Optimization and Numerical Methods

Bachelor of Statistical Data Science (BSDS)

Course instructor: Dr. Kaushik Jana
SQC & OR Unit, Delhi
Indian Statistical Institute
Email: kaushikjana11@gmail.com

Today's Overview: Lecture 1, Jan 27

1. **Teaching Team**

2. **Course logistics**

3. **Introduction**

About the Instructor

- From Digha, 150 KM from Kolkata, West Bengal
- Bachelors and Masters in Statistics

Figure: Indian Statistical Institute, Kolkata (2010-17)

- PhD in Statistics from Indian Statistical Institute, Kolkata (picture in the next page)
- A heavy rainy day in Kolkata, inspired me to work on modeling satellite-based rainfall imagery.

Figure: Imperial College London and British Library (2018-21, in picture)

- joined Imperial College London, UK for post-doctoral research and worked at the Alan Turing Institute housed in the British Library.

- Taught in Ahmedabad University in 2021-24 as an assistant professor
- Teaching Assistants
  - Subhajit Pramanick (Kolkata, email: spramanick104@gmail.com)
  - Somnath Jana (Bangalore, email: janasomnath364@gmail.com)

Course logistics

- Check google classroom frequently for updates and announcements. Pre-lecture notes will be posted before the lecture. Cumulative notes will be updated and posted after the lecture.
- Class starts are 12 noon sharp.
- My office hours: Wednesday 11.30 am to 1pm or by appointment. Meeting will be online or in-person when I am at your centre. At Delhi Centre my office number 319.
- Tutorial: Friday 12.30pm to 1.30pm
- TA office hours: will be added for each center.
- Homework assignments: every week except first week with Friday 11pm as submission deadline. Deadline can be extended to atmost 24 hrs.
- Final grade 30+20+50.

Topics to be studied

1. Role of Optimization and Numerical Methods in Statistical Data Science

   Optimization

2. Basics of Convex Optimization
3. Optimization Problems
4. Optimality Condition
5. Linear Programming
6. Quadratic Programming
7. Gradient-based methods
8. Second order method

   Numerical Methods

9. Numerical Solution
10. Numerical Interpolation
11. Numerical Integration

Course references

- Test book 'Convex Optimization' by Stephen Boyd and Lieven Vandenberghe
- The above book is available from the author website at their Stanford website: https://stanford.edu/ boyd/cvxbook/
- The notes and presentation slides are borrowed form the above author's course offered at Stanford

Introduction

- mathematical optimization
- least-squares and linear programming
- convex optimization
- example
- course goals and topics
- nonlinear optimization
- brief history of convex optimization.

Mathematical optimization

(mathematical) optimization problem

$$\begin{array}{ll} \text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq b_i, \quad i = 1, \ldots, m \end{array}$$

- $x = (x_1, \ldots, x_n)$: optimization variables
- $f_0 : \mathbf{R}^n \to \mathbf{R}$: objective function
- $f_i : \mathbf{R}^n \to \mathbf{R}$, $i = 1, \ldots, m$: constraint functions

optimal solution $x^\star$ has smallest value of f_0 among all vectors that satisfy the constraints

Examples

portfolio optimization

- variables: amounts invested in different assets
- constraints: budget, max./min. investment per asset, minimum return
- objective: overall risk or return variance

device sizing in electronic circuits

- variables: device widths and lengths
- constraints: manufacturing limits, timing requirements, maximum area
- objective: power consumption

data fitting

- variables: model parameters
- constraints: prior information, parameter limits
- objective: measure of misfit or prediction error

Solving optimization problems

general optimization problem

- very difficult to solve
- methods involve some compromise, $e.g.$, very long computation time, or not always finding the solution

exceptions: certain problem classes can be solved efficiently and reliably

- least-squares problems
- linear programming problems
- convex optimization problems

Least-squares

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

solving least-squares problems

- analytical solution: $x^\star = (A^T A)^{-1} A^T b$
- reliable and efficient algorithms and software
- computation time proportional to $n^2 k$ ($A \in \mathbf{R}^{k \times n}$); less if structured
- a mature technology

using least-squares

- least-squares problems are easy to recognize
- a few standard techniques increase flexibility ($e.g.$, including weights, adding regularization terms)

Linear programming

$$\begin{array}{ll} \text{minimize} & c^T x \\ \text{subject to} & a_i^T x \le b_i, \quad i = 1, \ldots, m \end{array}$$

solving linear programs

- no analytical formula for solution
- reliable and efficient algorithms and software
- computation time proportional to $n^2 m$ if $m \ge n$; less with structure
- a mature technology

using linear programming

- not as easy to recognize as least-squares problems
- a few standard tricks used to convert problems into linear programs ($e.g.$, problems involving ℓ_1- or ℓ_∞-norms, piecewise-linear functions)

Convex optimization problem

$$\begin{array}{ll} \text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq b_i, \quad i = 1, \ldots, m \end{array}$$

- objective and constraint functions are convex:

$$f_i(\alpha x + \beta y) \leq \alpha f_i(x) + \beta f_i(y)$$

  if $\alpha + \beta = 1$, $\alpha \geq 0$, $\beta \geq 0$

- includes least-squares problems and linear programs as special cases

solving convex optimization problems

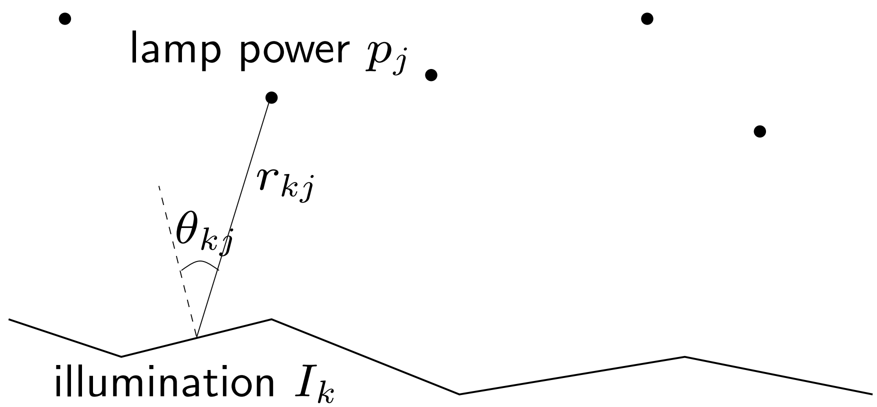
- no analytical solution
- reliable and efficient algorithms
- computation time (roughly) proportional to $\max\{n^3, n^2m, F\}$, where F is cost of evaluating f_i's and their first and second derivatives
- almost a technology

using convex optimization

- often difficult to recognize
- many tricks for transforming problems into convex form
- surprisingly many problems can be solved via convex optimization

Example

m lamps illuminating n (small, flat) patches



intensity I_k at patch k depends linearly on lamp powers p_j:

$$I_k = \sum_{j=1}^{m} a_{kj} p_j, \qquad a_{kj} = r_{kj}^{-2} \max\{\cos\theta_{kj}, 0\}$$

problem: achieve desired illumination I_{des} with bounded lamp powers

$$\begin{array}{ll} \text{minimize} & \max_{k=1,\ldots,n} |\log I_k - \log I_{\mathsf{des}}| \\ \text{subject to} & 0 \le p_j \le p_{\mathsf{max}}, \quad j = 1, \ldots, m \end{array}$$

how to solve?

1. use uniform power: $p_j = p$, vary p
2. use least-squares:

$$\text{minimize} \quad \sum_{k=1}^{n} (I_k - I_{\text{des}})^2$$

   round p_j if $p_j > p_{\text{max}}$ or $p_j < 0$

3. use weighted least-squares:

$$\text{minimize} \quad \sum_{k=1}^{n} (I_k - I_{\text{des}})^2 + \sum_{j=1}^{m} w_j (p_j - p_{\text{max}}/2)^2$$

   iteratively adjust weights w_j until $0 \le p_j \le p_{\text{max}}$

4. use linear programming:

$$\begin{array}{ll} \text{minimize} & \max_{k=1,\ldots,n} |I_k - I_{\text{des}}| \\ \text{subject to} & 0 \le p_j \le p_{\text{max}}, \quad j = 1, \ldots, m \end{array}$$

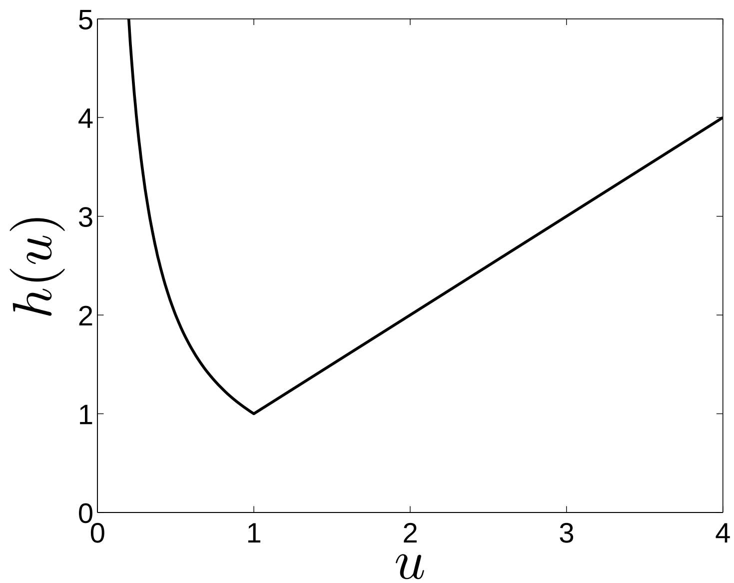
   which can be solved via linear programming

of course these are approximate (suboptimal) 'solutions'

5. use convex optimization: problem is equivalent to

$$\begin{array}{ll} \text{minimize} & f_0(p) = \max_{k=1,\ldots,n} h(I_k/I_{\mathsf{des}}) \\ \text{subject to} & 0 \leq p_j \leq p_{\mathsf{max}}, \quad j = 1, \ldots, m \end{array}$$

with $h(u) = \max\{u, 1/u\}$



f_0 is convex because maximum of convex functions is convex

exact solution obtained with effort $\approx$ modest factor $\times$ least-squares effort

additional constraints: does adding 1 or 2 below complicate the problem?

1. no more than half of total power is in any 10 lamps
2. no more than half of the lamps are on ($p_j > 0$)

- answer: with (1), still easy to solve; with (2), extremely difficult
- moral: (untrained) intuition doesn't always work; without the proper background very easy problems can appear quite similar to very difficult problems

Course goals and topics

goals

1. recognize/formulate problems (such as the illumination problem) as convex optimization problems
2. develop code for problems of moderate size (1000 lamps, 5000 patches)
3. characterize optimal solution (optimal power distribution), give limits of performance, etc.

topics

1. convex sets, functions, optimization problems
2. examples and applications
3. algorithms

Nonlinear optimization

traditional techniques for general nonconvex problems involve compromises

local optimization methods (nonlinear programming)

- find a point that minimizes f_0 among feasible points near it
- fast, can handle large problems
- require initial guess
- provide no information about distance to (global) optimum

global optimization methods

- find the (global) solution
- worst-case complexity grows exponentially with problem size

these algorithms are often based on solving convex subproblems

Brief history of convex optimization

theory (convex analysis): ca1900–1970

algorithms

- 1947: simplex algorithm for linear programming (Dantzig)
- 1960s: early interior-point methods (Fiacco & McCormick, Dikin, . . .)
- 1970s: ellipsoid method and other subgradient methods
- 1980s: polynomial-time interior-point methods for linear programming (Karmarkar 1984)
- late 1980s–now: polynomial-time interior-point methods for nonlinear convex optimization (Nesterov & Nemirovski 1994)

applications

- before 1990: mostly in operations research; few in engineering
- since 1990: many new applications in engineering (control, signal processing, communications, circuit design, . . .); new problem classes (semidefinite and second-order cone programming, robust optimization)

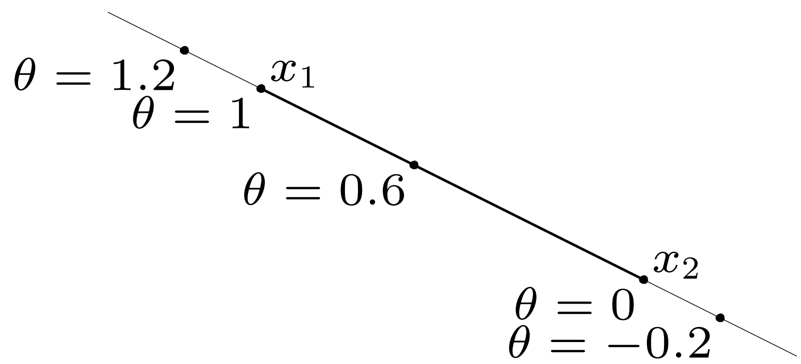
Lecture 2, Jan 30, 2025: Convex sets

- Definition of Affine and Convex sets
- Some important example:
  - Convex cone, Hyperplanes and halfspaces
  - Euclidean balls, Ellipsoids and Norm balls
  - Polyhedra
- Convexity Preserving Operations
- Reading reference: Chapter 2 of Boyd's book on Convex Optimization.
- Homework

Affine set

line through x_1, x_2: all points

$$x = \theta x_1 + (1 - \theta) x_2 \qquad (\theta \in \mathbf{R})$$



affine set: contains the line through any two distinct points in the set

example: solution set of linear equations $\{x \mid Ax = b\}$

(conversely, every affine set can be expressed as solution set of system of linear equations)

Convex set

line segment between x_1 and x_2: all points

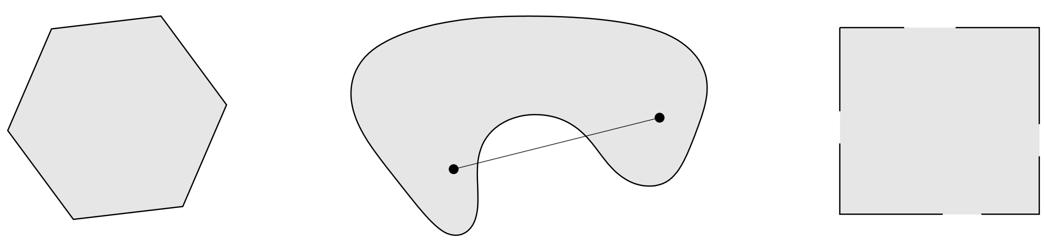
$$x = \theta x_1 + (1 - \theta)x_2$$

with $0 \leq \theta \leq 1$

convex set: contains line segment between any two points in the set

$$x_1, x_2 \in C, \quad 0 \leq \theta \leq 1 \quad \Longrightarrow \quad \theta x_1 + (1 - \theta)x_2 \in C$$

examples (one convex, two nonconvex sets)



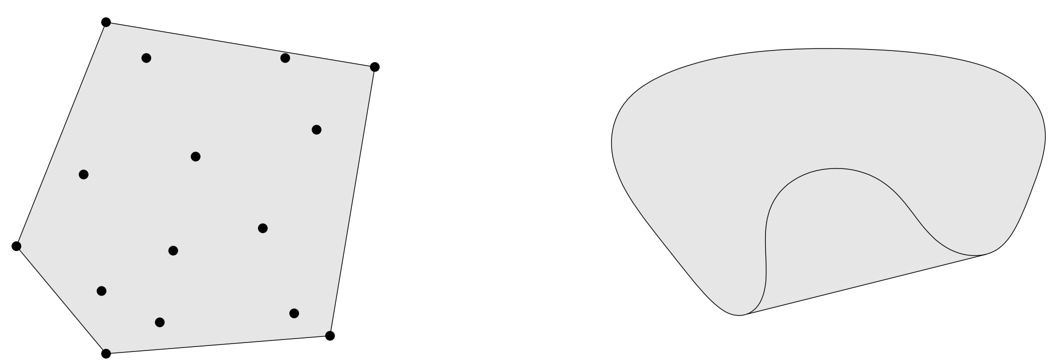
Convex combination and convex hull

convex combination of x_1,. . . , x_k: any point x of the form

$$x = \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_k x_k$$

with $\theta_1 + \cdots + \theta_k = 1$, $\theta_i \geq 0$

convex hull $\mathbf{conv}\, S$: set of all convex combinations of points in S

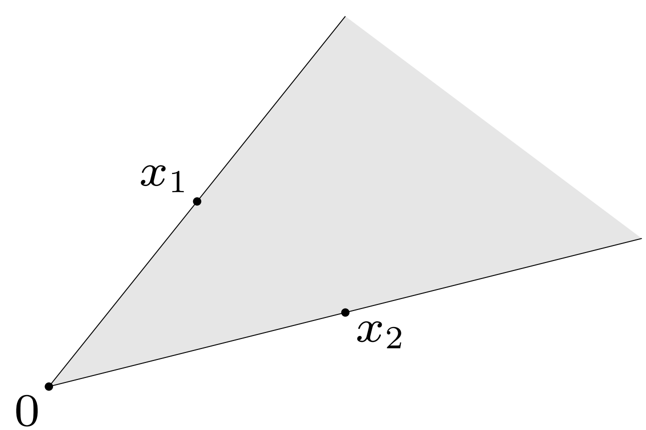


Convex cone

conic (nonnegative) combination of x_1 and x_2: any point of the form

$$x = \theta_1 x_1 + \theta_2 x_2$$

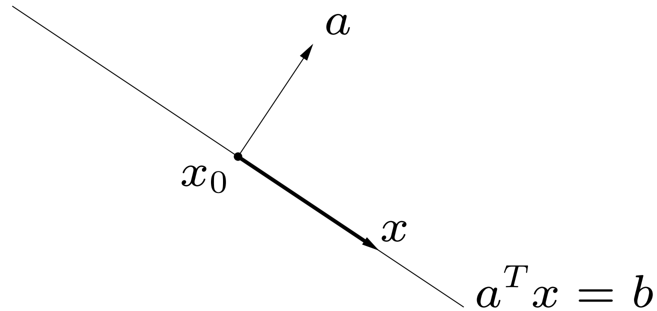
with $\theta_1 \geq 0$, $\theta_2 \geq 0$



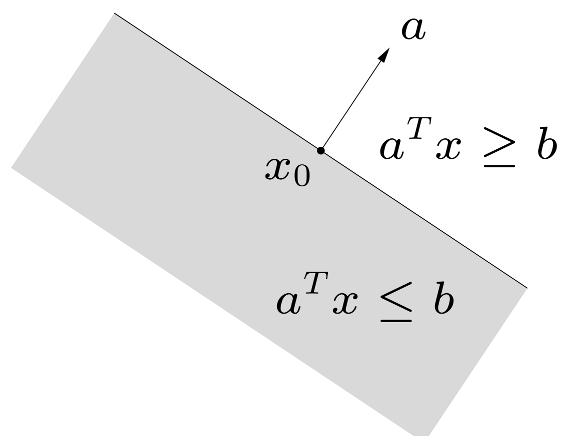
convex cone: set that contains all conic combinations of points in the set

Hyperplanes and halfspaces

hyperplane: set of the form $\{x \mid a^T x = b\}$ $(a \neq 0)$



halfspace: set of the form $\{x \mid a^T x \leq b\}$ $(a \neq 0)$



- a is the normal vector
- hyperplanes are affine and convex; halfspaces are convex

Euclidean balls and ellipsoids

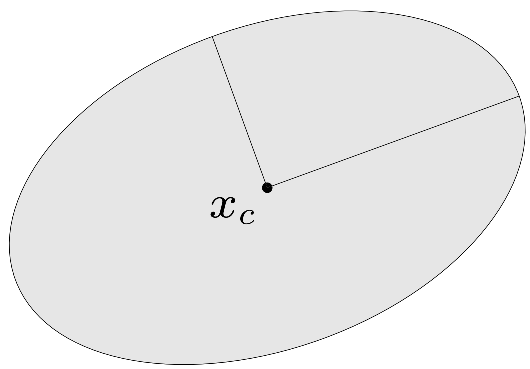
(Euclidean) ball with center x_c and radius r:

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

ellipsoid: set of the form

$$\{x \mid (x - x_c)^T P^{-1}(x - x_c) \leq 1\}$$

with $P \in \mathbf{S}^n_{++}$ (*i.e.*, P symmetric positive definite)



other representation: $\{x_c + Au \mid \|u\|_2 \leq 1\}$ with A square and nonsingular

Norm balls and norm cones

norm: a function $\|\cdot\|$ that satisfies

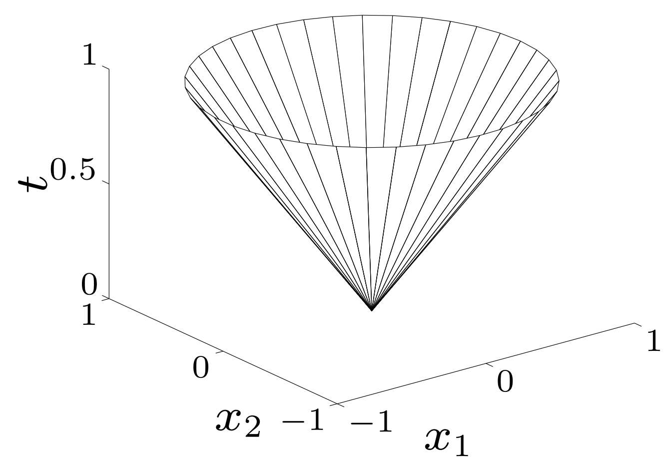
- $\|x\| \geq 0$; $\|x\| = 0$ if and only if $x = 0$
- $\|tx\| = |t|\,\|x\|$ for $t \in \mathbf{R}$
- $\|x + y\| \leq \|x\| + \|y\|$

notation: $\|\cdot\|$ is general (unspecified) norm; $\|\cdot\|_{\text{symb}}$ is particular norm

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

norm cone: $\{(x, t) \mid \|x\| \leq t\}$

Euclidean norm cone is called second-order cone



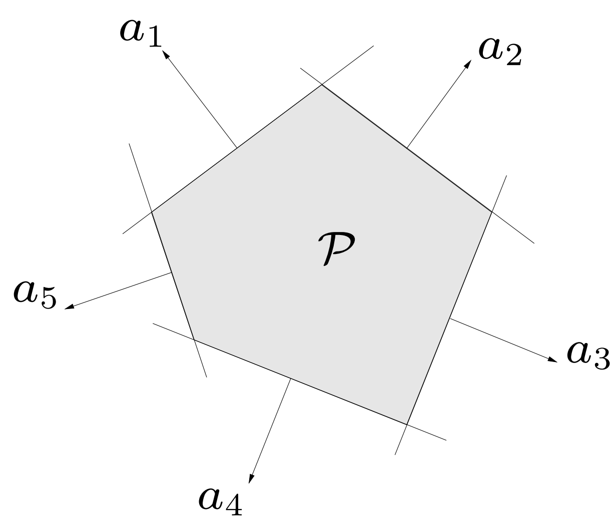
norm balls and cones are convex

Polyhedra

solution set of finitely many linear inequalities and equalities

$$Ax \preceq b, \qquad Cx = d$$

($A \in \mathbf{R}^{m \times n}$, $C \in \mathbf{R}^{p \times n}$, $\preceq$ is componentwise inequality)



polyhedron is intersection of finite number of halfspaces and hyperplanes

Positive semidefinite cone

notation:

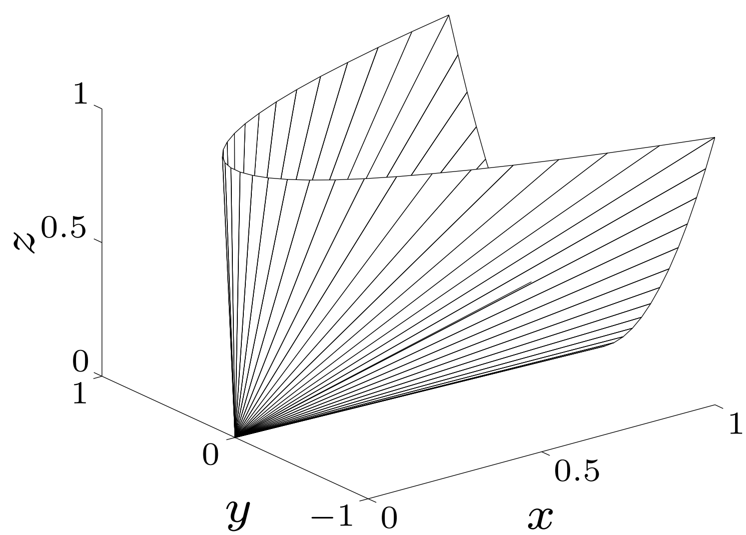
- $\mathbf{S}^n$ is set of symmetric $n \times n$ matrices
- $\mathbf{S}^n_+ = \{X \in \mathbf{S}^n \mid X \succeq 0\}$: positive semidefinite $n \times n$ matrices

$$X \in \mathbf{S}^n_+ \quad \iff \quad z^T X z \geq 0 \text{ for all } z$$

  $\mathbf{S}^n_+$ is a convex cone

- $\mathbf{S}^n_{++} = \{X \in \mathbf{S}^n \mid X \succ 0\}$: positive definite $n \times n$ matrices

example: $\begin{bmatrix} x & y \\ y & z \end{bmatrix} \in \mathbf{S}^2_+$



Operations that preserve convexity

practical methods for establishing convexity of a set C

1. apply definition

$$x_1, x_2 \in C, \quad 0 \le \theta \le 1 \quad \Longrightarrow \quad \theta x_1 + (1-\theta)x_2 \in C$$

2. show that C is obtained from simple convex sets (hyperplanes, halfspaces, norm balls, . . .) by operations that preserve convexity

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

Intersection

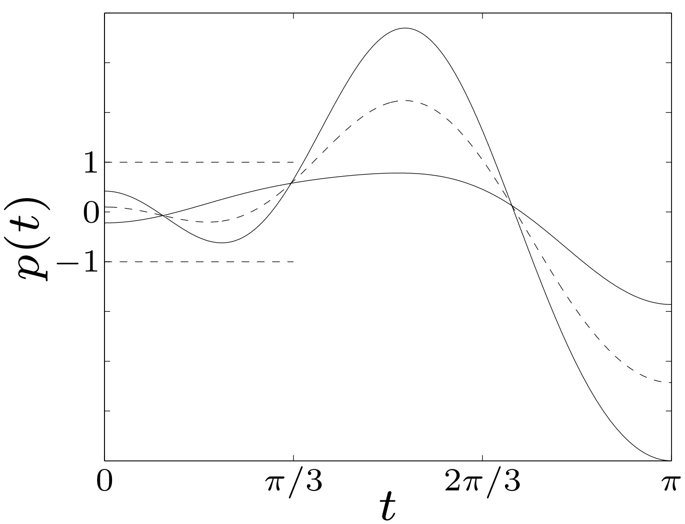
the intersection of (any number of) convex sets is convex

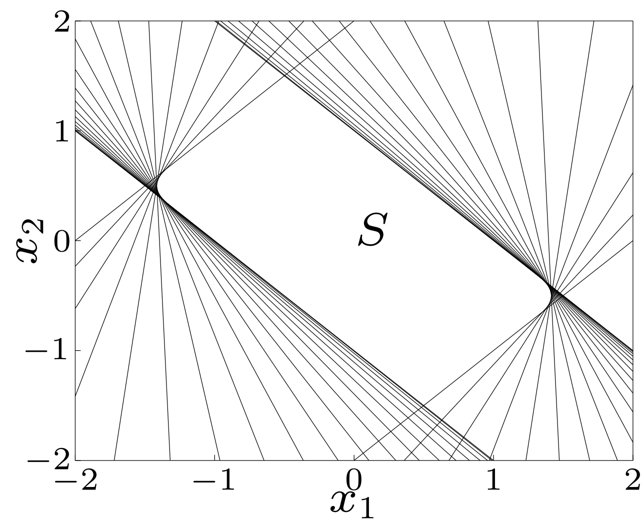
example:

$$S = \{x \in \mathbf{R}^m \mid |p(t)| \leq 1 \text{ for } |t| \leq \pi/3\}$$

where $p(t) = x_1 \cos t + x_2 \cos 2t + \cdots + x_m \cos mt$

for $m = 2$:





Affine function

suppose $f : \mathbf{R}^n \to \mathbf{R}^m$ is affine ($f(x) = Ax + b$ with $A \in \mathbf{R}^{m\times n}$, $b \in \mathbf{R}^m$)

- the image of a convex set under f is convex

$$S \subseteq \mathbf{R}^n \text{ convex} \quad \Longrightarrow \quad f(S) = \{f(x) \mid x \in S\} \text{ convex}$$

- the inverse image $f^{-1}(C)$ of a convex set under f is convex

$$C \subseteq \mathbf{R}^m \text{ convex} \quad \Longrightarrow \quad f^{-1}(C) = \{x \in \mathbf{R}^n \mid f(x) \in C\} \text{ convex}$$

examples

- scaling, translation, projection
- solution set of linear matrix inequality $\{x \mid x_1A_1 + \cdots + x_mA_m \preceq B\}$ (with $A_i, B \in \mathbf{S}^p$)
- hyperbolic cone $\{x \mid x^TPx \le (c^Tx)^2,\ c^Tx \ge 0\}$ (with $P \in \mathbf{S}^n_+$)

Perspective and linear-fractional function

perspective function $P : \mathbf{R}^{n+1} \to \mathbf{R}^n$:

$$P(x,t) = x/t, \qquad \mathbf{dom}\, P = \{(x,t) \mid t > 0\}$$

images and inverse images of convex sets under perspective are convex

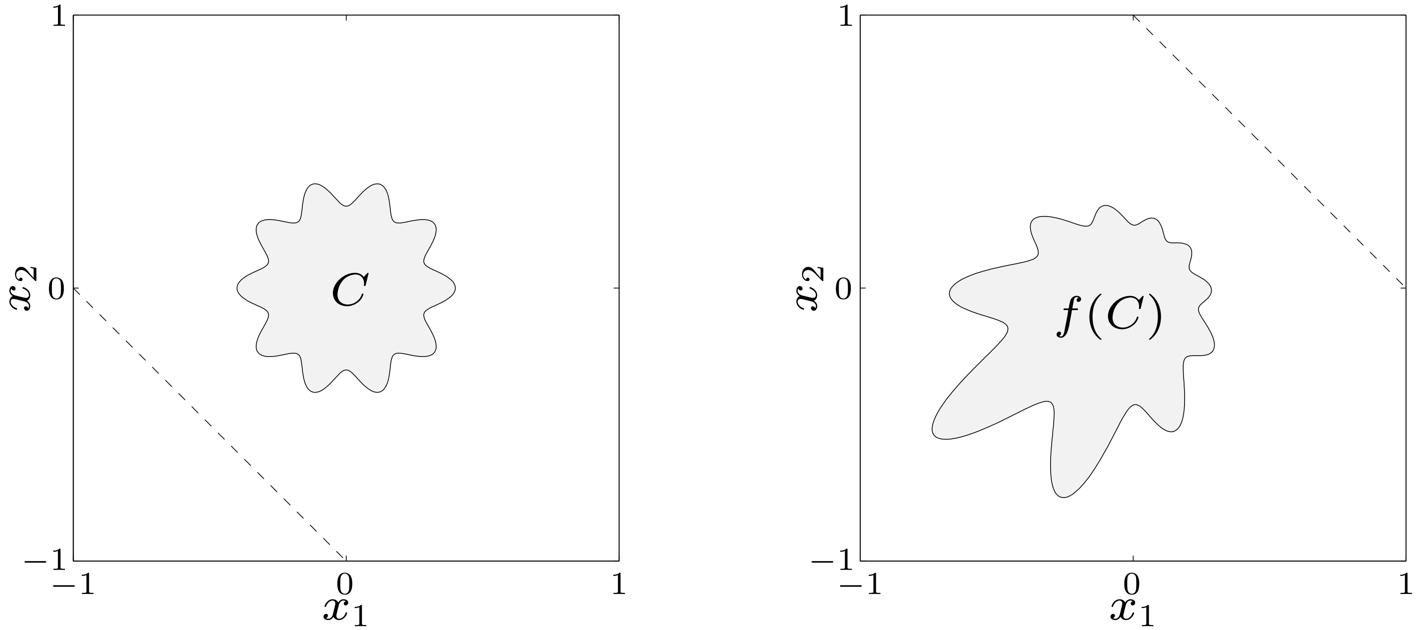
linear-fractional function $f : \mathbf{R}^n \to \mathbf{R}^m$:

$$f(x) = \frac{Ax+b}{c^T x + d}, \qquad \mathbf{dom}\, f = \{x \mid c^T x + d > 0\}$$

images and inverse images of convex sets under linear-fractional functions are convex

example of a linear-fractional function

$$f(x) = \frac{1}{x_1 + x_2 + 1} x$$



Lecture 3, February 04: Today's overview

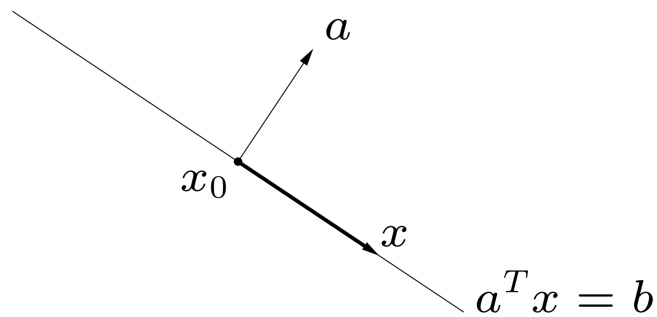
- Some announcement
- Questions from the last class (Polyhedra)
- Euclidean balls, Ellipsoids and Norm balls.
- Separating hyperplane theorem.
- Supporting hyperplane theorem.

Some announcements

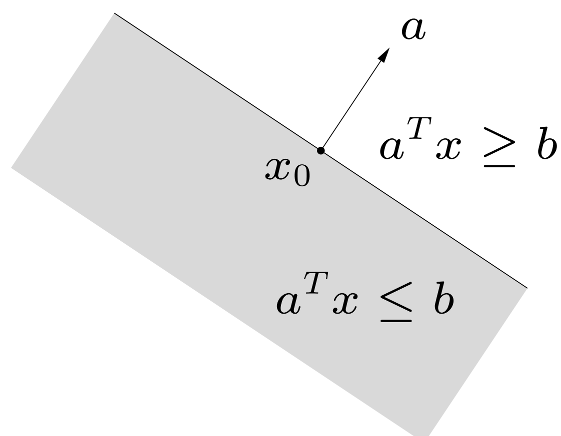
- No late entry and more than 5 minutes late may miss the attendance
- No mobile during class
- Separate workbook for assignment with week number and dates.
  - 10-20 marks for assignment.
  - scanned copy weekly in google classroom (weekly on Saturday)
  - hardcopy monthly (last week of the month).

Hyperplanes and halfspaces

hyperplane: set of the form $\{x \mid a^T x = b\}$ $(a \neq 0)$



halfspace: set of the form $\{x \mid a^T x \leq b\}$ $(a \neq 0)$



- a is the normal vector
- hyperplanes are affine and convex; halfspaces are convex

Euclidean balls and ellipsoids

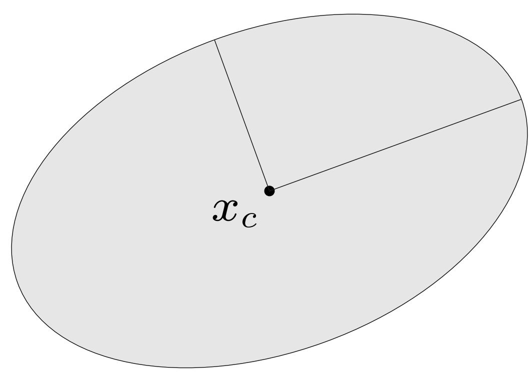
(Euclidean) ball with center x_c and radius r:

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

ellipsoid: set of the form

$$\{x \mid (x - x_c)^T P^{-1} (x - x_c) \le 1\}$$

with $P \in \mathbf{S}^n_{++}$ (*i.e.*, P symmetric positive definite)



other representation: $\{x_c + Au \mid \|u\|_2 \le 1\}$ with A square and nonsingular

Norm balls and norm cones

norm: a function $\|\cdot\|$ that satisfies

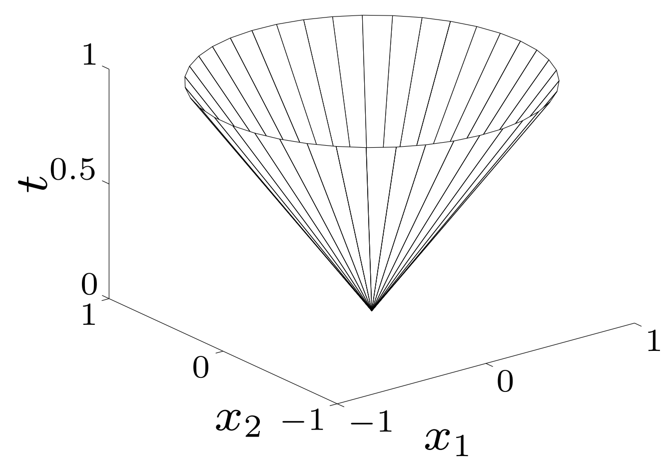
- $\|x\| \geq 0$; $\|x\| = 0$ if and only if $x = 0$
- $\|tx\| = |t|\,\|x\|$ for $t \in \mathbf{R}$
- $\|x + y\| \leq \|x\| + \|y\|$

notation: $\|\cdot\|$ is general (unspecified) norm; $\|\cdot\|_{\text{symb}}$ is particular norm

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

norm cone: $\{(x, t) \mid \|x\| \leq t\}$

Euclidean norm cone is called second-order cone



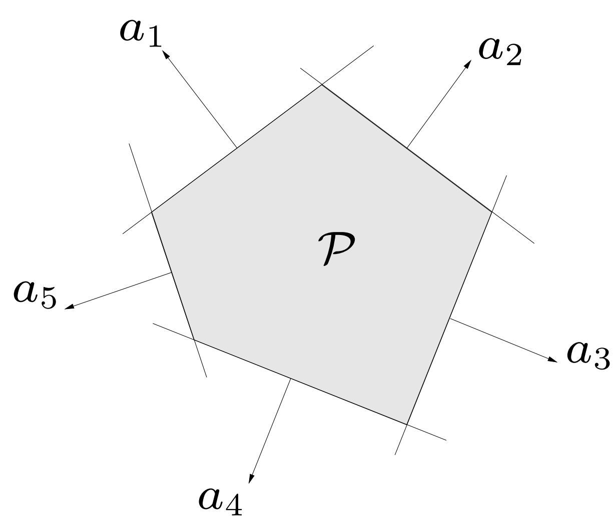
norm balls and cones are convex

Polyhedra

solution set of finitely many linear inequalities and equalities

$$Ax \preceq b, \qquad Cx = d$$

($A \in \mathbf{R}^{m\times n}$, $C \in \mathbf{R}^{p\times n}$, $\preceq$ is componentwise inequality)

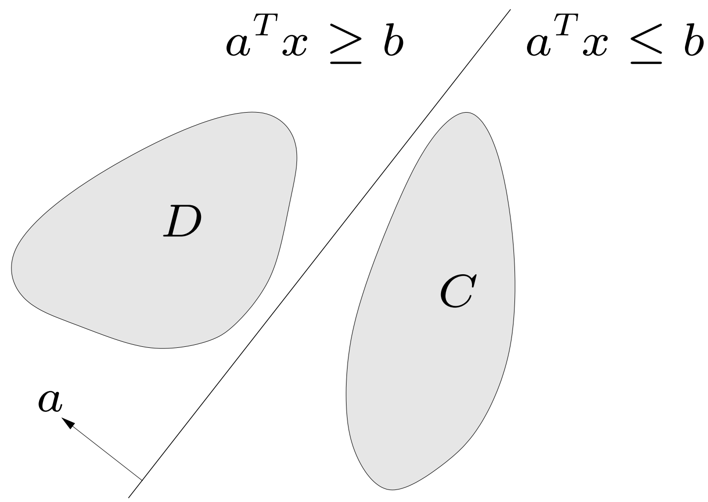


polyhedron is intersection of finite number of halfspaces and hyperplanes

Separating hyperplane theorem

if C and D are nonempty disjoint convex sets, there exist $a \neq 0$, b s.t.

$$a^T x \leq b \text{ for } x \in C, \qquad a^T x \geq b \text{ for } x \in D$$



the hyperplane $\{x \mid a^T x = b\}$ separates C and D

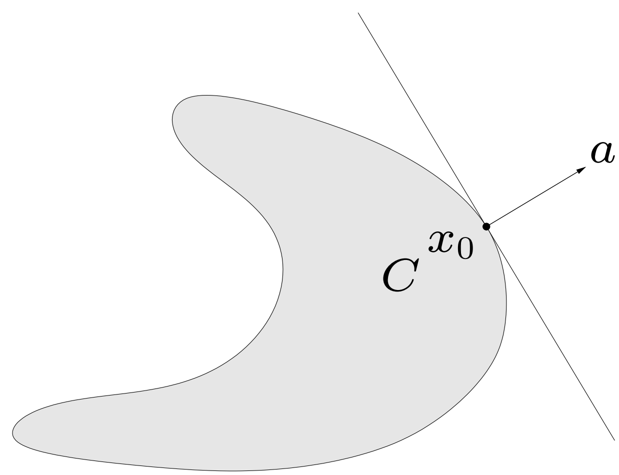
strict separation requires additional assumptions ($e.g.$, C is closed, D is a singleton)

Supporting hyperplane theorem

supporting hyperplane to set C at boundary point x_0:

$$\{x \mid a^T x = a^T x_0\}$$

where $a \neq 0$ and $a^T x \leq a^T x_0$ for all $x \in C$



supporting hyperplane theorem: if C is convex, then there exists a supporting hyperplane at every boundary point of C

Lecture 4, February 06: Today's overview

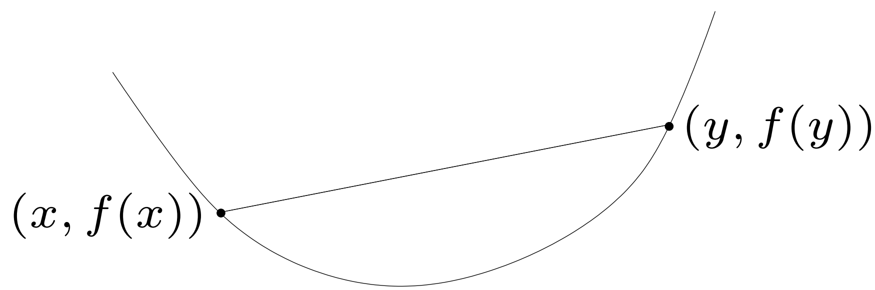
- Convex function
- Concave function
- Examples of convex/concave function
- First order condition (Gradient)
- Second order condition (Hessian)
- Reference: Chapter 3 of Convex Optimization

Definition

$f : \mathbf{R}^n \to \mathbf{R}$ is convex if $\mathbf{dom}\, f$ is a convex set and

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

for all $x, y \in \mathbf{dom}\, f$, $0 \leq \theta \leq 1$



- f is concave if $-f$ is convex
- f is strictly convex if $\mathbf{dom}\, f$ is convex and

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

for $x, y \in \mathbf{dom}\, f$, $x \neq y$, $0 < \theta < 1$

Examples on $\mathbf{R}$

convex:

- affine: $ax + b$ on $\mathbf{R}$, for any $a, b \in \mathbf{R}$
- exponential: e^{ax}, for any $a \in \mathbf{R}$
- powers: x^α on $\mathbf{R}_{++}$, for $\alpha \geq 1$ or $\alpha \leq 0$
- powers of absolute value: $|x|^p$ on $\mathbf{R}$, for $p \geq 1$
- negative entropy: $x \log x$ on $\mathbf{R}_{++}$

concave:

- affine: $ax + b$ on $\mathbf{R}$, for any $a, b \in \mathbf{R}$
- powers: x^α on $\mathbf{R}_{++}$, for $0 \leq \alpha \leq 1$
- logarithm: $\log x$ on $\mathbf{R}_{++}$

Examples on $\mathbf{R}^n$ and $\mathbf{R}^{m\times n}$

affine functions are convex and concave; all norms are convex

examples on $\mathbf{R}^n$

- affine function $f(x) = a^T x + b$
- norms: $\|x\|_p = (\sum_{i=1}^n |x_i|^p)^{1/p}$ for $p \geq 1$; $\|x\|_\infty = \max_k |x_k|$

examples on $\mathbf{R}^{m\times n}$ ($m \times n$ matrices)

- affine function

$$f(X) = \mathbf{tr}(A^T X) + b = \sum_{i=1}^m \sum_{j=1}^n A_{ij} X_{ij} + b$$

- spectral (maximum singular value) norm

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

First-order condition

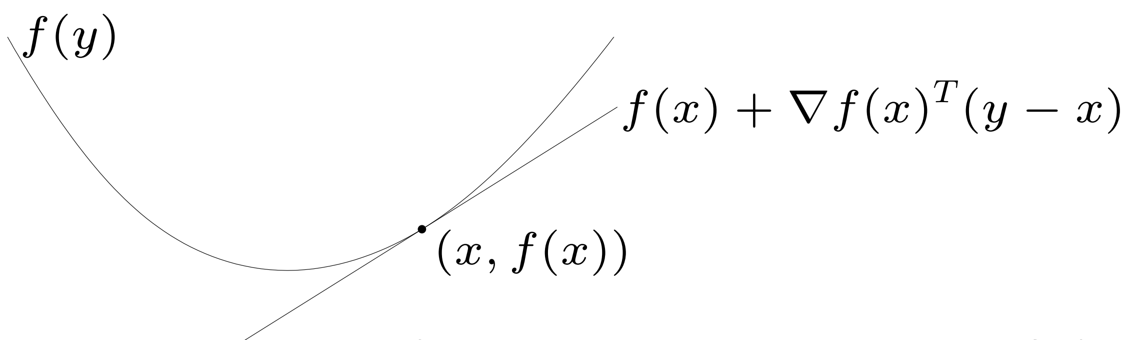
f is **differentiable** if $\mathbf{dom}\, f$ is open and the gradient

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

exists at each $x \in \mathbf{dom}\, f$

1st-order condition: differentiable f with convex domain is convex iff

$$f(y) \geq f(x) + \nabla f(x)^T (y - x) \quad \text{for all } x, y \in \mathbf{dom}\, f$$



first-order approximation of f is global underestimator

Second-order conditions

f is **twice differentiable** if $\mathbf{dom}\, f$ is open and the Hessian $\nabla^2 f(x) \in \mathbf{S}^n$,

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

exists at each $x \in \mathbf{dom}\, f$

2nd-order conditions: for twice differentiable f with convex domain

- f is convex if and only if

$$\nabla^2 f(x) \succeq 0 \quad \text{for all } x \in \mathbf{dom}\, f$$

- if $\nabla^2 f(x) \succ 0$ for all $x \in \mathbf{dom}\, f$, then f is strictly convex

Examples

quadratic function: $f(x) = (1/2)x^T Px + q^T x + r$ (with $P \in \mathbf{S}^n$)

$$\nabla f(x) = Px + q, \qquad \nabla^2 f(x) = P$$

convex if $P \succeq 0$

least-squares objective: $f(x) = \|Ax - b\|_2^2$

$$\nabla f(x) = 2A^T(Ax - b), \qquad \nabla^2 f(x) = 2A^T A$$

convex (for any A)

quadratic-over-linear: $f(x, y) = x^2/y$

$$\nabla^2 f(x, y) = \frac{2}{y^3} \begin{bmatrix} y \\ -x \end{bmatrix} \begin{bmatrix} y \\ -x \end{bmatrix}^T \succeq 0$$

convex for $y > 0$