Radial basis function approximation

PhD student course in Approximation Theory

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Outline

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RBF–QR

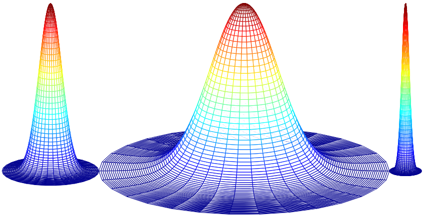
Short introduction to (global) RBF methods

Basis functions: $\phi_j(\underline{x}) = \phi(\|\underline{x} - \underline{x}_j\|)$. Translates of one single function rotated around a center point.

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

Approximation:
$s_\varepsilon(\underline{x}) = \sum_{j=1}^{N} \lambda_j \phi_j(\underline{x})$

Collocation:
$s_\varepsilon(\underline{x}_i) = f_i \;\Rightarrow\; A\underline{\lambda} = \underline{f}$



Advantages:

- Flexibility with respect to geometry.
- As easy in d dimensions.
- Spectral accuracy / exponential convergence.
- Continuosly differentiable approximation.

Commonly used RBFs

Global infinitely smooth

Gaussian	$\exp(-\varepsilon^2 r^2)$,	$\varepsilon > 0$
(Inverse) multiquadric	$(1+\varepsilon^2 r^2)^{\beta/2}$,	$\varepsilon > 0,\ \lvert\beta\rvert \in \mathbb{N}$

Global piecewise smooth

Polyharmonic spline (odd)	$\lvert r\rvert^{2m-1}$,	$m \in \mathbb{N}$
Polyharmonic spline (even)	$r^{2m}\log(r)$,	$m \in \mathbb{N}$
Matérn/Sobolev	$r^{\nu} K_{\nu}(r)$,	$\nu > 0$
C^2 Matérn	$(1+r)\exp(-r)$,	$v = 3/2$

Compactly supported Wendland functions

C^2 and pos def for $d \leq 3$,	$(1-\frac{r}{\rho})_+^4(4\frac{r}{\rho}+1)$,	$\rho > 0$
C^2 and pos def for $d \leq 5$,	$(1-\frac{r}{\rho})_+^4(5\frac{r}{\rho}+1)$,	$\rho > 0$

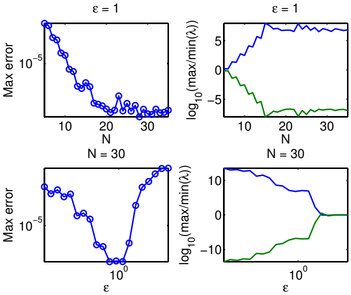
demo1.m

(RBF interpolation in 1-D)

Observations from the results of demo1.m

- As N grows for fixed ε, convergence stagnates.
- As ε decreases for fixed N, the error blows up.
- $\lambda_{\text{min}} = -\lambda_{\text{max}}$ means cancellation.
- Coefficients $\lambda \to \infty$ means that $\text{cond}(A) \to \infty$.

- For small ε, the RBFs are nearly flat, and almost linearly dependent. That is, they form a **bad basis**.



Why is it interesting to use small values of ε?

Driscoll & Fornberg [DF02]

Somewhat surprisingly, in 1-D for small ε

$$s(x,\varepsilon) = P_{N-1}(x) + \varepsilon^2 P_{N+1}(x) + \varepsilon^4 P_{N+3}(x) + \cdots,$$

where P_j is a polynomial of degree j and $P_{N-1}(x)$ is the Lagrange interpolant.

Implications

- It can be shown that $\text{cond}(A) \sim \mathcal{O}(N\varepsilon^{-2(N-1)})$, but the limit interpolant is well behaved.
- It is the intermediate step of computing $\underline{\lambda}$ that is ill-conditioned.
- By choosing the corresponding nodes, the flat RBF limit reproduces pseudo-spectral methods.
- This is a **good** approximation **space**.

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RBF–QR

The multivariate flat RBF limit

Larsson & Fornberg [LF05], Schaback [Sch05]

In n-D the flat limit can either be

$$s(\underline{x},\varepsilon) = P_K(\underline{x}) + \varepsilon^2 P_{K+2}(\underline{x}) + \varepsilon^4 P_{K+4}(\underline{x}) + \cdots,$$

where $\binom{(K-1)+d}{d} < N \leq \binom{K+d}{d}$ and P_K is a polynomial interpolant or

$$\begin{aligned} s(\underline{x},\varepsilon) &= \varepsilon^{-2q} P_{M-2q}(\underline{x}) + \varepsilon^{-2q+2} P_{M-2q+2}(\underline{x}) + \cdots \\ &+ P_M(\underline{x}) + \varepsilon^2 P_{M+2}(\underline{x}) + \varepsilon^4 P_{M+4}(\underline{x}) + \cdots. \end{aligned}$$

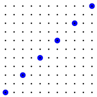
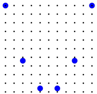
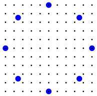
The questions of uniqueness and existence are connected with multivariate polynomial uni-solvency.

Schaback [Sch05]

Gaussian RBF limit interpolants always converge to the de Boor/Ron least polynomial interpolant.

The multivariate flat RBF limit: Divergence

Necessary condition: $\exists\ Q(\underline{x})$ of degree N_0 such that $Q(\underline{x}_j) = 0,\ j = 1, \ldots, N$.
Then divergence as ε^{-2q} may occur, where $q = \lfloor (M - N_0)/2 \rfloor$ and M = min non-degenerate degree.

Points	Q	N_0	Basis	M	q
	$x - y$	1	$1, x, x^2, x^3, x^4, x^5$	5	2
	$x^2 - y - 1$	2	$1, x, y, xy, y^2 xy^2$	3	0
	$x^2 + y^2 - 1$	2	$1, x, y, x^2, xy, x^3, x^2y, x^4$	4	1

Divergence actually only occurs for the first case as ε^{-2}.

The multivariate flat RBF limit, contd

Schaback [Sch05], Fornberg & Larsson [LF05]

Example: In two dimensions, the eigenvalues of A follow a pattern: $\mu_1 \sim \mathcal{O}(\varepsilon^0)$, $\mu_{2,3} \sim \mathcal{O}(\varepsilon^2)$, $\mu_{4,5,6} \sim \mathcal{O}(\varepsilon^4)$,...

In general, there are $\left(\begin{array}{c} k+n-1 \\ n-1 \end{array}\right) = \frac{(k+1)\cdots(k+n-1)}{(n-1)!}$ eigenvalues $\mu_j \sim \mathcal{O}(\varepsilon^{2k})$ in n dimensions.

Implications

- There is an opportunity for pseudo-spectral-like methods in n-D.
- There is no amount of variable precision that will save us.
- For "smooth" functions, a small ε can lead to very high accuracy.

Multivariate interpolation

Theorem (Mairhuber–Curtis)

For a domain $\Omega \subset \mathbb{R}^d$, $d \geq 2$ that has an interior point, there is no basis of continuous functions $f_1(\underline{x}), \ldots f_N(\underline{x})$, $N \geq 2$ such that an interpolation matrix $A = \{f_j(\underline{x}_i)\}_{i,j=1}^N$ is guaranteed to be non-singular (no Haar basis).

Proof.

Let two of the points $\underline{x}_i$ and $\underline{x}_k$ change places along a closed continuous path in Ω. When the two points have changed places, two rows in A are interchanged, and $\det(A)$ has changed sign. Then $\det(A) = 0$ somewhere along the path. □

- For RBF approximation, $A = \{\phi(\|\underline{x}_i - \underline{x}_j\|)\}_{i,j=1}^N$. If two points change place, two rows and two columns are swapped. Determinant does not change sign.

Positive definite functions

Definition (Positive definite function)

A real valued continuous function Φ is positive definite on $\mathbb{R}^d \Leftrightarrow$ it is even and

$$\sum_{j=1}^{N}\sum_{k=1}^{N} c_j c_k \Phi(\underline{x}_j - \underline{x}_k) \geq 0$$

for any parwise distinct points $\underline{x}_1, \ldots, \underline{x}_N \in \mathbb{R}^d$, $c_j \in \mathbb{R}$.

Theorem (Bochner 1933)

A function $\Phi \in C(\mathbb{R}^d)$ is positive definite on $\mathbb{R}^d \Leftrightarrow$ it is the Fourier transform of a finite non-negative Borel measure μ on $\mathbb{R}^d$

$$\Phi(\underline{x}) = \frac{1}{\sqrt{(2\pi)^d}} \int_{\mathbb{R}^d} e^{-i\underline{x}\cdot\underline{\omega}} d\mu(\underline{\omega}).$$

Bochner Theorem contd

Partial proof

$$\sum_{j=1}^{N}\sum_{k=1}^{N} c_j\overline{c_k}\Phi(\underline{x}_j-\underline{x}_k) =$$

$$= \frac{1}{\sqrt{(2\pi)^d}}\sum_{j=1}^{N}\sum_{k=1}^{N}\left(c_j\overline{c_k}\int_{\mathbb{R}^d} e^{-i(\underline{x}_j-\underline{x}_k)\cdot\underline{\omega}}d\mu(\underline{\omega})\right)$$

$$= \frac{1}{\sqrt{(2\pi)^d}}\int_{\mathbb{R}^d}\left(\sum_{j=1}^{N} c_j e^{-i\underline{x}_j\cdot\underline{\omega}}\sum_{k=1}^{N}\overline{c_k}e^{i\underline{x}_k\cdot\underline{\omega}}\right)d\mu(\underline{\omega})$$

$$= \frac{1}{\sqrt{(2\pi)^d}}\int_{\mathbb{R}^d}\left|\sum_{j=1}^{N} c_j e^{-i\underline{x}_j\cdot\underline{\omega}}\right|^2 d\mu(\underline{\omega}) \geq 0.$$

Example

The Gaussian is positive definite in any dimension

$$e^{-\varepsilon^2\|\underline{x}\|^2} = \frac{1}{\sqrt{(2\pi)^d}} \int_{\mathbb{R}^d} \frac{1}{(\sqrt{2}\varepsilon)^d} e^{-\|\omega\|^2/(4\varepsilon^2)} e^{i\underline{x}\cdot\underline{\omega}} d\underline{\omega}$$

Theorem (Schoenberg 1938)

A cont function $\varphi : [0,\infty) \to \mathbb{R}$ is strictly pos def and radial on $\mathbb{R}^d$ for all d $\Leftrightarrow$

$$\varphi(r) = \int_0^\infty e^{-r^2t^2} d\mu(t),$$

where μ is a finite non-negative Borel measure not concentrated at the origin.

Results and consequences for RBF approximation

- Non-singularity of RBF interpolation is guaranteed for distinct node points and strictly pos def functions such as the Gaussian and the inverse multiquadric.
- There are no *oscillatory* or *compactly supported* RBFs that are strictly pos def for all d.

  Because $\phi(r_0) = 0$ *breaks theorem, cf. Bessel and Wendland.*
- Non-singularity/positive definiteness of interpolation matrix holds also for *conditionally positive definite* RBFs augmented with polynomials.

  Micchelli [Mic86], cf. multiquadric RBFs

Tensor product vs multivariate basis

Tensor product basis

$$s(\underline{x}) = \sum_{i=0}^{n} \sum_{j=0}^{n} c_{ij} p_i(x_1) p_j(x_2)$$

Number of unknowns $N_T = (n+1)^d$.

Multivariate basis

Thinking in terms of polynomials, a multivariate polynomial space of degree n has dimension

$$N_M = \begin{pmatrix} n+d \\ d \end{pmatrix} = \frac{(n+1)\cdots(n+d)}{d!}$$

Degrees of freedom for $n = 8$:

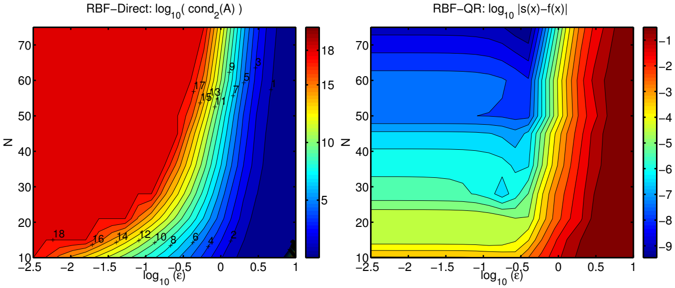
d	1	2	3
N_T	9	81	729
N_M	9	45	165

`demo2.m`

(Conditioning and errors)

Comments on the results of `demo2`

- Error is small where condition is high and vice versa.
- Interesting region only reachable with stable method.
- Best results for small ε.



Teaser: Conditioning for RBF–QR is perfect...

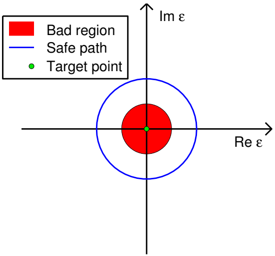
The Contour-Padé method

Fornberg & Wright [FW04]

- Think of ε as a complex variable.
- The limit $\varepsilon = 0$ is a removable singularity.
- Complex ε for which A is singular lead to poles.
- Pole location only depend on the location of nodes.

Example

- Evaluate $f(\varepsilon) = \frac{1-\cos(\varepsilon)}{\varepsilon^2}$
- Numerically unstable.
- Removable singularity at 0.
- Compute $f(0)$ as average of $f(\varepsilon)$ around "safe path".



The Contour-Padé method: Algorithm

- Compute $s(\underline{x},\varepsilon) = A_e A^{-1} f$ at M points around a "safe path" (circle).
- Inverse FFT of the M values gives a Laurent expansion

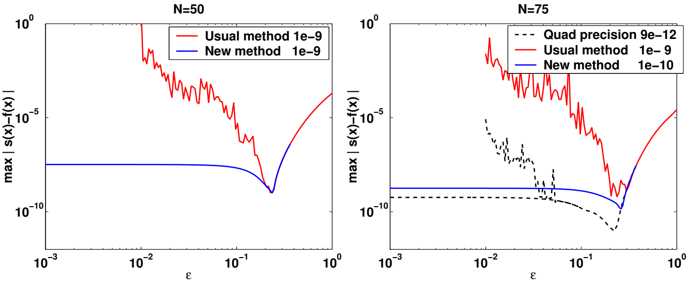
$$u(\underline{x}) = \underbrace{\ldots + s_{-2}(\underline{x})\varepsilon^{-4} + s_{-1}(\underline{x})\varepsilon^{-2}}_{\text{Needs to be converted}} + s_0(\underline{x}) + s_1(\underline{x})\varepsilon^2 + s_2(\underline{x})\varepsilon^4 + \ldots$$

- Convert the negative power expansion into Padé form and find the correct number of poles and their locations

$$s_{-1}\varepsilon^{-2} + s_{-2}\varepsilon^{-4} + \ldots = \frac{p_1\varepsilon^{-2} + \cdots + p_m\varepsilon^{-2m}}{1 + q_1\varepsilon^{-2} + \cdots + q_n\varepsilon^{-2n}}.$$

- Evaluate $u(\underline{x})$ using Taylor + Padé for any ε inside the circle.

The Contour-Padé method: Results



- Stable computation for all ε with Contour-Padé.
- Limited number of nodes, otherwise general.
- Expensive to compute A^{-1} at M points.
- Tricky to find poles.
- Modern efficient version RBF-RA [WF17].

Expansions of (Gaussian) RBFs

On the surface of the sphere

Hubbert & Baxter [BH01]

For different RBFs there are expansions

$$\phi(\|\underline{x}-\underline{x}_k\|)=\sum_{j=0}^{\infty}\varepsilon^{2j}\sum_{m=-j}^{j}c_{j,m}Y_j^m(\underline{x})$$

Cartesian space, polynomial expansion

For Gaussians

$$\begin{aligned}\phi(\|\underline{x}-\underline{x}_k\|) &= e^{-\varepsilon^2(\underline{x}-\underline{x}_k)\cdot(\underline{x}-\underline{x}_k)} \\ &= e^{-\varepsilon^2(\underline{x}\cdot\underline{x})}e^{-\varepsilon^2(\underline{x}_k\cdot\underline{x}_k)}e^{2\varepsilon^2(\underline{x}\cdot\underline{x}_k)} \\ &= e^{-\varepsilon^2(\underline{x}\cdot\underline{x})}e^{-\varepsilon^2(\underline{x}_k\cdot\underline{x}_k)}\sum_{j=0}^{\infty}\varepsilon^{2j}\frac{2^j}{j!}(\underline{x}\cdot\underline{x}_k)^j\end{aligned}$$

Expansions of (Gaussian) RBFs contd

Mercer expansion (Mercer 1909)

For a positive definite kernel $K(\underline{x}, \underline{x}_k) = \phi(\|\underline{x} - \underline{x}_k\|)$, there is an expansion

$$\phi(\|\underline{x} - \underline{x}_k\|) = \sum_{j=0}^{\infty} \lambda_j \varphi_j(\underline{x}) \varphi_j(\underline{x}_k),$$

where λ_j are positive eigenvalues, and $\varphi_j(\underline{x})$ are eigenfunctions of an associated compact integral operator.

The RBF-QR method on the sphere

Fornberg & Piret [FP07]

$$\phi(\|\underline{x}-\underline{x}_k\|) = \sum_{j=0}^{\infty} \varepsilon^{2j} \sum_{m=-j}^{j} c_{j,m} Y_j^m(\underline{x})$$

The number of SPH functions/power matches the RBF eigenvalue pattern on the sphere.

If we collect RBFs and expansion functions in vectors, and coefficients in the matrix B, we have a relation

$$\Phi(\underline{x}) = B \cdot Y = Q \cdot E \cdot R \cdot Y(\underline{x})$$

The new basis $\Psi(\underline{x}) = R \cdot Y(\underline{x})$ spans the same space as $\Phi(\underline{x})$, but the ill-conditioning has been absorbed in E.

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The RBF-QR method in Cartesian space

Fornberg, Larsson, Flyer [FLF11]

The expansion of the Gaussian

$$\phi(\|\underline{x} - \underline{x}_k\|) = e^{-\varepsilon^2(\underline{x}\cdot\underline{x})} e^{-\varepsilon^2(\underline{x}_k\cdot\underline{x}_k)} \sum_{j=0}^{\infty} \varepsilon^{2j} \frac{2^j}{j!} (\underline{x} \cdot \underline{x}_k)^j$$

\+ The number of expansion functions for each power of ε matches the eigenvalue pattern in A.

– The expansion functions are the monomials.

Better expansion functions in 2-D

- Change to polar coordinates.
- Trigs in the angular direction are perfect.
- Necessary to preserve powers of $\varepsilon \Rightarrow$ Partial conversion to Chebyshev polynomials.

The RBF-QR method in Cartesian space contd

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New expansion functions

$$\begin{cases} T^c_{j,m}(\underline{x}) = e^{-\varepsilon^2 r^2} r^{2m} T_{j-2m}(r)\cos((2m+p)\theta), \\ T^s_{j,m}(\underline{x}) = e^{-\varepsilon^2 r^2} r^{2m} T_{j-2m}(r)\sin((2m+p)\theta), \end{cases}$$

Matrix form of factorized expansion

Express $\Phi(\underline{x}) = (\phi(\|\underline{x}-\underline{x}_1\|),\ldots,\phi(\|\underline{x}-\underline{x}_N\|))^T$ in terms of expansion functions $T(\underline{x}) = (T^c_{0,0}, T^c_{1,0},\ldots)^T$ as.

$$\Phi(\underline{x}) = C \cdot D \cdot T(\underline{x}),$$

where c_{ij} is $\mathcal{O}(1)$ and $D = \mathrm{diag}(\mathcal{O}(\varepsilon^0, \varepsilon^2, \varepsilon^2, \varepsilon^4, \ldots))$.

Note that C has an infinite number of columns etc.

The RBF-QR method in Cartesian space contd

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RBF–QR

The QR part

The coefficient matrix C is QR-factorized so that $\Phi(\underline{x}) = Q \cdot \begin{bmatrix} R_1 & R_2 \end{bmatrix} \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix} \cdot T(\underline{x})$, where R_1 and D_1 are of size $(N \times N)$.

The change of basis

Make the new basis (same space) close to T

$$\Psi(\underline{x}) = D_1^{-1} R_1^{-1} Q^H \Phi(\underline{x}) = \begin{bmatrix} I & \tilde{R} \end{bmatrix} \cdot T(\underline{x}).$$

Analytical scaling of $\tilde{R} = D_1^{-1} R_1^{-1} R_2 D_2$

Any power of ε in $D_1 \leq$ any power of ε in $D_2 \Rightarrow$
Scaling factors $\mathcal{O}(\varepsilon^0)$ or smaller, truncation is possible.

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`demo3.m`

(RBF interpolation in 2-D with and without RBF–QR)

Stable computation as $\varepsilon \to 0$ and $N \to \infty$

The RBF-QR method allows stable computations for small ε. *(Fornberg, Larsson, Flyer [FLF11])*

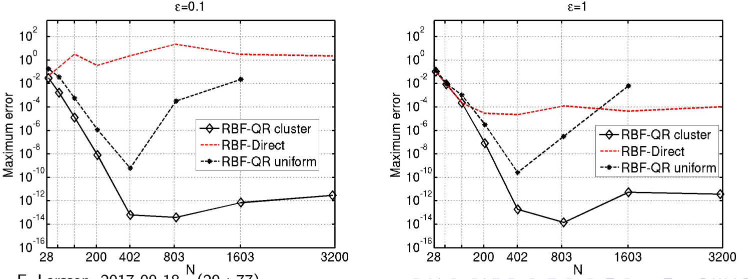
Consider a finite non-periodic domain.

Theorem (Platte, Trefethen, and Kuijlaars [PTK11]):

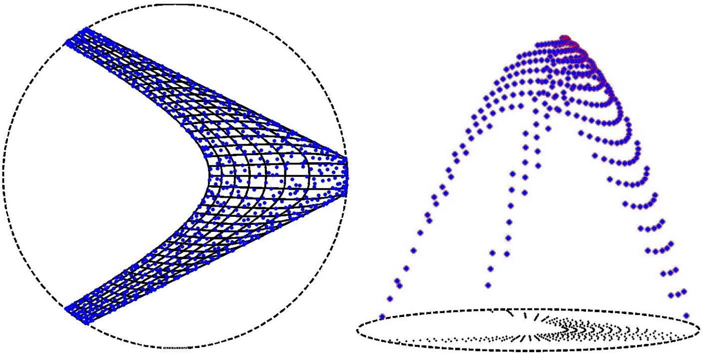
Exponential convergence on equispaced nodes $\Rightarrow$ exponential ill-conditioning.

Solution #1:

Cluster nodes towards the domain boundaries.



An RBF-QR example with clustered nodes in a non-trivial domain



$f(x, y) = \exp(-(x - 0.1)^2 - 0.5y^2)$
N=793 node points
Cosine-stretching towards each boundary
Maximum error 2.2e-10

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RBF–QR

`demo4.m`

(RBF interpolation in 2-D with clustered nodes)

Brief survey of Mercer based methods

Fasshauer & McCourt [FM12]

Eigenvalues and eigenfunctions in 1-D can be chosen as

$$\lambda_n = \sqrt{\frac{\alpha^2}{\alpha^2+\delta^2+\varepsilon^2}}\left(\frac{\varepsilon^2}{\alpha^2+\delta^2+\varepsilon^2}\right)^{n-1},$$

$$\phi_n = \gamma_n e^{-\delta^2 x^2} H_{n-1}(\alpha\beta x),$$

where $\beta = \left(1+\left(\frac{2\varepsilon}{\alpha}\right)^2\right)^{\frac{1}{4}}$, $\gamma_n = \sqrt{\frac{\beta}{2^{n-1}\Gamma(n)}}$, $\delta^2 = \frac{\alpha^2}{2}(\beta^2-1)$.

- Eigenfunctions are orthogonal in a weighted norm.
- The QR-step is similar to that of previous methods.
- Tensor product form is used in higher dimensions $\Rightarrow$ The powers of ε do not match the eigenvalues of A.
- New parameter α to tune.

Brief survey of Mercer based methods contd

De Marchi & Santin [DMS13]

- Discrete numerical approximation of eigenfunctions.
- W diagonal matrix with cubature weights.
  Perform SVD $\sqrt{W} \cdot A \cdot \sqrt{W} = Q \cdot \Sigma^2 \cdot Q^T$.
  The eigenbasis is given by $\sqrt{W^{-1}} \cdot Q \cdot \Sigma$.
- Rapid decay of singular values $\Rightarrow$ Basis can be truncated $\Rightarrow$ Low rank approximation of A.

De Marchi & Santin [DMS15]

- Faster: Lanczos algorithm on Krylov space $\mathcal{K}(A, f)$.
- Eigenfunctions through SVD of H_m from Lanczos.
- Computationally efficient.
- Basis depends on f. Potential trouble for $f \notin \mathcal{N}_K(X)$

For details it is a good idea to ask the authors :-)

Differentiation matrices and RBF-QR

Larsson, Lehto, Heryudono, Fornberg [LLHF13]

Let $\underline{u}_X$ be an RBF approximation evaluated at the nodes.

To compute $\underline{u}_Y$ evaluated at the set of points Y, we use

$$A\underline{\lambda} = \underline{u}_X \quad \Rightarrow \quad \underline{\lambda} = A^{-1}\underline{u}_X \text{ to get}$$

$$\underline{u}_Y = A_Y\underline{\lambda} = A_Y A^{-1}\underline{u}_X$$

where $A_Y(i,j) = \phi_j(y_i)$.

To instead evaluate a differential operator applied to $\underline{u}$,

$$\underline{u}_Y = A_Y^{\mathcal{L}} A^{-1}\underline{u}_X,$$

where $A_Y^{\mathcal{L}}(i,j) = \mathcal{L}\phi_j(y_i)$.

To do the same thing using RBF–QR, replace ϕ_j with ψ_j.

Solving PDEs with RBFs/RBF-QR

Domain defined by: $r_b(\theta) = 1 + \frac{1}{10}(\sin(6\theta) + \sin(3\theta))$.

PDE: $\begin{cases} \Delta u = f(\underline{x}), & \underline{x} \in \Omega, \\ u = g(\underline{x}), & \underline{x} \text{ on } \partial\Omega, \end{cases}$

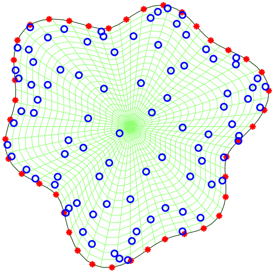
Solution: $u(\underline{x}) = \sin(x_1^2 + 2x_2^2) - \sin(2x_1^2 + (x_2 - 0.5)^2)$.

Collocation:

$$\begin{pmatrix} A^{\Delta}_{X^i} A_X^{-1} \\ I \end{pmatrix} \begin{pmatrix} \underline{u}^i_X \\ \underline{u}^b_X \end{pmatrix} = \begin{pmatrix} \underline{f}^i_X \\ \underline{g}^b_X \end{pmatrix}$$

Evaluation:

$\underline{u}_Y = A_Y A_X^{-1} \underline{u}_X$



Domain + nodes

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(Solving the Poisson problem in 2-D using RBFs)

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RBF–QR

Reproducing Kernel Hilbert spaces and optimality

Let $\mathcal{N}(\Omega)$ be a real Hilbert space of functions $u : \Omega \to \mathbb{R}$, where $\Omega \subseteq \mathbb{R}^d$ with inner product $(\cdot,\cdot)_{\mathcal{N}(\Omega)}$.

Consider an RBF as a kernel $K(\underline{x}, \underline{y})$. The following holds

(i) $K(\cdot, \underline{x}) \in \mathcal{N}(\Omega)$ for all $\underline{x} \in \Omega$.

(ii) $(u, K(\cdot, \underline{x}))_{\mathcal{N}(\Omega)} = u(\underline{x})$.

Let $I(u)$ be the interpolant of $u \in \mathcal{N}(\Omega)$. Then

$$\|I(u)\|_{\mathcal{N}(\Omega)} \leq \|u\|_{\mathcal{N}(\Omega)}$$

Consider a finite dimensional subspace $\mathcal{N}(X)$ of the *native space* $\mathcal{N}(\Omega)$. Then

$$(I(u) - u, v)_{\mathcal{N}(\Omega)} = 0 \text{ for all } v \in \mathcal{N}(X).$$

Ingredients for exponential convergence estimates

- Dependence on geometry through interior cone conditions.

  Approximation quality depends on boundary shape.
- General sampling inequalities based on polynomial approximation.

  These tell us how much a smooth error can grow between nodes.
- Embedding constants relating Native spaces to Sobolev spaces.

  These are needed to go from algebraic to exponential estimates.

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Interior cone conditions

Definition (Interior cone condition)

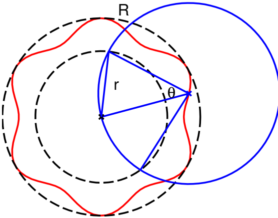
A domain $\Omega \subset \mathbb{R}^d$ satisfies an interior cone condition with radius r and angle θ if every $x \in \Omega$ is the vertex of such a cone that is contained entirely within Ω.

Definition (Star shaped)

A domain $\Omega \subset \mathbb{R}^d$ is star shaped with respect to $B(x_c, r)$ if for every $x \in \Omega$, the convex hull of x and $B(x_c, r)$ is entirely enclosed in Ω.

Example

A star shaped domain wrt $B(x_c, r)$, enclosed by $B(x_c, R)$ satisfies an interior cone condition with radius r and angle $\theta = 2\arcsin(\frac{r}{2R})$.



Narcowich, Ward, Wendland [NWW05]

General sampling inequalitites

Rieger & Zwicknagl [RZ10]

Bound derivatives of u through polynomial bounds

$$|D^{\alpha}u(\underline{x})| \leq |D^{\alpha}u(\underline{x}) - D^{\alpha}p(\underline{x})| + |D^{\alpha}p(\underline{x})|$$

Detailed computations with averaged Taylor polys

$$\begin{aligned} \|D^{\alpha}u\|_{L_q(\Omega)} &\leq \frac{C_S^k \delta_\Omega^{k-d(\frac{1}{p}-\frac{1}{q})}}{(k-|\alpha|)!}(\delta_\Omega^{-|\alpha|} + h^{-|\alpha|})|u|_{W_p^k(\Omega)} \\ &+ 2\delta_\Omega^{\frac{d}{q}} h^{-|\alpha|}\|u\|_{\ell_\infty(X)}, \end{aligned}$$

where δ_Ω is the diameter of Ω, h is the fill distance (largest ball empty of nodes from X), and the constant C_S depends on d, p, and θ, $1 \leq p < \infty$, $1 \leq q \leq \infty$.

Fill distance must be small enough and k large enough.

Embedding constants

Rieger & Zwicknagl [RZ10]

Assume there are embedding constants, for all k such that

$$\|u\|_{W_p^k(\Omega)} \leq E(k)\|u\|_{\mathcal{H}(\Omega)}$$

for some space $\mathcal{H}(\Omega)$ of smooth functions. Further assume that $E(k) \leq C_E^k k^{(1-\epsilon)k}$, for ϵ, $C_E > 0$.

Then, the general sampling inequality can be rewritten as

$$\|D^\alpha u\|_{L_q(\Omega)} \leq e^{C\frac{\log(h)}{\sqrt{h}}}\|u\|_{\mathcal{H}(\Omega)} + 2\delta_\Omega^{\frac{d}{q}} h^{-|\alpha|}\|u\|_{\ell_\infty(X)},$$

where $C = \epsilon\sqrt{c_0}/4$ and $c_0 = \min\{1, \frac{r\sin\theta}{4(1+sin\theta)}\}$.

We are still considering star shaped domains.

Lipschitz domains

Rieger & Zwicknagl [RZ10]

For a general Lipschitz domain that satisfies a uniform interior cone condition, we create a cover of Ω consisting of star shaped subdomains.

This affects the terms in front of the norms, but not the essentials.

For $E(k) \leq C_E^k k^{(1-\epsilon)k}$

$$\|D^\alpha u\|_{L_q(\Omega)} \leq e^{C\frac{\log(h)}{\sqrt{h}}} \|u\|_{\mathcal{H}(\Omega)} + C_2 h^{-|\alpha|} \|u\|_{\ell_\infty(X)}.$$

For $E(k) \leq C_E^k k^{sk}$, $s \geq 1$

$$\|D^\alpha u\|_{L_q(\Omega)} \leq e^{\frac{C}{h^{1/(1+s)}}} \|u\|_{\mathcal{H}(\Omega)} + C_2 h^{-|\alpha|} \|u\|_{\ell_\infty(X)}.$$

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Embedding constants for kernel spaces

Fourier characterization of spaces

$$\mathcal{N}_K(\mathbb{R}^d) = \left\{ u \in C(\mathbb{R}^d) \cap L_2(\mathbb{R}^d) : \|u\|^2_{\mathcal{N}_K} = \int_{\mathbb{R}^d} \frac{|\hat{u}(\omega)|^2}{|\hat{K}(\omega)|} d\omega < \infty \right\}$$

$$W_2^k(\mathbb{R}^d) = \left\{ u \in L_2(\mathbb{R}^d) : \int_{\mathbb{R}^d} |\hat{u}(\omega)|^2 (1 + \|\omega\|_2^2)^k d\omega < \infty \right\}$$

Finding a specific embedding constant

For a particular kernel function K find $E(k)$ such that

$$(1 + y)^k \leq \frac{E(k)^2}{\hat{K}(y)},$$

where $y = \|\omega\|_2^2$.

Embedding constants for kernel spaces contd

Rieger & Zwicknagl [RZ10]

For the Gaussian $\hat{K}(y) = (2\varepsilon^2)^{-\frac{d}{2}} e^{-\frac{y}{4\varepsilon^2}}$ and $E(k) = C^k k^{\frac{k}{2}}$.

For the inverse multiquadric
$$\hat{K}(y) = \frac{2^{1-\beta}}{\Gamma(\beta)} \left(\frac{\sqrt{y}}{\varepsilon}\right)^{\beta} (\varepsilon\sqrt{y})^{-d/2}\mathcal{K}_{d/2-\beta}\left(\frac{\sqrt{y}}{\varepsilon}\right),$$
where $\mathcal{K}$ is a modified Bessel function of the third kind, leading to $E(k) = C^k k^k$.

Using the embedding constants

We finally assume that there is an extension operator $\mathcal{E}$ such that $\|\mathcal{E}u\|_{\mathcal{N}(\mathbb{R}^d)} \leq \|u\|_{\mathcal{N}(\Omega)}$. Then

$$\|u\|_{W_2^k(\Omega)} \leq \|\mathcal{E}u\|_{W_2^k(\mathbb{R}^d)} \leq E(k)\|\mathcal{E}u\|_{\mathcal{N}(\mathbb{R}^d)} \leq E(k)\|u\|_{\mathcal{N}(\Omega)}$$

Wendland [Wen05, Theorem 10.46]

Implications for interpolation errors

Rieger & Zwicknagl [RZ10]

The interpolant $I(u)$ is zero at the node set X (discrete term goes away). Together with the optimality property $\|I(u)\|_{\mathcal{N}(\Omega)} \leq \|u\|_{\mathcal{N}(\Omega)}$, we get for the Gaussian

$$\|D^\alpha(I(u) - u)\|_{L_q(\Omega)} \leq e^{C\frac{\log(h)}{\sqrt{h}}}\|u\|_{\mathcal{N}(\Omega)},$$

and for the inverse multiquadric

$$\|D^\alpha(I(u) - u)\|_{L_q(\Omega)} \leq e^{\frac{C}{\sqrt{h}}}\|u\|_{\mathcal{N}(\Omega)}.$$

These estimates can be improved, e.g., for a compact cube.

Cost of global method

Global RBF approximations of smooth functions are very efficent.

A small number of node points per dimension are needed.

However $N = 15$ in 1-D becomes $N = 50\,625$ in 4-D.

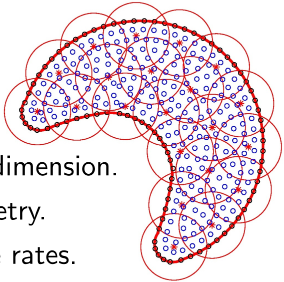
Up to three dimensions can be handled on a laptop, but not more.

Furthermore, for less smooth functions, the number of nodes per dimension grows quickly.

For a dense linear system: Direct solution $\mathcal{O}(N^3)$, storage $\mathcal{O}(N^2)$.

$\Rightarrow$ Move to localized methods.

Motivation for RBF-PUM



Global RBF approximation

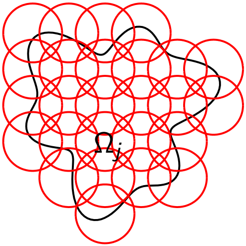
+ Ease of implementation in any dimension.
+ Flexibility with respect to geometry.
+ Potentially spectral convergence rates.
– Computationally expensive for large problems.

RBF partition of unity methods

- Local RBF approximations on patches are blended into a global solution using a partition of unity.
- Provides spectral or high-order convergence.
- Solves the computational cost issues.
- Allows for local adaptivity.

[Wen02, Fas07, HL12, Cav12, CDR14, CDR15, CDRP16, CRP16], [SVHL15, HLRvS16, SL16, LSH17]

The RBF partition of unity method

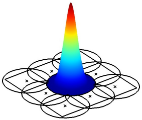


Global approximation

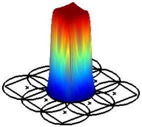
$$\tilde{u}(\underline{x}) = \sum_{j=1}^{P} w_j(\underline{x})\tilde{u}_j(\underline{x})$$

PU weight functions

Generate weight functions from
compactly supported C^2 Wendland functions



$$\psi(\rho) = (4\rho+1)(1-\rho)_+^4$$



using Shepard's method $w_i(\underline{x}) = \frac{\psi_i(\underline{x})}{\sum_{j=1}^{M}\psi_j(\underline{x})}$.

Cover

Each $\underline{x} \in \Omega$ must be in the interior of at least one Ω_j.
Patches that do not contain unique points are pruned.

Differentiating RBF-PUM approximations

Applying an operator globally

$$\Delta\tilde{u} = \sum_{i=1}^{M} \Delta w_i \tilde{u}_i + 2\nabla w_i \cdot \nabla \tilde{u}_i + w_i \Delta \tilde{u}_i$$

Local differentiation matrices

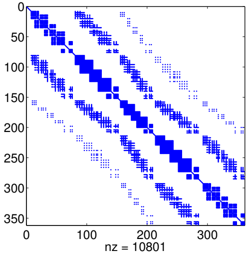
Let $\underline{u}_i$ be the vector of nodal values in patch Ω_i, then

$$\underline{u}_i = A\underline{\lambda}^i, \text{ where } A_{ij} = \phi_j(\underline{x}_i) \quad \Rightarrow$$

$$\mathcal{L}\underline{u}_i = A^{\mathcal{L}}A^{-1}\underline{u}_i, \text{ where } A^{\mathcal{L}}_{ij} = \mathcal{L}\phi_j(\underline{x}_i).$$

The global differentiation matrix

Local contributions are added into the global matrix.



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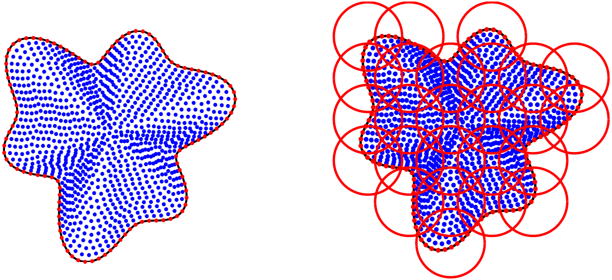
`demo6.m`

(Solving a Poisson problem in 2-D with RBF–PUM)

An RBF-PUM collocation method



Choices & Implications

- Nodes and evaluation points coincide.

  Square matrix, iterative solver available (Heryudono, Larsson, Ramage, von Sydow [HLRvS16]).

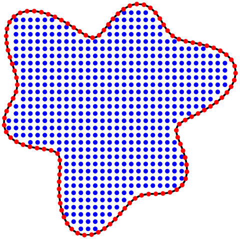
- Global node set.

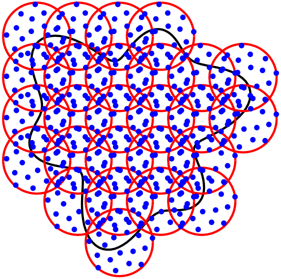
  Solutions $\tilde{u}_i(\underline{x}_k) = \tilde{u}_j(\underline{x}_k)$ *for* $\underline{x}_k$ *in overlap regions.*

- Patches are cut by the domain boundary.

  Potentially strange shapes and lowered local order.

An RBF-PUM least squares method





Choices & Implications

- Each patch has an identical node layout.
  Computational cost for setup is drastically reduced.
- Evaluation nodes are uniform.
  Easy to generate both local and global high quality node sets.
- Patches have nodes outside the domain.
  Good for local order, but requires denser evaluation points.

The RBF-PUM interpolation error

$$\mathcal{E}_\alpha = D^\alpha(I(u) - u) = \sum_{j=1}^{M} \sum_{|\beta| \leq |\alpha|} \binom{\alpha}{\beta} D^\beta w_j D^{\alpha-\beta}(I(u_j) - u_j)$$

The weight functions

For C^k weight functions and $|\alpha| \leq k$

$$\|D^\alpha w_j\|_{L_\infty(\Omega_j)} \leq \frac{C_\alpha}{H_j^{|\alpha|}}, \quad H_j = \mathrm{diam}(\Omega_j).$$

The local RBF interpolants (Gaussians)

Define the local fill distance h_j *(Rieger, Zwicknagl [RZ10])*

$$\|D^\alpha(I(u_j) - u_j)\|_{L_\infty(\tilde{\Omega}_j)} \leq c_{\alpha,j} h_j^{m_j - \frac{d}{2} - |\alpha|} \|u_j\|_{\mathcal{N}(\tilde{\Omega}_j)},$$

$$\|D^\alpha(I(u_j) - u_j)\|_{L_\infty(\tilde{\Omega}_j)} \leq e^{\gamma_{\alpha,j} \log(h_j)/\sqrt{h_j}} \|u_j\|_{\mathcal{N}(\tilde{\Omega}_j)}.$$

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RBF-PUM interpolation error estimates

Algebraic estimate for $H_j/h_j = c$

$\|\mathcal{E}_\alpha\|_{L_\infty(\Omega)} \leq K \max_{1\leq j\leq M} C_j H_j^{m_j-\frac{d}{2}-|\alpha|}\|u\|_{\mathcal{N}(\tilde{\Omega}_j)}$

K — Maximum # of Ω_j overlapping at one point

m_j — Related to the local # of points

$\tilde{\Omega}_j$ — $\Omega_j \cap \Omega$

Spectral estimate for fixed partitions

$\|\mathcal{E}_\alpha\|_{L_\infty(\Omega)} \leq K \max_{1\leq j\leq M} C e^{\gamma_j \log(h_j)/\sqrt{h_j}}\|u\|_{\mathcal{N}(\tilde{\Omega}_j)}$

Implications

- Bad patch reduces global order.
- Two refinement modes.
- Guidelines for adaptive refinement.

Error estimate for PDE approximation

Larsson, Shcherbakov, Heryudono [LSH17]

The PDE estimate

$$\|\tilde{u} - u\|_{L_\infty(\Omega)} \leq C_P \mathcal{E}_{\mathcal{L}} + C_P \|L_{\cdot,X} L^{+}_{Y,X}\|_\infty \left(C_M \delta_M + \mathcal{E}_{\mathcal{L}}\right),$$

where C_P is a well-posedness constant and $C_M\delta_M$ is a small multiple of the machine precision.

Implications

- Interpolation error $\mathcal{E}_{\mathcal{L}}$ provides convergence rate.
- Norm of inverse/pseudoinverse can be large.
- Matrix norm better with oversampling.
- Finite precision accuracy limit involves matrix norm.

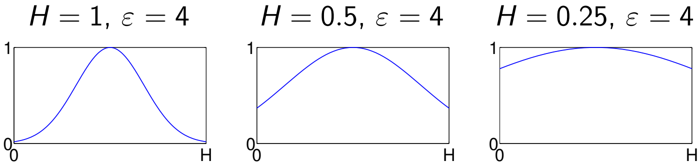
Follows strategies from Schaback [Sch07, Sch16]

Does RBF-PUM require stable methods?

In order to achieve convergence we have two options

- Refine patches such that diameter H decreases.
- Increase node numbers such that N_j increases.
- In both cases, theory assumes ε fixed.

The effect of patch refinement



The RBF–QR method: Stable as $\varepsilon \to 0$ for $N \gg 1$

Effectively a change to a stable basis.

Fornberg, Piret [FP07], Fornberg, Larsson, Flyer [FLF11], Larsson, Lehto, Heryudono, Fornberg [LLHF13]

Effects on the local matrices

Local contribution to a global Laplacian

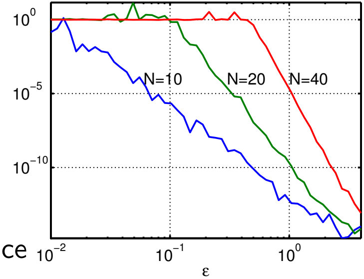
$$L_j = (W_j^{\Delta} A_j + 2W_j^{\nabla} \odot A_j^{\nabla} + W_j A_j^{\Delta}) A_j^{-1}.$$

Typically: A_j ill-conditioned, L_j better conditioned.

RBF-QR for accuracy

- Stable for small RBF shape parameters ε
- Change of basis $\tilde{A} = AQR_1^{-T} D_1^{-T}$
- Same result in theory $\tilde{A}^{\mathcal{L}} \tilde{A}^{-1} = A^{\mathcal{L}} A^{-1}$
- More accurate in practice

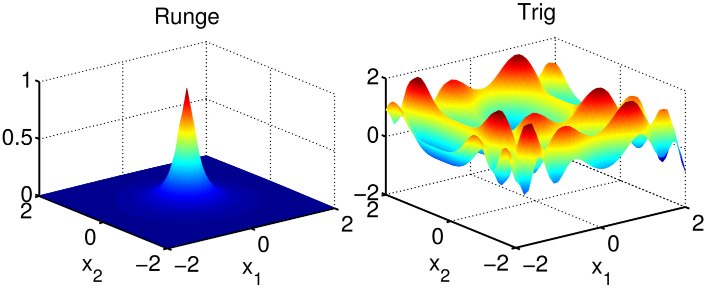
Relative error in $A_j^{\Delta} A_j^{-1}$ without RBF-QR



Poisson test problems in 2-D

Domain $\Omega = [-2,\, 2]^2$.

Uniform nodes in the collocation case.



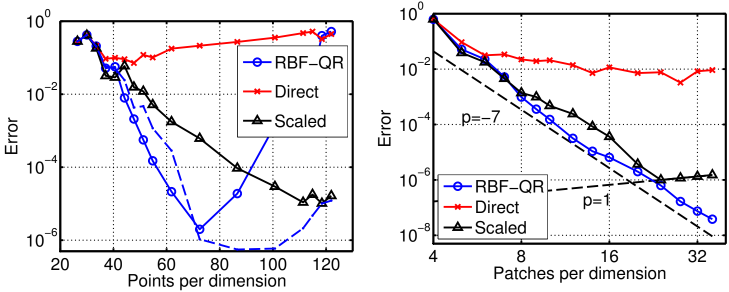
$$u_R(x,y) = \frac{1}{25x^2+25y^2+1}$$

$$u_T(x,y) = \sin(2(x-0.1)^2)\cos((x-0.3)^2)+\sin^2((y-0.5)^2)$$

Error results with and without RBF–QR

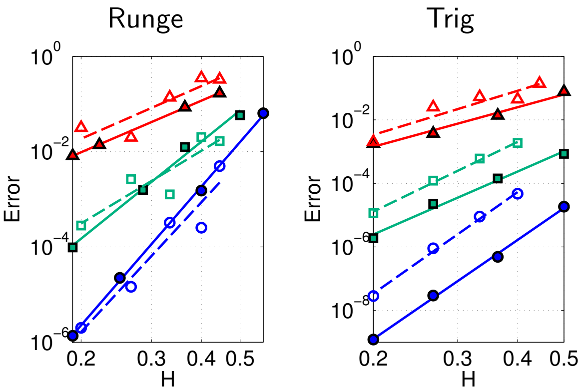
- Least squares RBF-PUM
- Fixed shape $\varepsilon = 0.5$ or scaled such that $\varepsilon h = c$
- Left: 5×5 patches   Right: 55 points per patch

Spectral mode   Algebraic mode



- With RBF–QR better results for H/h large.
- Scaled approach good until saturation.

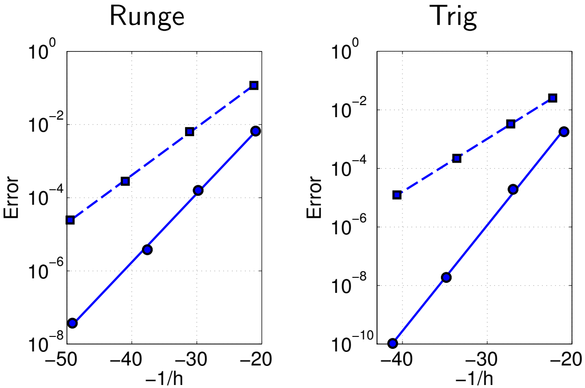
Convergence as a function of patch size



Collocation (dashed lines) and Least Squares (solid lines).

- Points per patch $n = 28, 55, 91$.
- Theoretical rates $p = 4, 7, 10$.
- Numerical rates $p \approx 3.9, 6.9, 9.8$.

Spectral convergence for fixed patches



Collocation (dashed lines) and Least Squares (solid lines).

LS-RBF-PU is significantly more accurate due to the constant number of nodes per patch.

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Robustness and large scale problems

The global error estimate

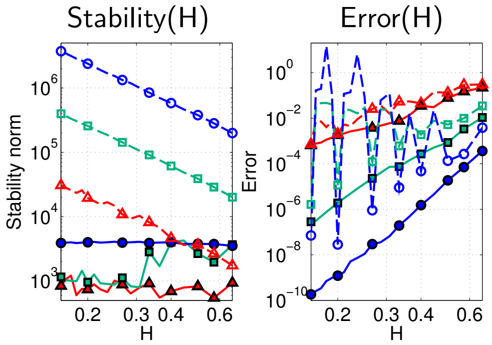
$$\|\tilde{u} - u\|_{L_\infty(\Omega)} \leq C_P \mathcal{E}_\mathcal{L} + C_P \|L_{\cdot,X} L^{+}_{Y,X}\|_\infty (C_M \delta_M + \mathcal{E}_\mathcal{L})$$

The dark horse is the 'stability matrix norm'

- The stability norm is related to conditioning.
- In the collocation case, $\|L^{-1}_{X,X}\|$ grows with N.
- How does it behave with least squares?

Stability norm: Patch size

- Fixed number of points per patch $n = 28, 55, 91$
- Results as a function of patch diameter H



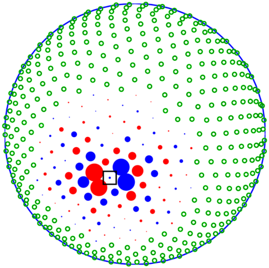
Collocation (dashed) and LS (solid)

- The norm does not grow for LS-RBF-PUM (!)

RBF-generated finite differences RBF–FD

Flyer et al. [FW09, FLB+12]

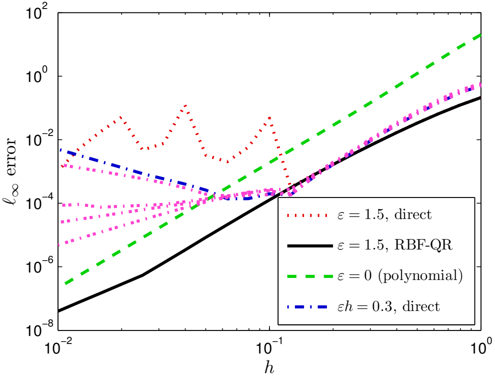
- Approximate $\mathcal{L}u(\underline{x}_c)$ using the n nearest nodes by
$$\mathcal{L}u(\underline{x}_c) \approx \sum_{k=1}^{n} w_k u(\underline{x}_k)$$
- Find weights w_k by asking exactness for RBF-interpolants.



$$\begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_1(\mathbf{x}_2) & \cdots & \phi_1(\mathbf{x}_n) \\ \phi_2(\mathbf{x}_1) & \phi_2(\mathbf{x}_2) & \cdots & \phi_2(\mathbf{x}_n) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_n(\mathbf{x}_1) & \phi_n(\mathbf{x}_2) & \cdots & \phi_n(\mathbf{x}_n) \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} \mathcal{L}\phi_1(\mathbf{x}_c) \\ \mathcal{L}\phi_2(\mathbf{x}_c) \\ \vdots \\ \mathcal{L}\phi_n(\mathbf{x}_c) \end{bmatrix}.$$

Is RBF-QR needed with RBF–FD?

Approximation of Δu with $n = 56$. Magenta lines are with added polynomial terms $p = 0, \ldots, 3$.



- Scaled ε: No ill-conditioning, but saturation/stagnation. *[LLHF13]*
- Fixed ε: RBF-QR is needed.
- Added terms: Compromise with partial recovery.

RBF-FD with PHS and polynomials

Combine polyharmonic splines, e.g, $\phi(r) = |r|^7$ with polynomial terms $1, x, y, \dots, x^2, \dots$ such that the number of polynomial terms $\approx$ the number of nodes.

- Contains both smooth and piecewise smooth components, that have different roles in the approximation.
- No shape parameter to tune.
- Heuristically, skewed stencils seem to behave well near boundaries.

Bayona, Flyer, Fornberg, Barnett [FFBB16, BFFB17]

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