Numerical Integration over unit sphere–by using spherical $t$-designs

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Outline

1. Well conditioned spherical designs
2. Numerical verification methods
3. Numerical results of verification methods
4. Numerical integration over unit sphere
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Numerical Integration over unit sphere–by using spherical $t$-designs

Notations

- $X_N = \{x_1, \ldots, x_N\} \subset S^2 = \{x, y, z \in \mathbb{R}^3 | x^2 + y^2 + z^2 = 1\}$
- $\mathbb{P}_t = \{\text{spherical polynomials of degree } \leq t\}$
  $= \{\text{polynomials in } x, y, z \text{ of degree } \leq t \text{ restricted to } S^2\}$
- $N = \text{Number of points}$
- $t = \text{Degree of polynomials}$
Spherical coordinates

\[ x_1 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad x_2 = \begin{bmatrix} \sin(\theta_2) \\ 0 \\ \cos(\theta_2) \end{bmatrix}, \quad x_i = \begin{bmatrix} \sin(\theta_i) \cos(\phi_i) \\ \sin(\theta_i) \sin(\phi_i) \\ \cos(\theta_i) \end{bmatrix}, \quad i = 3, \ldots, N \]
Part I

Background on spherical $t-$designs
Definition of Spherical $t$–design

Definition (Spherical $t$–design)

The set $X_N = \{x_1, \ldots, x_N\} \subset \mathbb{S}^2$ is a spherical $t$-design if

$$
\frac{1}{N} \sum_{j=1}^{N} p(x_j) = \frac{1}{4\pi} \int_{\mathbb{S}^2} p(x) d\omega(x) \quad \forall p \in \mathbb{P}_t,
$$

where $d\omega(x)$ denotes surface measure on $\mathbb{S}^2$.

The definition of spherical $t$–design was given by Delsarte, Goethals, Seidel in 1977 [10].
Numerical Integration over unit sphere—by using spherical $t$-designs

—Background on spherical $t$—designs

Real Spherical harmonics

Real Spherical harmonics[14]

$Y_{\ell k} : k = 1, \ldots, 2\ell + 1, \ell = 0, 1, \ldots, t$

- Basis
  \[ \mathbb{P}_t = \text{Span}\{Y_{\ell k} : k = 1, \ldots, 2\ell + 1, \ell = 0, 1, \ldots, t\} \]

- Orthonormality with respect to $L_2$ inner product
  \[ (p, q)_{L_2} = \int_{S^2} p(x)q(x)d\omega(x), \]

- Normalization
  \[ Y_{0,1} = \frac{1}{\sqrt{4\pi}} \]

- $\text{dim} \mathbb{P}_t = (t + 1)^2$

- Addition Theorem
  \[ \sum_{k=1}^{2\ell+1} Y_{\ell,k}(x)Y_{\ell,k}(y) = \frac{2\ell+1}{4\pi} P_\ell (x \cdot y), \; x, y \in S^2 \]
Spherical harmonic basis matrix

For $t \geq 1$, and $N \geq \dim(\mathbb{P}_t) = (t + 1)^2$, let $Y_t^0$ be the $((t + 1)^2 - 1)$ by $N$ matrix defined by

\[
Y_t^0(\mathcal{X}_N) := [Y_{\ell,k}(x_j)], \quad k = 1, \ldots, 2\ell + 1, \quad \ell = 1, \ldots, t; \quad j = 1, \ldots, N, \quad (3)
\]

\[
Y_t(\mathcal{X}_N) := \begin{bmatrix}
\frac{1}{\sqrt{4\pi}} e^T \\
Y_t^0(\mathcal{X}_N)
\end{bmatrix} \in \mathbb{R}^{(t+1)^2 \times N}, \quad (4)
\]

where $e = [1, \ldots, 1]^T \in \mathbb{R}^N$.

\[
G_t(\mathcal{X}_N) := Y_t(\mathcal{X}_N)^T Y_t(\mathcal{X}_N) \in \mathbb{R}^{N \times N},
\]

\[
H_t(\mathcal{X}_N) := Y_t(\mathcal{X}_N) Y_t(\mathcal{X}_N)^T \in \mathbb{R}^{(t+1)^2 \times (t+1)^2}.
\]
Nonlinear system $C_t(\mathcal{X}_N) = 0$

Let $N \geq (t + 1)^2$, define $C_t : (\mathbb{S}^d)^N \to \mathbb{R}$,

$$C_t(\mathcal{X}_N) = EG_t(\mathcal{X}_N)e$$

where the $N \times N$ Gram matrix $G_t$ for $\mathcal{X}_N \subset \mathbb{S}^2$

$$G_t(\mathcal{X}_N) = Y_t(\mathcal{X}_N)^T Y_t(\mathcal{X}_N)$$

$$e = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} \in \mathbb{R}^N, \ E = [1, -I] \in \mathbb{R}^{(N-1) \times N}, \ 1 = [1, \ldots, 1]^T \in \mathbb{R}^{N-1}$$
Nonlinear system \( C_t(\mathcal{X}_N) = 0 \)

Theorem (ACSW2010,[1])

Let \( N \geq (t + 1)^2 \). Suppose that \( \mathcal{X}_N = \{x_1, \ldots, x_N\} \) is a fundamental system for \( \mathbb{P}_t \). Then \( \mathcal{X}_N \) is a spherical \( t \)-design if and only if \( C_t(\mathcal{X}_N) = 0 \).

Definition (Fundamental system)

A point set \( \mathcal{X}_N = \{x_1, \ldots, x_N\} \subset S^2 \) is a fundamental system for \( \mathbb{P}_t \) if the zero polynomial is the only member of \( \mathbb{P}_t \) that vanishes at each point \( x_i, \ i = 1, \ldots, N \).

\( H_t(\mathcal{X}_N) \) is nonsingular \( \iff \) \( \mathcal{X}_N \) is a fundamental system for \( \mathbb{P}_t \).

Let \( N = (t + 1)^2 \), \( G_t(\mathcal{X}_N) \) is nonsingular \( \iff \) \( \mathcal{X}_N \) is a fundamental system for \( \mathbb{P}_t \).
Well conditioned spherical designs
Definition

Chen and Womersley [8], Chen, Frommer and Lang [9] verified that a spherical $t$-design exists in a neighborhood of an extremal system. This leads to the idea of *extremal spherical $t$-designs*, which first appeared in [8] in $N = (t + 1)^2$. We here extend the definition to $N \geq (t + 1)^2$.

**Definition (Extremal spherical designs[1])**

A set $\mathcal{X}_N = \{x_1, \ldots, x_N\} \subset \mathbb{S}^2$ of $N \geq (t + 1)^2$ points is a *extremal spherical $t$-design* if the determinant of the matrix

$\mathbf{H}_t(\mathcal{X}_N) := \mathbf{Y}_t(\mathcal{X}_N) \mathbf{Y}_t(\mathcal{X}_N)^T \in \mathbb{R}^{(t+1)^2 \times (t+1)^2}$

is maximal subject to the constraint that $\mathcal{X}_N$ is a spherical $t$-design.
Optimization Problem on $S^2$

$$\max \log \det (H_t(X_N))$$

$X_N \subset S^2$

subject to $C_t(X_N) = 0.$

$$\downarrow$$

Well conditioned spherical $t$-design.

The log of the determinant is bounded above by

$$\log \det (H_L(X_N)) \leq (t + 1)^2 \log \left(\frac{N}{4\pi}\right).$$
Numerical Integration over unit sphere—by using spherical $t$-designs

Numerical Verification method
Notations on Interval method

1. By $\mathbb{IR}^n$, denote $[a] = [a, \bar{a}]$, $a, \bar{a} \in \mathbb{R}^n$, $a \leq \bar{a}$

2. $+, -, \times, /$ can be extended from $\mathbb{R}^n$ to $\mathbb{IR}^n$ and from $\mathbb{R}^{n \times n}$ to $\mathbb{IR}^{n \times n}$.

3. Let $\text{mid}[a] = (a + \bar{a})/2$ in componentwise.

4. $\text{diam}[a] = \bar{a} - a = 2\text{rad}[a]$,

5. $F : D \subseteq \mathbb{R}^n \rightarrow \mathbb{R}^n$ be a continuously differentiable function. Let $[dF] \in \mathbb{IR}^{n \times n}$ be an interval matrix containing $F'(\xi)$ for all $\xi \in [x]$,

i.e.

$$\{F'(x) : x \in [x]\} \subseteq [dF]( [x] ).$$

(9)

Such $[dF]$ can be obtained by an interval arithmetic evaluation of (expressions for) the Jacobian $F'$ at the interval vector $[x]$. 
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Numerical Verification method

Krawczyk operator

Definition (Krawczyk operator,[11])

Given a nonsingular matrix $B_L \in \mathbb{R}^{n \times n}$, $\tilde{z} \in [z] \subseteq D$ and $[dF] \in \mathbb{I}\mathbb{R}^{n \times n}$, the Krawczyk operator [11] is defined by:

$$k_F(\tilde{z}, [z], B_L, [dF]) := \tilde{z} - B_L F(\tilde{z}) + (I_n - B_L \cdot [dF])([z] - \tilde{z}). \quad (10)$$

It is known that $k_F(\tilde{z}, [z], B_L, [dF])$ is an interval extension of the function $\psi(z) := z - B_L F(z)$ over $[z]$, that is, $z - B_L F(z) \in k_F(\tilde{z}, [z], B_L, [F])$ for all $z \in [z]$. 


Verification Theorem

Theorem (Krawczyk 1969 [11], Moore 1977[12])

Let $F : D \subset \mathbb{R}^n \to \mathbb{R}^n$ be a continuously differentiable function. Choose $[z] \in \mathbb{R}^n$, $\tilde{z} \in [z] \subseteq D$, an invertible matrix $B_L \in \mathbb{R}^{n \times n}$ and $[dF] \in \mathbb{R}^{n \times n}$ such that $F'(\xi) \in [dF]$ for all $\xi \in [z]$. Assume that

$$k_F(\tilde{z}, [z], B_L, [dF]) \subseteq [z].$$

Then $F$ has a zero $z^*$ in $k_F(\tilde{z}, [z], B_L, [dF])$. 
Deal with $C_t(\mathcal{X}_N)$

1. Represent the points $x_i$ on the sphere by spherical coordinates with $\phi$, $\theta$. That is

$$[x_i] = [\sin([\theta])\cos([\phi]), \sin([\theta])\sin([\phi]), \cos([\theta])]^T, \ i = 1, \ldots, N.$$ 

2. $C_t(\mathcal{X}_N)$ is redefined as a system of nonlinear equation

$$\tilde{\mathbf{F}}(\mathbf{y}) = 0.$$ 

The components of $\mathbf{y}$ are $y_{i-1} = \theta_i, \ i = 2, \ldots, N,$

$y_{N+i-3} = \varphi_i, \ i = 3, \ldots, N.$
1 Use a QR-factorization method at each step to determine the $N - 2$ least important components of $y$, which we label collectively by $y_N$, then write $y := (z, y_N)$, and define a new function $F(z) = \tilde{F}(z, y_N)$, where $F : \mathbb{R}^{N-1} \rightarrow \mathbb{R}^{N-1}$.

2 Using the Krawczyk operator with $B_L = (\text{mid}[dF])^{-1}$ we can verify the existence of a fixed point of $z - B_L F(z)$, which is a solution of $F(z) = 0$. 
The estimate on determinant

Theorem (ACSW2010,[1])

Let $U$ be a nonsingular upper triangular matrix. Assume that

$$
\|I_n - U^T[A]U\|_\infty \leq r < 1. \tag{11}
$$

Let $\beta = \left(\prod_{j=1}^{N} U_{jj}\right)^{-2}$. Then

$$
0 < \beta(1 - r)^N \leq \det(A) \leq \beta(1 + r)^N, \quad \text{for} \quad A \in [A] \quad \text{and} \quad A^T = A^a. \tag{12}
$$

---

Proof. We consider a symmetric matrix $A \in [A]$. Noting that $U^T A U$ preserves the symmetric structure, we denote its (real) eigenvalues by $\lambda_i(U^T A U)$. Since

$$\max_{1 \leq i \leq N} |1 - \lambda_i(U^T A U)| = \rho \left( I_n - U^T A U \right) \leq \|I_n - U^T A U\|_\infty \leq r,$$

where $\rho$ is the spectral radius, we have

$$0 < 1 - r \leq \lambda_i(U^T A U) \leq 1 + r, \quad i = 1, \ldots, N.$$

Hence,

$$(1 - r)^N \leq \det(U^T A U) \leq (1 + r)^N.$$

Noting that $\det(U) \det(U^T) = \left( \prod_{j=1}^{N} U_{jj} \right)^2 = \beta^{-1}$, from

$$0 < (1 - r)^N \leq \beta^{-1} \det(A) \leq (1 + r)^N,$$

we obtain (12).
In practical computation for $H_t$

1. Choose a preconditioning matrix $U$ s.t \((U^{-1})^T U^{-1} = \text{mid}[H_t]\)

2. Conduct all operations in machine interval arithmetic and get an interval enclosing \(\|I_n - U^T [H_t] U\|_\infty\).

\[
\|I_n - U^T [H_t] U\|_\infty = \|U^T ((U^{-1})^T U^{-1} - [H_t]) U\|_\infty \quad (13a)
\]

\[
= \|U^T (\text{mid}(H_t) - [H_t]) U\|_\infty \quad (13b)
\]

\[
\leq \|U^T\|_\infty \|\text{rad}(H_t)\|_\infty \|U\|_\infty < 1, \quad (13c)
\]

3. \[
[\log \det (H_t(\mathcal{X}_N))] \subseteq [\underline{b}, \bar{b}] \quad (14)
\]

for all $\mathcal{X}_N \in [\mathcal{X}_N]$, where

\[
\underline{b} = \log \beta + N \log (1 - r) \quad \text{and} \quad \bar{b} = \log \beta + N \log (1 + r).
\]
Numerical results of verification method

IV

Numerical results of verification method

- For $N = (t + 1)^2$, $\det(G_t(X_N)) = \det(H_t(X_N))$.
  Using an Extremal system $^1$ as a initial point set.
- Based on the MATLAB toolbox INTLAB $^2$, $^3$.


Numerical Integration over unit sphere—by using spherical $t$-designs

Numerical results of verification method

For $t = 1, \ldots, 151$ with $N = (t + 1)^2$

1. $\max \text{diam}(\mathcal{X}_N)$ represents the maximum diameter of all computed enclosures for the parametrization of the respective spherical $t$-design.

2. $[\log \det(G_t(\mathcal{X}_N))]$ is over $10^4$ for the largest $t$. 
Numerical Integration over unit sphere—by using spherical $t$-designs

Numerical results of verification method

Figure: The diameters of $[\mathcal{X}_N]$
Numerical Integration over unit sphere by using spherical $t$-designs

Numerical results of verification method

Figure: Middle point values and diameters of $\log \det(G_t(X_N))$
Geometry

Separation distance—well separated spherical $t$-design

$$\delta x_N := \min_{x_i, x_j \in x_N, i \neq j} \text{dist} (x_i, x_j) \geq \frac{\pi}{2t} \geq \frac{\pi}{2\sqrt{N}}.$$
Numerical Integration over unit sphere—by using spherical $t$-designs

Existence of well separated spherical $t$-designs

For each even $N \geq C_d t^d$, there exists of a well separated spherical $t$-design in the sphere $S^d$ consisting of $N$ points, where $C_d$ is a constant depending only on $d^4$.

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Geometry

Mesh norm

\[ h_{\mathcal{X}_N} := \max_{y \in S^2} \min_{x_i \in \mathcal{X}_N} \text{dist}(y, x_i) \leq \frac{4.8097}{t}, \]

Figure: The mesh norm of \( \mathcal{X}_N \) with \( N = (t + 1)^2 \)
Geometry

Mesh ratio \( \rho x_N := \frac{2h x_N}{\delta x_N} \geq 1 \)

Figure: The mesh ratio of extremal spherical t-designs with \( N = (t + 1)^2 \)
Conjecture on $S^2$

Let $C_\delta$, $C_h$ be constants. A lower bound on the separation of well conditioned spherical $t$-designs for

$$\delta \chi_N \geq C_\delta N^{-\frac{1}{2}},$$

combined with the known upper bounds on mesh norm

$$h \chi_N \leq C_h N^{\frac{1}{2}}$$

would give the uniform bound

$$\rho \chi_N \leq \frac{2C_h}{C_\delta}$$

independent of $t, N$. (15)
Numerical Integration over unit sphere—by using spherical $t$-designs

Numerical results of verification method

An example

Figure: Well conditioned 49 design with 2500 points
A question

Can we verify Womersley’s efficient spherical $t$-designs successfully by using Interval analysis?
Numerical Integrations over unit sphere

1. Bivariate trapezoidal rule\(^5\), with \(q = 2.5\).

2. Well conditioned spherical \(t\)-designs

3. Equal area points\(^6\)

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Numerical Integrations over unit sphere

Bivariate trapezoidal rule

For the problem of approximate

\[ I(f) = \int_{S^2} f(\mathbf{x}) d\omega(\mathbf{x}) \]

in which \( f \) is several times continuously differentiable over the unit sphere \( S^2 \), we can use spherical coordinates to rewrite it as

\[ I(f) = \int_{0}^{\pi} \int_{0}^{2\pi} f(\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta) \sin \theta d\phi d\theta \]
We use a transformation $\mathcal{L} : S^2 \rightarrow \tilde{S}^2$ With respect to spherical coordinates on $S^2$

\[
\mathcal{L} : x = (\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta) \mapsto \tilde{x} = (\cos \phi \sin^q \theta, \sin \phi \sin^q \theta, \cos \theta) = L(\theta, \phi). \tag{16}
\]

\[
\frac{\sqrt{\cos^2 \theta + \sin^2 q \theta}}{\cos \theta} = L(\theta, \phi). \tag{17}
\]

In this transformation, $q \geq 1$ is a ‘grading parameter’, The north and south poles of $S^2$ remain fixed, while the region around them is distorted by the mapping. If we chose a higher $q$, the area near two poles will have more points and equator area are more sparser.
The integral $I(f)$ becomes

$$I(f) = \int_{S^2} f(Lx) J_L(\tilde{x}) d\omega(\tilde{x})$$

with $J_L(\tilde{x})$ the jacobian of the mapping $L$,

$$J_L(\tilde{x}) = |D_\phi L(\theta, \phi) \times D_\theta L(\theta, \phi)| = \frac{\sin^{2q-1} \theta (q \cos^2 \theta + \sin^2 \theta)}{(\cos^2 \theta + \sin^{2q} \theta)^{\frac{3}{2}}}.$$ 

In spherical coordinates,

$$I(f) = \int_0^\pi \sin^{2q-1} \theta (q \cos^2 \theta + \sin^2 \theta) \int_0^{2\pi} f(\xi, \eta, \zeta) d\phi d\theta,$$

$$(\xi, \eta, \zeta) = \frac{(\cos \phi \sin^q \theta, \sin \phi \sin^q \theta, \cos \theta)}{\sqrt{\cos^2 \theta + \sin^{2q} \theta}}.$$
For $n \geq 1$, let $h = \pi / n$, and

$$
\phi_j = \theta_j = jh
$$

$$
\int_0^\pi \int_0^{2\pi} g(\sin \theta, \cos \theta, \sin \phi, \cos \phi) \, d\phi \, d\theta
\approx h^2 \sum_{k=1}^{n-1} \sum_{j=1}^{2n} g(\sin \theta_k, \cos \theta_k, \sin \phi_j, \cos \phi_j) \equiv I_n,
$$

$$
g = \frac{\sin^{2q-1} \theta (q \cos^2 \theta + \sin^2 \theta)}{(\cos^2 \theta + \sin^{2q} \theta)^{3/2}} f(\xi, \eta, \zeta).
$$

Error satisfies

$$
I - I_n = O(h^k) \quad f \in C^k(S^2)
$$
Equal-Area Points

The equal-area points aim to achieve a partition $T$ of the sphere into a user-chosen number of $N$ of subsets $T_j$ each of which has the same area

$$|T_j| = \frac{4\pi}{N}, \quad j = 1, \ldots, N,$$

and

$$diam(T_j) \leq \frac{c}{\sqrt{N}},$$

Then we obtain the equal weight rule

$$I_N f := \frac{4\pi}{N} \sum_{j=1}^{N} f(x_j).$$

We have

$$|I f - I_N f| \leq \frac{4\pi \sigma c}{\sqrt{N}}.$$
Geometry of different nodes

(a) Bi. trapezoidal rule  (b) Equal area points  (c) spherical $t$-design
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Numerical Integrations over unit sphere

Franke1 function

\[ f_1(x, y, z) = 0.75 \exp\left(-\frac{(9x - 2)^2}{4} - \frac{(9y - 2)^2}{4} - \frac{(9z - 2)^2}{4}\right) \\
+ 0.75 \exp\left(-\frac{(9x + 1)}{49} - \frac{(9y + 1)}{10} - \frac{(9z + 1)}{10}\right) \\
+ 0.5 \exp\left(-\frac{(9x - 7)^2}{4} - \frac{(9y - 3)^2}{4} - \frac{(9z - 5)^2}{10}\right) \\
+ 0.2 \exp\left(-\frac{(9x - 4)^2}{10} - \frac{(9y - 7)^2}{10} - \frac{(9z - 5)^2}{10}\right) \]
Numerical Integrations over unit sphere

$C_0$ function

$$f_2(x) = \sin^2(1 + \|x\|_1)/10$$

is not continuously differentiable at points where any component of $x$ is zero.

**Figure**: $f_2$
Nearby singular function

\[ f_3(x, y, z) = \frac{1}{101 - 100z} \]

is analytic over \( \mathbb{S}^2 \), it has a pole just off the surface of the sphere at \( x = (0, 0, 1.01) \), in other word, \( f_3((0, 0, 1.01)) = \infty \).

Figure: \( f_3 \)
Numerical Integrations over unit sphere

Cap function with $R = \frac{1}{3}$, center $x_0 = (0, 0, 1)^T$.

$$f_4(x) = \begin{cases} \cos^2\left(\frac{\pi}{2} \frac{\text{dist}(x, x_0)}{R}\right) & \text{if } \text{dist}(x, x_0) < R \\ 0 & \text{if } \text{dist}(x, x_0) \geq R, \end{cases}$$

**Figure:** $f_4$
Performance of Numerical Integrations
Performance of Numerical Integrations

<table>
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<th>function</th>
<th>exact integration values</th>
</tr>
</thead>
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<td>$f_1$</td>
<td>6.6961822200736179523</td>
</tr>
<tr>
<td>$f_2$</td>
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<tr>
<td>$f_3$</td>
<td>$\pi \log 201/50^*$</td>
</tr>
<tr>
<td>$f_4$</td>
<td>0.103351*</td>
</tr>
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Absolute error = $|I_f - I_nf|$  \hspace{1cm} (19)
Numerical Integration over unit sphere by using spherical \( t \)-designs

Performance of Numerical Integrations

Integration Error of \( f_1 \)

Franke1 Function

Figure: \( f_1 \)
Numerical Integration over unit sphere by using spherical $t$-designs

Performance of Numerical Integrations

Integration Error of $f_2$

$$\sin^2 \left(1 + \frac{\| (x, y, z) \|_1}{10} \right)$$

**Figure:** $f_2$
Numerical Integration over unit sphere by using spherical t-designs

Performance of Numerical Integrations

Integration Error of $f_3$

Figure: $f_3$
Numerical Integration over unit sphere by using spherical $t$-designs

Performance of Numerical Integrations

Figure: $f_4$
Final Remark

1. Well conditioned Spherical t-design is a useful tool to deal with numerical integration over the sphere.

2. Can we give a sharp error analysis for numerical integration (with different nodes) over the sphere as results on $[-1, 1]$?

3. How to set up a efficient quadrature rule when integrand with special properties? such as highly oscillatory integrals, potential integrals....
Thank you very much!
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REFERENCES
Numerical Integration over unit sphere—by using spherical \( t \)-designs

**REFERENCES**


