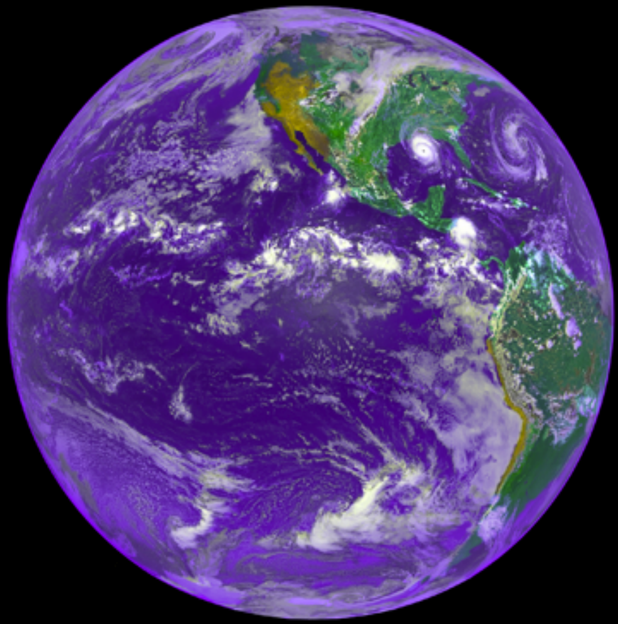
2014 Montestigliano Workshop

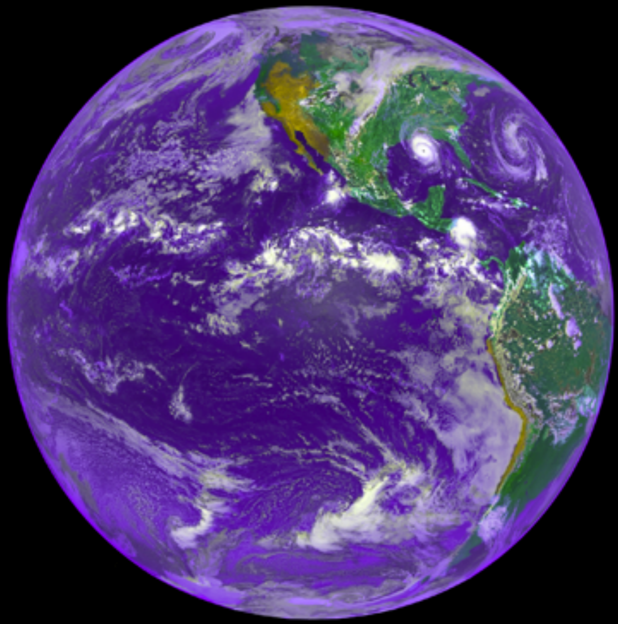
Radial Basis Functions for Scientific Computing



Grady B. Wright
Boise State University

*This work is supported by NSF grants DMS 0934581

2014 Montestigliano Workshop



Part I: Introduction

Grady B. Wright
Boise State University

*This work is supported by NSF grants DMS 0934581

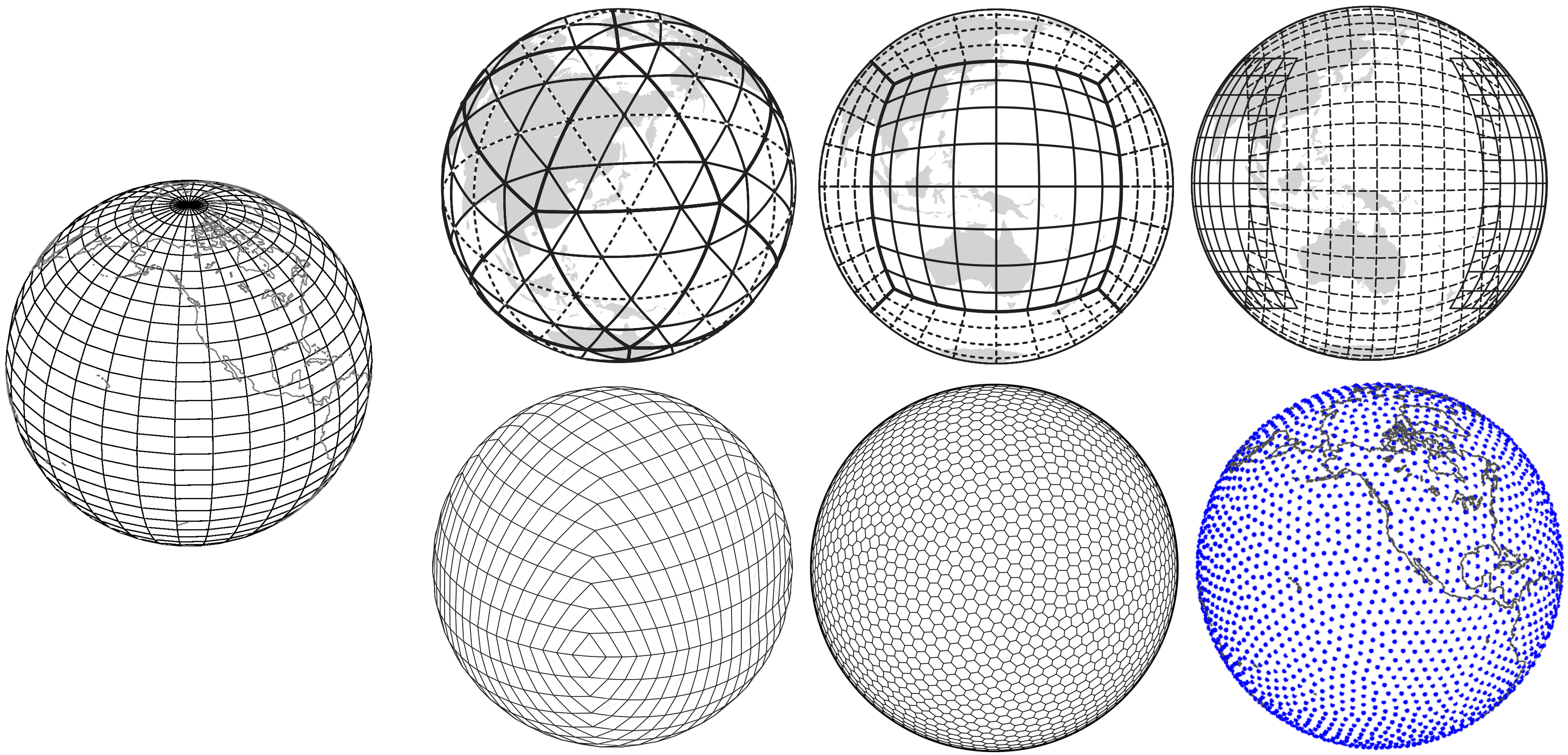
Overview

- Scattered data interpolation in $\mathbb{R}^d$
  - Positive definite radial kernels: radial basis functions (RBF)
  - Some theory
- Scattered data interpolation on the sphere $\mathbb{S}^2$
  - Positive definite (PD) zonal kernels
  - Brief review of spherical harmonics
  - Characterization of PD zonal kernels
  - Conditionally positive definite zonal kernels
  - Examples
- Error estimates:
  - Reproducing kernel Hilbert spaces
  - Sobolev spaces
  - Native spaces
  - Geometric properties of node sets
- Optimal nodes on the sphere

Grids, meshes, nodes, used for spherical geometries

Part 1

- Some examples of grids/meshes/nodes used in numerical methods:

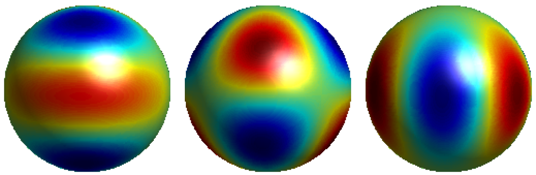


- Methods used:
  - Finite-difference, finite-element, finite-volume, semi-Lagrangian
  - Double Fourier, spherical harmonics, spectral elements, discontinuous Galerikin (DG), and radial basis functions (RBF)

Overview of some high-order methods for the sphere *Part 1*

Spherical harmonics (SPH):

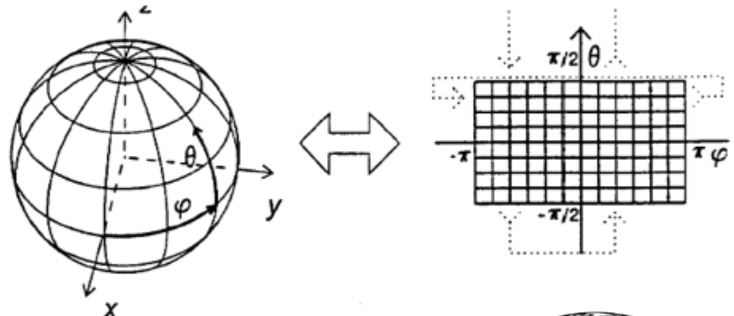
Expand solution in a set of orthogonal trig-like basis functions which give an entirely uniform resolution over the sphere.



Strengths: Exponential accuracy

Weakness: No practical option for local mesh refinement,
Relatively high computational cost,
Poor scalability on massively parallel machines

Double Fourier series (SPH):

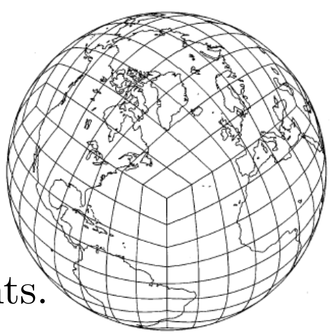


Strengths: Exponential accuracy,
Computationally fast due to FFT

Weakness: No option for local mesh refinement

Spectral elements

Map sphere to a cube.
Form elements on each face of cube.
Approximate on elements.



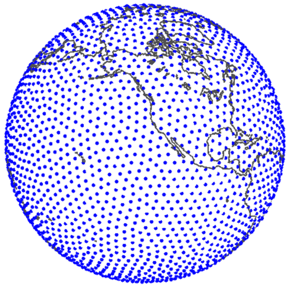
Strengths:
Accuracy approaching exponential,
Local mesh refinement feasible,
Scalable on massively parallel machines,
Mass conserving (DG)

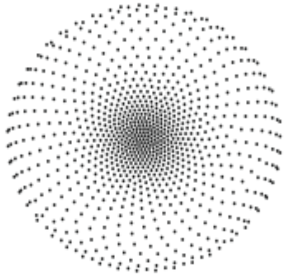
Weakness:
Loss of efficiency due to unphysical element boundaries,
Restrictive time-stepping due to clustered grids,
High algorithmic complexity, and preprocessing cost

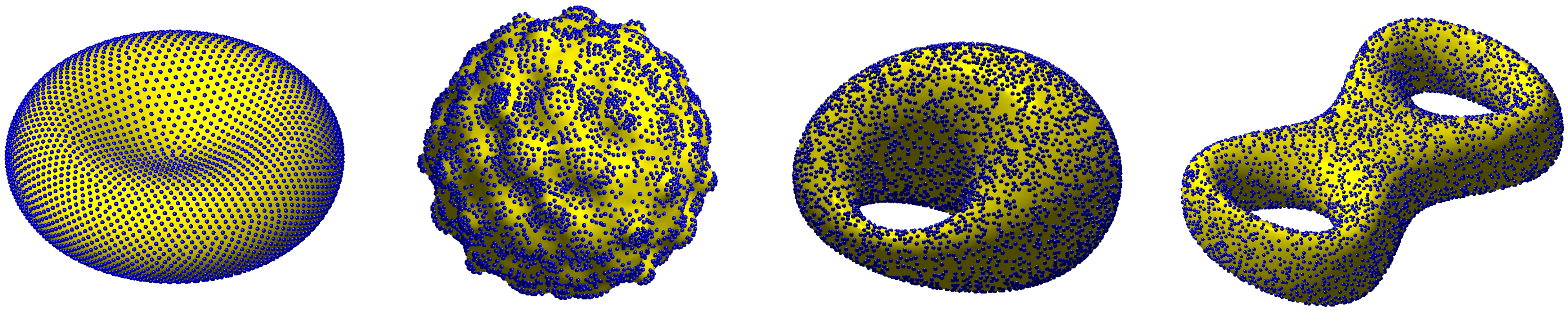
RBFs for the sphere

Strengths:

- High-order, even exponential, accuracy
- No grids or meshes: nodes can be scattered
- Local refinement is feasible
- No unphysical boundaries
- No unphysical clustering of nodes, allowing large time-steps for purely hyperbolic problems.
- No coordinate singularities to worry about
- Scalable on massively parallel machines (when using "local methods")
- Generalizes easily to other surfaces:







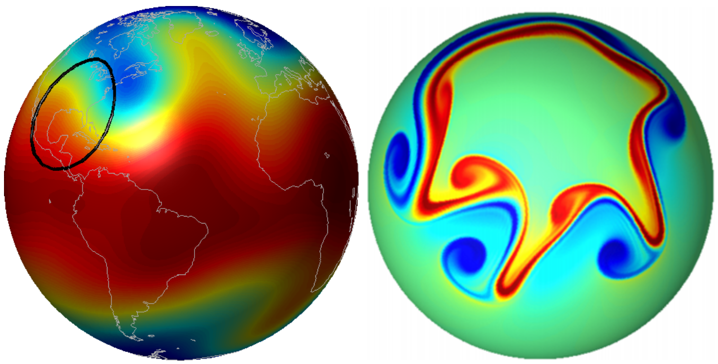
Weakness:

- Tuning of "shape parameter" is required
- Special algorithms required for small shape parameters
- Tuning of stabilization parameter for purely hyperbolic problems is required
- No inherent conservation

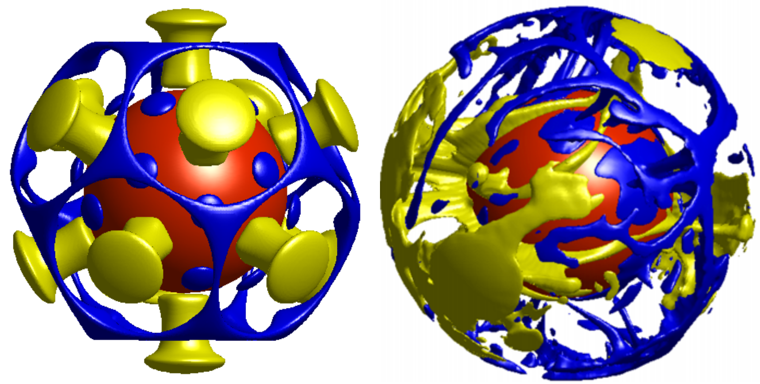
Applications of RBF methods on the sphere

- A visual overview:

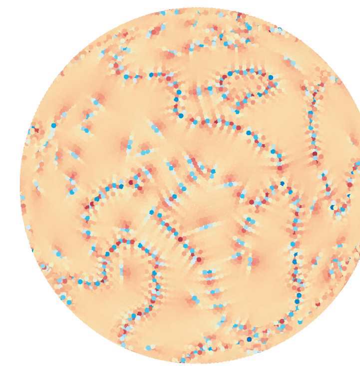
Shallow water flows:
numerical weather prediction



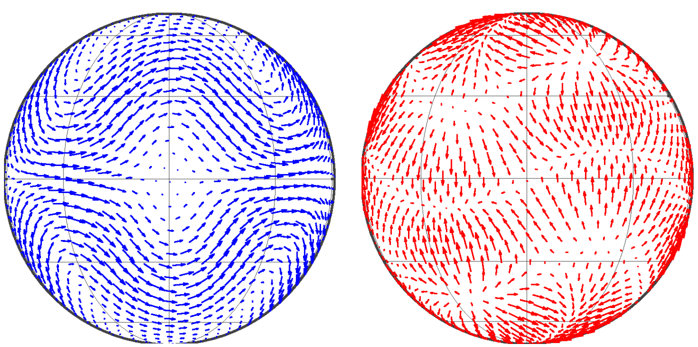
Rayleigh-Bénard convection:
Mantle convection



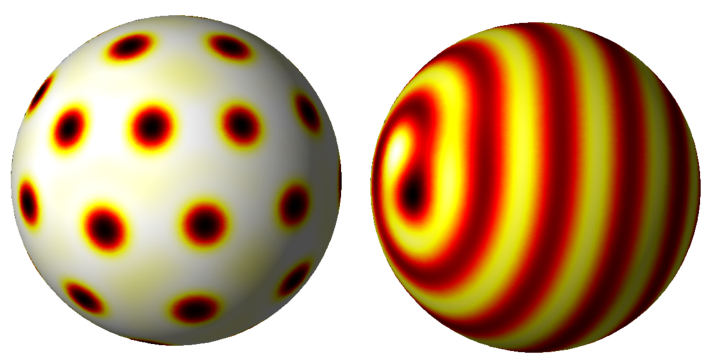
Numerical
integration



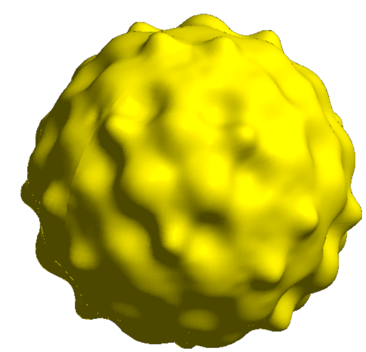
Vector fields on the sphere:
Helmholtz decomposition



Pattern formation:
Turing systems



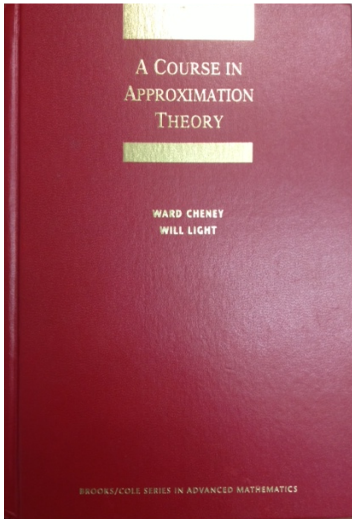
Geometric modeling



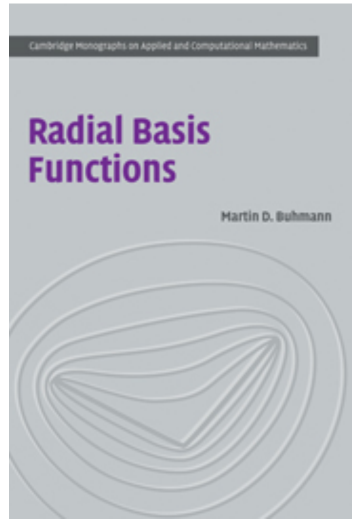
RBF References

- Many good books to consult on RBF theory and applications:

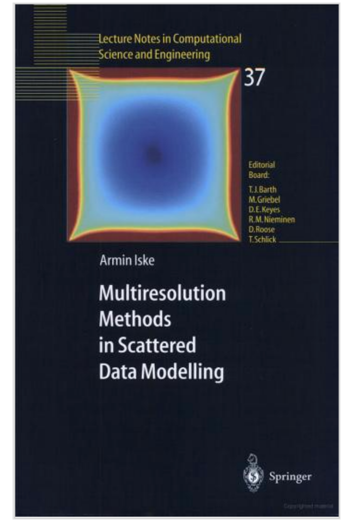
1999



2003

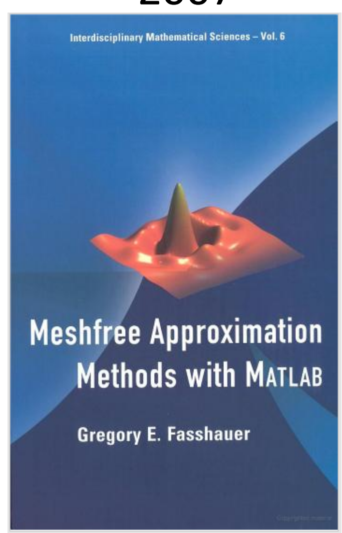


2004



2005

2007



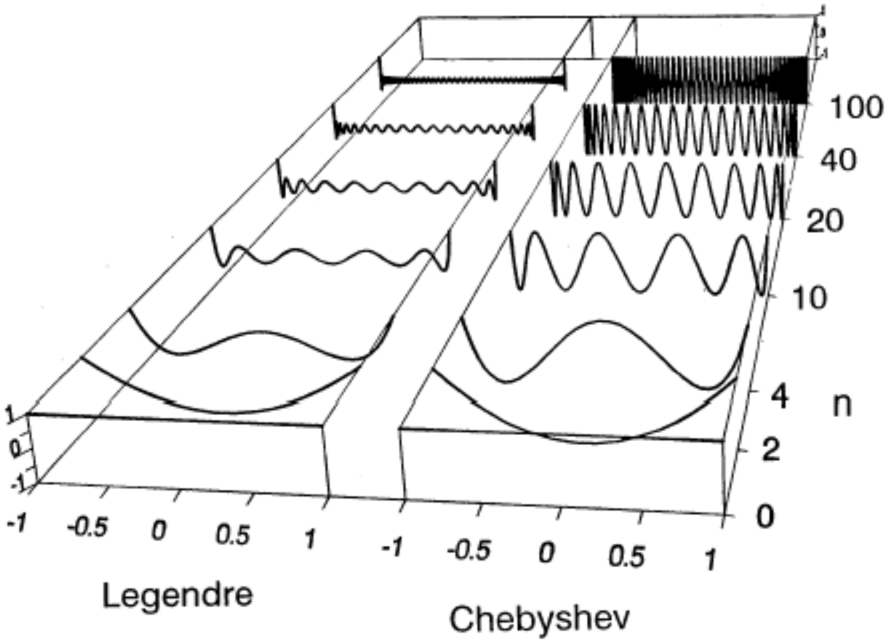
2014: SIAM

A Primer on
Radial Basis
Functions with
Applications to
the Geosciences

Bengt Fornberg
Natasha Flyer

Interpolation in 1-D with polynomials

- Orthogonal polynomial basis functions:
  Increasingly oscillatory as the degree increases



Data can be sampled at

1) Equally spaced points:

2) Boundary clustered points:

3) Irregular spaced points:

Interpolant: $I_N f = \sum_{k=0}^{N} c_k T_k(x), \;\; I_N f\Big|_{x=x_j} = f_j, \;\; j = 0, \ldots, N$

Expansion coefficients:

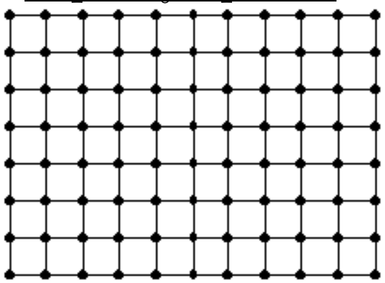
$$\begin{bmatrix} T_0(x_0) & T_1(x_0) & \cdots & T_N(x_0) \\ T_0(x_1) & T_1(x_1) & \cdots & T_N(x_1) \\ \vdots & \vdots & \ddots & \vdots \\ T_0(x_N) & T_1(x_N) & \cdots & T_N(x_N) \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_N \end{bmatrix} = \begin{bmatrix} f_0 \\ f_1 \\ \vdots \\ f_N \end{bmatrix}$$

System is non-singular provided the nodes are distinct

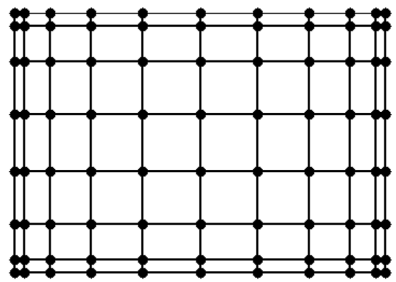
Polynomial interpolation in higher dimensions *Part 1*

- Tensor product grids:

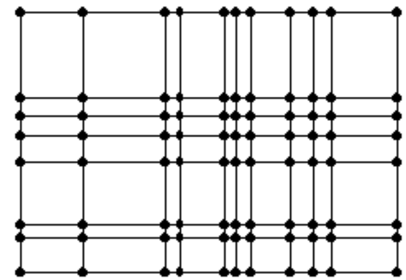
Equally spaced



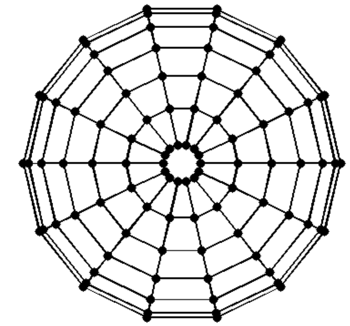
Boundary clustered



Irregular

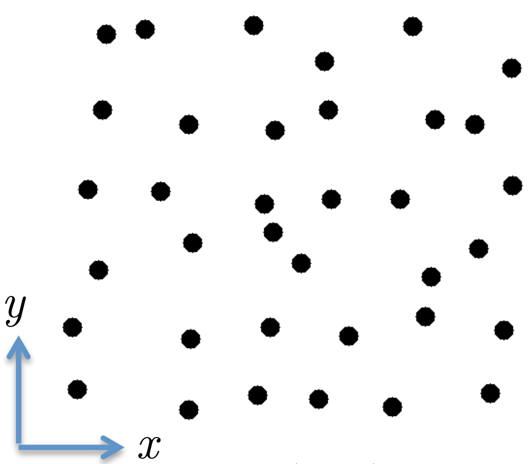


Polar grid:



Use standard 1-D interpolation in each direction and combine as a tensor product.

- What happens for scattered data?



$\mathbf{x} = (x, y)$

$\{T_k\}_{k=0}^N$ some bivariate polynomial basis

Interpolant: $I_N f = \sum_{k=0}^{N} c_k T_k(\mathbf{x}), \quad I_N f\Big|_{\mathbf{x}=\mathbf{x}_j} = f_j$

Expansion coefficients:

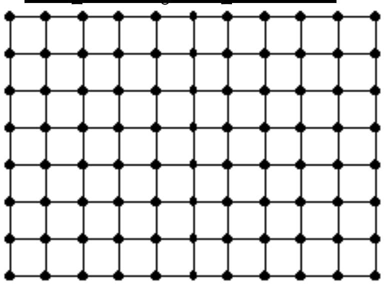
$$\begin{bmatrix} T_0(\mathbf{x}_0) & T_1(\mathbf{x}_0) & \cdots & T_N(\mathbf{x}_0) \\ T_0(\mathbf{x}_1) & T_1(\mathbf{x}_1) & \cdots & T_N(\mathbf{x}_1) \\ \vdots & \vdots & \ddots & \vdots \\ T_0(\mathbf{x}_N) & T_1(\mathbf{x}_N) & \cdots & T_N(\mathbf{x}_N) \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_N \end{bmatrix} = \begin{bmatrix} f_0 \\ f_1 \\ \vdots \\ f_N \end{bmatrix}$$

Depending on nodes, the system can be singular

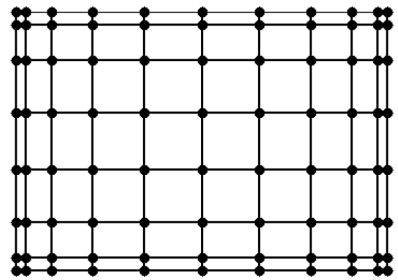
Polynomial interpolation in higher dimensions *Part 1*

- Tensor product grids:

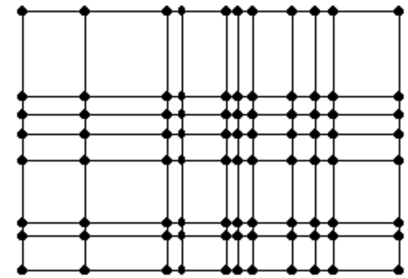
Equally spaced



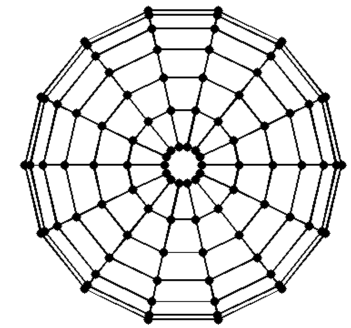
Boundary clustered



Irregular

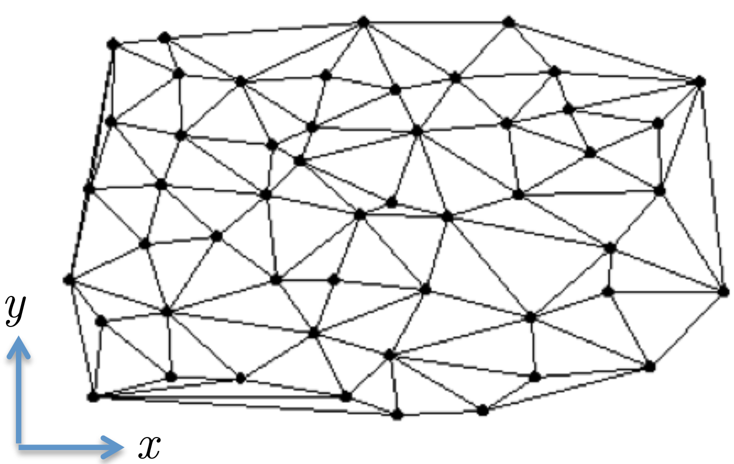


Polar grid:



Use standard 1-D interpolation in each direction and combine as a tensor product.

- What happens for scattered data?



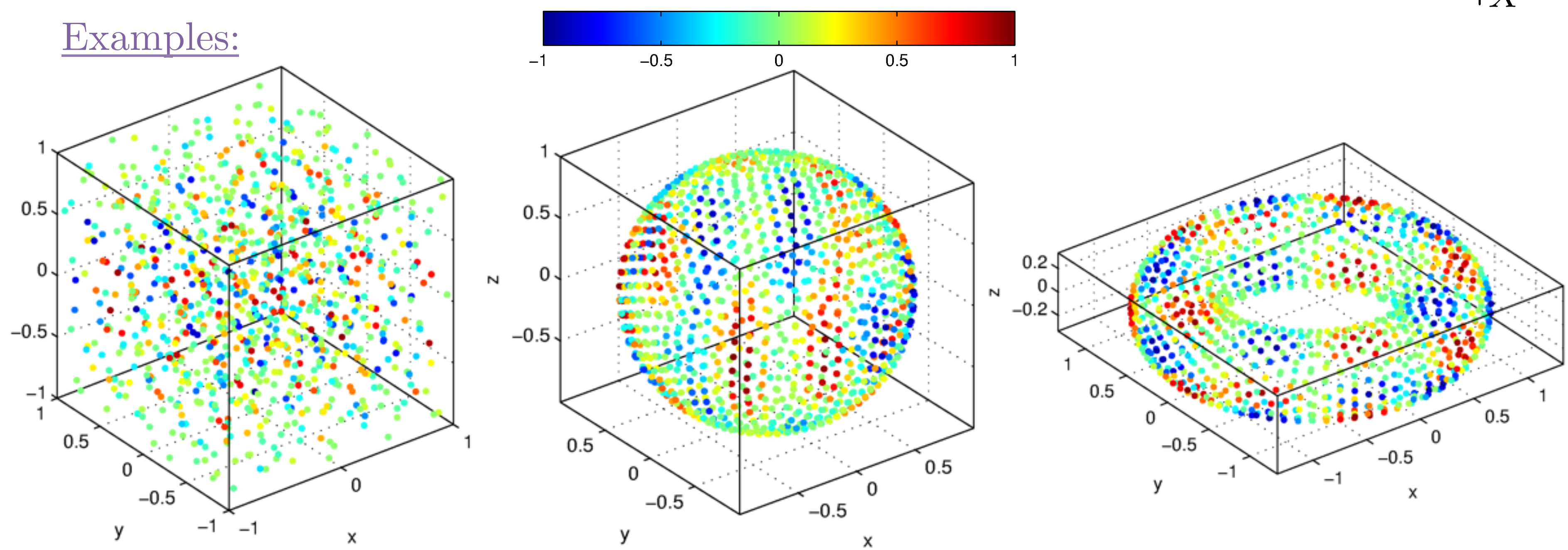
- Can triangulate the nodes and use splines.
- Achieving high orders of accuracy then becomes and difficult/impossible.
- Extensions to higher dimensions becomes increasingly complex.

Interpolation with kernels

- Let $\Omega \subset \mathbb{R}^d$ and $X = \{\mathbf{x}_j\}_{j=1}^N$ a set of nodes on Ω.

- Consider a continuous target function $f : \Omega \to \mathbb{R}$ sampled at X: $f\big|_X$.

Examples:



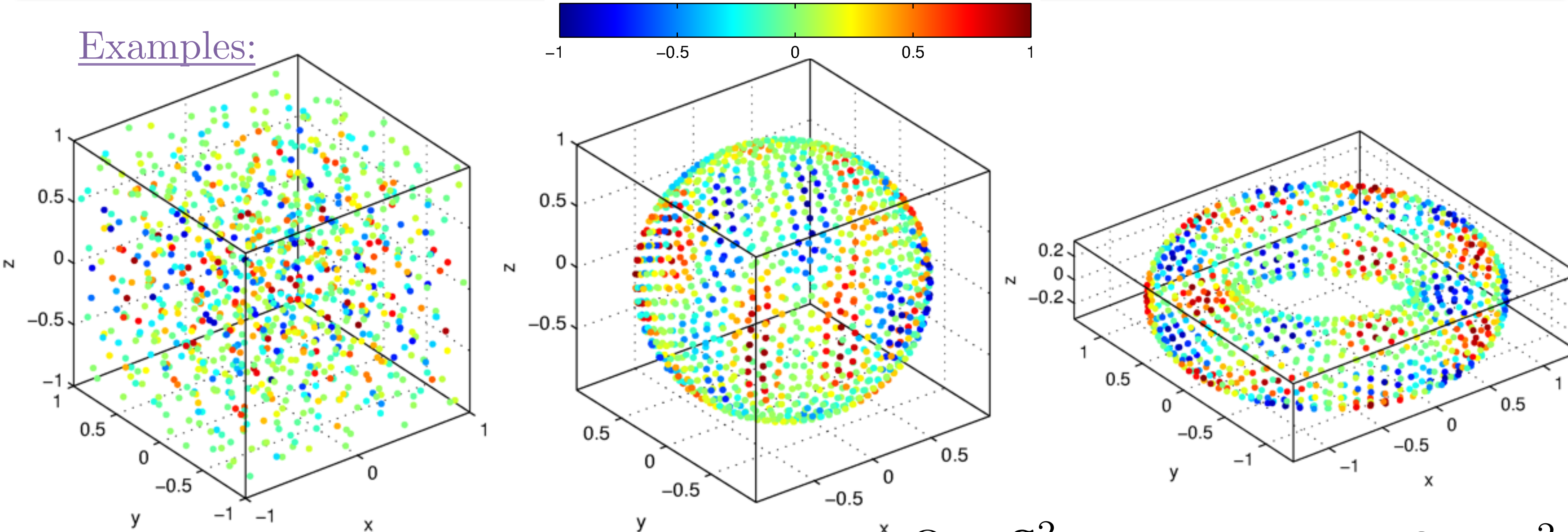
$\Omega = [-1, 1]^3$ $\qquad$ $\Omega = \mathbb{S}^2$ $\qquad$ $\Omega = \mathbb{T}^2$

- Kernel interpolant to $f\big|_X$: $\qquad I_X f = \sum_{j=1}^{N} c_j \Phi(\cdot, \mathbf{x}_j)$

  where $\Phi : \Omega \times \Omega \to \mathbb{R}$ and c_j come from requiring $I_X f\big|_X = f\big|_X$

Interpolation with kernels

Examples:



$\Omega = [-1,1]^3$ $\Omega = \mathbb{S}^2$ $\Omega = \mathbb{T}^2$

- Kernel interpolant to $f\Big|_X$: $\quad I_X f = \sum_{j=1}^{N} c_j \Phi(\cdot, \mathbf{x}_j)$

- Definition: Φ is a positive definite kernel on Ω if the matrix $A = \{\Phi(\mathbf{x}_i, \mathbf{x}_j)\}$ is positive definite for any distinct $X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega$, i.e.

$$\sum_{i=1}^{N}\sum_{j=1}^{N} b_i \Phi(\mathbf{x}_i, \mathbf{x}_j) b_j > 0, \text{ provided } \{b_i\}_{i=1}^N \not\equiv 0.$$

- In this case c_j are uniquely determined by X and $f\Big|_X$.

Interpolation with kernels

- Kernel interpolant to $f\big|_X$: $\quad I_X f = \sum_j c_j \Phi(\cdot, \mathbf{x}_j)$.
- Some considerations for choosing the kernel $\Phi : \Omega \times \Omega \to \mathbb{R}$

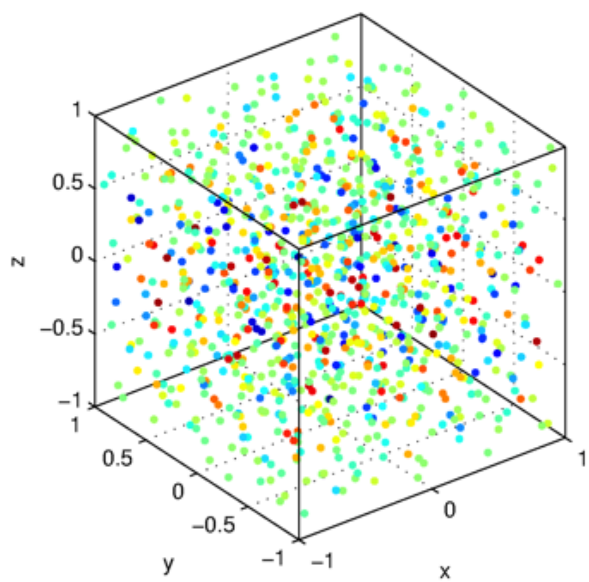
   1. The kernel should be easy to compute.
   2. The kernel interpolant should be uniquely determined by X and $f\big|_X$.
   3. The kernel interpolant should accurately reconstruct f.

Interpolation with kernels

- Kernel interpolant to $f\big|_X$: $\quad I_X f = \sum_j c_j \Phi(\cdot, \mathbf{x}_j)$.
- Some considerations for choosing the kernel $\Phi : \Omega \times \Omega \to \mathbb{R}$

  1. The kernel should be easy to compute.
  2. The kernel interpolant should be uniquely determined by X and $f\big|_X$.
  3. The kernel interpolant should accurately reconstruct f.

- For problems like



$\Omega = [-1, 1]^3$

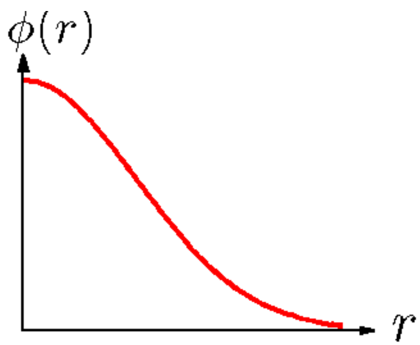
Good choice: ϕ is a (conditionally) positive definite radial kernel

$$\Phi(\mathbf{x}, \mathbf{x}_j) = \phi(\|\mathbf{x} - \mathbf{x}_j\|_2) = \phi(r)$$

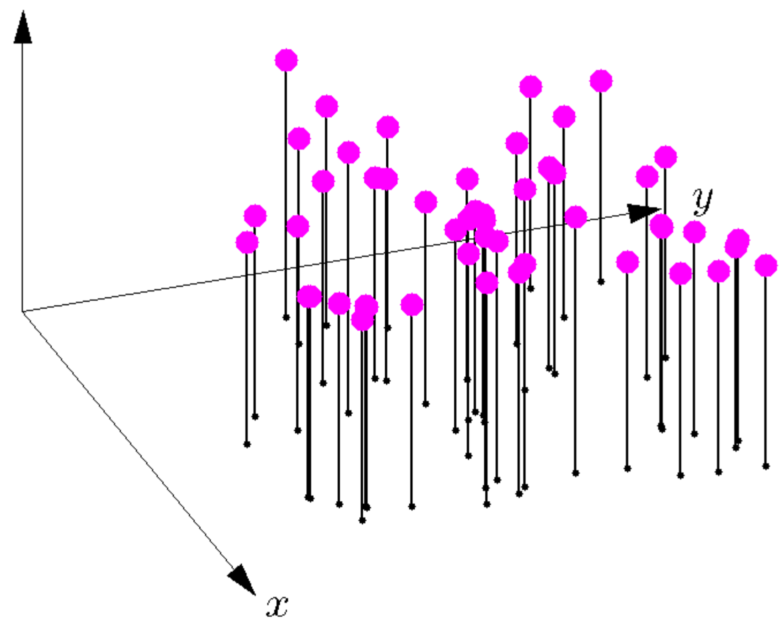
- Leads to RBF interpolation.

RBF interpolation

Key idea: linear combination of translates and rotations of a single radial kernel:



$f \qquad X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega, \quad f\big|_X = \{f_j\}_{j=1}^N$



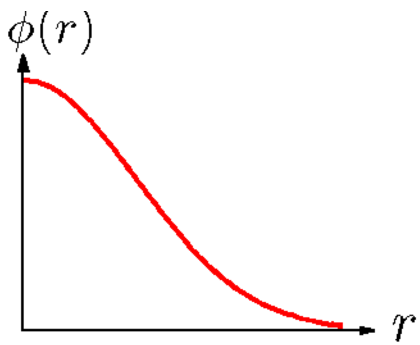
Basic RBF Interpolant for $\Omega \subseteq \mathbb{R}^2$

$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \phi(\|\mathbf{x} - \mathbf{x}_j\|)$$

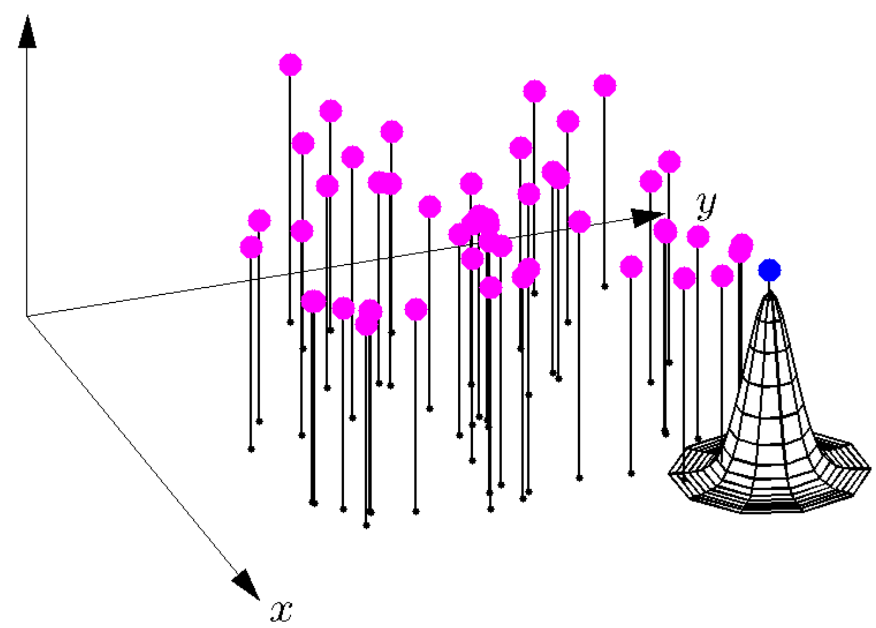
where $\|\mathbf{x} - \mathbf{x}_j\| = \sqrt{(x - x_j)^2 + (y - y_j)^2}$

RBF interpolation

Key idea: linear combination of translates and rotations of a single radial kernel:



$X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega, \quad f\Big|_X = \{f_j\}_{j=1}^N$



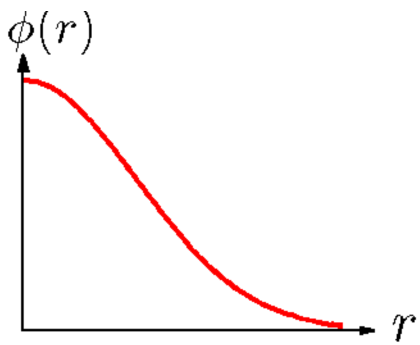
Basic RBF Interpolant for $\Omega \subseteq \mathbb{R}^2$

$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \phi(\|\mathbf{x} - \mathbf{x}_j\|)$$

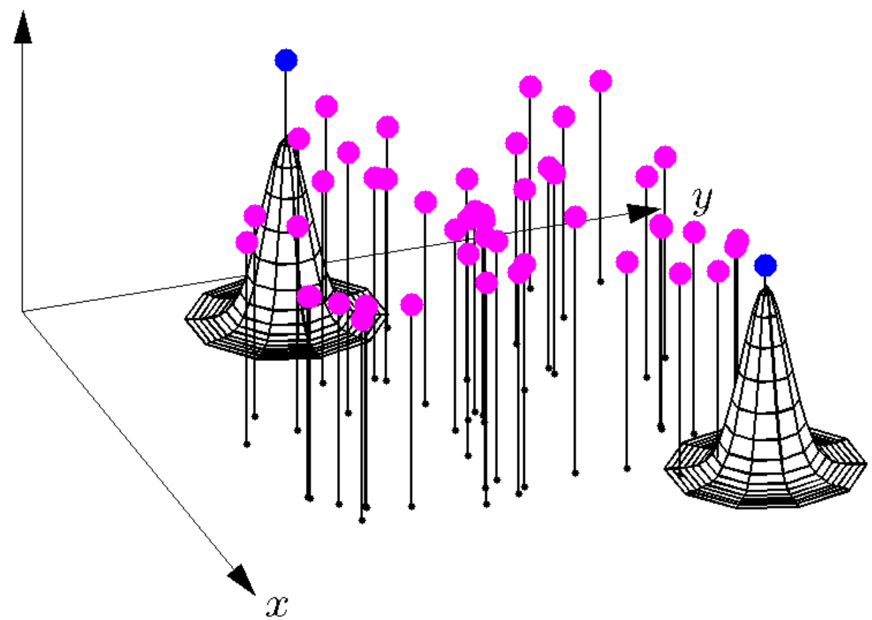
where $\|\mathbf{x} - \mathbf{x}_j\| = \sqrt{(x - x_j)^2 + (y - y_j)^2}$

RBF interpolation

<u>Key idea</u>: linear combination of translates and rotations of a single radial kernel:



$X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega, \quad f\Big|_X = \{f_j\}_{j=1}^N$



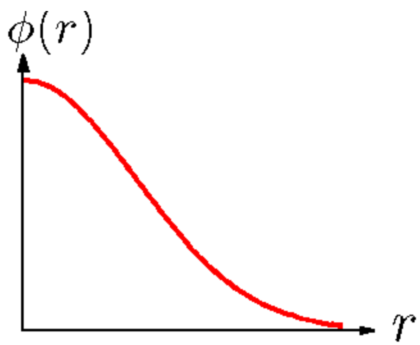
<u>Basic RBF Interpolant for $\Omega \subseteq \mathbb{R}^2$</u>

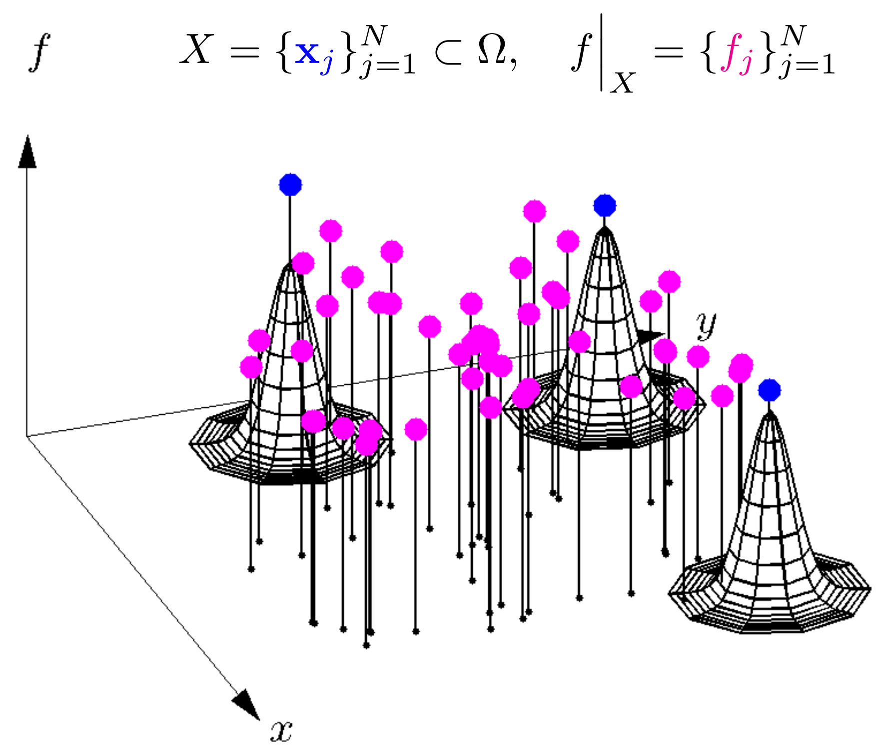
$$I_X f(\mathbf{x}) = \sum_{j=1}^N c_j \phi(\|\mathbf{x} - \mathbf{x}_j\|)$$

where $\|\mathbf{x} - \mathbf{x}_j\| = \sqrt{(x - x_j)^2 + (y - y_j)^2}$

RBF interpolation

Key idea: linear combination of translates and rotations of a single radial kernel:





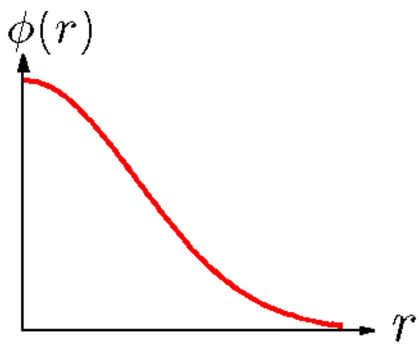
Basic RBF Interpolant for $\Omega \subseteq \mathbb{R}^2$

$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \phi(\|\mathbf{x} - \mathbf{x}_j\|)$$

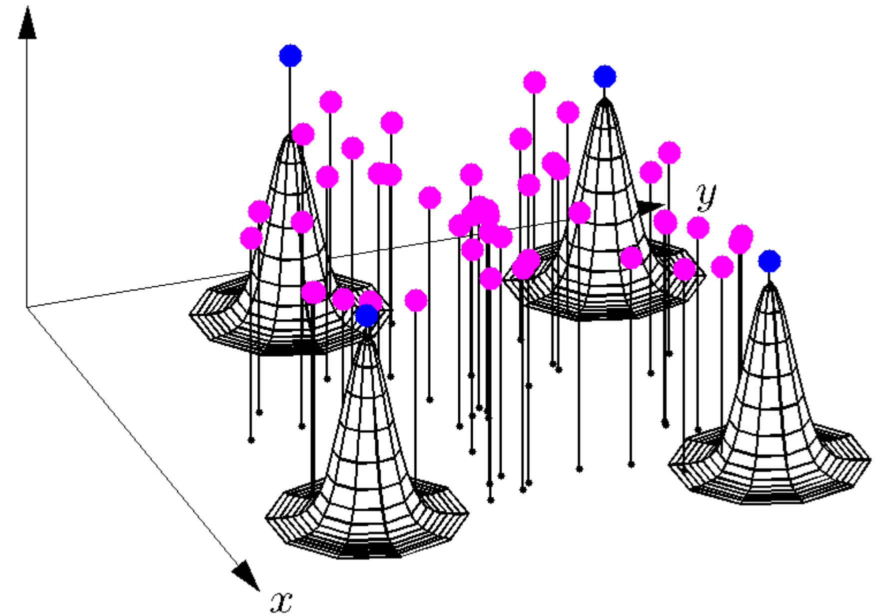
where $\|\mathbf{x} - \mathbf{x}_j\| = \sqrt{(x - x_j)^2 + (y - y_j)^2}$

RBF interpolation

Key idea: linear combination of translates and rotations of a single radial kernel:



$$X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega, \quad f\Big|_X = \{f_j\}_{j=1}^N$$



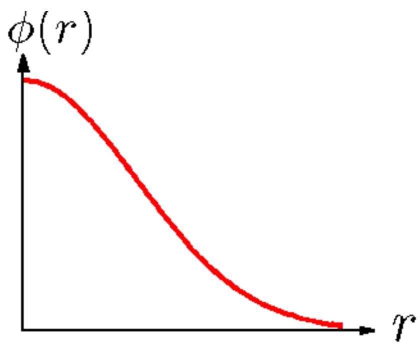
Basic RBF Interpolant for $\Omega \subseteq \mathbb{R}^2$

$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \phi(\|\mathbf{x} - \mathbf{x}_j\|)$$

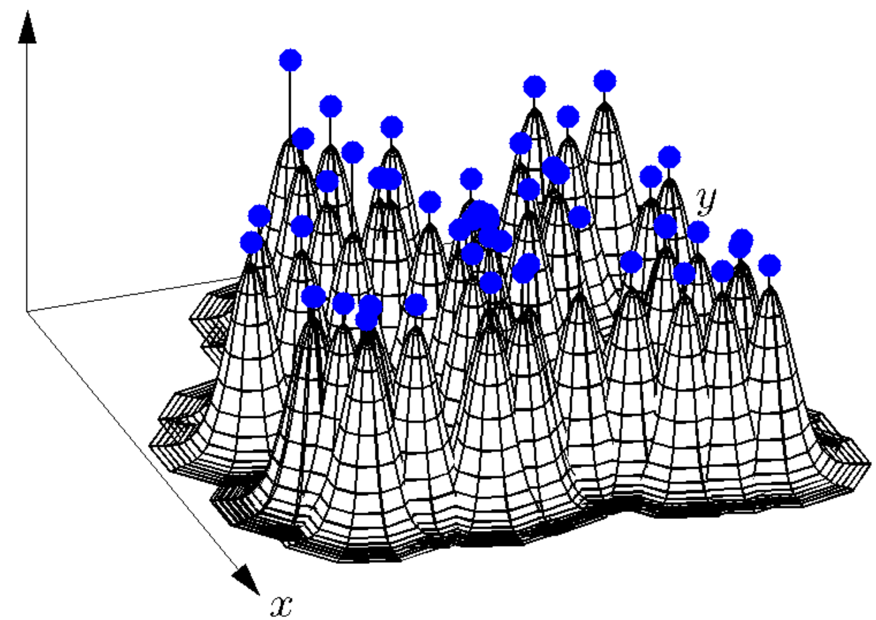
where $\|\mathbf{x} - \mathbf{x}_j\| = \sqrt{(x - x_j)^2 + (y - y_j)^2}$

RBF interpolation

Key idea: linear combination of translates and rotations of a single radial kernel:



$f \qquad X = \{\mathbf{x}_j\}_{j=1}^{N} \subset \Omega, \quad f\Big|_X = \{f_j\}_{j=1}^{N}$



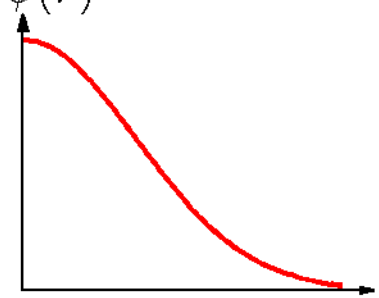
Basic RBF Interpolant for $\Omega \subseteq \mathbb{R}^2$

$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \phi(\|\mathbf{x} - \mathbf{x}_j\|)$$

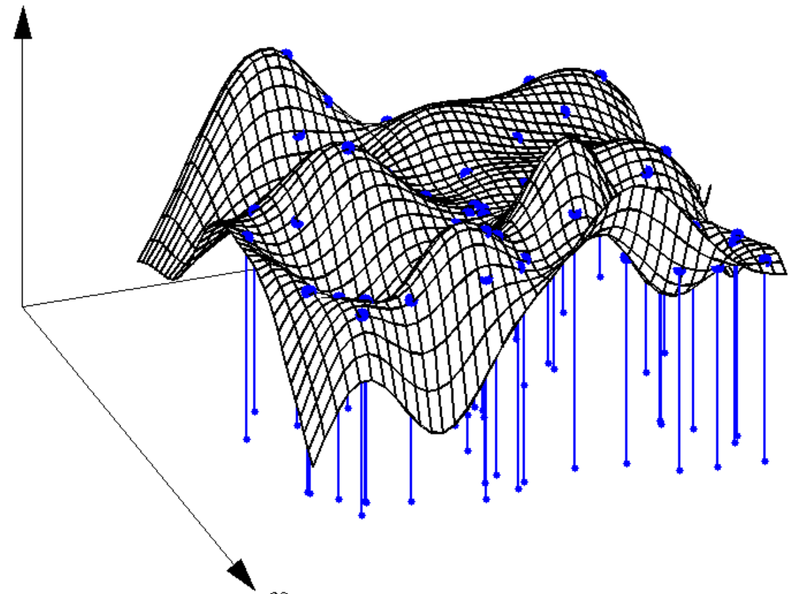
where $\|\mathbf{x} - \mathbf{x}_j\| = \sqrt{(x - x_j)^2 + (y - y_j)^2}$

RBF interpolation

Key idea: linear combination of translates and rotations of a single radial kernel:



$X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega, \quad f\big|_X = \{f_j\}_{j=1}^N$



Basic RBF Interpolant for $\Omega \subseteq \mathbb{R}^2$

$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \phi(\|\mathbf{x} - \mathbf{x}_j\|)$$

Linear system for determining the interpolation coefficients

$$\underbrace{\begin{bmatrix} \phi(\|\mathbf{x}_1 - \mathbf{x}_1\|) & \phi(\|\mathbf{x}_1 - \mathbf{x}_2\|) & \cdots & \phi(\|\mathbf{x}_1 - \mathbf{x}_N\|) \\ \phi(\|\mathbf{x}_2 - \mathbf{x}_1\|) & \phi(\|\mathbf{x}_2 - \mathbf{x}_2\|) & \cdots & \phi(\|\mathbf{x}_2 - \mathbf{x}_N\|) \\ \vdots & \vdots & \ddots & \vdots \\ \phi(\|\mathbf{x}_N - \mathbf{x}_1\|) & \phi(\|\mathbf{x}_N - \mathbf{x}_2\|) & \cdots & \phi(\|\mathbf{x}_N - \mathbf{x}_N\|) \end{bmatrix}}_{A_X} \underbrace{\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{bmatrix}}_{\underline{c}} = \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{bmatrix}}_{\underline{f}}$$

A_X is guaranteed to be positive definite if ϕ is positive definite.

Positive definite radial kernels

- Important result on positive definite kernels:

  Theorem (General kernel). Let ϕ be a continuous kernel in $L_1(\mathbb{R}^d)$. Then ϕ is positive definite if and only if ϕ is bounded and its d-dimensional Fourier transform $\hat{\phi}(\boldsymbol{\omega})$ is non-negative and not identically equal to zero.

  Remark: Related to Bochner's theorem (1933). Theorem and proof can be found in Wendland (2005).

- To make the result specific to radial kernels, we apply the d-dimensional Fourier transform and use radial symmetry to get (Hankel transform):

$$\hat{\phi}(\boldsymbol{\omega}) = \hat{\phi}(\|\boldsymbol{\omega}\|_2) = \frac{1}{\|\boldsymbol{\omega}\|_2^{\nu}} \int_0^{\infty} \phi(t) t^{d/2+1} J_{\nu}(\|\boldsymbol{\omega}\|_2 t) dt,$$

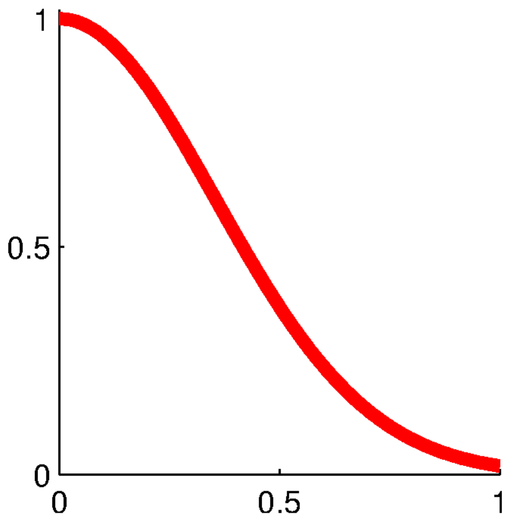
  where $\nu = d/2 - 1$ and J_ν is the J-Bessel function of order ν.

- Note that if ϕ is positive definite on $\mathbb{R}^d$ then it is positive definite on $\mathbb{R}^k$ for any $k \leq d$.

Positive definite radial kernels

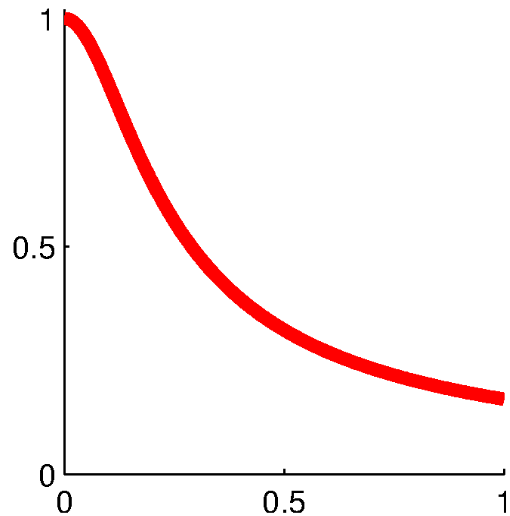
- Examples of positive definite kernels on $\mathbb{R}^d$, for any d

Gaussian



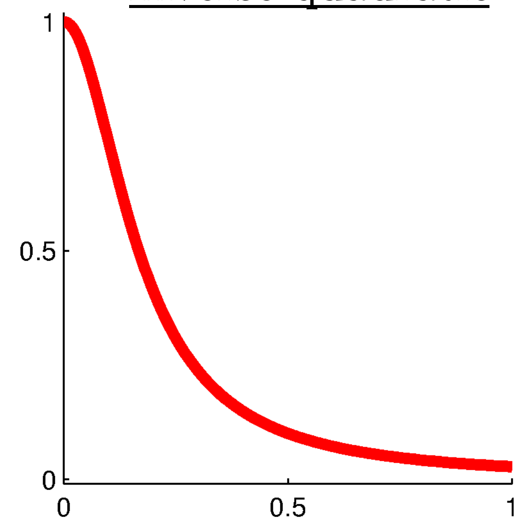
$$\phi(r) = \exp(-(\varepsilon r)^2)$$

Inverse multiquadric



$$\phi(r) = \frac{1}{\sqrt{1+(\varepsilon r)^2}}$$

Inverse quadratic



$$\phi(r) = \frac{1}{1+(\varepsilon r)^2}$$

- ε is called the shape parameter (more on this later).
- These kernels are infinitely smooth.

Positive definite radial kernels

- Examples of dimension specific positive definite kernels

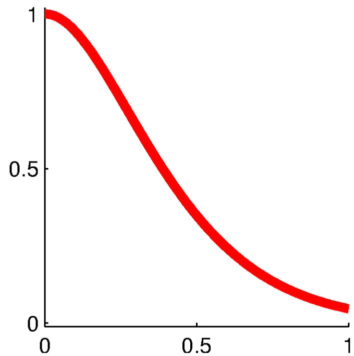
Finite-smoothness

Matérn

$(\varepsilon r)^{\nu-d/2} K_{\nu-d/2}(\varepsilon r)$

PD for $2\nu > d$

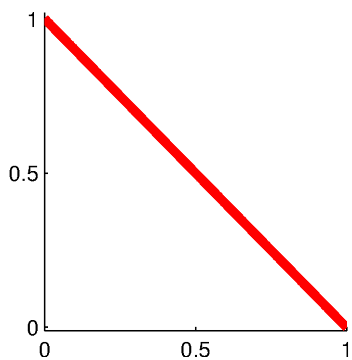
Ex: $e^{-r}(r^2 + 3r + 3)$



Truncated powers

$(1 - \varepsilon r)_+^{\ell}$

PD for $\ell \geq \lfloor d/2 \rfloor + 1$

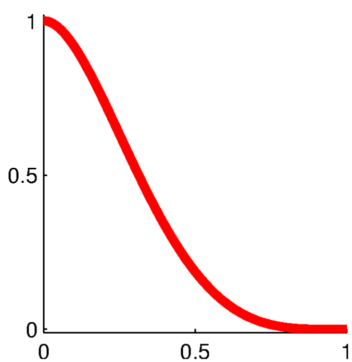


Wendland (1995)

$(1 - \varepsilon r)_+^k p_{d,k}(\varepsilon r)$

$p_{d,k}$ is a polynomial whose degree depends on d and k.

Ex: $(1 - \varepsilon r)_+^4 (4\varepsilon r + 1)$

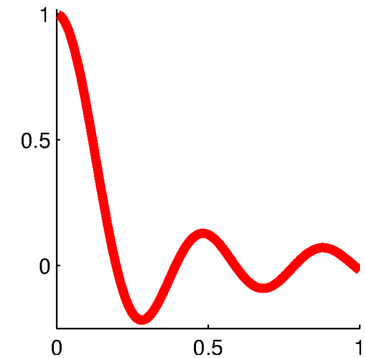


Infinite-smoothness

J-Bessel

$$\frac{J_{d/2-1}(\varepsilon r)}{(\varepsilon r)^{d/2}}$$

Ex $(d = 3)$: $\dfrac{\sin(\varepsilon r)}{\varepsilon r}$

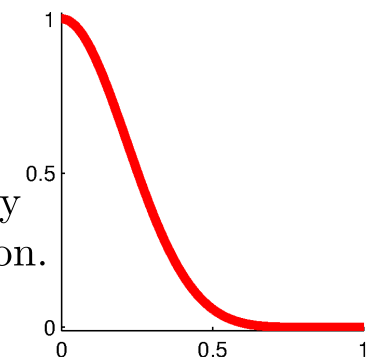


Platte

$(\varphi * \varphi)(r)$

φ is a $C^\infty(\mathbb{R})$ compactly supported radial function.

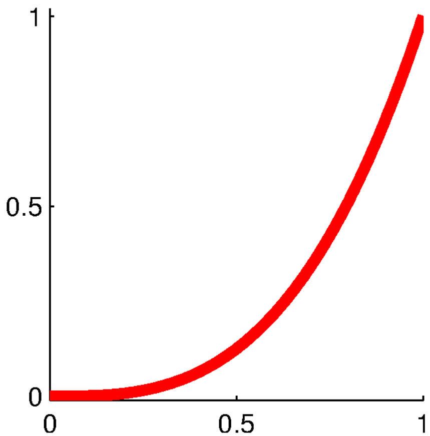
PD dimension depends on convolution dimension.



Conditionally positive definite kernels

- Discussion thus far does not cover many important radial kernels:

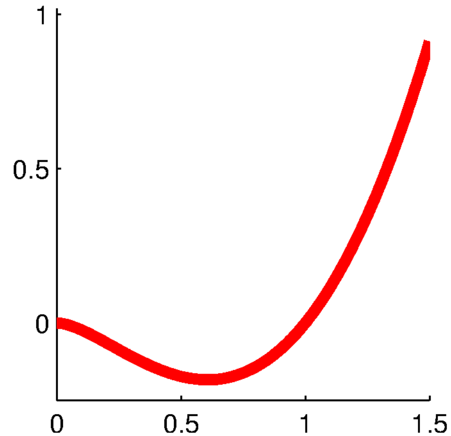
Cubic



$\phi(r) = r^3$

Cubic spline in 1-D

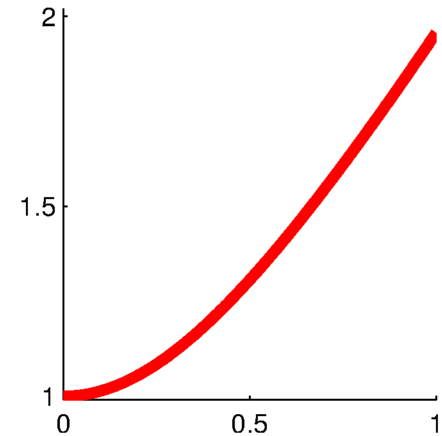
Thin plate spline



$\phi(r) = r^2 \log r$

Generalization of energy minimizing spline in 2D

Multiquadric



$\phi(r) = \sqrt{1 + (\varepsilon r)^2}$

Popular kernel and first used in any RBF application; Hardy 1971

- These can covered under the theory of conditionally positive definite kernels.

- CPD kernels can be characterized similar to PD kernels but, using generalized Fourier transforms; see Ch. 8 Wendland 2005 for details.

- See the supplementary lecture slides for details for a characterization of these kernels.

Conditionally positive definite kernels

Definition. A continuous radial kernel $\phi : [0, \infty) \to \mathbb{R}$ is said to be conditionally positive definite of order k on $\mathbb{R}^d$ if, for any distinct $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{R}^d$, and all $\mathbf{b} \in \mathbb{R}^N \backslash \{\mathbf{0}\}$ satisfying

$$\sum_{j=1}^{N} b_j p(\mathbf{x}_j) = 0$$

for all d-variate polynomials of degree $< k$, the following is satisfied:

$$\sum_{i=1}^{N} \sum_{j=1}^{N} b_i \phi(\|\mathbf{x}_i - \mathbf{x}_j\|) b_j > 0.$$

Conditionally positive definite kernels

Definition. A continuous radial kernel $\phi : [0, \infty) \to \mathbb{R}$ is said to be conditionally positive definite of order k on $\mathbb{R}^d$ if, for any distinct $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{R}^d$, and all $\mathbf{b} \in \mathbb{R}^N \backslash \{\mathbf{0}\}$ satisfying

$$\sum_{j=1}^{N} b_j p(\mathbf{x}_j) = 0$$

for all d-variate polynomials of degree $< k$, the following is satisfied:

$$\sum_{i=1}^{N} \sum_{j=1}^{N} b_i \phi(\|\mathbf{x}_i - \mathbf{x}_j\|) b_j > 0.$$

- Alternatively, ϕ is positive definite on the subspace $V_{k-1} \subset \mathbb{R}^N$:

$$V_{k-1} = \left\{ \mathbf{b} \in \mathbb{R}^N \middle| \sum_{j=1}^{N} b_j p(\mathbf{x}_j) = 0 \text{ for all } p \in \Pi_{k-1}(\mathbb{R}^d) \right\},$$

  where $\Pi_m(\mathbb{R}^d)$ is the space of all d-variate polynomials of degree $\leq m$.

- The case $k = 0$, corresponds to standard positive definite kernels on $\mathbb{R}^d$.

Conditionally positive definite kernels

Definition. Let $\phi : [0, \infty) \to \mathbb{R}$ be continuous and $\{p_i(\mathbf{x})\}_{i=1}^n$ be a basis for $\Pi_{k-1}(\mathbb{R}^d)$ $(k > 1)$. The general RBF interpolant for the distinct nodes $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{R}^d$ and some target, f, sampled on X, $\{f_j\}_{j=1}^N$ is

$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \phi(\|\mathbf{x} - \mathbf{x}_j\|) + \sum_{\ell=1}^{n} d_\ell p_\ell(\mathbf{x}),$$

where $I_X f(\mathbf{x}_i) = f_i$, $i = 1, \ldots, N$ and $\sum_{j=1}^{N} c_j p_\ell(\mathbf{x}_j) = 0$, $\ell = 1, \ldots, n$.

In linear system form, these constraints are

$$\begin{bmatrix} A & P \\ P^T & 0 \end{bmatrix} \begin{bmatrix} \underline{c} \\ \underline{d} \end{bmatrix} = \begin{bmatrix} \underline{f} \\ \underline{0} \end{bmatrix}, \text{ where } a_{i,j} = \phi(\|\mathbf{x}_i - \mathbf{x}_j\|), \; p_{i,\ell} = p_k(\mathbf{x}_i)$$

Conditionally positive definite kernels

Definition. Let $\phi : [0, \infty) \to \mathbb{R}$ be continuous and $\{p_i(\mathbf{x})\}_{i=1}^{n}$ be a basis for $\Pi_{k-1}(\mathbb{R}^d)$ $(k > 1)$. The general RBF interpolant for the distinct nodes $X = \{\mathbf{x}_j\}_{j=1}^{N} \subset \mathbb{R}^d$ and some target, f, sampled on X, $\{f_j\}_{j=1}^{N}$ is

$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \phi(\|\mathbf{x} - \mathbf{x}_j\|) + \sum_{\ell=1}^{n} d_\ell p_\ell(\mathbf{x}),$$

where $I_X f(\mathbf{x}_i) = f_i$, $i = 1, \ldots, N$ and $\sum_{j=1}^{N} c_j p_\ell(\mathbf{x}_j) = 0$, $\ell = 1, \ldots, n$.

In linear system form, these constraints are

$$\begin{bmatrix} A & P \\ P^T & 0 \end{bmatrix} \begin{bmatrix} \underline{c} \\ \underline{d} \end{bmatrix} = \begin{bmatrix} \underline{f} \\ \underline{0} \end{bmatrix}, \text{ where } a_{i,j} = \phi(\|\mathbf{x}_i - \mathbf{x}_j\|),\ p_{i,\ell} = p_k(\mathbf{x}_i)$$

Theorem (Micchelli (1986)). The above linear system is invertible for any distinct X, provided

- $\text{rank}(P) = n$ (i.e. X is unisolvent on $\Pi_{k-1}(\mathbb{R}^d)$),
- ϕ is conditionally positive definite of order k.

Conditionally positive definite kernels

Definition. Let $\phi : [0,\infty) \to \mathbb{R}$ be continuous and $\{p_i(\mathbf{x})\}_{i=1}^{n}$ be a basis for $\Pi_{k-1}(\mathbb{R}^d)$ $(k > 1)$. The general RBF interpolant for the distinct nodes $X = \{\mathbf{x}_j\}_{j=1}^{N} \subset \mathbb{R}^d$ and some target, f, sampled on X, $\{f_j\}_{j=1}^{N}$ is

$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \phi(\|\mathbf{x} - \mathbf{x}_j\|) + \sum_{\ell=1}^{n} d_\ell p_\ell(\mathbf{x}),$$

where $I_X f(\mathbf{x}_i) = f_i$, $i = 1, \ldots, N$ and $\sum_{j=1}^{N} c_j p_\ell(\mathbf{x}_j) = 0$, $\ell = 1, \ldots, n$.

In linear system form, these constraints are

$$\begin{bmatrix} A & P \\ P^T & 0 \end{bmatrix} \begin{bmatrix} \underline{c} \\ \underline{d} \end{bmatrix} = \begin{bmatrix} \underline{f} \\ \underline{0} \end{bmatrix}, \text{ where } a_{i,j} = \phi(\|\mathbf{x}_i - \mathbf{x}_j\|),\ p_{i,\ell} = p_k(\mathbf{x}_i)$$

Example (Multiquadric, $\mathbb{R}^d$). $\phi(r) = \sqrt{1 + (\varepsilon r)^2}$

- Conditionally positive definite of order 1.
- $p_1(x, y, z) = 1$.

The system has a unique solution.

Conditionally positive definite kernels

Definition. Let $\phi : [0,\infty) \to \mathbb{R}$ be continuous and $\{p_i(\mathbf{x})\}_{i=1}^{n}$ be a basis for $\Pi_{k-1}(\mathbb{R}^d)$ $(k > 1)$. The general RBF interpolant for the distinct nodes $X = \{\mathbf{x}_j\}_{j=1}^{N} \subset \mathbb{R}^d$ and some target, f, sampled on X, $\{f_j\}_{j=1}^{N}$ is

$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \phi(\|\mathbf{x} - \mathbf{x}_j\|) + \sum_{\ell=1}^{n} d_\ell p_\ell(\mathbf{x}),$$

where $I_X f(\mathbf{x}_i) = f_i$, $i = 1, \ldots, N$ and $\sum_{j=1}^{N} c_j p_\ell(\mathbf{x}_j) = 0$, $\ell = 1, \ldots, n$.

In linear system form, these constraints are

$$\begin{bmatrix} A & P \\ P^T & 0 \end{bmatrix} \begin{bmatrix} \underline{c} \\ \underline{d} \end{bmatrix} = \begin{bmatrix} \underline{f} \\ \underline{0} \end{bmatrix}, \text{ where } a_{i,j} = \phi(\|\mathbf{x}_i - \mathbf{x}_j\|),\ p_{i,\ell} = p_k(\mathbf{x}_i)$$

Example (Thin plate spline, $\mathbb{R}^3$). $\phi(r) = r^2 \log(r)$

- Conditionally positive definite of order 2.
- $p_1(x,y,z) = 1$, $p_2(x,y,z) = x$, $p_3(x,y,z) = y$, and $p_4(x,y,z) = z$.

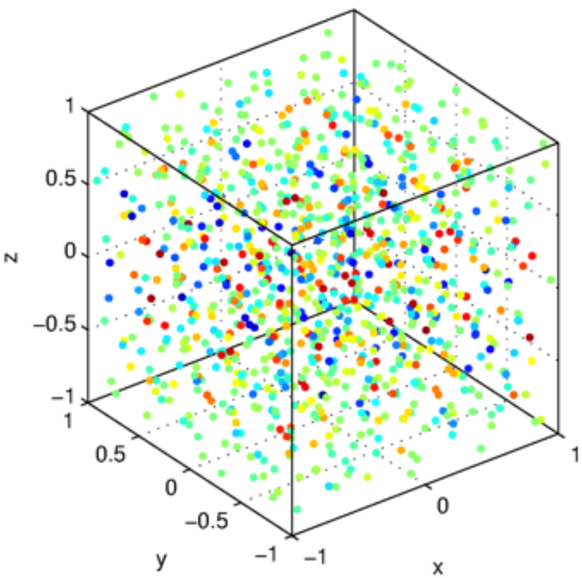
The system has a unique solution provided the nodes are not collinear.

Interpolation with kernels (revisited)

- Kernel interpolant to $f\big|_X$: $\qquad I_X f = \sum_j c_j \Phi(\cdot, \mathbf{x}_j)$.
- Some considerations for choosing the kernel $\Phi : \Omega \times \Omega \to \mathbb{R}$

  1. The kernel should be easy to compute.
  2. The kernel interpolant should be uniquely determined by X and $f\big|_X$.
  3. The kernel interpolant should accurately reconstruct f.

- For problems like



$\Omega = [-1, 1]^3$

Obvious choice: ϕ is a (conditionally) positive definite radial kernel

$$\Phi(\mathbf{x}, \mathbf{x}_j) = \phi(\|\mathbf{x} - \mathbf{x}_j\|_2) = \phi(r)$$

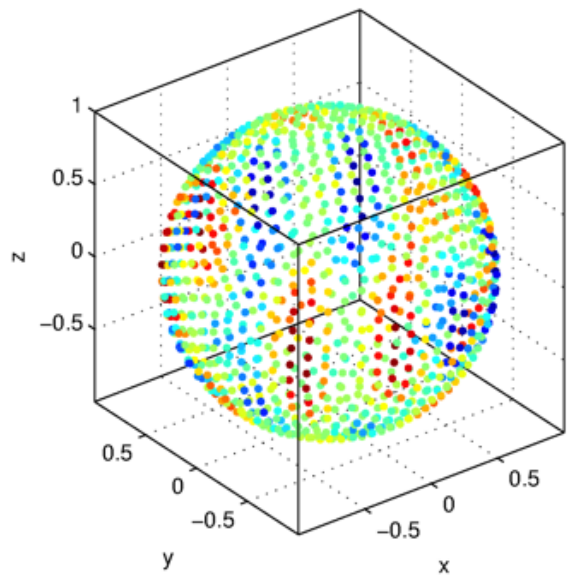
- Leads to RBF interpolation.

Interpolation with kernels on the sphere

- Kernel interpolant to $f\big|_X$: $\quad I_X f = \sum_j c_j \Phi(\cdot, \mathbf{x}_j)$.
- Some considerations for choosing the kernel $\Phi : \Omega \times \Omega \to \mathbb{R}$

   1. The kernel should be easy to compute.
   2. The kernel interpolant should be uniquely determined by X and $f\big|_X$.
   3. The kernel interpolant should accurately reconstruct f.

- For problems like



$\Omega = \mathbb{S}^2$

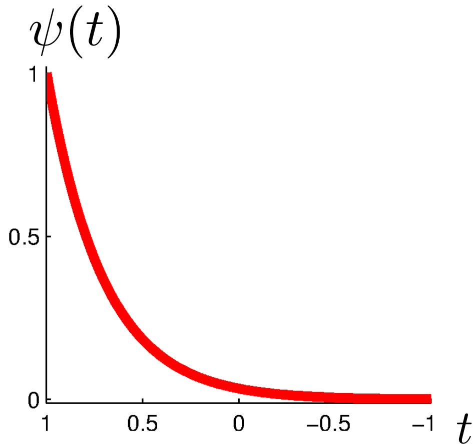
Obvious(?) choice: Φ is a (conditionally) positive definite zonal kernel:

$$\Phi(\mathbf{x}, \mathbf{x}_j) = \psi(\mathbf{x}^T \mathbf{x}_j) = \psi(t), \; t \in [-1, 1]$$

- Analog of RBF interpolation for the sphere: SBF interpolation.

SBF interpolation

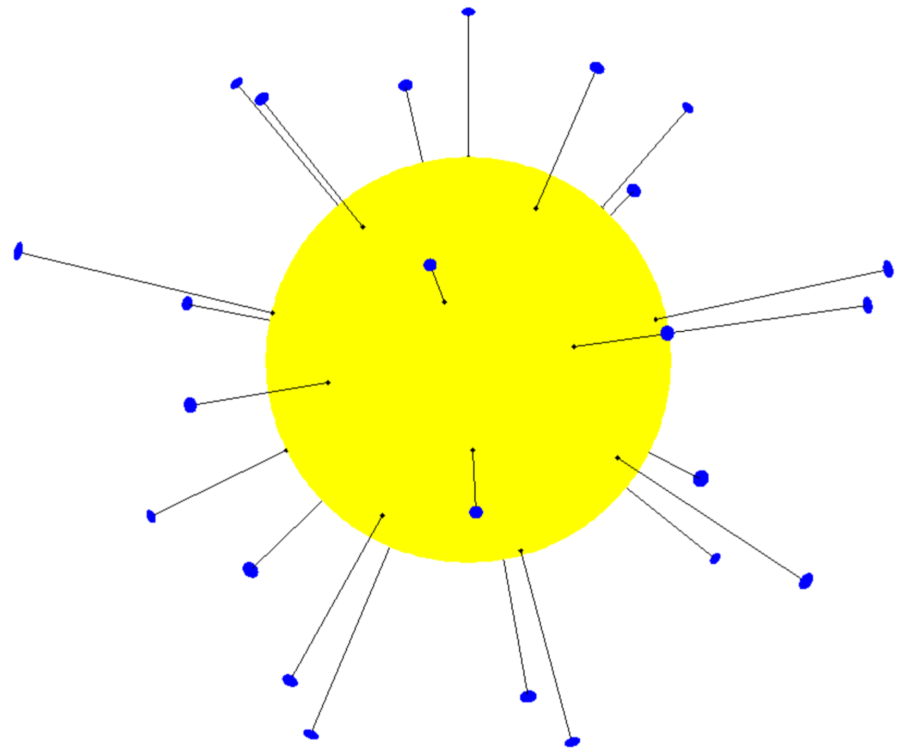
Key idea: linear combination of translates and rotations of a single zonal kernel on $\mathbb{S}^2$



Basic SBF Interpolant for $\mathbb{S}^2$

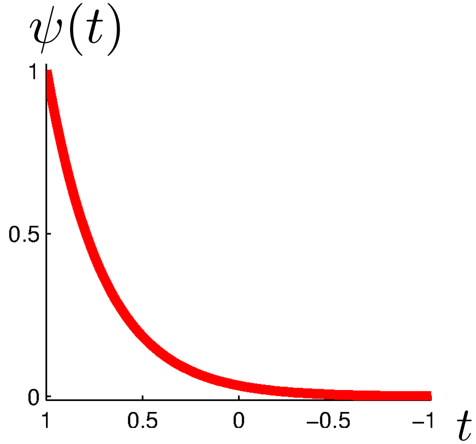
$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \psi(\mathbf{x}^T \mathbf{x}_j)$$

$X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega, \quad f\Big|_X = \{f_j\}_{j=1}^N$

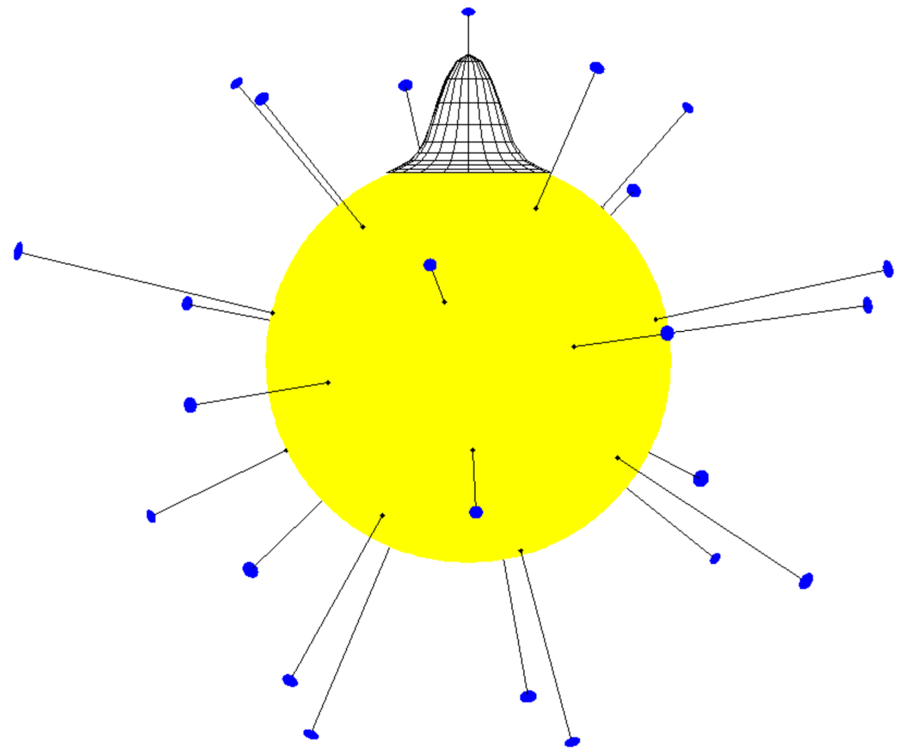


SBF interpolation

Key idea: linear combination of translates and rotations of a single zonal kernel on $\mathbb{S}^2$



$X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega, \quad f\Big|_X = \{f_j\}_{j=1}^N$

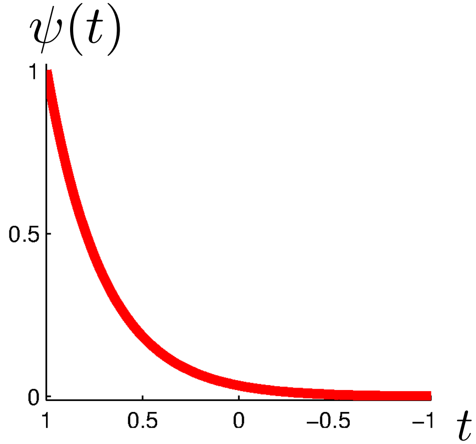


Basic SBF Interpolant for $\mathbb{S}^2$

$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \psi(\mathbf{x}^T \mathbf{x}_j)$$

SBF interpolation

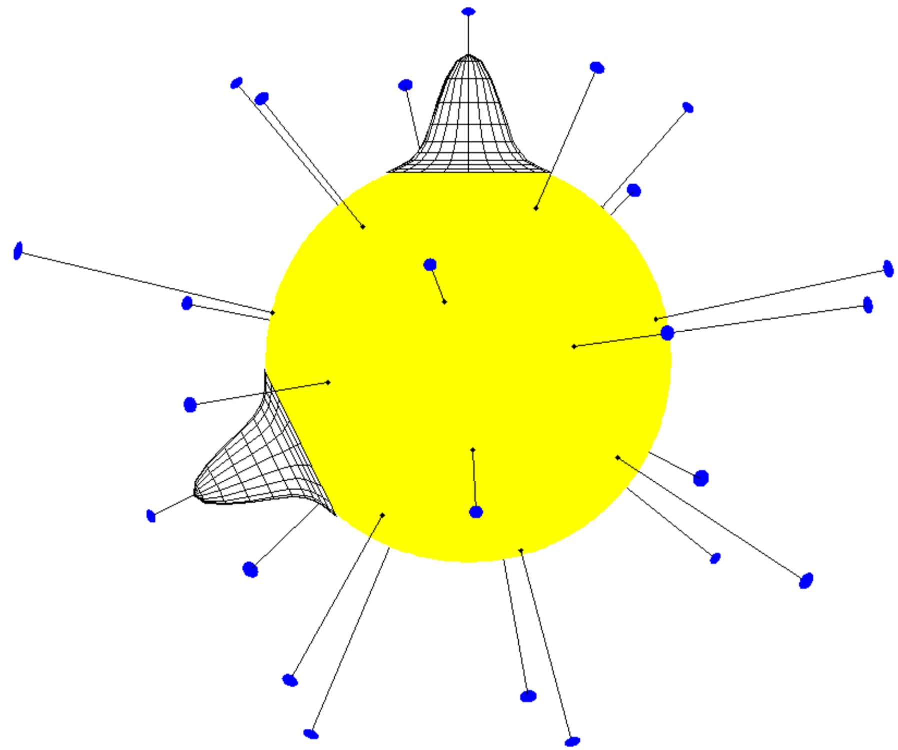
Key idea: linear combination of translates and rotations of a single zonal kernel on $\mathbb{S}^2$



Basic SBF Interpolant for $\mathbb{S}^2$

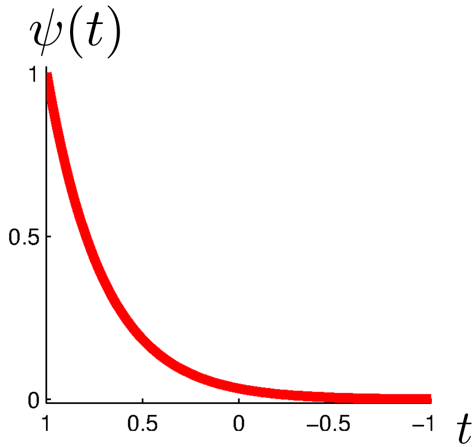
$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \psi(\mathbf{x}^T \mathbf{x}_j)$$

$$X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega, \quad f\Big|_X = \{f_j\}_{j=1}^N$$



SBF interpolation

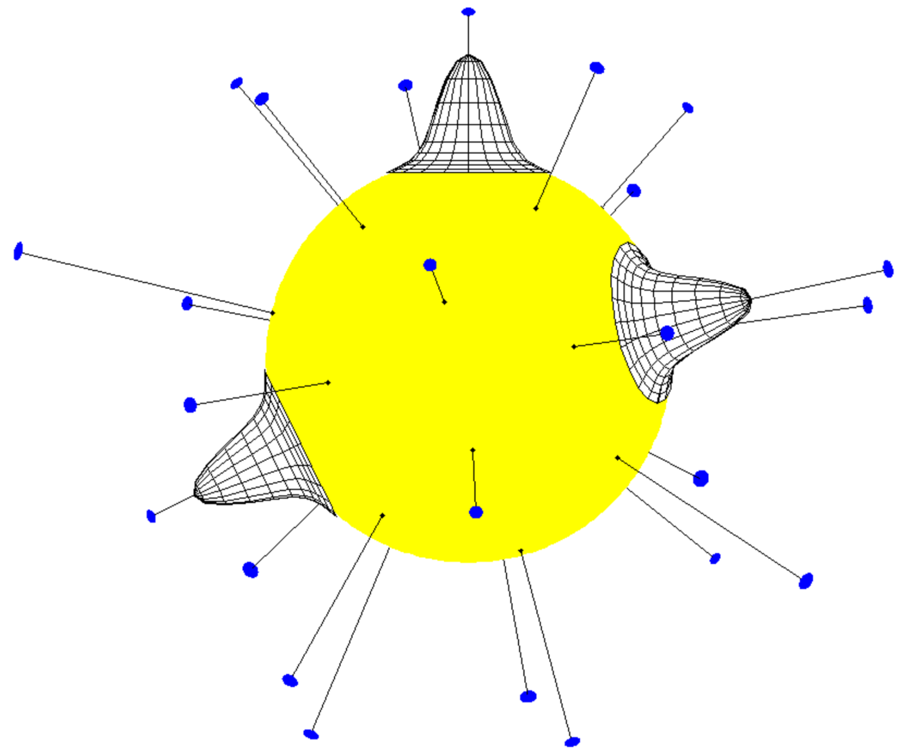
Key idea: linear combination of translates and rotations of a single zonal kernel on $\mathbb{S}^2$



Basic SBF Interpolant for $\mathbb{S}^2$

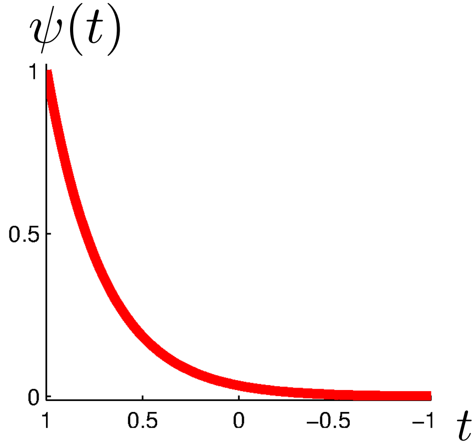
$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \psi(\mathbf{x}^T \mathbf{x}_j)$$

$$X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega, \quad f\Big|_X = \{f_j\}_{j=1}^N$$

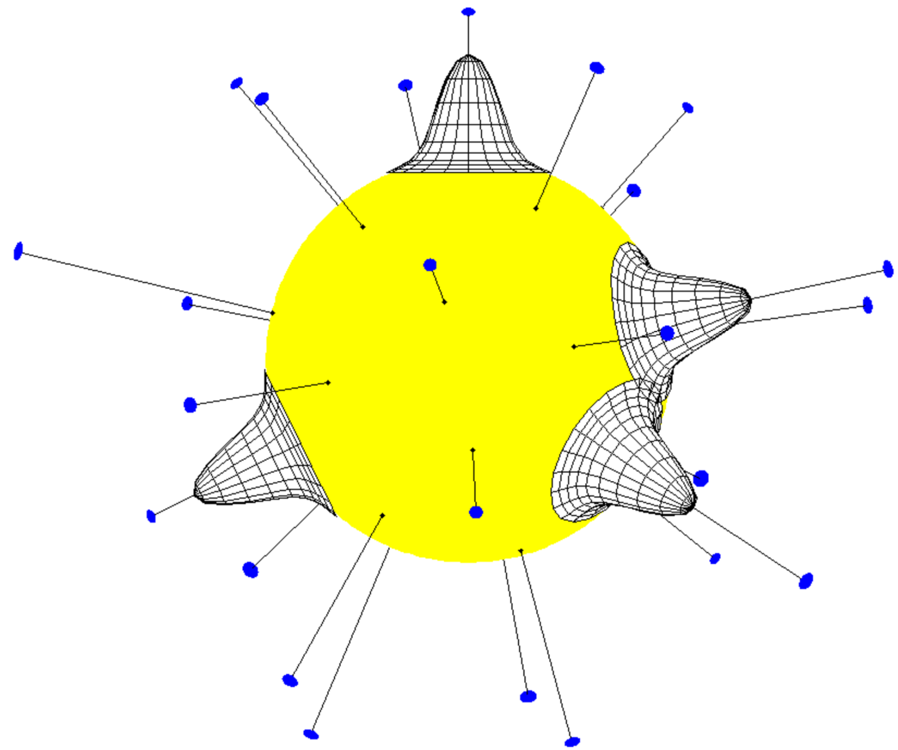


SBF interpolation

Key idea: linear combination of translates and rotations of a single zonal kernel on $\mathbb{S}^2$



$X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega, \quad f\Big|_X = \{f_j\}_{j=1}^N$

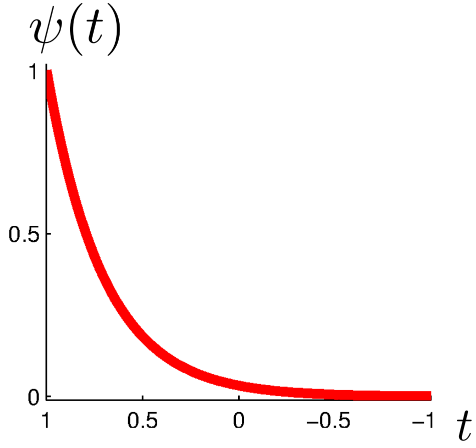


Basic SBF Interpolant for $\mathbb{S}^2$

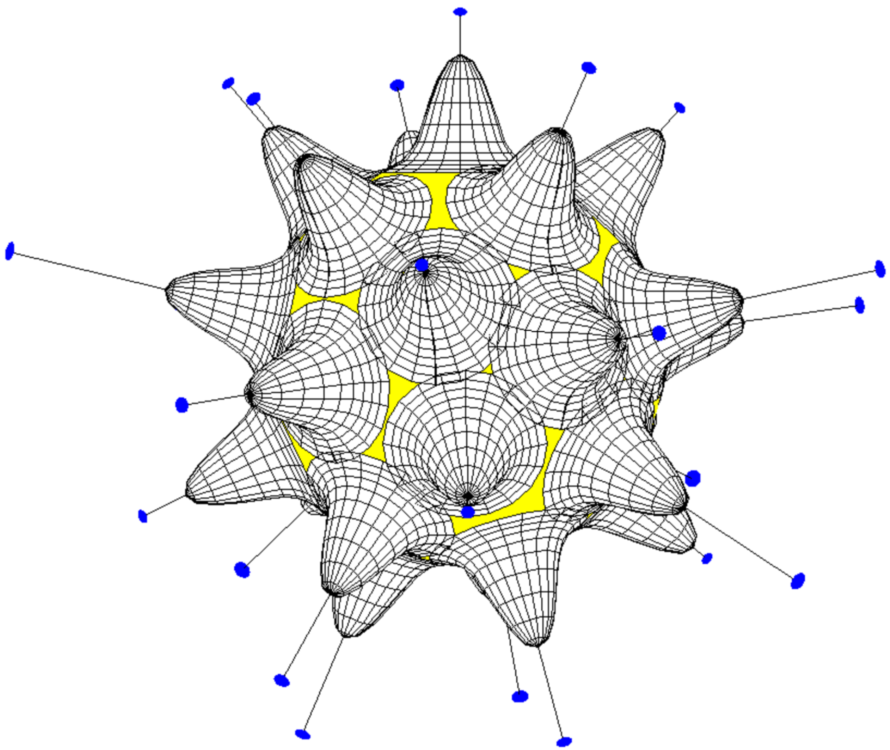
$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \psi(\mathbf{x}^T \mathbf{x}_j)$$

SBF interpolation

Key idea: linear combination of translates and rotations of a single zonal kernel on $\mathbb{S}^2$



$$X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega, \quad f\Big|_X = \{f_j\}_{j=1}^N$$



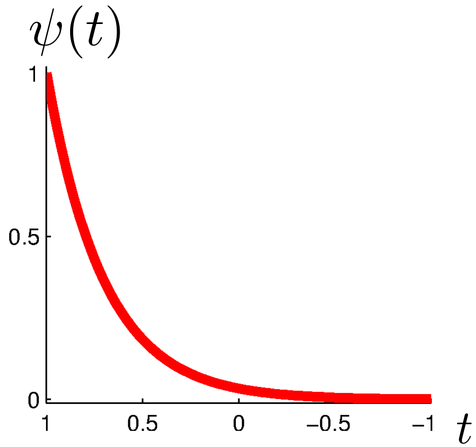
Basic SBF Interpolant for $\mathbb{S}^2$

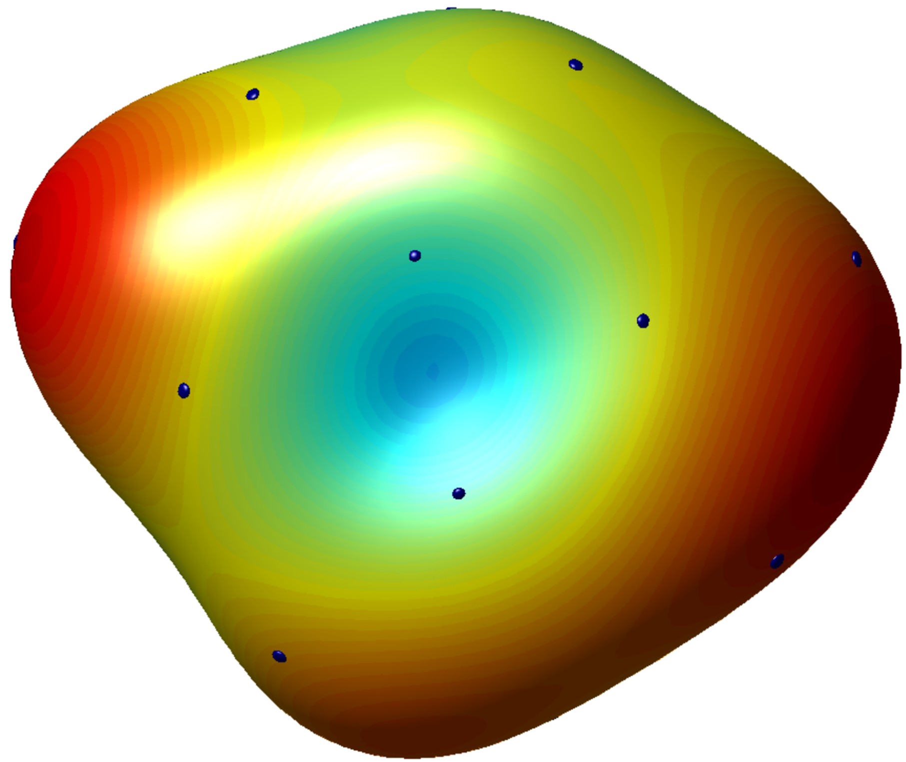
$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \psi(\mathbf{x}^T \mathbf{x}_j)$$

SBF interpolation

Key idea: linear combination of translates and rotations of a single zonal kernel on $\mathbb{S}^2$

$X = \{\mathbf{x}_j\}_{j=1}^{N} \subset \Omega, \quad f\big|_X = \{f_j\}_{j=1}^{N}$





Basic SBF Interpolant for $\mathbb{S}^2$

$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \psi(\mathbf{x}^T \mathbf{x}_j)$$

Linear system for determining the interpolation coefficients

$$\underbrace{\begin{bmatrix} \psi(\mathbf{x}_1^T\mathbf{x}_1) & \psi(\mathbf{x}_1^T\mathbf{x}_2) \cdots & \psi(\mathbf{x}_1^T\mathbf{x}_N) \\ \psi(\mathbf{x}_2^T\mathbf{x}_1) & \psi(\mathbf{x}_2^T\mathbf{x}_2) \cdots & \psi(\mathbf{x}_2^T\mathbf{x}_N) \\ \vdots & \vdots \quad \ddots & \vdots \\ \psi(\mathbf{x}_N^T\mathbf{x}_1) & \psi(\mathbf{x}_N^T\mathbf{x}_2) \cdots & \psi(\mathbf{x}_N^T\mathbf{x}_N) \end{bmatrix}}_{A_X} \underbrace{\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{bmatrix}}_{\underline{c}} = \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{bmatrix}}_{\underline{f}}$$

A_X is guaranteed to be positive definite if ψ is a positive definite zonal kernel

Positive definite zonal kernels

Definition. A kernel $\Psi : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{R}$ is called radial or zonal on $\mathbb{S}^{d-1}$ if $\Psi(\mathbf{x}, \mathbf{y}) = \psi(\mathbf{x}^T \mathbf{y})$, where $\psi : [-1, 1] \to \mathbb{R}$. In this case, ψ is simply referred to as the zonal kernel and no reference is made to Ψ.

Positive definite zonal kernels

Definition. A kernel $\Psi : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{R}$ is called radial or zonal on $\mathbb{S}^{d-1}$ if $\Psi(\mathbf{x}, \mathbf{y}) = \psi(\mathbf{x}^T\mathbf{y})$, where $\psi : [-1, 1] \to \mathbb{R}$. In this case, ψ is simply referred to as the zonal kernel and no reference is made to Ψ.

Definition. A zonal kernel $\psi : [-1, 1] \to \mathbb{R}$ is said to be a positive definite zonal kernel on $\mathbb{S}^{d-1}$ if for any distinct set of nodes $X = \{\mathbf{x}_j\}_{j=1}^{N} \subset \mathbb{S}^{d-1}$ and $\underline{b} \in \mathbb{R}^N \backslash \{0\}$ the matrix $A = \{\psi(\mathbf{x}_i^T\mathbf{x}_j)\}$ is positive definite, i.e.

$$\sum_{i=1}^{N}\sum_{j=1}^{N} b_i \psi(\mathbf{x}_i^T\mathbf{x}_j) b_j > 0.$$

Remark: PD zonal kernels are sometimes called spherical basis functions (SBFs).

Positive definite zonal kernels

Definition. A kernel $\Psi : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{R}$ is called radial or zonal on $\mathbb{S}^{d-1}$ if $\Psi(\mathbf{x}, \mathbf{y}) = \psi(\mathbf{x}^T\mathbf{y})$, where $\psi : [-1, 1] \to \mathbb{R}$. In this case, ψ is simply referred to as the zonal kernel and no reference is made to Ψ.

Definition. A zonal kernel $\psi : [-1, 1] \to \mathbb{R}$ is said to be a positive definite zonal kernel on $\mathbb{S}^{d-1}$ if for any distinct set of nodes $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{S}^{d-1}$ and $\underline{b} \in \mathbb{R}^N \backslash \{0\}$ the matrix $A = \{\psi(\mathbf{x}_i^T \mathbf{x}_j)\}$ is positive definite, i.e.

$$\sum_{i=1}^{N} \sum_{j=1}^{N} b_i \psi(\mathbf{x}_i^T \mathbf{x}_j) b_j > 0.$$

Remark: PD zonal kernels are sometimes called spherical basis functions (SBFs).

- The study of positive definite kernels on $\mathbb{S}^{d-1}$ started with Schoenberg (1940).
- Extension of this work, including to conditionally positive definite kernels, began in the 1990s (Cheney and Xu (1992)), and continues today.
- Our interest is strictly in $\mathbb{S}^2$ and we will only present results for this case.

Conditionally positive definite zonal kernels

- Similar to $\mathbb{R}^d$, we can define conditionally positive definite zonal kernels.

  Definition. A continuous zonal kernel $\psi : [-1,1] \to \mathbb{R}$ is said to be conditionally positive definite of order k on $\mathbb{S}^2$ if, for any distinct $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{S}^2$, and all $\mathbf{b} \in \mathbb{R}^N \backslash \{\mathbf{0}\}$ satisfying

$$\sum_{j=1}^{N} b_j p(\mathbf{x}_j) = 0$$

  for all spherical harmonics of degree $< k$, the following is satisfied:

$$\sum_{i=1}^{N} \sum_{j=1}^{N} b_i \psi(\mathbf{x}_i^T \mathbf{x}_j) b_j > 0.$$

- See the supplementary lecture slides for
  - Brief introduction to spherical harmonics
  - A full characterization for conditionally positive definite zonal kernels.

Conditionally positive definite zonal kernels

Definition. Let $\psi : [-1,1] \to \mathbb{R}$ be a continuous zonal kernel and $\{p_i(\mathbf{x})\}_{i=1}^{k^2}$ be a basis for the space of all spherical harmonics of degree $k-1$. The general SBF interpolant for the distinct nodes $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{S}^2$ and some target, f, sampled on X, $\{f_j\}_{j=1}^N$ is

$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \psi(\mathbf{x}^T \mathbf{x}_j) + \sum_{\ell=1}^{k^2} d_\ell p_\ell(\mathbf{x}),$$

where $I_X f(\mathbf{x}_i) = f_i$, $i = 1, \ldots, N$ and $\sum_{j=1}^{N} c_j p_\ell(\mathbf{x}_j) = 0$, $\ell = 1, \ldots, k^2$.

In linear system form, these constraints are

$$\begin{bmatrix} A & P \\ P^T & 0 \end{bmatrix} \begin{bmatrix} \underline{c} \\ \underline{d} \end{bmatrix} = \begin{bmatrix} \underline{f} \\ \underline{0} \end{bmatrix}, \text{ where } a_{i,j} = \psi(\mathbf{x}_i^T \mathbf{x}_j),\ p_{i,\ell} = p_\ell(\mathbf{x}_i)$$

Theorem. The above linear system is invertible for any distinct X, provided

- $\text{rank}(P) = k^2$,
- ψ is conditionally positive definite of of order k.

Conditionally positive definite zonal kernels

Definition. Let $\psi : [-1,1] \to \mathbb{R}$ be a continuous zonal kernel and $\{p_i(\mathbf{x})\}_{i=1}^{k^2}$ be a basis for the space of all spherical harmonics of degree $k-1$. The general SBF interpolant for the distinct nodes $X = \{\mathbf{x}_j\}_{j=1}^{N} \subset \mathbb{S}^2$ and some target, f, sampled on X, $\{f_j\}_{j=1}^{N}$ is

$$I_X f(\mathbf{x}) = \sum_{j=1}^{N} c_j \psi(\mathbf{x}^T \mathbf{x}_j) + \sum_{\ell=1}^{k^2} d_\ell p_\ell(\mathbf{x}),$$

where $I_X f(\mathbf{x}_i) = f_i$, $i = 1, \ldots, N$ and $\displaystyle\sum_{j=1}^{N} c_j p_\ell(\mathbf{x}_j) = 0$, $\ell = 1, \ldots, k^2$.

In linear system form, these constraints are

$$\begin{bmatrix} A & P \\ P^T & 0 \end{bmatrix} \begin{bmatrix} \underline{c} \\ \underline{d} \end{bmatrix} = \begin{bmatrix} \underline{f} \\ \underline{0} \end{bmatrix}, \text{ where } a_{i,j} = \psi(\mathbf{x}_i^T \mathbf{x}_j),\ p_{i,\ell} = p_\ell(\mathbf{x}_i)$$

Example (Restricted thin plate spline, or surface spline). Let

- $\psi(t) = (1-t)\log(2-2t)$
- $p_1(\mathbf{x}) = 1$, $p_2(\mathbf{x}) = x$, $p_3(\mathbf{x}) = y$, and $p_4(\mathbf{x}) = z$.

The system has a unique solution provided X are distinct.

Restricted radial kernels

- Any (conditionally) positive definite radial kernel ϕ on $\mathbb{R}^3$ is also (conditionally) positive definite on $\mathbb{S}^2$.

- In fact, they are (conditionally) positive definite zonal kernels, since

$$\phi(\|\mathbf{x}-\mathbf{y}\|) = \phi\left(\sqrt{2-2\mathbf{x}^T\mathbf{y}}\right) = \psi(\mathbf{x}^T\mathbf{y}), \text{ for any } \mathbf{x},\mathbf{y} \in \mathbb{S}^2$$

- So, standard RBF methods can be used for problems on the sphere $\mathbb{S}^2$.

- Cheney (1995) appears to have been the first to mathematically study the specialization of RBFs to the sphere. Many others have followed suit, e.g. Fasshauer & Schumaker (1998); Baxter & Hubbert (2001); Levesley & Hubbert (2001); Hubbert & Morton (2004); zu Castel & Filbir (2005); Narcowich, Sun, & Ward (2007); Narcowich, Sun, Ward, & Wendland (2007); Fornberg & Piret (2007); Narcowich, Ward, & W (2007); Fuselier, Narcowich, Ward, & W (2009); Fuselier & W (2009)

Restricted radial kernels

- Any (conditionally) positive definite radial kernel ϕ on $\mathbb{R}^3$ is also (conditionally) positive definite on $\mathbb{S}^2$.

- In fact, they are (conditionally) positive definite zonal kernels, since

$$\phi(\|\mathbf{x}-\mathbf{y}\|) = \phi\left(\sqrt{2-2\mathbf{x}^T\mathbf{y}}\right) = \psi(\mathbf{x}^T\mathbf{y}),\ \text{for any } \mathbf{x},\mathbf{y} \in \mathbb{S}^2$$

- So, standard RBF methods can be used for problems on the sphere $\mathbb{S}^2$.

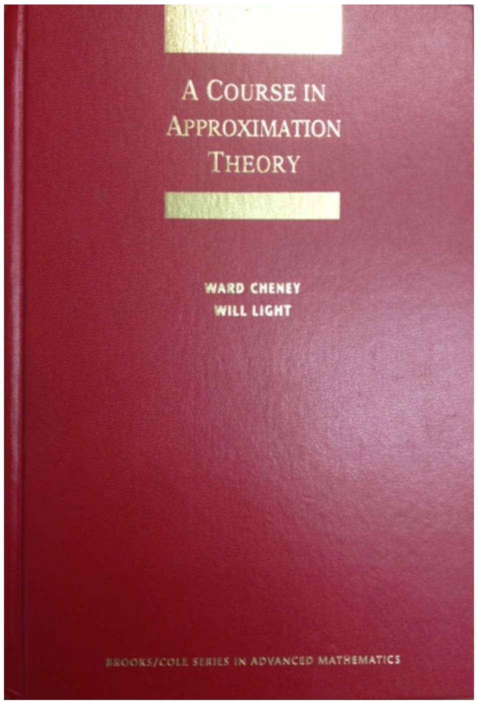
- Cheney (1995) appears to have been the first to mathematically study the specialization of RBFs to the sphere. Many others have followed suit, e.g. Fasshauer & Schumaker (1998); Baxter & Hubbert (2001); Levesley & Hubbert (2001); Hubbert & Morton (2004); zu Castel & Filbir (2005); Narcowich, Sun, & Ward (2007); Narcowich, Sun, Ward, & Wendland (2007); Fornberg & Piret (2007); Narcowich, Ward, & W (2007); Fuselier, Narcowich, Ward, & W (2009); Fuselier & W (2009)

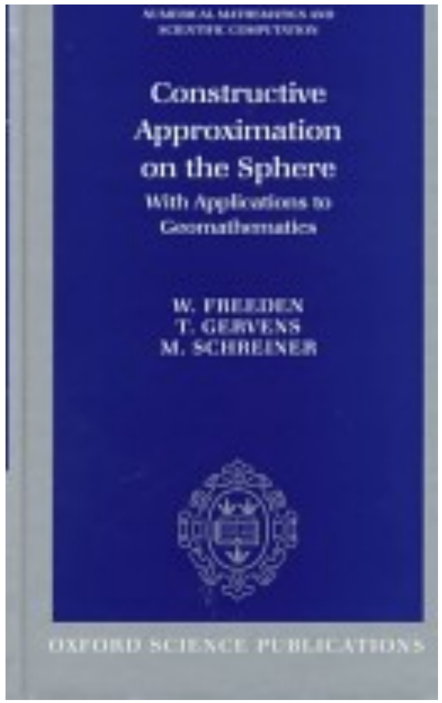
- Open question (Baxter & Hubbert (2001)): Are there any advantages to using a purely PD or CPD zonal kernel to a restricted PD or CPD radial kernel?

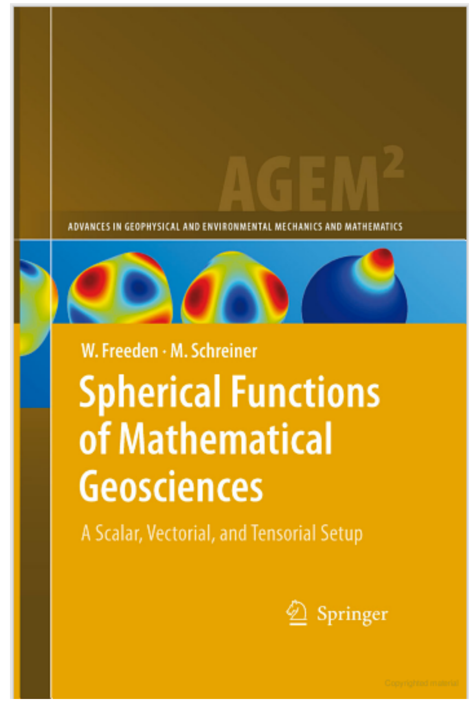
- In this workshop we will focus on restricted radial kernels.

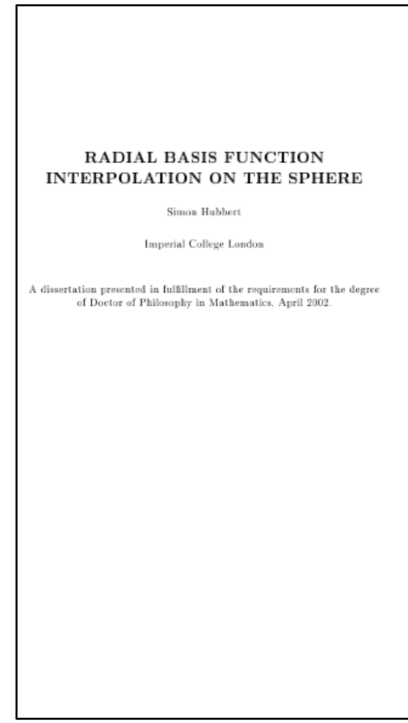
References for ZBF or SBF method

- For details on interpolation with more general zonal kernels, see








RADIAL BASIS FUNCTION
INTERPOLATION ON THE SPHERE

Simon Hubbert

Imperial College London

A dissertation presented in fulfillment of the requirements for the degree of Doctor of Philosophy in Mathematics, April 2002.

- Also see the supplementary lecture slides.

Error estimates

- Goal: Present some known results on error estimates for RBF interpolants on the sphere for target function of various smoothness.

- The supplementary lecture slides contain many of the technical details including:
  - Reproducing kernel Hilbert spaces (RKHS)
  - Sobolev spaces on $\mathbb{S}^2$;
  - Native spaces;

- Brief historical notes regarding error estimates:
  - Earliest results appear to be Freeden (1981), but do not depend on ψ or target.
  - First Sobolev-type estimates were given in Jetter, Stöckler, & Ward (1999).
  - Since then many more results have appeared, e.g.
    Levesley, Light, Ragozin, & Sun (1999), v. Golitschek & Light (2001), Morton & Neamtu (2002), Narcowich & Ward (2002), Hubbert & Morton (2004,2004), Levesley & Sun (2005), Narcowich, Sun, & Ward (2007), Narcowich, Sun, Ward, & Wendland (2007), Sloan & Sommariva (2008), Sloan & Wendland (2009), Hangelbroek (2011).

Geometric properties of node sets

- The following properties for node sets on the sphere appear in the error estimates:

- Mesh norm

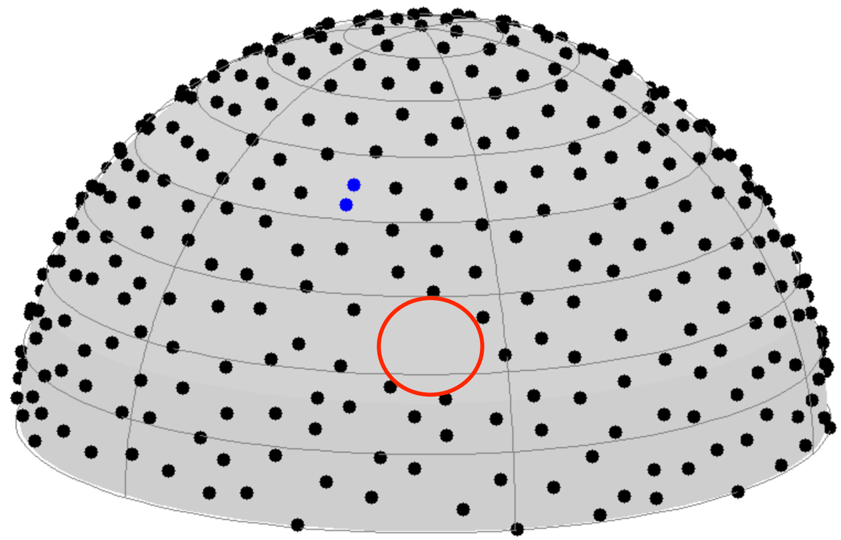
$$h_X = \sup_{\mathbf{x}\in\mathbb{S}^2} \operatorname{dist}_{\mathbb{S}^2}(\mathbf{x}, X)$$

- Separation radius

$$q_X = \frac{1}{2}\min_{i\neq j} \operatorname{dist}_{\mathbb{S}^2}(\mathbf{x}_i, \mathbf{x}_j)$$

- Mesh ratio

$$\rho_X = \frac{h_X}{q_X}$$

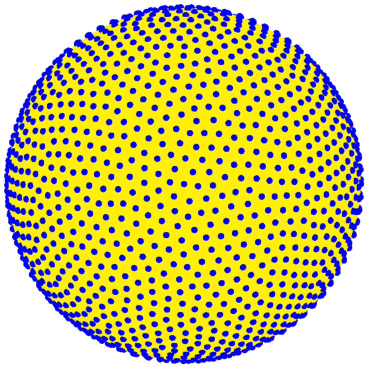


$$X = \{\mathbf{x}_j\}_{j=1}^{N} \subset \mathbb{S}^2$$

(Only part of the sphere is shown)

Interpolation error estimates

- We start with known error estimates for kernels of finite smoothness.
  Jetter, Stöckler, & Ward (1999), Morton & Neamtu (2002), Hubbert & Morton (2004,2004), Narcowich, Sun, Ward, & Wendland (2007)



<u>Notation:</u>

- ϕ is a restricted radial kernel
- $\hat{\phi}(\omega) \sim (1 + \|\omega\|_2^2)^{-(\tau+1/2)}$, $\tau > 1$
- $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{S}^2$
- $I_X f$ is RBF interpolant of $f\big|_X$
- h_X = mesh-norm
- q_X = separation radius
- $\rho_X = h_X / q_X$, mesh ratio

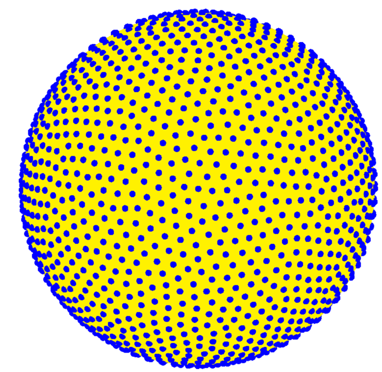
Theorem. Target function as smooth as the kernel

If $f \in H^\tau(\mathbb{S}^2)$ then $\|f - I_X f\|_{L_p(\mathbb{S}^2)} = \mathcal{O}(h_X^{\tau - 2(1/2-1/p)_+})$ for $1 \le p \le \infty$.
In particular,

$$\|f - I_X f\|_{L_1(\mathbb{S}^2)} = \mathcal{O}(h_X^\tau)$$
$$\|f - I_X f\|_{L_2(\mathbb{S}^2)} = \mathcal{O}(h_X^\tau)$$
$$\|f - I_X f\|_{L_\infty(\mathbb{S}^2)} = \mathcal{O}(h_X^{\tau-1})$$

Interpolation error estimates

- We start with known error estimates for kernels of finite smoothness.
  Jetter, Stöckler, & Ward (1999), Morton & Neamtu (2002), Hubbert & Morton (2004,2004), Narcowich, Sun, Ward, & Wendland (2007)



Notation:

- ϕ is a restricted radial kernel
- $\hat{\phi}(\omega) \sim (1 + \|\omega\|_2^2)^{-(\tau+1/2)}$, $\tau > 1$
- $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{S}^2$
- $I_X f$ is RBF interpolant of $f\big|_X$
- h_X = mesh-norm
- q_X = separation radius
- $\rho_X = h_X/q_X$, mesh ratio

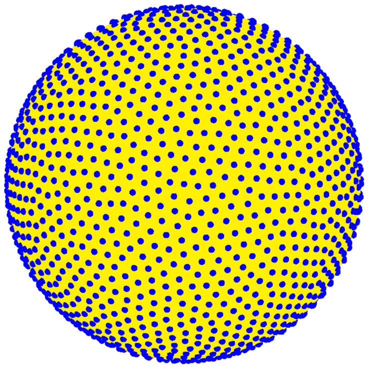
Theorem. Target functions twice as smooth as the kernel

$$\text{If } f \in H^{2\tau}(\mathbb{S}^2) \text{ then } \|f - I_X f\|_{L_p(\mathbb{S}^2)} = \mathcal{O}(h_X^{2\tau}) \text{ for } 1 \leq p \leq \infty.$$

Remark. Known as the "doubling trick" from spline theory. (Schaback 1999)

Interpolation error estimates

- We start with known error estimates for kernels of finite smoothness.
  Jetter, Stöckler, & Ward (1999), Morton & Neamtu (2002), Hubbert & Morton (2004,2004), Narcowich, Sun, Ward, & Wendland (2007)



Notation:

- ϕ is a restricted radial kernel
- $\hat{\phi}(\omega) \sim (1 + \|\omega\|_2^2)^{-(\tau+1/2)}$, $\tau > 1$
- $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{S}^2$
- $I_X f$ is RBF interpolant of $f\big|_X$
- h_X = mesh-norm
- q_X = separation radius
- $\rho_X = h_X/q_X$, mesh ratio

Theorem. Target functions rougher than the kernel.

If $f \in H^\beta(\mathbb{S}^2)$ for $\tau > \beta > 1$ then $\|f - I_X f\|_{L_p(\mathbb{S}^2)} = \mathcal{O}(\rho^{\tau-\beta} h_X^{\tau-2(1/2-1/p)_+})$ for $1 \le p \le \infty$.

Remark.

(1) Referred to as "escaping the native space". (Narcowich, Ward, & Wendland (2005, 2006)).

(2) These rates are the best possible.

Interpolation error estimates

- Example values of τ for some radial kernels:

Name	RBF (use $r = \sqrt{2-2t}$ to get SBF ψ)	τ
Matern	$\phi_2(r) = e^{-\varepsilon r}$	1.5
TPS(1)	$\phi(r) = r^2 \log(r)$	2
Cubic	$\phi(r) = r^3$	2
TPS(2)	$\phi(r) = r^4 \log(r)$	3
Wendland	$\phi_{3,2}(r) = (1-\varepsilon r)_+^6 (3 + 18(\varepsilon r) + 15(\varepsilon r)^2)$	3.5
Matern	$\phi_5(r) = e^{-\varepsilon r}(15 + 15(\varepsilon r) + 6(\varepsilon r)^2 + (\varepsilon r)^3)$	4.5

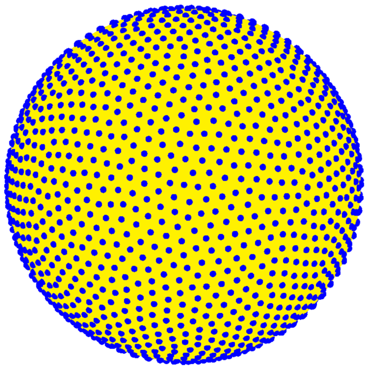
- For infinitely smooth kernels $\hat{\phi}$ decays faster than any polynomial power, and special error estimates are required.
- In this case the target functions have to be very smooth ($C^\infty(\mathbb{S}^2)$).

Interpolation error estimates

- Error estimates for infinitely smooth kernels (e.g. Gaussian, inverse multiquadric). Jetter, Stöckler, & Ward (1999)

Notation:

- ϕ is a restricted radial kernel
- $\hat{\phi}(\omega)$ decays faster than any polynomial power
- $X = \{\mathbf{x}_j\}_{j=1}^{N} \subset \mathbb{S}^2$
- $I_X f$ is RBF interpolant of $f\big|_X$



- h_X = mesh-norm

Theorem. Target function as smooth as the kernel

If $f \in \mathcal{N}_\phi(\mathbb{S}^2)$ then $\|f - I_X f\|_{L_\infty(\mathbb{S}^2)} = \mathcal{O}(h_X^{-1}\exp(-\alpha/2h_X))$, for some $\alpha > 0$ that depends on ϕ.

Remarks:

(1) This is called spectral (or exponential) convergence.

(2) Function space may be small, but does include all band-limited functions.

(3) Only known result I am aware of (too bad there are not more).

(4) Numerical results indicate convergence is also fine for less smooth functions.

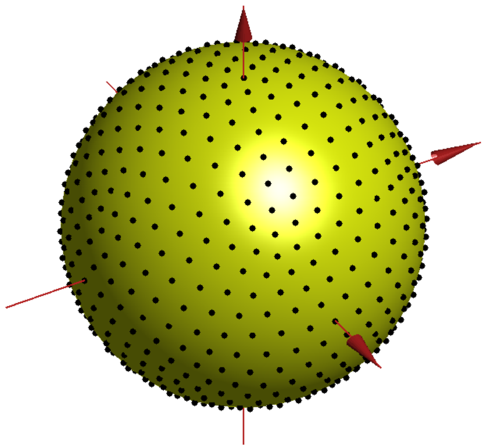
Optimal nodes

- If one has the freedom to choose the nodes, then the error estimates indicate they should be roughly as evenly spaced as possible.

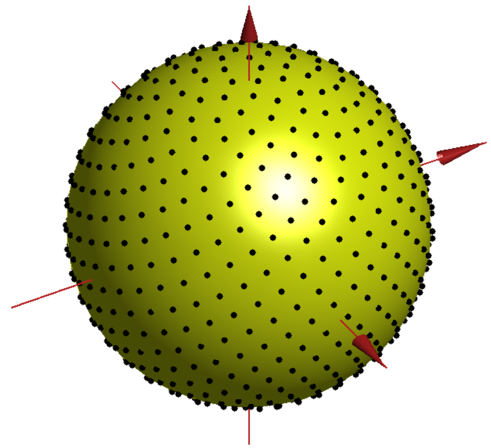
Examples:

Deterministic

Icosahedral

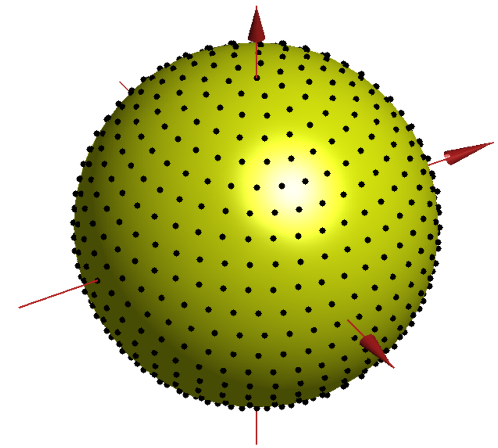


Fibonacci



Swinbank & Purser (2006)

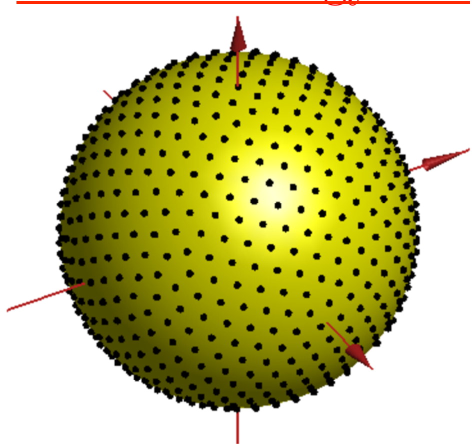
Equal area



Saff & Kuijlaars (1997)

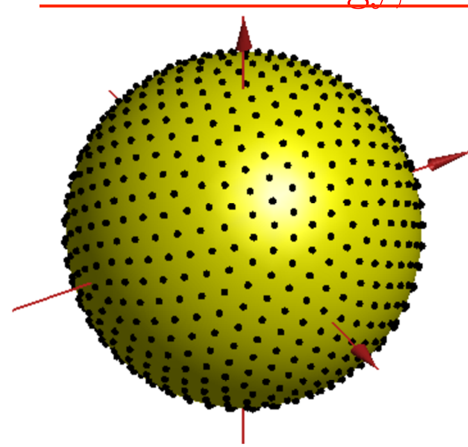
Non-deterministic

Minimum energy s=2



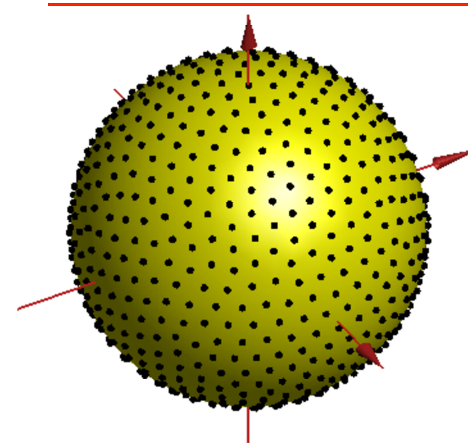
Hardin & Saff (2004)

Minimum energy, s=3



Riesz energy: $\|\mathbf{x}-\mathbf{y}\|_2^{-s}$

Maximal determinant



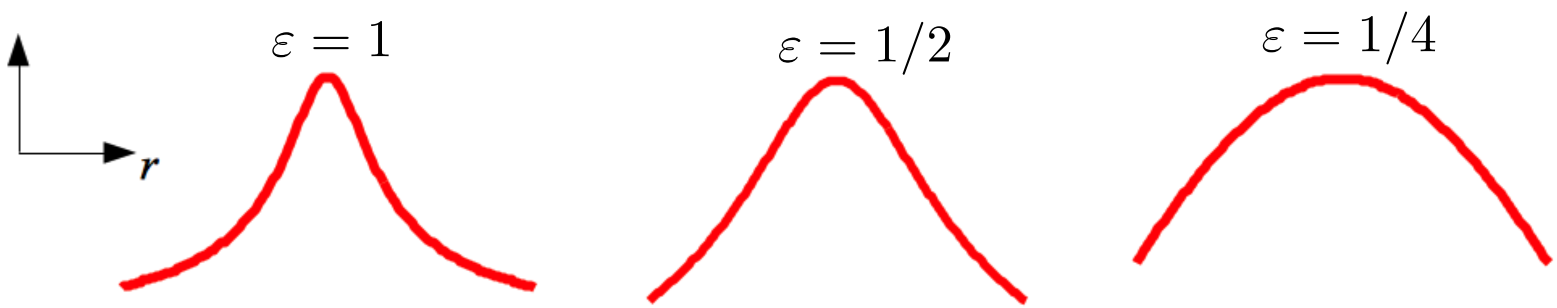
Womersley & Sloan (2001)

What about the shape parameter?

- Smooth kernels with a shape parameter.

Ex: $\phi(r) = \exp(-(\varepsilon r)^2)$ $\quad \phi(r) = \dfrac{1}{\sqrt{1+(\varepsilon r)^2}}$ $\quad \phi(r) = \sqrt{1+(\varepsilon r)^2}$

Issue: Effect of decreasing ε leads to severe ill-conditioning of interp. matrices



Basis functions get flatter as $\varepsilon \longrightarrow 0$

Linear system for determining the interpolation coefficients

$$\underbrace{\begin{bmatrix} \phi(\|\mathbf{x}_1-\mathbf{x}_1\|) & \phi(\|\mathbf{x}_1-\mathbf{x}_2\|) & \cdots & \phi(\|\mathbf{x}_1-\mathbf{x}_N\|) \\ \phi(\|\mathbf{x}_2-\mathbf{x}_1\|) & \phi(\|\mathbf{x}_2-\mathbf{x}_2\|) & \cdots & \phi(\|\mathbf{x}_2-\mathbf{x}_N\|) \\ \vdots & \vdots & \ddots & \vdots \\ \phi(\|\mathbf{x}_N-\mathbf{x}_1\|) & \phi(\|\mathbf{x}_N-\mathbf{x}_2\|) & \cdots & \phi(\|\mathbf{x}_N-\mathbf{x}_N\|) \end{bmatrix}}_{A_X} \underbrace{\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{bmatrix}}_{\underline{c}} = \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{bmatrix}}_{\underline{f}}$$

A_X is guaranteed to be positive definite if ϕ is positive definite.

RBF-Direct

RBF interpolation in the "flat" limit

RBF interpolant: $$I_{X,\varepsilon} f(\mathbf{x}) = \sum_{j=1}^{N} c_j(\varepsilon)\phi_\varepsilon(\|\mathbf{x} - \mathbf{x}_j\|)$$

Theorem (Driscoll & Fornberg (2002)). For N nodes in 1-D, the RBF interpolant (for certain smooth kernels) converges to the standard Lagrange interpolant as $\varepsilon \longrightarrow 0$ (flat limit)

- Higher dimensions: Limit usually exits and takes the form of a multivariate polynomial as $\varepsilon \longrightarrow 0$.
  - Fornberg, W, & Larsson (2004), Larsson & Fornberg (2005), Schaback (2005,2006), Lee, Yoon, & Yoon (2007)
  - In the case of the Gaussian kernel, the interpolant always converges to the de Boor & Ron "least polynomial interpolant".
- Sphere: Limit (usually) exits and converges to a spherical harmonic interpolant (Fornberg & Piret (2007)).

Base vs. space

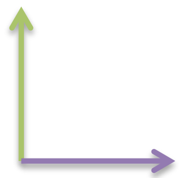
- Key observation: The space spanned by linear combinations of positive definite radial kernels (in $\mathbb{R}^d$ or $\mathbb{S}^2$) is good for approximation

  BUT, the standard basis $\{\phi(\cdot,\mathbf{x}_1),\ldots,\phi(\cdot,\mathbf{x}_N)\}$ can be problematic.

Analogy:
(Fornberg)

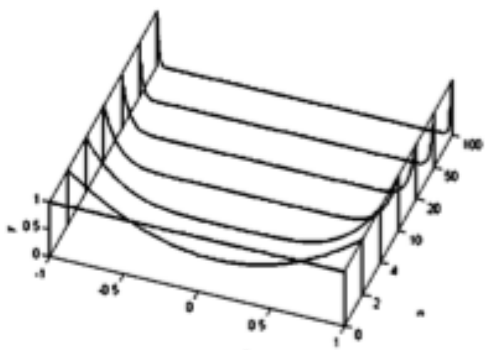
Vectors

Bad basis for $\mathbb{R}^2$

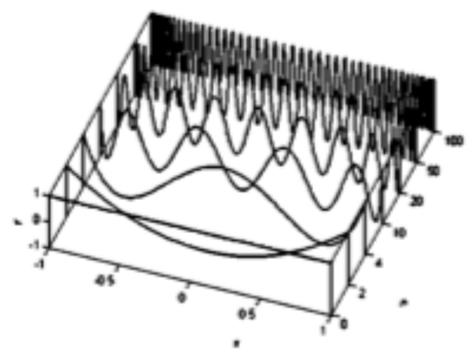


Good basis for $\mathbb{R}^2$

Polynomials

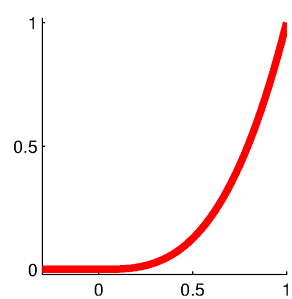


Bad basis: x^n, $n = 0, 1, \ldots$

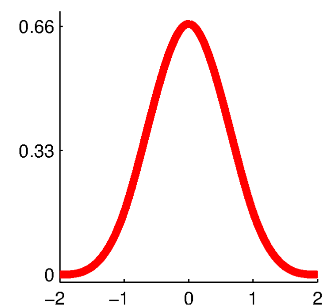


Chebyshev basis: $T_n(x)$, $n = 0, 1, \ldots$

Splines

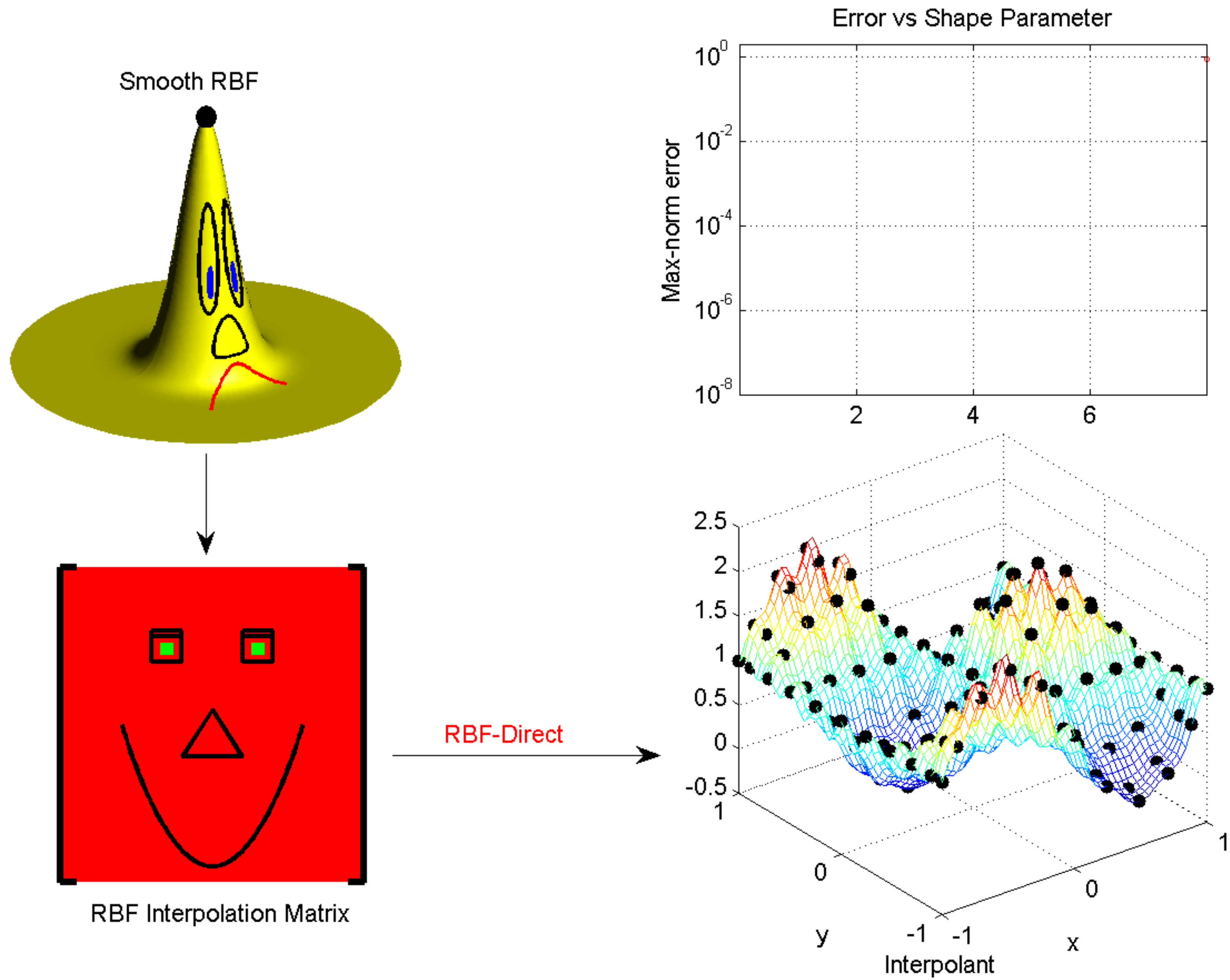


Truncated powers: $(x)_+^3$

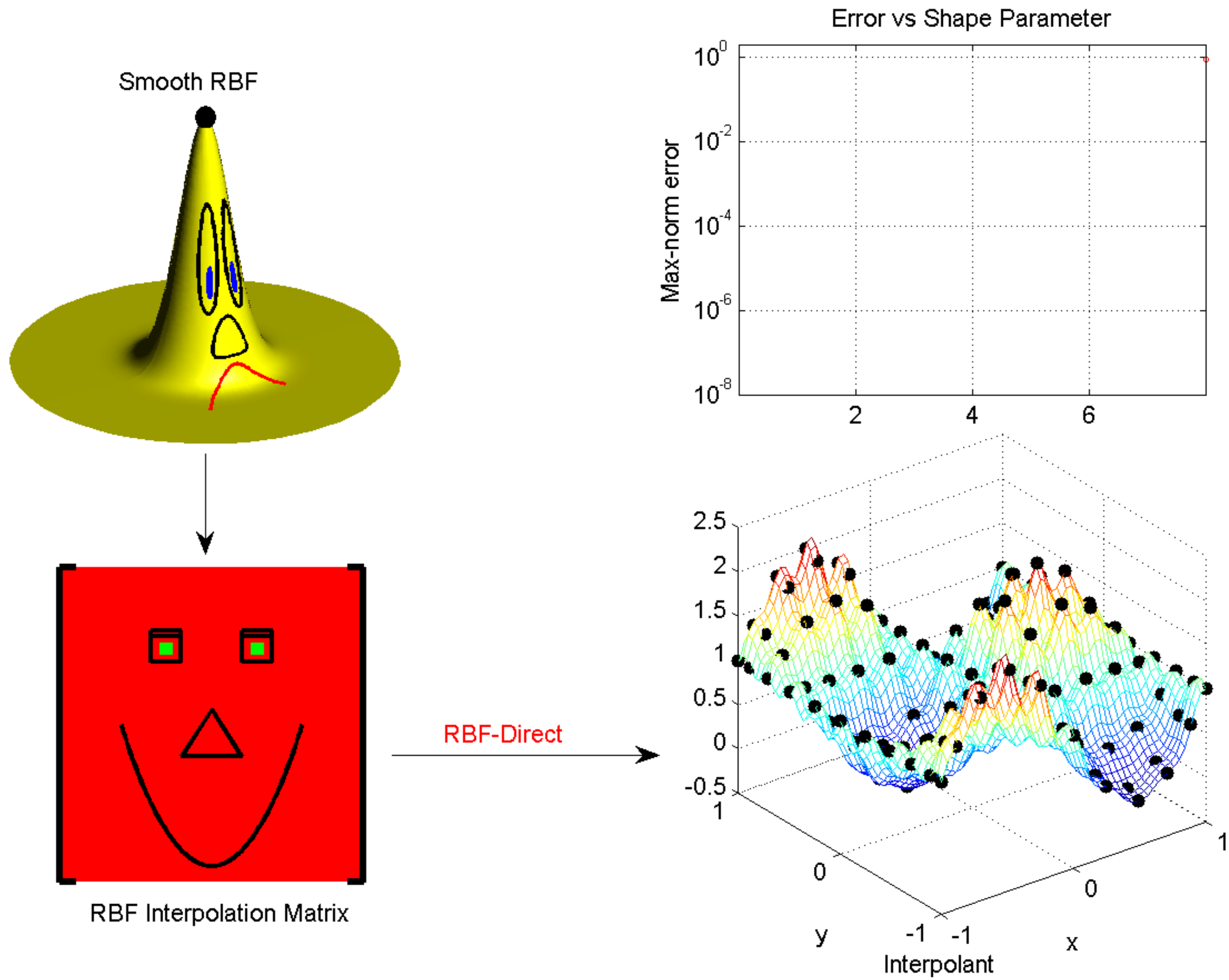


Bspline basis: $b_3(x)$

Using a bad basis for flat kernels:



Using a good basis for flat kernels:



Uncertainty principle misconception

- Schaback's uncertainty principle:

  Principle: *One cannot simultaneously achieve good conditioning and high accuracy.*

  Misconception: Accuracy that can be achieved is limited by ill-conditioning.

  Restatement:

  One cannot simultaneously achieve good conditioning and high accuracy when using the standard basis.

- It's a matter of base vs. space.
- Literature for interpolation with "flat" kernels is growing:

Theory:
Driscoll & Fornberg (2002)
Larsson & Fornberg (2003; 2005)
Fornberg, Wright, & Larsson (2004)
Schaback (2005; 2008)
Platte & Driscoll (2005)
Fornberg, Larsson, & Wright (2006)
deBoor (2006)
Fornberg & Zuev (2007)
Lee, Yoon, & Yoon (2007)
Fornberg & Piret (2008)
Buhmann, Dinew, & Larsson (2010)
Platte (2011)
Song, Riddle, Fasshauer, & Hickernell (2011)

Stable algorithms:
Fornberg & Wright (2004)
Fornberg & Piret (2007)
Fornberg, Larsson, & Flyer (2011)
Fasshauer & McCourt (2011)
Gonnet, Pachon, & Trefethen (2011)
Pazouki & Schaback (2011)
De Marchi & Santin (2013)
Fornberg, Letho, Powell (2013)
Wright & Fornberg (2013)

RBF-QR Algorithm

- RBF-QR algorithm developed by Fornberg and Piret allows one to stably compute “flat” kernel interpolants on the sphere.

- Idea is to create a new basis for the space spanned by shifts of a smooth radial kernel that removes the problems with small shape parameters (see supplementary lecture material for details).

- One can reach full numerical precision when interpolating a function using this procedure (for smooth enough target functions and large enough N)

- It is more expensive than standard approach (RBF-Direct).

- Work has gone into extending this idea to general Euclidean space, but the procedure is much more complicated.

- Matlab Code for RBF-QR is provided in the **rbfsphere** package.

- See Problem 2

Concluding remarks

- This was general background material for getting started in this area.
- There is still much more to learn and many interesting problems:
  - Approximation (and decomposition) of vector fields.
  - Fast algorithms for interpolation using localized bases
  - Numerical integration
  - RBF generated finite differences
  - RBF partition of unity methods
  - Numerical solution of partial differential equations on spheres.
  - Generalizations to other manifolds.

❖ If you have any questions or want to chat about research ideas, please come and talk to me.

Grazie per la vostra attenzione.