# Introduction to Optimization

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# Outline

# What is optimization?

- Finding (one or more) minimizer of a function subject to constraints

$$\begin{aligned} \underset{x}{\operatorname{argmin}} \quad & f_0(x) \\ \text{s.t.} \quad & f_i(x) \leq 0, i = \{1, ..., k\} \\ & h_j(x) = 0, j = \{1, ..., l\} \end{aligned} \tag{1}$$

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\end{aligned} \tag{1}
$$

- Most of the machine learning problems are, in the end, optimization problems.

# Examples

- (Soft) Linear SVM

$$
\begin{aligned}
\underset{w}{\operatorname{argmin}} \quad & \sum_{i=1}^{n} \|w\|^2 + C \sum_{i=1} n\epsilon_i \\
\text{s.t.} \quad & 1 - y_i x_i^T w \leq \epsilon_i \\
& \epsilon_i \geq 0
\end{aligned} \tag{2}
$$

- Maximum Likelihood

$$
\underset{\theta}{\operatorname{argmax}} \sum_{i=1}^{n} \log p_\theta(x_i) \tag{3}
$$

- K-means

$$
\underset{\mu_1,\mu_2,\ldots,\mu_k}{\operatorname{argmin}} J(\mu) = \sum_{j=1}^{k} \sum_{i \in C_j} \|x_i - \mu_j\|^2 \tag{4}
$$

# Outline

# Convex sets

## Definition

*A set $C \subseteq \mathbb{R}^n$ is convex if for $x, y \in C$ and any $\alpha \in [0,1]$, $\alpha x + (1-\alpha)y \in C$.*

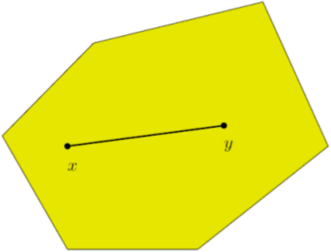



Figure: Convex Set

# Convex sets

## Example

- All of $\mathbb{R}^n$
- Non-negative orthant, $\mathbb{R}^n_+$: let $x \geq 0, y \geq 0$, clearly $\alpha x + (1-\alpha)y \geq 0$.
- Affine subspaces: $Ax = b, Ay = b$, then

$$A(\alpha x + (1-\alpha)y) = \alpha Ax + (1-\alpha)Ay = b$$

.

- Arbitrary intersections of convex sets: let $C_i$ be convex for $i \in \mathcal{I}, C = \bigcap_i C_i$, then

$$x \in C, y \in C \Rightarrow \alpha x + (1 - \alpha y) \in C_i \subseteq C, \forall i \in \mathcal{I}$$

.

# Convex functions

## Definition

*A function $f : \mathbb{R}^n \to \mathbb{R}$ is convex if for $x, y \in$ dom $f$ and any $a \in [0, 1]$,*

$$f(ax + (1-a)y) \leq af(x) + (1-a)f(y)$$

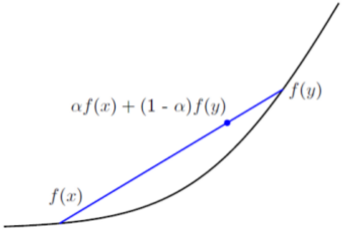


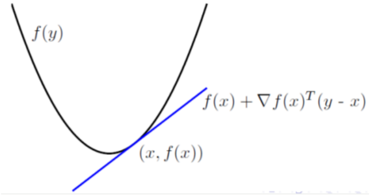

Figure: Convex Function

# Convexity condition 1

## Theorem

*Suppose $f : \mathbb{R}^n \to \mathbb{R}$ is differentiable. Then $f$ is convex if and only if for all $x, y \in$ dom $f$.*

$$f(y) \geq f(x) + \nabla f(x)^T (y - x)$$



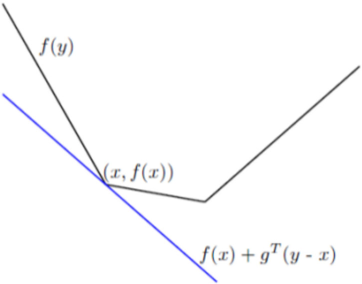
# Subgradient

## Definition

*The subgradient set, or subdifferential set, $\partial f(x)$ of f at x is*

$$\partial f(x) = \{g : f(y) \geq f(x) + g^T(y - x) \quad \forall y\}$$

.




## Theorem

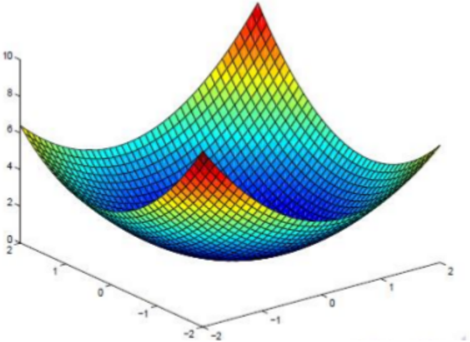
*$f : \mathbb{R}^n \to \mathbb{R}$ is convex iff it has ono-empty subdifferential set everywhere.*

# Convexity condition 2

## Theorem

*Suppose $f : \mathbb{R}^n \to \mathbb{R}$ is twice differentiable, Then $f$ is convex iff for all $x \in$ dom $f$,*

$$\nabla^2 f(x) \succeq 0.$$



# Examples of convex functions

- Linear/affine functions: $f(x) = b^T x + c$
- Quadratic function: $f(x) = \frac{1}{2} x^T A x + b^T x + c$, for $A \succeq 0$.
  *e.g.*, for regression:

$$\frac{1}{2}\|\mathbf{X}w - y\|^2 = \frac{1}{2} w^T \mathbf{X}^T \mathbf{X} w - y^T \mathbf{X} w + \frac{1}{2} y^T y$$

.

# Examples of convex functions

- Norms (like $l_l$ or $l_2$ for regularization):

$$\|ax + (1-a)y\| \leq \|ax\| + \|(1-a)y\| = a\|x\| + (1-a)\|y\|$$

.

- Composition with an affine function $f(Ax + b)$:

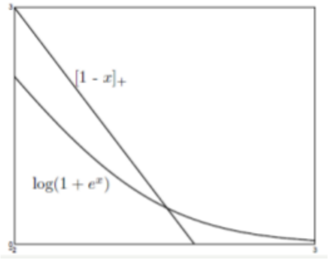
$$\begin{aligned} f(A(ax + (1-a)y) + b) &= f(a(Ax + b) + (1-a)(Ay + b)) \\ &\leq af(Ax + b) + (1-a)f(Ay + b) \end{aligned}$$

- Log-sum-exp (via $\nabla^2 f(x)$ PSD):

$$f(x) = \log\left(\sum_{i=1}^{n} \exp(x_i)\right)$$

# Examples in machine learning

- SVM loss: $f(w) = [1 - y_i x_i^T w]_+$
- Binary logistic loss: $f(w) = \log(1 + \exp(-y_i x_i^T w))$



# Convex optimization

## Definition

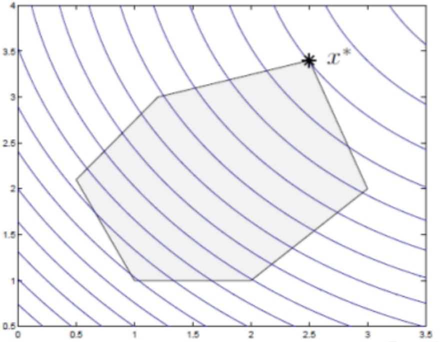
*An optimization problem is convex if its objective is a convex function. The inequality constrains $f_j$ are convex, and the equality constraints $h_j$ are affine.*

$$
\begin{aligned}
\min_{x} \quad & f_0(x) && \text{(Convex function)} \\
\text{s.t.} \quad & f_i(x) \leq 0, i = \{1, ..., k\} && \text{(Convex sets)} \\
& h_j(x) = 0, j = \{1, ..., l\} && \text{(Affine)}
\end{aligned}
\tag{5}
$$

# Convex Problems are nice ...

## Theorem

*If $\hat{x}$ is a local minimizer of a convex optimization problem, it is a global minimizer.*



# For smooth functions

## Theorem

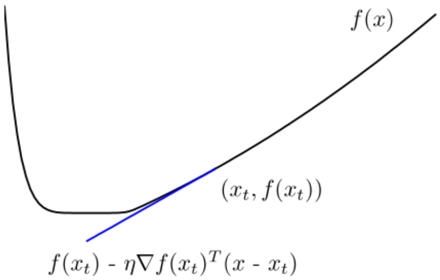
- $\nabla f(x) = 0$. *We have* $f(y) \geq f(x) + \nabla f(x)^T(y - x) = f(x)$.
- $\nabla f(x) \neq 0$. *There is a direction of descent.*

# Outline

# Gradient descent

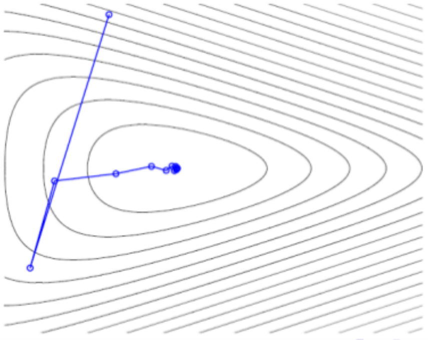
- Consider convex and unconstrained optimization.
- Solve $\min_x f(x)$.
- One of the simplest approach:
  - For $t = 1, ..., T$, $x_{t+1} \leftarrow x_t - \eta_t \nabla f(x_t)$
  - Until convergence
  - $\eta_t$ is called step-size of learning rate.

# Single step in gradient descent



# Full gradient descent

$$f(x) = \log(\exp(x_1 + 3x_2 - .1) + \exp(x_1 - 3x_2 - .1) + \exp(-x_1 - .1))$$



## How to choose step size?

- Idea 1: exact line search

$$\eta_t = \operatorname*{argmin}_{\eta} f(x - \eta \nabla f(x))$$

  Too expensive to be practical.

- Idea 2: backtracking (Armijo) line search. Let $\alpha \in (0, 1/2), \beta \in (0, 1)$. Multiply $\eta = \beta\eta$ until

$$f(x - \eta \nabla f(x)) \leq f(x) - \alpha\eta \|\nabla f(x)\|^2$$

  Works well in practice.

# Newton's method

Idea: use a second-order approximation to function.

$$f(x+\Delta x) \approx f(x) + \nabla f(x)^T \Delta x + 1/2 \Delta x^T \nabla^2 f(x) \Delta x$$

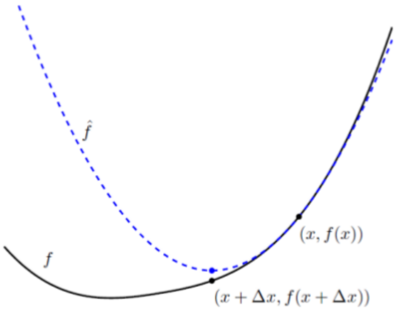
Choose $\Delta x$ to minimize above:

$$\Delta x = -[\nabla^2 f(x)]^{-1} \nabla f(x)$$

This is descent direction:

$$\nabla f(x)^T \Delta x = -\nabla f(x)^T [\nabla^2 f(x)]^{-1} \nabla f(x) \leq 0$$

# Single step in Newton's method




$\hat{f}$ is 2nd-order approximation, $f$ is true function.

# Convergence rate

- Strongly convex case: $\nabla^2 f(x) \succeq mI$, then "Linear convergence". For some $\gamma \in (0,1), f(x_t) - f(x^*) \leq \gamma^t, \gamma \leq 1$.

$$f(x_t) - f(x^*) \leq \gamma^t, t \geq \frac{1}{\gamma} \log \frac{1}{\epsilon} \Rightarrow f(x_t) - f(x^*) \leq \epsilon$$

.

- Smooth case: $\|\nabla f(x) - \nabla f(y)\| \leq C\|x - y\|$.

$$f(x_t) - f(x^*) \leq \frac{K}{t^2}$$

- Newton's method often is faster, especially when $f$ has "long valleys".

# Newton's method

- Inverting a Hessian is very expensive: $O(d^3)$
- Approximate inverse Hessian: BFGS, Limited-memory BFGS
- Or use Conjugate Gradient Descent.
- For unconstrained problems, you can use these off-the-shelf optimization methods
- For unconstrained non-convex problems, these methods will find local optima

# Optimization for machine learning

- Goal of machine learning
  - Minimize expected loss $L(h) = \mathbf{E}[\mathrm{loss}(h(x), y)]$ given samples $(x_i, y_i), i = 1, 2, ..., m$
  - But we don't know $P(x, y)$, nor can we estimate it well.
- Empirical risk minimization
  - Substitute sample mean for expectation.
  - Minimize empirical loss: $L(h) = 1/n \sum_i \mathrm{loss}(h(x_i), y_i)$
  - *a.k.a.* Sample Average Approximation.

# Batch gradient descent

Minimize empirical loss, assuming it's convex and unconstrained

- Gradient descent on the empirical loss:
- At each step,

$$w^{k+1} \leftarrow w^k - \eta_t \left( \frac{1}{n} \sum_{i=1}^{n} \frac{\partial L(w, x_i, y_i)}{\partial w} \right)$$

- Note: at each step, gradient is the average of the gradient for all samples $(i = 1, ..., n)$.
- Very slow when $n$ is very large.

# Stochastic Gradient Descent

- Alternative: compute gradient from just one (or a few samples)
- Known as SGD: At each step,

$$w^{k+1} \leftarrow w^k - \eta_t \frac{\partial L(w, x_i, y_i)}{\partial w}$$

  (choose one sample $i$ and compute gradient for that sample only)
- the gradient of one random sample is not the gradient of the objective function.
- Q1: Would this work at all?
- Q2: How good is it?

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  (choose one sample $i$ and compute gradient for that sample only)
- the gradient of one random sample is not the gradient of the objective function.
- Q1: Would this work at all?
- Q2: How good is it?
- A1: SGD converges to not only thy empirical loss minimum, but also to the expected loss minimum!
- A2: Convergence (to expected loss) is slow: $f(w_t) - E[f(w^*)] \leq O(1/t)$ or $O(1/\sqrt{t})$

# Practically speaking ...

- If the training set is small, we should use batch learning using quasi-Newton or conjugate gradient descent.
- If the training set is large, we should use SGD.
- If the size of training set is somewhere in between, we use mini-batch SGD.
- Convergence is very sensitive to learning rate, which needs to be determined by trial-and-error (model selection or cross-validation)

# Outline

Constrained optimization will be continued on Thursday, March 8.

- Lagrange duality
- SVM in primal and dual forms
- Constrained methods

# Thank you!