Kernel Interpolation and Quadrature with Localized Bases

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joint work with:

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Localized kernel bases

- Desired to treat large problems where standard basis is inadequate – often used as a pre-conditioner
- Local elements obtained by a difference operator applied to kernel – considered by Dyn-Levin-Rippa, Rabut, Buhmann-Dai, Beatson & Powell
- We consider local Lagrange functions of Beatson and Powell – showing rapid decay and L_p stability & most of all that this method scales: decay of basis elements is stationary & construction is nearly stationary.

Kernel based quadrature

- High performance quadrature rules for a variety of manifolds – based on an idea for spheres by Sommariva and Womersley
- Weights can be easily calculated
- In conjunction with localized bases – calculation of weights is fast and scales appropriately

Positive definite kernels

- For any set of centers Ξ, the collocation matrix
$$\mathsf{C}_\Xi := \big(k(\xi,\zeta)\big)_{(\xi,\zeta)\in\Xi\times\Xi}$$
is symmetric, positive definite.
- Interpolation: For any $f \in C(\mathbb{M})$ there is a unique $I_\Xi f \in S(\Xi)$ so that $I_\Xi f\,|_\Xi = f\,|_\Xi$. In this case: $I_\Xi f = \sum_{\xi\in\Xi} c_\xi k(\cdot,\xi)$ with $\mathsf{C}_\Xi \vec{c} = f\,|_\Xi$
- Native space: There is a Hilbert space of continuous functions $\mathcal{N}$ with k as its reproducing kernel: $f(x) = \langle f, k(x,\cdot)\rangle_\mathcal{N}$
- The interpolant $I_\Xi f$ to f is the best interpolant from $\mathcal{N}$ in the sense that any $s \in \mathcal{N}$ for which $s\,|_\Xi = f\,|_\Xi$ has
$$\|I_\Xi f\|_\mathcal{N} \le \|s\|_\mathcal{N}.$$

Positive definite kernels

- $\big(k(\cdot,\xi)\big)_{\xi\in\Xi}$ forms a basis for the space

$$S(\Xi) = \operatorname*{span}_{\xi\in\Xi} k(\cdot,\xi)$$

- So does the Lagrange basis $\big(\chi_\xi\big)_{\xi\in\Xi}$, where $\chi_\xi = \sum_{\eta\in\Xi} A_{\xi,\eta} k(\cdot,\eta)$ and for all $\zeta \in \Xi$, $\chi_\xi(\zeta) = \delta(\xi,\zeta)$.
- The matrix of Lagrange coefficients $\big(A_{\xi,\zeta}\big)_{(\xi,\zeta)\in\Xi\times\Xi}$ is the inverse of the collocation matrix C_Ξ.
- The Lagrange function coefficients satisfy $A_{\xi,\eta} = \langle \chi_\xi, \chi_\zeta\rangle_{\mathcal{N}}$.

$$\langle \chi_\xi, \chi_\zeta\rangle_{\mathcal{N}} = \sum_{\eta\in\Xi} A_{\zeta,\eta}\langle \chi_\xi, k(\cdot,\eta)\rangle_{\mathcal{N}} = \sum_{\eta\in\Xi} A_{\zeta,\eta}\delta(\xi,\eta) = A_{\xi,\eta}.$$

Sobolev spaces

Assume $\mathbb{M}$ is a d dimensional, compact Riemannian manifold without boundary.

- $\mathbb{M}$ is a metric space. Basic characteristics of Ξ apply:
  - fill distance $h := \max_{x\in\mathbb{M}} \mathrm{dist}(x, \Xi)$,
  - separation radius $q := \min_{\xi\in\Xi} \mathrm{dist}(\xi, \Xi \setminus \{\xi\})$,
  - mesh-ratio $\rho = h/q$.
- $\mathbb{M}$ is also a measure space, with $|B(x,r)| \sim r^d$ (for small r).
- Sobolev spaces $W_2^\tau(\mathbb{M})$ can also be defined easily – either via partition of unity and charts or by way of an elliptic differential operator (like the Laplace–Beltrami operator).
- If $\tau > d/2$, then $W_2^\tau(\mathbb{M})$ is a reproducing kernel Hilbert space. Its kernel is positive definite and $\mathcal{N} = W_2^\tau(\mathbb{M})$.
- [Fuselier-Wright, '11] If $\mathbb{M} \subset \mathbb{R}^{d+n}$ and $\phi \in C(\mathbb{R}^{d+n})$ is an RBF with native space $W_2^N(\mathbb{R}^d)$, then $k : (x,y) \mapsto \phi(x-y)$ has native space $W_2^\tau(\mathbb{M})$, $\tau = N - \frac{n}{2}$.

Kernels with $\mathcal{N} = W_2^\tau(\mathbb{M})$

If $k : \mathbb{M} \times \mathbb{M} \to \mathbb{R}$ has native space $W_2^\tau(\mathbb{M})$

- Lagrange function is bounded in native space norm

$$\|\chi_\xi\|_{\mathcal{N}} \le Cq^{d/2-\tau}.$$

  This is a bump estimate – compare χ_ξ to an interpolant with support in $B(\xi, q)$.

- Lagrange coefficients are uniformly bounded:

$$|A_{\xi,\zeta}| = |\langle \chi_\xi, \chi_\zeta \rangle_{\mathcal{N}}| \le Cq^{d-2\tau}$$

$$\longrightarrow \|(\mathrm{C}_\Xi)^{-1}\|_\infty \le Cq^{d-2\tau}(\#\Xi)$$

- [De Marchi-Schaback, '10] If Ξ is sufficiently dense in $\mathbb{M}$, then a zeros lemma ensures that the Lagrange function is bounded, independent of $\#\Xi$:

$$|\chi_\xi(x)| \le Cq^{d/2-\tau} h^{\tau-d/2} = C\rho^{\tau-d/2}$$

Sobolev kernels (or Sobolev-Matérn kernels)

- For open $\Omega \subset \mathbb{M}$, $m \in \mathbb{N}$ and $m > d/2$ define the $W_2^m(\Omega)$ inner product as

$$\langle f, g \rangle_{W_2^m(\Omega)} = \sum_{j=0}^{m} \int_{\Omega} \langle \nabla^j f, \nabla^j g \rangle_x \mathrm{d}x$$

- For $\Omega = \mathbb{M}$, this is the same as the other definitions of $W_2^m(\mathbb{M})$.
- The Sobolev kernel κ_m is the reproducing kernel for $\mathcal{N} = W_2^m(\mathbb{M})$.
- Equivalently, κ_m is the fundamental solution for the elliptic differential operator $\mathcal{L}_m = \sum_{j=0}^{m} (\nabla^j)^* \nabla^j$.

Lagrange function bounds

- For sufficiently dense Ξ, we have the energy bound for $R > 0$:

$$\text{For } R > 0, \quad \|\chi_\xi\|_{W_2^m(\mathbb{M}\setminus B(\xi,R))} \le C q^{d/2-m} e^{-\nu \frac{R}{h}}$$

- Lagrange functions have pointwise bounds

$$|\chi_\xi(x)| \le C\rho^{m-d/2} e^{-\nu \frac{\mathrm{dist}(\xi,x)}{h}} \quad (\text{H}-\text{Narcowich}-\text{Ward}, \text{`10})$$

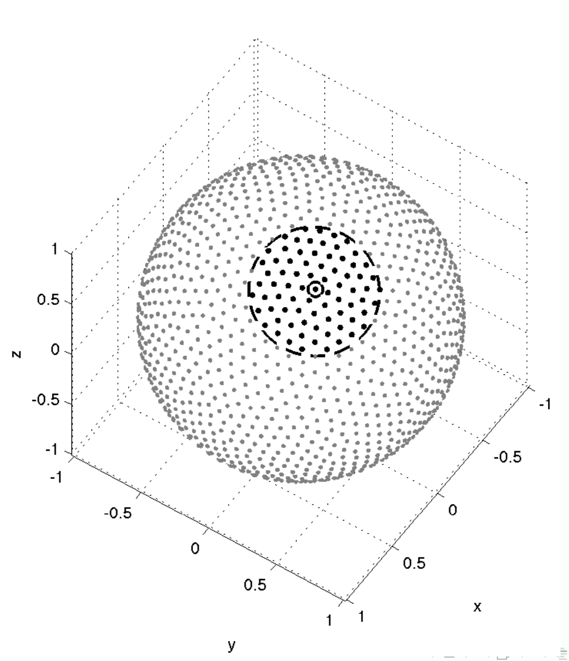
  - (H-N-W, '10) Boundedness of Lebesgue constant ,
  - (H-N-Sun-W, '11) Stability: $\|\sum_{\xi\in\Xi} a_\xi \chi_\xi\|_p \sim q^{\frac{d}{p}} \|\vec{a}\|_{\ell_p(\Xi)}$,
  - (H-N-S-W, '11) L_p boundedness of L_2 projector.
- Lagrange coefficients are bounded by

$$|A_{\xi,\zeta}| = |\langle \chi_\xi, \chi_\zeta\rangle_{W_2^m(\mathbb{M})}| \le C q^{d-2m} e^{-\frac{\nu}{2h}\mathrm{dist}(\xi,\zeta)}$$

- Centers more than $Kh|\log h|$ away from ξ:

$$|A_{\xi,\zeta}| \le C q^{d-2m} h^{\frac{\nu K}{2}} \le C_\rho h^{\frac{\nu K}{2}+d-2m}$$

Let $\Upsilon_\xi := \Xi \cap B(\xi, Kh|\log h|)$. If $N = \#\Xi$, then $\#\Upsilon_\xi \sim (\log N)^d$.



Better bases: truncated and local Lagrange bases

From [Fuselier - H - Narcowich - Ward - Wright, '13]

- Let $\Upsilon_\xi := \Xi \cap B(\xi, Kh|\log h|)$.
- Consider the truncated Lagrange basis $(\chi_\xi)_{\xi\in\Xi}$

$$\widetilde{\chi_\xi} := \sum_{\zeta\in\Upsilon_\xi} A_{\xi,\zeta}\kappa_m(\cdot,\zeta)$$

$$\longrightarrow \|\widetilde{\chi_\xi} - \chi_\xi\|_\infty \leq C_\rho h^{(\frac{K\nu}{2} - 2m)}$$

(Because there are at most $N \leq |\mathbb{M}|q^{-d}$ centers)

- Uses only a fraction of the total centers. but requires calculating all coefficients.

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(Because there are at most $N \le |\mathbb{M}|q^{-d}$ centers)

- Uses only a fraction of the total centers. but requires calculating all coefficients.
- Use instead $b_\xi \in S(\Upsilon_\xi)$, the local Lagrange functions: $b_\xi(\zeta) = \delta(\xi,\zeta)$ for all $\zeta \in \Upsilon_\xi$.
- Complexity of constructing each b_ξ is $\mathcal{O}(K^{3d}|\log N|^{3d})$. The full family $(b_\xi)_{\xi\in\Xi}$ costs $\mathcal{O}(K^{3d}N|\log N|^{3d})$.

Local Lagrange bounds: $\|\chi_\xi - b_\xi\|_\infty \le C_\rho h^J$

- Since $r = (\widetilde{\chi_\xi} - b_\xi) \in S(\Upsilon_\xi)$,

$$(\widetilde{\chi_\xi} - b_\xi) = \sum_{\xi \in \Upsilon_\xi} c_\xi \kappa_m(\cdot, \xi), \qquad \text{where} \quad \mathrm{C}_{\Upsilon_\xi} \vec{c} = r\big|_{\Upsilon_\xi}$$

- At the nodes, the error is small:

$$\max_{\zeta \in \Upsilon_\xi} |r(\zeta)| \le C_\rho h^{\frac{\nu K}{2} - 2m}$$

- The inverse collocation matrix $(\mathrm{C}_{\Upsilon_\xi})^{-1} = (A_{\eta,\zeta})_{(\eta,\zeta) \in \Upsilon_\xi \times \Upsilon_\xi}$ has $\ell_\infty \to \ell_\infty$ norm

$$\|(\mathrm{C}_{\Upsilon_\xi})^{-1}\|_\infty \le C q^{d-2m} (\#(\Upsilon_\xi)) \le C q^{-2m}$$

- Coefficients are small:

$$\|\vec{c}\|_\infty \le C_\rho q^{-2m} h^{\frac{\nu K}{2} - 2m} \le C_\rho h^{\frac{\nu K}{2} - 4m}$$

- The uniform error is small:

$$\|\widetilde{\chi_\xi} - b_\xi\|_\infty \le \sum_{\xi \in \Upsilon_\xi} |c_\xi| \|\kappa_m(\cdot, \xi)\|_\infty \le C_\rho h^{\frac{\nu K}{2} - 4m - d}$$

Local Lagrange basis summary

- Each element uses $K|\log N|^d$ centers
- For sufficiently large K, $(b_\xi)_{\xi\in\Xi}$ is an L_p-stable, rapidly decaying basis for $S(\Xi)$:

$$\|b_\xi - \chi_\xi\|_\infty \le C_\rho h^J \quad \text{when} \quad K = \frac{2}{\nu}(J+4m)$$

- Drawback: ν is not known.
- Can be used as a preconditioner for interpolation:

$$\mathrm{C}_\Xi \mathcal{A}\vec{c} = f|_\Xi\ .$$

- For sufficiently large K, $Q_\Xi f = \sum_{\xi\in\Xi} f(\xi) b_\xi$ behaves like $I_\Xi f = \sum_{\xi\in\Xi} f(\xi)\chi_\xi$. Namely,

$$\|Q_\Xi f - f\|_\infty \le \Lambda \mathrm{dist}(f, S(\Xi))_\infty + C_\rho h^{J-d}\|f\|_\infty$$

- Drawback: κ_m is hard to compute.

Quadrature on homogeneous spaces

From [Fuselier - H - Narcowich - Ward - Wright, to appear]

- G is a Lie group of isometries of $\mathbb{M}$ acting transitively
  $\forall x, y \in \mathbb{M}, \exists g \in G \quad y = gx$.

$$\forall g \in G, \int_{\mathbb{M}} f(gx)\mathrm{d}x = \int_{\mathbb{M}} f(x)\mathrm{d}x.$$

- G-invariant, positive definite kernel: $k(gx, gy) = k(x, y)$

$$\longrightarrow \forall y \in \mathbb{M}, \int_{\mathbb{M}} k(x, y)\mathrm{d}x = J_0$$

- For $s \in S(\Xi)$, $s = \sum_{\xi \in \Xi} a_\xi k(\cdot, \xi)$

$$\begin{aligned}
\int_{\mathbb{M}} s(x)dx &= \sum_{\xi} a_\xi \int_{\mathbb{M}} k(x, \xi)\mathrm{d}x \\
&= J_0(\mathbf{1}^T)\mathbf{a} \\
&= J_0 \mathbf{1}^T \left\{ \mathrm{C}_{\Xi}^{-1} s|_{\Xi} \right\} \\
&= J_0 \left\{ \mathrm{C}_{\Xi}^{-1} \mathbf{1} \right\}^T s|_{\Xi} = \mathbf{c}^T s|_{\Xi}
\end{aligned}$$

Quadrature error decays rapidly if $\mathcal{N} = W_2^\tau(\mathbb{M})$.

- Let k have $\mathcal{N} = W_2^\tau(\mathbb{M})$. For every $s \in S(\Xi)$

$$\left| \int_{\mathbb{M}} f(x) \mathrm{d}x - \sum_{\xi \in \Xi} c_\xi f(\xi) \right| \leq \int_{\mathbb{M}} |f(x) - s(x)| \mathrm{d}x + \sum_{\xi \in \Xi} |c_\xi| |f(\xi) - s(\xi)|$$

Choose $s = I_\Xi f$:

$$\left| \int_{\mathbb{M}} f(x) \mathrm{d}x - \sum_{\xi \in \Xi} c_\xi f(\xi) \right| \leq \|f - I_\Xi f\|_{L_1(\mathbb{M})} \leq h^\tau \|f\|_{W_2^\tau(\mathbb{M})}$$

- Using Sobolev kernel κ_m: Preconditioner solves interpolation problem and

$$\left| \int_{\mathbb{M}} f(x) \mathrm{d}x - \sum_{\xi \in \Xi} c_\xi f(\xi) \right| \leq C \begin{cases} h^\sigma \|f\|_{C^\sigma(\mathbb{M})} & 0 < \sigma \leq 2m \\ h^\sigma \|f\|_{W_2^\sigma(\mathbb{M})} & \frac{d}{2} < \sigma \leq m \end{cases}$$

Polyharmonic (and related) kernels

- $Q \in \Pi_m(\mathbb{R})$ with $\lim_{\lambda \to -\infty} Q(\lambda) = +\infty$.
- Fundamental solution to $\mathcal{L}_m = \sum_{j=0}^{m} a_j \Delta^j = Q(\Delta)$

$$f(x) = \int_{\mathbb{M}} [\mathcal{L}_m(f - p_f)](\alpha) k(x, \alpha) \mathrm{d}\alpha + p_f(x)$$

$p_f \in \Pi_{\mathcal{J}} = \mathrm{span}_{j \in \mathcal{J}}(\psi_j)$ with $\#\mathcal{J} < \infty$

- ψ_j eigenfunctions of Δ

$$k(x, y) = \sum_{j=1}^{\infty} \alpha_j \psi_j(x) \psi_j(y) \quad \left(\alpha_j = \left(Q(\lambda_j)\right)^{-1} \text{for } j \notin \mathcal{J}\right)$$

- $\mathcal{L}_m$ is positive on the eigenfunctions not in $\Pi_{\mathcal{J}}$.
- Conditionally positive definite w.r.t. $\Pi_{\mathcal{J}}$
- Reproducing kernel semi-Hilbert space $\mathcal{H}_k := \{f = \sum_{j=0}^{\infty} \hat{f}_j \psi_j \mid \sum_{j \notin \mathcal{J}} |\hat{f}_j|^2 Q(\lambda_j) < \infty\}$

2-point homogeneous spaces

- Restricted surface splines on $\mathbb{S}^d$: $k(x,\alpha) = \phi(x\cdot\alpha)$

$$\phi(t) = \begin{cases} (1-t)^{m-d/2} & \text{for } d \text{ odd} \\ (1-t)^{m-d/2}\log(1-t) & \text{for } d \text{ even} \end{cases}$$

  (Baxter & Hubbert, Levesley & Odell)
- Surface splines on $SO(3)$: $k(x,\alpha) = \phi(\omega(\alpha^{-1}x))$

$$\phi(t) = \big(\sin(t/2)\big)^{m-3/2}$$

  (H. & Schmid)
- On two point homogeneous spaces,

$$\mathcal{L}_m = \sum_{j=0}^{m} a_j \Delta^j = \sum_{j=0}^{m} \tilde{a}_j (\nabla^j)^* \nabla^j$$

- Special case: sometimes $\mathcal{L}_m \Pi_{\mathcal{J}} = \{0\}$,

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- Special case: sometimes $\mathcal{L}_m \Pi_{\mathcal{J}} = \{0\}$, When $\mathcal{L}_m \Pi_{\mathcal{J}} = \{0\}$...

1. Lagrange basis is local [H-N-W, '12]:

$$|\chi_\xi(x)| \le C_\rho \exp\left[-\nu\left(\frac{\mathrm{dist}(\xi, x)}{h}\right)\right].$$

2. The Lagrange basis is stable [H-N-W,'12]:

$$c_1 q^{d/p}\|a\|_{\ell_p} \le \|\sum_{\xi\in\Xi} a_\xi \chi_\xi\|_p \le c_2 q^{d/p}\|a\|_{\ell_p}$$

3. The local Lagrange function $b_\xi \in S(\Upsilon_\xi)$ using $\Upsilon_\xi \subset B(\xi, Kh|\log h|)$ is local and stable:

$$\|b_\xi - \chi_\xi\|_\infty \le C_\rho h^J$$

Benefits:

- Use as a preconditioner for interpolation, $I_\Xi f = \sum_{\xi\in\Xi} a_\xi b_\xi$:

$$\begin{bmatrix} \mathsf{C}_\Xi & \Psi \end{bmatrix} \begin{bmatrix} \mathcal{A} \\ \mathcal{B} \end{bmatrix} \begin{bmatrix} \mathbf{a} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \end{bmatrix}.$$

  $\mathcal{A} = (A_{\xi,\eta})$ and $\mathcal{B} = (B_{\xi,j})$ matrices of coefficients for each b_ξ. ($\mathcal{A}$ is sparse.)

- Basis collocation matrix $(b_\xi(\zeta))_{(\xi,\zeta)\in\Xi\times\Xi} = (\mathsf{C}_\Xi\mathcal{A} + \Psi\mathcal{B})$ has nice decay.

- Quasi-interpolation $Q_\Xi f = \sum_{\xi\in\Xi} f(\xi) b_\xi$ performs like I_Ξ

$$\|Q_\Xi f - f\|_\infty \le Ch^s \|f\|_{C^s}, \text{ for } s \le 2m$$

Quadrature on $\mathbb{S}^2$

Quadrature with $k(x,\alpha) = (1 - x\cdot\alpha)^{m-1}\log(1 - x\cdot\alpha)$

$$\int_{\mathbb{S}^2} f(x)\mathrm{d}x \sim \sum_{\xi\in\Xi} c_\xi f(\xi)$$

correct for $f \in S(\Xi)$

- Need to know $J_0 := \int_{\mathbb{S}^2} k(x,y)\mathrm{d}x$ – independent of y
- Need to know moment vector $J = (J_1, \dots J_m)$ where $J_j = \int_{\mathbb{S}^2} \psi_j(x)\mathrm{d}x$
- Weights are obtained from

$$\mathrm{K}_\Xi \begin{pmatrix} \mathbf{c} \\ \mathbf{d} \end{pmatrix} = \begin{pmatrix} \mathrm{C}_\Xi & \Psi \\ \Psi^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{c} \\ \mathbf{d} \end{pmatrix} = \begin{pmatrix} J_0\mathbf{1} \\ \mathbf{J} \end{pmatrix}$$

Quadrature with $k(x,\alpha) = (1 - x\cdot\alpha)^{m-1}\log(1 - x\cdot\alpha)$

For $s \in S(k,\Xi)$, $s = \sum a_\xi k(\cdot,\xi) + \sum b_j \psi_j$,

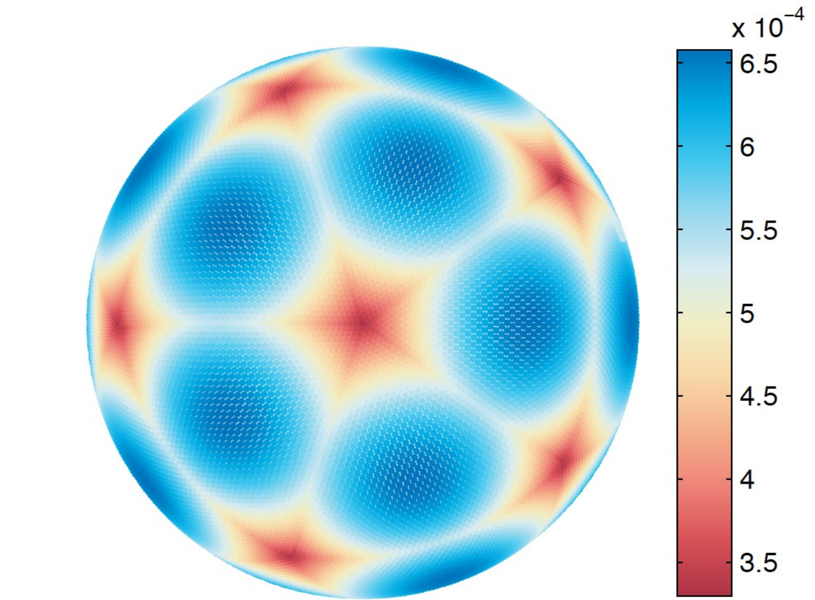
$$\begin{aligned}
\int_{\mathbb{S}^2} s(x)dx &= \sum_\xi a_\xi \int_{\mathbb{S}^2} k(x,\xi)\mathrm{d}x + \sum b_j \int_{\mathbb{S}^2} \psi_j(x)\mathrm{d}x \\
&= \begin{pmatrix} J_0\mathbf{1} \\ \mathbf{J} \end{pmatrix}^T \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix} \\
&= \left\{ \mathrm{K}_\Xi^{-1} \begin{pmatrix} J_0\mathbf{1} \\ \mathbf{J} \end{pmatrix} \right\}^T \begin{pmatrix} s|_\Xi \\ \mathbf{0} \end{pmatrix} = \mathbf{c}^T s|_\Xi
\end{aligned}$$

- $\mathrm{K}_\Xi \begin{pmatrix} \mathbf{c} \\ \mathbf{d} \end{pmatrix} = \begin{pmatrix} J_0\mathbf{1} \\ \mathbf{J} \end{pmatrix}$ not directly solvable – need to decompose $\mathbf{c}$ into $\mathrm{ran}\Psi$ and $\ker \Psi^T$.
- Each c_ξ can be obtained as $\int_{\mathbb{S}^2} \chi_\xi(x)\mathrm{d}x = B_{\xi,1}\mathrm{vol}(\mathbb{S}^2)$ where

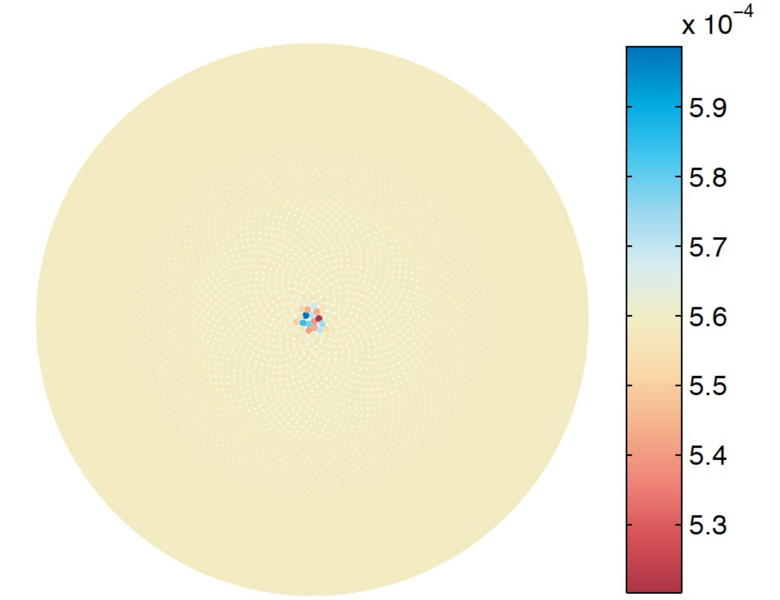
$$\chi_\xi = \sum_\zeta A_{\xi,\zeta} k(\cdot,\zeta) + \sum B_{\xi,j}\psi_j$$

Using the first coefficient from b_ξ may be faster.

Quadrature weights for 23042 icosahedral nodes



Quadrature weights for 22501 Fibonacci nodes



Quadrature weights for 22500 minimal energy nodes