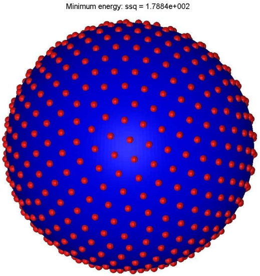
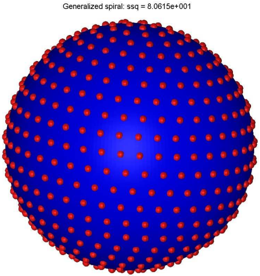
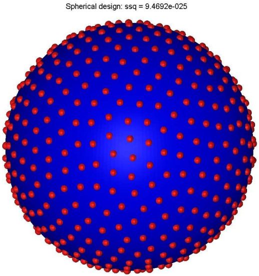
Spherical Designs and Approximate Spherical Designs

Rob Womersley, R.Womersley@unsw.edu.au
School of Mathematics and Statistics, University of New South Wales







The Fields Institute
Thematic Program on Discrete Geometry and Applications
Workshop on Sphere Arrangements, November 14–18, 2011

November 14–18, 2011

Outline

Definition - Spherical t-design

- Unit sphere $\mathbb{S}^2 := \left\{\mathbf{x} \in \mathbb{R}^3 : |\mathbf{x}| = 1\right\}$
- Standard Euclidean inner product $\mathbf{x} \cdot \mathbf{y}$ in $\mathbb{R}^3$: $|\mathbf{x}|^2 = \mathbf{x} \cdot \mathbf{x}$
- $\omega_2 = |\mathbb{S}^2| = \int_{\mathbb{S}^2} d\omega(\mathbf{x}) = 4\pi$
- Set $\mathcal{X}_N = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subset \mathbb{S}^2$
- Space $\mathbb{P}_t \equiv \mathbb{P}_t\left(\mathbb{S}^2\right)$ of spherical polynomials of degree at most t
  - $\dim(\mathbb{P}_t) = (t+1)^2$
- Spherical t-design is a set $\mathcal{X}_N$ of N points such that

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

  - $\mathcal{X}_N$ equal weight N point quadrature rule with degree of precision t

Spherical designs – Number of points

- Delsarte, Goethals and Seidel (1977) [10]
- For $\mathbb{S}^2$

$$N \geq N_0(t) := \begin{cases} \frac{(t+1)(t+3)}{4} & \text{if } t \text{ odd,} \\ \frac{(t+2)^2}{4} & \text{if } t \text{ even.} \end{cases} \tag{2}$$

- Bannai and Damerell (1979, 1980) [4, 5]
  - Tight spherical t-designs if achieve lower bounds
  - Cannot exist on $\mathbb{S}^2$ except for $t = 1, 2, 3, 5$
- Seymour and Zaslavsky (1984) [16]: Spherical t designs exist for N sufficiently large
- Bannai and Bannai (2009) [3] Survey on spherical designs and algebraic combinatorics on spheres
- Bondarenko, Radchenko and Viazovska (2010) [6] spherical t-designs on $\mathbb{S}^d$ exist for $N \geq c_d t^d$

Existence Results for $\mathbb{S}^2$

- Bajnok (1991) [2] construction with $N = O(t^3)$
  - n points $z_1, \ldots, z_n$, t-design on $[-1, 1]$
  - Regular m-gon at latitudes z_j
  - $N = mn$ point t-design if $m \geq t + 1$
- Korevaar and Meyers (1993) [14] - Faraday Cage
  - $N = O(t^3)$
- Both depend on t-designs for interval $[-1, 1]$
  - Set of n points $z_j \in [-1, 1]$:

$$\frac{2}{n} \sum_{j=1}^{n} p(z_j) = \int_{-1}^{1} p(z) dz \quad \forall p \in \mathbb{P}_t([-1, 1])$$

  - Equal weights $\Longrightarrow n = O(t^2)$ points
  - Survey Gautschi [11]
- Tensor product constructions based on 1-D existence result

Evidence for $\mathbb{S}^2$

- Hardin and Sloane (1996) [13]
  - Summary of known results for $\mathbb{S}^2$
  - Conjecture
  $$N = \frac{t^2}{2}\,(1 + o(1))$$
- $N = (t+1)^2 = \dim\left(\mathbb{P}_t(\mathbb{S}^2)\right)$
  - Start from extremal (maximum determinant) points
    Sloan, Womersley (2004) [17]
  - **Under-determined** system of equations
  - Use interval methods to verify a nearby solution
    - Chen and Womersley (2006) [8]
    - Chen, Frommer, Lang (2009) [7]
    - An, Chen, Sloan, Womersley (2010) [1]

Spherical designs – nonlinear equations

Delsarte, Goethals and Seidel (1977) [10]

$\mathcal{X}_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^2$ is a spherical t-design if and only if

$$r_{\ell,k}(\mathcal{X}_N) := \sum_{j=1}^{N} Y_{\ell,k}(\mathbf{x}_j) = 0 \tag{3}$$

for $k = 1, \ldots, 2\ell + 1, \quad \ell = 1, \ldots, t$.

- Spherical harmonics $\{Y_{\ell,k} : k = 1, \ldots, 2\ell + 1,\ \ell = 0, 1, \ldots, t\}$
  - Orthonormal basis for $\mathbb{P}_t(\mathbb{S}^2)$
  - $Y_{\ell,k}$ a spherical harmonic of degree ℓ
- Constant ($\ell = 0$) polynomial $Y_{0,1} = 1/\sqrt{4\pi}$ not included in (3)
- Integral of all spherical harmonics of degree $\ell \geq 1$ is zero

Polynomials with positive Legendre coefficients

- Polynomial $\psi_t \in \mathbb{P}_t[-1,1]$ with positive Legendre coefficients

$$\psi_t(z) := \sum_{\ell=1}^{t} a_{t,\ell} P_\ell(z), \tag{4}$$

$$a_{t,\ell} > 0 \quad \text{for} \quad \ell = 1, \ldots, t. \tag{5}$$

  - Legendre polynomial $P_\ell(z)$ for $z \in [-1,1]$
  - $\int_{-1}^{1} \psi_t(z) dz = 0$

- Variational form

$$A_{t,N,\psi}(\mathcal{X}_N) := \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \psi_t(\mathbf{x}_i \cdot \mathbf{x}_j)$$

Spherical designs – variational characterizations

$t \geq 1$, $\mathcal{X}_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^2$, ψ_t as in (4), (5). Then

$$0 \leq A_{t,N,\psi}(\mathcal{X}_N) \leq \sum_{\ell=1}^{t} a_{t,\ell} = \psi_t(1)$$

$$\overline{A}_{t,N,\psi} := \frac{1}{(\omega_2)^N} \int_{\mathbb{S}^2} \cdots \int_{\mathbb{S}^2} A_{t,N,\psi}(\mathbf{x}_1, \ldots, \mathbf{x}_N) d\omega(\mathbf{x}_1) \cdots d\omega(\mathbf{x}_N) = \frac{\psi_t(1)}{N}.$$

$\mathcal{X}_N$ is a spherical design if and only if

$$A_{t,N,\psi}(\mathcal{X}_N) = 0.$$

- Weighted sum of squares, strictly positive coefficients

$$A_{t,N,\psi}(\mathcal{X}_N) = \frac{4\pi}{N^2} \sum_{\ell=1}^{t} \frac{a_{t,\ell}}{2\ell+1} \sum_{k=1}^{2\ell+1} \left(r_{\ell,k}(\mathcal{X}_N)\right)^2 \tag{6}$$

- $A_{t,N,\psi}(\mathcal{X}_N) = 0 \iff \mathcal{X}_N$ spherical t-design
- Global min $A_{t,N,\psi}(\mathcal{X}_N) > 0 \Longrightarrow$ no spherical t-design with N points

Specific cases

- Grabner and Tichy (1993) [12]

$$\psi_t(z) = z^t + z^{t-1} - a_{t,0} \tag{7}$$

$$a_{t,0} = \begin{cases} \frac{1}{t} & t \text{ odd}, \\ \frac{1}{t+1} & t \text{ even}. \end{cases}$$

- Cohn and Kumar (2007) [9]

$$\psi_t(z) = (1+z)^t - \frac{2^t}{t+1}. \tag{8}$$

- Sloan and Womersley (2009) [18]

$$\psi_t(z) = \frac{1}{4\pi} P_t^{(1,0)}(z) - 1 = \sum_{\ell=1}^{t} (2\ell+1) P_\ell(z) \tag{9}$$

  - $P_t^{(1,0)}$ Jacobi polynomial

Evaluating $A_{t,N,\psi}(\mathcal{X}_N)$

- Matrix $\mathbf{\Psi}$: $\quad \mathbf{\Psi}_{ij} = \psi_t(\mathbf{x}_i \cdot \mathbf{x}_j), \qquad i,j = 1,\ldots,N$
- Spherical harmonic basis matrix $\mathbf{Y}$ of size $(t+1)^2 - 1$ by N:

$$\mathbf{Y} = \left[Y_{\ell,k}(\mathbf{x}_j)\right], \qquad \ell = 1,\ldots,t,\ k = 1,\ldots,2\ell+1; \quad j = 1,\ldots,N,$$

- Spherical t-design $\iff$ $(t+1)^2 - 1$ equations (3)

$$\mathbf{r} := \mathbf{Y}\mathbf{e} = \mathbf{0},$$

- Diagonal matrix $\mathbf{D}$ of weights from (6)

$$\mathbf{\Psi} = (4\pi)\mathbf{Y}^T\mathbf{D}\mathbf{Y}$$

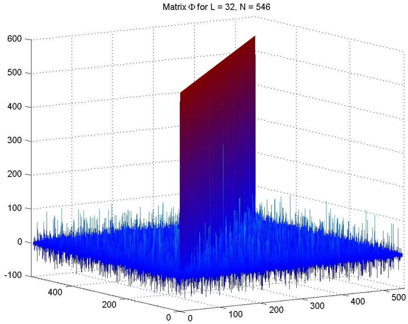
$$\mathbf{D} = \text{diag}\left(\frac{a_{t,\ell}}{2\ell+1}, k = 1,\ldots,2\ell+1, \ell = 1,\ldots,t\right)$$

- Any symmetric positive definite $\mathbf{D}$ possible
- Minimize

$$A_{t,N,\psi}(\mathcal{X}_N) = \frac{1}{N^2}\mathbf{e}^T\mathbf{\Psi}\mathbf{e} = \frac{4\pi}{N^2}\mathbf{e}^T\mathbf{Y}^T\mathbf{D}\mathbf{Y}\mathbf{e} = \frac{4\pi}{N^2}\mathbf{r}^T\mathbf{D}\mathbf{r}$$

Evaluating $A_{t,N,\psi}(\mathcal{X}_N)$ using $\boldsymbol{\Psi}$

- N by N matrix $\boldsymbol{\Psi}_{ij} = \psi_t(\mathbf{x}_i \cdot \mathbf{x}_j)$
- Constant diagonal elements $\psi_t(1) = \sum_{\ell=1}^{t} a_{t,\ell}$
- Matrix $\boldsymbol{\Psi}$ for $a_{t,\ell} = 2\ell + 1 \iff \mathbf{D} = \mathbf{I}$



- Advantages: simple, (trivially) parallel
- Issue: cancelation errors in summing off diagonal elements

Standard results

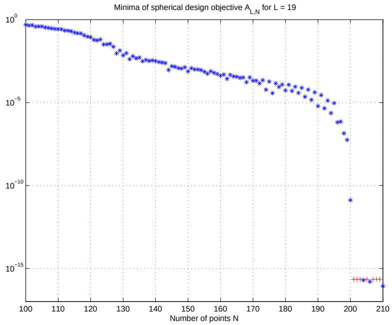
- System of equations $\mathbf{r}(x) = \mathbf{0}$, $\quad \mathbf{r} : \mathbb{R}^n \to \mathbb{R}^m$
- n variables, m equations
  - Under-determined $m < n$
  - Well-determined $m = n$
  - Over-determined $m > n$
- Sum of squares $f(x) = \mathbf{r}^T(x)\mathbf{r}(x) = \sum_{j=1}^m r_j(x)^2$
  - $f(x) \geq 0$ for all x, $f(x^*) = 0 \iff \mathbf{r}(x^*) = \mathbf{0}$
  - x^* global minimizer $f(x^*) > 0 \iff$ no solution exists
  - x^* local minimizer $f(x^*) > 0 \Longrightarrow$?
- Derivatives
  - Jacobian $J \in \mathbb{R}^{m\times n}$: $J_{ij}(x) = \frac{\partial r_i(x)}{\partial x_j}$, $i = 1, \ldots, m$, $j = 1, \ldots, n$
  - Gradient $\nabla f(x) = 2J^T\mathbf{r} \in \mathbb{R}^n$
  - Hessian $\nabla^2 f(x) = 2J^TJ + 2\sum_{i=1}^m r_i \nabla^2 r_i \in \mathbb{R}^{n\times n}$
- Newton's method: Correction $\mathbf{d} : J\mathbf{d} + \mathbf{r} \approx \mathbf{0}$
  - $x^* : \mathbf{r}(x^*) = \mathbf{0}$, J^* full rank $\Longrightarrow$ quadratic convergence if start sufficiently close

Degrees of freedom

- Spherical parametrization, normalization $\Longrightarrow n = 2N - 3$ variables
- $m = \dim(\mathbb{P}_t) - 1 = (t+1)^2 - 1$ equations
- Threshold $n \geq m \Longrightarrow$

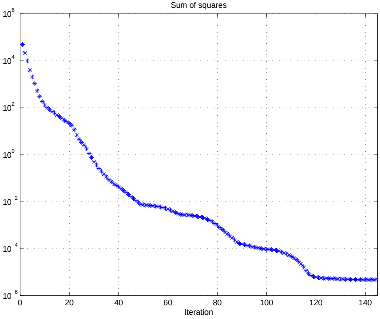
$$N \geq N_1(t) := \left\lceil (t+1)^2)/2 \right\rceil + 1$$

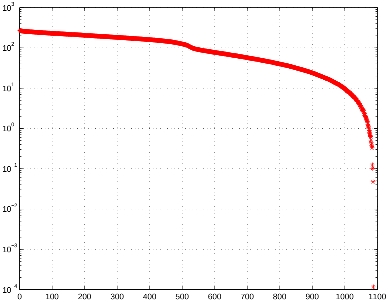
- Sum of squares for $t = 19$, varying N ($N_1(19) = 201$)



Example: $t = 32$, $N = N_1(32) = 546$

- $m = 1088$, $n = 1089$, under-determined
- Iterations: $f \to 4.8 \times 10^{-6}$, $\sigma_m = 1.16 \times 10^{-4}$, $\kappa = 2.3 \times 10^{6}$

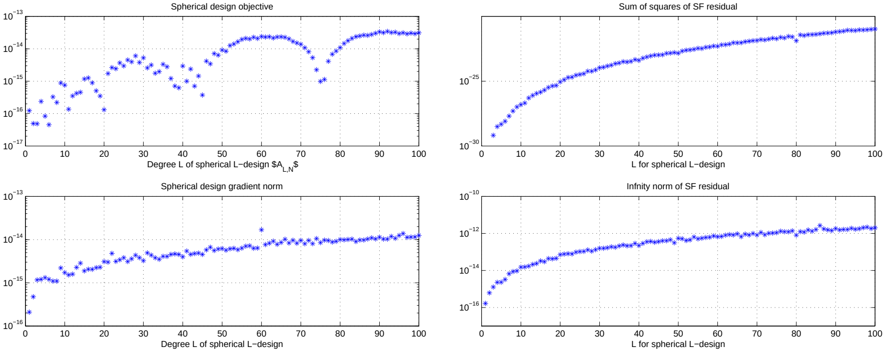




- Local minimum, but close to zero
- Jacobian at solution nearly singular
- Other starting points give a global minimizer with $f = 0$

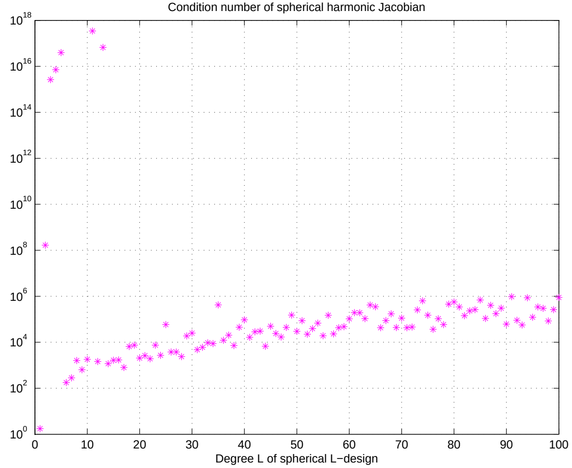
Spherical designs - numerical results

- Aim: Use $N = N_1(t)$, $\Longrightarrow n = m, t$ odd, $\quad n = m+1, t$ even
- Rounding error limits achievable accuracy in $A_{t,N}$
- Both $A_{t,N,\psi}(\mathcal{X}_N)$, $\mathbf{r}^T\mathbf{r}$ order of rounding error $\Longrightarrow$ what confidence?
- $t = 100 \Longrightarrow N_1(t) = 5102$, $m = 10200$, $n = 10201$



Condition numbers

- Condition numbers of Jacobian $J(\hat{x})$



Mesh norm and Separation

- Mesh norm (covering radius)

$$h_{\mathcal{X}_N} = \max_{\mathbf{x}\in\mathbb{S}^2} \min_{j=1,\dots,N} \text{dist}\left(\mathbf{x}, \mathbf{x}_j\right) \geq \frac{c_{\text{cov}}}{\sqrt{N}}$$

  - Stationary point of $A_{t,N,\psi}(\mathcal{X}_N)$ with $h_X < 1/(t+1)$ $\Longrightarrow A_{t,N,\psi}(\mathcal{X}_N) = 0$
  - But $h_X < 1/(t+1) \Longrightarrow N > c(t+1)^2$ where $c > 4$
  - Yudin [19] Mesh norm h given by largest zero $z_t = \cos(h)$ of $P^{(1,0)}(z)$
  - Reimer [15] extended to any positive weight cubature rule with degree of precision t

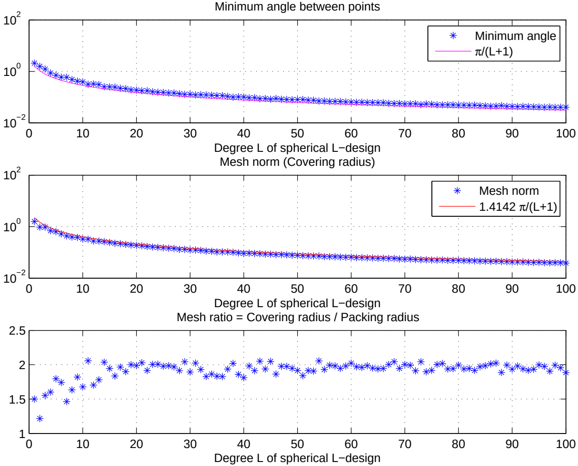
- Separation (twice packing radius)

$$\delta_{\mathcal{X}_N} = \min_{i\neq j} \text{dist}\left((,\mathbf{x})_i, \mathbf{x}_j\right) \leq \frac{c_{\text{pack}}}{\sqrt{N}}$$

  - Union of two spherical t-designs is a spherical t-design
  - $\mathcal{X}_N \cup Q\mathcal{X}_N$ is $2N$ point spherical t-design with arbitrary separation

Mesh ratio

$$\text{Mesh ratio } \rho_{\mathcal{X}_N} = \frac{2h_{\mathcal{X}_N}}{\delta_{\mathcal{X}_N}} = \frac{\text{Covering radius}}{\text{Packing radius}} \geq 1$$



Symmetric designs

- N even, $\mathbf{x} \in \mathcal{X}_N \iff -\mathbf{x} \in \mathcal{X}_N$
- Equal weights, ℓ odd $\implies Y_{\ell,k}$ integrated exactly
- Constraints from even degrees $\leq t$, t odd

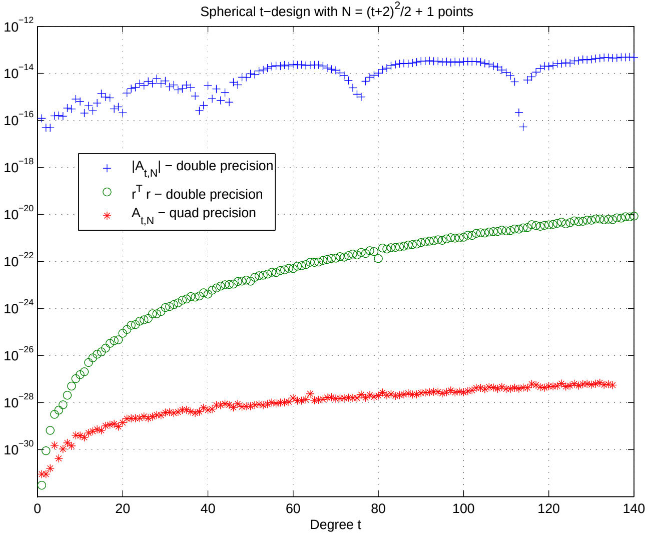
$$m = \sum_{k=1}^{(t-1)/2} 2(2k) + 1 = \frac{(t-1)(t+2)}{2}$$

- $N = 2K$ points $\implies 2K - 3 = N - 3$ degrees of freedom
- Degrees of freedom $\geq$ number of equations $\implies$

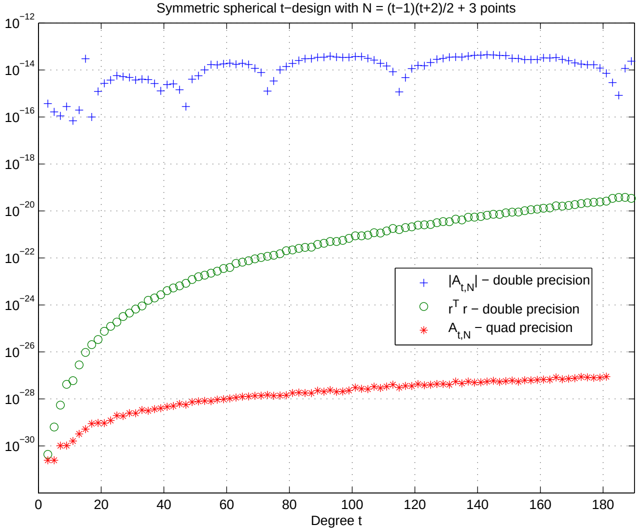
$$N \geq N_2(t) := 2\left\lceil \frac{(t-1)(t+2)+6}{4} \right\rceil \geq \frac{(t-1)(t+2)}{2} + 3$$

- Slightly less than $N_1(t)$
- Roughly half storage for Jacobian and time

Extended precision – Spherical designs

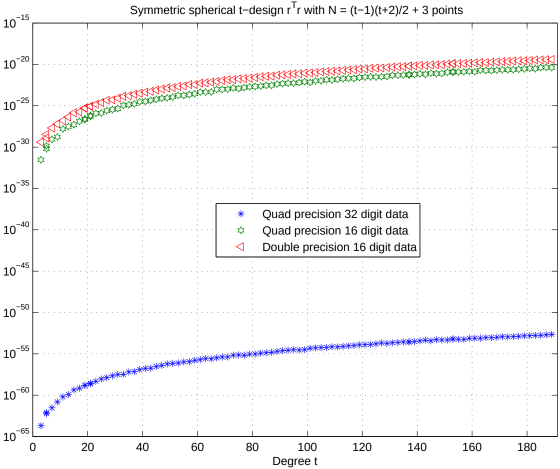


Extended precision – Symmetric spherical designs



Extended precision – Refinement

- Refine with Gauss-Newton steps in Quad precision
- Store as 16 digit or 32 digit files



Well-conditioned spherical designs

- When N is larger, eg $N > N_1(t)$, $\quad N \geq (t+1)^2$
- Use degrees of freedom to optimize other criteria
- Optimization problem

$$\max_{\mathcal{X}_N \subset \mathbb{S}^2} \prod_{j=1}^{\min(N,(t+1)^2)} \sigma_j(\mathbf{Y}_t(\mathcal{X}_N))$$

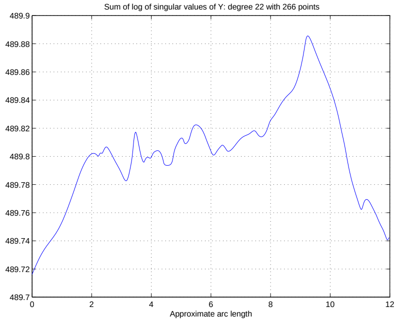
$$\text{Subject to} \quad \mathbf{r}(\mathcal{X}_N) = \mathbf{0}$$

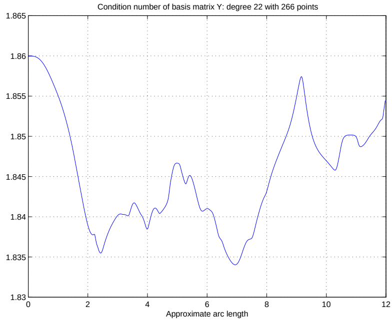
  - Spherical harmonic basis matrix $\mathbf{Y}_t = \begin{bmatrix} \frac{1}{4\pi}\mathbf{e}^T \\ \mathbf{Y} \end{bmatrix}, \quad (t+1)^2$ by N
  - Singular values

$$\sum_{j=1}^{\min(N,(t+1)^2)} \sigma_j^2(\mathbf{Y}_t(\mathcal{X}_N)) = \frac{N(t+1)^2}{4\pi}.$$

Example with one degree of freedom

- Degree $t = 22 \Longrightarrow m = 528$ equations
- Number of points $N = 266 \Longrightarrow n = 529$ variables
- One degree of freedom
- Continuation to follow spherical design constraint





Worst case error

Cubature rule: nodes $\mathcal{X}_N = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$, weights $w_1, \dots, w_N$

$$Q_N(f) := \sum_{j=1}^{N} w_j f(\mathbf{x}_j)$$

Approximate integral

$$I(f) := \int_{\mathbb{S}^d} f(\mathbf{x}) d\omega(\mathbf{x})$$

Sobolev space $\mathbb{H}^s = \mathbb{H}^s(\mathbb{S}^d)$ of functions, norm $\|f\|_{\mathbb{H}^s}$, $s > d/2$
Worst case cubature error

$$\mathsf{wce}(Q_N, \mathbb{H}^s) := \sup_{\|f\|_{\mathbb{H}^s} \leq 1} |I(f) - Q_N(f)|$$

Positive weight rule with degree of precision t

$$c(d,s)\ N^{-s/d} \leq \mathsf{wce}(Q_N, \mathbb{H}^s) \leq C(d,s)\ t^{-s}$$

Same order if $N = O(t^d)$

Approximate spherical designs

Sequence of $N = N(t)$ point configurations.
As $t \to \infty$

$$\sup_{\|f\|_{\mathbb{H}^s} \le 1} \left| I(f) - \frac{|\mathbb{S}^d|}{N} \sum_{j=1}^{N} f(\mathbf{x}_j) \right| = O\left(\frac{1}{t^s}\right)$$

Key: For $s > d/2$ Sobolev space $\mathbb{H}^s_{\mathbf{a}}$ with reproducing kernel

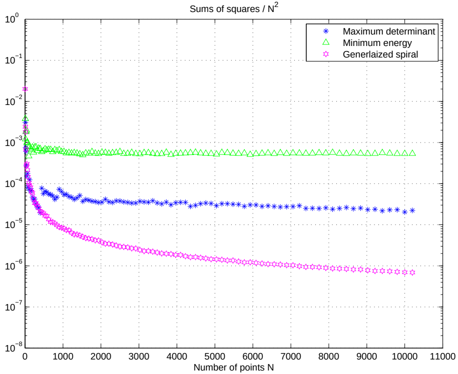
$$K(\mathbf{a}; \mathbf{x}, \mathbf{y}) = \sum_{\ell=1}^{\infty} a_\ell^{(s)} Z(d,\ell) P_\ell^{(d)}(\mathbf{x} \cdot \mathbf{y})$$

- $a_\ell^{(s)}$ define inner product in $\mathbb{H}^s_{\mathbf{a}}$
- For $d \ge 2$

Approximate spherical designs

$$\frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} K_t(\mathbf{a}, \mathbf{x}_i, \mathbf{x}_j) - a_0^{(s)} = O\left(t^{-2s}\right)$$

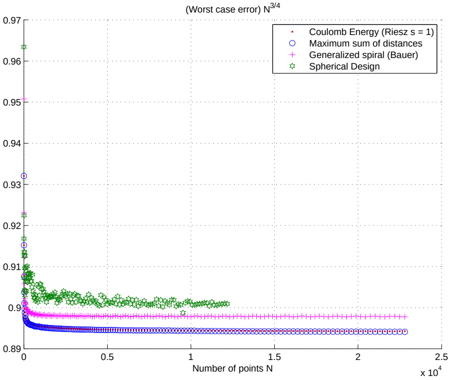
Spherical design functions



Worst case error for $s = 3/2$

For $d = 2$, $s = (d+1)/2 = 3/2$: choose $\mathbf{a}^{(s)}$ to get

- Cui and Freeden generalized discrepancy
- Sums of distances.



Conclusions

- Good points: $\mathbb{S}^2$
  - Numerical spherical t-designs for $t = 1, \ldots, 140$
  - Equal weight cubature rule, degree of precision t with $N = (t+1)^2/2 + O(1)$ points
  - Symmetric equal weight cubature rule, degree of precision t with $N = (t-1)(t+2)/2 + O(1)$ points for $t = 1, \ldots, 181$
  - Good geometric properties: mesh norm, separation
  - Larger N: Use degrees of freedom to satisfy other criteria
  - Approximate designs: more flexibility
- Issues
  - Rounding errors in evaluating criteria, speed of extended precision
  - Convergence difficulties with close to singular Jacobians
  - No proof of nearby exact spherical designs when $N < (t+1)^2$
  - No proof of existence for all t
  - There exist t-designs with $N < N_1(t)$; special symmetries
  - Calculation by optimization for each t, N
  - Point sets $\mathcal{X}_N$ not nested

Selected references

C. An, X. Chen, I. H. Sloan, and R. S. Womersley, *Well-conditioned spherical designs for integration and interpolation on the two-sphere*, SIAM Journal on Numerical Analysis, (2010), pp. 2135–2157.

B. Bajnok, *Construction of designs on the 2-sphere*, Europ. J. Combinatorics, 12 (1991), pp. 377–382.

E. Bannai and E. Bannai, *A survey on spherical designs and algebraic combinatorics on spheres*, Europ. J. Combinatorics, 30 (2009), pp. 1392–1425.

E. Bannai and R. M. Damerell, *Tight spherical design I*, Math. Soc. Japan, 31 (1979), pp. 199–207.

——, *Tight spherical design II*, J. London Math. Soc., 21 (1980), pp. 13–30.

A. Bondarekno, D. Radchenko, and M. Viazovska, *Optimal asymptotic bounds for spherical designs*, tech. report, arXiv:1009.4407 [math.MG], 2010.

X. Chen, A. Frommer, and B. Lang, *Computational existence proofs for spherical t-deisgins*, tech. report, Department of Applied Mathematics, Hong Kong Polytechnic University, 2009.

X. Chen and R. S. Womersley, *Existence of solutions to systms of underdetermined equations and sspherical designs*, SIAM Journal of Numerical

W. Gautschi, *Orthogonal polynomials: Computation and approximation*, Oxford University Press, Oxford, New York, 2004.

P. J. Grabner and R. F. Tichy, *Spherical designs, discrepancy and numerical integration*, Mathematics of Computation, 60 (1993), pp. 327–336.

R. H. Hardin and N. J. A. Sloane, *McLaren's improved Snub cube and other new spherical designs in three dimesnions*, Discrete and Computational Geometry, 15 (1996), pp. 429–441.

J. Korevaar and J. L. H. Meyers, *Spherical Faraday cage for the case of equal point charges and Chebyshev-type quadrature on the sphere*, Integral Transforms and Special Functions, 1 (1993), pp. 105–117.

M. Reimer, *Multivariate Polynomial Approximation*, vol. 144 of International Series of Numerical Mathematics, Birkhäuser Verlag, Basel, 2003.

P. D. Seymour and T. Zaslavsky, *Averaging sets: A generalization of mean values and spherical designs*, Adv. Math., 52 (1984), pp. 213–240.

I. H. Sloan and R. S. Womersley, *Extremal systems of points and numerical integration on the sphere*, Adv. Comp. Math., 21 (2004), pp. 107–125.

——, *A variational characterisation of spherical*