

MINIMIZING THE CONDITION NUMBER OF A GRAM MATRIX

XIAOJUN CHEN*, ROBERT S. WOMERSLEY†, AND JANE J. YE‡

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Abstract. The condition number of a Gram matrix defined by a polynomial basis and a set of points is often used to measure the sensitivity of the least squares polynomial approximation. Given a polynomial basis, we consider the problem of finding a set of points and/or weights which minimizes the condition number of the Gram matrix. The objective function f in the minimization problem is nonconvex and nonsmooth. We present an expression of the Clarke generalized gradient of f and show that f is Clarke regular and strongly semismooth. Moreover, we develop a globally convergent smoothing method to solve the minimization problem by using the exponential smoothing function. To illustrate applications of minimizing the condition number, we report numerical results for the Gram matrix defined by the weighted Vandermonde-like matrix for least squares approximation on an interval, and the Gram matrix defined by an orthonormal set of real spherical harmonics for least squares approximation on the sphere.

Key words: Condition number, Gram matrix, least squares, interpolation, smoothing method, generalized gradient, semi-smooth, spherical harmonics.

1. Introduction. We denote by S_n the space of symmetric $n \times n$ matrices with the standard inner products

$$\langle A, B \rangle = \sum_{i,j=1}^n a_{ij}b_{ij}, \quad \forall A = (a_{ij}), B = (b_{ij}) \in S_n.$$

We denote by S_n^+ and S_n^{++} , the cone of symmetric positive semidefinite $n \times n$ matrices and the cone of symmetric positive definite $n \times n$ matrices, respectively.

For $A \in S_n$, we denote by $\lambda(A) \in R^n$ the vector of its eigenvalues ordered in a decreasing order:

$$\lambda_1(A) \geq \dots \geq \lambda_n(A).$$

The Euclidean condition number of a nonzero matrix $A \in S_n^+$ is defined by [16]

$$\kappa(A) = \begin{cases} \frac{\lambda_1(A)}{\lambda_n(A)} & \text{if } A \text{ is nonsingular} \\ \infty & \text{if } A \text{ is singular.} \end{cases}$$

*Department of Applied Mathematics, The Hong Kong Polytechnic University, Kowloon, Hong Kong. Email: maxjchen@polyu.edu.hk. The research of this author is partially supported by the Hong Kong Research Grants Council (PolyU5003/08P).

†School of Mathematics and Statistics, University of New South Wales, Sydney, NSW, 2052, Australia (r.womersley@unsw.edu.au)

‡Department of Mathematics and Statistics, University of Victoria, P.O. Box 3060, STN CSC, Victoria, BC, V8W 3R4, Canada (janeye@Math.Uvic.CA). The research of this author is partially supported by NSERC.

Optimizing eigenvalue functions have been studied for decades [17, 21, 24, 25, 26, 27]. In a recent paper [18], Maréchal and Ye studied the following optimization problem

$$\begin{aligned} & \text{minimize} && \kappa(A) \\ & \text{subject to} && A \in \Omega, \end{aligned} \tag{1.1}$$

where Ω is a compact convex subset of S_n^+ . From the definition, it is clear that if $\Omega \cap S_n^{++}$ is not empty, then a minimizer for (1.1) must belong to S_n^{++} . However, if $\Omega \cap S_n^{++}$ is empty, then (1.1) has no optimal solution. The optimization problem (1.1) has several applications. See [18], for an example arising from the Markovitz portfolio selection.

In this paper, we are interested in the minimal condition number for matrices in the form $A = V^T V$, where $V \in R^{\ell \times n}$ with $\ell \geq n$, and $\text{rank}(V) = n$. Obviously $A \in S_n^{++}$.

Let $\|\cdot\|$ denote the Euclidean vector norm and matrix norm. The Euclidean condition number of V is defined by [14]

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

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

The quantity $\kappa(V)$ has been widely used in the sensitivity analysis of interpolation and approximation, for example [2, 3], the least squares polynomial approximation on an interval. In many least squares problems, V is a weighted Vandermonde-like matrix with $\text{rank}(V) = n$. Each element of V is defined by the weights and a set of node points. Estimation of upper bounds and lower bounds for $\kappa(V)$ with respect to the matrix size n have been studied extensively. However, there is little work on efficient optimization methods to find optimal weights and nodes which minimize $\kappa(V)$ with a fixed n .

Suppose each entry of $V(x)$ is a continuously differentiable function of $x \in R^m$. Then each entry of $A(x) = V(x)^T V(x)$ is also a continuously differentiable function of x . We consider the following minimization problem

$$\begin{aligned} & \text{minimize} && \kappa(A(x)) \\ & \text{subject to} && x \in \mathcal{X}, \end{aligned} \tag{1.2}$$

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

The objective function $\kappa(A(x))$ in (1.2) is neither convex nor smooth. Problem (1.2) can be considered as a special case of fractional programming [11, 12]. Applying the Dinkelbach method for fractional programming to (1.2), at each iteration, we need to solve a minimization problem

$$\begin{aligned} & \text{minimize} && \lambda_1(A(x)) - \kappa_k \lambda_n(A(x)) \\ & \text{subject to} && x \in \mathcal{X}, \end{aligned} \tag{1.3}$$

where $\kappa_k > 0$ is an approximation of the optimal value of (1.2). If λ_1 and λ_n are linear functions of x , then (1.3) is relatively easy to solve. However, in general, $\lambda_1(A(x))$ and $-\lambda_n(A(x))$ are nonconvex and nonsmooth functions of x . The Dinkelbach method for

(1.2) needs to solve a nonconvex and nonsmooth minimization problem (1.3) at each iteration.

Most optimization methods and softwares are only efficient for convex and smooth problems. To develop efficient algorithms to solve (1.2), we adopt the Clarke generalized gradient [10] and the exponential smoothing function [4, 20, 21]. At each iteration, we use the function value of the smoothing approximation of the objective function in (1.2) and update the smoothing parameter.

In section 2, we present an expression of the Clarke generalized gradient of $\kappa(A(x))$. We show that $\kappa(A(x))$ is Clarke regular and strongly semismooth.

In section 3, we propose a smoothing function for $\kappa(A(x))$ and show various properties of the smoothing function which ensure that a class of smoothing algorithms for solving (1.2) converge to a Clarke stationary point globally.

In section 4, we numerically investigate the condition number $\kappa(A(x))$ of a Gram matrix arising from the least squares polynomial approximation on an interval and on the sphere with x corresponding to a set of node points or weights. We compare the optimal solutions of (1.2) defined by the Vandermonde-like matrix with equally spaced points, Gauss points, Gauss-Lobatto points, Chebyshev points and Clenshaw-Curtis points on the interval $[-1, 1]$. Moreover, we compare the optimal solutions of (1.2) defined by the spherical harmonics with the extremal points, the minimum energy points and the points of spherical t -designs on the unit sphere.

Throughout this paper, we let $e_i \in R^n$ ($i = 1, \dots, n$) denote the i th column of the identity matrix in $R^{n \times n}$ and I_n denote the identity matrix in $R^{n \times n}$. We denote by D_n^+ (D_n^{++}) the set of all $n \times n$ diagonal matrices with nonnegative (positive) diagonal entries. Let

$$R_{++}^n := \{y \in R^n : y_i > 0, i = 1, \dots, n\} \quad \text{and} \quad R_+^n := \{y \in R^n : y_i \geq 0, i = 1, \dots, n\}.$$

2. Generalized gradient of $\kappa(A(x))$. In this section, we present an expression of the Clarke generalized gradient of $\kappa(A(x))$. In order to explain the expression clearly, we divide this section into three subsections. In subsection 2.1, we recall existing expressions for the generalized gradient $\partial\kappa(A)$ and give a new expression for $\partial\kappa(A)$. In subsection 2.2, we present an expression of the generalized gradient for $\kappa(A(V))$ with $A(V) = V^T V$. In subsection 2.3, we give an expression of the generalized gradient for $\kappa(A(x))$ with $A(x) = V(x)^T V(x)$.

2.1. $\kappa(A)$. For $A \in S_n$, the notation $\text{diag}(\lambda(A)) \in S_n$ is used for the diagonal matrix with the vector $\lambda(A) \in R^n$ on the main diagonal.

It is known that any $A \in S_n^+$ admits an eigenvalue decomposition:

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

with a square orthogonal matrix $U(A)$, $U(A)^T U(A) = I_n$, whose columns are eigenvectors of A . Let $u_i(A)$ be the i th column of matrix $U(A)$.

PROPOSITION 2.1 (The Clarke generalized gradient). ([17, 25, 20]) *Let $A \in S_n$. The Clarke generalized gradient of $\lambda_1(A)$ is given by*

$$\partial\lambda_1(A) = \left\{ G = \sum_{i=1}^{d(A)} \tau_i u_i(A) u_i(A)^T : \tau_i \geq 0, \quad i = 1, \dots, d(A), \quad \sum_{i=1}^{d(A)} \tau_i = 1 \right\}$$

where $d(A)$ is the multiplicity of the largest eigenvalue of the matrix A .

The Clarke generalized gradient of $\lambda_n(A)$ is given by

$$\partial\lambda_n(A) = \left\{ H = \sum_{i=1}^{b(A)} \gamma_i u_{n-i+1}(A) u_{n-i+1}(A)^T : \gamma_i \geq 0, \quad i = 1, \dots, b(A), \quad \sum_{i=1}^{b(A)} \gamma_i = 1 \right\}$$

where $b(A)$ is the multiplicity of the smallest eigenvalue of the matrix A .

Using [10, Proposition 2.3.14] for the Clarke generalized gradient of quotients, we have the following proposition for $\kappa(A)$.

PROPOSITION 2.2. ([18, Proposition 4.2]) *Assume that $A \in S_n^{++}$. Then κ is Clarke regular at A and its Clarke generalized gradient at A is given by*

$$\partial\kappa(A) = \lambda_n(A)^{-1}(\partial\lambda_1(A) - \kappa(A)\partial\lambda_n(A)).$$

The following two submatrices of $U(A)$

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

are formed by the orthonormal bases for the eigenspaces corresponding to the largest eigenvalue and the smallest eigenvalue of A .

Applying Propositions 2.1 and 2.2, we have the following formula for $\partial\kappa(A)$.

PROPOSITION 2.3. *For $A \in S_n^{++}$, let $d(A)$ be the multiplicity of the largest eigenvalue of matrix A , and $b(A)$ be the multiplicity of the smallest eigenvalue of matrix A . Then*

$$\begin{aligned} \partial\kappa(A) &= \lambda_n(A)^{-1}(\partial\lambda_1(A) - \kappa(A)\partial\lambda_n(A)) \\ &= \left\{ Y \in R^{n \times n} : Y_{pq} = \frac{1}{\lambda_n(A)} \langle U_\alpha^T(A) e_p e_q^T U_\alpha(A), P_\alpha \rangle - \frac{\kappa(A)}{\lambda_n(A)} \langle U_\beta^T(A) e_p e_q^T U_\beta(A), P_\beta \rangle, \right. \\ &\quad \left. p = 1, \dots, n, q = 1, \dots, n, \text{ where } P_\alpha \in D_{d(A)}^+, \text{tr}(P_\alpha) = 1, P_\beta \in D_{b(A)}^+, \text{tr}(P_\beta) = 1 \right\}. \end{aligned}$$

Proof. By Proposition 2.1, for any $G \in \partial\lambda_1(A)$, there is a $P_\alpha \in D_{d(A)}^+$, with $\text{tr}(P_\alpha) = 1$ such that each element G_{pq} of G can be written as

$$G_{pq} = \langle (e_p^T U_\alpha(A))^T e_q^T U_\alpha(A), P_\alpha \rangle = \langle U_\alpha^T(A) e_p e_q^T U_\alpha(A), P_\alpha \rangle.$$

Similarly, for any $H \in \partial\lambda_n(A)$, there is $P_\beta \in D_{b(A)}^+$, with $\text{tr}(P_\beta) = 1$ such that each element H_{pq} of H can be written as

$$H_{pq} = \langle U_\beta^T(A) e_p e_q^T U_\beta(A), P_\beta \rangle.$$

The desired formula follows from Proposition 2.2. \square

Remark 2.1 In the case where $\lambda_1(A) = \lambda_n(A)$, we have $U = U_\alpha = U_\beta$, and

$$\begin{aligned} \partial\kappa(A) &= \left\{ Y \in R^{n \times n} : Y_{pq} = \frac{1}{\lambda_n(A)} \langle U(A)e_p e_q^T U(A), P_\alpha \rangle - \frac{1}{\lambda_n(A)} \langle U(A)e_p e_q^T U(A), P_\beta \rangle, \right. \\ &\quad \left. p = 1, \dots, n, q = 1, \dots, n, \text{ where } P_\alpha \in D_n^+, \text{tr}(P_\alpha) = 1, P_\beta \in D_n^+, \text{tr}(P_\beta) = 1 \right\} \\ &= \left\{ Y \in R^{n \times n} : Y_{pq} \in \frac{1}{\lambda_n(A)} \max_{1 \leq i \leq n} |U(A)e_p e_q^T U(A)|_{ii} [-1, 1], \right. \\ &\quad \left. p = 1, \dots, n, q = 1, \dots, n \right\}. \end{aligned}$$

Such a matrix A would have the global minimal condition number 1 and it is clear that $0 \in \partial\kappa(A)$.

2.2. $\kappa(A(V))$ with $A(V) = V^T V$. We denote by $M_{\ell, n}$ the space of $\ell \times n$ matrices with the standard inner products

$$\langle V, U \rangle = \sum_{i=1}^{\ell} \sum_{j=1}^n V_{ij} U_{ij}, \quad \forall V, U \in M_{\ell, n}.$$

For $V \in M_{\ell, n}$, let $v_i^T \in R^n$ denote the i -th row of V , $i = 1, \dots, \ell$, that is, $V^T = (v_1, \dots, v_\ell) \in R^{n \times \ell}$.

Now we consider $V \in M_{\ell, n}$ with $\ell \geq n$ and $\text{rank}(V) = n$. Let $A(V) = V^T V$. Denote

$$(\mathcal{A}_{pq}(V)) = \frac{\partial A(V)}{\partial V_{pq}} \in R^{n \times n}, \quad p = 1, \dots, \ell, \quad q = 1, \dots, n.$$

By the definition of V and A , we have

$$\frac{\partial A(V)}{\partial V_{pq}} = \frac{\partial(\sum_{j=1}^{\ell} v_j v_j^T)}{\partial V_{pq}} = \frac{\partial v_p v_p^T}{\partial V_{pq}} = e_q v_p^T + v_p e_q^T.$$

Let $d(V)$ be the multiplicity of the largest eigenvalues of $A(V)$, and $b(V)$ be the multiplicity of the smallest eigenvalue of $A(V)$. Let $A(V)$ admit an eigenvalue decomposition

$$A(V) = U(V) \text{diag}(\lambda(A(V))) U(V)^T$$

with $U(V)^T U(V) = I_n$. Let

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

PROPOSITION 2.4. *Suppose that $\text{rank}(V) = n$. Then $\kappa(A(V))$ is Clarke regular and the Clarke generalized gradient of $\kappa(A(V))$ is*

$$\begin{aligned} \partial\kappa(A(V)) &= \left\{ Y \in R^{\ell \times n} : Y_{pq} = \frac{1}{\lambda_n(A(V))} \langle U_\alpha^T \mathcal{A}_{pq} U_\alpha, P_\alpha \rangle - \frac{\kappa(A(V))}{\lambda_n(A(V))} \langle U_\beta^T \mathcal{A}_{pq} U_\beta, P_\beta \rangle, \right. \\ &\quad \left. p = 1, \dots, \ell, q = 1, \dots, n, \text{ where } P_\alpha \in D_{d(V)}^+, \text{tr}(P_\alpha) = 1, P_\beta \in D_{b(V)}^+, \text{tr}(P_\beta) = 1 \right\}. \end{aligned}$$

Proof. Since $\kappa(A(V))$ is the composition of a Clarke regular function with a strictly differentiable function, by the chain rule, $\kappa(A(V))$ is Clarke regular and

$$\partial\kappa(A(V)) = \{Y \in R^{\ell \times n} : Y_{pq} = \langle G, \mathcal{A}_{pq}(V) \rangle \text{ for some } G \in \partial\kappa(A)\}.$$

The desired result follows immediately from applying Proposition 2.3. \square

2.3. $\kappa(A(x))$ with $A(x) = V(x)^T V(x)$. Let $V(x)$ be an $\ell \times n$ matrix with each entry being a continuously differentiable function of $x \in R^m$. The differentiability of V implies that each entry of $A(x) = V(x)^T V(x) \in R^{n \times n}$ is a continuously differentiable function of x .

Let $\mathcal{X} \subset R^m$ be a nonempty, compact and convex set. It is convenient to define a function $f : \mathcal{X} \rightarrow R$ by

$$f(x) = \kappa(A(x)). \quad (2.1)$$

We assume that for any $x \in \mathcal{X}$, $\text{rank}(V(x)) = n$. We consider (1.2) in the following version

$$\begin{aligned} & \text{minimize} && f(x) \\ & \text{subject to} && x \in \mathcal{X}. \end{aligned} \quad (2.2)$$

Since $\lambda_1(A)$ is a convex function of A and $\lambda_n(A)$ is a concave function of A , $\lambda_1(A)$ and $\lambda_n(A)$ are Lipschitz continuous functions of A . By the continuous differentiability of $A(x)$, $\lambda_1(A(x))$ and $\lambda_n(A(x))$ are Lipschitz continuous functions on \mathcal{X} . Moreover, there are positive constants $\underline{\lambda}_n$ and $\bar{\lambda}_1$, such that

$$\underline{\lambda}_n \leq \lambda_n(A(x)) \quad \text{and} \quad \lambda_1(A(x)) \leq \bar{\lambda}_1 \quad \forall x \in \mathcal{X}.$$

Hence f is Lipschitz continuous and satisfies

$$1 \leq f(x) \leq \frac{\bar{\lambda}_1}{\underline{\lambda}_n}, \quad \forall x \in \mathcal{X}. \quad (2.3)$$

This, together with the continuity of f on \mathcal{X} , ensures the existence of a solution of (2.2).

Denote

$$A_k(x) = \frac{\partial A(x)}{\partial x_k} \in S_n, \quad k = 1, \dots, m.$$

By the definition of \mathcal{A}_{pq} , V and A , we have

$$\begin{aligned} A_k(x) &= \sum_{p=1}^{\ell} \sum_{q=1}^n \frac{\partial A(V)}{\partial V_{pq}} \frac{\partial V_{pq}}{\partial x_k} = \sum_{p=1}^{\ell} \sum_{q=1}^n \mathcal{A}_{pq}(V) \frac{\partial V_{pq}}{\partial x_k} \\ &= \sum_{p=1}^{\ell} \sum_{q=1}^n (e_q v_p^T + v_p e_q^T) \frac{\partial V_{pq}}{\partial x_k} \in S_n. \end{aligned}$$

Let $d(x)$ be the multiplicity of the largest eigenvalues of $A(x)$, and $b(x)$ be the multiplicity of the smallest eigenvalue of $A(x)$. Let $A(x)$ admit an eigenvalue decomposition

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

with $U(x)^T U(x) = I_n$. Let

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

PROPOSITION 2.5. *Suppose that $\text{rank}(V(x)) = n$. Then f is Clarke regular at x and the Clarke generalized gradient of f is*

$$\begin{aligned} \partial f(x) = \{g \in R^m : g_k = \frac{1}{\lambda_n(A(x))} \langle U_\alpha^T A_k(x) U_\alpha, P_\alpha \rangle - \frac{\kappa(A(x))}{\lambda_n(A(x))} \langle U_\beta^T A_k(x) U_\beta, P_\beta \rangle \\ k = 1, \dots, m, \text{ where } P_\alpha \in D_{d(x)}^+, \text{tr}(P_\alpha) = 1, P_\beta \in D_{b(x)}^+, \text{tr}(P_\beta) = 1\}. \end{aligned}$$

The proof is similar to the proof of Proposition 2.4.

DEFINITION 2.6. [19, 24] *Suppose that $\phi : \mathcal{X} \subseteq R^m \rightarrow R$ is a locally Lipschitz continuous function. ϕ is said to be semismooth at $x \in \text{int}\mathcal{X}$ if ϕ is directionally differentiable at x and for any $g \in \partial\phi(x + \Delta x)$,*

$$\phi(x + \Delta x) - \phi(x) - g^T \Delta x = o(\|\Delta x\|),$$

where $\text{int}\mathcal{X}$ denotes the interior of \mathcal{X} . ϕ is said to be strongly semismooth at x if ϕ is semismooth at x and

$$\phi(x + \Delta x) - \phi(x) - g^T \Delta x = O(\|\Delta x\|^2).$$

A function ϕ is said to be a (strongly) semismooth function on \mathcal{X} if it is (strongly) semismooth everywhere in $\text{int}\mathcal{X}$.

PROPOSITION 2.7. *The function f is semismooth on \mathcal{X} . Moreover if $A(x)$ is strongly semismooth then f is strongly semismooth on \mathcal{X}*

Proof. It is shown in [24] that the eigenvalues of a symmetric matrix are strongly semismooth everywhere. It is known that the composition of (strongly) semismooth functions is still a (strongly) semismooth function [13, 19]. Since $A(x)$ is assumed to be continuous differentiable and hence semismooth, so is f . Moreover if $A(x)$ is strongly semismooth then as a composition of two strongly semismooth functions, f is then strongly semismooth on \mathcal{X} . \square

DEFINITION 2.8. ([22]) *$A(x)$ is said to be positive semidefinite convex on \mathcal{X} if it is convex with respect to the order relation imposed by the cone S_+^n . That is the inequality*

$$tA(x) + (1-t)A(y) \succeq A(tx + (1-t)y)$$

holds for any $x, y \in R^m$ and all $t \in [0, 1]$.

PROPOSITION 2.9. *Suppose that $A(x)$ is positive semidefinite convex on \mathcal{X} . Then $\lambda_1(A(x))$ is convex on \mathcal{X} .*

Proof. By [22, Proposition 1], the mapping $A(x)$ is positive semidefinite convex if and only if for any $w \in R^n$, $\varphi(x) = w^T A(x)w$ is convex. Since $\lambda_1(A(x)) = \max_{\|w\|=1} w^T A(x)w$, it follows that $\lambda_1(A(x))$ is convex. \square

THEOREM 2.10. *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} .*

Proof. According to Proposition 2.9 and its proof, it suffices to prove that for any $w \in R^n$, the function $\varphi(x) = w^T V(x)^T V(x)w$ is convex on \mathcal{X} . Observe that

$$\varphi(x) = w^T V(x)^T V(x)w = \|V(x)w\|^2.$$

The convexity of $\varphi(x)$ follows from the fact that it is a composition of a linear mapping and a convex function. \square

Proposition 2.9 and Theorem 2.10 imply that the function f is convex in some domain $\mathcal{X}_1 \subseteq \mathcal{X}$ when $\lambda_n(A(x))$ is identical to a constant in \mathcal{X}_1 ; see Example 4.1. However, in general, f is not convex. Now we consider some special cases where (2.2) can be solved by using a quasi-convex and (strongly) pseudoconvex function.

DEFINITION 2.11. *Let \mathcal{A} be a finite dimensional space. A function $\phi : \mathcal{A} \rightarrow R$ is said to be quasi-convex if*

$$\phi(\tau x + (1 - \tau)y) \leq \max\{\phi(x), \phi(y)\}, \quad \forall x, y \in \mathcal{A}, \forall \tau \in (0, 1).$$

Let $\phi : \mathcal{A} \rightarrow R$ be lower semicontinuous and Lipschitz near a point $x \in \mathcal{A}$. We say that ϕ is pseudo-convex at x on \mathcal{A} if for every $y \in \mathcal{A}$,

$$\max\{\langle \xi, y - x \rangle : \xi \in \partial\phi(x)\} \geq 0 \implies \phi(y) \geq \phi(x).$$

We say that ϕ is strongly pseudo-convex at x on \mathcal{A} if for every $y \in \mathcal{A}$,

$$\langle \xi, y - x \rangle \geq 0 \text{ for some } \xi \in \partial\phi(x) \implies \phi(y) \geq \phi(x).$$

We say that ϕ is (strongly) pseudo-convex on \mathcal{A} if ϕ is (strongly) pseudo-convex at every x on \mathcal{A} .

It is easy to see that a strongly pseudo-convex function must be a pseudo-convex function.

PROPOSITION 2.12. *Let B be a fixed $m \times n$ matrix with $m \geq n$ and $\text{rank}(B) = n$. Define*

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

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

Proof. The quasi-convexity is equivalent to the condition that the level sets of the function are convex. For any $\gamma \geq 1$, the level set of h can be written as

$$\mathcal{L}_\gamma = \{W \in S_m^{++} : \lambda_1(B^T W B) - \gamma \lambda_n(B^T W B) \leq 0\}.$$

Since for any $W \in S_m^{++}$, we have

$$\lambda_1(B^T W B) = \max_{\|y\|=1} y^T (B^T W B) y \quad \text{and} \quad \lambda_n(B^T W B) = \min_{\|y\|=1} y^T (B^T W B) y.$$

From the linearity, we can easily find that $\lambda_1(B^T W B) - \gamma \lambda_n(B^T W B)$ is a convex function with respect to W . Hence \mathcal{L}_γ is a convex set and thus h is a quasi-convex function.

Moreover, from the convexity of $\lambda_1(B^T W B)$ and $-\gamma \lambda_n(B^T W B)$, for any $g_1 \in \partial \lambda_1(B^T \bar{W} B)$ and $g_n \in \partial \lambda_n(B^T \bar{W} B)$, we have

$$\lambda_1(B^T W B) - \lambda_1(B^T \bar{W} B) \geq \langle g_1, W - \bar{W} \rangle$$

and

$$-\lambda_n(B^T W B) + \lambda_n(B^T \bar{W} B) \geq \langle -g_n, W - \bar{W} \rangle.$$

By the quotient rule, for any $g \in \partial h(\bar{W})$, there are $g_1 \in \partial \lambda_1(B^T \bar{W} B)$ and $g_n \in \partial \lambda_n(B^T \bar{W} B)$ such that

$$g = \lambda_1(B^T \bar{W} B)^{-1} h(\bar{W}) (g_1 - h(\bar{W}) g_n).$$

It follows that

$$\begin{aligned} & \lambda_1(B^T W B) - h(\bar{W}) \lambda_n(B^T W B) \\ &= \lambda_1(B^T W B) - \lambda_1(B^T \bar{W} B) + h(\bar{W}) (-\lambda_n(B^T W B) + \lambda_n(B^T \bar{W} B)) \\ &\geq \langle g_1 - h(\bar{W}) g_n, W - \bar{W} \rangle \\ &= \lambda_1(B^T \bar{W} B) h(\bar{W})^{-1} \langle g, W - \bar{W} \rangle. \end{aligned}$$

Therefore, if $\langle g, W - \bar{W} \rangle \geq 0$, then $h(W) \geq h(\bar{W})$. \square

Suppose $m = \ell$ and $V(x) = XB$, where $X \in D_m^{++}$ with diagonal elements $x_i, i = 1, \dots, n$, and B is a fixed $m \times n$ matrix. Such a matrix arises from the weighted Vandermonde-like matrix [2, 3]. See Section 4. In this case, we can write $A(V(x)) = B^T X^T X B = B^T W B$, where $W = X^T X \in D_m^{++}$. Let $w \in R^m$ with $w_i = x_i^2, i = 1, \dots, m$ being the diagonal elements of W . By Proposition 2.12, we can find an optimal solution w^* by using a quasi-convex and strongly pseudo-convex function $h(W)$, and then obtain a solution x^* of (2.2) as $x_i^* = \sqrt{w_i^*}, i = 1, \dots, m$.

3. Smoothing approximation. The exponential smoothing function has been used for continuous min-max problem [4] and for minimizing the largest eigenvalue of a symmetric matrix [20, 21]. Applying the exponential smoothing function for the largest and the smallest eigenvalue functions, we introduce the smoothing function of the condition number as follows:

$$\tilde{f}(x, \mu) = -\frac{\ln(\sum_{i=1}^n e^{\lambda_i(A(x))/\mu})}{\ln(\sum_{i=1}^n e^{-\lambda_i(A(x))/\mu})}. \quad (3.1)$$

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 (3.1).

In this section we will show that this smoothing function has various nice properties including the gradient consistent property. These properties ensure that any

accumulation point of the sequence generated by some smoothing methods is a Clarke stationary point. For example, the smoothing projected gradient (SPG) method [29] and the smoothing conjugate gradient method [9] can be used to solve (2.2).

DEFINITION 3.1. [29] Let $f : \mathcal{X} \subset R^m \rightarrow R$ be a locally Lipschitz continuous function. We call $\tilde{f} : \mathcal{X} \times R_+ \rightarrow R$ a smoothing function of f , if $\tilde{f}(\cdot, \mu)$ is continuously differentiable in $\text{int}\mathcal{X}$ for any $\mu \in R_{++}$, and for any $\bar{x} \in \mathcal{X}$,

$$\lim_{x \rightarrow \bar{x}, \mu \downarrow 0} \tilde{f}(x, \mu) = f(\bar{x}) \quad (3.2)$$

and the set $\{\lim_{x \rightarrow \bar{x}, \mu \downarrow 0} \nabla_x \tilde{f}(x, \mu)\}$ is nonempty and bounded.

For a vector $y \in R_{++}^n$, let

$$\varphi_1(y) = \max_{1 \leq i \leq n} \{y_i\}, \quad \varphi_n(y) = \min_{1 \leq i \leq n} \{y_i\}$$

be the functions defined by the largest element and the smallest element respectively. Denote their quotient by

$$\varphi(y) := \frac{\varphi_1(y)}{\varphi_n(y)}. \quad (3.3)$$

We define the smoothing functions of φ_1 , φ_n and φ respectively as follows: for $\mu > 0$,

$$\phi_1(y, \mu) = \mu \ln \left(\sum_{i=1}^n e^{y_i/\mu} \right), \quad \phi_n(y, \mu) = -\mu \ln \left(\sum_{i=1}^n e^{-y_i/\mu} \right)$$

and

$$\phi(y, \mu) = \frac{\phi_1(y, \mu)}{\phi_n(y, \mu)}. \quad (3.4)$$

These functions are Lipschitz continuous and by using the pointwise maxima formula in [10, Proposition 2.3.12], we have

$$\begin{aligned} \partial\varphi_1(y) &= \text{conv} \left\{ g \in R^n : g_j = \begin{cases} 1, & \text{if } y_j = \varphi_1(y) > \max_{i \neq j} \{y_i\} \\ 0, & \text{if } y_j < \varphi_1(y) \\ \theta, & \text{otherwise, } \theta \in [0, 1] \end{cases} \right\} \\ \partial\varphi_n(y) &= \text{conv} \left\{ g \in R^n : g_j = \begin{cases} 1, & \text{if } y_j = \varphi_n(y) < \min_{i \neq j} \{y_i\} \\ 0, & \text{if } y_j > \varphi_n(y) \\ \theta, & \text{otherwise, } \theta \in [0, 1] \end{cases} \right\} \end{aligned}$$

where ‘‘conv’’ denotes the convex hull. Since the functions $\varphi_1(y)$ and $\varphi_n(y)$ are convex and concave respectively, $\varphi_1(y)$ and $-\varphi_n(y)$ are Clarke regular. By the quotient rule in [10, Proposition 2.3.14], the function $\varphi(y)$ defined in (3.3) is Clarke regular in any nonempty and bounded subset \mathcal{Y} of R_{++}^n and its Clarke generalized gradient is

$$\partial\varphi(y) = \frac{1}{\varphi_n(y)} (\partial\varphi_1(y) - \varphi(y)\partial\varphi_n(y)).$$

We now show that the function (3.4) is indeed a smoothing function for (3.3).

PROPOSITION 3.2. Let φ and $\phi(\cdot, \mu)$ be defined by (3.3) and (3.4) respectively. Then

(i) $\phi(\cdot, \mu)$ is a C^∞ function for any fixed $\mu > 0$ with the partial derivative

$$\begin{aligned}\frac{\partial \phi(y, \mu)}{\partial y_j} &= -\frac{1}{\mu \ln(\sum_{i=1}^n e^{-y_i/\mu})} \left[\frac{1}{\sum_{i=1}^n e^{y_i/\mu}} e^{y_j/\mu} - \frac{\phi(y, \mu)}{\sum_{i=1}^n e^{-y_i/\mu}} e^{-y_j/\mu} \right] \\ &= \frac{1}{\phi_n(y, \mu)} (\nabla_y \phi_1(y, \mu) - \phi(y, \mu) \nabla_y \phi_n(y, \mu))_j.\end{aligned}\quad (3.5)$$

(ii) For the given numbers $\underline{\lambda}_n > 0$ and $\bar{\lambda}_1 > 0$, let $\mathcal{Y} = \{y \in R^n : \underline{\lambda}_n \leq y_i \leq \bar{\lambda}_1, i = 1, \dots, n\}$. Then for any $y \in \mathcal{Y}$ and $\mu \leq \frac{\underline{\lambda}_n}{2 \ln n}$

$$0 \leq \phi(y, \mu) - \varphi(y) \leq c\mu \quad (3.6)$$

with $c = \frac{8\bar{\lambda}_1}{\underline{\lambda}_n^2} \ln n$. Moreover we have for any $y \in \mathcal{Y}$,

$$\lim_{y \rightarrow \bar{y}, \mu \downarrow 0} \phi(y, \mu) = \varphi(\bar{y}). \quad (3.7)$$

(iii) For any $\bar{y} \in \mathcal{Y}$, $\{\lim_{y \rightarrow \bar{y}, \mu \downarrow 0} \nabla_y \phi(y, \mu)\}$ is nonempty and bounded. Moreover, $\phi(\cdot, \mu)$ satisfies the gradient consistent property, that is,

$$\{\lim_{y \rightarrow \bar{y}, \mu \downarrow 0} \nabla_y \phi(y, \mu)\} \subset \partial \varphi(\bar{y}).$$

Proof. (i) The calculation of partial derivatives is routine and we omit it.

(ii) It is easy to find

$$0 \leq \phi_1(y, \mu) - \varphi_1(y) = \mu \ln \left(\sum_{i=1}^n e^{\frac{y_i - \varphi_1(y)}{\mu}} \right) \leq \mu \ln n$$

and

$$0 \geq \phi_n(y, \mu) - \varphi_n(y) = -\mu \ln \left(\sum_{i=1}^n e^{\frac{\varphi_n(y) - y_i}{\mu}} \right) \geq -\mu \ln n.$$

Hence for any $y \in \mathcal{Y}$ and $\mu < \frac{\underline{\lambda}_n}{2 \ln n}$, we have

$$1 \leq \varphi(y) = \frac{\varphi_1(y)}{\varphi_n(y)} \leq \frac{\phi_1(y, \mu)}{\phi_n(y, \mu)} = \phi(y, \mu) \leq \frac{\varphi_1(y) + \mu \ln n}{\varphi_n(y) - \mu \ln n} \leq \frac{2\bar{\lambda}_1 + \underline{\lambda}_n}{\underline{\lambda}_n}. \quad (3.8)$$

This implies that for any $\bar{y} \in \mathcal{Y}$,

$$0 \leq \lim_{y \rightarrow \bar{y}, \mu \downarrow 0} (\phi(y, \mu) - \varphi(y)) \leq \lim_{y \rightarrow \bar{y}, \mu \downarrow 0} \left(\frac{\varphi_1(y) + \mu \ln n}{\varphi_n(y) - \mu \ln n} - \varphi(y) \right) = 0. \quad (3.9)$$

Moreover, for any fixed $y \in \mathcal{Y}$, let

$$\psi_y(\mu) = \frac{\mu \ln n + \varphi_1(y)}{-\mu \ln n + \varphi_n(y)}.$$

Then we find

$$0 \leq \phi(y, \mu) - \varphi(y) \leq \psi_y(\mu) - \psi_y(0) = \psi'_y(\hat{\mu})\mu \quad \text{for some } \hat{\mu} \in [0, \mu] \quad (3.10)$$

and

$$\psi'_y(\mu) = \frac{\ln n(\varphi_n(y) + \varphi_1(y))}{(-\mu \ln n + \varphi_n(y))^2} \leq \frac{8\bar{\lambda}_1}{\underline{\lambda}_n^2} \ln n, \quad \forall \mu \leq \frac{\underline{\lambda}_n}{2 \ln n}. \quad (3.11)$$

By (3.10) and (3.11), we obtain (3.6). By (3.9) we find (3.7).

(iii) From the proof of (ii), we observe that

$$\frac{1}{2}\underline{\lambda}_n \leq \underline{\lambda}_n - \mu \ln n \leq \phi_n(y, \mu)$$

and all components of the vectors $\nabla_y \phi_1(y, \mu)$ and $\nabla_y \phi_n(y, \mu)$ satisfy

$$0 \leq \frac{1}{\sum_{i=1}^n e^{(y_i - \varphi_n(y))/\mu}} \leq (\nabla_y \phi_1(y, \mu))_j \leq \frac{1}{\sum_{i=1}^n e^{(y_i - \varphi_1(y))/\mu}} \leq \frac{1}{d(y)} \leq 1 \quad (3.12)$$

and

$$0 \leq \frac{1}{\sum_{i=1}^n e^{(\varphi_1(y) - y_i)/\mu}} \leq (\nabla_y \phi_n(y, \mu))_j \leq \frac{1}{\sum_{i=1}^n e^{(\varphi_n(y) - y_i)/\mu}} \leq \frac{1}{b(y)} \leq 1, \quad (3.13)$$

where $d(y)$ and $b(y)$ are the multiplicity of the largest and smallest elements of y , respectively. Hence, by (3.5), for any $\bar{y} \in \mathcal{Y}$, $\{\lim_{y \rightarrow \bar{y}, \mu \downarrow 0} \nabla_y \phi(y, \mu)\}$ is nonempty and bounded. Moreover, since

$$\begin{aligned} \frac{\partial \phi_1}{\partial y_j}(y, \mu) &= \frac{1}{\sum_{i=1}^n e^{(y_i - y_j)/\mu}} \\ \frac{\partial \phi_n}{\partial y_j}(y, \mu) &= \frac{1}{\sum_{i=1}^n e^{(y_j - y_i)/\mu}} \end{aligned}$$

for any convergent subsequence of $\nabla_y \phi_1(y^k, \mu_k)$ and $\nabla_y \phi_n(y^k, \mu_k)$ with $y^k \rightarrow \bar{y}$ and $\mu_k \rightarrow 0$, as $k \rightarrow \infty$, we have

$$\begin{aligned} \left(\lim_{k \rightarrow \infty} \nabla_y \phi_1(y^k, \mu_k) \right)_j &= \begin{cases} 1, & \text{if } \bar{y}_j = \varphi_1(\bar{y}) > \max_{i \neq j} \{\bar{y}_i\} \\ 0, & \text{if } \bar{y}_j < \varphi_1(\bar{y}) \\ \theta_1, & \text{otherwise,} \end{cases} \\ \left(\lim_{k \rightarrow \infty} \nabla_y \phi_n(y^k, \mu_k) \right)_j &= \begin{cases} 1, & \text{if } \bar{y}_j = \varphi_n(\bar{y}) < \min_{i \neq j} \{\bar{y}_i\} \\ 0, & \text{if } \bar{y}_j > \varphi_n(\bar{y}) \\ \theta_n, & \text{otherwise,} \end{cases} \end{aligned}$$

where $\theta_1, \theta_n \in [0, 1]$. Hence

$$\left\{ \lim_{y \rightarrow \bar{y}, \mu \downarrow 0} \nabla_y \phi(y, \mu) \right\} \subset \partial \varphi(\bar{y}).$$

Therefore ϕ satisfies the gradient consistent property. \square

Remark 3.1 If we fix $\bar{y} \in \mathcal{Y}$ and take $\mu \downarrow 0$, we have that

$$\left(\lim_{\mu \downarrow 0} \nabla_y \phi(\bar{y}, \mu) \right)_j = \frac{1}{\varphi_n(\bar{y})} \begin{cases} (1 - \varphi(\bar{y}))/n, & \text{if } \bar{y}_j = \varphi_1(\bar{y}) = \varphi_n(\bar{y}) \\ 1/d(\bar{y}), & \text{if } \bar{y}_j = \varphi_1(\bar{y}) > \varphi_n(\bar{y}) \\ -\varphi(\bar{y})/b(\bar{y}), & \text{if } \bar{y}_j = \varphi_n(\bar{y}) < \varphi_1(\bar{y}) \\ 0, & \text{otherwise.} \end{cases}$$

DEFINITION 3.3. ([17, Definition 1]) Let $\varphi : R^n \rightarrow [-\infty, +\infty]$ be a function that is invariant under coordinate permutations. Then the composition function

$$\varphi \circ \lambda : S_n \rightarrow [-\infty, +\infty]$$

is called an eigenvalue function.

PROPOSITION 3.4. Let $\varphi : \mathcal{Y} \rightarrow R$ be a locally Lipschitz function and let $\phi : \mathcal{Y} \times R_+ \rightarrow R$ be a smoothing function of φ . Suppose that the function $A \rightarrow \phi(\lambda(A), \mu)$ is an eigenvalue function and $A(x)$ is continuously differentiable. Then $\tilde{f}(x, \mu) := \phi(\lambda(A(x)), \mu)$ is a smoothing function of $f(x) := \varphi(\lambda(A(x)))$ and its partial derivative with respect to x_k is given by

$$\frac{\partial \tilde{f}(x, \mu)}{\partial x_k} = \langle \text{diag}(\nabla_y \phi(\lambda(A(x)), \mu)), U(x)^T A_k(x) U \rangle$$

where $U(x)^T U(x) = I$, $U(x) \text{diag}(\lambda(A(x))) U(x)^T = A(x)$.

Moreover if the function $\phi(\cdot, \mu)$ satisfies the gradient consistent property, then the function $\tilde{f}(\cdot, \mu)$ also satisfies the gradient consistent property.

Proof. By [17, Corollary 3], since $\phi(\cdot, \mu)$ is a smooth function for each $\mu > 0$, the eigenvalue function $\phi(\lambda(A), \mu)$ is also a smooth function in A . By [17, Theorem 6] its Fréchet differential at a matrix $A \in S_n$ is a linear mapping from S_n to R given by the formula

$$\nabla_A \phi(\lambda(A), \mu) = U \text{diag}(\nabla_y \phi(\lambda(A), \mu)) U^T$$

where $U^T U = I$, $U \text{diag}(\lambda(A)) U^T = A$. By the chain rule,

$$\begin{aligned} \frac{\partial \tilde{f}(x, \mu)}{\partial x_k} &= \langle \nabla_A \phi(\lambda(A(x)), \mu), A_k(x) \rangle \\ &= \langle \text{diag}(\nabla_y \phi(\lambda(A(x)), \mu)), U(x)^T A_k(x) U(x) \rangle. \end{aligned}$$

The rest of the results follow by the continuity of the function $x \rightarrow \lambda(A(x))$ and the definition of a smoothing function and the gradient consistent property. \square

THEOREM 3.5. Let f and $\tilde{f}(\cdot, \mu)$ be defined by (2.1) and (3.1) respectively. Then (i) $\tilde{f}(\cdot, \mu)$ is continuously differentiable for any fixed $\mu > 0$ with gradient

$$\begin{aligned} \frac{\partial \tilde{f}(x, \mu)}{\partial x_k} &= \frac{-1}{\mu \ln(\sum_{i=1}^n e^{-\lambda_i(A(x))/\mu})} \left[\frac{1}{\sum_{i=1}^n e^{\lambda_i(A(x))/\mu} \sum_{i=1}^n e^{-\lambda_i(A(x))/\mu} u_i(x)^T A_k(x) u_i(x)} \right. \\ &\quad \left. - \frac{\tilde{f}(x, \mu)}{\sum_{i=1}^n e^{-\lambda_i(A(x))/\mu} \sum_{i=1}^n e^{-\lambda_i(A(x))/\mu} u_i(x)^T A_k(x) u_i(x)} \right]. \end{aligned}$$

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

$$0 \leq \tilde{f}(x, \mu) - f(x) \leq c\mu. \quad (3.14)$$

Moreover (3.2) holds.

(iii) For any $\bar{x} \in \mathcal{X}$, $\{\lim_{x \rightarrow \bar{x}, \mu \downarrow 0} \nabla_x \tilde{f}(x, \mu)\}$ is nonempty and bounded. Moreover, $\tilde{f}(\cdot, \mu)$ satisfies the gradient consistent property, that is,

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

(iv) For any fixed $\mu > 0$, the gradient of $\tilde{f}(x, \mu)$ is Lipschitz continuous, that is, for any $x, y \in \mathcal{X}$, there exists a constant L_μ such that

$$\|\nabla \tilde{f}(x, \mu) - \nabla \tilde{f}(y, \mu)\| \leq L_\mu \|x - y\|. \quad (3.15)$$

Proof. Note that $\tilde{f}(x, \mu) = \phi(\lambda(A(x)), \mu)$ with ϕ defined by (3.4). It is easy to see that the function $\phi(\cdot, \mu)$ is a permutation-invariant function and hence (i)-(iii) follows from Proposition 3.2 (i)-(iii) and Proposition 3.4.

(iv) Since for any fixed $\mu > 0$, $\phi(\cdot, \mu)$ is a C^∞ function. There is a constant ℓ_μ such that $\|\nabla_y^2 \phi(y, \mu)\| \leq \ell_\mu$ for $y \in \mathcal{Y}$. Hence, we can find a L_μ such that (3.15) holds. \square

According to Theorem 3.5, we can construct globally convergent smoothing methods for solving (2.2). In the smoothing methods, we can update the iterates x^k and smoothing parameter μ_k in an appropriate way which depends on the method used for the smoothing problems. For instance, we can use the smoothing projected gradient method (SPG) proposed in [29] to solve (2.2), which uses the projected gradient method in [6] for the smoothing problem. We have the following global convergence theorem.

THEOREM 3.6. *From any starting point $x^0 \in \mathcal{X}$, the sequence $\{x^k\}$ generated by the SPG method [29] 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*

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

Proof. From Theorem 3.5, we know that Assumption 2.1 in [29] holds, and

$$\{\lim_{x^k \rightarrow \bar{x}, \mu_k \downarrow 0} \nabla_x \tilde{f}(x^k, \mu)\} \subset \partial f(\bar{x}).$$

By Theorem 2.1 in [29], we have the conclusion of this theorem. \square

By virtue of [18, Proposition 5.1], Theorem 3.6 has the following immediate consequences.

COROLLARY 3.7. *Under the assumptions of Theorem 3.6 if the function f 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 is pseudoconvex on \mathcal{X} , then the accumulation point is a global optimal solution.*

Remark 3.1 Following the discussion above, we can easily see that the smoothing functions $\phi_1(\lambda(A(x)), \mu)$ and $\phi_n(\lambda(A(x)), \mu)$ for $\lambda_1(A(x))$ and $\lambda_n(A(x))$ have the same properties in Theorem 3.5 as $\phi(\lambda(A(x)), \mu)$ for $f(x)$. Hence we can similarly construct globally convergent smoothing methods for minimizing the largest eigenvalues and maximizing the smallest eigenvalues. In particular in the case where $V(x)$ is a linear mapping of x on \mathcal{X} , since $\lambda_1(A(x))$ is a convex function by virtue of Theorem 2.10, the smoothing algorithm we proposed will converge to a global optimal solution.

4. Numerical examples. In this section, we first use a small example to illustrate some properties of the condition number function $f(x) = \kappa(A(x))$. Next we report numerical results for the least squares polynomial approximation using the Vandermonde-like matrix with the optimal solution of (1.2), equally spaced points, Gauss points, Gauss-Lobatto points, Chebyshev points and Clenshaw-Curtis points on the interval $[-1, 1]$. Finally, we present numerical results to compare the optimal solution of (1.2) defined by the spherical harmonics with the extremal points, the minimum energy points and the points of spherical t -designs on the unit sphere.

EXAMPLE 4.1. Consider the following weighted Vandermonde-like matrix with $\ell = 3, n = 2, m = 1$, and a point set $\{-x, 0, x\}$. Let $\mathcal{X} = [0.5, 1.5]$ and

$$V(x) = \begin{pmatrix} 1 & -x \\ 1 & 0 \\ 1 & x \end{pmatrix}.$$

Then we have

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

and

$$f(x) = \frac{\lambda_1(A(x))}{\lambda_n(A(x))} = \begin{cases} \frac{3}{2x^2}, & 0.5 \leq x \leq \sqrt{1.5} \\ \frac{2x^2}{3}, & \sqrt{1.5} \leq x \leq 1.5. \end{cases} \quad (4.1)$$

We consider the problem

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

We find $x^* = \sqrt{1.5}$ is the minimizer with the function value $f(x^*) = 1$. Moreover, f is convex and strongly semismooth in \mathcal{X} . However, f is not differentiable at x^* . Since $\lambda_1(A(x^*)) = \lambda_2(A(x^*)) = 3$, we have $d(x^*) = b(x^*) = 2$ and we can take $U_\alpha(x^*) = U_\beta(x^*) = I$. Let

$$A'(x^*) = 2\sqrt{6} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Using Proposition 2.5, we can write the Clarke generalized gradient as

$$\begin{aligned} \partial f(x^*) &= \{g \in R : g = \frac{1}{3} \langle A'(x^*), P_\alpha \rangle - \frac{1}{3} \langle A'(x^*), P_\beta \rangle, \\ & \quad P_\alpha = \text{diag}(\alpha, (1 - \alpha)), \alpha \in [0, 1], \\ & \quad P_\beta = \text{diag}(\beta, (1 - \beta)), \beta \in [0, 1]\} \\ &= 2\sqrt{\frac{2}{3}}[-1, 1]. \end{aligned}$$

Using (4.1), we also find

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

Note that if $\mathcal{X} = (0, 1]$ then the optimal solution is $x^* = 1$ with $f(x^*) = \frac{3}{2}$. In this case, f is differentiable at x^* , but x^* is on the boundary of \mathcal{X} .

4.1. Least squares approximation on the interval $[-1, 1]$. Let $\{p_j, j = 0, \dots, n-1\}$ be a basis for $\mathbb{P}_{n-1}[-1, 1]$, the linear space of polynomials of degree $\leq n-1$ on $[-1, 1]$. For a given vector $w \in R_{++}^\ell$, given ℓ distinct real numbers

$$-1 \leq a_1 < a_2 < \dots < a_\ell \leq 1, \quad a^T = (a_1, \dots, a_\ell)$$

and given ℓ function values at these points

$$F_1, F_2, \dots, F_\ell,$$

the weighted least squares approximation on the interval $[-1, 1]$ is to find a vector $c = (c_1, \dots, c_n)^T$ which minimizes

$$\sum_{i=1}^{\ell} w_i^2 \left| F_i - \sum_{j=1}^n c_j p_{j-1}(a_i) \right|^2.$$

The unique solution [14] is given by

$$c^* = V(w, a)^\dagger (w_1 F_1, \dots, w_\ell F_\ell)^T$$

where $V(w, a) \in R^{\ell \times n}$ is the weighted Vandermonde-like matrix

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

When the data F_i is perturbed slightly, the maximal factor of magnification of relative errors is given by $\kappa(V(w, a)^T V(w, a))$ [5, 14]. We define the condition number function $f(x)$ by setting $x = (w, a)$, or $x = a$ ($x = w$) with fixed weights (points).

For fixed weights $w_i = 1, i = 1, \dots, \ell$, and $p_i(\tau) = \tau^i, i = 0, \dots, n-1$, we choose the following six sets of points on the interval $[-1, 1]$:

- equally spaced points $a_i = -1 + \frac{2(i-1)}{\ell-1}, i = 1, \dots, \ell.$
- Gauss points $a_i = i$ th zero of the Legendre polynomial $P_\ell(\tau).$
- Gauss-Lobatto points $a_i = i$ th zero of $(\tau^2 - 1)P'_{\ell-1}(\tau).$
- Clenshaw-Curtis points $a_i = i$ th extrema of the Chebyshev polynomial $T_{\ell-1}(\tau).$
- Chebyshev points $a_i = i$ th zero of the Chebyshev polynomial $T_\ell(\tau).$
- minimum cond points $a =$ optimal solution of (1.2) .

The Gauss points and Gauss-Lobatto points can be efficiently calculated by a tridiagonal eigenvalue problem [15]. These points are frequently used as quadrature points. It is known that the Gauss points satisfy

$$\int_{-1}^1 p(\tau) d\tau = \sum_{i=1}^{\ell} \alpha_i p(a_i), \quad \forall p \in \mathbb{P}_{2\ell-1}$$

while the Gauss-Lobatto points include the end-points ± 1 and satisfy

$$\int_{-1}^1 p(\tau) d\tau = \sum_{i=1}^{\ell} \alpha_i p(a_i), \quad \forall p \in \mathbb{P}_{2\ell-3},$$

where $\alpha_i, i = 1, \dots, \ell$ are the values of the integrals of Lagrange interpolation polynomials on $[-1, 1]$. It is remarkable that in 1932, Fejér showed that the Gauss-Lobatto points are also the Fekete points for which the determinant of the square Vandermonde matrix $V(e, x)$ with $e = (1, \dots, 1)^T \in R^\ell, \ell = n, x = a$, and $p_i(\tau) = \tau^i, i = 0, \dots, n-1$ is maximal [5].

The Chebyshev points can be calculated explicitly

$$a_i = -\cos \frac{\pi(2i-1)}{2\ell}, \quad i = 1, \dots, \ell,$$

while the Clenshaw-Curtis points, which include -1 and 1 , are given by the formula

$$a_i = -\cos \frac{\pi(i-1)}{\ell-1}, \quad i = 1, \dots, \ell.$$

Figure 4.1 shows the distribution of these six sets of points for $\ell = n = 11$. Table 4.1 shows the values of the condition number and determinant at those points for $n = 11$ and $\ell = 11, 21$.

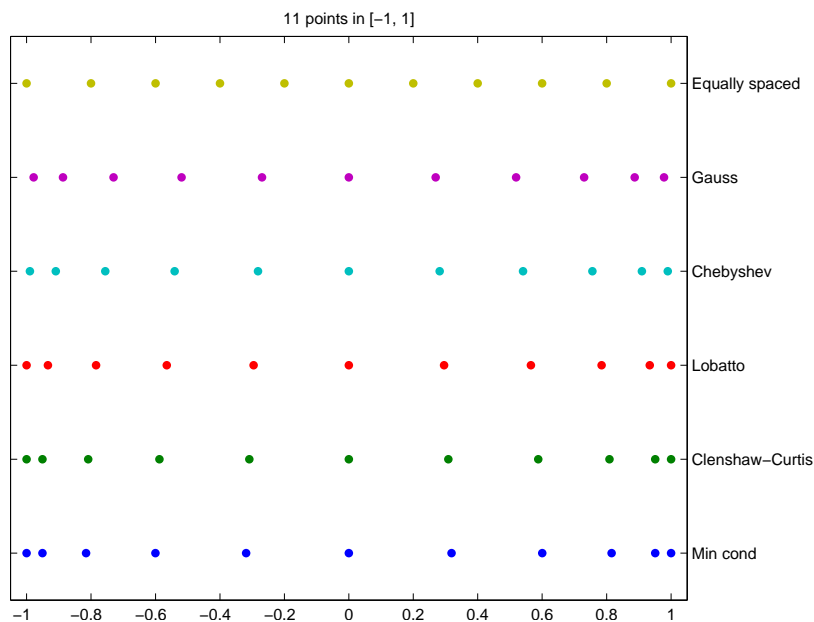


Fig. 4.1: Equally spaced points, Gauss Points, Chebyshev points, Gauss Lobatto points, Clenshaw-Curtis point and minimum condition number points in $[-1, 1]$ for interpolation using the monomial basis of degree 10.

For the least squares problem on $[-1, 1]$ with $\ell > n$, for example the degree 10 case with 21 points in Table 4.1, minimizing the condition number tended to make the nodes coalesce, so there were only $\ell = 11$ distinct nodes at the solution. It was also possible to converge to different local minima of the condition number by starting with different point sets. For example starting with $\ell = 21$ Chebyshev points gave $f(\bar{x}) = 6.235 \times 10^6$, while starting with $\ell = 21$ equally spaced points gave

sets of points	condition number		determinant	
	$\ell = 11$	$\ell = 21$	$\ell = 11$	$\ell = 21$
equally spaced points	1.946479e+8	1.093275e+7	5.755e-22	1.604e-16
Gauss points	1.767123e+7	1.271482e+7	4.616e-20	1.916e-16
Chebyshev points	1.287418e+7	1.287418e+7	2.251e-19	2.763e-16
Gauss-Lobatto points	9.606328e+6	1.325361e+7	7.968e-19	3.723e-16
Clenshaw-Curtis points	8.307060e+6	1.403922e+7	6.311e-19	3.756e-16
min cond points	8.176691e+6	5.246086e+6	5.826e-19	3.042e-16

Table 4.1: Values of the condition number and determinant of the Gram matrix using the monomial basis at different point sets for degree 10 and $\ell = 11$ and $\ell = 21$ points

$f(x^*) = 5.246 \times 10^6$. It should also be noted that the eigenvalues at the solution appeared to be distinct (in which case f is smooth), with some uncertainty in the smallest eigenvalue, for example $\lambda_{11}(x^*) = 6.048 \times 10^{-6}$ and $\lambda_{10}(x^*) = 1.485 \times 10^{-5}$.

Choosing good points does not overcome the well-known bad conditioning of the monomial basis. Table 4.2 gives the same data as Table 4.1, but using the Chebyshev basis $T_0 = 1/\sqrt{2}$, $T_j(x) = \cos(j \arccos(x))$, $j = 1, \dots, n-1$. For this basis the Chebyshev points give the optimal condition number of 1 as $V(x)^T V(x) = \frac{n}{2} I$. Minimizing the condition number of the Gram matrix obtained using the Chebyshev basis starting from one of the other point sets, except possibly the equally spaced points, converged to a point set which gives the optimal condition number of 1.

sets of points	condition number		determinant	
	$\ell = 11$	$\ell = 21$	$\ell = 11$	$\ell = 21$
equally spaced points	5.179192e+2	4.629276	3.562e+5	9.926e+10
Gauss points	3.237343	1.404429	2.858e+7	1.186e+11
Chebyshev points	1.000000	1.000000	1.393e+8	1.710e+11
Gauss-Lobatto points	2.523277	1.384010	4.932e+8	2.304e+11
Clenshaw-Curtis points	2.500000	1.550000	3.906e+8	2.325e+11

Table 4.2: Values of the condition number and determinant of the Gram matrix using the Chebyshev basis at different point sets for degree 10 and $\ell = 11$ and $\ell = 21$ points

Figure 4.2 shows the growth of the condition number as the degrees of the polynomial increases and the number of additional points also increases. For a good basis and a good point set the Gram matrix $A(w, a)$ can be well conditioned. Moreover we notice that with the same basis and the same choice of points, the condition number of $A(w, a)$ tends to be smaller as we add more points.

4.2. Least squares approximation on the sphere. Let $\mathbb{S}^2 = \{\mathbf{z} \in R^3 : \|\mathbf{z}\| = 1\}$ be the unit sphere in the Euclidean space R^3 . Let \mathbb{P}_t be the linear space of restrictions of polynomial of degree $\leq t$ in 3 variables to \mathbb{S}^2 . Let $Z_N = \{\mathbf{z}_1, \dots, \mathbf{z}_N\} \subset \mathbb{S}^2$ be a set of N -points on the sphere. The dimension of the linear space \mathbb{P}_t is $\dim(\mathbb{P}_t) = (t+1)^2$, and \mathbb{P}_t can be spanned by the orthonormal set of real spherical

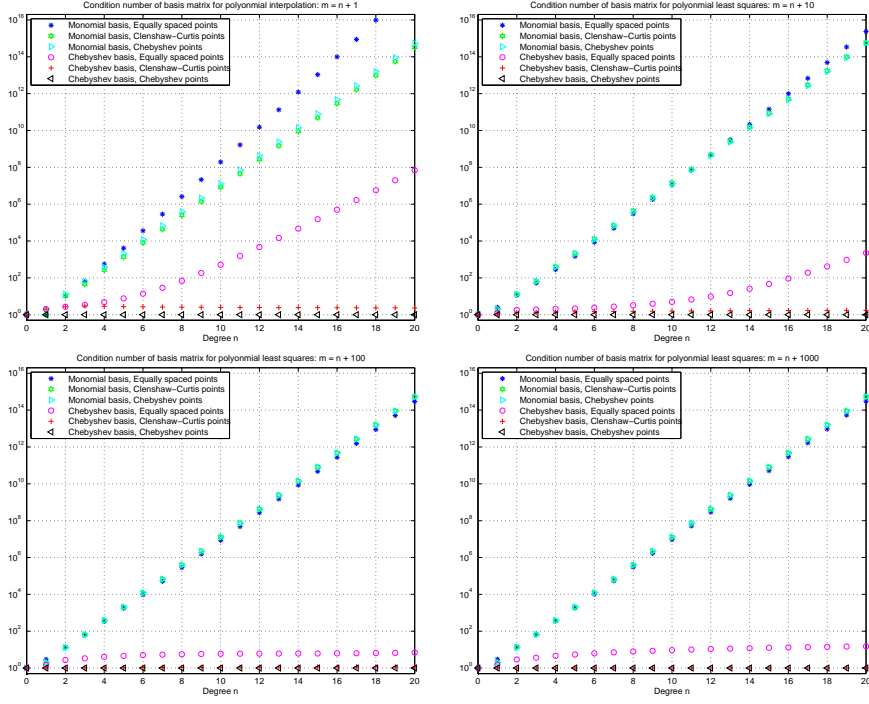


Fig. 4.2: Growth of condition numbers of the Gram matrix for Chebyshev and Monomial bases with degree n and m points.

harmonics with degree r and order k [23],

$$\{Y_{rk} \mid k = 1, \dots, 2r + 1, r = 0, 1, \dots, t\}.$$

The Gram matrix $G_t(Z_N)$ is

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

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

$$Y_{rk}(\mathbf{z}_j), \quad k = 1, \dots, 2r + 1, \quad r = 0, 1, \dots, t.$$

Given a function F defined on \mathbb{S}^2 , let

$$F = (F_1(\mathbf{z}_1), \dots, F_N(\mathbf{z}_N))^T.$$

Consider the problem of finding a polynomial $p \in \mathbb{P}_t$ which best approximates F in the Euclidean norm, which is to find a minimizer $c = (c_1, \dots, c_{(t+1)^2})^T \in R^{(t+1)^2}$ of the following least squares problem

$$\text{minimize } \|Y(Z_N)^T c - F\|_2^2. \quad (4.2)$$

An optimal solution of this problem can be given as

$$c^* = (Y(Z_N)^T)^\dagger F.$$

Let $A(Z_N) = Y(Z_N)Y(Z_N)^T$ and $N \geq (t+1)^2$. The Euclidean condition number of $A(Z_N)$ is

$$\kappa(A(Z_N)) = \|Y(Z_N)^T\|^2 \|(Y(Z_N)^T)^\dagger\|^2.$$

The condition number $\kappa(A(Z_N))$ measures the sensitivity of the least squares polynomial approximation. To have the best polynomial approximation, we choose a set Z_N of N -points on the sphere \mathbb{S}^2 which minimizes the condition number. By using the spherical parametrization [8], we can present the N points by using a vector $x \in R^m$, with $m = 2(t+1)^2 - 3$, and set $A(Z_N) = A(x)$. Hence we have an optimization problem in the form of (1.2). Note that $A(Z_N)$ and $G(Z_N)$ are polar similar and have same nonzero eigenvalues [16].

Let $N = (t+1)^2$. In this case, the number of points equals to the size of the Gram matrix. We consider the following four sets of points.

DEFINITION 4.1. Let $Z_N = \{\mathbf{z}_1, \dots, \mathbf{z}_N\} \subset \mathbb{S}^2$ be a set of N -points on the sphere.

<i>minimum energy system</i>	$\operatorname{argmin} \sum_{i \neq j}^N \frac{1}{\ \mathbf{z}_i - \mathbf{z}_j\ }.$
<i>extremal system</i>	$\operatorname{argmax} \det(Y(Z_N)Y(Z_N)^T).$
<i>spherical t-design</i>	$\int_{\mathbb{S}^2} p(z) dz = \frac{4\pi}{N} \sum_{i=1}^N p(\mathbf{z}_i), \quad \forall p \in \mathbb{P}_t.$
<i>minimum cond points</i>	<i>optimal solution of $\min \kappa(G_t(Z_N))$.</i>

These optimization problems on the sphere typically have many local solutions, so one has to settle for a good local solution, which is not necessarily a global solution. Also for a given t , a spherical t -design is not unique. Our numerical results use the one near the extremal system [1, 7, 8]. Let $t = 5$ and $N = (t+1)^2 = 36$. Consider the $N \times N$ Gram matrix $G_t(Z_N)$. The left plot in Figure 4.3 shows the values of the 36 eigenvalues of $G_t(Z_N)$ with the 36 extremal system points (initial point) and min cond points (final point found by the smoothing gradient method) on the sphere. It is clear to see that the multiplicity of the largest eigenvalue and smallest eigenvalue are four and five at the optimal solution $x^* \in R^{2N-3}$ of (1.2), respectively. Hence f is not differentiable at the solution x^* . The right plot in Figure 4.3 shows the function values of $f(x)$ and its smoothing function $f(x, \mu)$ with different values of μ for the same Gram matrix $G_t(Z_N)$ with $x = x^* - \alpha \nabla_x f(x^*, 0.0766)$ for $\alpha \in [-0.05, 0.1]$. It shows that the minimizers of smoothing functions approach x^* as $\mu \rightarrow 0$. Note that at x^* , the largest eigenvalue $\lambda_1(A(x^*))$ is 4.1949, the smallest eigenvalue $\lambda_n(A(x^*))$ is 1.3397 and the condition number $f(x^*)$ is 3.1312. By Theorem 3.5, the smoothing parameter μ should be chosen less than 0.3739.

In Figure 4.4, we show the log of the function values of the condition number function $f(x)$ with the degree $t = 9$ and $N = 100$ points over the sphere. We choose the extremal system

$$\hat{Z}_N = \{\hat{\mathbf{z}}_1, \dots, \hat{\mathbf{z}}_N\} = \operatorname{argmax} \det(G_t(Z_N)).$$

The first point of the set is the north pole $\hat{\mathbf{z}}_1 = (1, 0, 0)^T$. We consider $G_t(Z_N)$ with

$$Z_N = \{\mathbf{z}_1, \hat{\mathbf{z}}_2, \dots, \hat{\mathbf{z}}_N\}, \quad \mathbf{z}_1 \in \mathbb{S}^2,$$

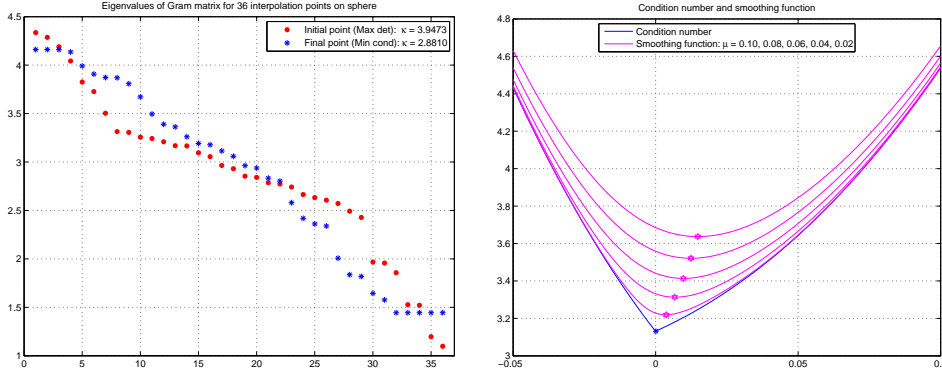


Fig. 4.3: Left: The 36 eigenvalues of the Gram matrix $G_t(Z_N)$ with degree $t = 5$ and $N = 36$ points on the sphere. Right: For the same Gram matrix, function values of $f(x^* - \alpha \nabla_x \tilde{f}(x^*, 0.0766))$ and $\tilde{f}(x^* - \alpha \nabla_x \tilde{f}(x^*, 0.0766), \mu)$ for $\alpha \in [-0.05, 0.1]$.

that is, we fix the $N - 1$ points $\hat{\mathbf{z}}_2, \dots, \hat{\mathbf{z}}_N$ and move \mathbf{z}_1 over the sphere. We find that the function $f(x) = \kappa(A(\mathbf{z}))$ has many local minimal points.

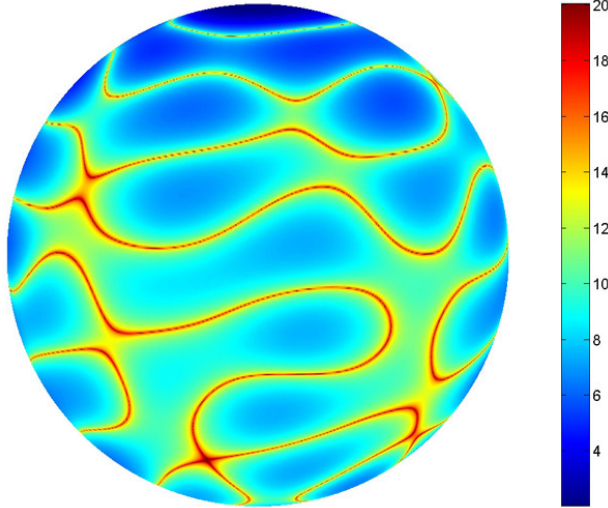


Fig. 4.4: The log of the condition number of the Gram matrix $G_t(X_N)$ for degree $t = 9$, $N = 100$ points. The first point is varied over the whole sphere, while the remaining 99 extremal points excluding the north pole are fixed.

Figure 4.5 shows the function values at those four sets of points in Definition 4.1 for different values of N and t with $N = (t + 1)^2$. It is worth noting that the Gram matrix $G_t(Z_N)$ is nearly singular at the minimum energy system for $t = 12$. The most striking feature of the plot of the condition numbers against degree of the interpolating polynomial in Figure 4.5 is that the minimum energy points obtained by minimizing the Coulomb energy can have very large condition numbers. In contrast,

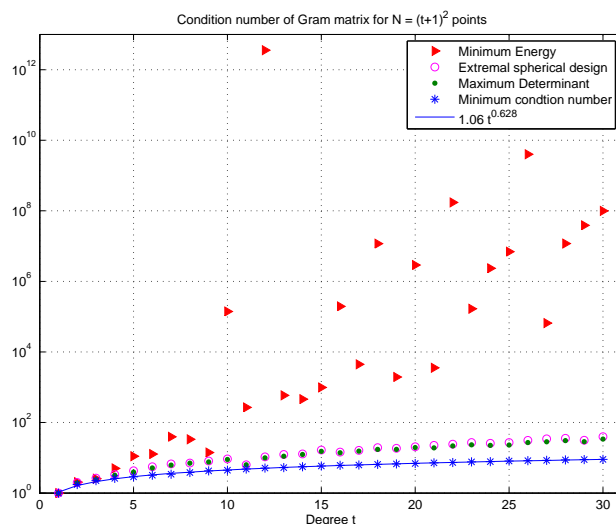


Fig. 4.5: Condition number on the minimum energy system, extremal system, spherical t -design, minimum cond points

for the extremal (maximum determinant) and new points obtained by minimizing the condition number, the condition number grows slowly. Indeed, for the points obtained by minimizing the condition number, the growth is less than linear in the degree t . Optimization problems on the sphere typically have many local minima, but the smallest possible condition number cannot be larger than those found so far.

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