Space-Time Kernels
8. Learned Kernels
9. Designer Kernels

Designer Kernels

Some ideas to obtain specially designed custom kernels (or designer kernels):

- Use the basic properties of kernels discussed in Chapter 2, such as adding, multiplying and taking positive linear combinations of kernels.
- Use ideas such as composition with multiply or completely monotone functions (see [Fas07]) to construct new radial kernels.
- Build a kernel via Mercer's theorem by combining an appropriate sequence of "eigenvalues" λ_n with a given set of orthogonal functions.
    - This may mean that the closed form of the kernel may not be known in this case.
    - Good example: iterated Brownian bridge kernels (see later).

References I

[Bax06] B. J. C. Baxter, *Scaling radial basis functions via Euclidean distance matrices*, Computers & Mathematics with Applications **51** (2006), no. 8, 1163–1170.

[BDL10] R. K. Beatson, O. Davidov, and J. Levesley, *Error bounds for anisotropic RBF interpolation.*, Journal of Approximation Theory **162** (2010), 512–527.

[BLRS14] Mira Bozzini, Licia Lenarduzzi, Milvia Rossini, and Robert Schaback, *Interpolation with variably scaled kernels*, IMA Journal of Numerical Analysis (2014).

[BTA04] A. Berlinet and C. Thomas-Agnan, *Reproducing Kernel Hilbert Spaces in Probability and Statistics*, Kluwer Academic Publishers, Dordrecht, 2004.

[CBM+03] J. C Carr, R. K Beatson, B. C McCallum, W. R Fright, T. J McLennan, and T. J Mitchell, *Smooth surface reconstruction from noisy range data*, Proceedings of the 1st international conference on Computer graphics and interactive techniques in Australasia and South East Asia (New York), GRAPHITE '03, ACM, 2003, pp. 119–126.

References II

[CH99] Noel Cressie and Hsin-cheng Huang, *Classes of nonseparable, spatio-temporal stationary covariance functions*, Journal of the American Statistical Association **94** (1999), 1330–1340.

[CH14] Andrew Chernih and Simon Hubbert, *Closed form representations and properties of the generalised Wendland functions*, Journal of Approximation Theory **177** (2014), 17–33.

[CL99] E. W. Cheney and W. A. Light, *A Course in Approximation Theory*, Brooks/Cole (Pacific Grove, CA), 1999.

[CLMM06] G. Casciola, D. Lazzaro, L. B. Montefusco, and S. Morigi, *Shape preserving surface reconstruction using locally anisotropic radial basis function interpolants*, Computers & Mathematics with Applications **51** (2006), no. 8, 1185–1198.

[CSW14] A. Chernih, I. H. Sloan, and R. S. Womersley, *Wendland functions with increasing smoothness converge to a Gaussian*, Advances in Computational Mathematics **40** (2014), no. 1, 185–200.

References III

[Fas07] G. E. Fasshauer, *Meshfree Approximation Methods with* MATLAB, Interdisciplinary Mathematical Sciences, vol. 6, World Scientific Publishing Co., Singapore, 2007.

[FHW12a] G. E. Fasshauer, F. J. Hickernell, and H. Woźniakowski, *On dimension-independent rates of convergence for function approximation with Gaussian kernels*, SIAM J. Numer. Anal. **50** (2012), no. 1, 247–271.

[FHW12b] G. E. Fasshauer, Fred J. Hickernell, and H. Woźniakowski, *Average case approximation: convergence and tractability of Gaussian kernels*, Monte Carlo and Quasi-Monte Carlo Methods 2010 (H. Woźniakowski and L. Plaskota, eds.), Springer Proceedings in Mathematics and Statistics, no. 23, Springer, Berlin, 2012, pp. 309—324.

[FLW06] B. Fornberg, E. Larsson, and G. Wright, *A new class of oscillatory radial basis functions*, Computers & Mathematics with Applications **51** (2006), no. 8, 1209–1222.

[Gen02] Marc G. Genton, *Classes of kernels for machine learning: A statistics perspective*, J. Mach. Learn. Res. **2** (2002), 299–312.

References IV

[GGG07] Tilmann Gneiting, Marc G. Genton, and Peter Guttorp, *Geostatistical space-time models, stationarity, separability and full symmetry*, Statistics of Spatio-Temporal Systems (B. Finkenstaedt, L. Held, and V. Isham, eds.), Chapman & Hall/CRC Press, 2007, pp. 151–175.

[Hub12] Simon Hubbert, *Closed form representations for a class of compactly supported radial basis functions*, Advances in Computational Mathematics **36** (2012), no. 1, 115–136.

[Joh12] Michael J. Johnson, *Compactly supported, piecewise polyharmonic radial functions with prescribed regularity*, Constructive Approximation **35** (2012), no. 2, 201–223.

[LCB$^+$04] Gert R. G. Lanckriet, Nello Cristianini, Peter Bartlett, Laurent El Ghaoui, and Michael I. Jordan, *Learning the kernel matrix with semidefinite programming*, Journal of Machine Learning Research **5** (2004), 27–72.

[LM11] Z. Li and X.-Z. Mao, *Global space-time multiquadric method for inverse heat conduction problem*, International Journal for Numerical Methods in Engineering **85** (2011), no. 3, 355–379.

References V

[LS75] B. F. Logan and L. A. Shepp, *Optimal reconstruction of a function from its projections*, Duke Mathematical Journal **42** (1975), no. 4, 645–659.

[Men99] V. A. Menegatto, *Strict positive definiteness on spheres*, Analysis **19** (1999), no. 3, 217—233.

[MP05] Charles A. Micchelli and Massimiliano Pontil, *Learning the kernel function via regularization*, J. Mach. Learn. Res. **6** (2005), 1099–1125.

[NW08] E. Novak and H. Woźniakowski, *Tractability of Multivariate Problems Volume 1: Linear Information*, EMS Tracts in Mathematics, no. 6, European Mathematical Society, 2008.

[Opf06] R. Opfer, *Multiscale kernels*, Advances in Computational Mathematics **25** (2006), no. 4, 357–380.

[Pin13] Allan Pinkus, *On ridge functions*, Azerbaijan Journal of Mathematics **3** (2013), no. 2.

References VI

[PMB07] E. Porcu, J. Mateu, and M. Bevilacqua, *Covariance functions that are stationary or nonstationary in space and stationary in time*, Statistica Neerlandica **61** (2007), no. 3, 358–382.

[RS96] A. Ron and X. Sun, *Strictly positive definite functions on spheres*, Math. Comp. **65** (1996), no. 216, 1513–1530.

[Sch11] Robert Schaback, *The missing Wendland functions*, Advances in Computational Mathematics **34** (2011), no. 1, 67–81.

[SS02] B. Schölkopf and A. J. Smola, *Learning with Kernels: Support Vector Machines, Regularization, Optimization, and Beyond*, The MIT Press, 2002.

[Ste05] Michael L Stein, *Space-time covariance functions*, Journal of the American Statistical Association **100** (2005), no. 469, 310–321.

[Ste13] Michael L. Stein, *On a class of space-time intrinsic random functions*, Bernoulli **19** (2013), no. 2, 387–408.

References VII

[Wah90] Grace Wahba, *Spline Models for Observational Data*, SIAM, Philadelphia, 1990.

[Wen95] H. Wendland, *Piecewise polynomial, positive definite and compactly supported radial functions of minimal degree*, Advances in Computational Mathematics **4** (1995), no. 1, 389–396.

[Wen05] ______, *Scattered Data Approximation*, Cambridge Monographs on Applied and Computational Mathematics, vol. 17, Cambridge University Press, 2005.

[XC92] Y. Xu and E. W. Cheney, *Strictly positive definite functions on spheres*, Proc. Amer. Math. Soc. **116** (1992), 977–981.

[ZS13] Barbara Zwicknagl and Robert Schaback, *Interpolation and approximation in Taylor spaces*, Journal of Approximation Theory **171** (2013), 65–83.

[Zwi08] B. Zwicknagl, *Power series kernels*, Constructive Approximation **29** (2008), no. 1, 61–84.