Minimizing the Condition Number of a Gram Matrix on the Sphere

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Joint work with

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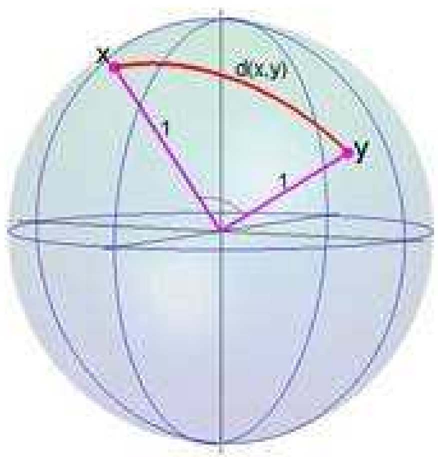
Least squares approximation on the sphere

$\mathbb{S}^2 = \{\mathbf{z} \in R^3 \ : \ \|\mathbf{z}\|_2 = 1\,\}$,   Area $|\mathbb{S}^2| = 4\pi$



$\mathbb{P}_t$: the linear space of restrictions of polynomials of degree $\leq t$ in 3 variables to $\mathbb{S}^2$.

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

Gram matrix

$\mathbb{P}_t$ can be spanned by an orthonormal set of real spherical harmonics with degree ℓ and order k,

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

Let $X_N = \{\mathbf{z}_1, \ldots, \mathbf{z}_N\} \subset S^2$ be a set of N-points on the sphere.
The Gram matrix is defined as

$$G_t(X_N) = Y(X_N)^T Y(X_N),$$

where $Y(X_N) \in R^{(t+1)^2 \times N}$ and the j-th column of $Y(X_N)$ is given by

$$Y_{\ell k}(\mathbf{z}_j), \qquad k = 1, \ldots, 2\ell + 1, \quad \ell = 0, 1, \ldots, t.$$

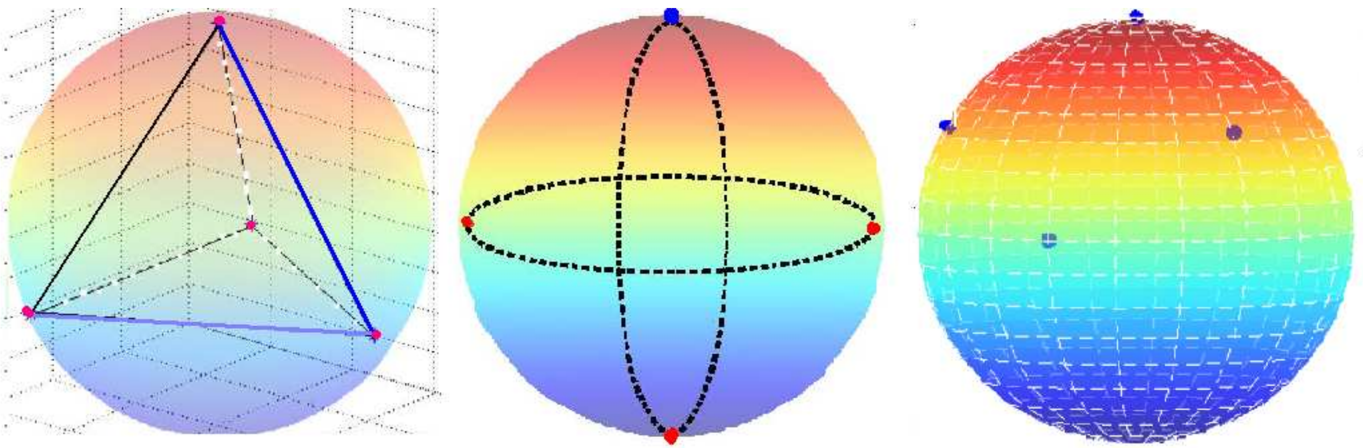
The Gram matrix G_t is a function of a set of N-points X_N.

Distribution of points on the sphere

$t = 1$,   dim$P_1 = 4$, $X_N = \{\mathbf{z}_1, \ldots, \mathbf{z}_4\} \subset S^2$,

$$G_1(X_N) \in R^{4\times 4}$$

$\det(G_1(X_N)) = \frac{1}{\pi^4}$	$\det(G_1(X_N)) = 0$	$\det(G(X_N)) = 0$



Regular tetrahedron: $G_1(X_N) = \frac{1}{\pi} I_4$,   cond$(G_1(X_N)) = 1$.

Four sets of points on the sphere

minimimum energy system $\qquad \operatorname{argmin} \sum_{i \neq j}^{N} \frac{1}{\|\mathbf{z}_i - \mathbf{z}_j\|}$

extremal system $\qquad \operatorname{argmax} \det(G_t(X_N))$

spherical design $\qquad \int_{\mathbb{S}^2} p(\mathbf{z}) d\mathbf{z} = \frac{4\pi}{N} \sum_{i=1}^{N} p(\mathbf{z}_i), \quad \forall p \in \mathbb{P}_t$

minimum cond points $\qquad$ optimal solution of problem:

$$\min \frac{\lambda_{\max}(G_t(X_N))}{\lambda_{\min}(G_t(X_N))}$$

Spherical t-Design

Definition 1 (Delsarte-Goethals-Seidel 1977)
A spherical t-design is a set of N points $X_N = \{\mathbf{z}_1, \ldots, \mathbf{z}_4\} \subset S^2$ such that

$$\frac{1}{4\pi} \int_{S^2} p(\mathbf{z}) d\mathbf{z} = \frac{1}{N} \sum_{i=1}^{N} p(\mathbf{z}_i)$$

for every polynomial $p \in \mathtt{P}_t$.

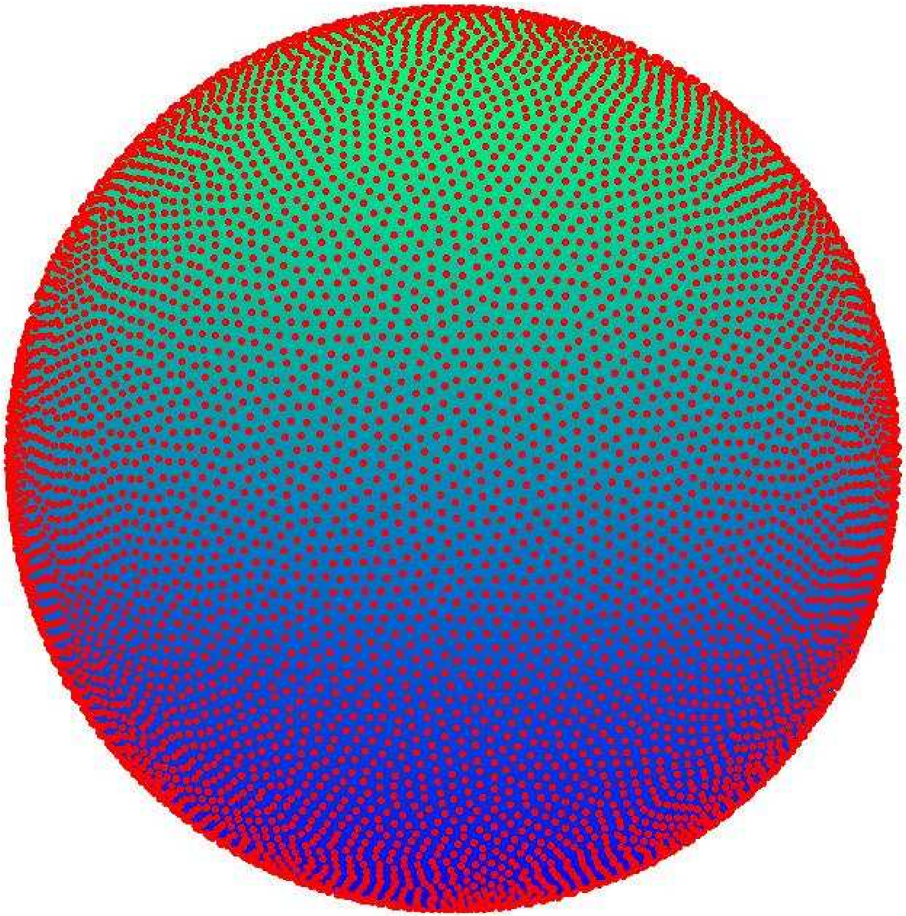
- The average value of $p \in \mathtt{P}_t$ on the whole sphere equals the average value of p on the set.
- The equally weighted cubature rule is exact for all $p \in \mathtt{P}_t$.

No answer to what is the number of points needed to construct a spherical t-design for any $t \geq 1$ **?** Whether $N = O(t^2)$ as $t \to \infty$ **?**

Can we guarantee the existence of spherical t-designs with $(t+1)^2$ points and well-conditioned Gram matrices **?**

Spherical 100-design

Chen-Frommer-Lang, to appear in Numer. Math.



Reformulation I: Parametrization

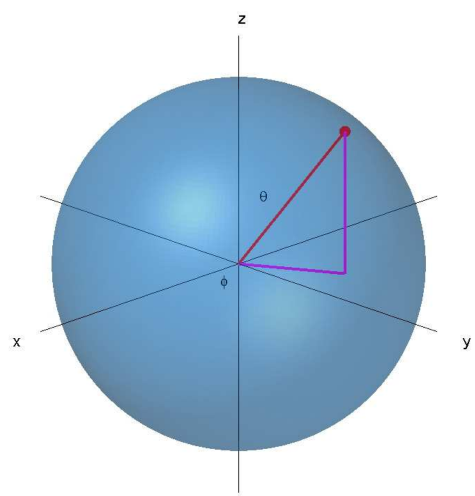
$$N = (t+1)^2, \quad m = 2N - 3, \quad X_N = \{\mathbf{z}_1, \dots, \mathbf{z}_4\} \subset S^2.$$

Represent $\mathbf{z}_i \in X_N \subset S^2$ using polar coordinates with angles θ_i, ϕ_i.

$$\mathbf{z}_i = [\sin(\theta_i)\cos(\phi_i), \quad \sin(\theta_i)\sin(\phi_i), \quad \cos(\theta_i)]^T, \quad \theta_1 = 0, \phi_1 = \phi_2 = 0$$

Fix $\mathbf{z}_1$ on the north pole and $\mathbf{z}_2$ on the zero meridian.

$x_\theta = [\theta_2, \dots, \theta_N]^T, \quad x_\phi = [\phi_3, \dots, \phi_N]^T, x = [x_\theta^T, x_\phi^T]^T \in R^m$



Reformulation II, Gram matrix

Define the Legendre polynomials by the recurrence

$p_0(u) = 1$
$p_1(u) = z$
$\ell p_\ell(z) = (2\ell - 1) u p_{\ell-1}(u) - (\ell - 1) p_{\ell-2}(u)$

for $\ell = 2, \ldots, t, \quad u \in [-1, 1]$.

Define the Jacobi polynomials

$$J_t(u) = \sum_{\ell=0}^{t} (2\ell + 1) p_\ell(u)$$

Define the Gram matrix $G(x) \in R^{N \times N}$

$$G_{i,j}(X_N(x)) = J_t(\mathbf{z}_i(x)^T \mathbf{z}_j(x))$$

Euclidean condition number

$V \in R^{\ell \times n}$ with $\ell \geq n$, and rank$(V) = n$. Let $A = V^T V$

The Euclidean condition number of V is defined by

$$\kappa(V) = \max_{y \neq 0} \frac{\|y\|}{\|Vy\|} \max_{z \neq 0} \frac{\|Vz\|}{\|z\|} = \|V\| \|V^\dagger\| = \sqrt{\kappa(A)} = \frac{\sqrt{\lambda_1(A)}}{\sqrt{\lambda_n(A)}},$$

$V^\dagger = (V^T V)^{-1} V^T$ is the Moore-Penrose generalized inverse of V.

Suppose each entry of $V(x)$ is a continuously differentiable function of $x \in R^m$. Let $A(x) = V(x)^T V(x)$.

We consider

$$\begin{array}{ll} \text{minimize} & \kappa(A(x)) \\ \text{subject to} & x \in \mathcal{X}, \end{array} \qquad (1)$$

where $\mathcal{X}$ is a convex set in R^m.

A small Vandermonde-like matrix

$$V(x) = \begin{pmatrix} 1 & -x \\ 1 & 0 \\ 1 & x \end{pmatrix}, \quad A(x) = V(x)^T V(x) = \begin{pmatrix} 3 & 0 \\ 0 & 2x^2 \end{pmatrix}$$

$$f(x) = \frac{\lambda_1(A(x))}{\lambda_n(A(x))} = \begin{cases} \dfrac{3}{2x^2}, & 0.5 \le x \le \sqrt{1.5} \\ \dfrac{2x^2}{3}, & \sqrt{1.5} \le x \le 1.5. \end{cases}$$

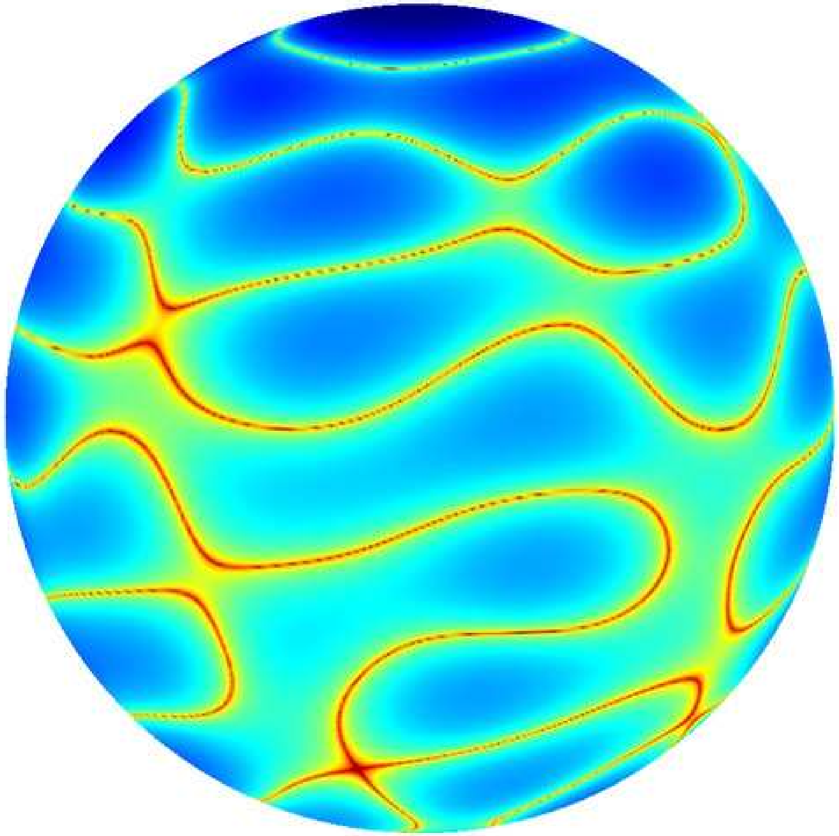
We consider

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & x \in [0.5, 1.5]. \end{array}$$

$x^* = \sqrt{1.5}$ is the minimizer. The Clarke generalized gradient at x^* is

$$\partial f(x^*) = \operatorname{conv}\left\{ -2\sqrt{\frac{2}{3}}, \quad 2\sqrt{\frac{2}{3}} \right\} = 2\sqrt{\frac{2}{3}}[-1, 1].$$

An example on the sphere



The condition number for degree $t = 9$, $N = 100$ extremal points. The plot is of the condition number of the Gram matrix G when the point at the north pole is moved to locations over the whole sphere.

Least squares approximation on $[-1,1]$

Let $\{p_j,\ j=0,\ldots,n-1\}$ be a basis for $\mathbb{P}_{n-1}[-1,1]$, the linear space of polynomials of degree $\leq n-1$.
For given ℓ distinct real numbers

$$-1 \leq a_1 < a_2 < \ldots < a_\ell \leq 1$$

we consider the weighted Vandermonde-like matrix

$$V(w,a) = \begin{pmatrix} w_1 p_0(a_1) & w_1 p_1(a_1) & w_1 p_2(a_1) & \ldots & w_1 p_{n-1}(a_1) \\ w_2 p_0(a_2) & w_2 p_1(a_2) & w_2 p_2(a_2) & \ldots & w_2 p_{n-1}(a_2) \\ \vdots & \vdots & \vdots & & \vdots \\ w_\ell p_0(a_\ell) & w_\ell p_1(a_\ell) & w_\ell p_2(a_\ell) & \ldots & w_\ell p_{n-1}(a_\ell) \end{pmatrix}.$$

$$w = (w_1,\ldots,w_\ell)^T \quad \text{and} \quad a = (a_1,\ldots,a_\ell)^T.$$

Generalized gradient

Let $d(x)$ be the multiplicity of $\lambda_1(A(x))$, and $b(x)$ be the multiplicity of $\lambda_n(A(x))$. Let $A(x)$ admit an eigenvalue decomposition

$$A(x) = U(x)\mathrm{diag}(\lambda(A(x)))U(x)^T$$

with $U(x)^T U(x) = I$. Denote

$$U_\alpha = (u_1(x), \ldots, u_{d(x)}(x)), \quad \text{and} \quad U_\beta = (u_{n-b(x)+1}(x), \ldots, u_n(x)).$$

Suppose that rank$(V(x)) = n$. Then f is Clarke regular and the Clarke generalized gradient $\partial f(x)$ is

$$\{g \in R^m : g_k = \frac{1}{\lambda_n(A(x))}\langle U_\alpha^T A_k(x) U_\alpha, P_\alpha\rangle - \frac{\kappa(A(x))}{\lambda_n(A(x))}\langle U_\beta^T A_k(x) U_\beta, P_\beta\rangle$$

$$k = 1, \ldots, m$$

$$\text{where } P_\alpha \in D^+_{d(x)}, \mathrm{tr}(P_\alpha) = 1, P_\beta \in D^+_{b(x)}, \mathrm{tr}(P_\beta) = 1\}.$$

Some properties

1. $f(x) = \kappa(A(x))$ is strongly semismooth on $\mathcal{X}$.

2. Suppose that $V(x)$ is a linear mapping of x on $\mathcal{X}$. Then $\lambda_1(A(x))$ with $A(x) = V(x)^T V(x)$ is a convex function on $\mathcal{X}$.

3. Let B be a fixed $m \times n$ matrix with $m \geq n$ and rank$(B) = n$. Define

$$h(W) = \kappa(B^T W B), \quad W \in S_m^{++}.$$

Then h is quasi-convex and strongly pseudo-convex.

Example: $V(x) = XB$, where $X \in D_m^{++}$ with diagonal elements $x_i, i = 1, \ldots, m$, $A(V(x)) = B^T X^T X B = B^T W B$.

Smoothing function I

We introduce the smoothing function of the condition number as follows:

$$\tilde{f}(x,\mu) = -\frac{\ln(\sum_{i=1}^{n} e^{\lambda_i(A(x))/\mu})}{\ln(\sum_{i=1}^{n} e^{-\lambda_i(A(x))/\mu})}. \qquad (2)$$

In numerical computations, we use an equivalent formula

$$\tilde{f}(x,\mu) = \frac{\lambda_1(A(x)) + \mu\ln(\sum_{i=1}^{n} e^{(\lambda_i(A(x))-\lambda_1(A(x)))/\mu})}{\lambda_n(A(x)) - \mu\ln(\sum_{i=1}^{n} e^{(\lambda_n(A(x))-\lambda_i(A(x)))/\mu})},$$

which is more numerically stable than (2).

Smoothing function II

(i) $\tilde{f}(\cdot, \mu)$ is continuously differentiable for any fixed $\mu > 0$.

(ii) There exists $c > 0$ such that for any $x \in \mathcal{X}$ and $\mu \leq \dfrac{\lambda_n}{2 \ln n}$

$$0 \leq \tilde{f}(x, \mu) - f(x) \leq c\mu. \tag{3}$$

$$\lim_{x \to \bar{x}, \mu \downarrow 0,} \tilde{f}(x, \mu) = f(\bar{x}).$$

(iii) For any $\bar{x} \in \mathcal{X}$, $\{\lim_{x \to \bar{x},\ \mu \downarrow 0} \nabla_x \tilde{f}(x, \mu)\}$ is nonempty and bounded.

$$\{\lim_{x \to \bar{x}, \mu \downarrow 0,} \nabla_x \tilde{f}(x, \mu)\} \subset \partial f(\bar{x}).$$

(iv) For any fixed $\mu > 0$, there exists a constant L_μ such that

$$\|\nabla \tilde{f}(x, \mu) - \nabla \tilde{f}(y, \mu)\| \leq L_\mu \|x - y\|. \tag{4}$$

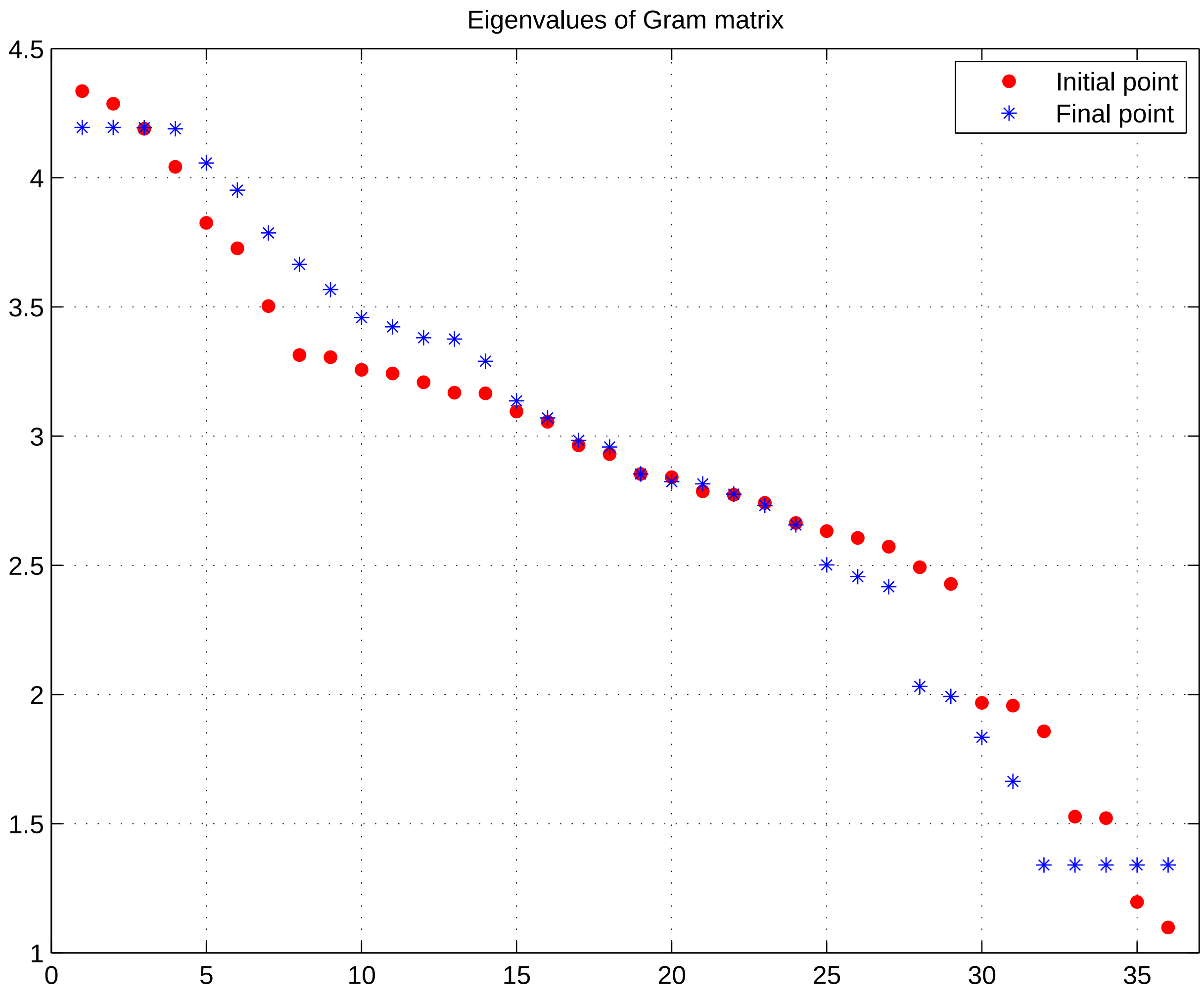
Convergence

Theorem From any staring point $x^0 \in \mathcal{X}$, the sequence $\{x^k\}$ generated by the SPG method is contained in $\mathcal{X}$ and any accumulation point $\bar{x}$ of $\{x^k\}$ is a Clarke stationary point, that is, there is $g \in \partial f(\bar{x})$ such that

$$\langle g, x - \bar{x} \rangle \geq 0, \quad \forall x \in \mathcal{X}.$$

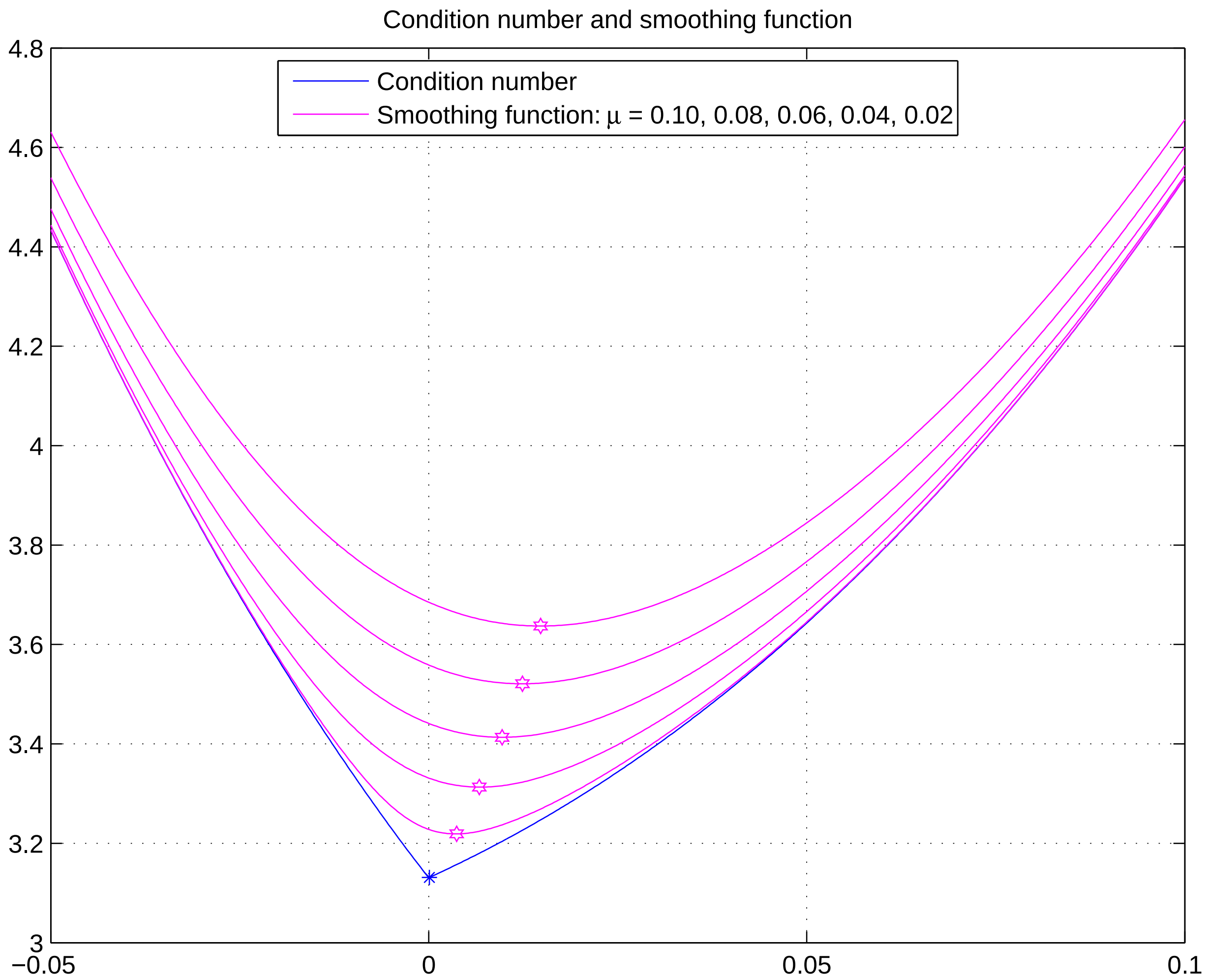
Corollary If the function $f(x)$ is pseudoconvex in a neighborhood $B(\bar{x}) \subset \mathcal{X}$, then the accumulation point is a local optimal solution and if the function $f(x)$ is pseudoconvex on $\mathcal{X}$, then the accumulation point is a global optimal solution over $\mathcal{X}$.

Eigenvalues of a Gram matrix on the sphere



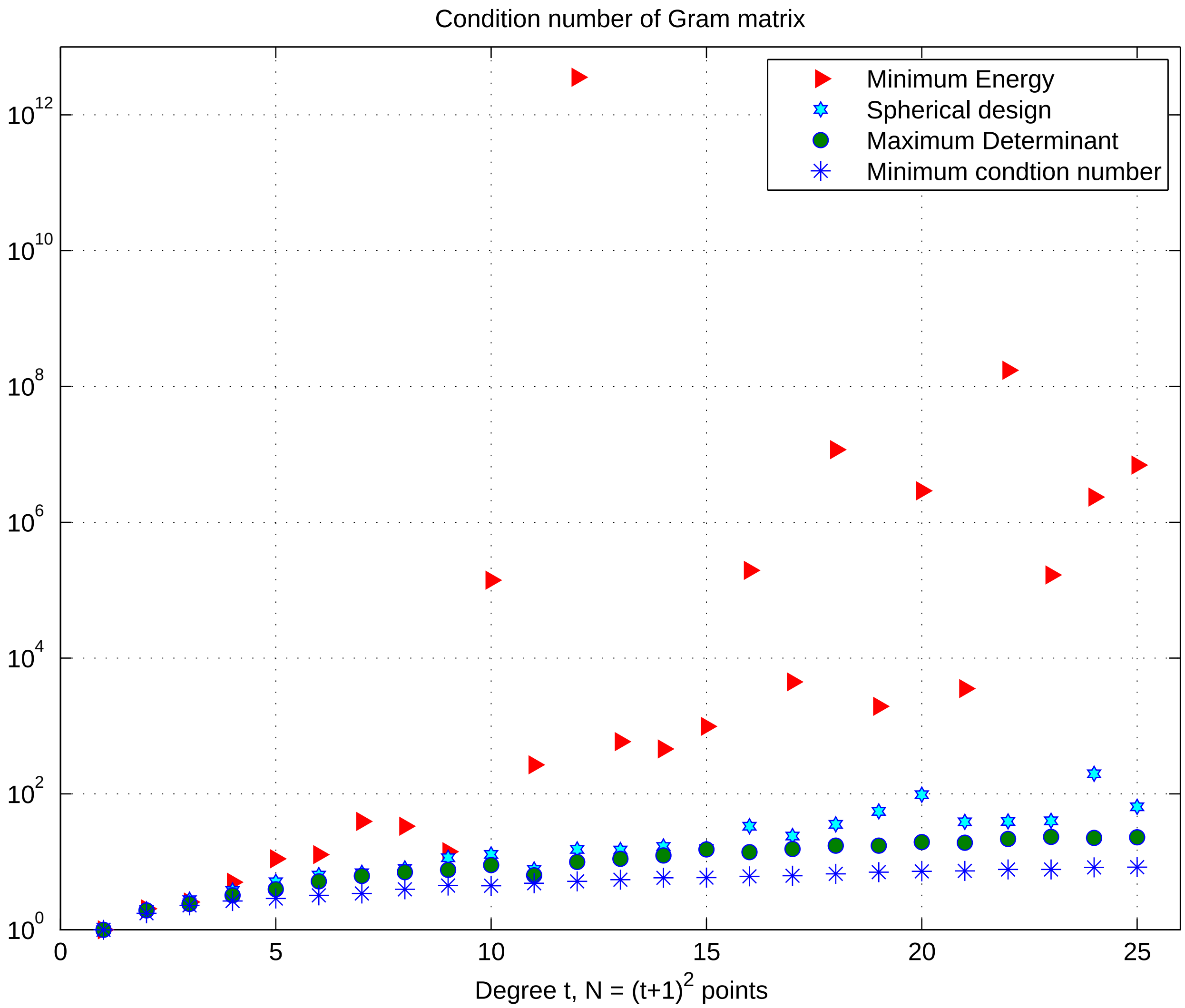
The eigenvalues of 36×36 Gram matrix for degree 5, with 36 points on the sphere.

Smoothing function



For the same Gram matrix, $f(x^* + \alpha \nabla_x \tilde{f}(x^*, 0.0766))$, $\alpha \in [-0.05, 0.1]$.

Condition number on the four sets of points



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2. X. Chen, A. Frommer and B. Lang, Computational existence proofs for spherical t-designs, to appear in Numer. Math.

$$\mathtt{www.math.uni-wuppertal.de/SciComp/SphericalTDesigns}$$

3. C. An, X. Chen, I.H. Sloan and R.S. Womersley, Well-conditioned spherical designs on 2-sphere, to appear in SIAM J. Numer. Anal.
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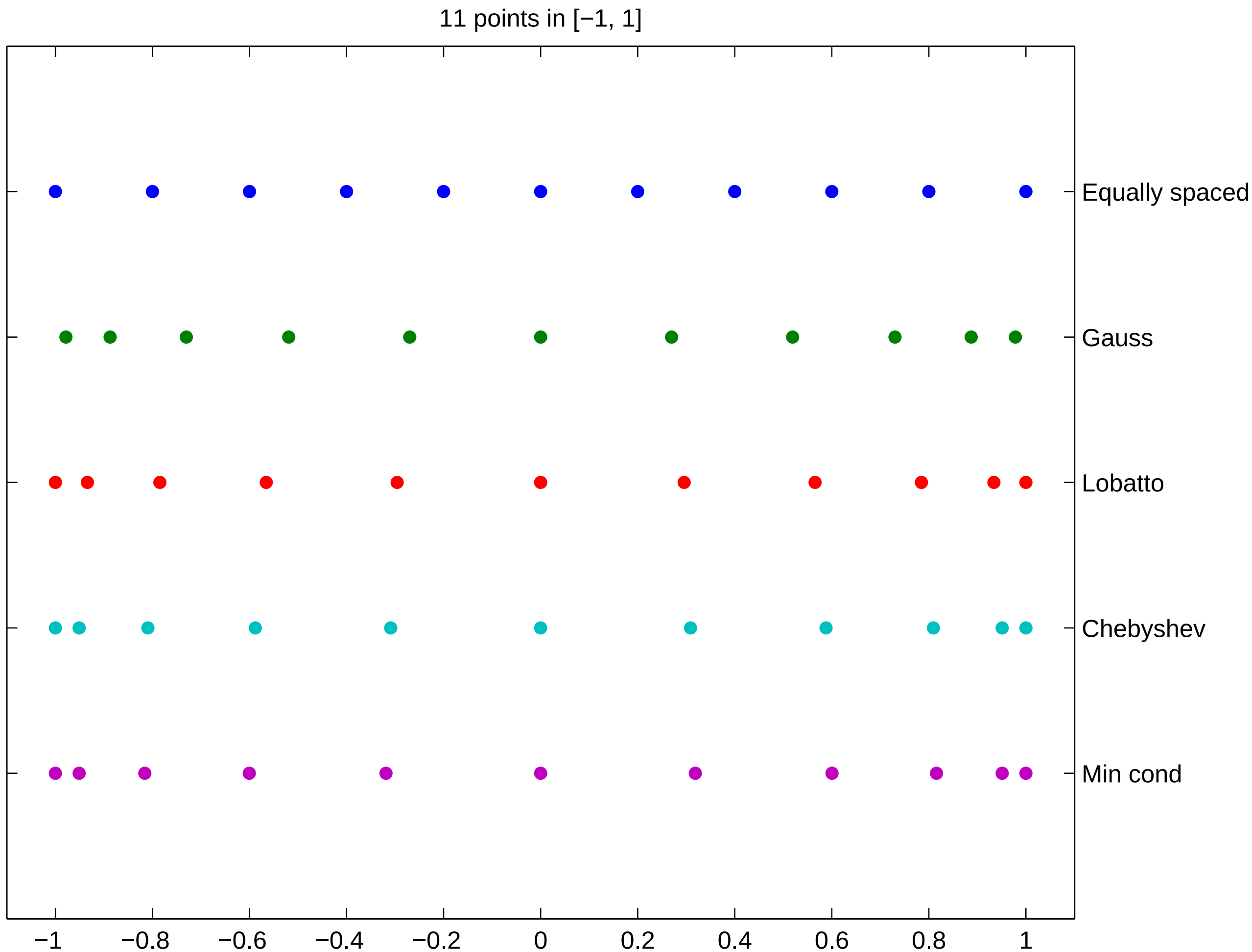
Thank you very much

Five sets of points in the interval $[-1, 1]$

equally spaced points	$a_i = -1 + \frac{2(i-1)}{\ell - 1}, \quad i = 1, \ldots, \ell.$
Gauss points	$\int_{-1}^{1} p(\tau) d\tau = \sum_{i=0}^{n-1} \alpha_i p(a_i), \quad \forall p \in \mathbb{P}_{2n}$
Gauss Lobatto points	$a = \operatorname{argmax} \det(V(x)^T V(x)).$
Chebyshev points	$a_i = \cos \frac{\pi(2i-1)}{2\ell}, \quad i = 1, \ldots, \ell.$
minimum cond points	$a =$ optimal solution of (1) .

Here $\alpha_i, i = 0, \ldots, n-1$ are the integral values of the Lagrange interpolation polynomials on $[-1, 1]$.

Distribution of points



condition number and determinant

	condition number	determinant
equally spaced points	1.946479e+008	5.755277e-022
Gauss points	1.767123e+007	4.616572e-020
Lobatto points	9.606328e+006	7.968101e-019
Chebyshev points	8.307060e+006	6.310887e-019
min cond points	8.176691e+006	5.826573e-019

Values of the condition number and determinant at equally spaced points, Gauss Points, Gauss Lobatto points, Chebyshev points and minimum cond points