# Computational Data Analysis

## Machine Learning

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## Basic Optimization

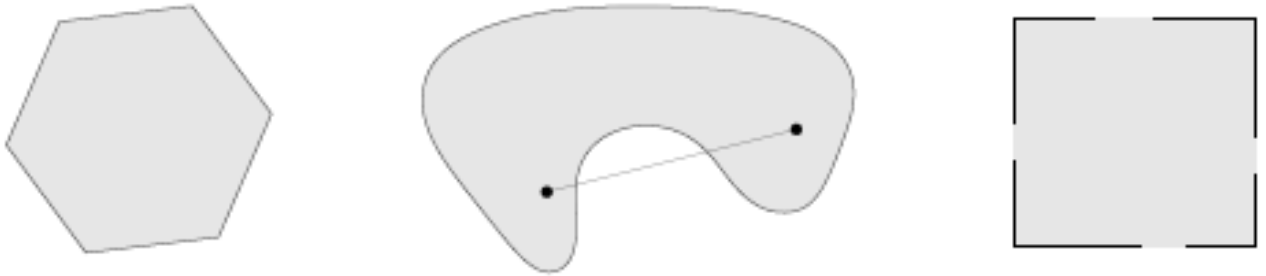
# Outline

- Convex set
- Convex/concave function
- First-order condition
- Second-order condition
- Theory under EM for GMM
- Langragian and dual function
- KKT conditions

The goal of this lecture is to build up necessary math background in developing algorithms for machine learning algorithms (previous and future lectures). You are not required to *master* everything.

# Convex Set

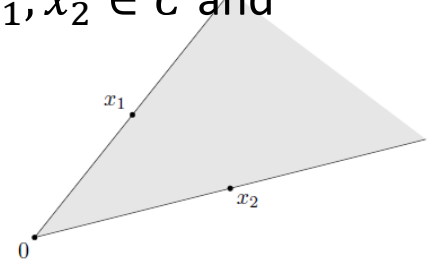
- Definition: A set $A$ is convex, if for every $0 \leq \alpha \leq 1$ it satisfies
  - $\forall x,\ y \in A \rightarrow \alpha x + (1-\alpha)y \in A$
- The line segment between any two points is also in the set.
- Examples of convex and non-convex sets



# Common Convex Set

- Cones: A set $C$ is a convex cone, if for any $x_1, x_2 \in C$ and $\theta_1, \theta_2 \geq 0$, we have

$$\theta_1 x_1 + \theta_2 x_2 \in C$$

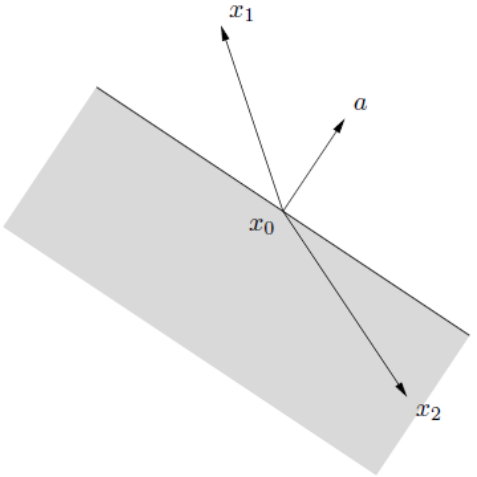



- Hyperplanes and halfspaces:
  A set is hyperplane if

$$\{x | a^\top (x - x_0) = 0, a \neq 0\}$$

  A halfspace is

$$\{x | a^\top (x - x_0) \leq 0, a \neq 0\}$$



# Common Convex Set

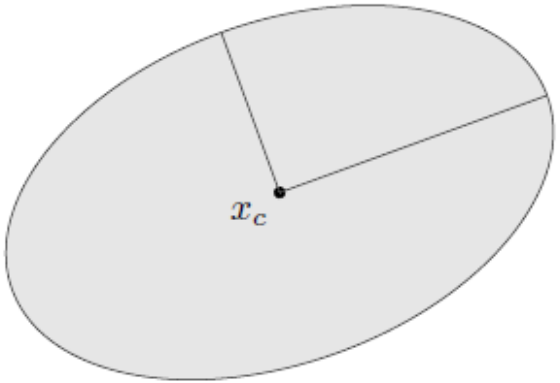
- Euclidean balls: A Euclidean ball has the form

$$B(x_c, r) = \{x | \|x - x_c\|_2 \leq r\}$$

- Ellipsoids:

$$E = \{x | (x - x_c)^\top P^{-1} (x - x_c) \leq 1\}$$

  - The eigen-vectors and eigen-values determine the direction and shape of the semi-axes



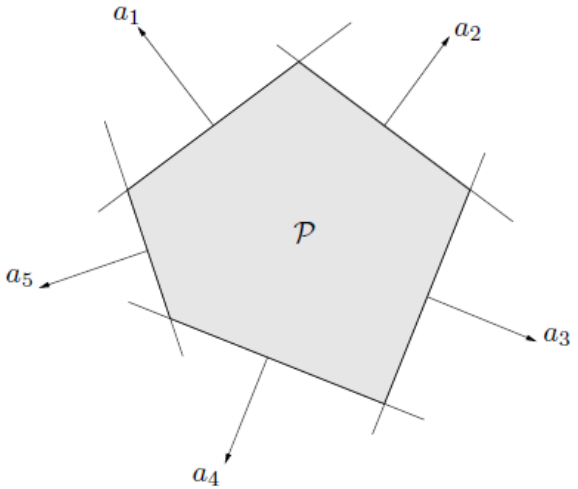

Used in support vector novelty detection

# Common Convex Set

- Polyhedra: Intersection of a *finite* set of halfspaces/hyperplanes

$$P = \{x | a_j^\top x \leq b_j, j = 1, \ldots, m, c_j^\top x = d_j, j = 1, \ldots, p\}$$

- It is defined by as the solution set of a finite number of linear equalities and inequalities




Used in SVM

# Operations that Preserve Convex Sets

- Intersections: In fact, *every* closed convex set $S$ is the intersection of all halfspaces that contain it:

$$S = \bigcap \{H | H \text{ is halfspace}, S \subset H\}$$

- Linear combination:

$$\alpha S = \{\alpha x | x \in S\},\ S + \alpha = \{x + a | x \in S\}$$

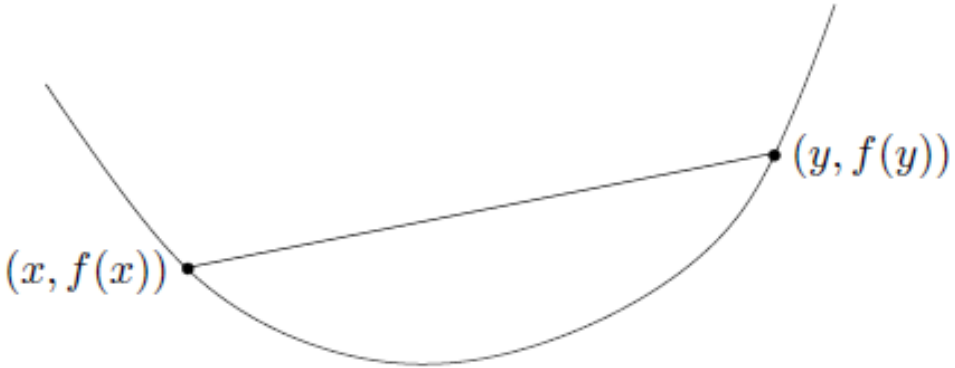
- Projection/Concatenation

# Convex Functions

- Definition: A function $f: R^n \rightarrow R$ is convex if the domain $\mathbf{dom} f$ is a convex set and if for all $x, y \in \mathbf{dom} f$, and $0 \leq \theta \leq 1$, we have

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

- Geometrically, the line segment between $(x, f(x))$ and $(y, f(y))$ lies above the graph of $f$

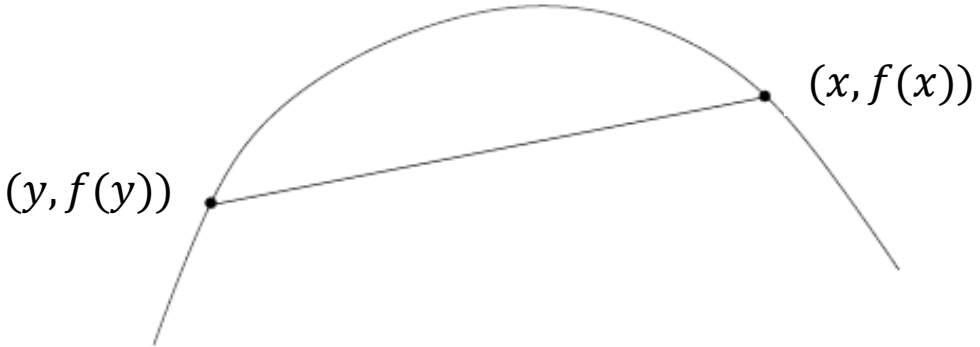


# Concave Functions

- Definition: A function $f: R^n \rightarrow R$ is concave if the domain $\mathbf{dom} f$ is a convex set and if for all $x, y \in \mathbf{dom} f$, and $0 \leq \theta \leq 1$, we have

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

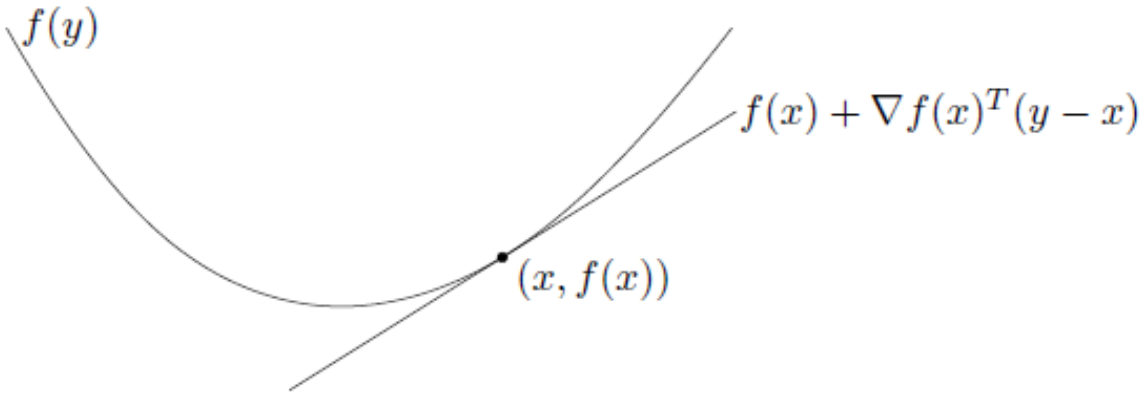
- Geometrically, the line segment between $(x, f(x))$ and $(y, f(y))$ lies below the graph of $f$



# First-order Condition

- If $f$ is differentiable, another way to characterize it is the first-order condition: $f$ is convex iff $\mathbf{dom} f$ is convex and
$$f(y) \geq f(x) + \nabla f(x)^{\mathsf{T}}(y - x)$$
holds for all $x, y \in \mathbf{dom} f$.

- Geometrically, it means that the tangent line of $f$ at point $x$ lies below the function



# Second-order Condition

- If $f$ is twice differential, the second-order condition is: $f$ is convex iff $\mathbf{dom} f$ is convex and for all $x \in \mathbf{dom} f$

$$\nabla^2 f(x) \succcurlyeq 0$$

positive semidefinite (symmetric and all eigenvalue nonnegative)

- That is the Hessian is positive semidefinite.

- Geometrically, the graph of the function has positive (upward) curvature at every point.

- Eg. $\mathrm{f(x)} = x^{\mathsf{T}} Ax$, for $A$ positive semidefinite

# Examples

- Exponential: $e^{ax}$ for every $a \in R$
- Powers: $x^a$ is convex on $R_{++}$ when $a \geq 1$ or $a \leq 0$; concave (i.e., $-f$ is convex) for $0 \leq a \leq 1$
- Powers of absolute vaue: $|x|^p$ for $p \geq 1$
- Logarithm: $\log x$ is concave on $R_{++}$
- Negative entropy: $x \log x$ is convex
- Norms: All norms are convex (nonnegative; homogeneous; triangular inequality)
- Max function: $f(x) = \max\{x_1, \ldots, x_n\}$ is convex
- Log-determinant: $f(X) = \log \det X$ is convex for all positive definite matrices

Used in EM

Used in multivariate Gaussian fit

# Operations that Preserve Convexity

- Nonnegative weighted sums: If $f_1, \dots, f_m$ are convex, and $w_1, \dots, w_m \geq 0$, then
$$f = w_1 f_1 + \cdots + w_m f_m$$
is convex

- Composition with an affine mapping: suppose $f$ is convex, then
$$g(x) = f(Ax + b)$$
with $\mathbf{dom} g = \{x | Ax + b \in \mathbf{dom} f\}$ is convex

- Pointwise maximum and supremum: If $f_1$ and $f_2$ are convex, then $f(x) = \max\{f_1, f_2\}$ is also convex. It easily extends to multiple functions.

# Operations that Preserve Convexity

- Composition: If $h$ is convex and nondecreasing, and $g$ is convex, then $f(x) = h(g(x))$ is convex
  - The second derivative of $f$ is
    $$f''(x) = h''\big(g(x)\big)g'(x)^2 + h'\big(g(x)\big)g''(x)$$
    for $f$ to be convex, $f''$ should be nonnegative

- Log-sum-exp: $f(x) = \log(e^{x_1} + \cdots + e^{x_n})$

# Theory underlying EM

- Recall that in MLE, we intend to learn the model parameter that would have maximize the likelihood of the data.
  - $l(\theta; D) = \log \sum_z p(x, z|\theta) = \log \sum_z p(x|\, z, \theta) P(z|\theta)$

- But we are iterating these:
  - Expectation step (E-step)
    - $f(\theta) = E_{q(z)}[\log p(x, z|\theta)], where\ q(z) = P(z|x, \theta^t)$
  - Maximization step (M-step)
    - $\theta^{t+1} = argmax_\theta\ f(\theta)$

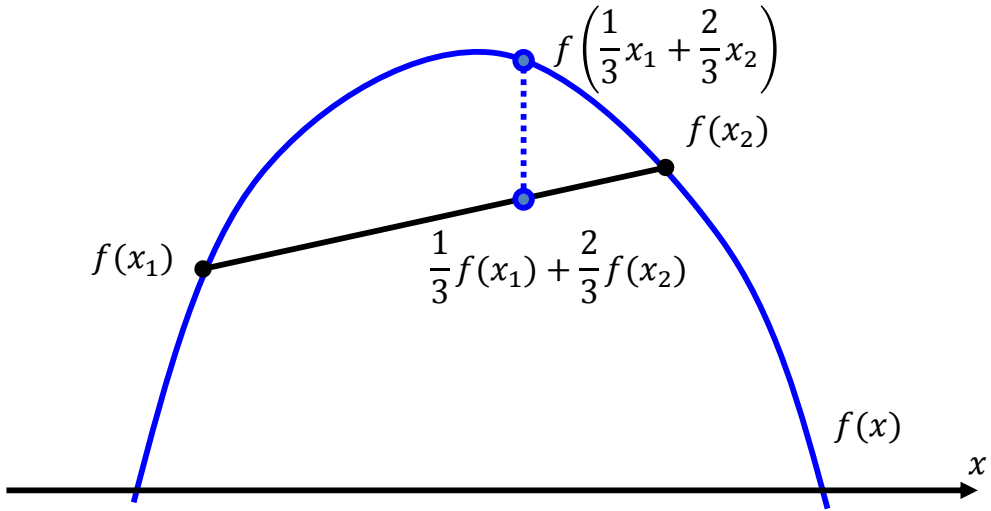
- Does maximizing this surrogate yield a maximizer of the likelihood?

# Jensen's inequality

- For concave function $f(x)$
  - $f(\sum_i \alpha_i x_i) \geq \sum_i \alpha_i f(x_i)\,, where\ \sum_i \alpha_i = 1, \alpha_i \geq 0$

- Most general case: If $x$ is a random variable, and $f$ is concave,

$$f(\mathbf{E}x) \geq \mathbf{E}f(x)$$



# Lower bound of log-likelihood

- Log-likelihood $l(x;\theta) = \log \sum_z p(x,z|\theta)$

$$= \log \sum_z q(z) \frac{p(x,z|\theta)}{q(z)} \text{ (arbitrary } q(z))$$

$$\geq \sum_z q(z) \log \frac{p(x,z|\theta)}{q(z)} \; (Jensen's\ inequality\ f\left(\sum_i \alpha_i x_i\right) \geq \sum_i \alpha_i f(x_i))$$

$$= \sum_z q(z) \log p(x,z|\theta) - \sum_z q(z) \log q(z)$$

$$= E_{q(z)}[\log p(x,z|\theta)] + H_{q(z)}$$

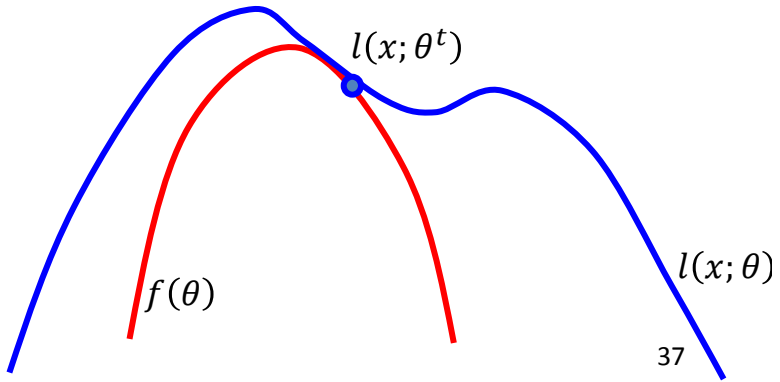
What $q$ to use?

# What attains equality?

- $q(z) = p(z|x, \theta^t)$: posterior of $z$ given $x$ attains the equality at $\theta^t$

Let $F(q, \theta) = \sum_z q(z|x) \log \frac{p(x,z|\theta)}{q(z|x)} \leq l(x; \theta) = \log \sum_z p(x, z|\theta)$

- $F(p(z|x, \theta^t), \theta^t) = \sum_z p(z|x, \theta^t) \log \frac{p(x,z|\theta^t)}{p(z|x,\theta^t)}$
- $= \sum_z p(z|x, \theta^t) \log p(x|\theta^t)$
- $= \log p(x|\theta^t)$
- $= \log \sum_z p(x, z|\theta^t)$



# Convex Optimization

- Definition: An optimization problem is specified by

$$\begin{aligned} &\text{minimize} && f_0(x) \\ &\text{subject to} && f_i(x) \leq 0,\ i = 1, \ldots, m \\ &&& h_i(x) = 0,\ i = 1, \ldots, p \end{aligned}$$

- A convex optimization problem has the following requirements
  - The objective function $f_0(x)$ must be convex
  - The inequality constraint functions $f_i(x)$ must be convex
  - The equality constraint functions $h_i(x)$ must be affine

- Eg. support vector machines (SVM), logistic regression, maximum likelihood, ridge regression, …

# Convex Optimization

- Global optimum: a point $x^*$ in the feasible set is a global optimum iff
$$f_0(x^*) \leq f_0(x)$$
for all $x$ in the feasible set

- Local optimum: a point $x^*$ in the feasible set is a local optimum iff there exists $r > 0$, such that for all $x \in \{x | \|x - x^*\| \leq r\}$ and also in the feasible set, we have $f_0(x^*) \leq f_0(x)$

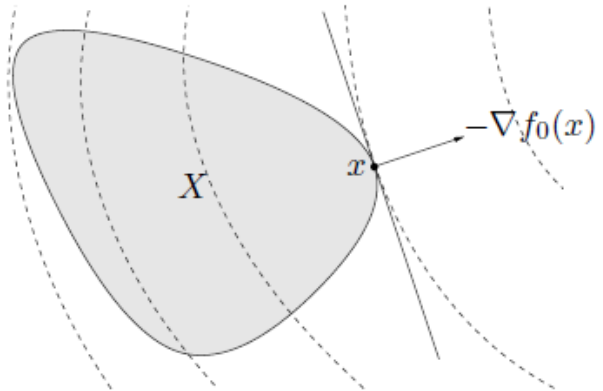
- For convex optimization problem, any local optimum is also a global optimum

# First order optimality condition

- Let $X$ denotes the feasible set, then $x$ is optimal iff
$$\nabla f_0(x)^\top (y - x) \geq 0 \text{ for all } y \in X$$

- For an unconstrained problem, the condition becomes
$$\nabla f_0(x) = 0$$

- Geometrically, if $\nabla f_0(x) \neq 0$, it means $-\nabla f_0(x)$ is orthogonal to the feasible set at $x$



# Operations that Preserve Convex Sets

- For an unconstrained problem, the condition becomes

$$\nabla f_0(x) = 0$$

- For an constrained problem, we need to use the Lagrangian

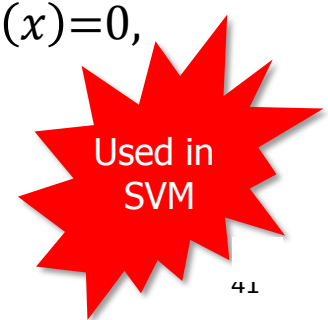
$$L(x, \mu, \lambda) = f_0(x) + \sum_{i=1}^{p} \mu_i h_i(x) + \sum_{i=1}^{m} \lambda_i f_i(x)$$

$$\text{s.t.} \quad \lambda_i \geq 0$$

to transform it into an unconstrained problem

- It is a lower bound of $f_0(x)$ for all $x \in X$, since $h_i(x)=0$, $f_i(x) \leq 0$ and $\lambda_i \geq 0$

$$L(x, \mu, \lambda) \leq f_0(x) \text{ for all } x \in X$$



# Lagrange dual function

- The Lagrange dual function is

$$g(\mu, \lambda) = \inf_x L(x, \mu, \lambda)$$

- It is a lower bound for the optimal value

$$g(\mu, \lambda) = \inf_x L(x, \mu, \lambda) \leq L(x^*, \mu, \lambda) \leq f_0(x^*)$$

- We want to maximize the lower bound to make it tight

$$g(\mu^*, \lambda^*) = \max g(\mu, \lambda)$$

# Primal and Dual problems

- Primal problem

$$\begin{aligned} &\text{minimize} && f_0(x) \\ &\text{subject to} && f_i(x) \leq 0, \ i = 1, \dots, m \\ &&& h_i(x) = 0, \ i = 1, \dots, p \end{aligned}$$

- Dual problem

$$\begin{aligned} &\text{maximize} && g(\mu, \lambda) \\ &\text{subject to} && \lambda_i \geq 0, \ i = 1, \dots, m \end{aligned}$$


- Strong duality (for convex problems, with mild condition)

$$g(\mu^*, \lambda^*) = f_0(x^*)$$

- Slater's condition: There exists an $x$ inside the relative interior of the domain $X$ such that, $f_i(x) < 0, \ i = 1, \dots, m$

# KKT Optimality conditions

- The following list of optimality conditions, for an optimal triplet $(x^*, \mu^*, \lambda^*)$, are called KKT conditions

- $\nabla f_0(x^*) + \sum_{i=1}^{m} \lambda_i^* \nabla f_i(x^*) + \sum_{i=1}^{p} \mu_i^* \nabla h_i(x^*) = 0$

- $\lambda_i^* f_i(x^*) = 0$

- $f_i(x^*) \leq 0$

- $h_i(x^*) = 0$

- $\lambda_i^* \geq 0$


SUMMARY