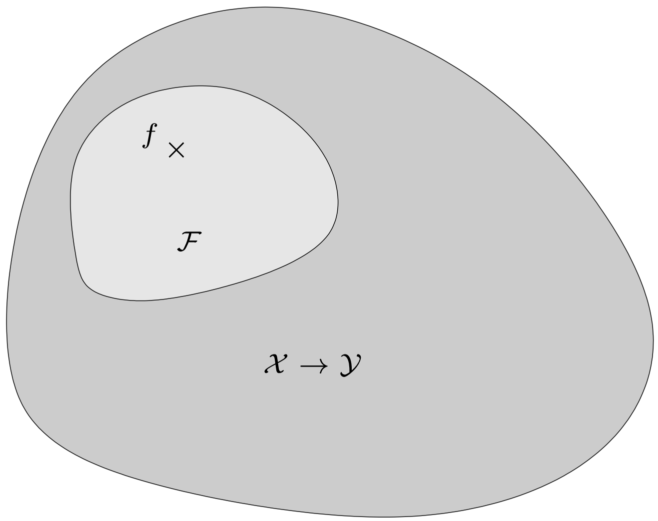
Convex Optimization & Machine Learning

Introduction to Optimization

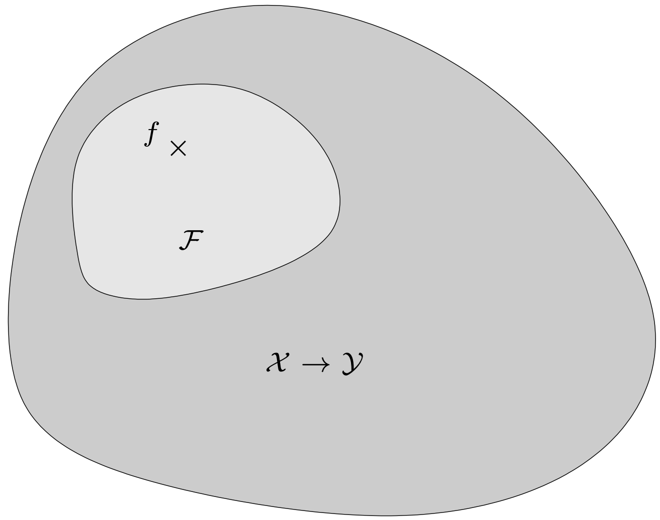
mcuturi@i.kyoto-u.ac.jp

Why do we need optimization in machine learning

- We want to find the best possible decision w.r.t. a problem
- In a supervised setting for instance, we want to **learn** a map $\mathcal{X} \to \mathcal{Y}$
- We consider a set of candidates $\mathcal{F}$ for such a decision



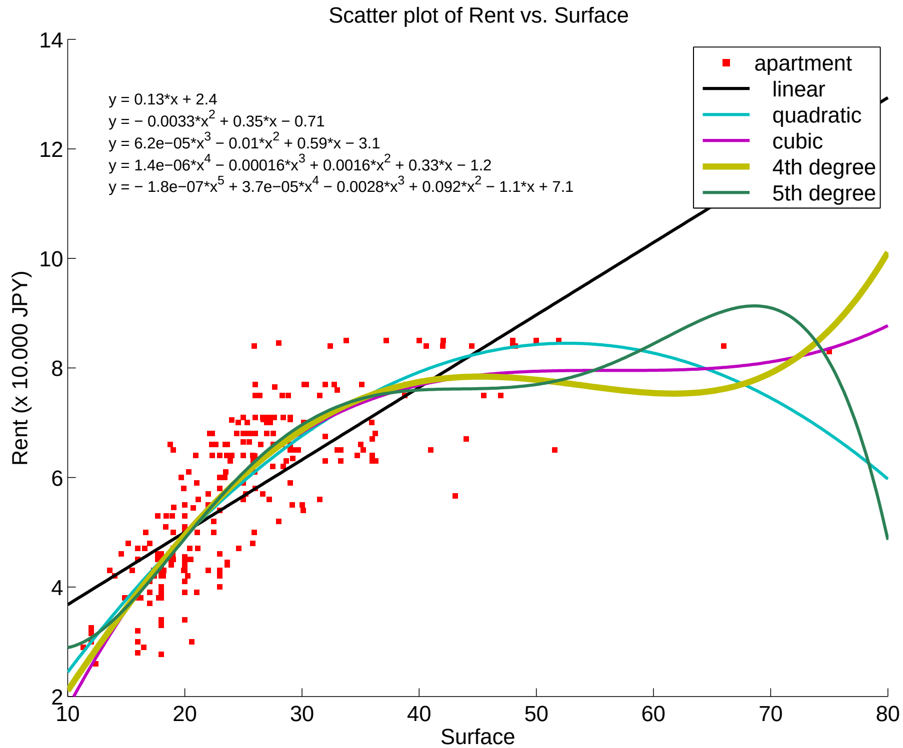
Why do we need optimization in machine learning



- **Quantify** how well a candidate function in $\mathcal{F}$ fits with the database
  - define a **data-dependent** criterion $C_{\textbf{data}}$
  - Typically, given a function f, $C_{\text{data}}(f)$ is **big** if f **not accurate** on the data.
- Given both $\mathcal{F}$ and C_{data}, a method to find an **optimal** candidate:

$$\min_{f \in \mathcal{F}} \quad C_{\text{data}}(f).$$

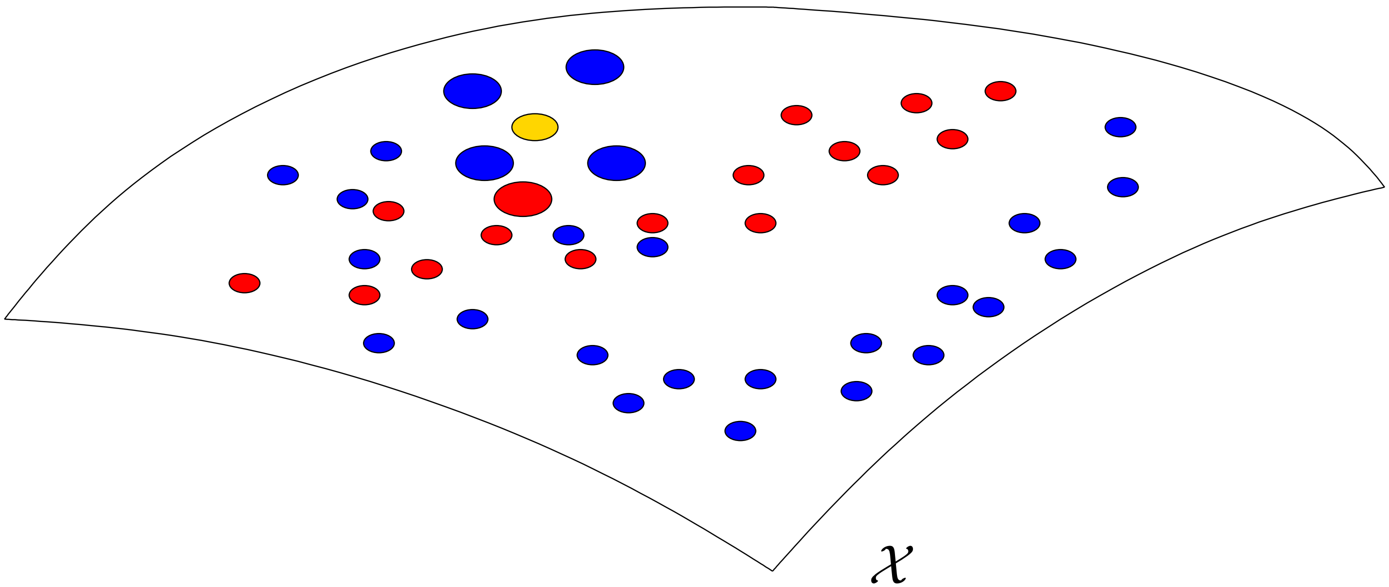
Quizz: Regression



Does Least-Square regression fall into this approach?

1. Yes   2. No

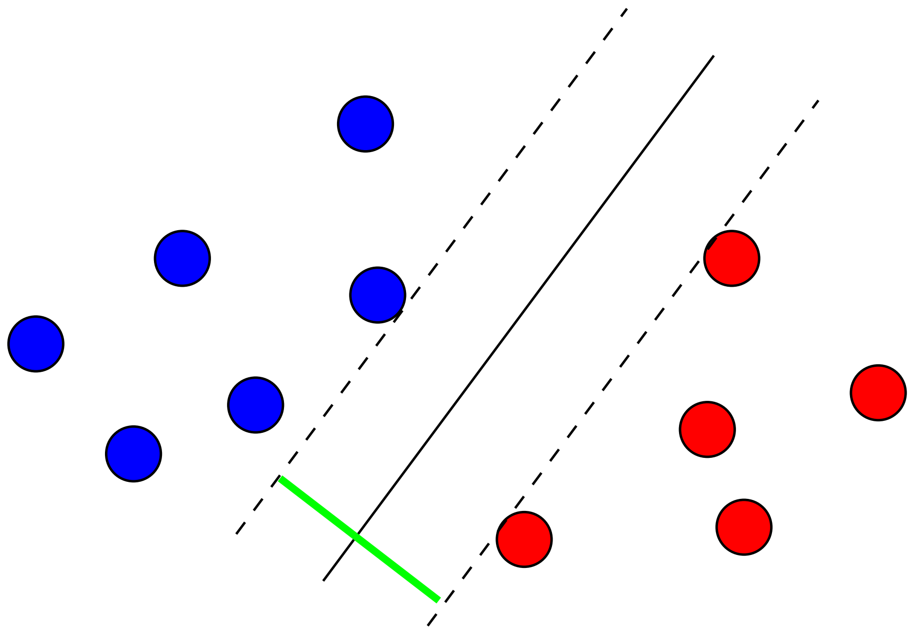
Quizz: k-nearest neighbors



Does k-nearest neighbors fall into this approach?

1. Yes   2. No

Quizz: SVM



Does the SVM fall into this approach?

1. Yes   2. No

What is optimization?

- A general formulation for optimization problem is that of defining
  - unknown variables $x_1, x_2, \cdots, x_n \in \mathcal{X}_1 \times \mathcal{X}_2 \times \cdots \times \mathcal{X}_n$, and solve

$$
\begin{array}{ll}
\text{minimize (or mazimize)} & \boldsymbol{f(x_1, x_2, \cdots, x_n)}, \\
\text{subject to} & \boldsymbol{f_i(x_1, x_2, \cdots, x_n)} \left\{ \begin{array}{c} <,> \\ = \\ \leq,\geq \end{array} \right\} \boldsymbol{b_i}, i = 1, 2, \cdots, m;
\end{array}
$$

What is optimization?

- A general formulation for optimization problem is that of defining
  - unknown variables $x_1, x_2, \cdots, x_n \in \mathcal{X}_1 \times \mathcal{X}_2 \times \cdots \times \mathcal{X}_n$, and solve

$$
\begin{array}{ll}
\text{minimize (or mazimize)} & \boldsymbol{f(x_1, x_2, \cdots, x_n)}, \\
\text{subject to} & \boldsymbol{f_i(x_1, x_2, \cdots, x_n)} \left\{ \begin{array}{c} <,> \\ = \\ \leq,\geq \end{array} \right\} \boldsymbol{b_i}, i = 1, 2, \cdots, m;
\end{array}
$$

- where
  - the $b_i \in \mathbb{R}$
  - functions $\boldsymbol{f}$ (objective) and $\boldsymbol{g_1, g_2, \cdots, g_m}$ (constraints) are functions

$$\mathcal{X}_1 \times \mathcal{X}_2 \times \cdots \times \mathcal{X}_n \to \mathbb{R}$$

What is optimization?

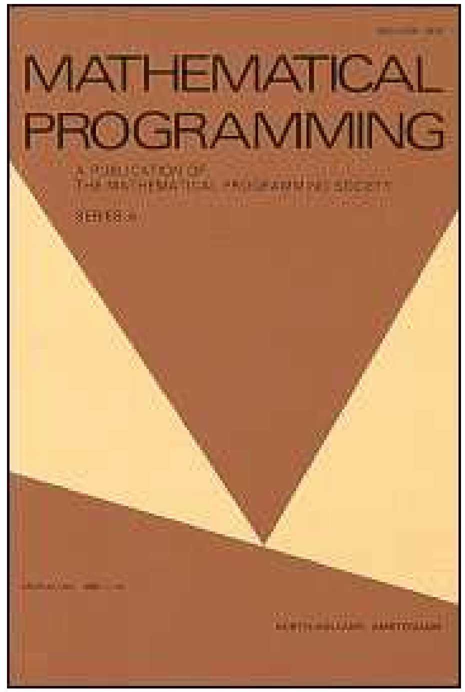
- A general formulation for optimization problem is that of defining
  - unknown variables $x_1, x_2, \cdots, x_n \in \mathcal{X}_1 \times \mathcal{X}_2 \times \cdots \times \mathcal{X}_n$, and solve

$$
\begin{array}{ll}
\text{minimize (or mazimize)} & \boldsymbol{f(x_1, x_2, \cdots, x_n)}, \\
\text{subject to} & \boldsymbol{f_i(x_1, x_2, \cdots, x_n)} \left\{ \begin{array}{c} <,> \\ = \\ \leq, \geq \end{array} \right\} \boldsymbol{b_i}, i = 1, 2, \cdots, m;
\end{array}
$$

- the sets $\mathcal{X}_i$ need not be the same, as $\mathcal{X}_i$ might be
  - $\mathbb{R}$ scalar numbers,
  - **Z** integers,
  - $\mathbf{S}_n^+$ positive definite matrices,
  - strings of letters,
  - $etc.$
- When the $\mathcal{X}_i$ are different, the adjective *mixed* usually comes in.

Optimization & Mathematical Programming

- Optimization is field of **applied mathematics** on its own.
- Also called **Mathematical Programming**.



Mathematical Programming is not about programming code for mathematics!

Optimization & Mathematical Programming

Mathematical Programming is not about programming code for mathematics!

- **George Dantzig**, who proposed the "first" optimization algorithm, explains:

  - `The military refer to their various plans or proposed schedules of training, logistical supply and deployment of combat units as a program. When I first analyzed the Air Force planning problem and saw that it could be formulated as a system of linear inequalities, I called my paper Programming in a Linear Structure. Note that the term program was used for linear programs long before it was used as the set of instructions used by a computer. In the early days, these instructions were called codes.`

Mathematical Programming

- In the summer of 1948, Koopmans and I visited the Rand Corporation. One day we took a stroll along the Santa Monica beach. Koopmans said: Why not shorten Programming in a Linear Structure to Linear Programming? I replied: Thats it! From now on that will be its name. Later that day I gave a talk at Rand, entitled Linear Programming; years later Tucker shortened it to Linear Program.

- The term Mathematical Programming is due to Robert Dorfman of Harvard, who felt as early as 1949 that the term Linear Programming was too restrictive.

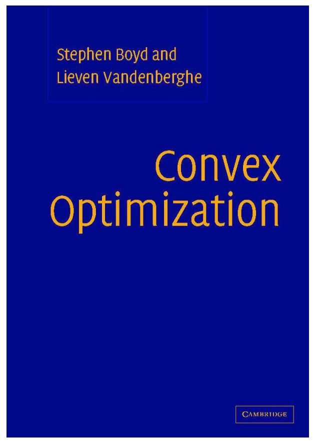
Mathematical Programming

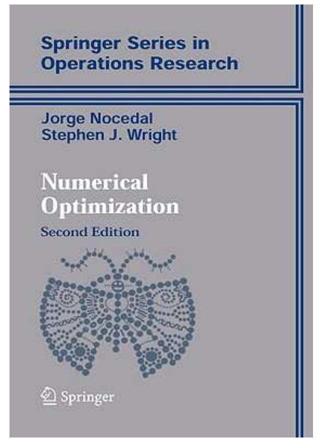
- Today mathematical programming = **optimization**. A relatively **new discipline**

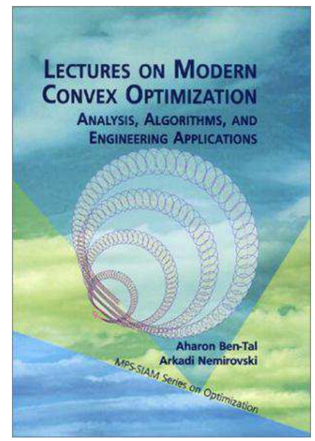
  - `What seems to characterize the pre-1947 era was lack of any interest in trying to optimize. T. Motzkin in his scholarly thesis written in 1936 cites only 42 papers on linear inequality systems, none of which mentioned an objective function.`

Before we move on to some reminders

- Keep in mind that optimization is hard. very hard in general.
- In 60 years, we have gone from nothing to quite a few successes.







- But always keep in mind that **most problems are intractable**.
- For **some particular problems** there is hope: **CONVEX problems**

Before we move on to some reminders

Evaluation = Programming Assignments

Reminders

Sources: Stephen Boyd's slides

Reminders: Convex set

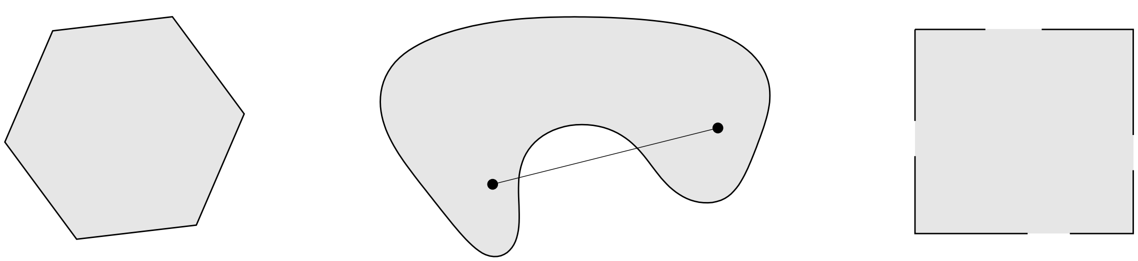
line segment between x_1 and x_2: all points

$$\{x = \lambda x_1 + (1-\lambda)x_2, \quad 0 \le \lambda \le 1\}$$

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

$$C \text{ is convex } \Leftrightarrow \forall x_1, x_2 \in C, 0 \le \lambda \le 1; \quad \lambda x_1 + (1-\lambda)x_2 \in C$$

examples (one convex, two nonconvex sets)



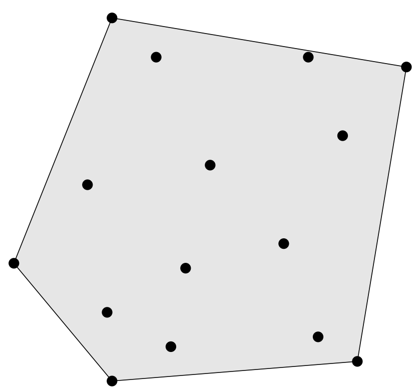
Convex combination and convex hull

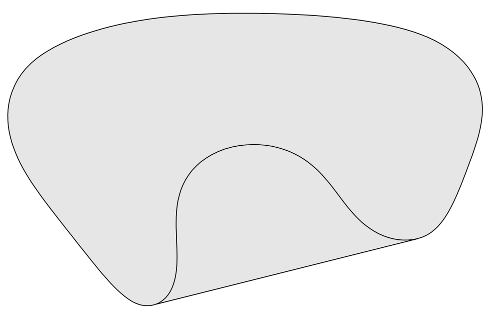
convex combination of x_1,. . . , x_k: any point x of the form

$$x = \lambda_1 x_1 + \lambda_2 x_2 + \cdots + \lambda_k x_k$$

with $\lambda_1 + \cdots + \lambda_k = 1$, $\lambda_i \geq 0$

convex hull $\langle S \rangle$: set of all convex combinations of points in S



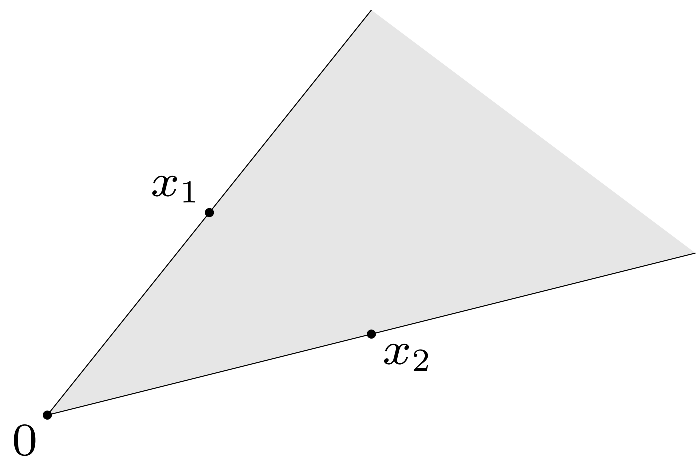


Convex cone

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

$$x = \lambda_1 x_1 + \lambda_2 x_2$$

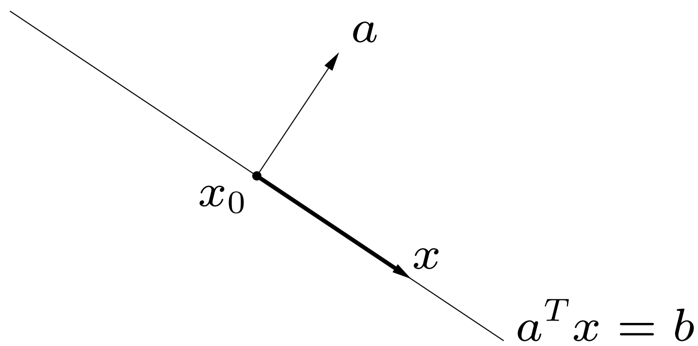
with $\lambda_1 \geq 0$, $\lambda_2 \geq 0$



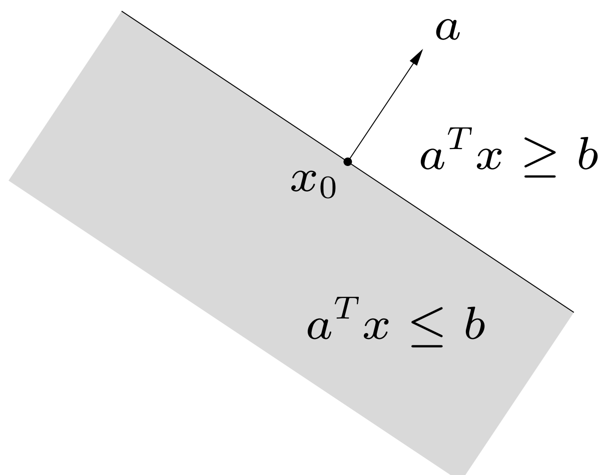
convex cone: set that contains all conic combinations of points in the set

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

Norm balls and norm cones

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

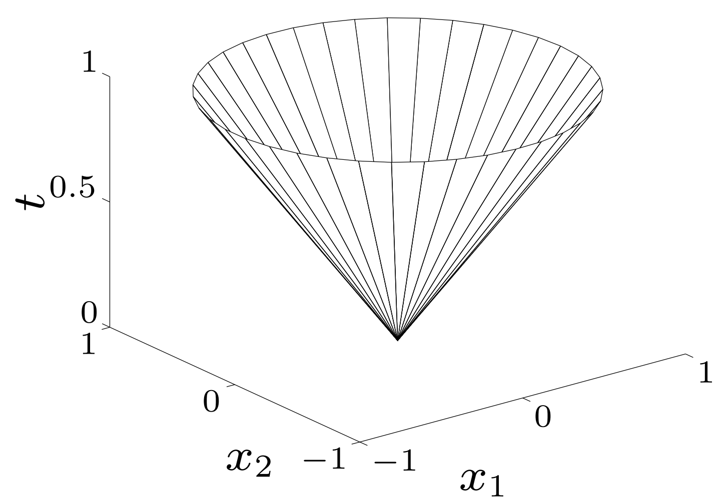
- $\|x\| \geq 0$; $\|x\| = 0$ if and only if $x = 0$
- $\|tx\| = |t| \, \|x\|$ for $t \in \mathbb{R}$
- $\|x + y\| \leq \|x\| + \|y\|$

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



cones are convex

Usual norms for vectors in $\mathbb{R}^d$

- l_2 norm:

$$\|x\|_2 = \sqrt{x^T x} = \sqrt{\sum_{i=1}^{d} x_i^2}$$

- l_1 norm:

$$\|x\|_1 = \sum_{i=1}^{d} |x_i|$$

- l_p norm:

$$\|x\|_p = \left(\sum_{i=1}^{d} |x_i|^p \right)^{\frac{1}{p}}$$

Quizz: l_p norms

The **unit ball** of the l_p norm is $\{x \mid \|x\|_p \leq 1\}$

The **unit ball** of the l_p norm is convex.

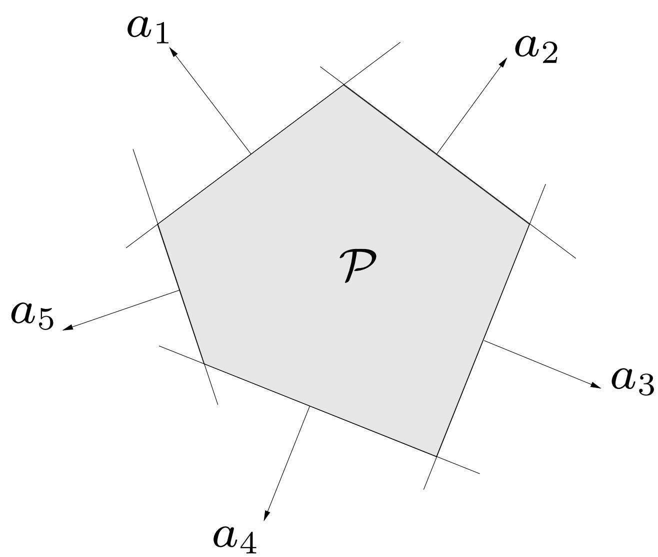
1. True   2. False

Polyhedra

solution set of finitely many linear inequalities and equalities

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

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



polyhedron is intersection of **finite** number of halfspaces and hyperplanes

Positive semidefinite cone

notation:

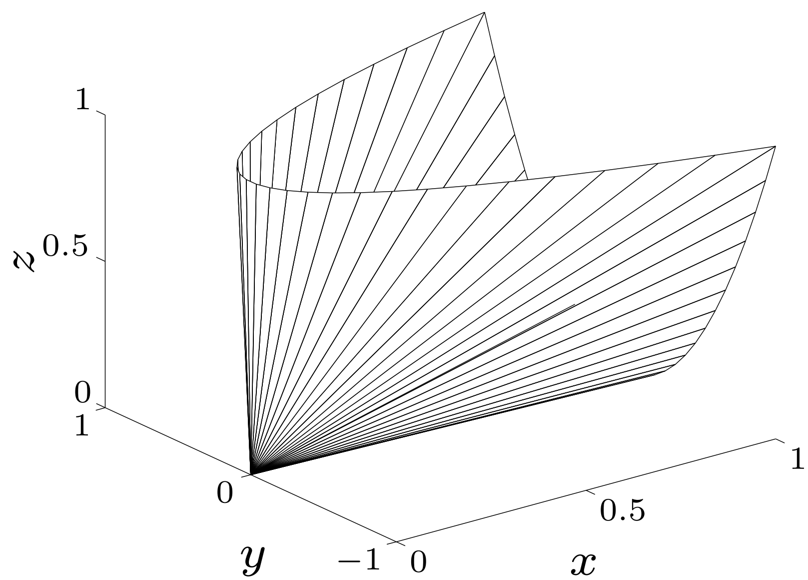
- $\mathbf{S}^n$ is set of symmetric $n \times n$ matrices
- $\mathbf{S}^n_+ = \{X \in \mathbf{S}^n \mid X \succeq 0\}$: positive semidefinite $n \times n$ matrices

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

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

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

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



Euclidean balls and ellipsoids

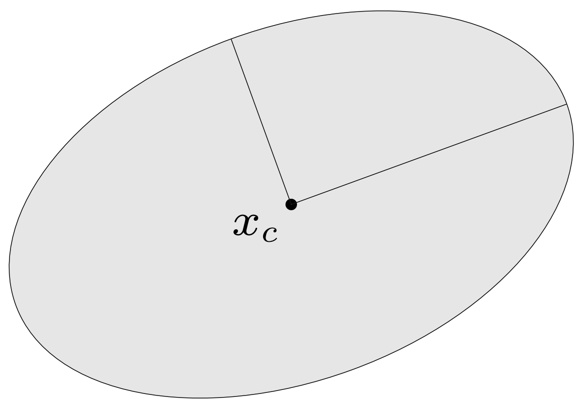
(Euclidean) ball with center x_c and radius r:

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

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

optimization problems

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

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

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

Quizz

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

If an optimization problem has an optimal solution $x^\star$, this solution is unique.

1. True   2. False

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 $n^2 k$ ($A \in \mathbb{R}^{k \times n}$); 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

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

solving linear programs

- no analytical formula for solution
- reliable and efficient algorithms and software
- computation time proportional to $n^2 m$ if $m \geq n$; 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

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

- 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

Convex optimization problem

$\boxed{\text{solving convex optimization problems}}$

- 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

$\boxed{\text{using convex optimization}}$

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