Radial Basis Functions III

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Radial Function in $\mathbb{R}^s$

Definition

Let $s \in \mathbb{N}$ and $\| \ \|$ a norm on $\mathbb{R}^s$. A function $\Phi : \mathbb{R}^s \to \mathbb{R}$ is called radial if

$$\Phi(\mathbf{x}) = \varphi(\|\mathbf{x}\|), \quad \mathbf{x} \in \mathbb{R}^s,$$

for some univariate function $\varphi : [0, \infty) \to \mathbb{R}$.

- The norm is often the Euclidian norm $\| \ \|_2$.
- $\| \ \| = \| \ \|_2$ when nothing else is said.
- Radial: $\Phi(\mathbf{x}) = \varphi(r)$ for all $\mathbf{x}$ with $\|\mathbf{x}\| = r$.

Examples $\Phi(\mathbf{x}) = \varphi(\|\mathbf{x}\|)$

$\varepsilon \in \mathbb{R}$, $\varepsilon \neq 0$

- **Gauss** $\varphi(r) = e^{-\varepsilon^2 r^2}$,
- **distance** $\varphi(r) = r$,
- **power** $\varphi(r) = r^{2m+1}$, $m \geq 0$,
- **thin plate spline** $\varphi(r) = r^2 \log r$
- **multiquadric** $\varphi(r) = \sqrt{1 + (\varepsilon r)^2}$,
- **inverse multiquadric** $\varphi(r) = 1/\sqrt{1 + (\varepsilon r)^2}$,
- **Wendland's** C^0 **compactly supported** $\varphi(r) = (1 - r)_+^2$
- **Wendland's** C^2 **compactly supported** $\varphi(r) = (1 - r)_+^4(4r + 1)$

RBF interpolation in $\mathbb{R}^s$ with polynomial precision

Given

- Distinct points $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathbb{R}^s$.
- Ordinate-values $f_j = f(\mathbf{x}_j)$ representing an unknown function f.
- A radial function $\Phi : \mathbb{R}^s \to \mathbb{R}$ given by $\Phi(\mathbf{x}) = \varphi(\|\mathbf{x}\|)$
- A basis $q_1, \ldots, q_M$ of $\Pi_m(\mathbb{R}^s)$ (for example the monomials)

Find

- $\mathbf{c} = [c_1, \ldots, c_N]$ and $\mathbf{d} = [d_1, \ldots, d_M]$ such that
- $P_f(\mathbf{x}) := \sum_{k=1}^{N} c_k \Phi(\mathbf{x} - \mathbf{x}_k) + \sum_{k=1}^{M} d_k q_k(\mathbf{x})$ satisfies

$$\begin{aligned} P_f(\mathbf{x}_j) = \sum_{k=1}^{N} c_k \Phi(\mathbf{x}_j - \mathbf{x}_k) + \sum_{k=1}^{M} d_k q_k(\mathbf{x}_j) &= f_j, \quad j = 1, \ldots, N \\ \sum_{k=1}^{N} c_k q_j(\mathbf{x}_k) &= 0, \quad j = 1, \ldots, M. \end{aligned}$$

- Note that $P_f = f$ for all $f \in \Pi_m(\mathbb{R}^s)$

Linear system

- $$\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{0} \end{bmatrix},$$
- $\mathbf{A} = [\Phi(\mathbf{x}_j - \mathbf{x}_k)] \in \mathbb{R}^{N,N}, \ \mathbf{B} = [q_j(\mathbf{x}_k)] \in \mathbb{R}^{M,N}$.
- $N + M$ linear equations in $N + M$ unknowns.
- Symmetric coefficient matrix.
- Positive definite? Nonsingular?

Positive definite on a subspace

Definition

Suppose $\mathbf{A} \in \mathbb{R}^{N,N}$ and $\mathcal{S}$ a subspace of $\mathbb{R}^N$. We say that $\mathbf{A}$ is positive definite on $\mathcal{S}$ if $\mathbf{A}^T = \mathbf{A}$ and $\mathbf{c}^T\mathbf{A}\mathbf{c} > 0$ for all nonzero $\mathbf{c} \in \mathcal{S}$.

- If $\mathbf{A}$ is positive definite on $\mathcal{S} = \ker(\mathbf{B}) := \{\mathbf{c} \in \mathbb{R}^N : \mathbf{B}\mathbf{c} = \mathbf{0}\}$ and $\mathbf{B} \in \mathbb{R}^{M,N}$ has linearly independent rows then the block matrix

$$\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix}$$

  is nonsingular.
- Suppose $\mathcal{S}, \mathcal{T}$ are subspaces of $\mathbb{R}^N$ with $\mathcal{S} \subset \mathcal{T}$. If $\mathbf{A}$ is positive definite on $\mathcal{S}$ then $\mathbf{A}$ is positive definite on $\mathcal{T}$.

$\mathbf{B}$ full rank?

- Definition
  We say that a set of points $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{R}^s$ is m-unisolvent if $p \in \Pi_m(\mathbb{R}^s)$ and $p(\mathbf{x}_k) = 0$ for $k = 1, \ldots, N$ implies $p = 0$.

- Lemma
  Let $\mathbf{B} = [q_j(\mathbf{x}_k)] \in \mathbb{R}^{M,N}$, where $N \geq M$, $q_1, \ldots, q_M$ is a basis for $\Pi_m(\mathbb{R}^s)$, and $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{R}^s$ are distinct points in $\mathbb{R}^s$. Then $\mathbf{B}$ has linearly independent rows if and only if $\mathbf{X}$ is m-unisolvent.
  - **Proof**: We have $\mathbf{a}^T\mathbf{B} = [p(\mathbf{x}_1), \ldots, p(\mathbf{x}_N)]$ where $p(\mathbf{x}) = \sum a_j q_j(\mathbf{x})$. Thus $\mathbf{a}^T\mathbf{B} = \mathbf{0} \Rightarrow \mathbf{a} = \mathbf{0}$ if and only if $p(\mathbf{x}_k) = 0 \quad k = 1, \ldots, N \Rightarrow p = 0$.

Non-singularity via Fourier Transform

Definition

For a function $f \in L_1(\mathbb{R}^s)$ we define the (symmetric) Fourier transform of f by

$$\hat{f}(\boldsymbol{\omega}) := \frac{1}{(2\pi)^{s/2}} \int_{\mathbb{R}^s} f(\mathbf{x}) e^{-i\boldsymbol{\omega}\cdot\mathbf{x}} d\mathbf{x}, \quad \boldsymbol{\omega} \in \mathbb{R}^s. \tag{1}$$

and the inverse Fourier transform

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{s/2}} \int_{\mathbb{R}^s} \hat{f}(\boldsymbol{\omega}) e^{i\boldsymbol{\omega}\cdot\mathbf{x}} d\boldsymbol{\omega}, \quad \mathbf{x} \in \mathbb{R}^s. \tag{2}$$

Non-negative Fourier transform

Theorem

Let $\Phi(\mathbf{x}) = \varphi(\|\mathbf{x}\|)$ be a radial function with nonnegative Fourier transform not identically zero. For any distinct points $\mathbf{x}_1, \ldots, \mathbf{x}_N$ the matrix

$$\mathbf{A} := [\varphi(\|\mathbf{x}_j - \mathbf{x}_k\|)] \in \mathbb{R}^{N,N},$$

is positive definite.

The Gauss Kernel

Theorem

Suppose that $\mathbf{x}_1, \ldots, \mathbf{x}_N$, $N \in \mathbb{N}$, *are distinct points in* $\mathbb{R}^s$, $s \in \mathbb{N}$. *Then the matrix*

$$\mathbf{A} := [e^{-\varepsilon \|\mathbf{x}_j - \mathbf{x}_k\|_2^2}] \in \mathbb{R}^{N,N}, \quad \varepsilon > 0$$

is positive definite.

Proof The Fourier transform can be calculated as

$$\Phi(\mathbf{x}) := e^{-\varepsilon^2 \|\mathbf{x}\|^2} \Rightarrow \hat{\Phi}(\boldsymbol{\omega}) := e^{-\|\boldsymbol{\omega}\|^2/(4\varepsilon^2)} \geq 0.$$

Thus **A** is positive definite.

Discussion

- The Fourier transform can be used for Gaussian- and compactly supported RBF's. But,
- The distance function and thin plate and other examples are not integrable so do not have a Fourier transform
- Can use nonnegativity of the generalized Fourier transform.
- Can use complete monmotonicity.

Completely monotone functions

Definition

A function $g \in C^\infty(0,\infty)$ that satisfies

$$(-1)^\ell g^{(\ell)}(r) \geq 0, \quad r > 0, \quad \ell = 0, 1, 2, \ldots$$

is called completely monotone on $(0,\infty)$. If in addition $g \in C[0,\infty)$ then g is said to be completely monotone on $[0,\infty)$.

Examples:

- $g(r) = e^{-\varepsilon r}$, $\varepsilon \geq 0$, $r \geq 0$
- $g(r) = r^{-1/2}$, $r > 0$
- $g(r) = \int_0^\infty w(x) e^{-xr} dx, \quad r > 0$, where w is the Laplace transform of a piecewise continuous, nonnegative, and nonzero function.

The main Theorem

Theorem

Let $\varphi \in C[0,\infty)$ and $\psi := \varphi(\sqrt{\cdot}) \in C^\infty(0,\infty)$ Suppose for a nonnegative integer m that the derivative $\psi^{(m+1)}$ is the Laplace transform of a function w that is piecewise continuous, nonnegative, and nonzero on $(0,\infty)$, i. e.,

$$\psi^{(m+1)}(r) = \int_0^\infty w(x) e^{-xr} dx, \quad r > 0.$$

Let $\mathbf{A} := [\Phi(\mathbf{x}_j - \mathbf{x}_k)] \in \mathbb{R}^{N,N}$, where $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ are distinct points in $\mathbb{R}^s$. Then $(-1)^{m+1}\mathbf{A}$, is positive definite on the subspace
$\mathcal{S}_m(\mathbf{X}) := \{\mathbf{c} \in \mathbb{R}^N : \sum_{k=1}^N c_k p(\mathbf{x}_k) = 0,\ p \in \Pi_m(\mathbb{R}^s)\}.$

Thin Plate

- $\varphi(r) = r^2 \log r$, $\psi(r) = \frac{1}{2} r \log r$.
- $\psi''(r) = \frac{1}{2r}$ is completely monotone
- $\psi''(r) = \frac{1}{2} \int_0^\infty e^{-xr} dx$, $w(x) = \frac{1}{2}$.
- $m = 1$, $\mathbf{A}$ is positive definite on $\mathcal{S}_1(\mathbf{X})$
- Interpolation problem with reproduction of linear polynomials non-singular for all $s \geq 1, N \geq 2$, and any distinct $\mathbf{x}_1, \ldots, \mathbf{x}_N$ in $\mathbb{R}^s$ that do not lie on a straight line.

Power

- $\varphi(r) = r^{2m+1}$, $\psi(r) = r^{m+1/2}$, $m \geq 0$.
- $\psi^{(m+1)}(r) = \text{const}\, r^{-1/2}$ is completely monotone
- $\psi^{(m+1)}(r) = \text{const} \int_0^\infty \frac{1}{\sqrt{\pi x}} e^{-xr} dx$.
- $(-1)^{m+1}\mathbf{A}$ is positive definite on $\mathcal{S}_m(\mathbf{X})$.
- Cubic: $m = 1$, $\mathbf{A}$ is positive definite on $\mathcal{S}_1(\mathbf{X})$
- Interpolation problem with reproduction of linear polynomials non-singular for all $s \geq 1, N \geq 2$, and any distinct $\mathbf{x}_1, \ldots, \mathbf{x}_N$ in $\mathbb{R}^s$ that do not lie on a straight line.

A Lemma

$$\mathbf{c}^T[\|\mathbf{x}_j - \mathbf{x}_k\|^{2\ell}]\mathbf{c} = 0,\ \mathbf{c} \in \mathcal{S}_m(\mathbf{X}),\ 0 \le \ell \le m.$$

This was proved last time.

"Proof" of Main Theorem

- Integrating we find $\psi^{(m)}(r) = \int_0^\infty w(x)e^{-xr}x^{-1}dx + a_m$, where a_m is a constant. and $\psi^{(m-1)}(r) = \int_0^\infty w(x)e^{-xr}x^{-2}dx + a_m r + a_{m-1}$, where a_{m-1} is another constant.
- continuing we find $\psi(r) = \int_0^\infty w(x)e^{-xr}x^{-m-1}dx + q(r)$, where $q(r) = a_m r^m + \cdots + a_0$ is a polynomial of degree $\leq m$.
- Assuming that the integral exists we find

$$
\begin{aligned}
&(-1)^{m+1}\sum_{j,k} c_j c_k \psi(\|\mathbf{x}_j - \mathbf{x}_k\|^2) \\
=&(-1)^{m+1}\sum_{j,k} c_j c_k \int_0^\infty w(x)e^{-x\|\mathbf{x}_j-\mathbf{x}_k\|^2}x^{-m-1}dx \\
&+ (-1)^{m+1}\sum_{j,k} c_j c_k q(\|\mathbf{x}_j - \mathbf{x}_k\|^2)
\end{aligned}
$$

"Proof" continued

- By lemma
- $\sum_{j,k} c_j c_k q(\|\mathbf{x}_j - \mathbf{x}_k\|^2) = \sum_{\ell=0}^{m} a_\ell \sum_{j,k} c_j c_k \|\mathbf{x}_j - \mathbf{x}_k\|^{2\ell} = 0$
- $(-1)^{m+1}\mathbf{c}^T\mathbf{A}\mathbf{c} = \int_0^\infty \frac{w(x)}{x^{m+1}}\Big(\sum_{j,k} c_j c_k e^{-x\|\mathbf{x}_j - \mathbf{x}_k\|^2}\Big)dx.$
- Since $[e^{-x\|\mathbf{x}_j - \mathbf{x}_k\|^2}]$ is positive definite for $x > 0$ the integral is positive "showing" the result.
- Need a refined argument to guarantee that the integrals exist.

Proof of Main Theorem

- Let $\delta_k : (0, \infty) \to \mathbb{R}$ for $k \geq 0$ be given by

$$(-1)^{k+1}\delta_k(r) := \int_0^1 w(x)\big(e^{-xr} - q_k(-xr)\big)x^{-k-1}dx + \int_1^\infty w(x)e^{-xr}x^{-k-1}dx,$$

  where $q_k(t) = \sum_{\ell=0}^{k} \frac{t^k}{k!}$.
- To see that this is well defined we observe that $q_k(t)$ is the first few terms in the Taylor expansion of e^t around $t = 0$. Thus for $t < 0$
- $e^t - q_k(t) = \frac{t^{k+1}}{(k+1)!}e^c$ with $t \leq c \leq 0$.
- Then for $0 < x \leq 1$,
  $|e^{-xr} - q_k(-xr)|x^{-k-1} = \frac{(xr)^{k+1}}{(k+1)!}x^{-k-1}e^c \leq \frac{r^{k+1}}{(k+1)!}$
- $|e^{-xr}x^{-k-1}| \leq e^{-xr}$, $x \geq 1$.
- We show that $\delta_0'(r) = \psi^{(m+1)}(r)$ and $\delta_k' = \delta_{k-1}$ for $k \geq 1$

δ_0'

- Since $q_0(t) = 1$ we find the derivative

$$\delta_0'(r) =$$
$$-\frac{d}{dr}\Big(\int_0^1 w(x)\big(e^{-xr} - 1\big)x^{-1}dx + \int_1^\infty w(x)e^{-xr}x^{-1}dx\Big)$$
$$= \int_0^1 w(x)e^{-xr}dx + \int_1^\infty w(x)e^{-xr}dx$$
$$= \int_0^\infty w(x)e^{-xr}dx = \psi^{(m+1)}(r)$$

δ_1'

- $$\begin{aligned}
&\delta_1'(r) \\
&= -\frac{d}{dr}\Big(\int_0^1 w(x)\big(e^{-xr} - 1 + xr\big)x^{-2}dx + \int_1^\infty w(x)e^{-xr}x^{-2}dx \\
&= \int_0^1 w(x)\big(e^{-xr} - 1\big)x^{-1}dx + \int_1^\infty w(x)e^{-xr}x^{-1}dx \\
&= \delta_0(r).
\end{aligned}$$

- Since $q_k'(t) = q_{k-1}(t)$ we find $\frac{d}{dr}q_k(-xr) = -xq_{k-1}(-xr)$
- So $\delta_k'(r) = \delta_{k-1}(r)$, $k \geq 1$
- Thus $\delta_m^{(m+1)}(r) = \delta_{m-1}^{(m)}(r) = \cdots = \delta_0'(r) = \psi^{(m+1)}(r)$

Proof

- $\psi(r) = \delta_m(r) + q(r), \quad r \geq 0$, where $q \in \Pi_m(\mathbb{R}^1)$
- For $\mathbf{c} \in \mathcal{S}_m(\mathbf{X})$

$$(-1)^{m+1}\mathbf{c}^T\mathbf{A}\mathbf{c} = (-1)^{m+1}\sum_{j,k} c_j c_k \psi(\|\mathbf{x}_j - \mathbf{x}_k\|^2)$$

$$=(-1)^{m+1}\sum_{j,k} c_j c_k \big(\delta_m(\|\mathbf{x}_j - \mathbf{x}_k\|^2) + q(\|\mathbf{x}_j - \mathbf{x}_k\|^2)\big)$$

$$=(-1)^{m+1}\sum_{j,k} c_j c_k \delta_m(\|\mathbf{x}_j - \mathbf{x}_k\|^2)$$

$$=\sum_{j,k} c_j c_k \Big(\int_0^1 w(x)\big(e^{-x\|\mathbf{x}_j-\mathbf{x}_k\|^2} - q_m(-x\|\mathbf{x}_j - \mathbf{x}_k\|^2)\big)x^{-m-1}dx$$

$$+ \int_1^\infty w(x)e^{-x\|\mathbf{x}_j-\mathbf{x}_k\|^2}x^{-m-1}dx\Big),$$

Proof

- $\sum_{j,k} c_j c_k q_m(\|\mathbf{x}_j - \mathbf{x}_k\|^2) = \sum_{\ell=0}^{m} \frac{(-x)^\ell}{\ell!} \sum_{j,k} c_j c_k \|\mathbf{x}_j - \mathbf{x}_k\|^{2\ell} = 0$
- $(-1)^{m+1}\mathbf{c}^T\mathbf{A}\mathbf{c} = \int_0^\infty \frac{w(x)}{x^{m+1}} \left(\sum_{j,k} c_j c_k e^{-x\|\mathbf{x}_j - \mathbf{x}_k\|^2} \right) dx > 0$
- Since $[e^{-x\|\mathbf{x}_j - \mathbf{x}_k\|^2}]$ is positive definite for $x > 0$ the integral is positive showing the result.