# Radial Basis Functions II

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December 2, 2008

# 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** $\varphi(r) = r$,
- **cubic power** $\varphi(r) = r^3$,
- **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** $\varphi(r) = (1 - r)_+^4 (4r + 1)$

# Subspaces of $\mathbb{R}^N$

The class of polynomials in $s$ variables with real coefficients and of total degree $\leq m$ are denoted by

$$\Pi_m(\mathbb{R}^s) := \operatorname{span}\{x_1^{i_1} \cdots x_s^{i_s} : i_1, \ldots, i_s \geq 0, \ \sum_{k=1}^{s} i_k \leq m\}.$$

- To given distinct points $\mathbf{X} := \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ in $\mathbb{R}^s$ and a nonnegative integer $m$ we define a subspace of $\mathbb{R}^N$ by

$$\mathcal{S}_m(\mathbf{X}) := \{\mathbf{c} \in \mathbb{R}^N : \sum_{k=1}^{N} c_k p(\mathbf{x}_k) = 0, \ p \in \Pi_m(\mathbb{R}^s)\}.$$

- We define $\mathcal{S}_{-1}(\mathbf{X}) := \mathbb{R}^N$.

# Subspaces of $\mathbb{R}^N$

$$\mathcal{S}_m(\mathbf{X}) := \{\mathbf{c} \in \mathbb{R}^N : \sum_{k=1}^{N} c_k p(\mathbf{x}_k) = 0,\ \ p \in \Pi_m(\mathbb{R}^s)\}.$$

- $\mathcal{S}_0(\mathbf{X}) = \{\mathbf{c} \in \mathbb{R}^N : \sum_{k=1}^{N} c_k = 0\}$
- Given a basis $q_1, \ldots, q_M$ of $\Pi_m(\mathbb{R}^s)$
- Then
  $\mathcal{S}_m(\mathbf{X}) := \{\mathbf{c} \in \mathbb{R}^N : \sum_{k=1}^{N} c_k q_j(\mathbf{x}_k) = 0,\ \ j = 1, \ldots, M\}.$

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

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 powers)
- Linear combinations $P_f(\mathbf{x}) := \sum_{k=1}^{N} c_k \Phi(\mathbf{x} - \mathbf{x}_k) + \sum_{k=1}^{M} d_k q_k(\mathbf{x})$

Find

- $\mathbf{c} = [c_1, \ldots, c_N]$ and $\mathbf{d} = [d_1, \ldots, d_M]$ such that

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

# 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.

# 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*

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

*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
- Alternatives:
  - Nonnegativity of the generalized Fourier transform.
  - Complete monotonicity

# 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 $p(\mathbf{x}_k) = 0 \quad k = 1, \ldots, N \Rightarrow p = 0$.

# Example, Univariate natural cubic spline interpolation

- $\varphi(r) = r^3$, $\Phi(x) = |x|^3$
- $P_f(x_j) = \sum_{k=1}^{N} c_k |x_j - x_k|^3 + d_0 + d_1 x_j = f_j$, $j = 1, \ldots, N$
- $\sum_k c_k = 0$, $\sum_k c_k x_k = 0$.
- Matrix form

$$\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{0} \end{bmatrix}, \mathbf{A} = [|x_j - x_k|^3],\ \mathbf{B} = \begin{bmatrix} 1 & \cdots & 1 \\ x_1 & \cdots & x_N \end{bmatrix}.$$

- $N + 2$ equations in $N + 2$ unknowns.
- If $\mathbf{A}$ is positive definite on $\ker(\mathbf{B})$ and $x_1, \ldots, x_N$ are distinct then $\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix}$ is non-singular.

# Example Cubic power in $\mathbb{R}^3$, $N \geq 4$

- $\varphi(r) = r^3$; $\Phi(\mathbf{x}) = \|\mathbf{x}\|^3 = (x^2 + y^2 + z^2)^{3/2}$
- $P_f(\mathbf{x}) := \sum_{k=1}^{N} c_k \Phi(\mathbf{x} - \mathbf{x}_k) + d_1 + d_2 x + d_3 y + d_4 z$,
- $\sum_{k=1}^{N} c_k \Phi(\mathbf{x}_j - \mathbf{x}_k) + d_1 + d_2 x_j + d_3 y_j + d_4 z_j = f_j, \; j = 1, \ldots, N$

  $$\sum_k c_k = 0, \quad \sum_k c_k x_k = 0, \quad \sum_k c_k y_k = 0, \quad \sum_k c_k z_k = 0$$
- $N + 4$ equations in $N + 4$ unknowns.
- $\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{0} \end{bmatrix}$, $\mathbf{A} = [\Phi(\mathbf{x}_j - \mathbf{x}_k)]$

  $$\mathbf{B} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_N \\ y_1 & y_2 & \cdots & y_N \\ z_1 & z_2 & \cdots & z_N \end{bmatrix} \in \mathbb{R}^{4,N},$$
- If $\mathbf{A}$ is positive definite on $\mathcal{S}_1(\mathbf{X})$ and the $\mathbf{x}_j$ are not on a straight line then $\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix}$ is nonsingular.

# 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:

- $g(r) = e^{-\varepsilon r}$, $\varepsilon \geq 0$, $r \geq 0$
- $g(r) = r^{-1/2}$, $r > 0$

# Characterization of completely monotone functions

- There is a general result stating that $g$ is completely monotone if and only if it is the Laplace transform of a finite nonnegative Borel measure on $[0, \infty)$. This is known as the Hausdorff-Bernstein-Widdler theorem, see Wendland 2005.
- We will only use a sufficient condition, namely that many completely monotone functions $g$ are the Laplace transform of an admissible function $w$

$$g : [0, \infty) \to \mathbb{R}, \quad g(r) := \int_0^\infty w(x) e^{-xr} dx.$$

- We say that $w : (0, \infty) \to \mathbb{R}$ is admissible, if it is piecewise continuous, nonnegative, nonzero and the Laplace transform $g$ of $w$ exists.

# Positive definite on a subspace

## 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 an admissible function $w$, 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*
$\mathcal{S}_m(\mathbf{X}) := \{\mathbf{c} \in \mathbb{R}^N : \sum_{k=1}^N c_k p(\mathbf{x}_k) = 0,\ p \in \Pi_m(\mathbb{R}^s)\}$.

# Example Distance in $\mathbb{R}^s$

- $\varphi(r) = r$, $\psi(r) = \sqrt{r}$.
- $\psi'(r) = \frac{1}{2} r^{-1/2}$ is completely monotone
- $\psi'(r) = \int_0^\infty w(x) e^{-xr} dx$, $w(x) = \frac{1}{2\sqrt{\pi x}}$.
- For $\int_0^\infty = \frac{e^{-x}}{\sqrt{x}} dx = 2 \int_0^\infty e^{-y^2} dy = \int_{-\infty}^\infty e^{-y^2} dy = \sqrt{\pi}$
- so $\int_0^\infty \frac{e^{-rx}}{\sqrt{\pi x}} dx = \frac{r^{-1/2}}{\sqrt{\pi}} \int_0^\infty \frac{e^{-y}}{\sqrt{y}} dy = r^{-1/2}$.
- $w$ is admissible.
- $m = 0$, $-\mathbf{A}$ is positive definite on $\mathcal{S}_0 = \{\mathbf{c} : \sum_k c_k = 0\}$
- From theorem last time it follows that $\mathbf{A}$ is nonsingular (nonzero eigenvalues) for all $s \geq 1, N \geq 2$, and any distinct $\mathbf{x}_1, \ldots, \mathbf{x}_N$ in $\mathbb{R}^s$.
- Interpolation problem with reproduction of $\Pi_m$ also non-singular for all $m \geq 0$, $s \geq 1, N \geq 2$, and any distinct $\mathbf{x}_1, \ldots, \mathbf{x}_N$ in $\mathbb{R}^s$.

# Example Cubic

- $\varphi(r) = r^3$, $\psi(r) = r^{3/2}$.
- $\psi''(r) = \frac{3}{4} r^{-1/2}$ is completely monotone
- $\psi''(r) = \int_0^\infty w(x) e^{-xr} dx$, $w(x) = \frac{3}{4\sqrt{\pi x}}$.
- $w$ is admissible.
- $m = 1$, $\mathbf{A}$ 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.

# Example Thin plate

- $\varphi(r) = r^2 \log r$, $\psi(r) = \frac{1}{2} r \log r$.
- $\psi''(r) = \frac{1}{2r}$ is completely monotone
- $\psi''(r) = \frac{1}{2} \int_0^\infty e^{-xr} dx$, $w(x) = \frac{1}{2}$.
- $w$ is admissible.
- $m = 1$, $\mathbf{A}$ 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.

# Example Inverse Multiquadrics

- $\varphi(r) = 1/\sqrt{1+(\varepsilon r)^2}$, $\psi(r) = 1/\sqrt{1+\varepsilon^2 r}$, $\varepsilon \neq 0$
- $\psi$ is completely monotone.
- $\psi(r) = \int_0^\infty w(x) e^{-xr} dx$, $w$ admissible.
- $\mathbf{A}$ is positive definite.

# Example Multiquadrics

- $\varphi(r) = \sqrt{1 + (\varepsilon r)^2}$, $\psi(r) = \sqrt{1 + \varepsilon^2 r}$,
- $\psi'$ is completely monotonic and the Laplace transform of an admissible function $w$.
- $-\mathbf{A}$ is positive definite on $\mathcal{S}_0$.
- $\mathbf{A}$ is non-singular with $N - 1$ positive and one negative eigenvalue.

# Summary of Examples

- **Gauss** $\varphi(r) = e^{-\varepsilon^2 r^2}$, $m = -1$, $\mathbf{A}$ is positive definite
- **inverse multiquadric** $\varphi(r) = 1/\sqrt{1 + (\varepsilon r)^2}$, $m = -1$, $\mathbf{A}$ is positive definite
- **multiquadric** $\varphi(r) = \sqrt{1 + (\varepsilon r)^2}$, $m = 0$ $-\mathbf{A}$ is positive definite on $\mathcal{S}_0$
- **distance** $\varphi(r) = r$, $m = 0$ $-\mathbf{A}$ is positive definite on $\mathcal{S}_0$
- **cubic power** $\varphi(r) = r^3$, $m = 1$ $\mathbf{A}$ is positive definite on $\mathcal{S}_1$
- **thin plate spline** $\varphi(r) = r^2 \log r$ $m = 1$ $\mathbf{A}$ is positive definite on $\mathcal{S}_1$.

# Lemma

## Lemma

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

- **Proof**:
- $\|\mathbf{x}_j - \mathbf{x}_k\|^{2\ell} = \left(\|\mathbf{x}_j\|^2 + \|\mathbf{x}_k\|^2 - 2\mathbf{x}_j^T\mathbf{x}_k\right)^{\ell}$,
- $\|\mathbf{x}_j - \mathbf{x}_k\|^{2\ell} = \sum_{\alpha+\beta+\gamma=\ell} \frac{\ell!}{\alpha!\beta!\gamma!}\|\mathbf{x}_j\|^{2\alpha}\|\mathbf{x}_k\|^{2\beta}(-2\mathbf{x}_j^T\mathbf{x}_k)^{\gamma}$
- 

$$\begin{aligned}
&\mathbf{c}^T[\|\mathbf{x}_j - \mathbf{x}_k\|^{2\ell}]\mathbf{c} \\
&= \sum_{j,k} c_j c_k \sum_{\alpha+\beta+\gamma=\ell} \frac{\ell!}{\alpha!\beta!\gamma!}\|\mathbf{x}_j\|^{2\alpha}\|\mathbf{x}_k\|^{2\beta}(-2\mathbf{x}_j^T\mathbf{x}_k)^{\gamma} \\
&= \sum_{\alpha+\beta+\gamma=\ell} \frac{\ell!}{\alpha!\beta!\gamma!} \sum_{j,k} c_j c_k \|\mathbf{x}_j\|^{2\alpha}\|\mathbf{x}_k\|^{2\beta}(-2\mathbf{x}_j^T\mathbf{x}_k)^{\gamma}
\end{aligned}$$

# Proof continued

- Divide $\alpha, \beta, \gamma$ sum into two sums $\alpha \leq \beta$ and $\beta < \alpha$. Consider first the $\alpha \leq \beta$ sum.
- $q_{\alpha\beta\gamma}(\mathbf{x}) := \sum_{k=1}^{N} c_k \|\mathbf{x}\|^{2\alpha} \|\mathbf{x}_k\|^{2\beta} (-2\mathbf{x}^T \mathbf{x}_k)^\gamma$, $\mathbf{x} \in \mathbb{R}^s$.
- $q_{\alpha\beta\gamma} \in \Pi_{2\alpha+\gamma}(\mathbb{R}^s) \subset \Pi_m(\mathbb{R}^s)$ for $\alpha \leq \beta$.
- Indeed, If $\alpha \leq \beta$ then $2\alpha + \gamma = 2\alpha + 2\beta + \gamma - 2\beta = \ell + \alpha - \beta \leq m$.
- So $\sum_{j=1}^{N} q_{\alpha\beta\gamma}(\mathbf{x}_j) = 0$
- $\sum_{j,k} c_j c_k \|\mathbf{x}_j\|^{2\alpha} \|\mathbf{x}_k\|^{2\beta} (-2\mathbf{x}_j^T \mathbf{x}_k)^\gamma = 0$ for $\alpha \leq \beta$
- By symmetry this also holds for $\alpha > \beta$ and the lemma follows.