Spherical configurations and quadrature methods for integral equations of the second kind†

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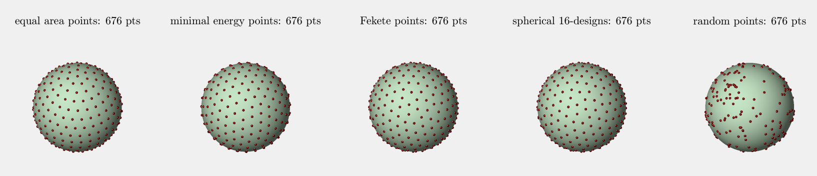
Point distributions on spheres



☞ Many **point distributions** $\{\boldsymbol{x}_j\}_{j=1}^m \subset \mathbb{S}^2$ are investigated:

- Equal area points;
- Minimal energy points: $\{\boldsymbol{x}_j\}_{j=1}^m$ that minimizes the Coulomb energy;
- Fekete points: $\{\boldsymbol{x}_j\}_{j=1}^m$ that maximizes the determinant for polynomial interpolation;
- Spherical t-designs: $\{\boldsymbol{x}_j\}_{j=1}^m$ that satisfies (quadrature exactness)

$$\frac{1}{m}\sum_{j=1}^{m} g(\boldsymbol{x}_j) = \frac{1}{4\pi}\int_{\mathbb{S}^2} g \, d\omega \quad \forall g \in \mathbb{P}_t;$$

- Even random points.

Marcinkiewicz–Zygmund inequality: A characterization

✍ Marcinkiewicz and Zygmund (1937): There exists $\eta \in [0,1)$ such that

$$(1-\eta)\int_{\Omega}\chi^2 \mathrm{d}\omega_d \le \sum_{j=1}^{m} w_j \chi(x_j)^2 \le (1+\eta)\int_{\Omega}\chi^2 \mathrm{d}\omega_d \quad \forall \chi \in \mathbb{P}_n.$$

- MZ on spheres: Mhaskar, Narcowich, & Ward (2001)
- MZ on compact manifolds: Filbir & Mhaskar (2011)

In particular on $\mathbb{S}^2$, $[h_{\mathcal{X}_m} := \max_{\boldsymbol{x}\in\mathbb{S}^2} \min_{\boldsymbol{x}_j\in\mathcal{X}_m} \mathrm{dist}(\boldsymbol{x}, \boldsymbol{x}_j)]$

- **Spherical t-designs**: MZ holds with $\eta = 0$ if $n^2 \le t$;
- **Scattered data**: MZ holds if $n \lesssim \eta / h_{\mathcal{X}_m}$, where $h_{\mathcal{X}_m}$ is the mesh norm of $\{x_j\}_{j=1}^m$
- **Random data** (Le Gia & Mhaskar '09): If $\{x_j\}$ are i.i.d drawn from the distribution ω_d, then there exists a constant $\bar{c} := \bar{c}(\gamma)$ such that MZ holds on $\mathbb{S}^2$ with probability $\ge 1 - \bar{c}N^{-\gamma}$ on the condition $m \ge \bar{c}N^2 \log N/\eta^2$

Fredholm integral equations of the second kind

☞ Consider the Fredholm integral equation of the second kind

$$\boxed{\varphi(\boldsymbol{x}) - \int_{\mathbb{S}^2} h(|\boldsymbol{x}-\boldsymbol{y}|)K(\boldsymbol{x},\boldsymbol{y})\varphi(\boldsymbol{y})d\omega(\boldsymbol{y}) = f(\boldsymbol{x})}$$

on $\mathbb{S}^2$, where $|\boldsymbol{x}-\boldsymbol{y}| := \sqrt{2(1-\boldsymbol{x}\cdot\boldsymbol{y})}$ denotes the Euclidean distance between points $\boldsymbol{x}$ and $\boldsymbol{y}$ on $\mathbb{S}^2$.

- The inhomogeneous term f, the kernel K, and the solution φ are **continuous**, and K may be **oscillatory**.
- The weight function $h : (0,\infty) \to \mathbb{R}$ is allowed to be **weakly singular**, i.e., h is continuous for all $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{S}^2$ with $\boldsymbol{x} \neq \boldsymbol{y}$, and there exists positive constants M and $\alpha \in (0,2]$ such that

$$|h(|\boldsymbol{x}-\boldsymbol{y}|)| \leq M|\boldsymbol{x}-\boldsymbol{y}|^{\alpha-2};$$

- It is assumed that the homogeneous equation has no non-trivial solution: **classic Riesz theory** $\Rightarrow$ the inhomogeneous equation has a unique solution continuously depending on f.

Dangerous: Applying a quadrature rule to discretize the integral op.

☞ Consider a quadrature rule $\sum_{j=1}^{m} w_j g(\boldsymbol{x}_j) \approx \int_\Omega g \mathrm{d}\omega$ and evaluate the integral operator in terms of

$$\int_{\mathbb{S}^2} h(|\boldsymbol{x}-\boldsymbol{y}|) K(\boldsymbol{x},\boldsymbol{y}) \varphi(\boldsymbol{y}) d\omega(\boldsymbol{y}) \approx \sum_{j=1}^{m} w_j h(|\boldsymbol{x}-\boldsymbol{x}_j|) K(\boldsymbol{x},\boldsymbol{x}_j) \varphi(\boldsymbol{x}_j),$$

resulting

$$\varphi(\boldsymbol{x}_i) - \sum_{j=1}^{m} w_j h(|\boldsymbol{x}_i-\boldsymbol{x}_j|) K(\boldsymbol{x}_i,\boldsymbol{x}_j) \varphi(\boldsymbol{x}_j) = f(\boldsymbol{x}_i), \quad i = 1, 2, \ldots, m.$$

☞ Numerically evaluating singular integrals is **risky**: as quadrature points approach the singularity, the scheme becomes increasingly unstable.

(Think about $\boldsymbol{x}_i = \boldsymbol{x}_j$ and thus $h(|\boldsymbol{x}_i - \boldsymbol{x}_j|) = \infty$)

Wise: A semi-analytical approach for the singular kernel

☞ Let $\{Y_{\ell,k}:\ \ell=0,\dots,n,\ k=1,\dots,2\ell+1\}$ be the set of **spherical harmonics** of degree $\le n$. They are orthogonal polynomials on spheres.

☞ **Funk–Hecke formula:** Let $g\in L^1(-1,1)$ and $\boldsymbol{x}\in\mathbb{S}^2$. Then

$$\int_{\mathbb{S}^2} g(\boldsymbol{x}\cdot\boldsymbol{y})Y_{\ell,k}(\boldsymbol{y})d\omega(\boldsymbol{y})=\mu_\ell Y_{\ell,k}(\boldsymbol{x}),$$

where

$$\mu_\ell := 2\pi\int_{-1}^{1} g(t)P_\ell(t)dt,$$

and $P_\ell(t)$ is the standard Legendre polynomial of degree ℓ.

☞ **Modified moments:** Computing the singular part analytically

$$\boxed{\int_{\mathbb{S}^2} h(|\boldsymbol{x}-\boldsymbol{y}|)Y_{\ell,k}(\boldsymbol{y})d\omega(\boldsymbol{y})=\mu_\ell Y_{\ell,k}(\boldsymbol{x}),}$$

where $\quad (|\boldsymbol{x}-\boldsymbol{y}|:=\sqrt{2(1-\boldsymbol{x}\cdot\boldsymbol{y})}$ and $h(|\boldsymbol{x}-\boldsymbol{y}|)=(2^{1/2}(1-\boldsymbol{x}\cdot\boldsymbol{y})^{1/2}))$

$$\boxed{\mu_\ell := 2\pi\int_{-1}^{1} h(2^{1/2}(1-t)^{1/2})P_\ell(t)dt.}$$

☞ **Example 1:** $h(|\boldsymbol{x}-\boldsymbol{y}|) = |\boldsymbol{x}-\boldsymbol{y}|^\nu$ with $-2<\nu<0$. Then

$$\boxed{\mu_\ell = 2^{\nu+2}\pi\left(-\frac{\nu}{2}\right)_\ell \frac{\Gamma\left(\frac{\nu+2}{2}\right)}{\Gamma\left(\ell+\frac{\nu}{2}+2\right)}} \text{ with } (x)_n := \frac{\Gamma(x+n)}{\Gamma(x)} \text{ for } x>0.$$

☞ **Example 2:** $h(|\boldsymbol{x}-\boldsymbol{y}|) = \log|\boldsymbol{x}-\boldsymbol{y}|$. Then

$$\boxed{\mu_\ell = 2\pi\int_{-1}^{1}\log(2^{1/2}(1-t)^{1/2})P_\ell(t)\,dt} = \pi\int_{-1}^{1}\log(2(1-t))P_\ell(t)\,dt.$$

☞ **Example 3:** $h(|\boldsymbol{x}-\boldsymbol{y}|) = |\boldsymbol{x}-\boldsymbol{y}|^{\nu_1}|\boldsymbol{x}+\boldsymbol{y}|^{\nu_2}$ with $-2\le\nu_1,\nu_2<0$. Then

$$\boxed{\mu_\ell = 2^{(\nu_1+\nu_2)/2}(2\pi)\int_{-1}^{1}(1-t)^{\nu_1/2}(1+t)^{\nu_2/2}P_\ell(t)\,dt.}$$

A new quadrature rule for the integral operator

☞ For the integral operator $\int_{\mathbb{S}^2} h(|\boldsymbol{x}-\boldsymbol{y}|)K(\boldsymbol{x},\boldsymbol{y})\varphi(\boldsymbol{y})d\omega(\boldsymbol{y})$:

- We approximate $K(\boldsymbol{x},\boldsymbol{y})\varphi(\boldsymbol{y})$ using spherical harmonics $\{Y_{\ell,k}(\boldsymbol{y})\}$;
- The approximation should be produced using information on the point set $\{\boldsymbol{x}_j\}_{j=1}^m$.

☞ Approximation of f with only $\{f(\boldsymbol{x}_j)\}_{j=1}^m$ available:

Sloan (1995): Hyperinterpolation

The **hyperinterpolation** of $f \in C(\mathbb{S}^2)$ onto $\mathbb{P}_n$ is defined as

$$\mathcal{L}_n f := \sum_{\ell=0}^{n}\sum_{k=1}^{2\ell+1}\langle f, Y_{\ell,k}\rangle_m Y_{\ell,k},$$

where $\langle f, Y_{\ell,k}\rangle_m := \sum_{j=1}^m w_j f(\boldsymbol{x}_j)Y_{\ell,k}(\boldsymbol{x}_j)$ with all $w_j > 0$.

Hyperinterpolation and Marcinkiewicz–Zygmund inequality

Theorem (Sloan '95 JAT)

Assume the quadrature rule has **exactness degree** $2n$. Then for any $f \in C(\Omega)$,

$$\|\mathcal{L}_n f - f\|_2 \leq 4\pi^{1/2} E_n(f),$$

where $E_n(f) := \inf_{\chi \in \mathbb{P}_n} \|f - \chi\|_\infty$.

Theorem (An & W. '24 JoC)

Assume the quadrature rule **satisfies the MZ property**. Then for any $f \in C(\Omega)$,

$$\|\mathcal{L}_n f - f\|_{L^2} \leq \left(\sqrt{1+\eta} \left(\sum_{j=1}^{m} w_j \right)^{1/2} + 2\pi^{1/2} \right) E_n(f) + \sqrt{\eta^2 + 4\eta} \|\chi^*\|_{L^2},$$

where $E_n(f) = \|f - \chi^*\|$.

A new quadrature rule for the integral operator (cont.)

For the integral operator $\int_{\mathbb{S}^2} h(|\boldsymbol{x}-\boldsymbol{y}|)K(\boldsymbol{x},\boldsymbol{y})\varphi(\boldsymbol{y})d\omega(\boldsymbol{y})$, we approximate it as

$$\begin{aligned}
&\int_{\mathbb{S}^2} h(|\boldsymbol{x}-\boldsymbol{y}|)\mathcal{L}_n\left(K(\boldsymbol{x},\cdot)\varphi(\cdot)\right)d\omega(\boldsymbol{y})\\
&=\int_{\mathbb{S}^2} h(|\boldsymbol{x}-\boldsymbol{y}|)\left(\sum_{\ell=0}^{n}\sum_{k=1}^{2\ell+1}\left\langle K(\boldsymbol{x},\cdot)\varphi, Y_{\ell,k}\right\rangle_m Y_{\ell,k}(\boldsymbol{y})\right)d\omega(\boldsymbol{y})\\
&=\sum_{\ell=0}^{n}\sum_{k=1}^{2\ell+1}\boxed{\left(\int_{\mathbb{S}^2} h(|\boldsymbol{x}-\boldsymbol{y}|)Y_{\ell,k}(\boldsymbol{y})d\omega(\boldsymbol{y})\right)}\left\langle K(\boldsymbol{x},\cdot)\varphi, Y_{\ell,k}\right\rangle_m\\
&=\sum_{j=1}^{m} w_j\left(\sum_{\ell=0}^{n}\sum_{k=1}^{2\ell+1}\left(\int_{\mathbb{S}^2} h(|\boldsymbol{x}-\boldsymbol{y}|)Y_{\ell,k}(\boldsymbol{y})d\omega(\boldsymbol{y})\right)Y_{\ell,k}(\boldsymbol{x}_j)\right)K(\boldsymbol{x},\boldsymbol{x}_j)\varphi(\boldsymbol{x}_j)\\
&=:\sum_{j=1}^{m} W_j(\boldsymbol{x})K(\boldsymbol{x},\boldsymbol{x}_j)\varphi(\boldsymbol{x}_j),
\end{aligned}$$

Two-stage numerical scheme for the integral equation

Let φ_γ denotes the numerical solution:

$$\varphi_\gamma(\boldsymbol{x}) - \sum_{j=1}^{m} W_j(\boldsymbol{x}) K(\boldsymbol{x}, \boldsymbol{x}_j) \varphi_\gamma(\boldsymbol{x}_j) = f(\boldsymbol{x})$$

☞ **First stage** We set $\boldsymbol{x} = \boldsymbol{x}_j$, $j = 1, \ldots, m$, then numerically solves the obtained system of linear equations

$$\varphi_\gamma(\boldsymbol{x}_i) - \sum_{j=1}^{m} W_j(\boldsymbol{x}_i) K(\boldsymbol{x}_i, \boldsymbol{x}_j) \varphi_\gamma(\boldsymbol{x}_j) = f(\boldsymbol{x}_i), \quad i = 1, \ldots, m$$

for the quantities $\varphi_\gamma(\boldsymbol{x}_j)$, $j = 1, \ldots, m$.

☞ **Second stage** The value of $\varphi_\gamma(\boldsymbol{t})$ at any $\boldsymbol{t} \in \mathbb{S}^2$ can be evaluated by the direct usage of

$$\varphi_\gamma(\boldsymbol{t}) = f(\boldsymbol{t}) + \sum_{j=1}^{m} W_j(\boldsymbol{t}) K(\boldsymbol{t}, \boldsymbol{x}_j) \varphi_\gamma(\boldsymbol{x}_j).$$

Numerical analysis for the numerical scheme

Let

$$(A\varphi)(\boldsymbol{x}) := \int_{\mathbb{S}^2} h(|\boldsymbol{x}-\boldsymbol{y}|)K(\boldsymbol{x},\boldsymbol{y})\varphi(\boldsymbol{y})d\omega(\boldsymbol{y})$$

and

$$(A_\gamma\varphi)(\boldsymbol{x}) := \sum_{j=1}^{m} W_j(\boldsymbol{x})K(\boldsymbol{x},\boldsymbol{x}_j)\varphi(\boldsymbol{x}_j).$$

☞ For $\varphi - A\varphi = f$: Riesz theory $\Rightarrow (I-A)^{-1} : C(\mathbb{S}^2) \to C(\mathbb{S}^2)$ exists and is bounded ✓

☞ For $\varphi_\gamma - A_\gamma\varphi_\gamma = f$ and $(I-A_\gamma)(\varphi_\gamma - \varphi) = (A_\gamma - A)\varphi$: The existence of φ_γ and the error bound of $\|\varphi_\gamma - \varphi\|_{L^\infty}$ depend on the **existence and boundedness of $(I-A_\gamma)^{-1}$ (?)**.

☞ The identity $(I-A)^{-1} = I + (I-A)^{-1}A$ suggests that

$$(I - A_\gamma)^{-1} \approx B_\gamma := I + (I-A)^{-1}A_\gamma$$

☞ Note that

$$(I-A)B_\gamma(I-A_\gamma) = \cdots = (I-A) - (A_\gamma - A)A_\gamma,$$

which is equivalent to

$$B_\gamma(I-A_\gamma) = I - (I-A)^{-1}(A_\gamma - A)A_\gamma =: I - S_\gamma.$$

☞ If we **assume** $\|(I-A)^{-1}(A_\gamma - A)A_\gamma\| < 1$, Neumann series $\Rightarrow$ $(I-S_\gamma)^{-1}$ exists and is bounded by

$$\|(I-S_\gamma)^{-1}\| \le \frac{1}{1-\|S_\gamma\|}.$$

Then $I - A_\gamma$ is an injection. If we **assume A_γ is compact**, then A_γ is also a surjection (and hence bijection) $\Rightarrow$ $(I-A_\gamma)^{-1}$ exists and

$$(I-A_\gamma)^{-1} = (I-S_\gamma)^{-1}B_\gamma.$$

Key Lemma

Assume that operators A_γ are compact and the sequence $\{A_\gamma\}$ satisfies

$$\|(I-A)^{-1}(A_\gamma - A)A_\gamma\| < 1,$$

Then the inverse operators $(I-A_\gamma)^{-1} : C(\mathbb{S}^2) \to C(\mathbb{S}^2)$ exist and are bounded by

$$\|(I-A_\gamma)^{-1}\| \le \frac{1+\|(I-A)^{-1}A_\gamma\|}{1-\|(I-A)^{-1}(A_\gamma - A)A_\gamma\|}.$$

For solutions of the equations

$$\varphi - A\varphi = f \quad \text{and} \quad \varphi_\gamma - A_\gamma \varphi_\gamma = f,$$

we have the error estimate

$$\|\varphi_\gamma - \varphi\|_{L^\infty} \le \frac{1+\|(I-A)^{-1}A_\gamma\|}{1-\|(I-A)^{-1}(A_\gamma - A)A_\gamma\|}\|(A_\gamma - A)\varphi\|_{L^\infty}.$$

- Applying previous approximation results of hyperinterpolation, we can verify A_γ is compact and $\|(I-A)^{-1}(A_\gamma - A)A_\gamma\| < 1$.
- We need $h(2^{1/2}(1-t)^{1/2}) \in L^1(-1,1) \cap L^2(-1,1)$ to apply the theory of hyperinterpolation.

Theorem (An & W. - arXiv :2408.14392)

Let $\gamma = (m, n, \eta) \in \Gamma$ with sufficiently large n and sufficiently small η. Then

$$\|\varphi_\gamma\|_{L^\infty} \leq C_1(m,n,\eta)\|f\|_{L^\infty},$$

where $C_1(m,n,\eta) > 0$ is some constant decreasing as n grows or η decreases. Moreover, there exists $\boldsymbol{x}_0 \in \mathbb{S}^2$ such that

$$\|\varphi_\gamma - \varphi\|_{L^\infty} \leq C_2(m,n,\eta)\left(E_n(K(\boldsymbol{x}_0,\cdot)\varphi) + \sqrt{\eta^2+4\eta}\|\chi^*\|_{L^2}\right),$$

where $C_2(m,n,\eta) > 0$ is some constant decreasing as n grows or η decreases, and χ^* stands for the best approximation polynomial of $K(\boldsymbol{x}_0,\cdot)\varphi(\cdot)$ in $\mathbb{P}_n$.

Numerical experiments for the integral equation solver

☞ **Toy example setting:** For various singular kernel h and continuous kernel K, let $\varphi \equiv 1 \Rightarrow$ value of $f \Rightarrow$ Solve for φ_γ and compare with 1.

☞ **Point sets** $\{\boldsymbol{x}_j\}_{j=1}^m$ for the first stage: We investigate four kinds of point distributions on sphere:

- Spherical t-designs;
- Minimal energy points;
- Fekete points;
- Equal area points.

☞ **Validation points** for the second stage: 5,000 uniformly distributed points on $\mathbb{S}^2$.

Example 1: $h(\boldsymbol{x},\boldsymbol{y}) = |\boldsymbol{x}-\boldsymbol{y}|^{-0.5}$ with modified moments (and hence $W_j(\boldsymbol{x})$) analytically evaluated. We let $K(\boldsymbol{x},\boldsymbol{y}) = \cos(10|\boldsymbol{x}-\boldsymbol{y}|)$, thus

$$f(\boldsymbol{x},\boldsymbol{y}) \equiv 1 - 2\pi \int_{-1}^{1} \left(\sqrt{2(1-t)}\right)^{-0.5} \cos\left(10\sqrt{2(1-t)}\right) dt$$
$$\approx 0.303738699125466.$$

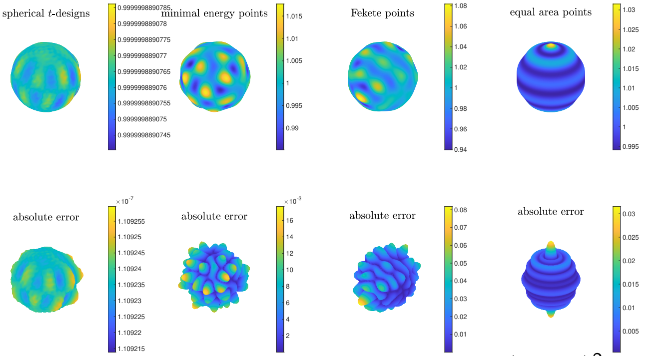


Figure: Numerical solutions with $n = 20$ and $m = (2n+1)^2$.

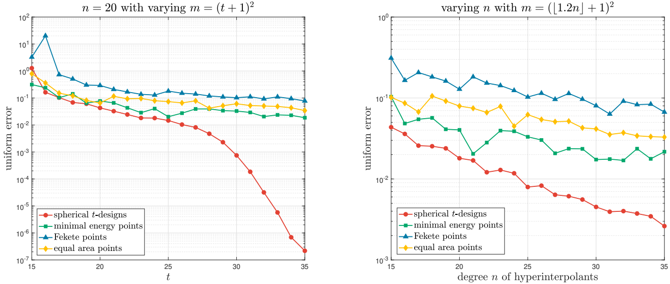


Figure: Singular $h(\boldsymbol{x}, \boldsymbol{y}) = |\boldsymbol{x} - \boldsymbol{y}|^{-0.5}$ and oscillatory $K(\boldsymbol{x}, \boldsymbol{y}) = \cos(10|\boldsymbol{x} - \boldsymbol{y}|)$: Uniform errors with different n and m.

Example 2: $h(\boldsymbol{x},\boldsymbol{y}) = \log|\boldsymbol{x}-\boldsymbol{y}|$ with modified moments (and hence $W_j(\boldsymbol{x})$) stably evaluated. We let $K=1$ and

$$f(\boldsymbol{x},\boldsymbol{y}) \equiv 1 - 2\pi \int_{-1}^{1} \log\left(\sqrt{2(1-t)}\right) dt = 1 - \pi(4\log 2 - 2).$$

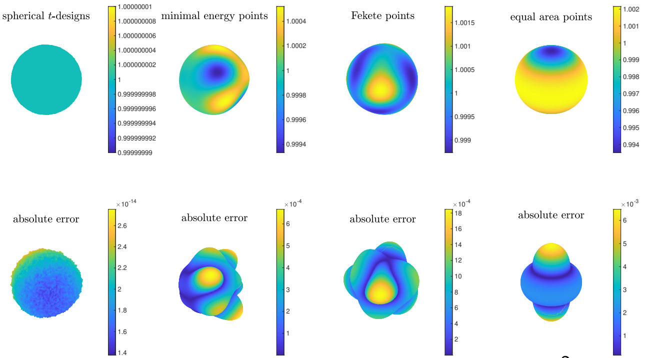


Figure: Numerical solutions $n=5$ and $m=(2n+1)^2$.

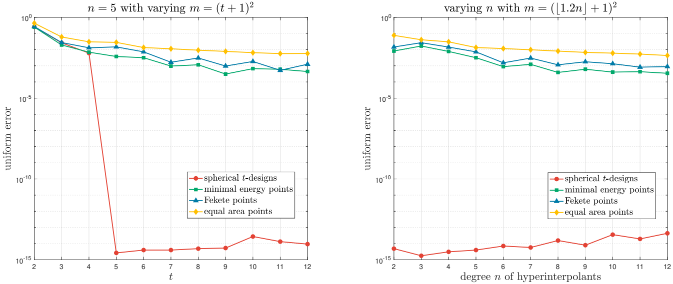


Figure: Singular $h(\boldsymbol{x}, \boldsymbol{y}) = \log |\boldsymbol{x} - \boldsymbol{y}|$ and non-oscillatory $K = 1$: Uniform errors with different n and m.

Thanks for your attention.

Photo taken from the State Botanical Garden of Georgia/Athens, GA.