

CS295: Convex Optimization

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Course information

- ▶ Prerequisites: multivariate calculus and linear algebra
- ▶ Textbook: Convex Optimization by Boyd and Vandenberghe
- ▶ Course website:
[http://eee.uci.edu/wiki/index.php/CS_295_Convex_Optimization_\(Winter_2011\)](http://eee.uci.edu/wiki/index.php/CS_295_Convex_Optimization_(Winter_2011))
- ▶ Grading based on:
 - ▶ final exam (50%)
 - ▶ final project (50%)

Mathematical optimization

Mathematical **optimization problem**:

$$\begin{aligned} & \text{minimize } f_0(\mathbf{x}) \\ & \text{subject to } f_i(\mathbf{x}) \leq \mathbf{b}_i, \quad i = 1, \dots, m \end{aligned}$$

where

- ▶ $\mathbf{x} = (x_1, \dots, x_n) \in \mathbb{R}^n$: optimization variables
- ▶ $f_0 : \mathbb{R}^n \rightarrow \mathbb{R}$: objective function
- ▶ $f_i : \mathbb{R}^n \rightarrow \mathbb{R}$: constraint function

Optimal solution \mathbf{x}^* has smallest value of f_0 among all vectors that satisfy the constraints.

Examples

- ▶ transportation - product transportation plan
- ▶ finance - portfolio management
- ▶ machine learning - support vector machines, graphical model structure learning

Transportation problem

We have a product that can be produced in amounts a_i at location i with $i = 1, \dots, m$. The product must be shipped to n destinations, in quantities b_j to destination j with $j = 1, \dots, n$. The amount shipped from origin i to destination j is x_{ij} , at a cost of c_{ij} per unit.

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To find the transportation plan that minimizes the total cost, we solve an LP:

$$\begin{aligned} \min \quad & \sum_{i=1}^m \sum_{j=1}^n x_{ij} c_{ij} \\ \text{s. t.} \quad & \sum_{j=1}^n x_{ij} = a_i \quad i = 1, \dots, m \\ & \sum_{i=1}^m x_{ij} = b_j \quad j = 1, \dots, n \\ & x_{ij} \geq 0 \end{aligned}$$

Markowitz portfolio optimization

Consider a simple portfolio selection problem with n stocks held over a period of time:

- ▶ $\mathbf{x} = (x_1, \dots, x_n)$: the optimization variable with x_i denoting the amount to invest in stock i
- ▶ $\mathbf{p} = (p_1, \dots, p_n)$: a random vector with p_i denoting the reward from stock i . Suppose its mean μ and covariance matrix Σ are known.
- ▶ $r = \mathbf{p}^T \mathbf{x}$: the overall return on the portfolio. r is a random variable with mean $\mu^T \mathbf{x}$ and variance $\mathbf{x}^T \Sigma \mathbf{x}$.

Markowitz portfolio optimization

The Markowitz portfolio optimization problem is the QP

$$\begin{aligned} \min \quad & \mathbf{x}^T \Sigma \mathbf{x} \\ \text{s. t.} \quad & \mu^T \mathbf{x} \geq r_{\min} \\ & \mathbf{1}^T \mathbf{x} = B \\ & x_i \geq 0, \quad i = 1, \dots, n \end{aligned}$$

which find the portfolio that minimizes the return variance subject to three constraints:

- ▶ achieving a minimum acceptable mean return r_{\min}
- ▶ satisfying the total budget B
- ▶ no short positions ($x_i \geq 0$)

Support vector machines (SVMs)

Input: a set of training data,

$$\mathcal{D} = \{(\mathbf{x}_i, y_i) \mid \mathbf{x}_i \in \mathbb{R}^p, y_i \in \{-1, 1\}, i = 1, \dots, n\}$$

where y_i is either 1 or -1 , indicating the class to which \mathbf{x}_i belongs.

Problem: find the **optimal separating hyperplane** that separates the two classes and maximizes the distance to the closet point from either class.

Support vector machines (SVMs) 2

Define a hyperplane by $w^T x - b = 0$. Suppose the training data are linearly separable. So we can find w and b such that $w^T x_i - b \geq 1$ for all x_i from class 1 and $w^T x_i - b \leq -1$ for all x_i from class -1 .

The distance between the two parallel hyperplanes, $w^T x_i - b = 1$ and $w^T x_i - b = -1$, is $\frac{2}{\|w\|}$, called **margin**.

To find the optimal separating hyperplane, we choose w and b that maximize the margin:

$$\begin{aligned} \min \quad & \|w\|^2 \\ \text{s. t.} \quad & y_i(w^T x_i - b) \geq 1, \quad i = 1, \dots, n \end{aligned}$$

Undirected graphical models

Input: a set of training data,

$$\mathcal{D} = \{(\mathbf{x}_i) \mid \mathbf{x}_i \in \mathbb{R}^p \ i = 1, \dots, n\}$$

Assume the data were sampled from a Gaussian graphical model with mean $\mu \in \mathbb{R}^p$ and covariance matrix $\Sigma \in \mathbb{R}^{p \times p}$. The inverse covariance matrix, Σ^{-1} , encodes the structure of the graphical model in the sense that the variables i and j are connected only if the (i, j) -entry of Σ^{-1} is nonzero.

Problem: Find the maximum likelihood estimation of Σ^{-1} with a sparsity constraint, $\|\Sigma^{-1}\|_1 \leq \lambda$.

Undirected graphical models 2

Let S be the empirical covariance matrix:

$$S := \frac{1}{n} \sum_{k=1}^n (\mathbf{x}_k - \mu)(\mathbf{x}_k - \mu)^T.$$

Denote $\Theta = \Sigma^{-1}$.

The convex optimization problem:

$$\begin{aligned} \min \quad & -\log \det \Theta + \text{tr}(S\Theta) \\ \text{s. t.} \quad & \|\Theta\|_1 \leq \lambda \\ & \Theta \succ 0 \end{aligned}$$

Solving optimization problems

The optimization problem is in general difficult to solve: taking very long long time, or not always finding the solution

Exceptions: certain classes of problems can be solved efficiently:

- ▶ least-square problems
- ▶ linear programming problems
- ▶ convex optimization problems

Least-squares

$$\text{minimize } \|Ax - b\|_2^2$$

where $x \in \mathbb{R}^n$, $b \in \mathbb{R}^k$ and $A \in \mathbb{R}^{k \times n}$.

- ▶ analytical solution: $x^* = (A^T A)^{-1} A^T b$ (assuming $k > n$ and **rank** $A = n$)
- ▶ reliable and efficient algorithms available
- ▶ computational time proportional to $n^2 k$, and can be further reduced if A has some special structure

Linear programming

$$\begin{aligned} \min \quad & c^T x \\ \text{s.t.} \quad & a_i^T x \leq b_i, \quad i = 1, \dots, m \end{aligned}$$

where the optimization variable $x \in \mathbb{R}^n$, and $c, a_i, b_i \in \mathbb{R}^n$ are parameters.

- ▶ no analytical formula for solution
- ▶ reliable and efficient algorithms available (e.g., Dantzig's simplex method, interior-point method)
- ▶ computational time proportional to $n^2 m$ if $m \leq n$ (interior-point method); less with structure

Linear programming: example

The Chebyshev approximation problem:

$$\text{minimize } \|Ax - b\|_\infty$$

with $x \in \mathbb{R}^n$, $b \in \mathbb{R}^k$ and $A \in \mathbb{R}^{k \times n}$. The problem is similar to the least-square problem, but with the ℓ_∞ -norm replacing the ℓ_2 -norm:

$$\|Ax - b\|_\infty = \max_{i=1, \dots, k} |a_i^T x - b_i|$$

where $a_i \in \mathbb{R}^n$ is the i th column of A^T .

Linear programming: example

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An equivalent linear programming:

$$\begin{aligned} \min \quad & t \\ \text{s.t.} \quad & a_i^T x - t \leq b_i, \quad i = 1, \dots, k \\ & -a_i^T x - t \leq -b_i, \quad i = 1, \dots, k \end{aligned}$$

Convex optimization problems

$$\begin{aligned} & \text{minimize } f_0(\mathbf{x}) \\ & \text{subject to } f_i(\mathbf{x}) \leq \mathbf{b}_i, \quad i = 1, \dots, m \end{aligned}$$

where $x \in \mathbb{R}^n$.

- ▶ both objective and constraint functions are convex

$$f(\theta x + (1 - \theta)y) \leq \theta f(x) + (1 - \theta)f(y)$$

for any $0 \leq \theta \leq 1$, and any x and y in the domain of f_0 and f_i for all i .

- ▶ includes least-square and linear programming problems as special cases.
- ▶ no analytical formula for solution
- ▶ reliable and efficient algorithms available

Topics to be covered

- ▶ Convex sets and convex functions
- ▶ Duality
- ▶ Unconstrained optimization
- ▶ Equality constrained optimization
- ▶ Interior-point methods
- ▶ Semidefinite programming

Brief history of optimization

- ▶ 1700s: theory for unconstrained optimization (Fermat, Newton, Euler)
- ▶ 1797: theory for equality constrained optimization (Lagrange)
- ▶ 1947: simplex method for linear programming (Dantzig)
- ▶ 1960s: early interior-point methods (Fiacco, McCormick, Dikin, etc)
- ▶ 1970s: ellipsoid method and other subgradient methods
- ▶ 1980s: polynomial-time interior-point methods for linear programming (Karmarkar)
- ▶ 1990s: polynomial-time interior-point methods for nonlinear convex optimization (Nesterov & Nemirovski)
- ▶ 1990-now: many new applications in engineering (control, signal processing, communications, etc); new problem classes (semidefinite and second-order cone programming, robust optimization, convex relaxation, etc)

Convex set

Definition

A set C is called **convex** if

$$\mathbf{x}, \mathbf{y} \in C \implies \theta \mathbf{x} + (1 - \theta) \mathbf{y} \in C \quad \forall \theta \in [0, 1]$$

In other words, a set C is convex if the line segment between any two points in C lies in C .

Convex combination

Definition

A **convex combination** of the points x_1, \dots, x_k is a point of the form

$$\theta_1 x_1 + \dots + \theta_k x_k,$$

where $\theta_1 + \dots + \theta_k = 1$ and $\theta_i \geq 0$ for all $i = 1, \dots, k$.

A set is convex if and only if it contains every convex combinations of the its points.

Convex hull

Definition

The **convex hull** of a set C , denoted $\mathbf{conv} C$, is the set of all convex combinations of points in C :

$$\mathbf{conv} C = \left\{ \sum_{i=1}^k \theta_i x_i \mid x_i \in C, \theta_i \geq 0, i = 1, \dots, k, \sum_{i=1}^k \theta_i = 1 \right\}$$

Properties:

- ▶ A convex hull is always convex
- ▶ $\mathbf{conv} C$ is the smallest convex set that contains C , i.e.,
 $B \supseteq C$ is convex $\implies \mathbf{conv} C \subseteq B$

Convex cone

A set C is called a **cone** if $x \in C \implies \theta x \in C, \forall \theta \geq 0$.

A set C is a **convex cone** if it is convex and a cone, i.e.,

$$x_1, x_2 \in C \implies \theta_1 x_1 + \theta_2 x_2 \in C, \quad \forall \theta_1, \theta_2 \geq 0$$

The point $\sum_{i=1}^k \theta_i x_i$, where $\theta_i \geq 0, \forall i = 1, \dots, k$, is called a **conic combination** of x_1, \dots, x_k .

The **conic hull** of a set C is the set of all conic combinations of points in C .

Hyperplanes and halfspaces

A **hyperplane** is a set of the form $\{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{a}^T \mathbf{x} = b\}$ where $a \neq 0, b \in \mathbb{R}$.

A (closed) **halfspace** is a set of the form $\{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{a}^T \mathbf{x} \leq b\}$ where $a \neq 0, b \in \mathbb{R}$.

- ▶ \mathbf{a} is the normal vector
- ▶ hyperplanes and halfspaces are convex

Euclidean balls and ellipsoids

Euclidean ball in R^n with center x_c and radius r :

$$B(x_c, r) = \{x \mid \|x - x_c\|_2 \leq r\} = \{x_c + ru \mid \|u\|_2 \leq 1\}$$

Euclidean balls and ellipsoids

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ellipsoid in R^n with center x_c :

$$\mathcal{E} = \left\{x \mid (x - x_c)^T P^{-1} (x - x_c) \leq 1\right\}$$

where $P \in S_{++}^n$ (i.e., symmetric and positive definite)

- ▶ the lengths of the semi-axes of \mathcal{E} are given by $\sqrt{\lambda_i}$, where λ_i are the eigenvalues of P .
- ▶ An alternative representation of an ellipsoid: with $A = P^{1/2}$

$$\mathcal{E} = \{x_c + Au \mid \|u\|_2 \leq 1\}$$

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Euclidean balls and ellipsoids are convex.

Norms

A function $f : R^n \rightarrow R$ is called a **norm**, denoted $\|x\|$, if

- ▶ nonnegative: $f(x) \geq 0$, for all $x \in R^n$
- ▶ definite: $f(x) = 0$ only if $x = 0$
- ▶ homogeneous: $f(tx) = |t|f(x)$, for all $x \in R^n$ and $t \in R$
- ▶ satisfies the triangle inequality: $f(x + y) \leq f(x) + f(y)$

notation: $\| \cdot \|$ denotes a general norm; $\| \cdot \|_{\text{symb}}$ denotes a specific norm

Distance: $dist(x, y) = \|x - y\|$ between $x, y \in R^n$.

Examples of norms

- ▶ l_p -norm on R^n : $\|x\|_p = (|x_1|^p + \dots + |x_n|^p)^{1/p}$
 - ▶ l_1 -norm: $\|x\|_1 = \sum_i |x_i|$
 - ▶ l_∞ -norm: $\|x\|_\infty = \max_i |x_i|$
- ▶ Quadratic norms: For $P \in S_{++}^n$, define the P -quadratic norm as

$$\|x\|_P = (x^T P x)^{1/2} = \|P^{1/2} x\|_2$$

Equivalence of norms

Let $\|\cdot\|_a$ and $\|\cdot\|_b$ be norms on R^n . Then $\exists \alpha, \beta > 0$ such that $\forall x \in R^n$,

$$\alpha\|x\|_a \leq \|x\|_b \leq \beta\|x\|_a.$$

Norms on any finite-dimensional vector space are equivalent (define the same set of open subsets, the same set of convergent sequences, etc.)

Norm balls and norm cones

norm ball with center x_c and radius r : $\{x \mid \|x - x_c\| \leq r\}$

norm cone: $C = \{(x, t) \mid \|x\| \leq t\} \subseteq \mathbb{R}^{n+1}$

- ▶ the second-order cone is the norm cone for the Euclidean norm

norm balls and cones are convex

Polyhedra

A **polyhedron** is defined as the solution set of a finite number of linear equalities and inequalities:

$$\mathcal{P} = \{x \mid Ax \preceq b, Cx = d\}$$

where $A \in \mathbb{R}^{m \times n}$, $C \in \mathbb{R}^{p \times n}$, and \preceq denotes *vector inequality* or *componentwise inequality*.

A polyhedron is the intersection of finite number of halfspaces and hyperplanes.

Simplexes

The **simplex** determined by $k + 1$ affinely independent points $v_0, \dots, v_k \in \mathbb{R}^n$ is

$$C = \mathbf{conv}\{v_0, \dots, v_k\} = \left\{ \theta_0 v_0 + \dots + \theta_k v_k \mid \theta \succeq 0, \mathbf{1}^T \theta = 1 \right\}$$

The affine dimension of this simplex is k , so it is often called k -dimensional simplex in \mathbb{R}^n .

Some common simplexes: let e_1, \dots, e_n be the unit vectors in R^n .

- ▶ **unit simplex:** $\mathbf{conv}\{0, e_1, \dots, e_n\} = \{x \mid x \succeq 0, \mathbf{1}^T \theta \leq 1\}$
- ▶ **probability simplex:** $\mathbf{conv}\{e_1, \dots, e_n\} = \{x \mid x \succeq 0, \mathbf{1}^T \theta = 1\}$

Positive semidefinite cone

notation:

- ▶ S^n : the set of symmetric $n \times n$ matrices
- ▶ $S_+^n = \{X \in S^n \mid X \succeq 0\}$: symmetric positive semidefinite matrices
- ▶ $S_{++}^n = \{X \in S^n \mid X \succ 0\}$ symmetric positive definite matrices

S_+^n is a convex cone, called positive semidefinite cone. S_{++}^n comprise the cone interior; all singular positive semidefinite matrices reside on the cone boundary.

Example:

$$X = \begin{bmatrix} x & y \\ y & z \end{bmatrix} \in S_+^2 \iff x \geq 0, z \geq 0, xz \geq y^2$$

Operations that preserve complexity

- ▶ intersection
- ▶ affine function
- ▶ perspective function
- ▶ linear-fractional functions



Inner product, Euclidean norm

- ▶ Standard inner product on R^n : $\langle x, y \rangle = x^T y = \sum_i x_i y_i$
- ▶ Euclidean norm (ℓ_2 norm): $\|x\|_2 = \langle x, x \rangle^{1/2}$
- ▶ Cauchy-Schwartz inequality: $\langle x, y \rangle \leq \|x\|_2 \|y\|_2$
- ▶ Standard inner product on $R^{m \times n}$:

$$\langle X, Y \rangle = \text{tr}(X^T Y) = \sum_{i=1}^m \sum_{j=1}^n X_{ij} Y_{ij}$$

- ▶ Frobenius norm: $\|X\|_F = \langle X, X \rangle^{1/2}$

Norms and distance

- ▶ A function $f : R^n \rightarrow R$ with $\text{dom } f = R^n$ is called a *norm*, written as $f(x) = \|x\|$, if
 - ▶ $f(x) \geq 0$, for all $x \in R^n$
 - ▶ $f(x) = 0$ only if $x = 0$
 - ▶ $f(tx) = |t|f(x)$, for all $x \in R^n$ and $t \in R$
 - ▶ $f(x + y) \leq f(x) + f(y)$
- ▶ Distance: $\text{dist}(x, y) = \|x - y\|$ between $x, y \in R^n$.
- ▶ Unit ball: $B = \{x \in R^n \mid \|x\| \leq 1\}$
 - ▶ B is convex
 - ▶ B is closed, bounded, and has nonempty interior
 - ▶ B is symmetric about the origin, i.e., $x \in B$ iff $-x \in B$.

Examples of norms

- ▶ l_p -norm on R^n : $\|x\|_p = (|x_1|^p + \dots + |x_n|^p)^{1/p}$
 - ▶ l_1 -norm: $\|x\|_1 = \sum_i |x_i|$
 - ▶ l_∞ -norm: $\|x\|_\infty = \max_i |x_i|$
- ▶ Quadratic norms: For $P \in S_{++}^n$, define the P -quadratic norm as

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$$\alpha\|x\|_a \leq \|x\|_b \leq \beta\|x\|_a.$$

In fact, norms on any finite-dimensional vector space are equivalent (define the same set of open subsets, the same set of convergent sequences, etc.)

- ▶ Let $\|\cdot\|$ be a norm on R^n . Then \exists a quadratic norm $\|\cdot\|_P$ such that $\forall x \in R^n$,

$$\|x\|_P \leq \|x\| \leq \sqrt{n}\|x\|_P$$

“Minimum Norms” Lemma

Lemma

Suppose X is an n -dimensional normed vector space over \mathbb{R} or (\mathbb{C}) with basis $\{x_1, \dots, x_n\}$. There exists a $c > 0$ such that

$$\|\alpha_1 x_1 + \dots + \alpha_n x_n\| \geq c(|\alpha_1| + \dots + |\alpha_n|)$$

for any selection of $\alpha_1, \dots, \alpha_n$ in the field.

Operator norms

Let $\|\cdot\|_a$ and $\|\cdot\|_b$ be norms on R^m and R^n , respectively. The operator norm of $X \in R^{m \times n}$, induced by $\|\cdot\|_a$ and $\|\cdot\|_b$, is defined to be

$$\|X\|_{a,b} = \sup \{ \|Xu\|_a \mid \|u\|_b \leq 1 \}$$

- ▶ Spectral norm (ℓ_2 -norm):

$$\|X\|_2 = \|X\|_{2,2} = \sigma_{\max}(X) = (\lambda_{\max}(X^T X))^{1/2}$$

- ▶ Max-row-sum norm:

$$\|X\|_{\infty} = \|X\|_{\infty,\infty} = \max_{i=1,\dots,m} \sum_{j=1}^n |X_{ij}|$$

- ▶ Max-column-sum norm:

$$\|X\|_1 = \|X\|_{1,1} = \max_{j=1,\dots,n} \sum_{i=1}^m |X_{ij}|$$

Dual norm

Let $\|\cdot\|$ be a norm on R^n . The associated dual norm, denoted $\|\cdot\|_*$, is defined as

$$\|z\|_* = \sup \{z^T x \mid \|x\| \leq 1\}.$$

- ▶ $z^T x \leq \|x\| \|z\|_*$ for all $x, z \in R^n$
- ▶ $\|x\|_{**} = \|x\|$ for all $x \in R^n$
- ▶ The dual of the Euclidean norm is the Euclidean norm
- ▶ The dual of the ℓ_∞ norm is the ℓ_1 norm
- ▶ The dual of the ℓ_p -norm is the ℓ_q -norm, where $1/p + 1/q = 1$
- ▶ The dual of the ℓ_2 -norm on $R^{m \times n}$ is the nuclear norm,

$$\begin{aligned}\|Z\|_{2*} &= \sup \{tr(Z^T X) \mid \|X\|_2 \leq 1\} \\ &= \sigma_1(Z) + \cdots + \sigma_r(Z) = tr(Z^T Z)^{1/2},\end{aligned}$$

where $r = \text{rank } Z$.

Continuity

A function $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is continuous at $x \in \text{dom } f$ if $\forall \epsilon > 0 \exists \delta > 0$ such that

$$\|y - x\| < \delta \implies \|f(y) - f(x)\| < \epsilon.$$

Continuity can also be described in terms of limits: whenever the sequence (x_i) converges to a point $x \in \text{dom } f$, the sequence $(f(x_i))$ converges to $f(x)$,

$$\lim_{i \rightarrow \infty} f(x_i) = f(\lim_{i \rightarrow \infty} x_i).$$

A function f is **continuous** if it is continuous at every point in its domain.

Derivatives

The function $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is **differentiable** at $x \in \text{int } \text{dom } f$ if there exists a matrix $Df(x) \in \mathbb{R}^{m \times n}$ that satisfies

$$\lim_{z \rightarrow x} \frac{\|f(z) - f(x) - Df(x)(z - x)\|}{\|z - x\|} = 0,$$

with $z \in \text{dom } f \setminus \{x\}$. $Df(x)$ is called the **derivative** of f at x . The function f is differentiable if $\text{dom } f$ is open, and it is differentiable at every point in its domain.

The derivative can be found from partial derivatives:

$$Df(x)_{ij} = \frac{\partial f_i(x)}{\partial x_j},$$

for all $i = 1, \dots, m$, and $j = 1, \dots, n$.

Gradient

The gradient of the function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is

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

which is a (column) vector in \mathbb{R}^n . Its components are the partial derivatives of f :

$$\nabla f(x)_i = \frac{\partial f(x)}{\partial x_j}, \quad i = 1, \dots, n.$$

The first-order approximation of f at $x \in \text{int dom } f$ is

$$f(x) + \nabla f(x)^T(z - x).$$

Chain rule

Suppose $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is differentiable at $x \in \text{int dom } f$, and $g : \mathbb{R}^m \rightarrow \mathbb{R}^p$ are differentiable at $f(x) \in \text{int dom } g$. Define the composition $h : \mathbb{R}^n \rightarrow \mathbb{R}^p$ by $h(x) = g(f(x))$. Then h is differentiable at x , with derivative

$$Dh(x) = Dg(f(x)) Df(x).$$

Examples:

- ▶ $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and $g : \mathbb{R} \rightarrow \mathbb{R}$:

$$\nabla(g \circ f)(x) = g'(f(x)) \nabla f(x)$$

- ▶ $h(x) = f(Ax + b)$, where $A \in \mathbb{R}^{n \times m}$ and $g : \mathbb{R}^m \rightarrow \mathbb{R}$:

$$\nabla h(x) = A^T \nabla f(Ax + b)$$

Second derivative

The second derivative or Hessian matrix of $f : \mathbb{R}^n \rightarrow \mathbb{R}$ at $x \in \text{int dom } f$, denoted $\nabla^2 f(x)$, is given by

$$\nabla^2 f(x)_{ij} = \frac{\partial^2 f(x)}{\partial x_i \partial x_j}, \quad i = 1, \dots, n, \quad j = 1, \dots, n,$$

provided f is twice differentiable at x .

The second-order approximation of f , at or near x , is:

$$\hat{f}(z) = f(x) + \nabla f(x)^T (z - x) + \frac{1}{2} (z - x)^T \nabla^2 f(x) (z - x).$$

Chain rule for second derivative

Some special cases:

- ▶ $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and $g : \mathbb{R} \rightarrow \mathbb{R}$:

$$\nabla^2(g \circ f)(x) = g'(f(x))\nabla^2 f(x) + g''(f(x))\nabla f(x)\nabla f(x)^T$$

- ▶ $h(x) = f(Ax + b)$, where $A \in \mathbb{R}^{n \times m}$ and $g : \mathbb{R}^m \rightarrow \mathbb{R}$:

$$\nabla^2 h(x) = A^T \nabla^2 f(Ax + b)A$$

Matrix calculus

Suppose $A \in \mathbb{R}^{n \times n}$. $\text{adj}(A)$ denotes the adjugate of A , the transpose of the cofactor matrix of A . The derivative of $\det(A)$,

$$\frac{d \det(A)}{d\alpha} = \text{tr} \left(\text{adj}(A) \frac{dA}{d\alpha} \right).$$

If A is invertible,

$$\frac{d \det(A)}{d\alpha} = \det(A) \text{tr} \left(A^{-1} \frac{dA}{d\alpha} \right).$$

In particular,

$$\frac{\partial \det(A)}{\partial A_{ij}} = \text{adj}(A)_{ji} = \det(A)(A^{-1})_{ji}$$

$$\frac{\partial \log \det(A)}{\partial A_{ij}} = (A^{-1})_{ji}$$

Derivative of $\det(A)$

Proof.

Denote C the cofactor matrix of A . $\det(A) = \sum_k A_{ik} C_{ik}$.

$$\begin{aligned}\frac{d \det(A)}{d\alpha} &= \sum_i \sum_j \frac{\partial \det(A)}{\partial A_{ij}} \frac{dA_{ij}}{d\alpha} \\ &= \sum_i \sum_j \frac{\partial}{\partial A_{ij}} \sum_k A_{ik} C_{ik} \frac{dA_{ij}}{d\alpha} \\ &= \sum_i \sum_j C_{ij} \frac{dA_{ij}}{d\alpha} \\ &= \text{tr} \left(\text{adj}(A) \frac{dA}{d\alpha} \right).\end{aligned}$$



Example: the gradient of the log det function

Consider the function $f : S_{++}^n \rightarrow \mathbb{R}$, given by $f(X) = \log \det X$.
The first-order approximation of f is

$$\log \det(X + \Delta X) = \log \det(X) + \text{tr}(X^{-1}\Delta X),$$

which implies that

$$\nabla f(X) = X^{-1}.$$

Example: the gradient of the log det function II

The result can be proved using the formula on the derivative of $\det(X)$ function. But here we use a different technique based on the first-order approximation.

$$\begin{aligned}\log \det(X + \Delta X) &= \log \det \left(X^{1/2} (I + X^{-1/2} \Delta X X^{-1/2}) X^{1/2} \right) \\ &= \log \det X + \log \det (I + X^{-1/2} \Delta X X^{-1/2}) \\ &= \log \det X + \sum_i \log(1 + \lambda_i) \\ &\approx \log \det X + \sum_i \lambda_i \\ &= \log \det X + \text{tr}(X^{-1/2} \Delta X X^{-1/2}) \\ &= \log \det X + \text{tr}(X^{-1} \Delta X),\end{aligned}$$

where λ_i is the i th eigenvalue of $X^{-1/2} \Delta X X^{-1/2}$.