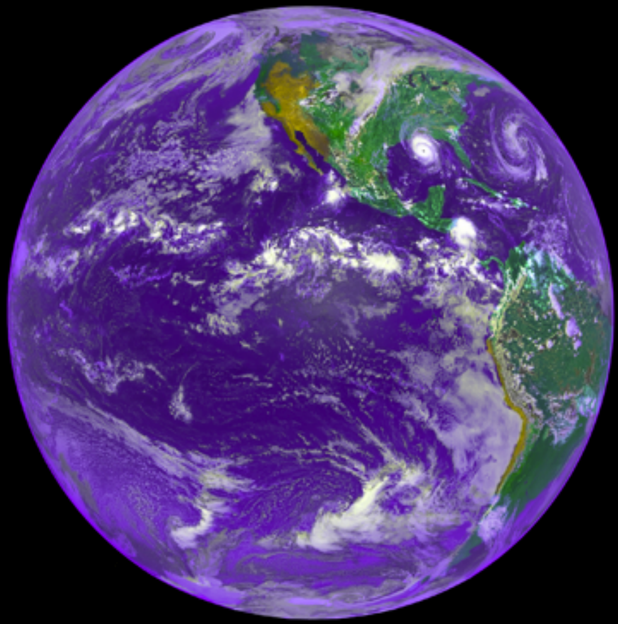
2013 Dolomites Research Week on Approximation

Kernel approximation on the sphere with applications to computational geosciences



Grady B. Wright
Boise State University

*This work is supported by NSF grants DMS 0934581

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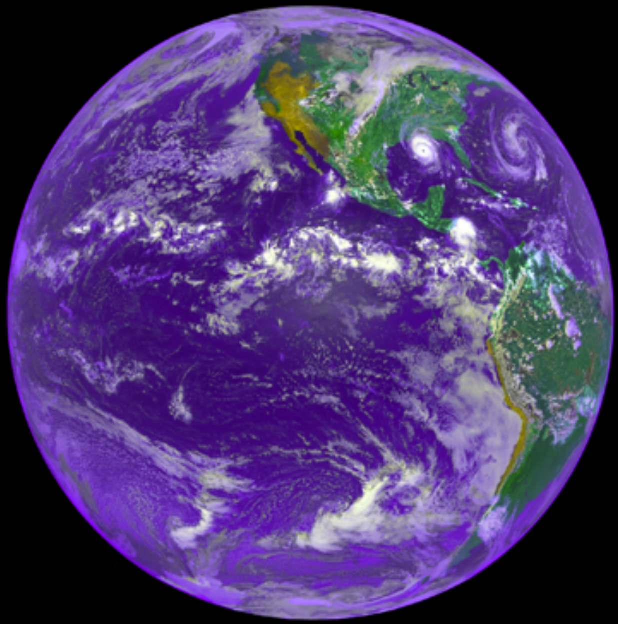
Lecture 1: Introduction to kernels and approximation on the sphere



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Overview

- Applications in spherical geometries
- 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

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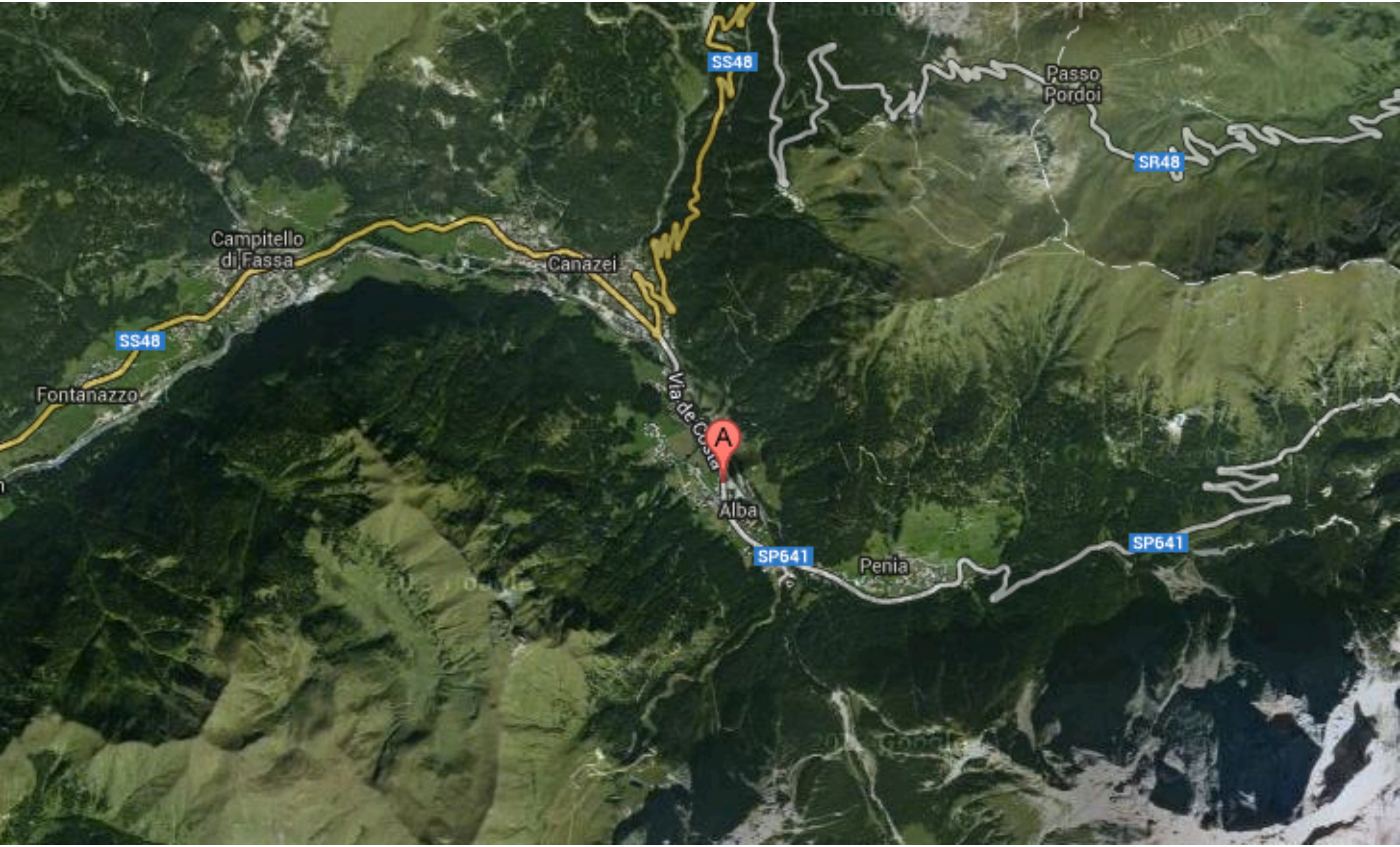

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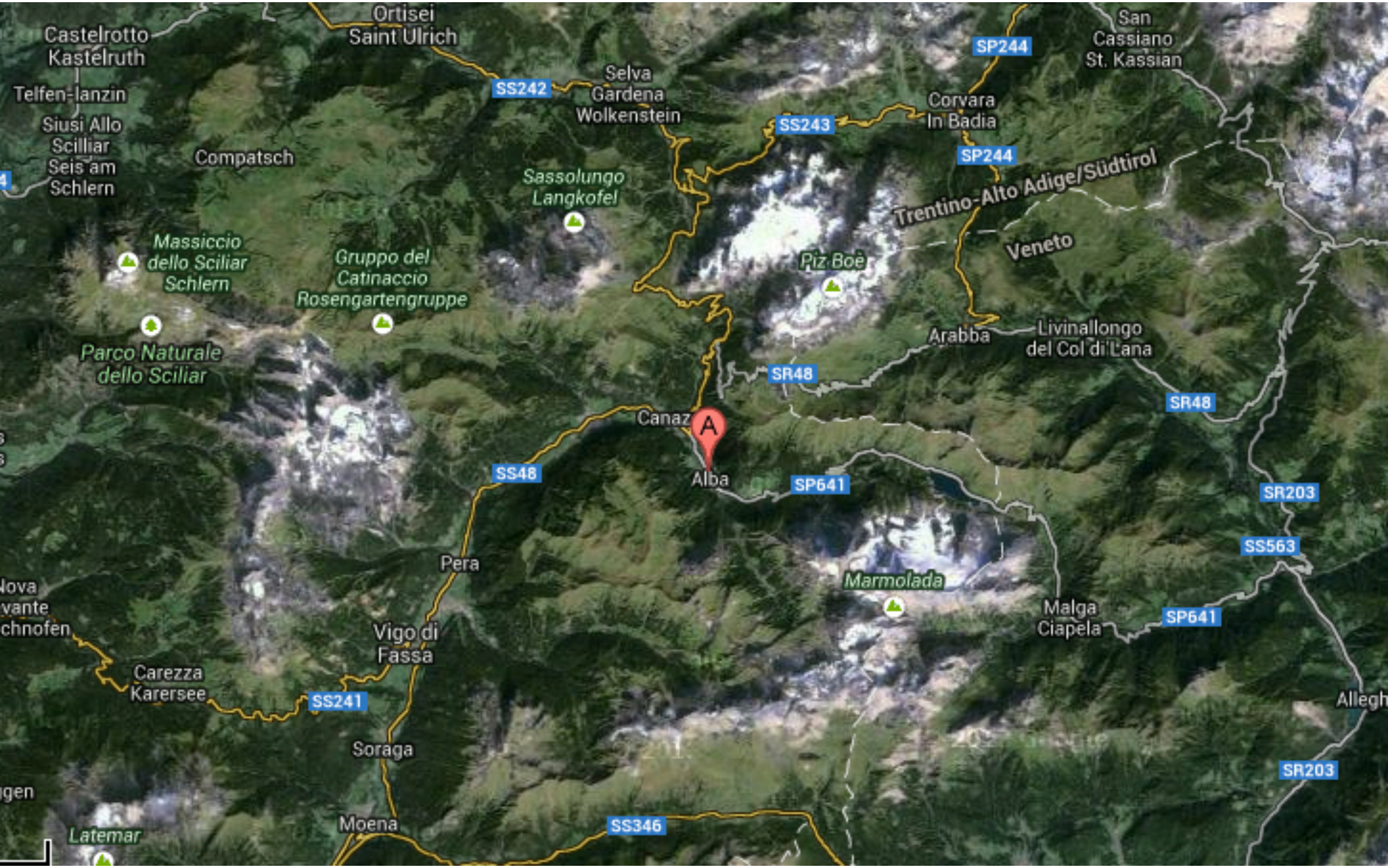

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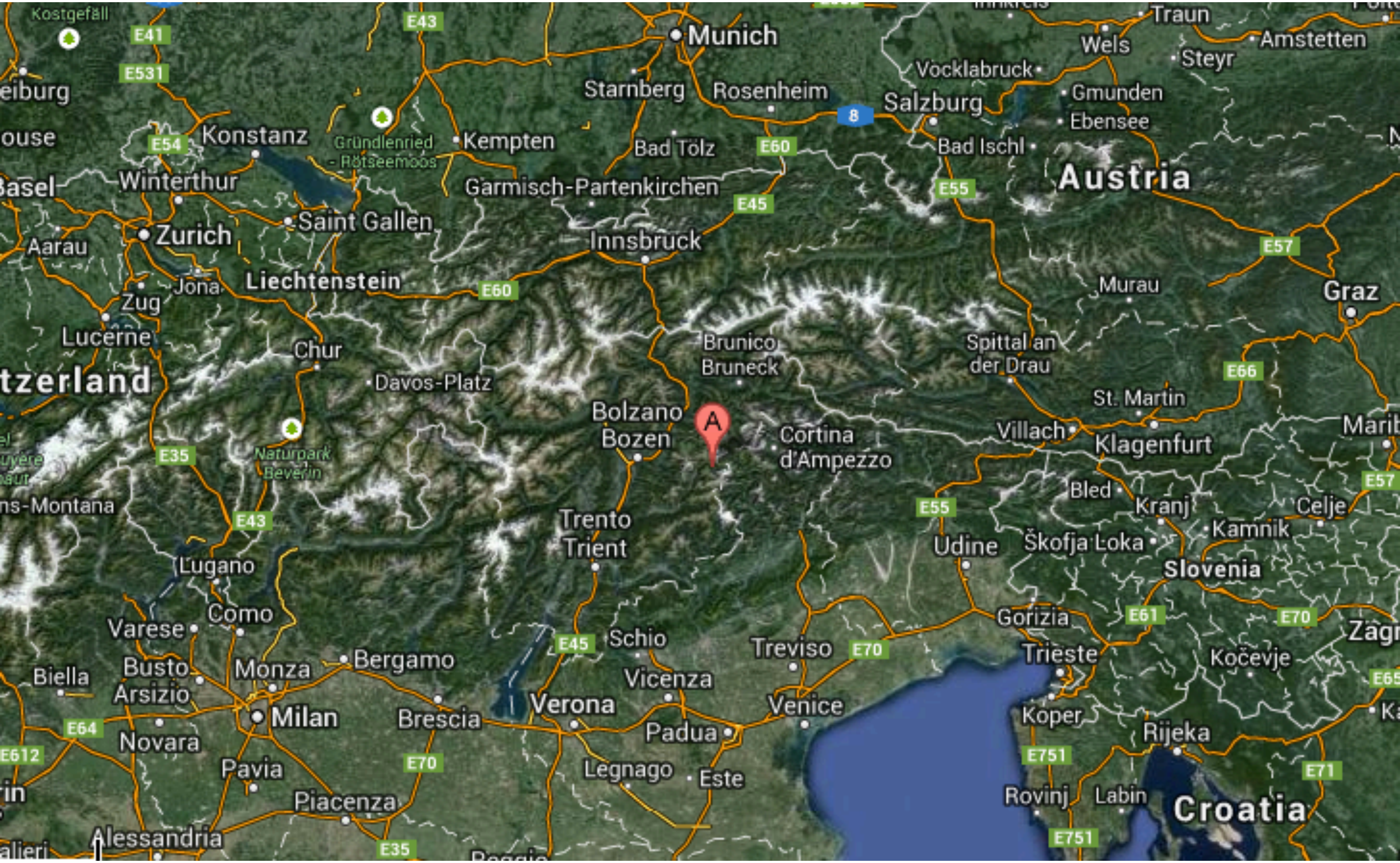

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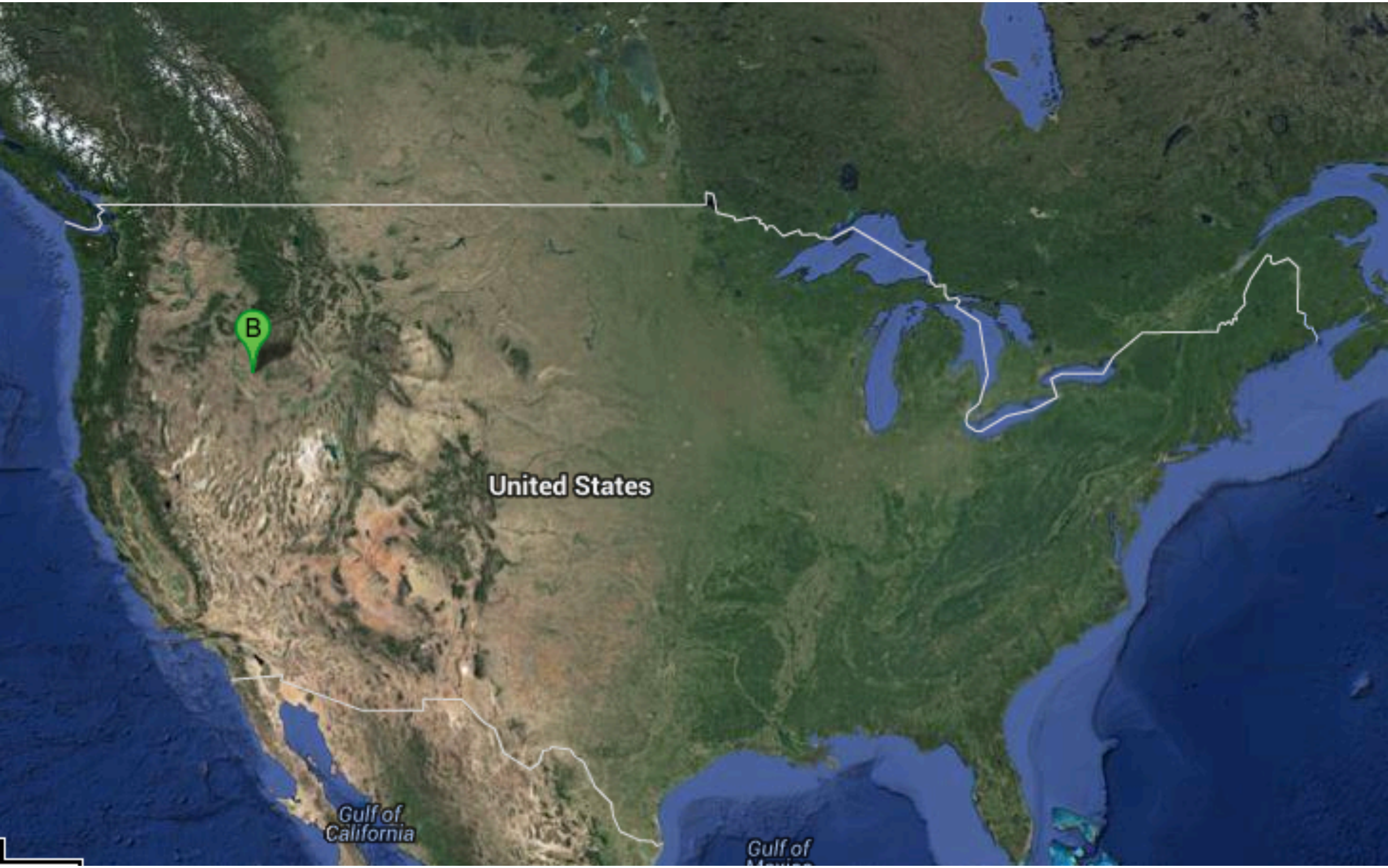

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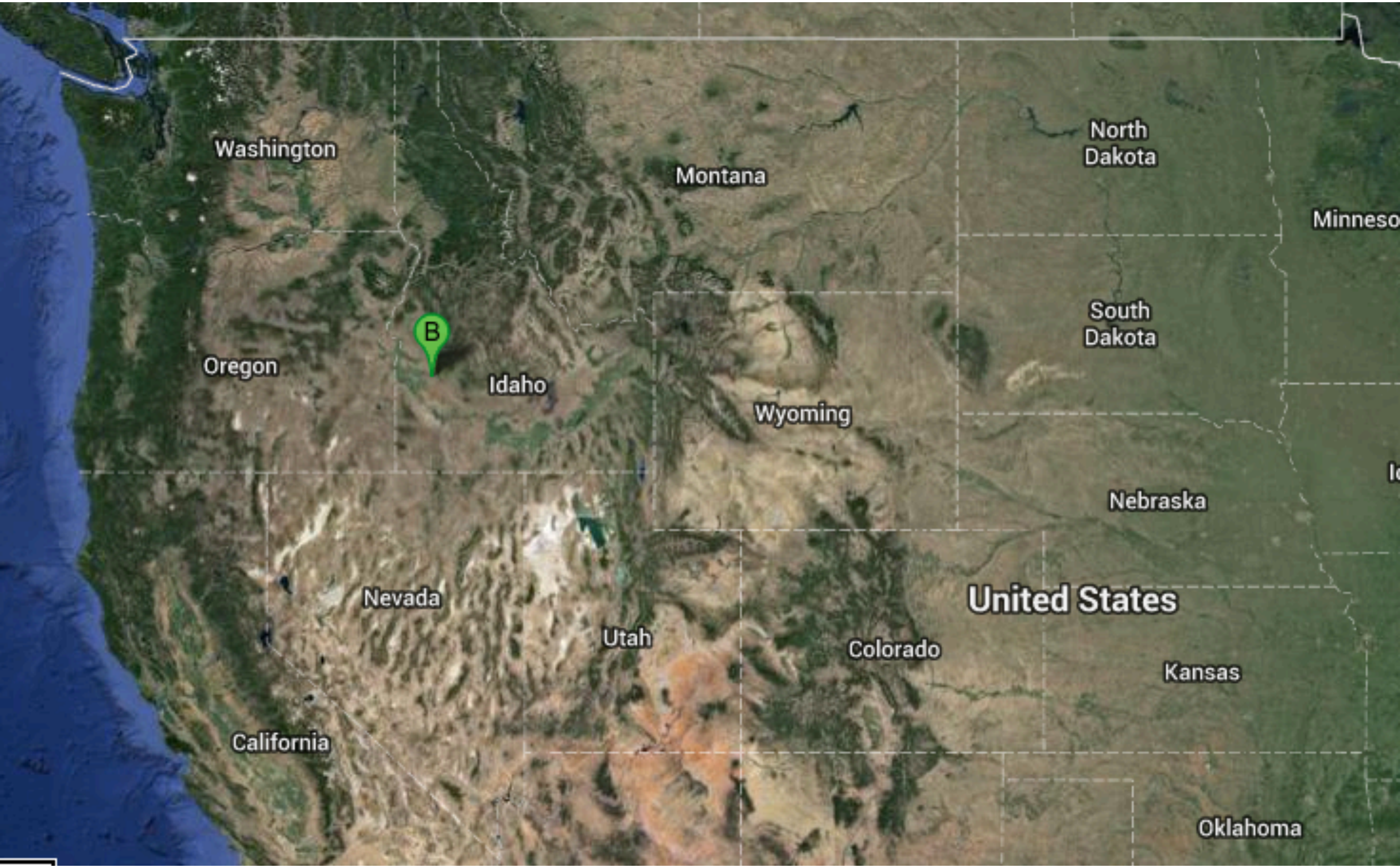

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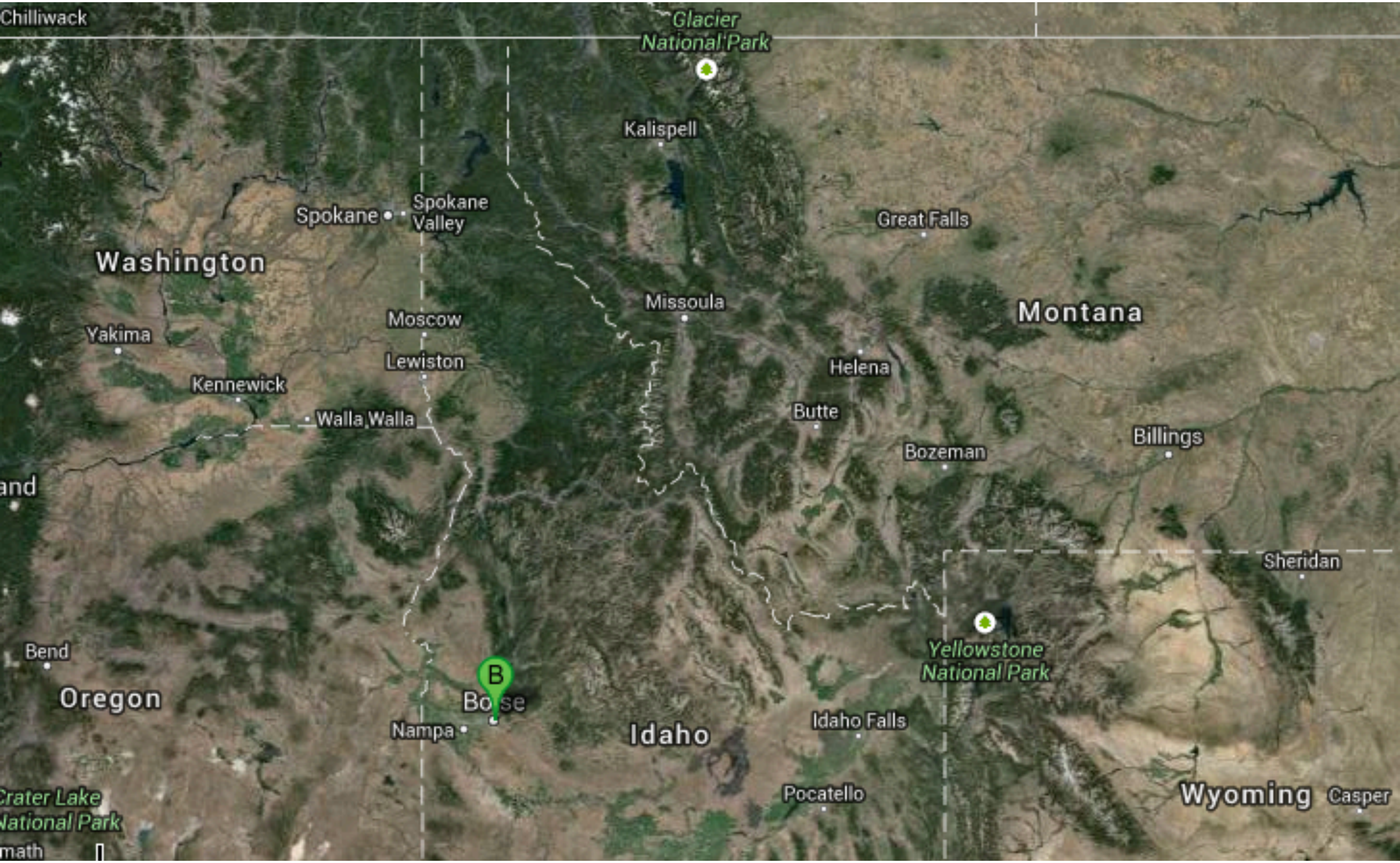

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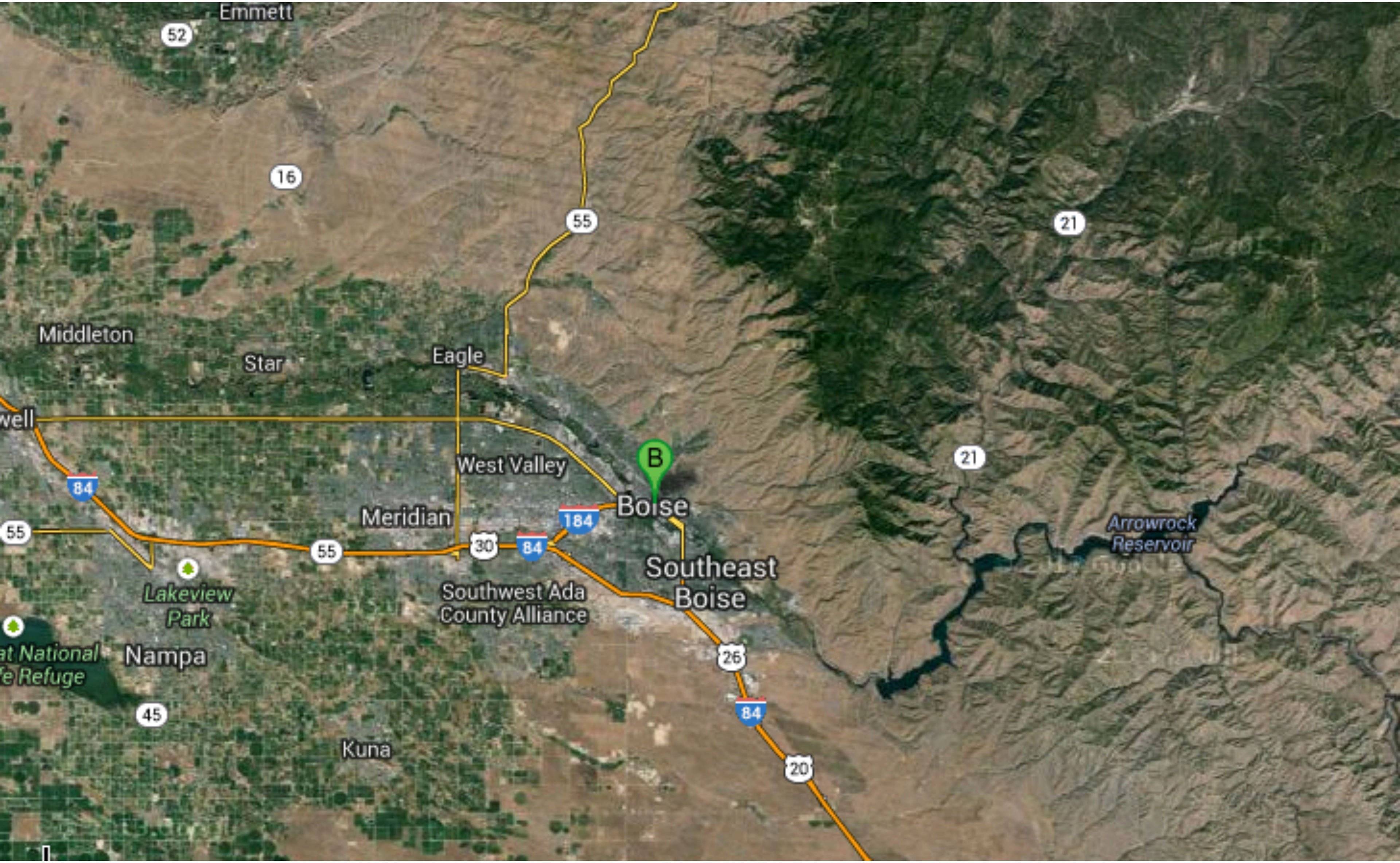

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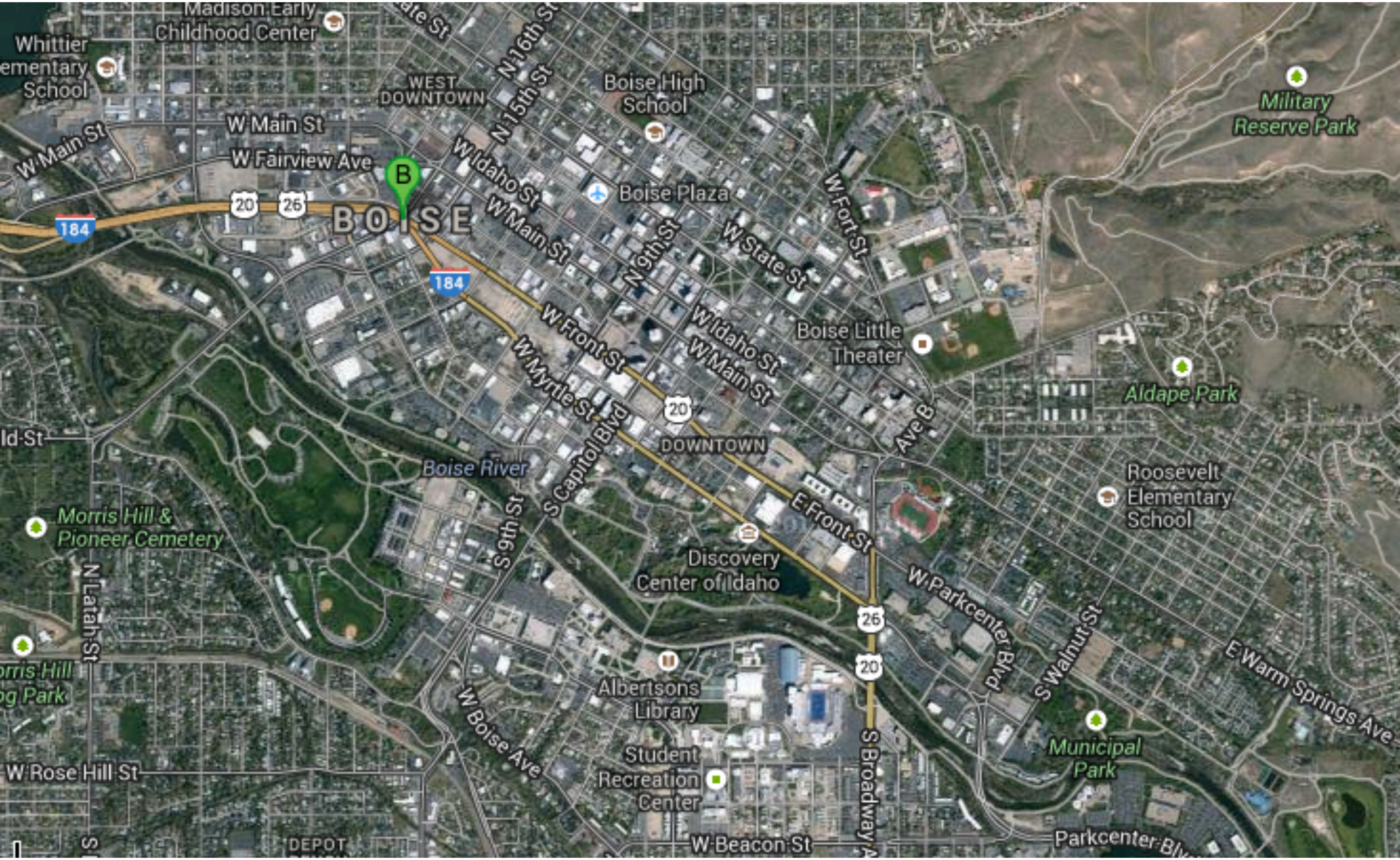

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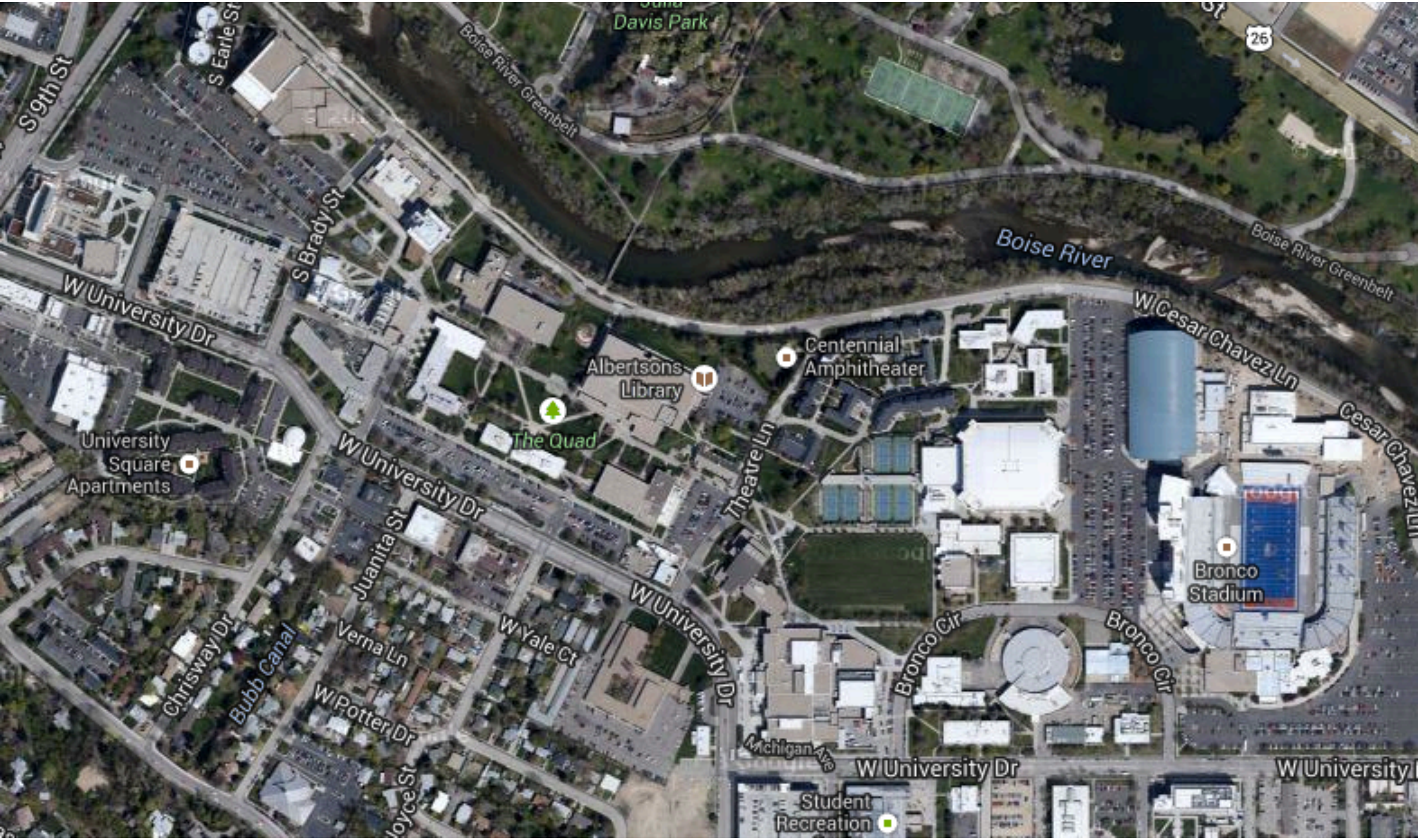
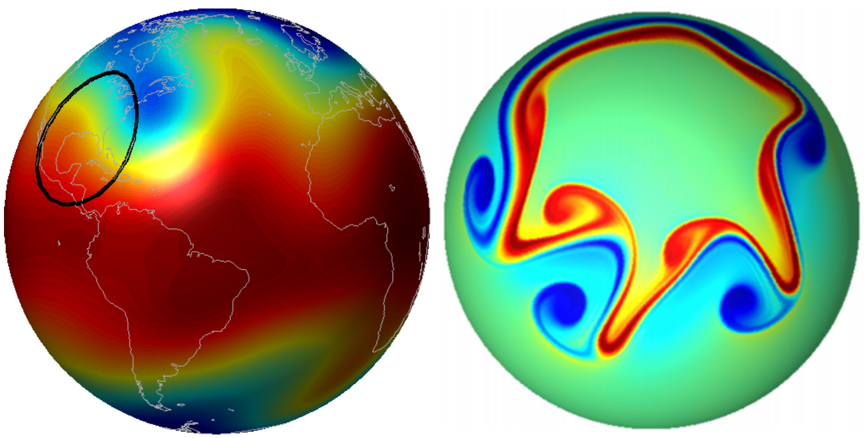


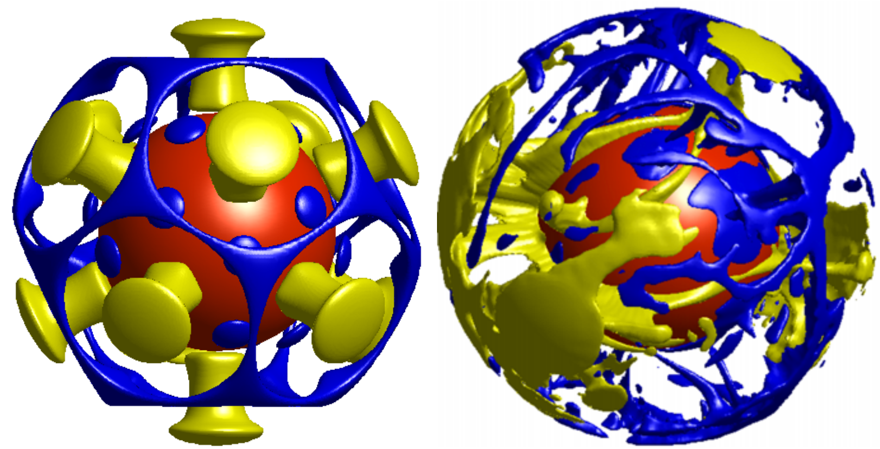
Applications in spherical geometries

- A visual overview: applications in the geosciences

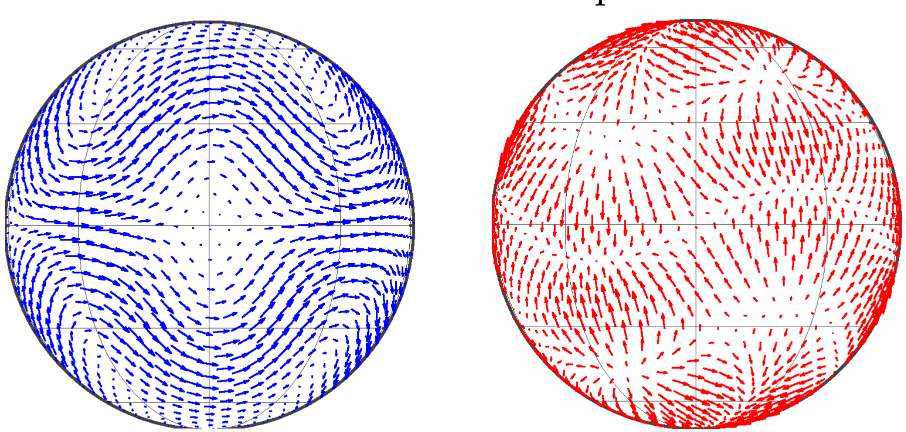
Shallow water flows:
numerical weather prediction



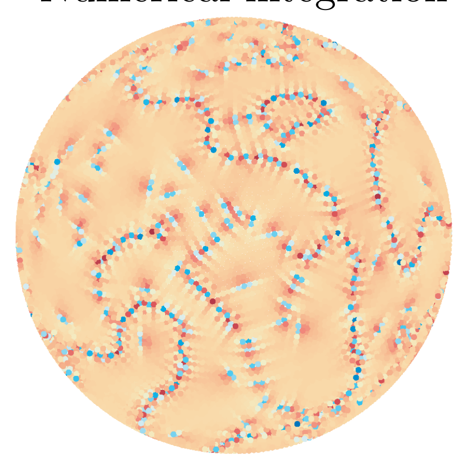
Rayleigh-Bénard Convection:
Mantle convection



Vector fields on the sphere



Numerical integration

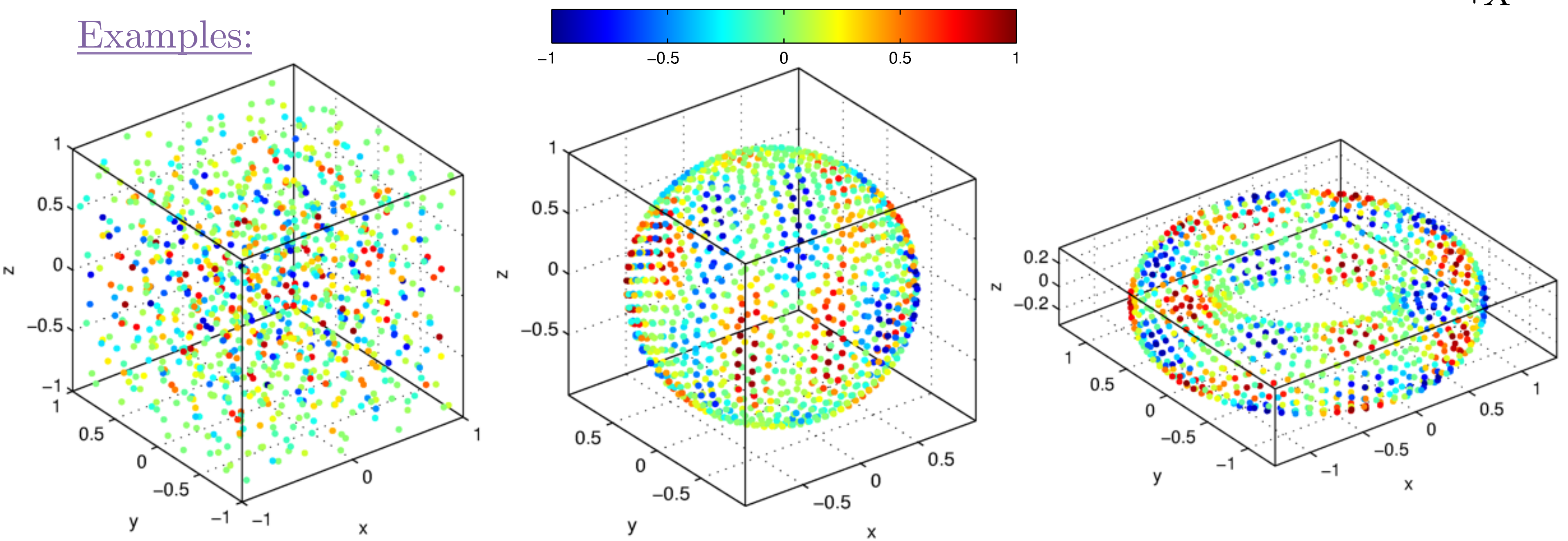


Interpolation with kernels

- 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:



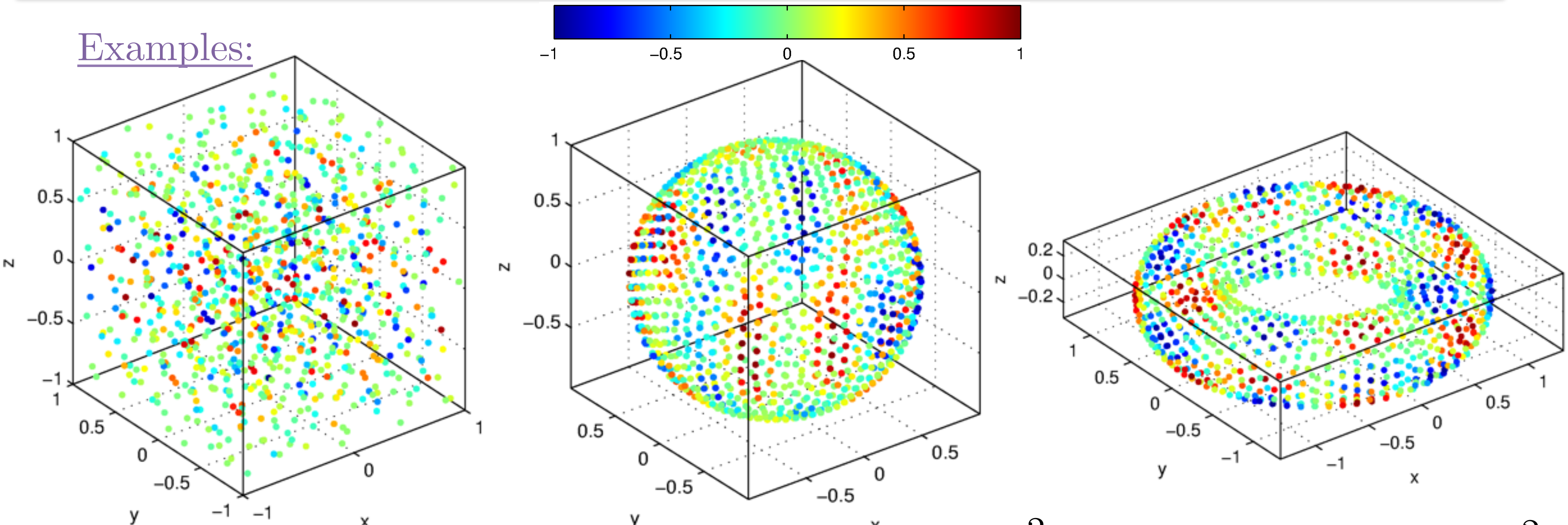
$\Omega = [-1, 1]^3$ $\Omega = \mathbb{S}^2$ $\Omega = \mathbb{T}^2$

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

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

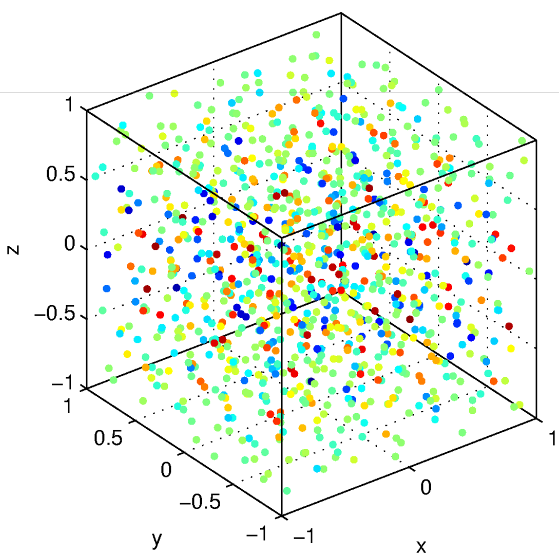
Interpolation with kernels

- 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 $f\big|_X$: $\quad I_X f = \sum_j c_j \Phi(\cdot, \mathbf{x}_j).$

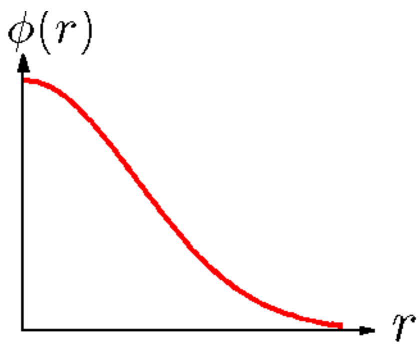


$$\Omega = [-1, 1]^3$$

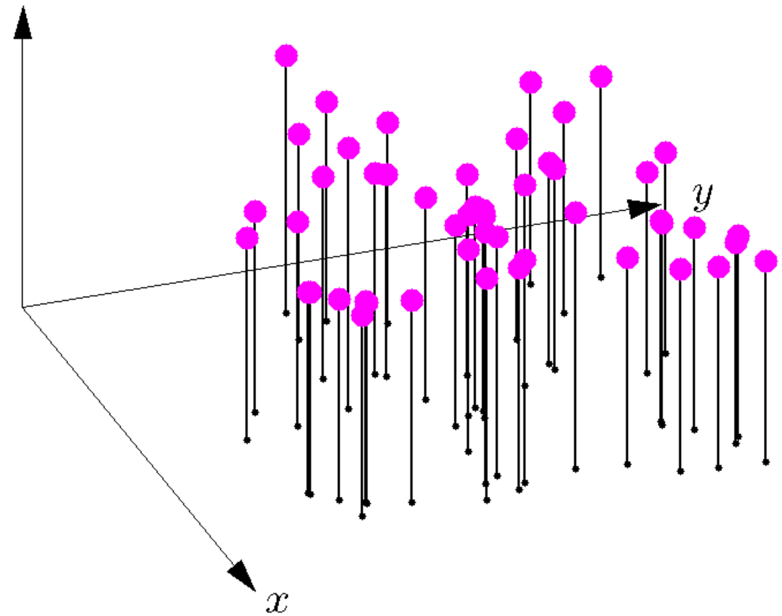
- Leads to radial basis function (RBF) interpolation.

Radial basis function (RBF) interpolation

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



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



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

Radial basis function (RBF) interpolation

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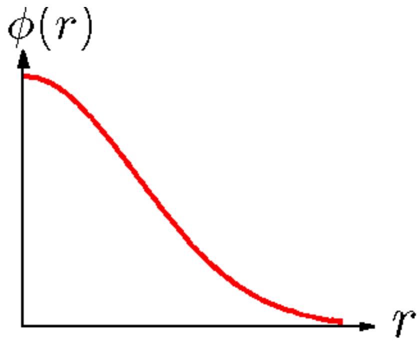

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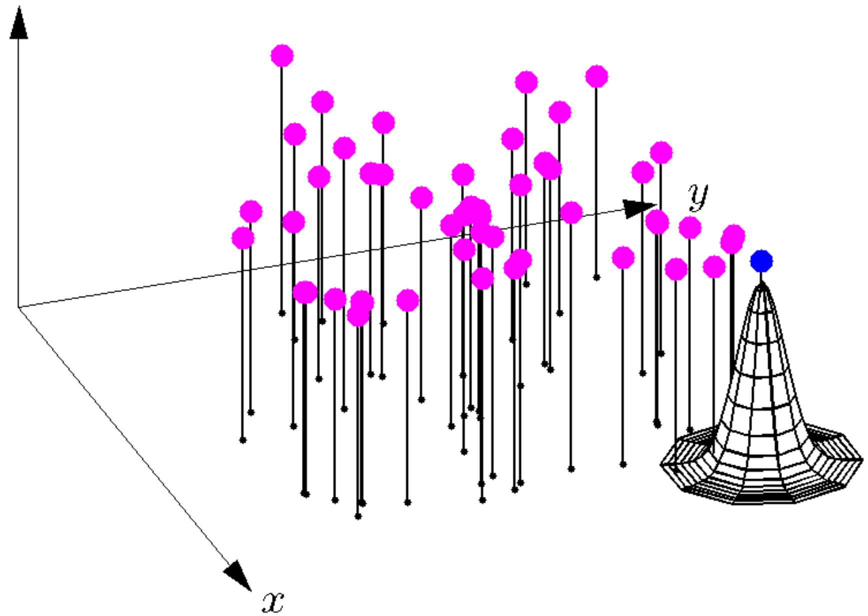

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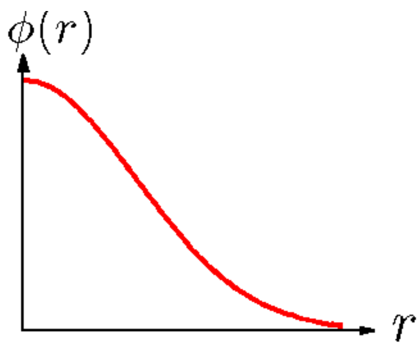

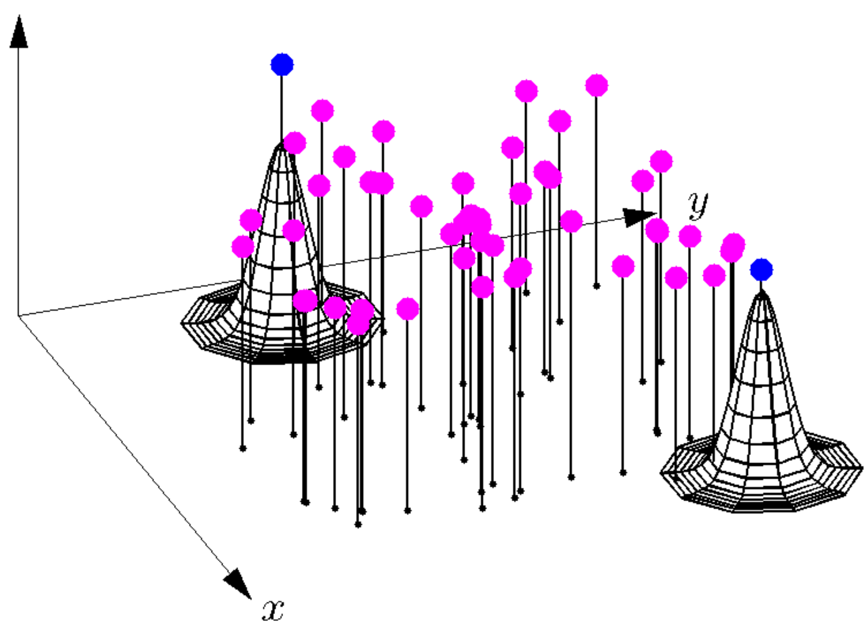

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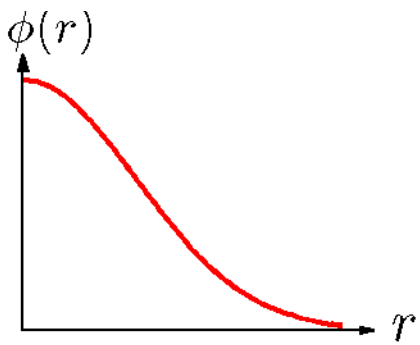

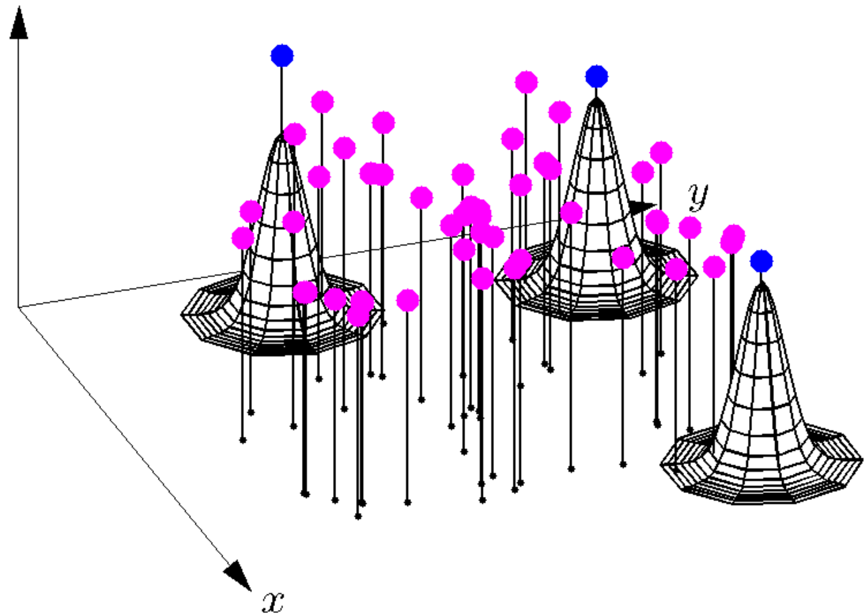

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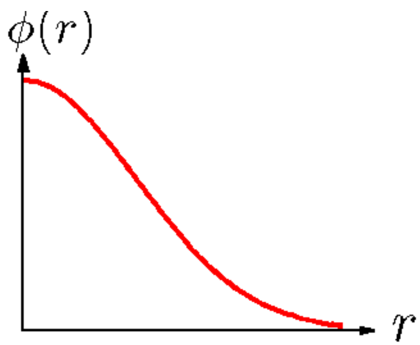

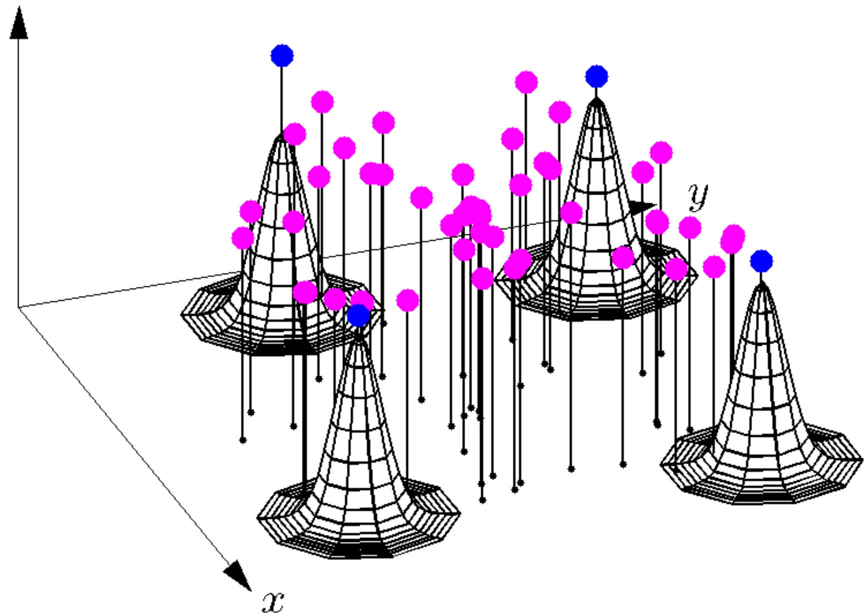

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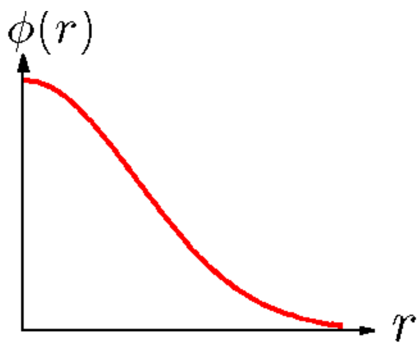

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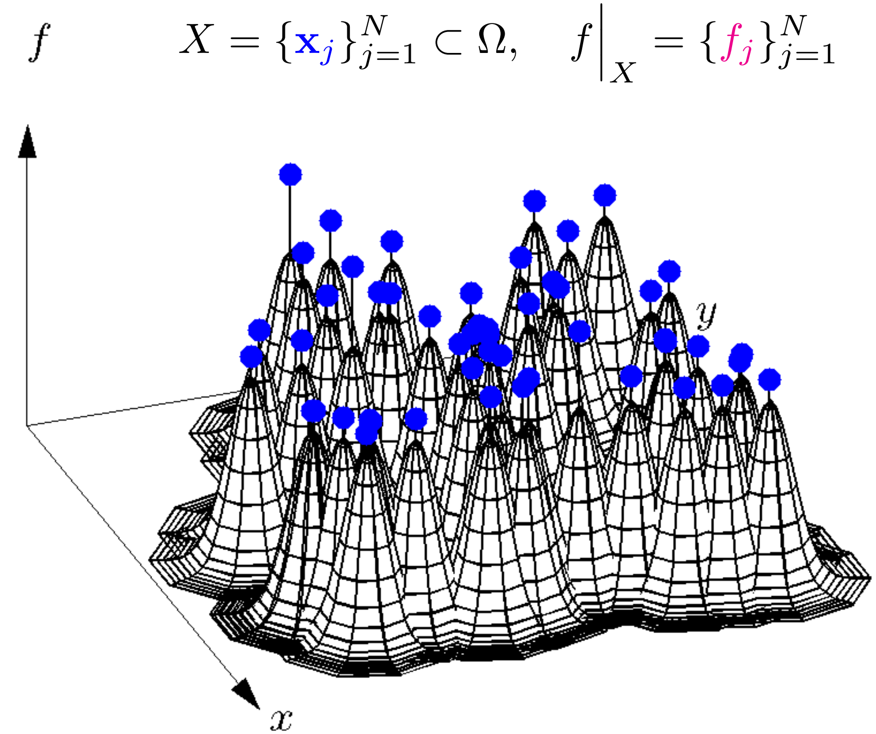

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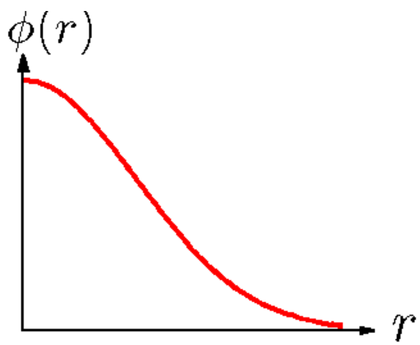

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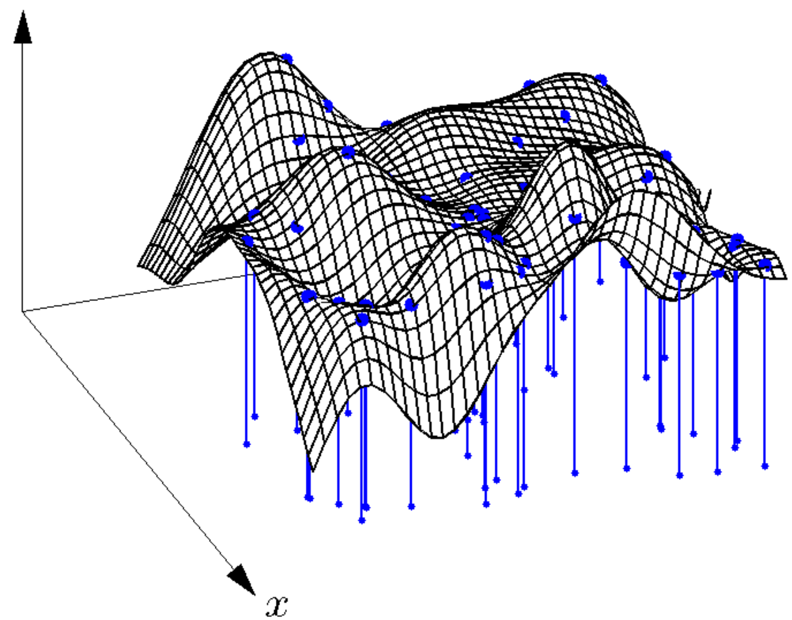

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Linear system for determining the interpolation coefficients

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

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

Positive definite radial kernels

- Some results on positive definite radial kernels.

  Theorem. If $\phi \in C[0,\infty)$ with $\phi(0) > 0$ and $\phi(\rho) < 0$ for some $\rho > 0$, then ϕ cannot be positive definite in $\mathbb{R}^d$ for all d.

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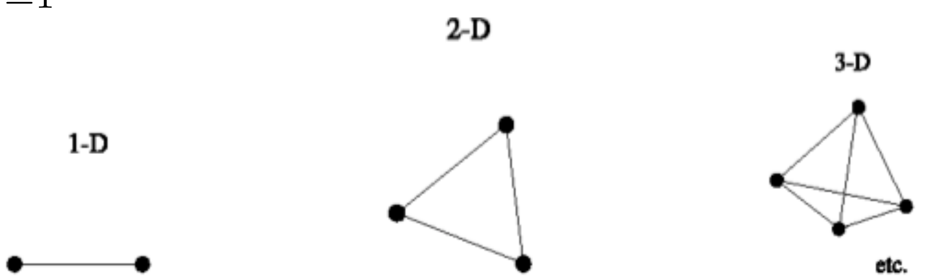
  Theorem. If $\phi \in C[0,\infty)$ with $\phi(0) > 0$ and $\phi(\rho) < 0$ for some $\rho > 0$, then ϕ cannot be positive definite in $\mathbb{R}^d$ for all d.

  Proof

  Consider X to be the vertices of an m dimensional simplex with spacing ρ, i.e. $X = \{\mathbf{x}\}_{j=1}^{m+1} \subset \mathbb{R}^m$



  Then

$$\sum_{i=1}^{m+1}\sum_{j=1}^{m+1}\phi(\|\mathbf{x}_i - \mathbf{x}_j\|) = \sum_{i=1}^{m+1}\phi(0) + \sum_{i=1}^{m+1}\sum_{j=1, j\neq i}^{m+1}\phi(\rho)$$
$$= (m+1)[\phi(0) + m\phi(\rho)].$$

  Given $\phi(0) > 0$, we can find a ρ for which $\phi(\rho) < 0$ and an m to make this sum zero.

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Definition. A function $\Phi : [0, \infty) \to \mathbb{R}$ is said to be completely monotone on $[0, \infty)$ if

$$(1)\ \Phi \in C[0,\infty), \quad (2)\ \Phi \in C^{\infty}(0,\infty), \quad (3)\ (-1)^k \Phi^{(k)}(t) \geq 0,\ t > 0,\ k = 0, 1, \ldots$$

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Theorem (Hausdorff-Bernstien-Widder)**.** A function Φ is completely monotone if and only if it can be written in the form

$$\Phi(t) = \int_0^\infty e^{-st} d\gamma(s),$$

where $\gamma(s)$ is bounded, non-decreasing, and not concentrated at zero.

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$$\Phi(t) = \int_0^{\infty} e^{-st} d\gamma(s),$$

where $\gamma(s)$ is bounded, non-decreasing, and not concentrated at zero.

Theorem (Schoenberg 1938). Let $\phi : [0, \infty) \to \mathbb{R}$ be a radial kernel and $\Phi(r) = \phi(\sqrt{r})$. Then ϕ is positive definite on $\mathbb{R}^d$, for all d, if and only if Φ is completely monotone on $[0, \infty)$ and not constant.

Proof: Use Bernstein-Hausdorff-Widder result and the fact the Gaussian is positive definite.

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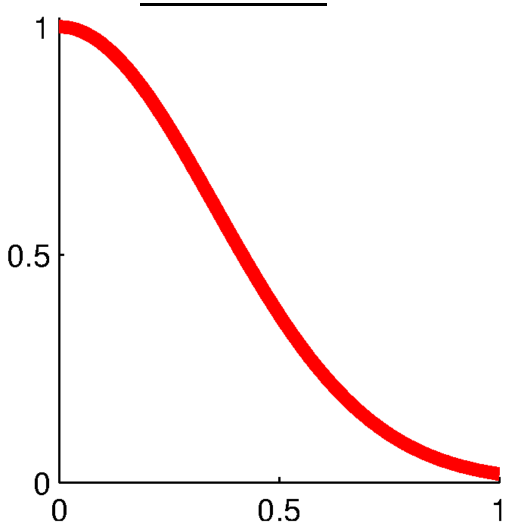
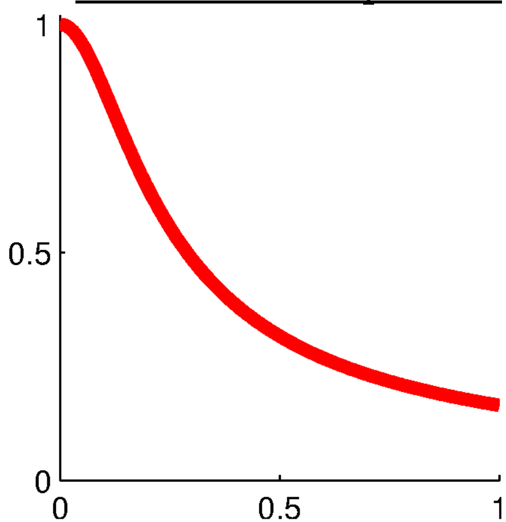
Examples:

Gaussian



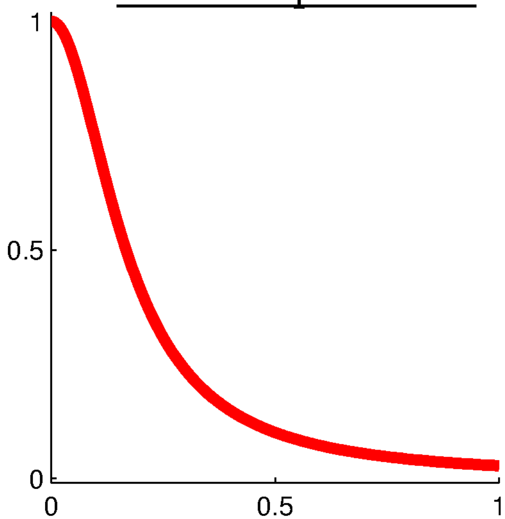
$$\phi(r) = \exp(-(\varepsilon r)^2)$$

Inverse multiquadric



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

Inverse quadratic



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

Here ε is called the shape parameter (more on this later).

Positive definite radial kernels

- Results on dimensions specific positive definite radial 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

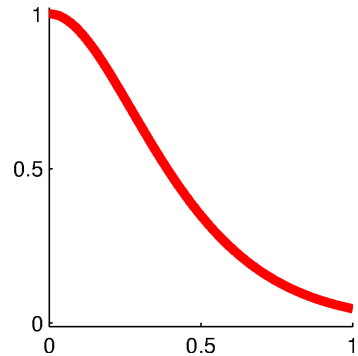
Finite-smoothness

Matérn

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

PD for $2\nu > d$

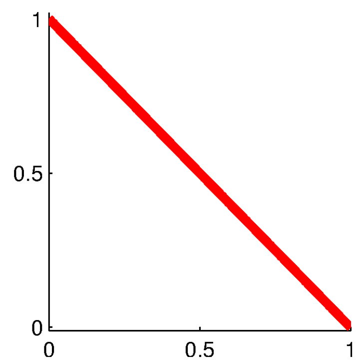
Ex: $e^{-r}(r^2+3r+3)$



Truncated powers

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

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

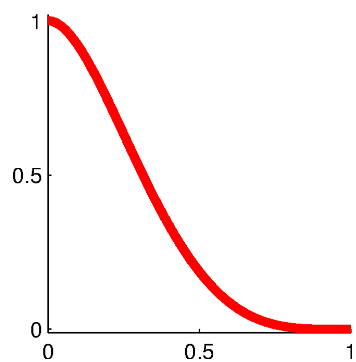


Wendland (1995)

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

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

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

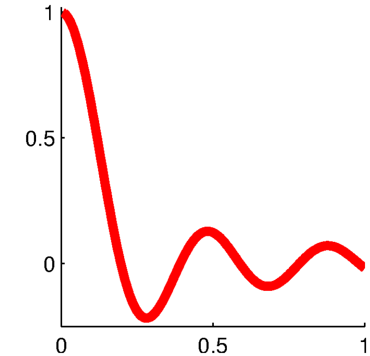


Infinite-smoothness

J-Bessel

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

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

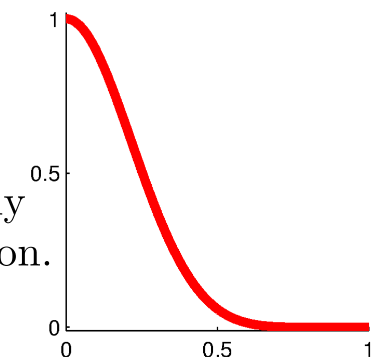


Platte

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

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

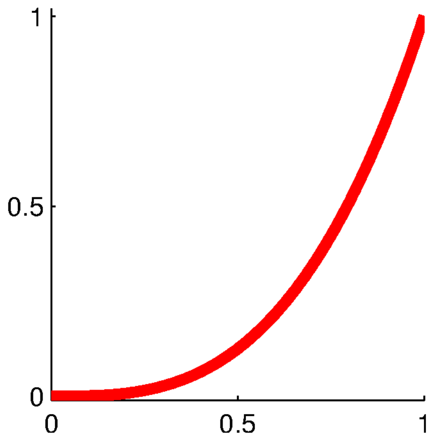
PD dimension depends on convolution dimension.



Conditionally positive definite kernels

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

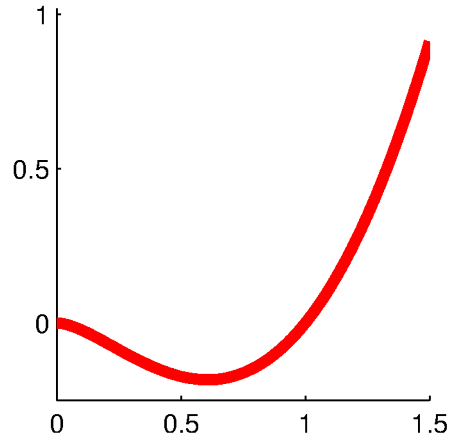
Cubic



$$\phi(r) = r^3$$

Cubic spline in 1-D

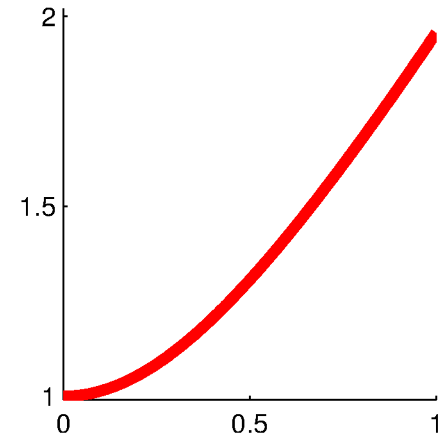
Thin plate spline



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

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. We will not take this approach; see Ch. 8 Wendland 2005 for details.

- We will instead use a generalization of completely monotone functions.

Conditionally positive definite kernels

Definition. A continuous 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:

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

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

- 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. A continuous kernel $\Phi : [0, \infty) \to \mathbb{R}$ is said to be completely monotone *of order k* on $(0, \infty)$ if $(-1)^k \Phi^{(k)}$ is completely monotone on $(0, \infty)$.

Examples:

k=1: $\Phi(t) = \sqrt{t}$ $\quad \Phi(t) = \sqrt{1+t}$

k=2: $\Phi(t) = t^{3/2}$ $\quad \Phi(t) = \frac{1}{2} t \log t$

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Examples:

$k=1$		$k=2$	
$\Phi(t) = \sqrt{t}$	$\Phi(t) = \sqrt{1+t}$	$\Phi(t) = t^{3/2}$	$\Phi(t) = \frac{1}{2} t \log t$

Theorem (Micchelli (1986); Guo, Hu, & Sun (1993))**.** The radial kernel $\phi : [0,\infty)$ is conditionally positive definite on $\mathbb{R}^d$, for all d, if and only if $\Phi = \phi(\sqrt{\cdot})$ is completely monotone of order k on $(0,\infty)$ and $\Phi^{(k)}$ is not constant.

Remark:

- This is one of the BIG theorems that launched the RBF field.
- It says, for example, that linear, cubic, thin-plate splines, and the multiquadric are conditionally positive definite on $\mathbb{R}^d$ for any d.
- Next, its consequences on RBF interpolation of scattered data...

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

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

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

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

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

- $\text{rank}(P) = n$ (i.e. X is unisolvent on $\Pi_{k-1}(\mathbb{R}^d)$),
- $\Phi = \phi(\sqrt{\cdot})$ is completely monotone of order k on $(0, \infty)$,
- $\Phi^{(k)}$ is not constant.

Conditionally positive definite kernels

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Example (Thin plate spline, $\mathbb{R}^2$). Let

- $\phi(r) = r^2 \log(r)$
- $p_1(x, y) = 1$, $p_2(x, y) = x$, and $p_3(x, y) = y$.

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

Conditionally positive definite kernels

Theorem (Micchelli (1986)). Suppose $\Phi = \phi(\sqrt{\cdot})$ is completely monotone of order 1 on $(0,\infty)$ and Φ' is not constant. Then for any distinct set of nodes $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{R}^d$, and any d, the matrix A with entries $a_{i,j} = \phi(\|\mathbf{x}_i - \mathbf{x}_j\|)$, $i,j = 1,\ldots,N$, has $N-1$ positive eigenvalues and 1 negative eigenvalue. Hence it is invertible.

Remark:

- This theorem means that for kernels like the popular multiquadric $\phi(r) = \sqrt{1+(\varepsilon r)^2}$ the basic RBF interpolant

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

  has a unique solution for any distinct set of nodes $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{R}^d$ and sampled target function f on X.

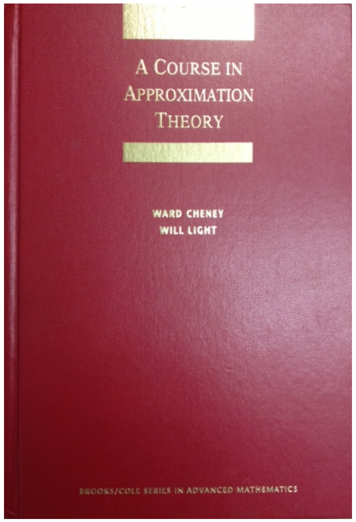
- Augmenting the RBF interpolant with polynomials is not necessary to guarantee uniqueness for order 1 CPD kernels.

- This theorem answered a conjecture from Franke (1983) regarding the multiquadric.

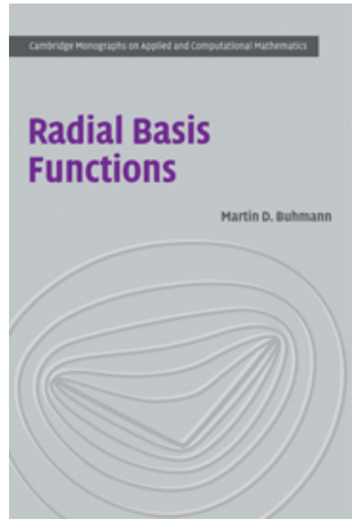
Radial basis function (RBF) interpolation

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

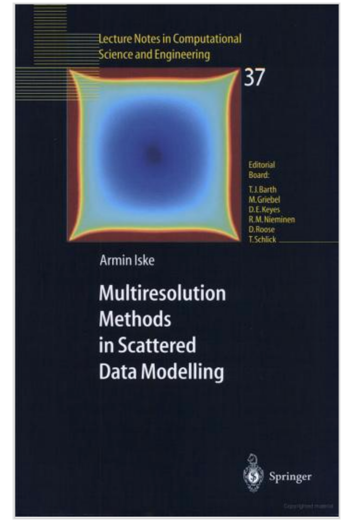
1999



2003

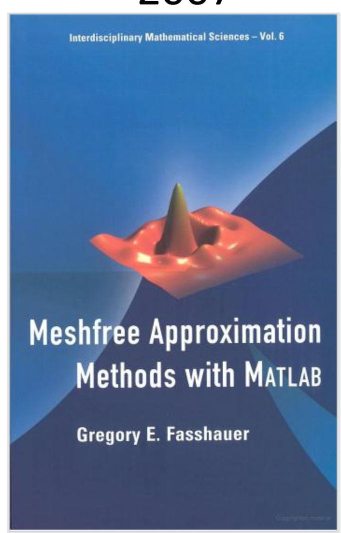


2004



2005

2007



2014: SIAM

A Primer on Radial Basis Functions with Applications to the Geosciences

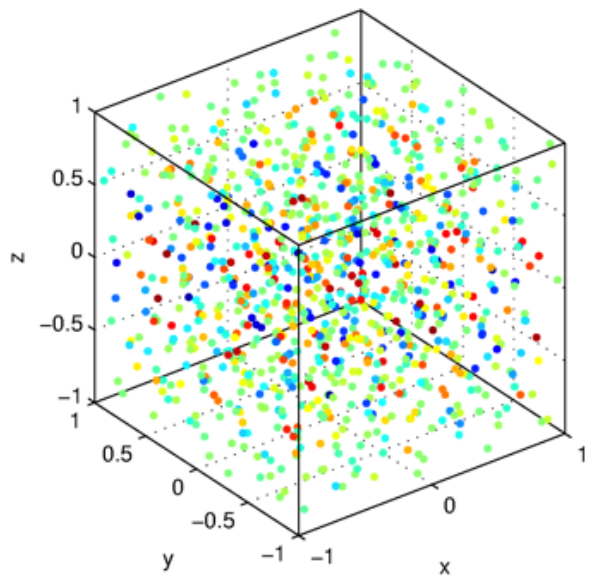
Bengt Fornberg
Natasha Flyer

Interpolation 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 radial basis function (RBF) interpolation.

Interpolation with kernels on the sphere

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

  1. The kernel should be easy to compute.
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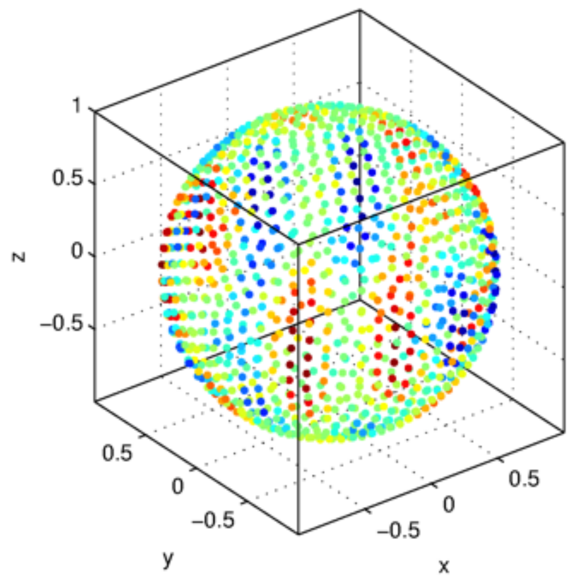
  3. The kernel interpolant should accurately reconstruct f.

- For problems like



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

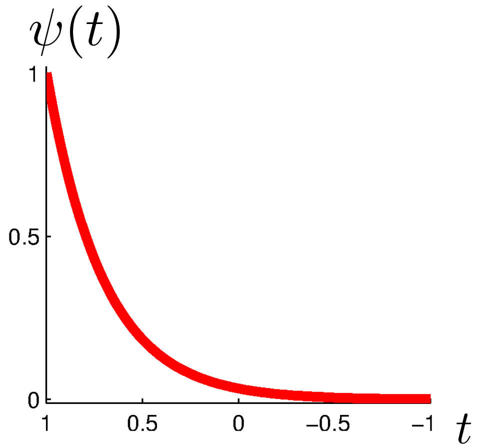
Obvious(?) choice: Φ is a (conditionally) positive definite zonal kernel:

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

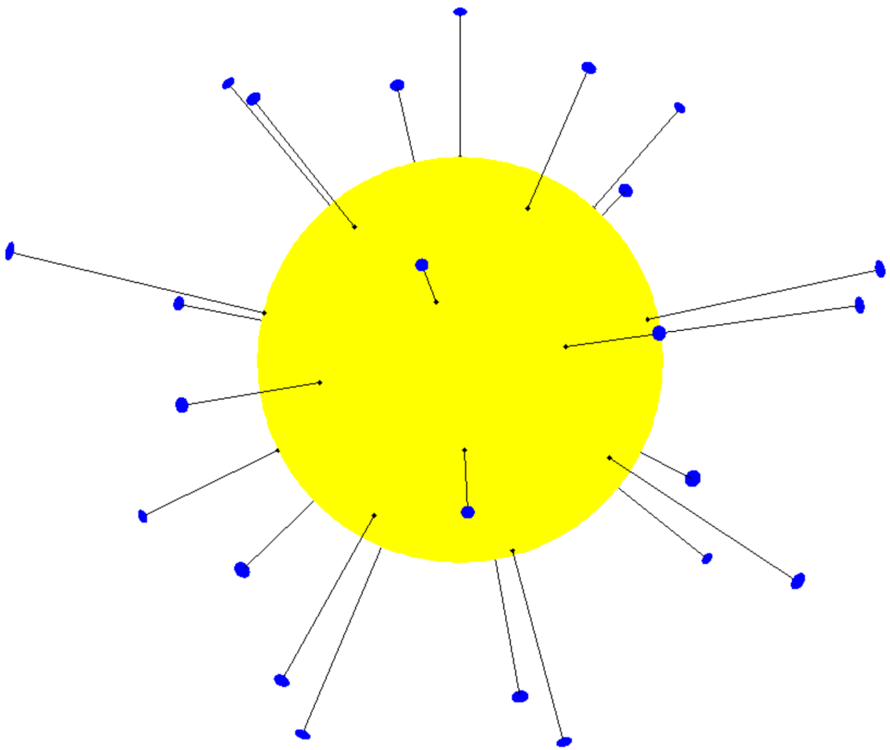
- Analog of RBF interpolation for the sphere: SBF interpolation.

SBF interpolation

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



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



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

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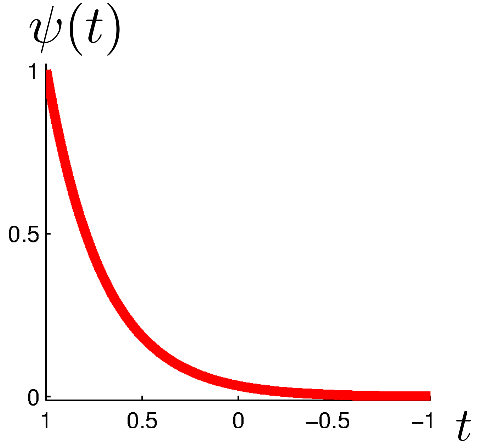

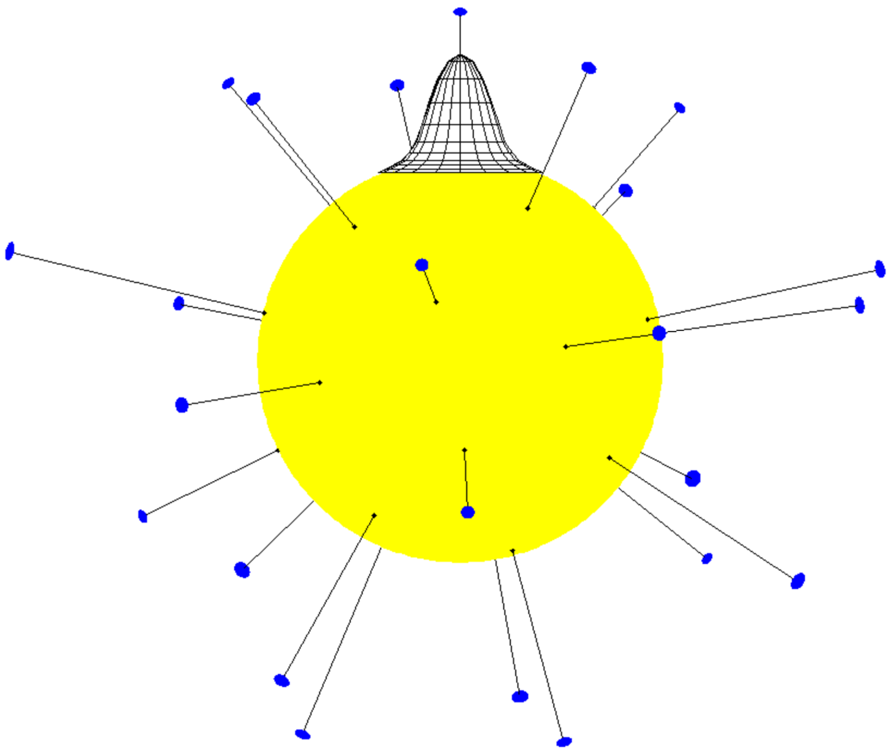

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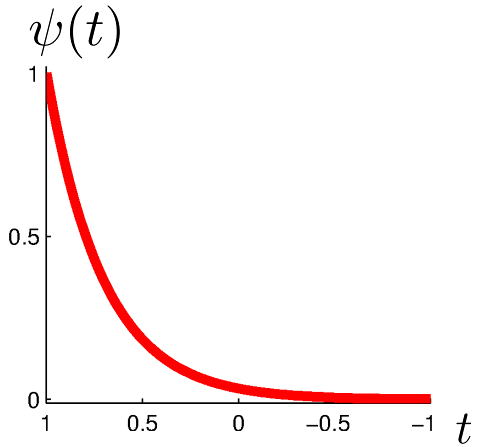

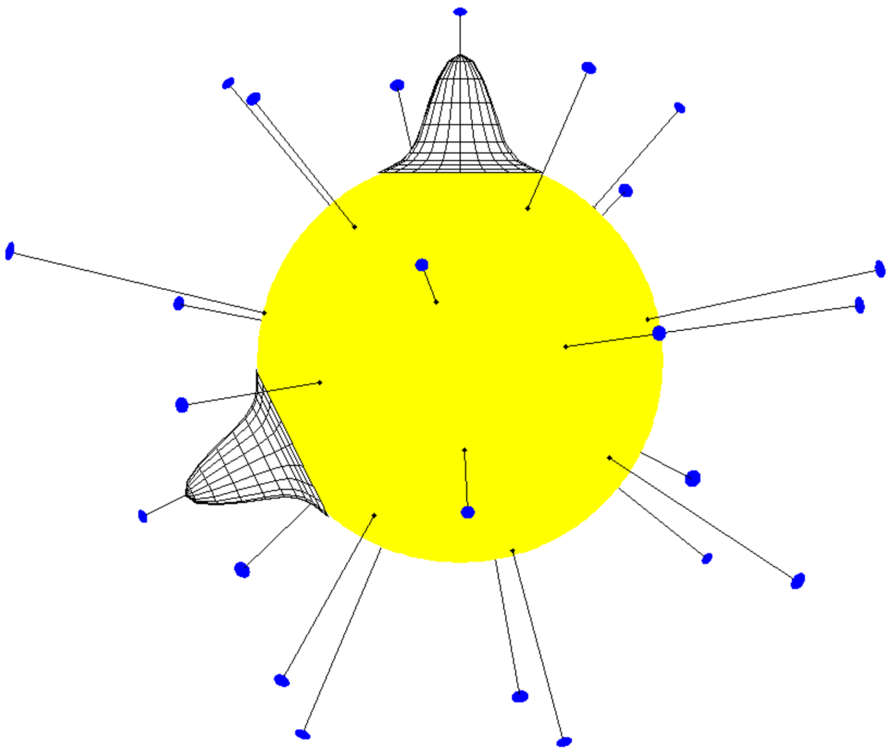

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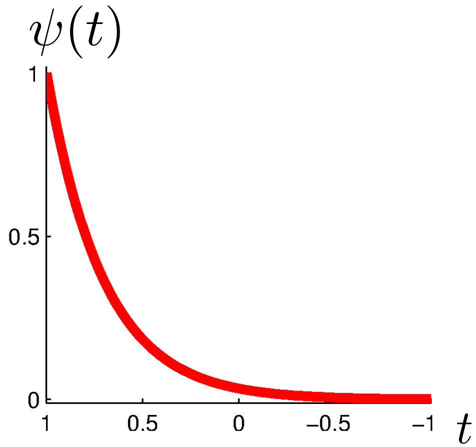

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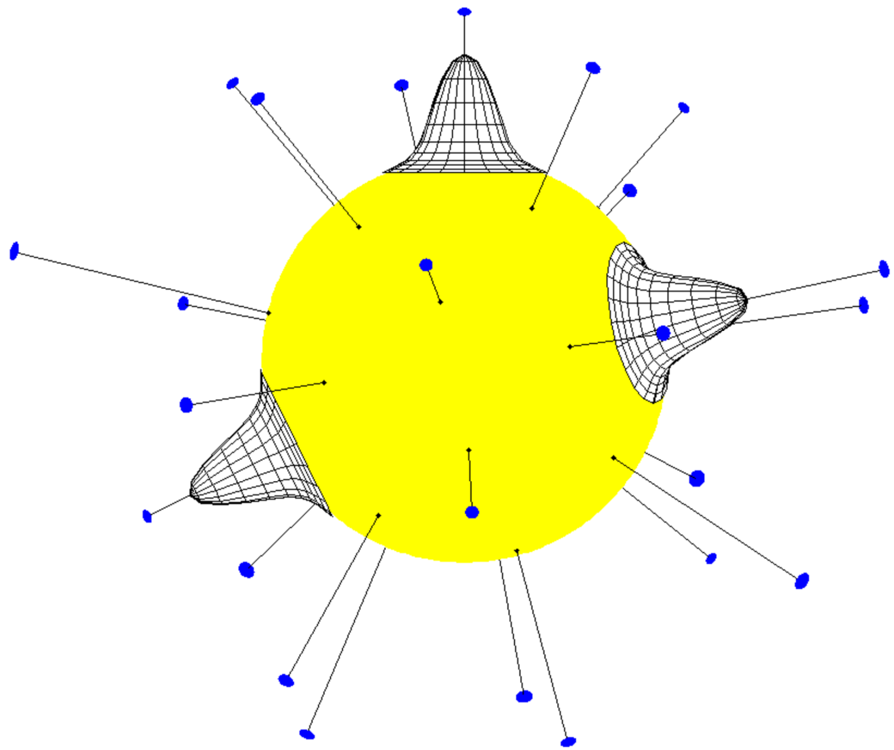

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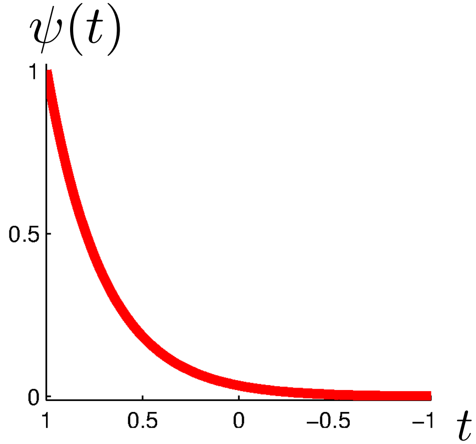

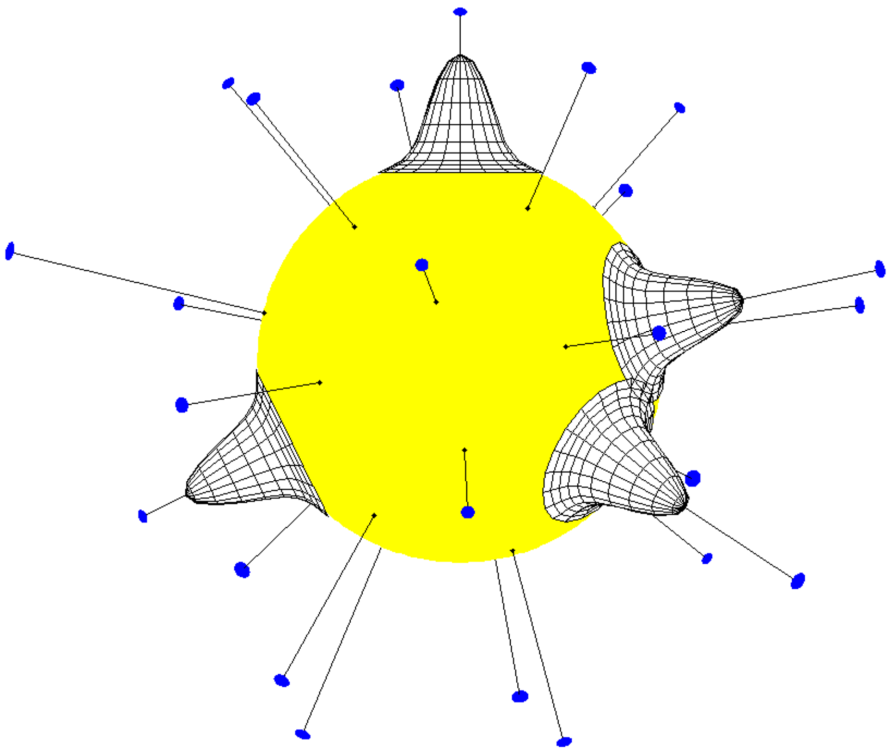

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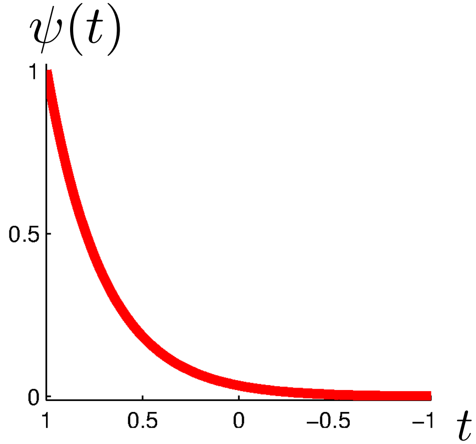

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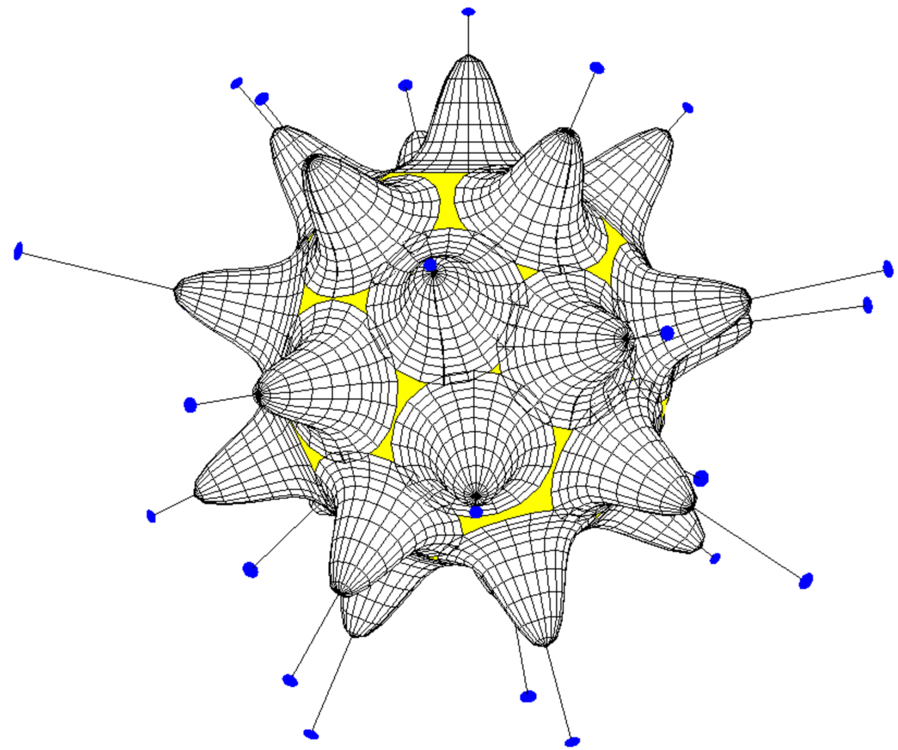

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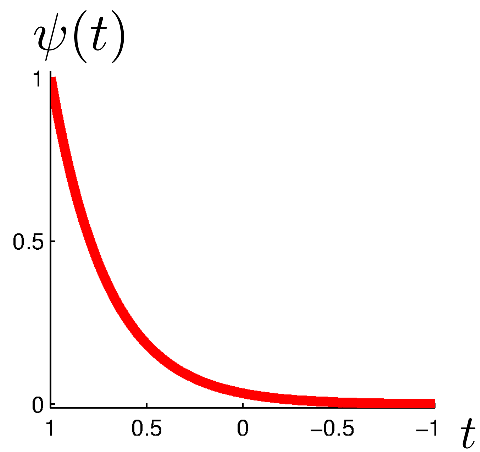

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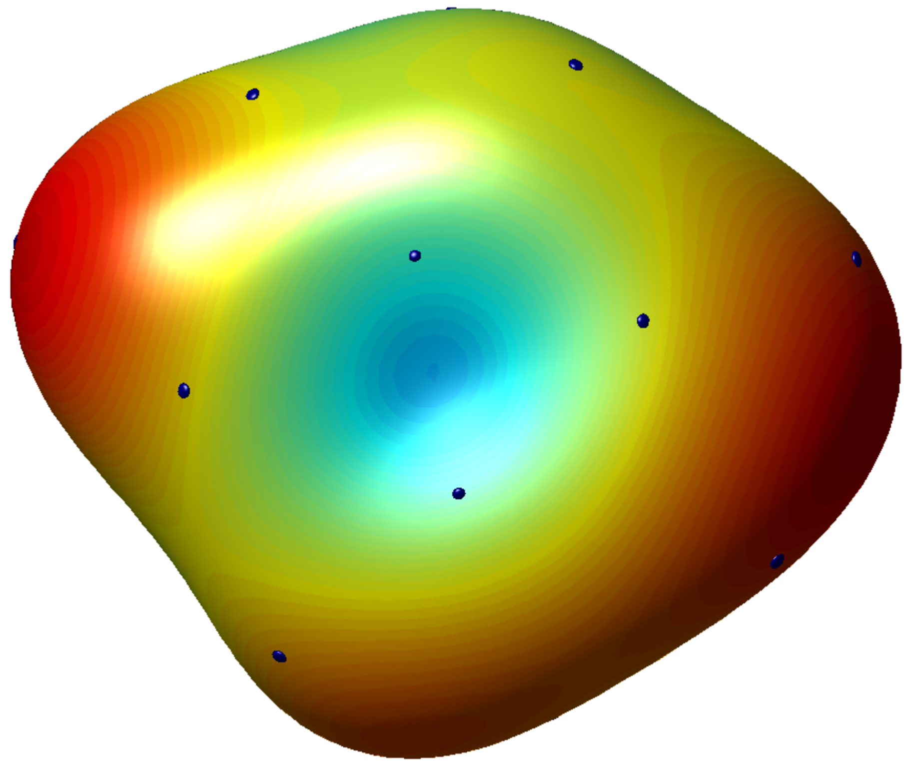

Basic SBF Interpolant for $\mathbb{S}^2$

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

Linear system for determining the interpolation coefficients

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

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.

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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).

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- 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.

Positive definite zonal kernels

- Any positive definite radial kernel ϕ on $\mathbb{R}^3$ is also positive definite on $\mathbb{S}^2$.
- In fact, they are positive definite zonal kernels, since for $\mathbf{x}, \mathbf{y} \in \mathbb{S}^2$

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- 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)

Positive definite zonal kernels

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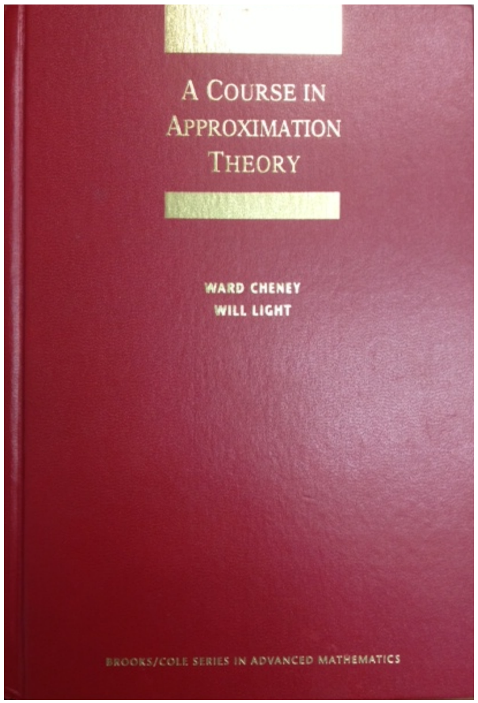
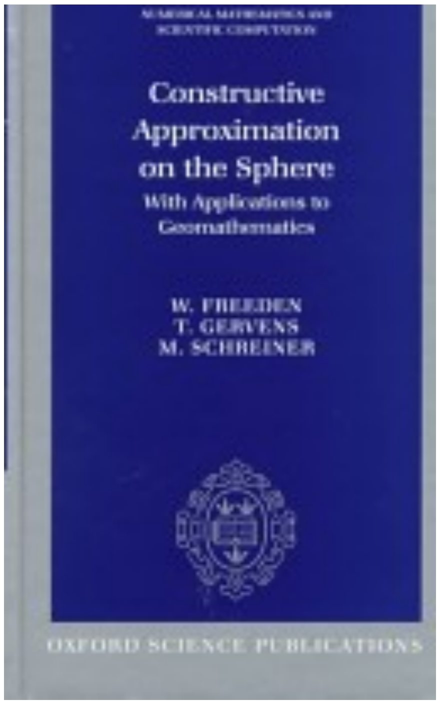
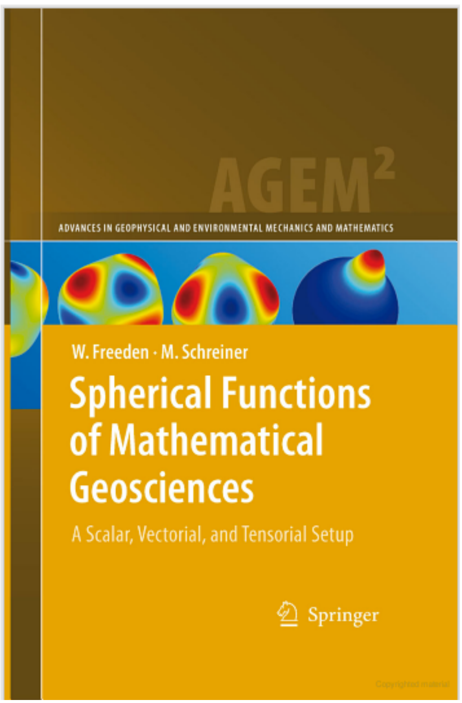
- Is there any advantage to using a purely PD zonal kernel to a restricted PD radial kernel? (Baxter & Hubbert (2001))
- Personally, I have always used restricted radial kernels.

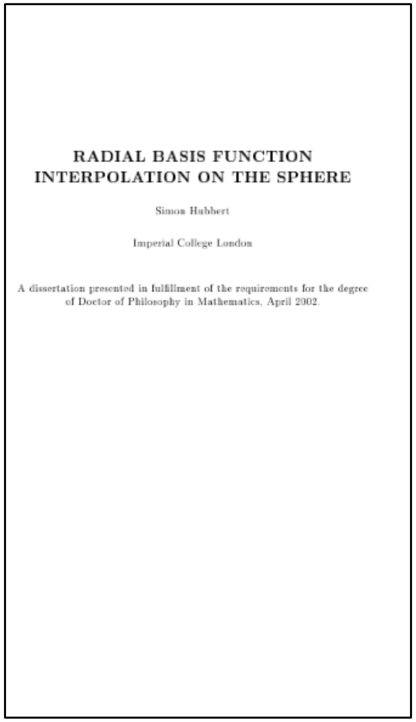
Positive definite zonal kernels

- Some references for the material to come:









Spherical harmonics

- A good understanding of functions on the sphere requires one to be well-versed in spherical harmonics.

- Spherical harmonics are the analog of 1-D Fourier series for approximation on spheres of dimension 2 and higher.

- Several ways to introduce spherical harmonics (Freeden & Schreiner 2008)

- We will use the eigenfunction approach and restrict our attention to the 2-sphere.

- Following this we review some important results about spherical harmonics.

Overview of spherical harmonics

- Laplacian in spherical coordinates ($x = r\cos\theta\cos\varphi$, $y = r\cos\theta\sin\varphi$, $z = r\sin\theta$)

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\underbrace{\left\{\frac{\partial^2}{\partial\theta^2} - \tan\theta\frac{\partial}{\partial\theta} + \frac{1}{\cos^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\}}_{\Delta_s = \text{Laplace-Beltrami operator}}$$

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- Spherical harmonics: Set of all functions bounded at $\theta = \pm\frac{\pi}{2}$ or $z = \pm 1$ such that $\Delta_s Y = \lambda Y$.

- Solve using separation of variables to arrive at:

$$Y_\ell^m(\theta,\varphi) = a_\ell^{|m|}P_\ell^{|m|}(\cos\theta)e^{im\varphi},\ \ell = 0,1,\ldots,\ \ m = -\ell,-\ell+1,\ldots,\ell-1,\ell.$$

- Here P_ℓ^k, for $k = 0,1,\ldots$, $\ell = k,k+1,\ldots$, are the Associated Legendre functions, given by Rodrigues' formula

$$P_\ell^k(z) = (1-z^2)^{k/2}\frac{d^k}{dz^k}\left(P_\ell(z)\right),$$

where P_ℓ is the standard Legendre polynomial of degree ℓ.

- The a_ℓ^k are normalization factors (e.g. $a_\ell^k = \sqrt{((2\ell+1)(\ell-k)!)/(4\pi(\ell+m)!)}$)

Overview of spherical harmonics

- Each spherical harmonic satisfies $\Delta_s Y_\ell^m = -\ell(\ell+1)Y_\ell^m$.
- For each $\ell = 0, 1, \ldots$, there are $2\ell+1$ harmonics with eigenvalue $-\ell(\ell+1)$.

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- Real-form of spherical harmonics:

$$Y_\ell^m(\theta,\varphi) = Y_\ell^m(z,\varphi) = \begin{cases} \sqrt{2}a_\ell^m P_\ell^m(z)\cos(m\varphi) & m > 0, \\ a_\ell^0 P_\ell(z) & m = 0, \\ \sqrt{2}a_\ell^{|m|} P_\ell^{|m|}(z)\sin(m\varphi) & m < 0. \end{cases}$$

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- Can also be expressed purely in Cartesian coordinates ($\mathbf{x} = (x,y,z) \in \mathbb{S}^2$):

$$Y_\ell^m(\mathbf{x}) = Y_\ell^m(x,y,z) = \begin{cases} \sqrt{2} a_\ell^m Q_\ell^m(z)\frac{1}{2}\left((x+iy)^m + (x-iy)^m\right) & m > 0, \\ a_\ell^0 P_\ell(z) & m = 0, \\ \sqrt{2} a_\ell^{|m|} Q_\ell^{|m|}(z)\frac{1}{2i}\left((x+iy)^{-m} - (x-iy)^{-m}\right) & m < 0. \end{cases}$$

where $Q_\ell^m(z) = (-1)^m \dfrac{\partial^m}{\partial z^m} P_\ell(z)$.

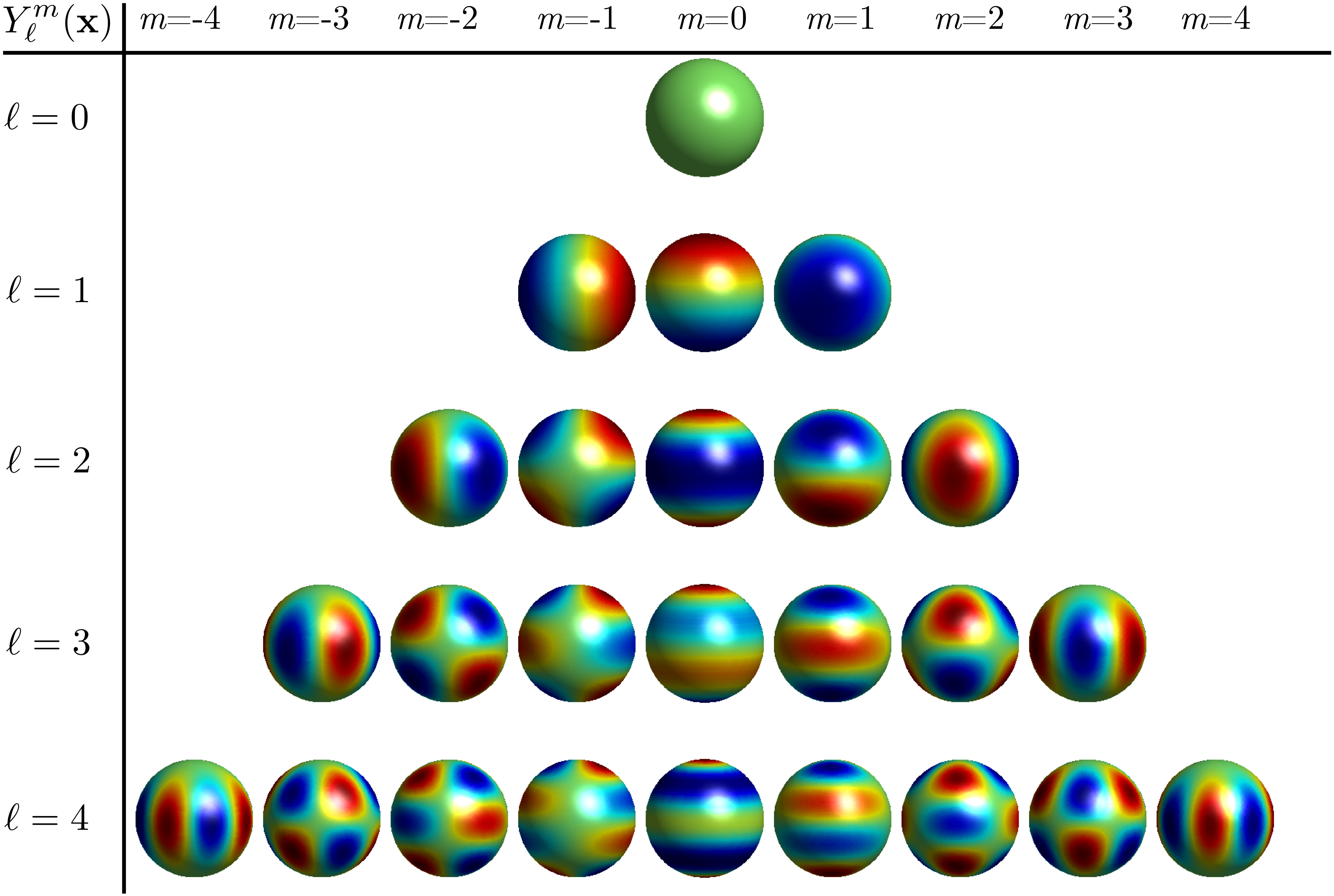
- We will sometimes switch notation from $Y_\ell^m(\theta,\varphi)$ to $Y_\ell^m(\mathbf{x})$.

Overview of spherical harmonics

- Spherical harmonics $Y_\ell^m(\mathbf{x})$ in Cartesian form, for $\ell = 0, 1, 2, 3$.

m=-3	m=-2	m=-1	m=0	m=1	m=2	m=3
			$\frac{1}{2\sqrt{\pi}}$			
		$-\frac{1}{2}\sqrt{\frac{3}{2\pi}}\,y$	$\frac{1}{2}\sqrt{\frac{3}{\pi}}\,z$	$-\frac{1}{2}\sqrt{\frac{3}{2\pi}}\,x$		
	$\frac{1}{2}\sqrt{\frac{15}{2\pi}}\,x\,y$	$-\frac{1}{2}\sqrt{\frac{15}{2\pi}}\,y\,z$	$\frac{1}{4}\sqrt{\frac{5}{\pi}}\left(3z^2-1\right)$	$-\frac{1}{2}\sqrt{\frac{15}{2\pi}}\,x\,z$	$\frac{1}{4}\sqrt{\frac{15}{2\pi}}\,(x-y)(x+y)$	
$-\frac{1}{8}\sqrt{\frac{35}{\pi}}\left(3x^2y-y^3\right)$	$\frac{1}{2}\sqrt{\frac{105}{2\pi}}\,x\,y\,z$	$-\frac{1}{4}\sqrt{\frac{7}{3\pi}}\,y\left(\frac{15z^2}{2}-\frac{3}{2}\right)$	$\frac{1}{2}\sqrt{\frac{7}{\pi}}\left(\frac{5z^3}{2}-\frac{3z}{2}\right)$	$-\frac{1}{4}\sqrt{\frac{7}{3\pi}}\,x\left(\frac{15z^2}{2}-\frac{3}{2}\right)$	$\frac{1}{4}\sqrt{\frac{105}{2\pi}}\,z\left(x^2-y^2\right)$	$-\frac{1}{8}\sqrt{\frac{35}{\pi}}\left(x^3-3xy^2\right)$

Overview of spherical harmonics



Overview of spherical harmonics

- Spherical harmonics satisfy the $L_2(\mathbb{S}^2)$ orthogonality condition:

$$\int_{\mathbb{S}^2} Y_\ell^m(\mathbf{x}) Y_k^n(\mathbf{x}) d\mu(\mathbf{x}) = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \int_{-\pi}^{\pi} Y_\ell^m(\theta,\varphi) Y_k^n(\theta,\varphi) \cos\theta d\varphi d\theta = \delta_{k\ell}\delta_{mn}$$

- They form a complete orthonormal basis for $L_2(\mathbb{S}^2)$.
- If $f \in L_2(\mathbb{S}^2)$ then

$$f(\mathbf{x}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \hat{f}_\ell^m Y_\ell^m(\mathbf{x}), \text{ where } \hat{f}_\ell^m = \int_{\mathbb{S}^2} f(\mathbf{x}) Y_\ell^m(\mathbf{x}) d\mu(\mathbf{x}).$$

- There is no counter part to the fast Fourier transform (FFT) for computing the spherical harmonic coefficients $\hat{f}_\ell^m$.
  - Fast methods of similar complexity ($\mathcal{O}(N \log N)$) have been developed, but have very large constants associated with them. So an actual computational advantage does not occur until N is extremely large.

Overview of spherical harmonics

- Two useful results on spherical harmonics we will use:
- Addition theorem: Let $\mathbf{x}, \mathbf{y} \in \mathbb{S}^2$, then for $\ell = 0, 1, \ldots$

$$\frac{4\pi}{2\ell + 1} \sum_{m=-\ell}^{\ell} Y_\ell^m(\mathbf{x}) Y_\ell^m(\mathbf{y}) = P_\ell(\mathbf{x}^T \mathbf{y}),$$

where P_ℓ is the standard Legendre polynomial of degree ℓ.

- Funk-Hecke formula: Let $f \in L_1(-1, 1)$ and have the Legendre expansion

$$f(t) = \sum_{k=0}^{\infty} a_k P_k(t), \text{ where } a_k = \frac{2k+1}{2} \int_{-1}^{1} f(t) P_k(t) dt.$$

Then for any spherical harmonic Y_ℓ^m the following holds:

$$\int_{\mathbb{S}^2} f(\mathbf{x} \cdot \mathbf{y}) Y_\ell^m(\mathbf{x}) d\mu(\mathbf{x}) = \frac{4\pi a_\ell}{2\ell + 1} Y_\ell^m(\mathbf{y}).$$

Theorems for positive definite zonal kernels

Definition. A zonal kernel $\psi : [-1,1] \to \mathbb{R}$ is said to be a positive definite zonal kernel on $\mathbb{S}^2$ if for any distinct set of nodes $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{S}^2$ 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.

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

Theorem (Schoenberg (1942))**.** If a zonal kernel $\psi : [-1,1] \to \mathbb{R}$ is expressible in a Legendre series as

$$\psi(t) = \sum_{\ell=0}^\infty a_\ell P_\ell(t)$$

where $a_\ell > 0$ for $\ell \geq 0$ and $\sum_{\ell=0}^\infty a_\ell < \infty$ then ψ is a positive definite zonal kernel on $\mathbb{S}^2$.

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Proof:

1. The condition $\sum_{\ell=0}^{\infty} a_\ell < \infty$ guarantees that $\psi \in C(\mathbb{S}^2)$.
2. Use the addition theorem: Let $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{S}^2$ and $\underline{b} \in \mathbb{R}^N \backslash \{0\}$ then

$$\begin{aligned}
\sum_{i=1}^N \sum_{j=1}^N b_i \psi(\mathbf{x}_i^T \mathbf{x}_j) b_j &= \sum_{i=1}^N \sum_{j=1}^N b_i b_j \sum_{\ell=0}^{\infty} a_\ell P_\ell(\mathbf{x}_i^T \mathbf{x}_j) \\
&= \sum_{\ell=0}^{\infty} \frac{4\pi a_\ell}{2\ell+1} \sum_{m=-\ell}^{\ell} \sum_{i=1}^N \sum_{j=1}^N b_i b_j Y_\ell^m(\mathbf{x}_i) Y_\ell^m(\mathbf{x}_j) \\
&= \sum_{\ell=0}^{\infty} \frac{4\pi a_\ell}{2\ell+1} \sum_{m=-\ell}^{\ell} \left| \sum_{j=1}^N b_j Y_\ell^m(\mathbf{x}_j) \right|^2 \geq 0
\end{aligned}$$

3. Show that the quadratic form must be strictly positive.

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where $a_\ell > 0$ for $\ell \geq 0$ and $\sum_{\ell=0}^{\infty} a_\ell < \infty$ then ψ is a positive definite zonal kernel on $\mathbb{S}^2$.

- Necessary and sufficient conditions on the Legendre coefficients a_ℓ were only given in 2003 by Chen, Menegatto, & Sun.
  - Their result says the set $\left\{ \ell \in \mathbb{N}_0 \middle| a_\ell > 0 \right\}$ must contain infinitely many odd and infinitely many even integers.

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:

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

Theorem. If the Legendre expansion coefficients of $\psi : [-1,1] \to \mathbb{R}$ satisfy $a_\ell > 0$ for $\ell \geq k$ and $\sum_{\ell=0}^{\infty} a_\ell < \infty$.

Proof: Use same ideas as the positive definite case.

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.

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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.

Spherical Fourier coefficients

- More useful to work with a zonal kernels spherical Fourier coefficients $\hat{\psi}_\ell$. These are related to Legendre coefficients through the Funk-Hecke formula:

$$\psi(\mathbf{x}^T\mathbf{y}) = \sum_{\ell=0}^{\infty} \hat{\psi}(\ell) \sum_{m=-\ell}^{\ell} Y_\ell^m(\mathbf{x}) Y_\ell^m(\mathbf{y}) \Longrightarrow \hat{\psi}(\ell) := \frac{4\pi a_\ell}{2\ell+1}$$

- Error estimates for SBF interpolants are governed by the asymptotic decay of $\hat{\psi}_\ell$.
- Stable algorithms (RBF-QR) also work with $\hat{\psi}_\ell$ (more on this later...)
- Baxter & Hubbert (2001) computed $\hat{\psi}_\ell$ for many standard RBFs restricted to $\mathbb{S}^2$.
- zu Castell & Filbir (2005) and Narcowich, Sun, & Ward (2007) linked the spherical Fourier coefficients of restricted RBFs to the standard Fourier coefficients in $\mathbb{R}^3$:

$$\hat{\psi}_\ell = \int_0^\infty u \hat{\phi}(u) J_{\ell+1/2}(u) du,$$

where $\hat{\phi}$ is the Hankel transform of the RBF in $\mathbb{R}^3$.

Examples of positive definite zonal kernels

- Examples of positive definite (PD) and order k conditionally positive definite (CPD(k)) zonal kernels with their spherical Fourier coefficients.

Name	Kernel $(r(t)=\sqrt{2-2t})$	Fourier coefficients $\hat{\psi}_\ell$ $(0<h<1,\ \varepsilon>0)$	Type
Legendre	$\psi(t)=(1+h^2-2ht)^{-1/2}$	$\hat{\psi}_\ell=\dfrac{2\pi h^\ell}{\ell+1/2}$	PD
Poisson	$\psi(t)=(1-h^2)(1+h^2-2ht)^{-3/2}$	$\hat{\psi}_\ell=4\pi h^\ell$	PD
Spherical	$\psi(t)=1-r(t)+\dfrac{(r(t))^2}{2}\log\left(\dfrac{r(t)+2}{r(t)}\right)$	$\hat{\psi}_\ell=\dfrac{2\pi}{(\ell+1/2)(\ell+1)(\ell+2)}$	PD
Gaussian	$\psi(t)=\exp(-(\varepsilon r(t))^2)$	$\varepsilon^{2\ell}\dfrac{4\pi^{3/2}}{\varepsilon^{2\ell+1}}e^{-2\varepsilon^2}I_{\ell+1/2}(2\varepsilon^2)$	PD
IMQ	$\psi(t)=\dfrac{1}{\sqrt{1+(\varepsilon r(t))^2)}}$	$\varepsilon^{2\ell}\dfrac{4\pi}{(\ell+1/2)}\left(\dfrac{2}{1+\sqrt{4\varepsilon^2+1}}\right)^{2\ell+1}$	PD
MQ	$\psi(t)=-\sqrt{1+(\varepsilon r(t))^2)}$	$\varepsilon^{2\ell}\dfrac{2\pi(2\varepsilon^2+1+(\ell+1/2)\sqrt{1+4\varepsilon^2})}{(\ell+3/2)(\ell+1/2)(\ell-1/2)}\left(\dfrac{2}{1+\sqrt{4\varepsilon^2+1}}\right)^{2\ell+1}$	CPD(1)
TPS	$\psi(t)=(r(t))^2\log(r(t))$	$\dfrac{8\pi}{(\ell+2)(\ell+1)\ell(\ell-1)}$	CPD(2)
Cubic	$\psi(t)=(r(t))^3$	$\dfrac{18\pi}{(\ell+5/2)(\ell+3/2)(\ell+1/2)(\ell-1/2)(\ell-3/2)}$	CPD(2)

- First three kernels are specific to $\mathbb{S}^2$, while the last 5 are RBFs restricted to $\mathbb{S}^2$.

Error estimates

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

- We will introduce (or review) some background notation and material that is necessary for the proofs of the estimates, but will not prove them.
  - Reproducing kernel Hilbert spaces (RKHS)
  - Sobolev spaces on $\mathbb{S}^2$;
  - Native spaces;
  - Geometric properties of node sets $X \subset \mathbb{S}^2$.

- Brief historical notes regarding SBF 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).

Reproducing kernel Hilbert spaces

- Reproducing kernel Hilbert spaces (RKHS) play a key role deriving error estimates for SBF (and more generally RBF) interpolants.

- They allow one to view the interpolation problem as the solution to a particular optimization problem.

Definition. Let $\mathcal{F}(\Omega)$ be a Hilbert space of functions $f : \Omega \to \mathbb{R}$ with inner product $\langle \cdot, \cdot \rangle_{\mathcal{F}}$. If there exists a kernel $\Phi : \Omega \times \Omega \to \mathbb{R}$ such that for all $\mathbf{y} \in \Omega$

$$f(\mathbf{y}) = \langle f, \Phi(\cdot, \mathbf{y}) \rangle_{\mathcal{F}} \text{ for all } f \in \mathcal{F},$$

then $\mathcal{F}$ is called a RKHS with reproducing kernel Φ.

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  then $\mathcal{F}$ is called a RKHS with reproducing kernel Φ.

- The reproducing kernel Φ of a RKHS is unique.

- Existence of Φ is equivalent to the point evaluation functional $\delta_{\mathbf{y}} : \mathcal{F} \to \mathbb{R}$ being continuous. (Implied by Reisz representation theorem).

- Φ also satisfies the following:
  (1) $\Phi(\mathbf{x}, \mathbf{y}) = \Phi(\mathbf{y}, \mathbf{x})$ for $x, y \in \Omega$; (2) Φ is positive semi-definite on Ω.

Reproducing kernel Hilbert spaces

Example. The space spanned by all spherical harmonics of degree n with the standard $L_2(\mathbb{S}^2)$ inner product $\langle \cdot, \cdot \rangle_{L_2}$ is a RKHS with reproducing kernel

$$\Phi_n(\mathbf{x}, \mathbf{y}) = \sum_{k=0}^{n} \frac{2k+1}{4\pi} P_k(\mathbf{x}^T \mathbf{y}).$$

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Let $\mathbf{x}, \mathbf{y} \in \mathbb{S}^2$ and $f(\mathbf{x}) = \sum_{\ell=0}^{n} \sum_{m=-\ell}^{\ell} c_\ell^m Y_\ell^m(\mathbf{x})$ for some coefficients c_ℓ^m. Then

$$\begin{aligned}
\langle f, \Phi_n(\cdot, \mathbf{y}) \rangle_{L_2} &= \int_{\mathbb{S}^2} f(\mathbf{x}) \Phi_n(\mathbf{x}, \mathbf{y}) d\mu(\mathbf{x}) \\
&= \int_{\mathbb{S}^2} \left(\sum_{\ell=0}^{n} \sum_{m=-\ell}^{\ell} c_\ell^m Y_\ell^m(\mathbf{x}) \right) \left(\sum_{k=0}^{n} \frac{2k+1}{4\pi} P_k(\mathbf{x}^T \mathbf{y}) \right) d\mu(\mathbf{x}) \\
&= \sum_{k=0}^{n} \frac{2k+1}{4\pi} \sum_{\ell=0}^{n} \sum_{m=-\ell}^{\ell} c_\ell^m \int_{\mathbb{S}^2} P_k(\mathbf{x}^T \mathbf{y}) Y_\ell^m(\mathbf{x}) d\mu(\mathbf{x}) \\
&= \sum_{k=0}^{n} \frac{2k+1}{4\pi} \sum_{m=-k}^{k} \frac{4\pi}{2k+1} c_k^m Y_k^m(\mathbf{y}) \qquad \text{(Funk-Hecke formula)} \\
&= \sum_{k=0}^{n} \sum_{m=-k}^{k} c_k^m Y_k^m(\mathbf{y}) = f(\mathbf{y})
\end{aligned}$$

Sobolev spaces

- Sobolev spaces on $\mathbb{S}^2$ can be defined in terms of spherical Harmonics.

Definition. The Sobolev space of order τ on $\mathbb{S}^2$ is given by

$$H^\tau(\mathbb{S}^2) = \left\{ f \in L_2(\mathbb{S}^2) \middle| \|f\|_{H^\tau}^2 = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (1 + \ell(\ell+1))^\tau \left| \hat{f}_\ell^m \right|^2 < \infty \right\}.$$

Here $\|\cdot\|_{H^\tau}$ is a norm induced by the inner product

$$\langle f, g \rangle_{H^\tau} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (1 + \ell(\ell+1))^\tau \hat{f}_\ell^m \hat{g}_\ell^m,$$

where $\hat{f}_\ell^m = \langle f, Y_\ell^m \rangle_{L_2} = \int_{\mathbb{S}^2} f(\mathbf{x}) Y_\ell^m(\mathbf{x}) d\mu(\mathbf{x})$.

- Compare to Sobolev spaces on $\mathbb{R}^3$:

$$H^\beta(\mathbb{R}^3) = \left\{ f \in L_2(\mathbb{R}^3) \middle| \|f\|_{H^\beta}^2 = \int_{\mathbb{R}^3} (1 + \|\boldsymbol{\omega}\|^2)^\beta \left| \hat{f}(\boldsymbol{\omega}) \right|^2 d\mathbf{x} < \infty \right\}.$$

Sobolev spaces

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- Sobolev embedding theorem implies $H^\tau(\mathbb{S}^2)$ is continuously embedded in $C(\mathbb{S}^2)$ for $\tau > 1$. Thus, $H^\tau(\mathbb{S}^2)$ is a RKHS.

- Can show the reproducing kernel is $\Phi_\tau(\mathbf{x}, \mathbf{y}) = \sum_{\ell=0}^{\infty} (1+\ell(\ell+1))^{-\tau} \frac{2\ell+1}{4\pi} P_\ell(\mathbf{x} \cdot \mathbf{y})$.

Native spaces

- Each positive definite zonal kernel ψ naturally gives rise to a RKHS on $\mathbb{S}^2$, which is called the native space of ψ.

- This is the natural space to understand approximation with shifts of ψ.

  Definition. Let ψ be a positive definite zonal kernel with spherical Fourier coefficients $\hat{\psi}_\ell$, $\ell = 0, 1, \ldots$. The native space $\mathcal{N}_\psi$ of ψ is given by

$$\mathcal{N}_\psi = \left\{ f \in L_2(\mathbb{S}^2) \,\middle|\, \|f\|_{\mathcal{N}_\psi} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{|\hat{f}_\ell^m|^2}{\hat{\psi}_\ell} < \infty \right\},$$

  with inner product

$$\langle f, g \rangle_{\mathcal{N}_\psi} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{\hat{f}_\ell^m \hat{g}_\ell^m}{\hat{\psi}_\ell}.$$

- A similar definition holds for conditionally positive definite kernels, but the inner product has to be slightly modified (see Hubbert, 2002).

Native spaces

- An important "optimality" result stems from $\mathcal{N}_\psi(\mathbb{S}^2)$ being a RKHS.
- Consider the following optimization problem:

  Problem. Let $X = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ be a distinct set of nodes on $\mathbb{S}^2$ and let $\{f_1, \ldots, f_N\}$ be samples of some target function f on X. Find $s \in \mathcal{N}_\psi(\mathbb{S}^2)$ that satisfies $s(\mathbf{x}_j) = f_j$, $j = 1, \ldots, N$ and has minimal native space norm $\|s\|_{\mathcal{N}_\psi}$, i.e.

  $$\text{minimize}\left\{\|s\|_{\mathcal{N}_\psi} \,\middle|\, s \in \mathcal{N}_\psi(\mathbb{S}^2) \text{ with } s\big|_X = f\big|_X\right\}.$$

  Solution: s is the unique SBF interpolant to $f\big|_X$ using the kernel ψ.

- SBF interpolants also have nice properties in their respective native spaces:

  1. $\|f - I_{\psi,X} f\|^2_{\mathcal{N}_\psi} + \|I_{\psi,X} f\|^2_{\mathcal{N}_\psi} = \|f\|^2_{\mathcal{N}_\psi}$
  2. $\|f - I_{\psi,X} f\|_{\mathcal{N}_\psi} \leq \|f\|_{\mathcal{N}_\psi}$

Native spaces

- Note similarity between Sobolev space $H^\tau(\mathbb{S}^2)$ and $\mathcal{N}_\psi(\mathbb{S}^2)$:

$$H^\tau(\mathbb{S}^2) = \left\{ f \in L_2(\mathbb{S}^2) \middle| \|f\|_{H^\tau}^2 = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (1+\ell(\ell+1))^\tau \left|\hat{f}_\ell^m\right|^2 < \infty \right\}$$

$$\mathcal{N}_\psi(\mathbb{S}^2) = \left\{ f \in L_2(\mathbb{S}^2) \middle| \|f\|_{\mathcal{N}_\psi} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{|\hat{f}_\ell^m|^2}{\hat{\psi}_\ell} < \infty \right\}$$

- If $\hat{\psi}_\ell \sim (1+\ell(\ell+1))^{-\tau}$, then it follows that $\mathcal{N}_\psi = H^\tau$, with equivalent norms.

- This is one reason we care about the asymptotic behavior of $\hat{\psi}_\ell$.

- For RBFs restricted to $\mathbb{S}^2$, we have the following nice result connecting the asymptotics of the spherical Fourier coefficients to the Fourier transform (Levesley & Hubbert (2001), zu Castell & Filbir (2005), Narcowich, Sun, & Ward (2007)):

> If ψ is an SBF obtained by restricting an RBF ϕ to $\mathbb{S}^2$ and if $\hat{\phi}(\boldsymbol{\omega}) \sim (1+\|\boldsymbol{\omega}\|_2^2)^{-(\tau+1/2)}$ then $\hat{\psi}_\ell \sim (1+\ell(\ell+1))^{-\tau}$.

Native spaces

- Examples of radial kernels ϕ and their norm-equivalent native spaces $\mathcal{N}_\psi$ when restricted to $\mathbb{S}^2$:

Name	RBF (use $r = \sqrt{2-2t}$ to get SBF ψ)	$\mathcal{N}_\psi(\mathbb{S}^2)$
Matern	$\phi_2(r) = e^{-\varepsilon r}$	$H^{1.5}(\mathbb{S}^2)$
TPS(1)	$\phi(r) = r^2 \log(r)$	$H^{2}(\mathbb{S}^2)$
Cubic	$\phi(r) = r^3$	$H^{2.5}(\mathbb{S}^2)$
TPS(2)	$\phi(r) = r^4 \log(r)$	$H^{3}(\mathbb{S}^2)$
Wendland	$\phi_{3,2}(r) = (1-\varepsilon r)_+^6(3+18(\varepsilon r)+15(\varepsilon r)^2)$	$H^{3.5}(\mathbb{S}^2)$
Matern	$\phi_5(r) = e^{-\varepsilon r}(15+15(\varepsilon r)+6(\varepsilon r)^2+(\varepsilon r)^3)$	$H^{4.5}(\mathbb{S}^2)$

- The spherical Fourier coefficients for all these restricted kernels have algebraic decay rates.

- For kernels with spherical Fourier coefficients with exponential decay rates (*e.g.* Gaussian and multiquadric) the Native spaces are no longer equivalent to Sobolev spaces.

- These natives spaces do satisfy: $\mathcal{N}_\psi(\mathbb{S}^2) \subset H^\tau(\mathbb{S}^2)$ for all $\tau > 1$.

- Error estimates for interpolants are directly linked to the native space of ψ.

Geometric properties of node sets

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

- Mesh norm

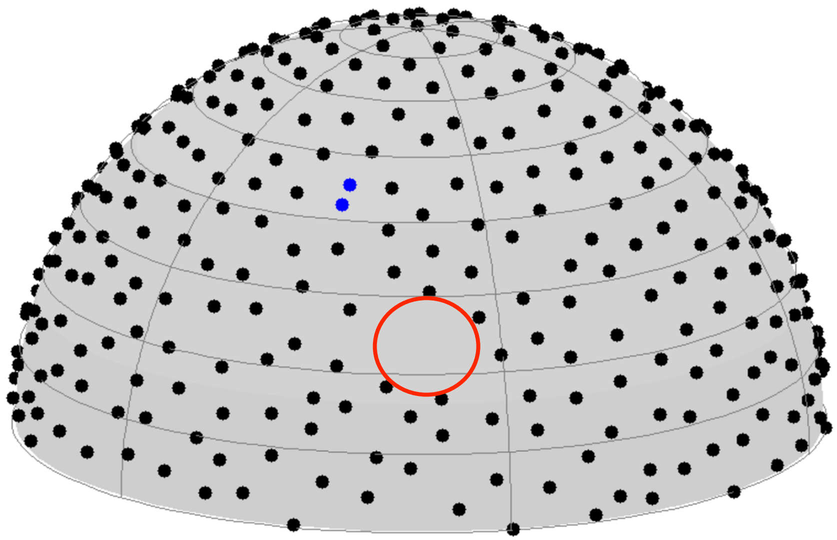
$$h_X = \sup_{\mathbf{x}\in\mathbb{S}^2} \mathrm{dist}_{\mathbb{S}^2}(\mathbf{x}, X)$$

- Separation radius

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

- Mesh ratio

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



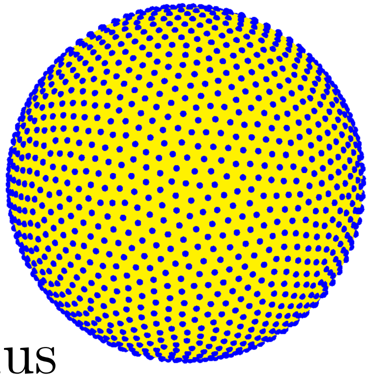
$$X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{S}^2$$

(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>



- ψ is the SBF
- $\hat{\psi}_\ell \sim (1 + \ell(\ell+1))^{-\tau}$, $\tau > 1$
- $\mathcal{N}_\psi(\mathbb{S}^2) = H^\tau(\mathbb{S}^2)$
- $I_X f$ is SBF interpolant of $f\big|_X$

- $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{S}^2$
- h_X = mesh-norm
- q_X = separation radius
- $\rho_X = h_X/q_X$, mesh ratio

Theorem. Target functions in the native space.

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,

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

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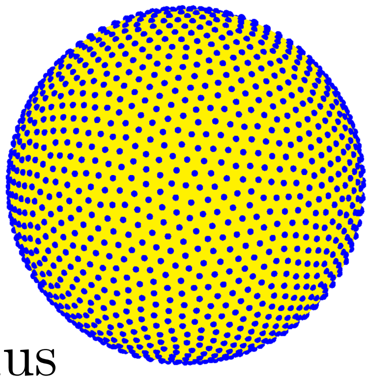

Theorem. Target functions twice as smooth as the native space.

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

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

Interpolation error estimates

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  Jetter, Stöckler, & Ward (1999), Morton & Neamtu (2002), Hubbert & Morton (2004,2004), Narcowich, Sun, Ward, & Wendland (2007)

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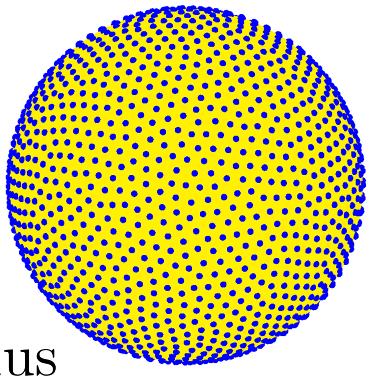


- ψ is the SBF
- $\hat{\psi}_\ell \sim (1+\ell(\ell+1))^{-\tau}$, $\tau > 1$
- $\mathcal{N}_\psi(\mathbb{S}^2) = H^\tau(\mathbb{S}^2)$
- $I_X f$ is SBF interpolant of $f\big|_X$
- $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{S}^2$
- h_X = mesh-norm
- q_X = separation radius
- $\rho_X = h_X/q_X$, mesh ratio

Theorem. Target functions rougher than the native space.

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).

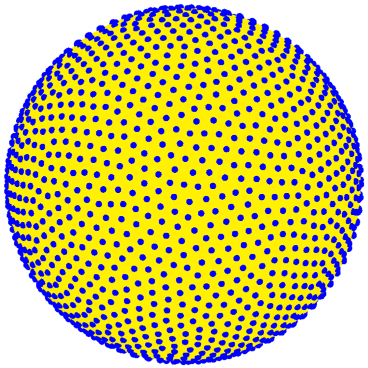
(2) These rates are the best possible.

Interpolation error estimates

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

Notation:

- ψ is the SBF
- $\hat{\psi}_\ell \sim \exp(-\alpha(2\ell+1))$, $\alpha > 0$
- $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{S}^2$
- h_X = mesh-norm



- $$\mathcal{N}_\psi(\mathbb{S}^2) = \left\{ f \in L_2(\mathbb{S}^2) \,\middle|\, \|f\|_{\mathcal{N}_\psi} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{|\hat{f}_\ell^m|^2}{\hat{\psi}_\ell} < \infty \right\}$$

Theorem. Target functions in the native space.

If $f \in \mathcal{N}_\psi(\mathbb{S}^2)$ then $\|f - I_X f\|_{L_\infty(\mathbb{S}^2)} = \mathcal{O}(h_X^{-1}\exp(-\alpha/2h))$.

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.

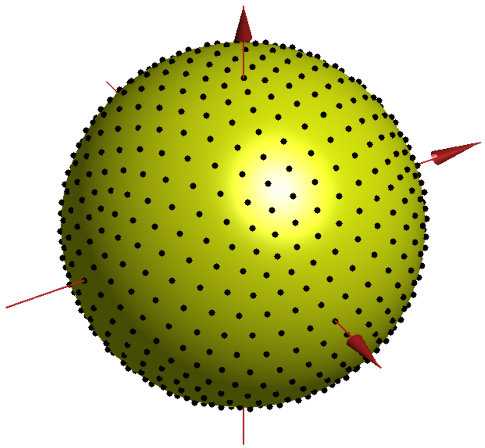
Optimal nodes

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

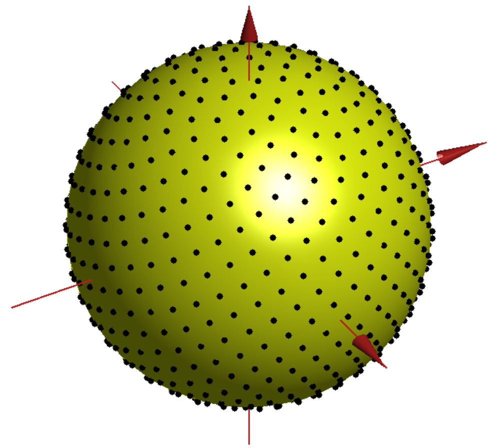
Examples:

Deterministic

Icosahedral

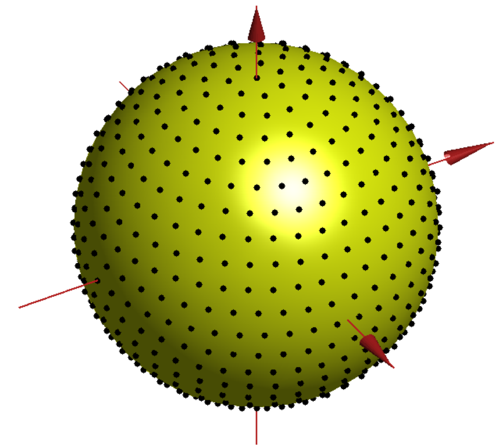


Fibonacci



Swinbank & Purser (2006)

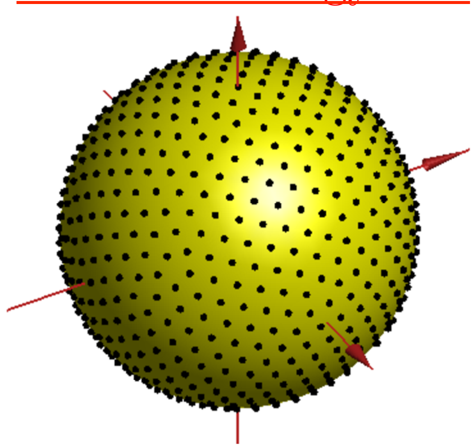
Equal area



Saff & Kuijlaars (1997)

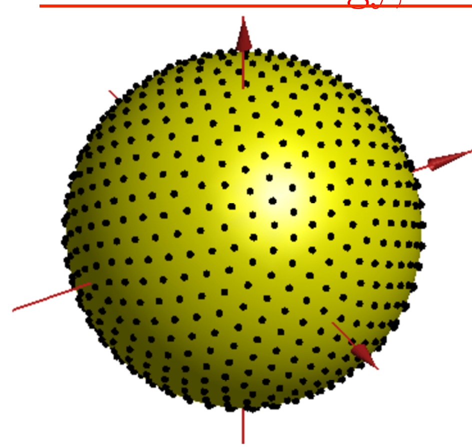
Non-deterministic

Minimum energy $s=2$



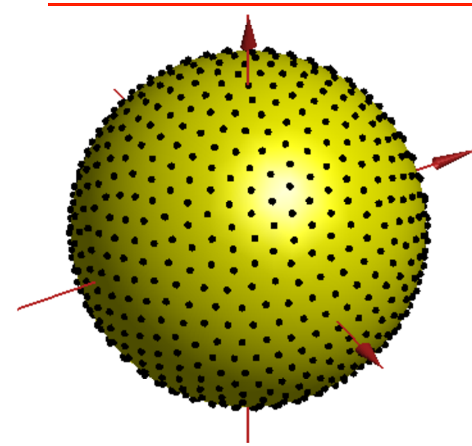
Hardin & Saff (2004)

Minimum energy, $s=3$



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

Maximal determinant



Womersley & Sloan (2001)

Concluding remarks

- This was general background material for getting started in this area.
- There is still much more to learn and many interesting problems.
- Remainder of the lectures will focus on:
  - Approximation (and decomposition) of vector fields.
  - Better bases for certain kernels (better=more stable).
  - Fast algorithms for interpolation (with applications to quadrature)
  - Numerical solution of partial differential equations on spheres.
    - ✧ Focus: non-linear hyperbolic equations.
    - ✧ Global and local methods.
  - Problems in spherical shells.
    - ✧ Mantle convection (Rayleigh-Bénard convection).
  - ✧ 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.