MA 5037: Optimization Methods and Applications Unconstrained Optimization



Suh-Yuh Yang (楊肅煜)

Department of Mathematics, National Central University Jhongli District, Taoyuan City 320317, Taiwan

First version: May 17, 2018/Last updated: June 13, 2025

Global minimum and global maximum

Definition: Let $f: S \to \mathbb{R}$ be a real-valued function defined on a nonempty set $S \subseteq \mathbb{R}^n$.

- (1) $x^* \in S$ is called a global minimum point (minimizer) of f over S if $f(x^*) \leq f(x)$, $\forall x \in S$.
- (2) $x^* \in S$ is called a strict global minimum point (minimizer) of f over S if $f(x^*) < f(x)$, $\forall x \in S$ and $x \neq x^*$. (for short, $\forall x^* \neq x \in S$)
- (3) $x^* \in S$ is called a global maximum point (maximizer) of f over S if $f(x) \le f(x^*)$, $\forall x \in S$.
- (4) $x^* \in S$ is called a strict global maximum point (maximizer) of f over S if $f(x) < f(x^*)$, $\forall x^* \neq x \in S$.
- (5) The set S on which the optimization of f is performed is called the feasible set, and any point $x \in S$ is called a feasible solution.

Note: We will frequently omit the adjective "global".

Minimal value and maximal value of f over S

Definition: Let $f: S \to \mathbb{R}$ be a real-valued function defined on a nonempty set $S \subseteq \mathbb{R}^n$.

- (1) $x^* \in S$ is called a global optimum of f over S if it is either a global minimizer or a global maximizer.
- (2) The minimal value of f over $S := \inf\{f(x) : x \in S\}$. If $x^* \in S$ is a global minimum of f over S, then $\inf\{f(x) : x \in S\} = f(x^*)$.
- (3) The maximal value of f over $S := \sup\{f(x) : x \in S\}$. If $x^* \in S$ is a global maximum of f over S, then $\sup\{f(x) : x \in S\} = f(x^*)$.
- (4) The set of all global minimizers of f over S is denoted by

$$\operatorname{argmin}\{f(x): x \in S\}.$$

The set of all global maximizers of f over S is denoted by

$$argmax{f(x) : x \in S}.$$

Find the global minimum and maximum points of f(x,y) = x + y over $S = B[\mathbf{0}, 1] = \{(x, y)^\top : x^2 + y^2 \le 1\}.$

Solution:

• By the Cauchy-Schwarz inequality, for any $(x,y)^{\top} \in S$, we have

$$x + y = (x, y) \begin{bmatrix} 1 \\ 1 \end{bmatrix} \le \sqrt{x^2 + y^2} \sqrt{1^2 + 1^2} \le \sqrt{2}.$$

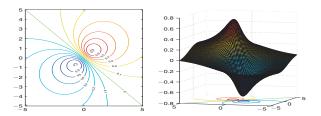
Therefore, the maximal value of f over S is upper bounded by $\sqrt{2}$. Note that $(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}) \in S$ and $f(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}) = \sqrt{2}$ and this is the *only* point that attains this value. Thus, $(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ is the *strict* global maximum point of f over S, and the maximal value is $\sqrt{2}$.

• Similarly, we can show that $-(x+y) \le \sqrt{2} \Longrightarrow x+y \ge -\sqrt{2}$. Thus, $(\frac{-1}{\sqrt{2}}, \frac{-1}{\sqrt{2}})$ is the strict global minimum point of f over S, and the minimal value is $-\sqrt{2}$.

Consider the following 2-D function defined over the entire space:

$$f(x,y) = \frac{x+y}{x^2 + y^2 + 1}.$$

The contour and surface plots of the function are given below:



- The global maximizer = $(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$, the maximal value = $\frac{1}{\sqrt{2}}$.
- The global minimizer $=(\frac{-1}{\sqrt{2}},\frac{-1}{\sqrt{2}})$, the minimal value $=\frac{-1}{\sqrt{2}}$.

The proof of these facts will be given later.

Local minimum and local maximum

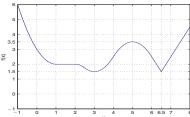
Definition: Let $f: S \to \mathbb{R}$ be a real-valued function defined on a nonempty set $S \subseteq \mathbb{R}^n$.

- (1) $x^* \in S$ is called a local minimum point of f over S if $\exists r > 0$ such that $f(x^*) \leq f(x), \forall x \in S \cap B(x^*, r)$.
- (2) $x^* \in S$ is called a strict local minimum point of f over S if $\exists r > 0$ such that $f(x^*) < f(x)$, $\forall x^* \neq x \in S \cap B(x^*, r)$.
- (3) $x^* \in S$ is called a local maximum point of f over S if $\exists r > 0$ such that $f(x) \le f(x^*)$, $\forall x \in S \cap B(x^*, r)$.
- (4) $x^* \in S$ is called a strict local maximum point of f over S if $\exists r > 0$ such that $f(x) < f(x^*), \forall x^* \neq x \in S \cap B(x^*, r)$.

Consider the following 1-D function defined over [-1,8]:

$$f(x) = \begin{cases} (x-1)^2 + 2, & -1 \le x \le 1, \\ 2, & 1 \le x \le 2, \\ -(x-2)^2 + 2, & 2 \le x \le 2.5, \\ (x-3)^2 + 1.5, & 2.5 \le x \le 4, \\ -(x-5)^2 + 3.5, & 4 \le x \le 6, \\ -2x + 14.5, & 6 \le x \le 6.5, \\ 2x - 11.5, & 6.5 \le x \le 8. \end{cases}$$

Classify each of the points x = -1, 1, 2, 3, 5, 6.5, 8 as strict/nonstrict, global/local, minimum/maximum points.



First order optimality condition for local optimum points

Theorem: Let $f: U \to \mathbb{R}$ be a function defined on a set $\emptyset \neq U \subseteq \mathbb{R}^n$. Assume that $x^* \in int(U)$ is a local optimum point and that all the partial derivatives of f exist at x^* . Then $\nabla f(x^*) = \mathbf{0}$. (Fermat's theorem in 1D)

Proof: Given $1 \le i \le n$, we define the function $g_i(t) := f(x^* + te_i)$. Then g_i is differentiable at t = 0 and $g_i'(0) = \nabla f(x^*) \cdot e_i = \frac{\partial f}{\partial x_i}(x^*)$. Since x^* is a local optimum point of f, it follows that t = 0 is a local optimum of g_i . By Fermat's theorem, we have $g_i'(0) = 0$, which implies that $\nabla f(x^*) = 0$.

Note: First order optimality condition is only *a necessary condition*.

Definition: Let $f: U \to \mathbb{R}$ be a function defined on a set $\emptyset \neq U \subseteq \mathbb{R}^n$. Assume that $x^* \in int(U)$ and all the partial derivatives of f exist over some neighborhood of x^* . If $\nabla f(x^*) = \mathbf{0}$, then x^* is called a stationary point of f.

Positive definiteness (review)

- Let $A \in \mathbb{C}^{n \times n}$ be a square matrix and $x, y \in \mathbb{C}^n$. Define $x^* := \overline{x}^\top$, $(x,y) := y^*x \in \mathbb{C}$. Then $(Ax,x) = x^*Ax$ is called a quadratic form.
- **Definition:** Let $A \in \mathbb{C}^{n \times n}$.

A is positive definite
$$\iff$$
 $(Ax, x) > 0$, $\forall 0 \neq x \in \mathbb{C}^n$.

- Note 1: $A = A^* (:= \overline{A}^\top) \iff (Ax, x) \in \mathbb{R}, \forall x \in \mathbb{C}^n$.
- Note 2: If $A \in \mathbb{C}^{n \times n}$ is positive definite, then $A = A^*$. (by Note 1)
- Note 3: Let $A \in \mathbb{R}^{n \times n}$. A is positive definite $\iff A = A^{\top}$ and (Ax, x) > 0, $\forall 0 \neq x \in \mathbb{R}^{n}$. Proof: (⇒) Trivial! (⇐) Let $0 \neq x := x_{1} + ix_{2} \in \mathbb{C}^{n}$. Then $x_{1} \neq 0$ or $x_{2} \neq 0$. $\therefore (A(x_{1} + ix_{2}), (x_{1} + ix_{2})) = (Ax_{1}, x_{1}) - i(Ax_{1}, x_{2}) + i(Ax_{2}, x_{1}) + (Ax_{2}, x_{2})$ $\because -i(Ax_{1}, x_{2}) = -i(x_{1}, A^{*}x_{2}) = -i(x_{1}, A^{\top}x_{2}) = -i(x_{1}, Ax_{2}) = -i(Ax_{2}, x_{1})$ $\therefore (A(x_{1} + ix_{2}), (x_{1} + ix_{2})) = (Ax_{1}, x_{1}) + (Ax_{2}, x_{2}) > 0$
- Note 4: Let $A \in \mathbb{C}^{n \times n}$ and $A = A^*$. Then A is positive definite \iff all of its eigenvalues are real and positive.

Proof of Note 1

$$(\Rightarrow) :: (Ax,x) = x^*Ax = (Ax)^*x = (x,Ax) = \overline{(Ax,x)}, \forall x \in \mathbb{C}^n$$

$$:: (Ax,x) \in \mathbb{R}, \forall x \in \mathbb{C}^n$$

- (⇐) $\forall x,y \in \mathbb{C}^n$, we have $\mathbb{R} \ni (x+y)^*A(x+y) = x^*Ax + y^*Ay + x^*Ay + y^*Ax$. $\therefore x^*Ay + y^*Ax \in \mathbb{R}$
 - Let $x = e_j \in \mathbb{R}^n$, $y = e_k \in \mathbb{R}^n$. Then $\mathbb{R} \ni x^*Ay + y^*Ax = a_{jk} + a_{kj}$ $\therefore Im(a_{jk}) = -Im(a_{kj})$ $\therefore a_{jk} := a + bi$ and $a_{kj} := c - bi$ for some $a, b, c \in \mathbb{R}$
 - Let $x = ie_i \in \mathbb{C}^n$, $y = e_k \in \mathbb{R}^n$. Then

$$\mathbb{R} \ni x^*Ay + y^*Ax = -ia_{jk} + ia_{kj} = (-ia + b) + (ci + b) = (c - a)i + 2b.$$

$$\therefore c = a$$
. Then $a_{jk} := a + bi = \overline{a - bi} = \overline{a_{kj}}$

$$A = \overline{A}^{\top} = A^*$$

Positive definiteness

- **Definition:** A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is called positive semidefinite, denoted by $A \succeq \mathbf{0}$, if $\mathbf{x}^{\top} A \mathbf{x} \geq 0$, $\forall \mathbf{x} \in \mathbb{R}^{n}$.
- **Definition:** A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is called positive definite, denoted by $A \succ \mathbf{0}$, if $\mathbf{x}^{\top} A \mathbf{x} > 0$, $\forall \mathbf{0} \neq \mathbf{x} \in \mathbb{R}^{n}$.
- **Example:** Let $A := \begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix}$. $\forall x = (x_1, x_2)^{\top} \in \mathbb{R}^2$, we have

$$\mathbf{x}^{\top} A \mathbf{x} = \begin{bmatrix} x_1, x_2 \end{bmatrix} \begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$
$$= 2x_1^2 - 2x_1x_2 + x_2^2 = x_1^2 + (x_1 - x_2)^2 \ge 0.$$

Since $x_1^2 + (x_1 - x_2)^2 = 0$ iff $x_1 = x_2 = 0$, we have A > 0.

• **Example:** Let $A := \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$. One can show that A is not positive definite. *Hint: consider* $\mathbf{x} = (1, -1)^{\top}$

The diagonal components of a positive definite matrix

- Note: Let $A \in \mathbb{R}^{n \times n}$ and $A \succ 0$. Then the diagonal elements of A are positive. Proof: $A_{ii} = e_i^{\top} A e_i > 0$, $\forall i$. \square Let $A \in \mathbb{R}^{n \times n}$ and $A \succeq 0$. Then the diagonal elements of A are nonnegative.
- **Definition:** $A \leq 0$ (negative semidefinite) iff $-A \succeq 0$. A < 0 (negative definite) iff $-A \succ 0$.
- Note: Let $A \in \mathbb{R}^{n \times n}$ and $A \prec 0$. Then the diagonal elements of A are negative.
 - Let $A \in \mathbb{R}^{n \times n}$ and $A \leq \mathbf{0}$. Then the diagonal elements of A are nonpositive.
- **Definition:** A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is called indefinite if $\exists x, y \in \mathbb{R}^n$ such that $x^\top Ax > 0$ and $y^\top Ay < 0$.
- Note: Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix. If there exist positive and negative elements in the diagonal of A, then A is indefinite.

Proof: Let *i* and *j* be the indices such that $A_{ii} > 0$ and $A_{jj} < 0$. Then $e_i^{\top} A e_i = A_{ii} > 0$ and $e_i^{\top} A e_j = A_{jj} < 0$.

Eigenvalue characterization theorem

Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix. Then

• $A \succ 0$ if and only if all its eigenvalues are positive.

Proof: By the spectral decomposition theorem, there exist an orthogonal matrix U and a diagonal matrix $D = diag(d_1, \cdots, d_n)$ whose diagonal elements are the eigenvalues of A, for which $U^{\top}AU = D$. For any $0 \neq x \in \mathbb{R}^n$, let $y = U^{-1}x$. Then

$$x^{\top}Ax = y^{\top}U^{\top}AUy = y^{\top}Dy = \sum_{i=1}^{n} d_i y_i^2.$$

Therefore, $x^{\top}Ax > 0$ for any $x \neq \mathbf{0}$ if and only if $\sum_{i=1}^{n} d_i y_i^2 > 0$ for any $y \neq \mathbf{0}$.

- (1) For any given i, let $y = e_i$, we have $d_i > 0$, i.e., all eigenvalues are positive.
- (2) If $d_i > 0 \ \forall i$, then $\sum_{i=1}^n d_i y_i^2 > 0$ for any $y \neq \mathbf{0}$, i.e., $x^\top A x > 0$ for any $x \neq \mathbf{0}$. \square
- $A \succeq 0$ if and only if all its eigenvalues are nonnegative.
- $A \prec 0$ if and only if all its eigenvalues are negative.
- $A \leq 0$ if and only if all its eigenvalues are nonpositive.
- A is indefinite if and only if it has at least one positive eigenvalue and at least one negative eigenvalue.

Trace and determinant

- If $A \succ \mathbf{0}(\succeq \mathbf{0})$, then $Tr(A) > (\geq)0$ and $det(A) > (\geq)0$.

 Idea of the proof: The trace and determinant of a symmetric matrix are the sum and product of its eigenvalues respectively.
- *Above two conditions are necessary and sufficient for* 2×2 *matrix A*. *Idea of the proof:* For any two real number $a, b \in \mathbb{R}$, one has $a, b > (\geq)0$ if and only if a + b > (>)0 and ab > (>)0.
- Example: Consider the matrices

$$A := \begin{bmatrix} 4 & 1 \\ 1 & 3 \end{bmatrix}, \qquad B := \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 0.1 \end{bmatrix}.$$

- (1) $A \succ \mathbf{0}$ since Tr(A) = 7 > 0 and det(A) = 11 > 0.
- (2) As for the matrix B, Tr(B) = 2.1 > 0 and det(B) = 0. Even so, we cannot conclude that the matrix B is positive semidefinite. In fact, B is indefinite since

$$e_1^{\mathsf{T}}Be_1 = 1 > 0$$
, $(e_2 - e_3)^{\mathsf{T}}B(e_2 - e_3) = -0.9 < 0$.

Positive semidefinite square root

Given $A \succeq \mathbf{0}$, let $A = \mathbf{U}\mathbf{D}\mathbf{U}^{\top}$ be the spectral decomposition, where \mathbf{U} is an orthogonal matrix, $\mathbf{D} = diag(d_1, d_2, \cdots, d_n)$ is a diagonal matrix whose diagonal elements are the eigenvalues of A. Since $A \succeq \mathbf{0}$, we have $d_1, d_2, \cdots, d_n \geq 0$. We define

$$A^{\frac{1}{2}} := \mathbf{U} \mathbf{E} \mathbf{U}^{\top}, \quad \mathbf{E} = diag(\sqrt{d_1}, \sqrt{d_2}, \cdots, \sqrt{d_n}).$$

Obviously,

$$A^{\frac{1}{2}}A^{\frac{1}{2}} = UEU^{\top}UEU^{\top} = UEEU^{\top} = UDU^{\top} = A.$$

The matrix $A^{\frac{1}{2}}$ *is called the positive semidefinite square root.*

Principal minors criterion

- **Definition:** Given an $n \times n$ matrix, the determinant of the upper left $k \times k$ submatrix is called the kth principal minor, denoted by $D_k(A)$.
- **Example:** The principal minors of the $k \times k$ matrix

$$A := \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

are $D_1(A) = a_{11}$,

$$D_2(A) = \det \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}, \ D_3(A) = \det \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}.$$

• **Principal minors criterion:** Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix. Then $A \succ \mathbf{0}$ if and only if $D_1(A) > 0$, $D_2(A) > 0$, \cdots , $D_n(A) > 0$.

Note: It cannot be used for detecting positive semidefiniteness!

Diagonally dominant matrices

- **Definition:** Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix. Then
 - (1) A is called diagonally dominant if $|A_{ii}| \ge \sum_{j \ne i} |A_{ij}|, \forall i$.
 - (2) A is called strictly diagonally dominant if $|A_{ii}| > \sum_{j \neq i} |A_{ij}|, \forall i$.
- **Theorem:** Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix.
 - (1) If A is a diagonally dominant matrix whose diagonal elements are nonnegative. Then $A \succeq 0$.
 - (2) If A is a strictly diagonally dominant matrix whose diagonal elements are positive. Then $A \succ 0$.

Proof: (1). Suppose $\exists \ \lambda < 0$ an eigenvalue of A. Let $\mathbf{u} = (u_1, \cdots, u_n)^\top$ be a corresponding eigenvector. Let $|u_i| = \max\{|u_1|, \cdots, |u_n|\}$. Then by $A\mathbf{u} = \lambda \mathbf{u}$,

$$|A_{ii} - \lambda||u_i| = \left|\sum_{i \neq i} A_{ij} u_i\right| \le \left(\sum_{i \neq i} |A_{ij}|\right) |u_i| \le |A_{ii}||u_i|,$$

implying $|A_{ii} - \lambda| \le |A_{ii}|$. This is a contradiction.

(2). From (1), we know that $A \succeq 0$. Thus, all we need to show is that A has no zero eigenvalues. Suppose \exists eigenvalue $\lambda = 0$, $u \neq 0$ such that Au = 0. Similar to part (1), we obtain

$$|A_{ii}||u_i| = \left|\sum_{j\neq i} A_{ij} u_j\right| \le \left(\sum_{j\neq i} |A_{ij}|\right) |u_i| < |A_{ii}||u_i|.$$

This is obviously a contradiction.

Necessary second order optimality condition

Theorem: Let $f: U \to \mathbb{R}$ be a function defined on an open set $U \subseteq \mathbb{R}^n$. Assume that f is twice continuously differentiable over U and that x^* is a stationary point. Then the following hold:

- (1) If x^* is a local minimum point of f over U, then $\nabla^2 f(x^*) \succeq \mathbf{0}$.
- (2) If x^* is a local maximum point of f over U, then $\nabla^2 f(x^*) \leq 0$.

Proof: (1). Since x^* is a local minimum point, $\exists B(x^*,r) \subseteq U$ for which $f(x^*) \le f(x)$, $\forall x \in B(x^*,r)$. Let $\mathbf{0} \ne d \in \mathbb{R}^n$. For any $0 < \alpha < \frac{r}{\|d\|}$, we have $x^*_\alpha := x^* + \alpha d \in B(x^*,r)$ and $f(x^*_\alpha) \ge f(x^*)$. By the linear approximation theorem, $\exists z_\alpha \in (x^*,x^*_\alpha)$ such that

$$f(x_{\alpha}^*) - f(x^*) = \underbrace{\nabla f(x^*)^{\top}}_{0} (x_{\alpha}^* - x^*) + \frac{1}{2} (x_{\alpha}^* - x^*)^{\top} \nabla^2 f(z_{\alpha}) (x_{\alpha}^* - x^*) = \frac{\alpha^2}{2} d^{\top} \nabla^2 f(z_{\alpha}) d.$$

Thus, $d^{\top}\nabla^2 f(z_{\alpha})d \geq 0$, $\forall \alpha \in (0, \frac{r}{\|d\|})$. Using the fact that $z_{\alpha} \to x^*$ as $\alpha \to 0^+$, and the continuity of the Hessian, we obtain $d^{\top}\nabla^2 f(x^*)d \geq 0$. We conclude that $\nabla^2 f(x^*) \geq 0$.

(2). Employing the result of part (1) on the function -f, we obtain (2).

Sufficient second order optimality condition

Theorem: Let $f: U \to \mathbb{R}$ be a function defined on an open set $U \subseteq \mathbb{R}^n$. Assume that f is twice continuously differentiable over U and that x^* is a stationary point. Then the following hold:

- (1) If $\nabla^2 f(x^*) > 0$, then x^* is a strict local minimum point of f over U.
- (2) If $\nabla^2 f(x^*) \prec 0$, then x^* is a strict local maximum point of f over U.

Proof: (1) Since the Hessian is continuous, it follows that there exists a ball $B(x^*,r) \subseteq U$ s.t. $\nabla^2 f(x) \succ 0$, $\forall x \in B(x^*,r)$ (using the principal minors criterion on page 16). By the linear approximation theorem, it follows that for any $x \in B(x^*,r)$, $\exists z_x \in (x^*,x) \subset B(x^*,r)$ such that

$$f(x) - f(x^*) = \frac{1}{2}(x - x^*)^{\top} \nabla^2 f(z_x)(x - x^*).$$

Since $\nabla^2 f(z_x) \succ \mathbf{0}$, it follows that

$$f(x) - f(x^*) > 0$$
, for $x \neq x^*$.

That is, x^* is a strict local minimum point of f over U.

(2) This part follows from part (1) by considering the function -f. \Box

Sufficient condition for a saddle point

- **Definition:** Let $f: U \to \mathbb{R}$ be a function defined on an open set $U \subseteq \mathbb{R}^n$. Assume that f is continuously differentiable over U. A stationary point x^* is called a saddle point of f over U if it is neither a local minimum point nor a local maximum point of f over U.
- Sufficient condition for a saddle point: Let $f: U \to \mathbb{R}$ be a function defined on an open set $U \subseteq \mathbb{R}^n$. Assume that f is twice continuously differentiable over U and that x^* is a stationary point. If $\nabla^2 f(x^*)$ is an indefinite matrix, then x^* is a saddle point of f over U.

Proof: Let $\lambda>0$ be an eigenvalue of $\nabla^2 f(x^*)$ with a normalized eigenvector v. Since U is open, $\exists \ r>0$ such that $x^*+\alpha v\in U, \ \forall \ \alpha\in(0,r)$. By the quadratic approximation theorem and $\nabla f(x^*)=\mathbf{0}$, we have

$$f(x^* + \alpha v) = f(x^*) + \frac{\alpha^2}{2} v^{\top} \nabla^2 f(x^*) v + o(\alpha^2 ||v||^2)$$

$$= f(x^*) + \frac{\lambda \alpha^2}{2} ||v||^2 + o(\alpha^2 ||v||^2) = f(x^*) + \frac{\lambda \alpha^2}{2} + o(\alpha^2).$$
Co $\frac{o(\alpha^2)}{2} \to 0$ as $\alpha \to 0^+$ is $\alpha \in (0, r)$ such that $\alpha(\alpha^2) > -\frac{\lambda}{2} \alpha^2 \forall \alpha \in (0, r)$.

Since $\frac{o(\alpha^2)}{\alpha^2} \to 0$ as $\alpha \to 0^+$, $\exists \ \epsilon_1 \in (0,r)$ such that $o(\alpha^2) > -\frac{\lambda}{2}\alpha^2$, $\forall \ \alpha \in (0,\epsilon_1)$.

Hence, $f(x^* + \alpha v) > f(x^*)$. This shows that x^* cannot be a local maximum point of f over U. Similarly, we can show that x^* cannot be a local minimum point of f over U. Therefore, x^* is a saddle point of f over U. \square

Weierstrass theorem

- Weierstrass Theorem: Let $f: \emptyset \neq C \subseteq \mathbb{R}^n \to \mathbb{R}$ be a continuous function and C is a compact set. Then there exist a global minimum point of f over C and a global maximum point of f over C.
- **Definition:** Let $f : \mathbb{R}^n \to \mathbb{R}$ be a continuous function defined over \mathbb{R}^n . The function f is called coercive if $\lim_{\|\mathbf{x}\| \to \infty} f(\mathbf{x}) = \infty$.
- Attainment under coerciveness: Let $f : \mathbb{R}^n \to \mathbb{R}$ be a continuous and coercive function and let $S \subseteq \mathbb{R}^n$ be a nonempty closed set. Then f has a global minimum point over S.

Proof:

- (1) Let $x_0 \in S$. Since f is coercive, $\exists M > 0$ such that $f(x) > f(x_0)$, $\forall x \in \mathbb{R}^n$ and ||x|| > M.
- (2) Since any global minimizer x^* of f over S satisfies $f(x^*) \le f(x_0)$, it follows that the set of global minimizers of f over S is the same as the set of global minimizers of f over $S \cap B[0, M]$.
- (3) The set $S \cap B[0, M]$ is compact and nonempty, by the Weierstrass theorem, there exists a global minimizer of f over $S \cap B[0, M]$ and hence also over S.

Consider $f(x_1, x_2) = x_1^2 + x_2^2$ over the set $C = \{(x_1, x_2) \in \mathbb{R}^2 : x_1 + x_2 \le -1\}$.

- Since C is not bounded, the Weierstrass theorem does not guarantee the existence of global minimizer and maximizer of f over C. Obviously, f has no global maximizer over C.
- *f* is coercive and *C* is closed, *f* has a global minimizer over *C*.
- In the interior of *C*: $\nabla f(x_1, x_2) = \mathbf{0} \Rightarrow (x_1, x_2) = (0, 0) \notin C$. At the boundary of *C*: $\{(x_1, x_2) : x_1 + x_2 = -1\} \Rightarrow x_1 = -x_2 - 1$. $g(x_2) := f(-x_2 - 1, x_2) = (-x_2 - 1)^2 + x_2^2$ $g'(x_2) = 2(1 + x_2) + 2x_2 \Rightarrow g'(x_2) = 0 \Rightarrow x_2 = -\frac{1}{2} \Rightarrow x_1 = -\frac{1}{2}$.

Thus, $(x_1, x_2) = (-\frac{1}{2}, -\frac{1}{2})$ is the only candidate for a global minimum point. Therefore, $(x_1, x_2) = (-\frac{1}{2}, -\frac{1}{2})$ is the global minimum point of f over C.

Consider the function $f(x_1, x_2) = 2x_1^3 + 3x_2^2 + 3x_1^2x_2 - 24x_2$ over \mathbb{R}^2 .

- $\nabla f(x_1, x_2) = \begin{bmatrix} 6x_1^2 + 6x_1x_2 \\ 6x_2 + 3x_1^2 24 \end{bmatrix} := \mathbf{0}$. Then the stationary points of the function f are $(x_1, x_2) = (0, 4), (4, -4), (-2, 2)$.
- The Hessian of f is given by $\nabla^2 f(x_1, x_2) = 6 \begin{bmatrix} 2x_1 + x_2 & x_1 \\ x_1 & 1 \end{bmatrix}$.
- $\nabla^2 f(0,4) = 6 \begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix} \succ \mathbf{0} \Rightarrow (0,4)$ is a strict local minimum point. It is not a global minimum point, since $f(x_1,0) = 2x_1^3 \to -\infty$ as $x_1 \to -\infty$.

$$\nabla^2 f(4, -4) = 6 \begin{bmatrix} 4 & 4 \\ 4 & 1 \end{bmatrix}$$
, $tr(A) > 0$ but $det(A) < 0$, an indefinite matrix.

 \therefore (4,-4) is a saddle point

$$abla^2 f(-2,2) = 6 \begin{bmatrix} -2 & -2 \\ -2 & 1 \end{bmatrix}$$
 is indefinite, since it has both positive and negative elements on its diagonal (cf. page 10).

 \therefore (-2,2) is a saddle point

Consider the function $f(x_1, x_2) = (x_1^2 + x_2^2 - 1)^2 + (x_2^2 - 1)^2$ over \mathbb{R}^2 .

•
$$\nabla f(x_1, x_2) = 4 \begin{bmatrix} (x_1^2 + x_2^2 - 1)x_1 \\ (x_1^2 + x_2^2 - 1)x_2 + (x_2^2 - 1)x_2 \end{bmatrix} := \mathbf{0}.$$

Then the stationary points are (0,0), (1,0), (-1,0), (0,1), (0,-1).

• The Hessian of the function is

$$\nabla^2 f(x_1,x_2) = 4 \begin{bmatrix} 3x_1^2 + x_2^2 - 1 & 2x_1x_2 \\ 2x_1x_2 & x_1^2 + 6x_2^2 - 2 \end{bmatrix}.$$

 \therefore (0,0) is a strict local maximum point (not global, $\because f(x_1,0) = (x_1^2 - 1)^2 + 1 \to \infty$)

$$\nabla^2 f(1,0) = \nabla^2 f(-1,0) = 4 \begin{bmatrix} 2 & 0 \\ 0 & -1 \end{bmatrix}$$
, indefinite matrix.

 \therefore (1,0), (-1,0) saddle points

$$\nabla^2 f(0,1) = \nabla^2 f(0,-1) = 4 \begin{bmatrix} 0 & 0 \\ 0 & 4 \end{bmatrix} \succeq \mathbf{0}$$
, no conclusion!

$$f(0,1) = f(0,-1) = 0$$
 and f is bounded below by 0

(0,1), (0,-1) are global minimum points

Contour and surface plots of Example 3

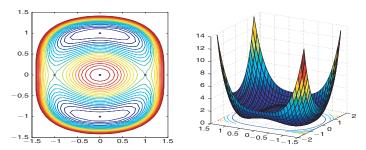


Figure 2.3. Contour and surface plots of $f(x_1, x_2) = (x_1^2 + x_2^2 - 1)^2 + (x_2^2 - 1)^2$. The five stationary points (0,0),(0,1),(0,-1),(1,0), are denoted by asterisks. The points (0,-1),(0,1) are strict local minimum points as well as global minimum points, (0,0) is a local maximum point, and (-1,0),(1,0) are saddle points.

```
ezsurfc('(x^2 + y^2 - 1)^2 + (y^2 - 1)^2', [-2 2 -1.5 1.5]) colorbar view(-30, 30)
```

Consider the function $f(x,y) = \frac{x+y}{x^2+y^2+1}$ over \mathbb{R}^2 .

•
$$\nabla f(x,y) = \frac{1}{(x^2 + y^2 + 1)^2} \begin{bmatrix} (x^2 + y^2 + 1) - 2(x + y)x \\ (x^2 + y^2 + 1) - 2(x + y)y \end{bmatrix} := \mathbf{0}. \Rightarrow$$

 $-x^2 - 2xy + y^2 = -1, x^2 - 2xy - y^2 = -1$
 $\Rightarrow xy = 1/2 \text{ (adding)}, x^2 = y^2 \text{ (subtracting)}$
 $\Rightarrow \text{ stationary points are } (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}), (\frac{-1}{\sqrt{2}}, \frac{-1}{\sqrt{2}})$

• For any $(x,y)^{\top} \in \mathbb{R}^2$, from the Cauchy-Schwarz inequality,

$$f(x,y) = \frac{(x,y)^{\top} \cdot (1,1)^{\top}}{x^2 + y^2 + 1} \le \sqrt{2} \frac{\sqrt{x^2 + y^2}}{x^2 + y^2 + 1} \le \sqrt{2} \max_{t \ge 0} \frac{t}{t^2 + 1} \le \frac{\sqrt{2}}{2}.$$

$$\therefore (t-1)^2 \ge 0 \Rightarrow t^2 + 1 \ge 2t$$

•
$$: f(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}) = \frac{\sqrt{2}}{2} : (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$$
 is the global maximum point
Similarly, $: \frac{(-x, -y)^{\top} \cdot (1, 1)^{\top}}{x^2 + y^2 + 1} \le \frac{\sqrt{2}}{2} : f(x, y) \ge \frac{-\sqrt{2}}{2}$
 $: f(\frac{-1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}) = \frac{-\sqrt{2}}{2} : (\frac{-1}{\sqrt{2}}, \frac{-1}{\sqrt{2}})$ is the global minimum point

Consider the function $f(x_1, x_2) = -2x_1^2 + x_1x_2^2 + 4x_1^4$ over \mathbb{R}^2 .

- $\nabla f(x_1, x_2) = \begin{bmatrix} -4x_1 + x_2^2 + 16x_1^3 \\ 2x_1x_2 \end{bmatrix} := \mathbf{0}.$ \Rightarrow stationary points are (0,0), (1/2,0), (-1/2,0).
- The Hessian of the function is $\nabla^2 f(x_1, x_2) = \begin{bmatrix} -4 + 48x_1^2 & 2x_2 \\ 2x_2 & 2x_1 \end{bmatrix}$.
- $\nabla^2 f(1/2,0) = \begin{bmatrix} 8 & 0 \\ 0 & 1 \end{bmatrix} \succ \mathbf{0}.$ \therefore (1/2,0) is a strict local minimum point (not global, $f(-1,x_2) = 2 x_2^2 \rightarrow -\infty$, $x_2 \rightarrow \infty$) $\nabla^2 f(-1/2,0) = \begin{bmatrix} 8 & 0 \\ 0 & -1 \end{bmatrix}$, indefinite. \therefore (-1/2,0) saddle point $\nabla^2 f(0,0) = \begin{bmatrix} -4 & 0 \\ 0 & 0 \end{bmatrix}$, a negative semidefinite matrix. $\therefore f(\alpha^4,\alpha) = \alpha^6(-2\alpha^2 + 1 + 4\alpha^{10}) > 0$ $f(-\alpha^4,\alpha) = \alpha^6(-2\alpha^2 1 + 4\alpha^{10}) < 0 \text{ for } 0 < \alpha \ll 1$ $\therefore (0,0) \text{ is a saddle point of } f$

Contour and surface plots of Example 5

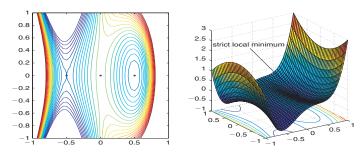


Figure 2.4. Contour and surface plots of $f(x_1, x_2) = -2x_1^2 + x_1 x_2^2 + 4x_1^4$. The three stationary point (0,0), (0.5,0), (-0.5,0) are denoted by asterisks. The point (0.5,0) is a strict local minimum, while (0,0) and (-0.5,0) are saddle points.

```
ezsurfc('-2*x^2 + x*y^2 + 4*x^4', [-1 1 -1 1]) colorbar view(-45, 30)
```

Global optimality conditions

• Theorem: Let $f: \mathbb{R}^n \to \mathbb{R}$ be a twice continuously differentiable function. Assume that $\nabla^2 f(x) \succeq \mathbf{0}$, $\forall x \in \mathbb{R}^n$. Let $x^* \in \mathbb{R}^n$ be a stationary point of f. Then x^* is a global minimum point of f.

Proof: By the linear approximation theorem, $\forall x \in \mathbb{R}^n$, $\exists z_x \in (x^*, x)$ such that

$$f(x) - f(x^*) = \frac{1}{2}(x - x^*)^{\top} \nabla^2 f(z_x)(x - x^*).$$

Since $\nabla^2 f(z_x) \succeq \mathbf{0}$, we have $f(x) \geq f(x^*)$. $\therefore x^*$ is a global minimum point of $f \square$

• Example:

$$f(\mathbf{x}) := x_1^2 + x_2^2 + x_3^2 + x_1x_2 + x_1x_3 + x_2x_3 + (x_1^2 + x_2^2 + x_3^2)^2.$$

$$\nabla f(\mathbf{x}) = \begin{bmatrix} 2x_1 + x_2 + x_3 + 4x_1(x_1^2 + x_2^2 + x_3^2) \\ 2x_2 + x_1 + x_3 + 4x_2(x_1^2 + x_2^2 + x_3^2) \\ 2x_3 + x_1 + x_2 + 4x_3(x_1^2 + x_2^2 + x_3^2) \end{bmatrix}.$$

Obviously, $(x_1, x_2, x_3) = (0, 0, 0)$ is a stationary point.

The Hessian is $\nabla^2 f(x) = A + B(x) + C(x)$, where

$$A = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} \succeq \mathbf{0}$$
, since it is diagnoally dominant with positive diagonal

elements, $B(x) = 4(x_1^2 + x_2^2 + x_3^2)I_3 \succeq \mathbf{0}$, and $C(x) = 8xx^{\top} \succeq \mathbf{0}$.

 $\nabla^2 f(x) \succeq \mathbf{0}$ $\therefore x = (0,0,0)^{\top}$ is a global minimum point of f over \mathbb{R}^3

Quadratic functions

Quadratic functions are an important class of functions that are useful in the modeling of many optimization problems.

• **Definition:** A quadratic function over \mathbb{R}^n is a function of the form

$$f(x) = x^{\top} A x + 2b^{\top} x + c,$$

where $A \in \mathbb{R}^{n \times n}$ is symmetric, $b \in \mathbb{R}^n$, and $c \in \mathbb{R}$.

• The gradient and Hessian of the above quadratic function f(x):

$$\nabla f(x) = 2Ax + 2b$$
, $\nabla^2 f(x) = 2A$.

- Properties of quadratic functions:
 - (1) x is a stationary point of f iff Ax = -b.
 - (2) If $A \succeq \mathbf{0}$, then x is a global minimum point of f iff $Ax = -\mathbf{b}$. *Proof*: By Theorems on page 8 and page 29. \square
 - (3) If $A \succ 0$, $x = -A^{-1}b$ is a strict global minimum point of f.

 Proof: If $A \succ 0$, then $x = -A^{-1}b$ is the unique solution to Ax = -b. Hence, it is the unique global minimum point of f.

Note: In (3), the minimal value of f is given by

$$f(x) = (-A^{-1}b)^{\top}A(-A^{-1}b) - 2b^{\top}A^{-1}b + c = c - b^{\top}A^{-1}b.$$

Coerciveness of quadratic functions

Theorem: Let $f(x) = x^{\top}Ax + 2b^{\top}x + c$, where $A \in \mathbb{R}^{n \times n}$ is symmetric, $b \in \mathbb{R}^n$, and $c \in \mathbb{R}$. Then f is coercive if and only if $A \succ 0$.

Proof:

(\Rightarrow) Assume that $A \succ 0$. Then $x^{\top}Ax \ge \alpha ||x||^2$ with $\alpha = \lambda_{\min}(A) > 0$. Thus,

$$f(x) \geq \alpha \|x\|^2 - 2\|b\| \|x\| + c = \alpha \|x\| \left(\|x\| - 2\frac{\|b\|}{\alpha} \right) + c \to \infty, \quad \text{as } \|x\| \to \infty.$$

Therefore, f is coercive.

(\Leftarrow) Assume that f is coercive. We need to prove that $A \succ \mathbf{0}$. We first show that there does not exist a negative eigenvalue. Suppose $\exists \ \mathbf{0} \neq v \in \mathbb{R}^n, \ \lambda < 0 \ \text{s.t.} \ Av = \lambda v$. Then for any $\alpha \in \mathbb{R}$,

$$f(\alpha v) = \lambda ||v||^2 \alpha^2 + 2(b^\top v)\alpha + c \to -\infty$$
 as $\alpha \to \infty$.

This is a contradiction. We now show that 0 cannot be an eigenvalue of A. Suppose $\exists \ \mathbf{0} \neq v \in \mathbb{R}^n$ s.t. $Av = \mathbf{0}$. Then for any $\alpha \in \mathbb{R}$,

$$f(\alpha \mathbf{v}) = 2(\mathbf{b}^{\top} \mathbf{v})\alpha + c.$$

If $\mathbf{b}^{\top}\mathbf{v} = 0$ then $f(\alpha \mathbf{v}) \to c$ as $\alpha \to \infty$. If $\mathbf{b}^{\top}\mathbf{v} > 0$ then $f(\alpha \mathbf{v}) \to -\infty$ as $\alpha \to -\infty$. If $\mathbf{b}^{\top}\mathbf{v} < 0$ then $f(\alpha \mathbf{v}) \to -\infty$ as $\alpha \to \infty$. All these contradict the coerciveness of f.

Characterization of the nonnegativity of quadratic functions

Theorem: Let $f(x) = x^{T}Ax + 2b^{T}x + c$, where $A \in \mathbb{R}^{n \times n}$ is symmetric. $b \in \mathbb{R}^n$, and $c \in \mathbb{R}$. Then the following two claims are equivalent:

(a)
$$f(x) = x^{\top}Ax + 2b^{\top}x + c \ge 0, \forall x \in \mathbb{R}^n$$
.

(b)
$$\begin{bmatrix} A & b \\ b^\top & c \end{bmatrix} \succeq \mathbf{0}.$$

Proof:

(b)
$$\Rightarrow$$
 (a): For any $x \in \mathbb{R}^n$, $0 \le \begin{bmatrix} x \\ 1 \end{bmatrix}^\top \begin{bmatrix} A & b \\ b^\top & c \end{bmatrix} \begin{bmatrix} x \\ 1 \end{bmatrix} = x^\top Ax + 2b^\top x + c \Rightarrow$ (a).

(a) \Rightarrow (b): We begin by showing that $A \succ 0$.

Suppose not. $\exists \mathbf{0} \neq v \in \mathbb{R}^n$ and $\lambda < 0$ s.t. $Av = \lambda v$. Thus, for any $\alpha \in \mathbb{R}$,

$$f(\alpha v) = \lambda ||v||^2 \alpha^2 + 2(b^\top v)\alpha + c \to -\infty$$
 as $\alpha \to -\infty$,

contradicting the nonnegativity of f. Our objective is to prove (b). We want to show that for any $y \in \mathbb{R}^n$ and $t \in \mathbb{R}$, $\begin{bmatrix} y \\ t \end{bmatrix}^{\top} \begin{bmatrix} A & b \\ b^{\top} & c \end{bmatrix} \begin{bmatrix} y \\ t \end{bmatrix} \ge 0$, which is equivalent to

$$\mathbf{y}^{\top} A \mathbf{y} + 2t \mathbf{b}^{\top} \mathbf{y} + c t^2 \ge 0. \qquad (\star)$$

If t = 0 then $\mathbf{y}^{\top} A \mathbf{y} + 2t \mathbf{b}^{\top} \mathbf{y} + c t^2 = \mathbf{y}^{\top} A \mathbf{y} > 0$, since $A \succeq \mathbf{0}$. We obtain (\star) . If $t \neq 0$ then $0 < t^2 f(\mathbf{y}/t) = \mathbf{y}^{\top} A \mathbf{y} + 2t \mathbf{b}^{\top} \mathbf{y} + c t^2$, we have (\star) .