Optimization Techniques
Lecture 2
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Gradient, Hessian, Convexity of functions, Definiteness

Gradient

- When f is real-valued (i.e.f:$R^n \rightarrow R$) the derivative Df(x) is a 1xn matrix, i.e. it is a row vector. Its transpose is called the gradient of the function:

$$\nabla f(x) = Df(x)^T$$

- which is a column vector, i.e. in R^n. Its components are the partial derivatives of f:

$$\nabla f(x)_i = \frac{\partial f(x)}{\partial x_i}, i = 1,2,\ldots,n$$

$$\nabla f(x) = \left[\frac{\partial f(x)}{\partial x_1}, \frac{\partial f(x)}{\partial x_2}, \ldots, \frac{\partial f(x)}{\partial x_n}\right]^T$$

The direction of ∇f is the orientation in which the directional derivative has the largest value and $|\nabla f|$ is the value of that directional derivative.

Hessian Matrix -Second Derivative

Given $f : \mathbb{R}^n \to \mathbb{R}$, if ∇f is differentiable, we say that f is *twice differentiable*, and we write the derivative of ∇f as

$$D^2 f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_2 \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_1} \\ \frac{\partial^2 f}{\partial x_1 \partial x_2} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_1 \partial x_n} & \frac{\partial^2 f}{\partial x_2 \partial x_n} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}.$$

The matrix $D^2 f(\boldsymbol{x})$ is called the *Hessian* matrix of f at $\boldsymbol{x}$, and is often also denoted $\boldsymbol{F}(\boldsymbol{x})$.

Find the Hessian Matrix of the function $f(x, y) = x^2y + xy^3$**.**

We need to first find the first partial derivatives of f. We have that:

$$\frac{\partial f}{\partial x} = 2xy + y^3 \quad , \quad \frac{\partial f}{\partial y} = x^2 + 3xy^2$$

We then calculate the second partial derivatives of f:

$$\frac{\partial^2 f}{\partial x^2} = 2y \quad , \quad \frac{\partial^2 f}{\partial y \partial x} 2x + 3y^2 \quad , \quad \frac{\partial^2 f}{\partial x \partial y} = 2x + 3y^2 \quad , \quad \frac{\partial^2 f}{\partial y^2} = 6xy$$

Therefore the Hessian Matrix of f is:

$$\mathcal{H}(x, y) = \begin{bmatrix} 2y & 2x + 3y^2 \\ 2x + 3y^2 & 6xy \end{bmatrix}$$

Example 6.1 Let $f(x_1, x_2) = 5x_1 + 8x_2 + x_1x_2 - x_1^2 - 2x_2^2$.

Theorem 21.2 *A function $f : \Omega \to \mathbb{R}$ defined on a convex set $\Omega \subset \mathbb{R}^n$ is convex if and only if for all $\boldsymbol{x}, \boldsymbol{y} \in \Omega$ and all $\alpha \in (0,1)$, we have*

$$f(\alpha \boldsymbol{x} + (1-\alpha)\boldsymbol{y}) \le \alpha f(\boldsymbol{x}) + (1-\alpha) f(\boldsymbol{y}).$$

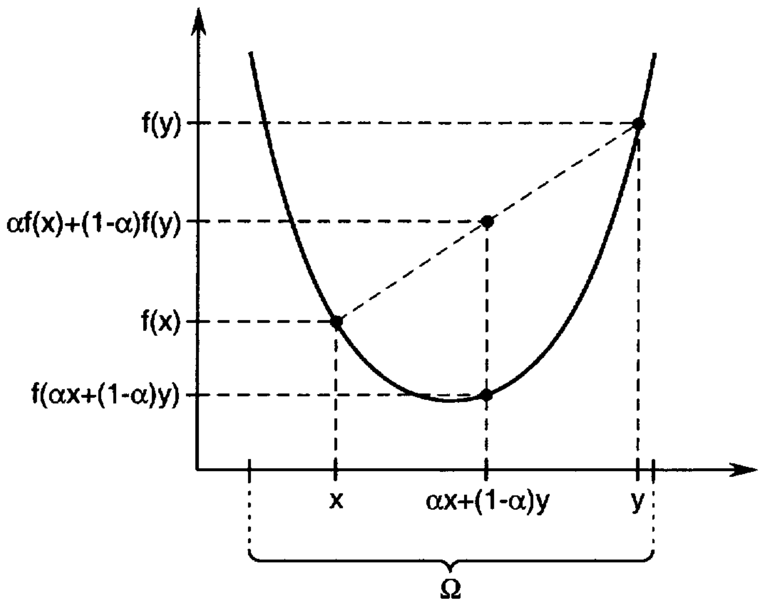


Figure 21.5 Geometric interpretation of Theorem 21.2

The line segment between any two points on the graph lies on or above the graph

Definition 21.4 A function $f : \Omega \to \mathbb{R}$ on a convex set $\Omega \subset \mathbb{R}^n$ is *strictly convex* if for all $\boldsymbol{x}, \boldsymbol{y} \in \Omega$, $\boldsymbol{x} \neq \boldsymbol{y}$, and $\alpha \in (0,1)$, we have

$$f(\alpha \boldsymbol{x} + (1-\alpha)\boldsymbol{y}) < \alpha f(\boldsymbol{x}) + (1-\alpha) f(\boldsymbol{y}).$$

Definition 21.5 A function $f : \Omega \to \mathbb{R}$ on a convex set $\Omega \subset \mathbb{R}^n$ is (strictly) *concave* if $-f$ is (strictly) convex. ∎

Definition 21.1 The *graph* of $f : \Omega \to \mathbb{R}$, $\Omega \subset \mathbb{R}^n$, is the set of points in $\Omega \times \mathbb{R} \subset \mathbb{R}^{n+1}$ given by

$$\{[\boldsymbol{x}, f(\boldsymbol{x})]^T : \boldsymbol{x} \in \Omega\}.$$

Definition 21.2 The *epigraph* of a function $f : \Omega \to \mathbb{R}$, $\Omega \subset \mathbb{R}^n$, denoted epi$(f)$, is the set of points in $\Omega \times \mathbb{R}$ given by

$$\text{epi}(f) = \{[\boldsymbol{x}, \beta]^T : \boldsymbol{x} \in \Omega, \beta \in \mathbb{R}, \beta \geq f(\boldsymbol{x})\}.$$

The epigraph epi(f) of a function f is simply the set of points in $\Omega \times \mathbb{R}$ on or above the graph of f (see Figure 21.4). We can also think of epi(f) as a subset of $\mathbb{R}^{n+1}$.

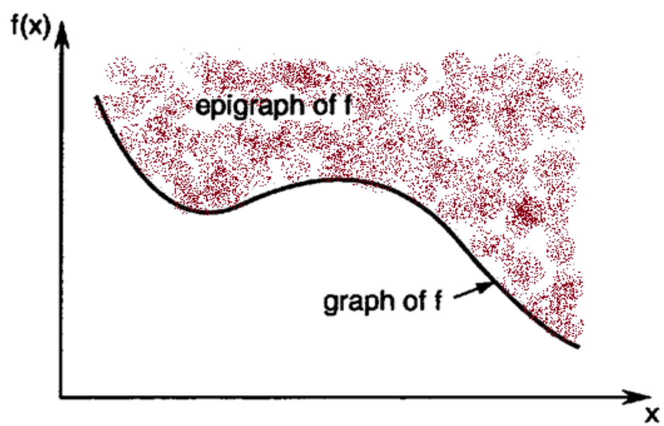


Figure 21.4 The graph and epigraph of a function $f : \mathbb{R} \to \mathbb{R}$

The hypograph of a function $f: \Omega \to R$, denoted *hyp(f)*, is the set of points in $\Omega \, x \, R$ given by

$$hyp(f) = \{[x, \beta]^T: \; x \,\epsilon\, \Omega, \beta \,\epsilon\, R, \beta \leq f(x)\}$$

Theorem (Characterization the convexity of a function in terms of graphs)

(a) A function f defined on a convex set is concave if and only if its hypograpf hyp f is convex.

(b) A function f defined on a convex set S is convex if and only if its epigraph epi f is convex.

Theorem 21.4 *Let $f : \Omega \to \mathbb{R}$, $f \in C^2$, be defined on an open convex set $\Omega \subset \mathbb{R}^n$. Then, f is convex on Ω if and only if for each $\boldsymbol{x} \in \Omega$, the Hessian $\boldsymbol{F}(\boldsymbol{x})$ of f at $\boldsymbol{x}$ is a positive semidefinite matrix.* □

DEFINITENESS of a MATRIX

- A matrix $H \in R^{nxn}$ (H is a real symmetric *nxn* matrix) is said to be positive definite if for all $h \neq 0$, $h^T H h > 0$.

- **The First Method (Definition)**

$$\forall h \in R^n, h \neq 0$$

i) $h^T H h \geq 0 \Rightarrow H$ is positive semidefinite

$h^T H h > 0 \Rightarrow H$ is positive definite

ii) $h^T H h \leq 0 \Rightarrow H$ is negative semidefinite

$h^T H h < 0 \Rightarrow H$ is negative definite

iii) Otherwise, H is indefinite matrix

The Second Method (Eigenvalues)

- Let the eigenvalues of *H* be $\lambda_1, \lambda_2, \ldots, \lambda_n$.

i) If all $\lambda_i \geq 0$; i=1,2,...,n, then *H* is positive semidefinite

If all $\lambda_i > 0$; i=1,2,...,n, then *H* is positive definite

ii) If all $\lambda_i \leq 0$; i=1,2,...,n, then *H* is negative semidefinite

If all $\lambda_i < 0$; i=1,2,...,n, then *H* is negative definite

iii) Otherwise, *H* is indefinite matrix

The Third Method (Principal Leading Minors)**

A minor of the matrix A of order k is **principal** if it is obtained by deleting $n-k$ rows and the $n-k$ columns with the same numbers.

Note that the definition does not specify which $n-k$ rows and columns to delete, only that their indices must be the same.

The **leading principal minor** of A of order k is the minor of order k obtained by deleting the **last** $n-k$ rows and the **last** $n-k$ columns.

Example 3 *For a general* 3×3 *matrix,*

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

All principal minors:

There is one third order principal minor, namely $|A|$.

There are three second order principal minors:

$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}$, *formed by deleting column 3 and row 3;*

$\begin{vmatrix} a_{11} & a_{13} \\ a_{31} & a_{33} \end{vmatrix}$, *formed by deleting column 2 and row 2;*

$\begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix}$, *formed by deleting column 1 and row 1*

And there are three first order principal minors:

$|a_{11}|$, *formed by deleting the last two rows and columns*

$|a_{22}|$, *formed by deleting the first and third rows and columns*

$|a_{33}|$, *formed by deleting the first two rows and columns*

The Leading principal minors:

The first order principal minor:

The second order principal minor:

The third order principal minor:

The algorithm for testing the definiteness of a symmetric matrix:

Let A *be* a symmetric $n \times n$ matrix, denote

its leading principal minors by Δ_i for $i \in \{1, 2, \dots, n\}$ and

its principal minors by D_i for each order $i \in \{1, 2, \dots, n\}$.

Remark: The matrix A has $\binom{n}{i}$ principal minors of order i.

The algorithm for testing the definiteness of a symmetric matrix:

1. A is **positive definite** if and only if all its n leading principal minors are positive, that is $\Delta_i > 0$ for all $i \in \{1, 2, \ldots, n\}$.
2. A is **negative definite** if and only if its n leading principal minors alternate in sign beginning by negative: $\Delta_1 < 0, \Delta_2 > 0, \Delta_3 < 0, \Delta_4 > 0, \ldots$
3. A is **positive semidefinite** if and only if all its principal minors are nonnegative, that is all $D_i \geq 0$ for all $i \in \{1, 2, \ldots, n\}$ considering all principal minors.
4. A is **negative semidefinite** if and only if every principal minors of odd order is nonpositive (≤ 0) and every principal minors of even order is nonnegative (≥ 0), that is $(-1)^i D_i \geq 0$ for all $i \in \{1, 2, \ldots, n\}$ considering all principal minors.
5. Otherwise A is **indefinite**.

Note:

- In the first two cases, it is enough to check the inequality for all the leading principal minors.
- If some $i-$th order leading principal minor of A is nonzero but does not fit either of the sign patterns in case 1 and case 2, then A is indefinite.
- When some leading principal minor of A is zero, but the others fit one of the patterns in case 1 and case 2: the matrix is not definite, but may or may not be semidefinite. In this case, we must unfortunately check not only the principle leading minors, but ***every*** principal minor (cases 3 and 4: we must check all principles minors that is for each i with $1 \leq i \leq n$ and for each of the $\begin{pmatrix} n \\ i \end{pmatrix}$ principal minors of order i.)

Example: Determine the definiteness of the following matrix with three methods

$$H = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$$

Example: Determine the definiteness of the following matrices

$$A = \begin{bmatrix} 6 & 4 \\ 4 & 5 \end{bmatrix}, \; B = \begin{bmatrix} -3 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & -1 \end{bmatrix}, C = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1/2 \end{bmatrix}$$

We have that $D_1 = 6 > 0$, and $D_2 = \begin{vmatrix} 6 & 4 \\ 4 & 5 \end{vmatrix} = 30 - 16 = 14 > 0$.

Therefore, A is a positive definite matrix.

We have that $D_1 = -3 < 0$ and $D_2 = \begin{vmatrix} -3 & 0 \\ 0 & -2 \end{vmatrix} = 6 > 0$. The matrix A is known as a diagonal matrix,

and the determinant $D_3 = \begin{vmatrix} -3 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & -1 \end{vmatrix}$

can be computed as the product of the entries in the main diagonal, that is $D_3 = (-3)(-2)(-1) = -6 < 0$.

Since $D_1, D_3 < 0$ and $D_2 > 0$, we have that A is a negative definite matrix.

$$C = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1/2 \end{bmatrix}$$

Theorem 21.4 *Let $f : \Omega \to \mathbb{R}$, $f \in \mathcal{C}^2$, be defined on an open convex set $\Omega \subset \mathbb{R}^n$. Then, f is convex on Ω if and only if for each $\boldsymbol{x} \in \Omega$, the Hessian $\boldsymbol{F}(\boldsymbol{x})$ of f at $\boldsymbol{x}$ is a positive semidefinite matrix.* □

Note that by definition of concavity, a function $f : \Omega \to \mathbb{R}$, $f \in \mathcal{C}^2$, is concave over the convex set $\Omega \subset \mathbb{R}^n$ if and only if for all $\boldsymbol{x} \in \Omega$, the Hessian $\boldsymbol{F}(\boldsymbol{x})$ of f is negative semidefinite.

positive semidefinite – convex
positive definite – strictly convex
negative semidefinite – concave
negative definite – strictly concave

Some exercises on convexity of sets and functions

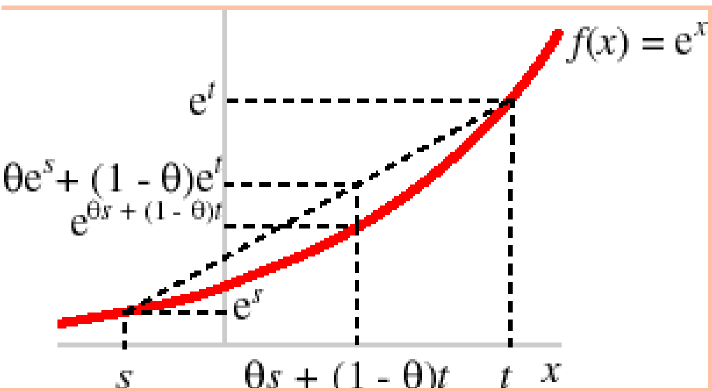
1. By drawing diagrams, determine which of the following sets is convex.

a. $\{(x, y): y = e^x\}$.

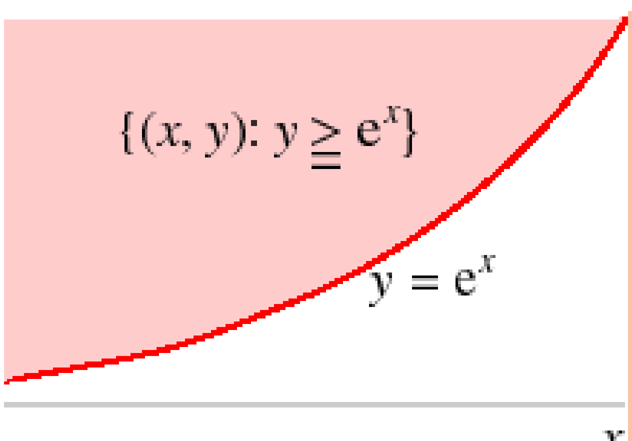
b. $\{(x, y): y \geq e^x\}$.

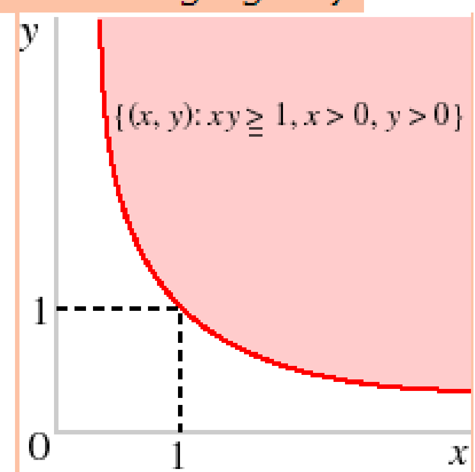
c. $\{(x, y): xy \geq 1, x > 0, y > 0\}$.

a. Not convex, because $e^{\theta x+(1-\theta)u} \neq \theta e^x + (1-\theta)e^u$, as illustrated in the following figure.



b. Convex, because $e^{\theta x+(1-\theta)u} < \theta e^x + (1-\theta)e^u$ (see the following figure).





c. Convex, because if $xy \geq 1$ and $uv \geq 1$ then $(\theta x + (1-\theta)u)(\theta y + (1-\theta)v) \geq 1$ (see figure).

2. For each of the following functions, determine which, if any, of the following conditions the function satisfies: concavity, strict concavity, convexity, strict convexity. (Use whatever technique is most appropriate for each case.)

a. $f(x, y) = x + y$.

b. $f(x, y) = x^2$. [Note: f is a function of two variables.]

c. $f(x, y) = x + y - e^x - e^{x+y}$.

d. $f(x, y, z) = x^2 + y^2 + 3z^2 - xy + 2xz + yz$.

3. Let $f(x_1, x_2) = x_1^2 - x_1x_2 + x_2^2 + 3x_1 - 2x_2 + 1$. Is f convex, concave, or neither?

4. Let $f(x_1, x_2) = x_1^3 + 2x_1^2 + 2x_1x_2 + (1/2)x_2^2 - 8x_1 - 2x_2 - 8$. Find the range of values of (x_1, x_2) for which f is convex, if any.

5. Determine the values of a (if any) for which the function $2x^2 + 2xz + 2ayz + 2z^2$ is concave and the values for which it is convex.

6. Show that the function $-w^2 + 2wx - x^2 - y^2 + 4yz - z^2$ (in the four variables w, x, y, and z) is not concave.