Radial Basis Functions I

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Today

- Reformulation of natural cubic spline interpolation
- Scattered data interpolation with RBF's
- Franke's example using Gaussian
- Non-singularity via nonnegative Fourier Transform
- RBF interpolation with polynomial precision
- Positive definite matrices on a subspace.

Cubic Splines

- Given $a < b$ and $\mathbf{x} = [x_0, \ldots, x_{N+1}]$ with $a =: x_0 < x_1 < \cdots < x_N < x_{N+1} := b$.
- Cubic Splines: $\mathbb{S}_3^2(\mathbf{x}) := \{g \in C^2[a,b] : g_{|_{(x_j, x_{j+1})}} \in \Pi_3,\ \text{for } j = 0, \ldots, N$
- $\Pi_d := \text{span}\{x^k : 0 \le k \le d\}$ polynomials of degree $\le d$.
- Unique representation of $g \in \mathbb{S}_3^2$ in terms of truncated powers $x_+^3 := \max\{x^3, 0\}$.
- $x_+^3 \in C^2(\mathbb{R})$.
- $g(x) = \sum_{k=1}^{N} c_k (x - x_k)_+^3 + \sum_{k=0}^{3} a_k x^k,\ x \in [a,b]$.
- $\mathbb{S}_3^2(\mathbf{x})$ is a linear space of functions of dimension $N + 4$.

Natural Cubic Splines

- $\mathbb{NS}_3^2(\mathbf{x}) := \{g \in \mathbb{S}_3^2(\mathbf{x}) : g|_{(a,x_1)}, g|_{(x_N,b)} \in \Pi_1\}$.
- Truncated power representation $g \in \mathbb{NS}_3^2(\mathbf{x}) \iff$
  - $g(x) = \sum_{k=1}^{N} c_k (x - x_k)_+^3 + a_0 + a_1 x, \; x \in [a, b]$,
  - $\sum_{k=1}^{N} c_k = 0, \quad \sum_{k=1}^{N} c_k x_k = 0$.
- **Proof** Choosing $x \in (a, x_1)$ shows that $a_2 = a_3 = 0$ in the truncated power representation.
- Choosing $x \in (x_N, b)$ shows the orthogonality conditions.
  - remove $+$'s:
    $g(x) = \sum_{k=1}^{N} c_k (x - x_k)^3 + a_0 + a_1 x, \; x \in (x_N, b)$.
  - Expand $(x - x_k)^3 = x^3 - 3x_k x^2 + 3x_k^2 x - x_k^3$
  - Expanded Sum: $\sum_k c_k (x - x_k)^3 =$
    $x^3 \sum_k c_k - 3(\sum_k c_k x_k) x^2 + 3(\sum_k c_k x_k^2) x - (\sum_k c_k x_k^3)$.

Radial basis function representation

- truncated power representation: $g \in \mathbb{NS}_3^2(\mathbf{x}) \Longleftrightarrow$
  - $g(x) = \sum_{k=1}^{N} c_k (x - x_k)_+^3 + a_0 + a_1 x, \ x \in [a, b]$,
  - $\sum_{k=1}^{N} c_k = 0, \quad \sum_{k=1}^{N} c_k x_k = 0.$
- Replace x_+^3 by $\frac{1}{2}(|x|^3 + x^3)$ in truncated power representation.
- $g(x) = \frac{1}{2} \sum_{k=1}^{N} c_k |x - x_k|^3 + \frac{1}{2} \sum_{k=1}^{N} c_k (x - x_k)^3 + a_0 + a_1 x, \ x \in [a, b]$,
- $g(x) = \frac{1}{2} \sum_{k=1}^{N} c_k |x - x_k|^3 + \frac{3}{2} (\sum_{k=1}^{N} c_k x_k^2) x - \frac{1}{2} (\sum_{k=1}^{N} c_k x_k^3) + a_0 + a_1 x, \ x \in [a, b]$,
- radial basis function representation
  - $g(x) = \sum_{k=1}^{N} c_k |x - x_k|^3 + d_0 + d_1 x, \ x \in [a, b]$,
  - $\sum_{k=1}^{N} c_k = 0, \quad \sum_{k=1}^{N} c_k x_k = 0.$

Natural cubic spline interpolation in a radial basis formulation

- Find $P_f \in \mathbb{NS}_3^2(\mathbf{x})$ such that $P_f(x_j) = f_j$, $j = 1, \ldots, N$.
- $\sum_{k=1}^{N} c_k \varphi(|x_j - x_k|) + d_0 + d_1 x_j = f_j$, $j = 1, \ldots, N$
- $\sum_k c_k = 0$, $\sum_k c_k x_k = 0$.
- Matrix form

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

- $N + 2$ equations in $N + 2$ unknowns.

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

Definition

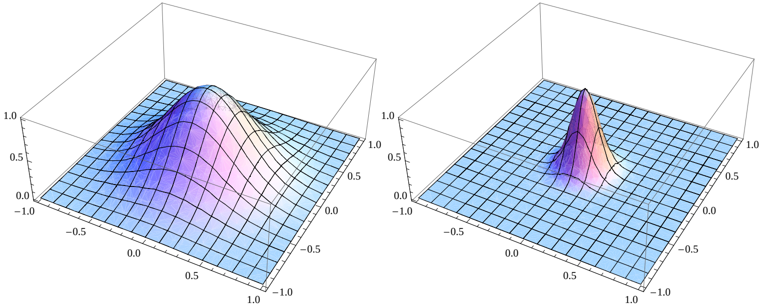
Let $s \in \mathbb{N}$ and $\| \ \|$ a norm on $\mathbb{R}^s$. A function $\Phi : \mathbb{R}^s \to \mathbb{R}$ is called radial if

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

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

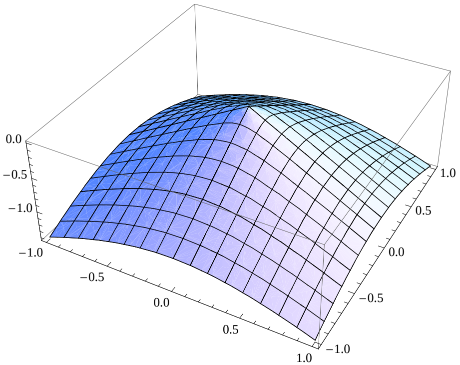
- The norm is often the Euclidian norm $\| \ \|_2$.
- $\| \ \| = \| \ \|_2$ when nothing else is said.
- Radial: $\Phi(\mathbf{x}) = \varphi(r)$ for all $\mathbf{x}$ with $\|\mathbf{x}\| = r$.

Gaussian, $\varphi(r) = e^{-\varepsilon^2 r^2}, \quad \varepsilon = 2, 6$



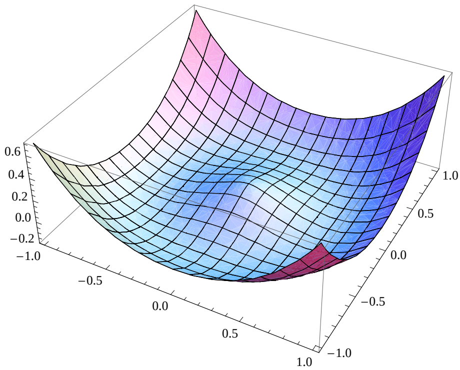
$$\Phi(\mathbf{x}) = \varphi(\|\mathbf{x}\|) = e^{-\varepsilon^2 \|\mathbf{x}\|^2}$$

Distance, $\varphi(r) = -r$



$$\Phi(\mathbf{x}) = \varphi(\|\mathbf{x}\|) = -\sqrt{x^2 + y^2}$$

Thin Plate, $\varphi(r) = r^2 \log r$



$$\Phi(\mathbf{x}) = \varphi(\|\mathbf{x}\|) = \frac{1}{2}(x^2 + y^2)\log(x^2 + y^2).$$

$$\nabla^4 \Phi(\mathbf{x}) = 0.$$

RBF Interpolation without polynomial precision

Given

- $N, s \in \mathbb{N}$ and 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 $\Phi(\mathbf{x}) = \varphi(\|\mathbf{x}\|)$
- Linear combinations $P_f(\mathbf{x}) := \sum_{k=1}^{N} c_K \Phi(\mathbf{x} - \mathbf{x}_k)$

Find

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

$$P_f(\mathbf{x}_j) := \sum_{k=1}^{N} c_k \Phi(\mathbf{x}_j - \mathbf{x}_k) = f_j, \quad j = 1, \ldots, N$$

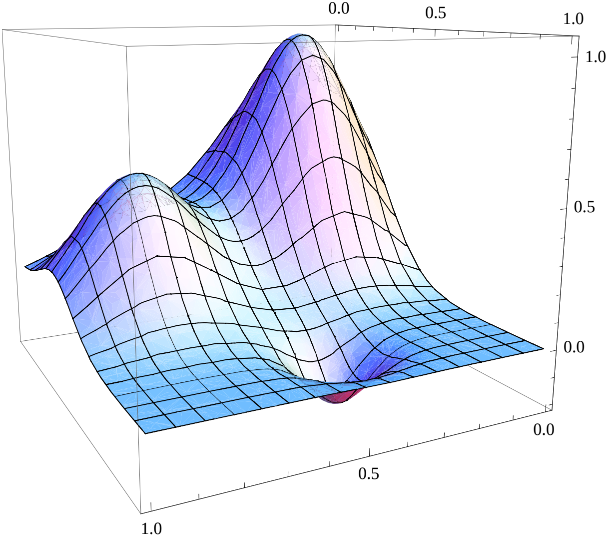
- Matrix Problem $\mathbf{Ac} = \mathbf{f}$, where $\mathbf{A} = [\varphi(\|\mathbf{x}_j - \mathbf{x}_k\|)] \in \mathbb{R}^{N,N}$, $\mathbf{f} = [f_1, \ldots, f_N]^T$.

$N = 2$

$$\mathbf{A} = \begin{bmatrix} \varphi(\|\mathbf{x}_1 - \mathbf{x}_1\|) & \varphi(\|\mathbf{x}_1 - \mathbf{x}_2\|) \\ \varphi(\|\mathbf{x}_2 - \mathbf{x}_1\|) & \varphi(\|\mathbf{x}_2 - \mathbf{x}_2\|) \end{bmatrix}.$$

- $\varphi(r) = e^{-\varepsilon^2 r^2}$, $\mathbf{A} = \begin{bmatrix} 1 & a \\ a & 1 \end{bmatrix}$, $a = e^{-\varepsilon^2 \|\mathbf{x}_1 - \mathbf{x}_2\|^2} < 1$ if $\varepsilon \neq 0$.
- $\mathbf{A}$ is symmetric and positive definite. (Positive eigenvalues by Gerschgorin or strict diagonal dominance).
- $\varphi(r) = r$, $\mathbf{A} = \begin{bmatrix} 0 & b \\ b & 0 \end{bmatrix}$, $b = \|\mathbf{x}_1 - \mathbf{x}_2\|$.
- $\mathbf{A}$ is symmetric with one positive and one negative eigenvalue.
- Nonsingular, but indefinite.
- Same for thin plate

Franke's test function

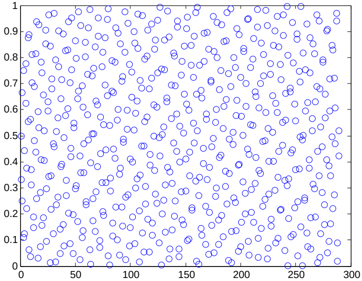


Franke's test function

$$
\begin{aligned}
f(x,y) :=& 0.75 * Exp\Big(-((9*x-2)^2 + (9*y-2)^2)/4\Big) \\
&+ 0.75 * Exp\Big(-((9*x+1)^2/49 + (9*y+1)^2/10)\Big) \\
&+ 0.5 * Exp\Big(-((9*x-7)^2 + (9*y-3)^2)/4\Big) \\
&- 0.2 * Exp\Big(-((9*x-4)^2 + (9*y-7)^2)\Big)
\end{aligned}
$$

Halton Points

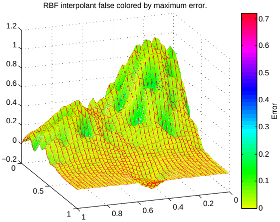
- $\mathbf{x}_1, \ldots, \mathbf{x}_N$ uniformly distributed points in $(0, 1)^s$.
- can be downloaded by searching for **haltonseq.m**.

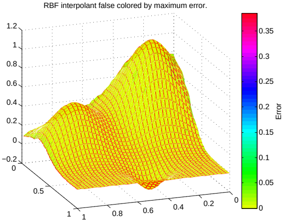


289 Halton Points in $\mathbb{R}^2$

Gaussian Example

- $$\Phi(\mathbf{x}) = e^{-\varepsilon^2 \|\mathbf{x}\|^2}, \quad \varepsilon = 21.1$$
- 289 (left) and 1089 right) Halton Points
- **f** sampled from Franke's test function.
- Matlab program RBFInterpolation2D.m by Fasshauer





Discussion

- Dense linear system
- Non-singular?
- Extremely ill-conditioned for ε not large.
- Polynomials of low degree not reproduced.
- But.. Can work for scattered data in high space dimension without triangulating the data.

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

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

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

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.

Proof

$$
\begin{aligned}
\mathbf{c}^T\mathbf{A}\mathbf{c} &= \sum_{j=1}^{N}\sum_{k=1}^{N} c_j c_k \Phi(\mathbf{x}_j - \mathbf{x}_k) \\
&= \frac{1}{(2\pi)^{s/2}} \sum_{j,k} c_j c_k \int_{\mathbb{R}^s} \hat{\Phi}(\boldsymbol{\omega}) e^{i\boldsymbol{\omega}\cdot(\mathbf{x}_j - \mathbf{x}_k)} d\boldsymbol{\omega} \\
&= \frac{1}{(2\pi)^{s/2}} \int_{\mathbb{R}^s} \sum_{j,k} \left(c_j e^{i\boldsymbol{\omega}\cdot\mathbf{x}_j} c_k e^{-i\boldsymbol{\omega}\cdot\mathbf{x}_k}\right) \hat{\Phi}(\boldsymbol{\omega}) d\boldsymbol{\omega} \\
&= \frac{1}{(2\pi)^{s/2}} \int_{\mathbb{R}^s} \sum_{j} |c_j e^{i\boldsymbol{\omega}\cdot\mathbf{x}_j}|^2 \hat{\Phi}(\boldsymbol{\omega}) d\boldsymbol{\omega} \geq 0.
\end{aligned}
$$

$$
\text{Equality } \Rightarrow \sum_j c_j e^{i\boldsymbol{\omega}\cdot\mathbf{x}_j} = 0, \ \boldsymbol{\omega} \in \mathbb{R}^s, \ \Rightarrow \mathbf{c} = \mathbf{0}.
$$

Discussion

- The Fourier transform can be used for some other examples. 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.
- We will instead look at the connection between positive definite matrices and completely monotone functions.

Polynomial reproduction

- Gaussian, distance and thin plate do not reproduce polynomials
- can add terms to achieve this.
- Example $\mathbf{x} = (x, y) \in \mathbb{R}^2$, add $1, x, y$ to reproduce linear polynomials
- $P_f(\mathbf{x}) := \sum_{k=1}^{N} c_k \varphi(\|\mathbf{x} - \mathbf{x}_k\|) + d_1 + d_2 x + d_3 y$,
- need 3 extra conditions
- $\sum_k c_k = 0$, $\sum_k c_k x_k = 0$, $\sum_k c_k y_k = 0$

Linear system

- $\sum_{k=1}^{N} c_k \varphi(\|\mathbf{x}_j - \mathbf{x}_k\|) + d_1 + d_2 x_j + d_3 y_j = f_j,\ j = 1, \ldots, N$
  $\sum_k c_k = 0, \quad \sum_k c_k x_k = 0, \quad \sum_k c_k y_k = 0$
- $$\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{0} \end{bmatrix},\ \mathbf{A} = [\varphi(\|\mathbf{x}_j - \mathbf{x}_k\|)],\ \mathbf{B}^T = \begin{bmatrix} 1 & x_1 & y_1 \\ \vdots & \vdots & \vdots \\ 1 & x_N & y_N \end{bmatrix}$$
- $\mathcal{S}_1 := \{\mathbf{c} \in \mathbb{R}^N : \mathbf{Bc} = \mathbf{0}\}$, is a subspace of $\mathbb{R}^N$.

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.

Proof

- $$\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix} = 0 \Rightarrow \begin{array}{r} \mathbf{A}\mathbf{c} + \mathbf{B}^T\mathbf{d} = 0 \\ \mathbf{B}\mathbf{c} = 0 \end{array}$$
$$\Rightarrow \begin{array}{r} \mathbf{c}^T\mathbf{A}\mathbf{c} + \mathbf{c}^T\mathbf{B}^T\mathbf{d} = 0 \\ \mathbf{c}^T\mathbf{B}^T = 0 \end{array}.$$
- So $\mathbf{c} = \mathbf{0}$ and then $\mathbf{d} = \mathbf{0}$ since $\mathbf{0} = \mathbf{A}\mathbf{c} + \mathbf{B}^T\mathbf{d} = \mathbf{B}^T\mathbf{d}$ and $\mathbf{B}$ has linearly independent rows.

Positive and negative eigenvalues

Theorem

If $\mathbf{A} \in \mathbb{R}^{N,N}$ *is positive definite on the subspace* $\mathcal{S} := \{\mathbf{c} \in \mathbb{R}^N : \sum_k c_k = 0\}$ *and* $\sum_i a_{ii} \le 0$*, then* $\mathbf{A}$ *has* $N-1$ *positive eigenvalues and one negative eigenvalue.*

- Proof
- $\mathcal{S}$ is a subspace of $\mathbb{R}^N$ of dimension $N-1$.
- Since $\mathbf{A}$ is symmetric it has real eigenvalues.
- Let $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_N$ be the eigenvalues of $\mathbf{A}$.
- Recall Courant-Fischer's characterization

$$\lambda_k = \max_{\dim \mathcal{T}=k} \min_{\substack{\mathbf{c}\in\mathcal{T} \\ \|\mathbf{c}\|=1}} \mathbf{c}^T\mathbf{A}\mathbf{c}.$$

- In particular

$$\lambda_{N-1} \ge \min_{\substack{\mathbf{c}\in\mathcal{S} \\ \|\mathbf{c}\|=1}} \mathbf{c}^T\mathbf{A}\mathbf{c} > 0.$$

- But $\sum_i \lambda_i = \sum_i a_{ii} \le 0$ so $\lambda_N < 0$.

Non-singularity without polynomial precision

Corollary

Let $\Phi(\mathbf{x}) := \varphi(\|\mathbf{x}\|)$ *be a radial function. If* $\mathbf{A} = [\varphi(\|\mathbf{x}_j - \mathbf{x}_k\|)] \in \mathbb{R}^{N,N}$ *is positive definite on the subspace* $\mathcal{S} := \{\mathbf{c} \in \mathbb{R}^N : \sum_k c_k = 0\}$ *and* $\varphi(0) = 0$ *then* $\mathbf{A}$ *is non-singular with* $N - 1$ *positive eigenvalues and one negative eigenvalue.*

Proof.

This follows immediately from the previous theorem. □

Distance matrix

- $\varphi(r) = -r$, $\Phi(\mathbf{x}) = \varphi(\|\mathbf{x}\|) = -\|\mathbf{x}\|$.
- $\mathbf{A} = [\|\mathbf{x}_j - \mathbf{x}_k\|]$ and
- $a_{jj} = \|\mathbf{x}_j - \mathbf{x}_j\| = 0$, $j = 1, \ldots, N$ since $\varphi(0) = 0$ so $\sum_j a_{jj} \leq 0$.
- We show next time that $\mathbf{A}$ is positive definite on $\mathcal{S} := \{\mathbf{c} \in \mathbb{R}^N : \sum_k c_k = 0\}$.
- It will then follow that the distance matrix is non-singular with $N - 1$ positive and one negative eigenvalue.