Sometimes scale matters – zooming in using multiscale Wendland RBFs

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Joint work with Q Thong Le Gia and Holger Wendland

The need for many scales

Physical phenomena often occur on many different scales.

An example: the topography of Earth







Radial basis functions

Radial basis functions (RBFs) in \mathbb{R}^3 :

$$\Psi(\mathbf{x},\mathbf{y}) = \psi(|\mathbf{x}-\mathbf{y}|)$$

RBFs with compact support:

$$\psi(t)=0$$
 for $t\geq 1.$

Example (Holger Wendland):

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



Wendland RBF restricted to the plane





Scaling the RBF

Suppose we replace $\psi(t)$ by

$$\psi_{\frac{1}{2}}(t) := c\psi\left(\frac{t}{1/2}\right) = c\psi(2t) = c(4 \times 2t + 1)(1 - 2t)_{+}^{4}.$$

The 'scaled' RBF $\psi_{\frac{1}{2}}(t)$ has support of radius $\frac{1}{2}$.

We say that $\psi_{\frac{1}{2}}$ has the scale $\delta = \frac{1}{2}$.



The scaled **RBF**





RBF approximation

An RBF approximation (with a single scale) has the form

$$f(\mathbf{x}) pprox \sum_{j=1}^{M} lpha_j \Psi(\mathbf{x}, \mathbf{x}_j), \qquad \mathbf{x} \in \mathbb{R}^3.$$



Example

Here's an example: It's a sum of nine RBF's on a 3 imes3 grid.



Now spherical basis functions

Starting with an RBF $\Psi(\mathbf{x}, \mathbf{y})$ in \mathbb{R}^3 , we obtain a **spherical radial basis function** (SBF) by restricting Ψ to the sphere \mathbb{S}^2 :

$$\Phi(\mathbf{x},\mathbf{y}) := \Psi(\mathbf{x},\mathbf{y})$$
 if $|\mathbf{x}| = |\mathbf{y}| = 1$.

 $\Phi(\mathbf{x},\mathbf{y})$ depends only on the angle between \mathbf{x} and \mathbf{y} , thus we can write

$$\Phi(\mathbf{x},\mathbf{y}) = \phi(\mathbf{x} \cdot \mathbf{y}).$$



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$$f(\mathbf{x}) pprox \sum_{j=1}^{M} \alpha_j \phi(\mathbf{x} \cdot \mathbf{x}_j), \qquad \mathbf{x} \in \mathbb{S}^2.$$



Positive definite RBFs

We often prefer RBFs that are (strictly) **positive definite**:

$$\sum_{j=1}^M \sum_{k=1}^M lpha_j lpha_k \Psi(\mathrm{x}_j,\mathrm{x}_k) \geq 0 \qquad orall M,\mathrm{x}_j,lpha_j,$$

with equality iff
$$\alpha_1 = \alpha_2 = \cdots = \alpha_M = 0$$
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.

The Wendland RBF is (strictly) positive definite.

Proof: (Wendland) By showing that its Fourier transform is positive.



How to choose the coefficients α_j ?

Recall: an SBF approximation (with a single scale) has the form

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How to find good coefficients α_j ?



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Recall: an SBF approximation (with a single scale) has the form

$$f(\mathbf{x}) \approx \sum_{j=1}^{M} \alpha_j \phi(\mathbf{x} \cdot \mathbf{x}_j), \quad \mathbf{x} \in \mathbb{S}^2.$$

How to find good coefficients α_j ?

One way is to interpolate at the points x_1, x_2, \ldots, x_M : then we have to solve

$$f(\mathbf{x}_i) = \sum_{j=1}^M lpha_j \phi(\mathbf{x}_i \cdot \mathbf{x}_j), \qquad i = 1, \dots, M,$$



a linear system with the $M \times M$ symmetric matrix $(\phi(\mathbf{x}_j \cdot \mathbf{x}_i))$.

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If δ is too large, then the approximation can be very good, but the **condition** of the matrix $\phi(\mathbf{x}_j \cdot \mathbf{x}_i)$ will be bad.



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If δ is too large, then the approximation can be very good, but the **condition** of the matrix $\phi(\mathbf{x}_j \cdot \mathbf{x}_i)$ will be bad.

If δ is too small, then the matrix will be well conditioned but the **approximation will be poor**.



Interpolation with $\delta = 1$ and 8000 points

Approximating 'topo', with $\delta = 1$.





The approximation is quite good, but the condition number is $4 imes 10^6$

Interpolation with $\delta = \frac{1}{16}$ and 8000 points

Approximating 'topo', with $\delta = \frac{1}{16}$.





The approximation is terrible, but the condition number is only 8.

Which points?

The examples use Rakhmanov-Saff-Zhou 'equal-area' points, rounded to nearest degree (because that is where the values of 'topo' are available.)

The figure shows 8000 equal area points:





Convergence of interpolation for a single scale

The (global) mesh norm of the point set $X = \{x_1, \ldots, x_N\}$ is:

$$h_X := \max_{\mathbf{x} \in \mathbb{S}^2} \min_{1 \le j \le M} \cos^{-1}(\mathbf{x} \cdot \mathbf{x}_j).$$



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The following is well known:

Theorem. Let X be a point set on \mathbb{S}^2 , with mesh norm h_X . Then

$$\|f-I_Xf\|_{L_2}\leq ch_X^\sigma\|f\|_{H^\sigma(\mathbb{S}^2)},\quad f\in H^\sigma.$$

where $\sigma>0$ depends on Φ ,

For the Wendland function $\psi(t) = (4t+1)(1-t)_+^4$ we have $\sigma = 5/2$. For smoother Wendland functions σ is larger.



What is H^{σ} ?

Think of $H^{\sigma}(\mathbb{S}^2)$ as the space of L^2 functions on the sphere with σ square-integrable derivatives.

For $f\in L^2(\mathbb{S}^2)$ we can write

$$f(\mathbf{x}) = \sum_{\ell=0}^{\infty} \sum_{k=1}^{2\ell+1} \widehat{f}_{\ell,k} Y_{\ell,k}(\mathbf{x}),$$

with $\{Y_{\ell,k}\}$ an orthonormal set of spherical harmonics, and

$$\widehat{f}_{\ell,k} = \int_{\mathbb{S}^2} f(\mathrm{x}) Y_{\ell,k(\mathrm{x})} \mathrm{d} \omega(\mathrm{x}).$$



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Then

$$\|f\|_{H^{\sigma}(\mathbb{S}^2)} := \left[\sum_{\ell=0}^{\infty} \sum_{k=1}^{2\ell+1} (1+\ell)^{2\sigma} |\widehat{f}_{\ell,k}|^2\right]^{1/2}.$$



Wendland functions and Sobolev spaces

Each Wendland function is associated with a particular Sobolev space:

Given
$$\psi(|\mathbf{x}-\mathbf{y}|) = \phi(\mathbf{x}\cdot\mathbf{y})$$
 for $\mathbf{x},\mathbf{y}\in\mathbb{S}^2$, define $\widehat{\phi}(\ell)$ by

$$\phi(t) = rac{1}{4\pi} \sum_{\ell=0}^{\infty} (2\ell+1) \, \widehat{\phi}(\ell) P_{\ell}(t), \quad t \in [-1,1].$$
 (1)

Then the Wendland functions have the property that for some $\sigma > 0$

$$\widehat{\phi}(\ell) \asymp (1+\ell)^{-2\sigma}.$$

Example: $\sigma = 5/2$ for $\phi(t) = (4t+1)(1-t)_{+}^{4}$.



The Sobolev space for a Wendland Φ

With a positive definite SBF kernel Φ we can associate a special Hilbert space (the "native space"), with norm

$$\|f\|_{\Phi} := \left[\sum_{\ell=0}^{\infty} \sum_{k=1}^{2\ell+1} \frac{|\widehat{f}_{\ell,k}|^2}{\widehat{\phi}(\ell)}\right]^{1/2}$$



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Thus for the Wendland functions, if $\hat{\phi}(\ell) \simeq (1+\ell)^{-2\sigma}$ then $\|f\|_{\Phi}$ is equivalent to $\|f\|_{H^{\sigma}(\mathbb{S}^2)}$.

So each Wendland function is associated with a unique Sobolev spaces $H^{\sigma}(\mathbb{S}^2)$.



Mixing of different scales is not often tried. The problem is that one loses symmetry and positive definiteness of the interpolation matrix, and hence may lose the unique solvability property.

(Bozzini, Lenarduzzi, Rossini and Schaback 2004 showed that unique solvability is retained if the matrix perturbation is small enough.)



uses scaled versions of a single compactly supported radial basis function (RBF) $\Psi(x, y) = \psi(|x - y|), x, y \in \mathbb{R}^3$ The scaled version, with scale δ , is $\Psi_{\delta}(x, y) = \delta^{-2}\psi\left(\left|\frac{x-y}{\delta}\right|\right)$.



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- It uses a sequence of scales $\delta_1, \delta_2, \ldots$ with $\delta_j \to 0$.
- And a sequence of ever denser point sets X_1, X_2, \ldots (which need not be nested).
- At stage *j* the error from the previous stage is approximated using radial basis functions of smaller scale δ_j , and with closer spaced centres $X_j = \{x_1, \dots, x_{N_j}\}.$



Schaback 1995 and Floater & Iske 1996 considered a special case with nested point sets (for the radial basis function centres).

Hales & Levesley 2002 used polyharmonic spines and special point sets.

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But theory was lacking, for multiscale based on scaled versions of a single compactly supported RBF on either Euclidean spaces or spheres, and scattered data points.



The following multilevel scheme achieves good approximation AND good (even constant!) condition number:

Suppose we have a sequence of point sets $X_1, X_2, \ldots \subset \mathbb{S}^2$, with mesh norm h_{X_j} of X_j approaching zero.

The mesh norm of \boldsymbol{X} is

$$h_X := \max_{\mathbf{x} \in \mathbb{S}^2} \min_{1 \le j \le M} \cos^{-1}(\mathbf{x} \cdot \mathbf{x}_j).$$

Correspondingly, we take scales $\delta_j = \text{const} \times h_{X_j}$.

Then the algorithm is ...



The algorithm

Step 1. The first approximation is $f_1 = s_1 := I_{X_1,\delta_1} f$

 $I_{X_1,\delta_1}f$ is the interpolant of f on the point set X_1 with scale δ_1 .

The error is $e_1 := f - f_1$.


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Step 2 computes $s_2 = I_{X_2,\delta_2}e_1$ (interpolant of e_1 on X_2 at scale δ_2). The new approximation is $f_2 := f_1 + s_2 = f_1 + I_{X_2,\delta_2}e_1$. The new error is $e_2 := e_1 - I_{X_2,\delta_2}e_1$.



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Finally, after n steps

$$f \approx f_n = s_1 + s_2 + \ldots + s_n.$$



The multiscale convergence theorem

Theorem (LeGia, IHS, Wendland, 2010).

Let X_1, X_2, \ldots be a sequence of point sets belonging to \mathbb{S}^2 , with mesh norms h_1, h_2, \ldots satisfying $h_{j+1} = \mu h_j$, for $\mu \in (0, 1)$. Let $\delta_1, \delta_2, \ldots$ be scales ≤ 1 satisfying $\delta_j = \frac{\beta}{\mu} h_j$ for some fixed $\beta > 0$. Let Φ be a Wendland function associated with $H^{\sigma}(\mathbb{S}^2)$, for some

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Then with $\alpha = C\mu^{\sigma}$ and $C = \dots$ we have

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And hence for μ sufficiently small f_n converges to f linearly .

Condition numbers

Theorem

Under the conditions in the theorem above, and provided the sequence of point sets is quasi-uniform, the condition number of the linear system at stage j is independent of j.

Quasiuniform means: Minimum separation distance scales like h_X .



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Quasiuniform means: Minimum separation distance scales like h_X .

Largest eigenvalue: the matrix becomes larger, but the number and size of non-zero entries in a row remain roughly constant.

Smallest eigenvalue: the smallest eigenvalue is essentially

unchanged because the minimum separation distance between points scales proportionally to δ .



A multiscale experiment with topo

The following experiment uses these values:

n	32	125	500	2000	8000
δ_j	1	$rac{1}{2}$	$rac{1}{4}$	$\frac{1}{8}$	$\frac{1}{16}$
j	1	2	3	4	5

and the Wendland basis function $\psi(t) = (4t+1)(1-t)_+^4$.



First approximation $f_1 = s_1$







Second approximation f_2







Third approximation f_3



-6000	-4000	-2000	0	2000	4000











 $\frac{5}{2}$ Condition number = 4.1

Fourth approximation f_4



		I	I	I		
-6000	-4000	-2000	0	2000	4000	











Fifth approximation f_5







^S The total number of points is 8000 + 2000 + 500 + 125 + 32 = 10,657.





	1	I	1	I	1	
-3000	-2000	-1000	0	1000	2000	3000





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In any case, do we REALLY want more precision everywhere? Why not just look only at places where the error is large?



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In any case, do we REALLY want more precision everywhere? Why not just look only at places where the error is large?

We should be able to "zoom in" anywhere we want to.





Le Gia, IHS and Wendland "Zooming from global to local: a multiscale RBF approach" (Advances in Computational Math., to appear).



A new example





The function is

$$f(\mathbf{x}) = 2 + \left[\sin t \cos(100t) + (1 - \pi s/144)_+^2 \cos(2000\theta)\right] S(\theta).$$

S(θ) is a cubic spline which equals 1 for $\theta \in [0, \pi/2]$ and equals
0 for $\theta \in [2\pi/3, \pi]$.

$$\bullet$$
 $t=\cos^{-1}(\mathbf{p}\cdot\mathbf{x})$, with $\mathbf{p}=(1/\sqrt{3},\ 1/\sqrt{3},\ 1/\sqrt{3})^T$

 \blacksquare $s = \cos^{-1}(\mathbf{q} \cdot \mathbf{x})$, with $\mathbf{q} = (-0.7476, \ 0.5069, \ 0.4289)^T$

It has both slowly varying and fine scale features.













TY OF NEW

RBF approximation after 3 global + 3 local + 3 superlocal levels



RBF approximation after 3 global + 3 local + 3 superlocal levels

3

2.8

2.6

2.4

2.2 2

1.8

1.6

1.4

1.2



Some numbers

Level	N	δ_j	h_j	$\ e_j\ _{L_2(\Omega_2)}$	κ_j
1	500	1/4	0.113	4.2e-02	1.7
2	2000	1/8	0.057	4.2e-02	1.7
3	8000	1/16	0.028	3.4e-02	1.7
4	500	1/32	0.019	1.2e-02	3.2
5	2000	1/64	0.0089	9.8e-03	3.4
6	8000	1/128	0.0041	8.9e-03	3.3
7	500	1/256	0.0018	7.9e-03	3.2
8	2000	1/512	0.0009	2.9e-03	3.4
9	8000	1/1024	0.0005	8.0e-04	3.3

Black: the global levels

Blue: The local levels (zooming to the large spherical cap Ω_1)



Red: The superlocal levels (zooming to the small spherical cap Ω_2) Here h_j is the global mesh norm or local mesh norm, as appropriate.

Algorithm 1: Multiscale global/local algorithm

Data: Right hand side f, total number of levels n, number of zoomed levels m < n, spherical cap Ω for zooming to, $X_j \in \mathbb{S}^2, \delta_j$ for $j = 1, \dots, m$, $X_j \in \Omega, \delta_j$ for $j = m + 1, \dots, n$.

begin

$$\begin{array}{|c|c|c|} & \operatorname{Set} f_0 = 0, \, e_0 = f. \\ & \text{for } j = 1, 2, \dots, n \text{ do} \\ & & \operatorname{Determine \ the \ (global \ or \ local) \ interpolant \ s_j \in W_j \ to \ e_{j-1}} \\ & & \operatorname{Set} \ f_j = f_{j-1} + s_j. \\ & & \operatorname{Set} \ e_j = e_{j-1} - s_j. \end{array} \\ \end{array}$$
 Result: Approximation solution $f_n|_{\Omega} = s_1 + s_2 + \dots + s_n$



Theorem

(LeGia, IHS, Wendland, Adv. Comp. Math., to appear).

Let X_1, X_2, \ldots, X_m be point sets belonging to \mathbb{S}^2 ,

 X_{m+1}, \ldots, X_n be point sets belonging to a spherical cap Ω , and h_j be the (global or local) mesh norm of X_j , where the mesh norms satisfy satisfy $h_{j+1} = \mu h_j$, for some $\mu \in (0, 1)$.

Let $\delta_1, \delta_2, \ldots$ be scales ≤ 1 satisfying $\delta_j = \frac{\beta}{\mu} h_j$ for some fixed $\beta > 0$.

Let Φ be a Wendland function associated with $H^{\sigma}(\mathbb{S}^2)$, for some $\sigma > 1$.



Theorem (continued)

Then with $\alpha = C\mu^{\sigma}$ and $C = \dots$ we have

 $\|f-f_k\|_{L_2(\Omega)} \leq c lpha^n \|f\|_{H^\sigma}$ for all $f \in H^\sigma$



Theorem (continued)

Then with $\alpha = C\mu^{\sigma}$ and $C = \dots$ we have

 $\|f-f_k\|_{L_2(\Omega)} \leq c lpha^n \|f\|_{H^\sigma}$ for all $f \in H^\sigma$

And hence for μ sufficiently small f_n converges to f linearly as $n \to \infty$.



Main ideas in the proof

First let's pretend that all levels are global, i.e. $\Omega = \mathbb{S}^2$.

1. Define $e_n := f - f_n$.

Because $e_n(\mathbf{x}) = 0$ for $\mathbf{x} \in X_n$, it follows from the zeros theorem

(Hangelbroek, Narcowich, Ward 2012, Le Gia, Narcowich, Ward, Wendland 2006) that

 $\|e_n\|_{L_2(\mathbb{S}^2)} \leq ch_n^{\sigma} \|e_n\|_{H^{\sigma}(\mathbb{S}^2)}.$



Main ideas - scaling

2. **Scaling**: All the scaled norms Φ_{δ_i} are equivalent, but different:

 $\|c_1\|u\|_{\Phi_\delta}\leq \|u\|_{H^\sigma(\mathbb{S}^2)}\leq c_2\delta^{-\sigma}\|u\|_{\Phi_\delta}$

$$\implies \|e_n\|_{L_2(\mathbb{S}^2)} \leq ch_n^{\sigma} \|e_n\|_{H^{\sigma}(\mathbb{S}^2)} \leq cc_2 h_n^{\sigma} \delta_{n+1}^{-\sigma} \|e_n\|_{\Phi_{\delta_{n+1}}}$$

and because $\delta_{n+1} = \frac{\beta}{\mu} h_{n+1} = \frac{\beta}{\mu} \cdot \mu h_n = \beta h_n$, we have now
 $\|e_n\|_{L_2(\mathbb{S}^2)} \leq c' \|e_n\|_{\Phi_{\delta_{n+1}}}.$



Main ideas - recursion

3. The key step is a (not-so-obvious) recursion:

$$\|e_{\boldsymbol{j}}\|_{\Phi_{\delta_{\boldsymbol{j}+1}}}\leq lpha\|e_{\boldsymbol{j}-1}\|_{\Phi_{\delta_{\boldsymbol{j}}}}, \hspace{1em} j=n,n-1,\dots 1,$$

with $\alpha = C\mu^{\sigma}$. So $\alpha < 1$ for μ sufficiently small.

Putting things together, we have $\|e_n\|_{L_2(\Omega)} \leq c' \|e_n\|_{\Phi_{n+1}}$, and now

$$\|e_n\|_{\Phi_{n+1}} \le \alpha \|e_{n-1}\|_{\Phi_n}$$

$$\leq lpha^n \|e_0\|_{\Phi_1}$$

 $\leq c lpha^n \|f\|_{H^{\sigma}}(\mathbb{S}^2)$.

Except for the local aspect, that's it!
Main ideas – extension

To get results for errors on $bos\Omega$ we need an

extension operator *E*:

$$E: H^{
u}(\Omega) o H^{
u}(\mathbb{S}^2), \quad 0 \leq
u \leq \sigma,$$

with E independent of ν , and such that

 $Eu|_{\Omega}=u|_{\Omega} \quad ext{for all } u\in H^{
u}(\Omega),$

and

 $\|Eu\|_{H^{\nu}(\mathbb{S}^2)} \leq c_{\nu}\|u\|_{H^{\nu}(\Omega)}.$

Proof of existence of E: Hubbert and Morton (2004) for integer ν , plus interpolation.



Applying zeros theorem and extension

So now we have

$$\begin{split} \|e_n\|_{L_2(\Omega)} &\leq ch_n^{\sigma} \|e_n\|_{H^{\sigma}(\Omega)} \\ &= ch_n^{\sigma} \|Ee_n\|_{H^{\sigma}(\Omega)} \\ &\leq ch_n^{\sigma} \|Ee_n\|_{H^{\sigma}(\mathbb{S}^2)} \\ &\leq \text{etc} \end{split}$$



Two alternative calculations

In the right picture we do one **single-scale interpolation** at the 9th level. The graininess is apparent!

In the left picture we do **three multiscale levels**, all on the superlocal cap (i.e. levels 7, 8, 9 of the 9-level calculation).









RBF approximation after 3 global + 3 local + 3 superlocal levels



Final L^2 errors

9-level:
$$||e||_{L^2(\Omega_2)} = 8.0e - 4$$

3-level:
$$||e||_{L^2(\Omega_2)} = 9.2e-3$$

1-level:
$$||e||_{L^2(\Omega_2)} = 2.0e-2$$



Final comments on "zooming in"

- The theory combines the ideas of the global theory for the sphere LeGia,S,Wendland 2010, AND the theory for bounded regions in Euclidean space Wendland, Numer Math 2010.
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In both theory and practice it seems we could continue zooming to smaller and smaller regions, without limit.

