

Optimization for Machine Learning

(Lecture 1)

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- My website (Teaching)
- Some references:
 - *Introductory lectures on convex optimization* – Nesterov
 - *Convex optimization* – Boyd & Vandenberghe
 - *Nonlinear programming* – Bertsekas
 - *Convex Analysis* – Rockafellar
 - *Fundamentals of convex analysis* – Urruty, Lemaréchal
 - *Lectures on modern convex optimization* – Nemirovski
 - *Optimization for Machine Learning* – Sra, Nowozin, Wright
 - *NIPS 2016 Optimization Tutorial* – Bach, Sra
- Some related courses:
 - EE227A, Spring 2013, (Sra, UC Berkeley)
 - 10-801, Spring 2014 (Sra, CMU)
 - EE364a,b (Boyd, Stanford)
 - EE236b,c (Vandenberghe, UCLA)
- Venues: NIPS, ICML, UAI, AISTATS, SIOPT, Math. Prog.

Lecture Plan

- Introduction
- Recap of convexity, sets, functions
- Recap of duality, optimality, problems
- First-order optimization algorithms and techniques
- Large-scale optimization (SGD and friends)
- Directions in non-convex optimization

Introduction

Supervised machine learning

- ▶ **Data:** n observations $(x_i, y_i)_{i=1}^n \in \mathcal{X} \times \mathcal{Y}$
- ▶ **Prediction function:** $h(x, \theta) \in \mathbb{R}$ parameterized by $\theta \in \mathbb{R}^d$

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- ▶ **Prediction function:** $h(x, \theta) \in \mathbb{R}$ parameterized by $\theta \in \mathbb{R}^d$
- ▶ **Motivating examples:**
 - **Linear predictions:** $h(x, \theta) = \theta^\top \Phi(x)$ using features $\Phi(x)$
 - **Neural networks:** $h(x, \theta) = \theta_m^\top \sigma(\theta_{m-1}^\top \sigma(\cdots \theta_2^\top \sigma(\theta_1^\top x)))$
- ▶ Estimating θ parameters is an optimization problem

Introduction

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Unsupervised and other ML setups

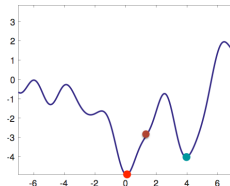
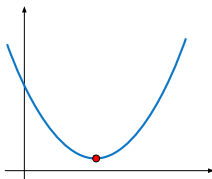
- ▶ Different formulations, but ultimately optimization at heart

The Problem!

$$\min_{\theta \in \mathcal{S}} f(\theta)$$

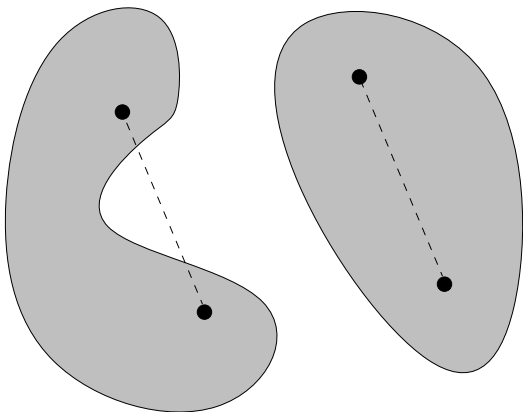
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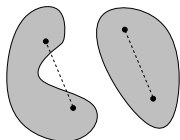
Convex analysis

Convex sets



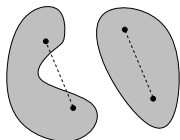
Convex sets

Def. Set $C \subset \mathbb{R}^n$ called **convex**, if for any $x, y \in C$, the line-segment $\lambda x + (1 - \lambda)y$, where $\lambda \in [0, 1]$, also lies in C .



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Combinations of points

- ▶ **Convex:** $\lambda_1 x + \lambda_2 y \in C$, where $\lambda_1, \lambda_2 \geq 0$ and $\lambda_1 + \lambda_2 = 1$.
- ▶ **Linear:** if restrictions on λ_1, λ_2 are dropped
- ▶ **Conic:** if restriction $\lambda_1 + \lambda_2 = 1$ is dropped

Different restrictions lead to different “algebra”

Recognizing / constructing convex sets

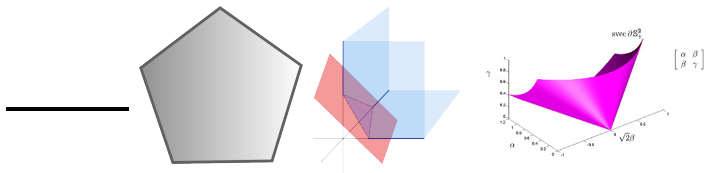
Theorem. (Intersection).

Let C_1, C_2 be convex sets. Then, $C_1 \cap C_2$ is also convex.

Proof.

- If $C_1 \cap C_2 = \emptyset$, then true vacuously.
- Let $x, y \in C_1 \cap C_2$. Then, $x, y \in C_1$ and $x, y \in C_2$.
- But C_1, C_2 are convex, hence $\theta x + (1 - \theta)y \in C_1$, and also in C_2 .
Thus, $\theta x + (1 - \theta)y \in C_1 \cap C_2$.
- Inductively follows that $\bigcap_{i=1}^m C_i$ is also convex.

Convex sets



(psdcone image from convexoptimization.com, Dattorro)

Convex sets

♡ Let $x_1, x_2, \dots, x_m \in \mathbb{R}^n$. Their **convex hull** is

$$\text{co}(x_1, \dots, x_m) := \left\{ \sum_i \theta_i x_i \mid \theta_i \geq 0, \sum_i \theta_i = 1 \right\}.$$

♡ Let $A \in \mathbb{R}^{m \times n}$, and $b \in \mathbb{R}^m$. The set $\{x \mid Ax = b\}$ is convex (it is an *affine space* over subspace of solutions of $Ax = 0$).

♡ *halfspace* $\{x \mid a^T x \leq b\}$.

♡ *polyhedron* $\{x \mid Ax \leq b, Cx = d\}$.

♡ *ellipsoid* $\{x \mid (x - x_0)^T A (x - x_0) \leq 1\}$, (A : semidefinite)

♡ *convex cone* $x \in \mathcal{K} \implies \alpha x \in \mathcal{K}$ for $\alpha \geq 0$ (and \mathcal{K} convex)

○

Exercise: Verify that these sets are convex.

Challenge 1

Let $A, B \in \mathbb{R}^{n \times n}$ be symmetric. Prove that

$$R(A, B) := \left\{ (x^T A x, x^T B x) \mid x^T x = 1 \right\}$$

is a compact convex set for $n \geq 3$.

Convex functions

Def. A function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is **convex** if and only if its *epigraph* $\{(x, t) \subseteq \mathbb{R}^{d+1} \mid x \in \mathbb{R}^d, t \in \mathbb{R}, f(x) \leq t\}$ is a convex set.

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Def. A function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is called **convex** if its domain $\text{dom}(f)$ is a convex set and for any $x, y \in \text{dom}(f)$ and $\lambda \geq 0$,

$$f((1 - \lambda)x + \lambda y) \leq (1 - \lambda)f(x) + \lambda f(y).$$

These functions also known as **Jensen convex**; named after J.L.W.V. Jensen (after his influential 1905 paper).

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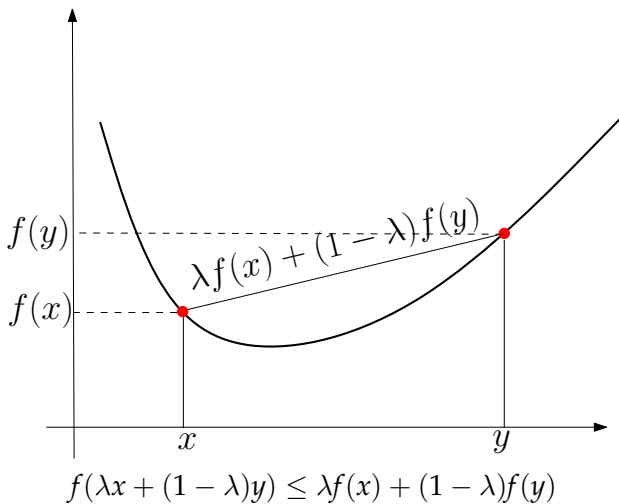
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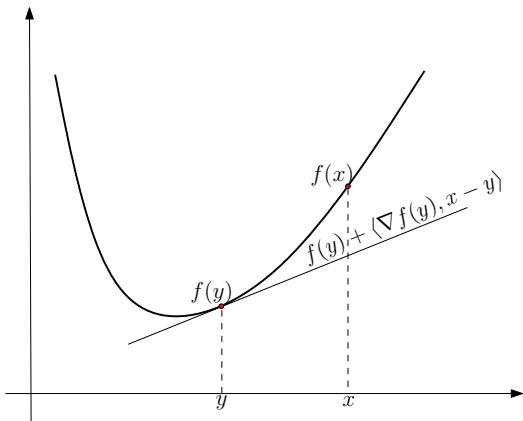
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Exercise: Why are we focusing on these functions?

Convex functions: Jensen's inequality

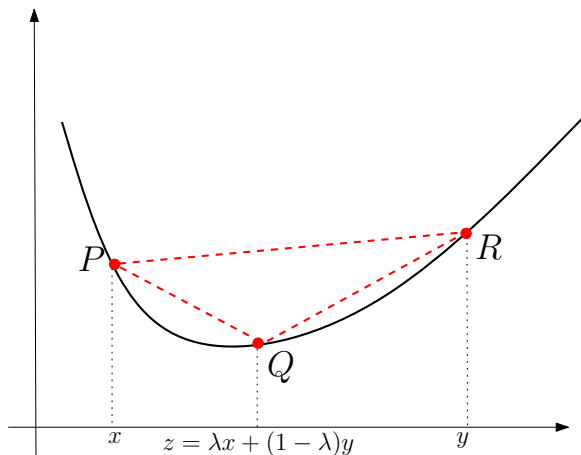


Convex functions: affine lower bounds



$$f(x) \geq f(y) + \langle \nabla f(y), x - y \rangle$$

Convex functions: increasing slopes



slope $PQ \leq$ slope $PR \leq$ slope QR

Recognizing convex functions

- ♠ If f is continuous and midpoint convex, then it is convex.
- ♠ If f is differentiable, then f is convex *if and only if* $\text{dom } f$ is convex and $f(x) \geq f(y) + \langle \nabla f(y), x - y \rangle$ for all $x, y \in \text{dom } f$.
- ♠ If f is twice differentiable, then f is convex *if and only if* $\text{dom } f$ is convex and $\nabla^2 f(x) \succeq 0$ at every $x \in \text{dom } f$.

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- ♠ By showing $f : \text{dom}(f) \rightarrow \mathbb{R}$ is convex *if and only if* its **restriction to any line** that intersects $\text{dom}(f)$ is convex. That is, for any $x \in \text{dom}(f)$ and any v , the function $g(t) = f(x + tv)$ is convex (on its domain $\{t \mid x + tv \in \text{dom}(f)\}$).

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- ♠ By showing f to be a pointwise max of convex functions
- ♠ See exercises (Ch. 3) in Boyd & Vandenberghe for more!

Operations preserving convexity

Example. Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be convex. Let $A \in \mathbb{R}^{m \times n}$, and $b \in \mathbb{R}^m$. Prove that $g(x) = f(Ax + b)$ is convex.

Exercise: Verify!

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Proof. Let $x, y \in I_1$, and let $\lambda \in (0, 1)$.

$$\begin{aligned} f(\lambda x + (1 - \lambda)y) &\leq \lambda f(x) + (1 - \lambda)f(y) \\ g(f(\lambda x + (1 - \lambda)y)) &\leq g(\lambda f(x) + (1 - \lambda)f(y)) \\ &\leq \lambda g(f(x)) + (1 - \lambda)g(f(y)). \end{aligned}$$

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► Do not miss out on several other important examples in BV!

Constructing convex functions: sup

Example. The *pointwise maximum* of a family of convex functions is convex. That is, if $f(x; y)$ is a convex function of x for every y in an arbitrary “index set” \mathcal{Y} , then

$$f(x) := \sup_{y \in \mathcal{Y}} f(x; y)$$

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Constructing convex functions: joint inf

Theorem. Let \mathcal{Y} be a nonempty convex set. Suppose $L(x, y)$ is convex in **both** (x, y) , then,

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Proof. Let $u, v \in \text{dom } f$. Since $f(u) = \inf_y L(u, y)$, for each $\epsilon > 0$, there is a $y_1 \in \mathcal{Y}$, s.t. $f(u) + \frac{\epsilon}{2}$ is **not** the infimum. Thus, $L(u, y_1) \leq f(u) + \frac{\epsilon}{2}$.

Similarly, there is $y_2 \in \mathcal{Y}$, such that $L(v, y_2) \leq f(v) + \frac{\epsilon}{2}$.

Now we prove that $f(\lambda u + (1 - \lambda)v) \leq \lambda f(u) + (1 - \lambda)f(v)$ directly.

$$\begin{aligned} f(\lambda u + (1 - \lambda)v) &= \inf_{y \in \mathcal{Y}} L(\lambda u + (1 - \lambda)v, y) \\ &\leq L(\lambda u + (1 - \lambda)v, \lambda y_1 + (1 - \lambda)y_2) \\ &\leq \lambda L(u, y_1) + (1 - \lambda)L(v, y_2) \\ &\leq \lambda f(u) + (1 - \lambda)f(v) + \epsilon. \end{aligned}$$

Since $\epsilon > 0$ is arbitrary, claim follows.

Convex functions – norms

Let $\Omega : \mathbb{R}^d \rightarrow \mathbb{R}$ be a function that satisfies

- 1 $\Omega(x) \geq 0$, and $\Omega(x) = 0$ if and only if $x = 0$ (**definiteness**)
- 2 $\Omega(\lambda x) = |\lambda|\Omega(x)$ for any $\lambda \in \mathbb{R}$ (**positive homogeneity**)
- 3 $\Omega(x + y) \leq \Omega(x) + \Omega(y)$ (**subadditivity**)

Such function called *norms*—usually denoted $\|x\|$.

Theorem. Norms are convex.

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Often used in “regularized” ML problems

$$\min_{\theta} f(\theta) + \mu\Omega(\theta).$$

Norms: important examples

Example. (ℓ_2 -norm): $\|x\|_2 = (\sum_i x_i^2)^{1/2}$

Example. (ℓ_p -norm): Let $p \geq 1$. $\|x\|_p = (\sum_i |x_i|^p)^{1/p}$

Example. (ℓ_∞ -norm): $\|x\|_\infty = \max_{1 \leq i \leq n} |x_i|$

Example. (Frobenius-norm): Let $A \in \mathbb{R}^{m \times n}$. $\|A\|_F := \sqrt{\sum_{ij} |a_{ij}|^2}$

Example. Let A be any matrix. Then, the **operator norm** of A is

$$\|A\| := \sup_{\|x\|_2 \neq 0} \frac{\|Ax\|_2}{\|x\|_2} = \sigma_{\max}(A).$$

Exercise: Verify that above functions are actually norms!

Convex functions – Indicator

Let $\mathbb{1}_{\mathcal{X}}$ be the *indicator function* for \mathcal{X} defined as:

$$\mathbb{1}_{\mathcal{X}}(x) := \begin{cases} 0 & \text{if } x \in \mathcal{X}, \\ \infty & \text{otherwise.} \end{cases}$$

Note: $\mathbb{1}_{\mathcal{X}}(x)$ is convex **if and only if** \mathcal{X} is convex.

► Also called “extended value” convex function.

Fenchel conjugate

Def. The **Fenchel conjugate** of a function f is

$$f^*(z) := \sup_{x \in \text{dom} f} x^T z - f(x).$$

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Example. $+\infty$ and $-\infty$ conjugate to each other.

Example. Let $f(x) = \|x\|$. We have $f^*(z) = \mathbb{1}_{\|z\|_* \leq 1}(z)$. That is, conjugate of norm is the indicator function of dual norm ball.

Proof. $f^*(z) = \sup_x z^T x - \|x\|$. If $\|z\|_* > 1$, by defn. of the dual norm, $\exists u$ such that $\|u\| \leq 1$ and $u^T z > 1$. Now select $x = \alpha u$ and let $\alpha \rightarrow \infty$. Then, $z^T x - \|x\| = \alpha(z^T u - \|u\|) \rightarrow \infty$. If $\|z\|_* \leq 1$, then $z^T x \leq \|x\| \|z\|_*$, which implies the sup must be zero.

Fenchel conjugate: examples

Example. $f(x) = \frac{1}{2}x^T Ax$, where $A \succ 0$. Then, $f^*(z) = \frac{1}{2}z^T A^{-1}z$.

Example. $f(x) = \max(0, 1 - x)$. Verify: $\text{dom } f^* = [-1, 0]$, and on this domain, $f^*(z) = z$.

Example. $f(x) = \mathbb{1}_{\mathcal{X}}(x)$: $f^*(z) = \sup_{x \in \mathcal{X}} \langle x, z \rangle$ (aka **support func**)

Example. If $f^{**} = f$, we say f is a **closed convex function**.

Exercise: Suppose $f(x) = (\sum_i |x_i|^{1/2})^2$. What is f^{**} ?

Exercise: Suppose $f(x) = x^T Ax + b^T x$ but $A \succeq 0$; what is f^* ?

Challenge 2

Consider the following functions on strictly positive variables:

$$h_1(x) := \frac{1}{x}$$

$$h_2(x, y) := \frac{1}{x} + \frac{1}{y} - \frac{1}{x+y}$$

$$h_3(x, y, z) := \frac{1}{x} + \frac{1}{y} + \frac{1}{z} - \frac{1}{x+y} - \frac{1}{y+z} - \frac{1}{x+z} + \frac{1}{x+y+z}$$

- ♡ Prove that $h_n(x) > 0$ (easy)
- ♡ Prove that h_1, h_2, h_3 , and in general h_n are convex (hard)
- ♡ Prove that in fact each $1/h_n$ is concave (harder).

Optimization

Optimization problems

Let $f_i : \mathbb{R}^n \rightarrow \mathbb{R}$ ($0 \leq i \leq m$). Generic **nonlinear program**

$$\begin{aligned} \min \quad & f_0(x) \\ \text{s.t.} \quad & f_i(x) \leq 0, \quad 1 \leq i \leq m, \\ & x \in \{\text{dom } f_0 \cap \text{dom } f_1 \cdots \cap \text{dom } f_m\}. \end{aligned}$$

Henceforth, we drop condition on domains for brevity.

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Henceforth, we drop condition on domains for brevity.

- If f_i are **differentiable** — smooth optimization
- If any f_i is **non-differentiable** — nonsmooth optimization
- If all f_i are **convex** — convex optimization
- If $m = 0$, i.e., only f_0 is there — **unconstrained** minimization

Convex optimization

Let \mathcal{X} be **feasible set** and p^* the **optimal value**

$$p^* := \inf \{f_0(x) \mid x \in \mathcal{X}\}$$

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- ▶ If \mathcal{X} is empty, we say problem is **infeasible**
- ▶ By **convention**, we set $p^* = +\infty$ for infeasible problems
- ▶ If $p^* = -\infty$, we say problem is **unbounded below**.
- ▶ Example, $\min x$ on \mathbb{R} , or $\min -\log x$ on \mathbb{R}_{++}
- ▶ Sometimes **minimum doesn't exist** (as $x \rightarrow \pm\infty$)
- ▶ Say $f_0(x) = 0$, problem is called **convex feasibility**

Optimality

Def. A point $x^* \in \mathcal{X}$ is **locally optimal** if $f(x^*) \leq f(x)$ for all x in a **neighborhood** of x^* . **Global** if $f(x^*) \leq f(x)$ for **all** $x \in \mathcal{X}$.

Theorem. For convex problems, local \implies global!

Exercise: Prove this theorem (*Hint*: try contradiction)

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Theorem. Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be continuously differentiable in an open set S containing x^* , a local min of f . Then, $\nabla f(x^*) = 0$.

If f is convex, then $\nabla f(x^*) = 0$ **sufficient** for global optimality.
(This property makes convex optimization special!)

Optimality – constrained

♠ For every $x, y \in \text{dom} f$, we have $f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle$.

Optimality – constrained

- ♠ For every $x, y \in \text{dom}f$, we have $f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle$.
- ♠ Thus, x^* is optimal **if** and only if

$$\langle \nabla f(x^*), y - x^* \rangle \geq 0, \quad \text{for all } y \in \mathcal{X}.$$

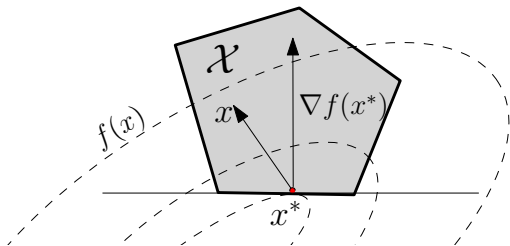
Optimality – constrained

♠ For every $x, y \in \text{dom}f$, we have $f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle$.

♠ Thus, x^* is optimal **if** and only if

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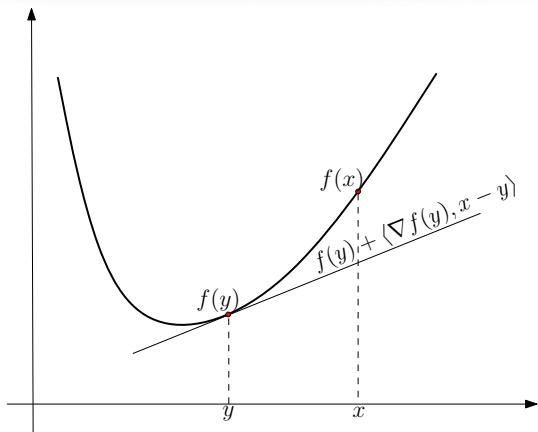
♠ If $\mathcal{X} = \mathbb{R}^n$, this reduces to $\nabla f(x^*) = 0$



♠ If $\nabla f(x^*) \neq 0$, it defines supporting hyperplane to \mathcal{X} at x^*

Optimization: via subgradients

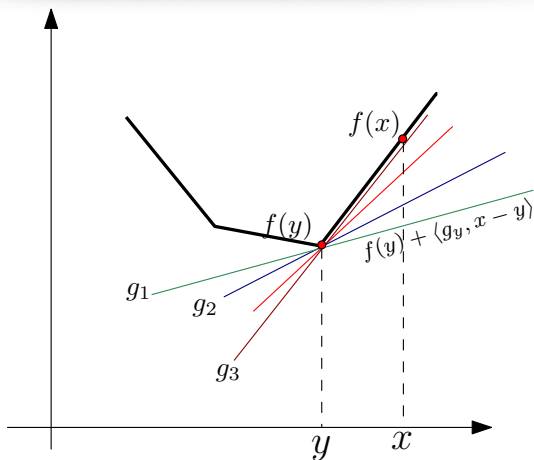
Subgradients: global underestimators



$$f(x) \geq f(y) + \langle \nabla f(y), x - y \rangle$$

Hence $\nabla f(y) = 0$ implies that y is global min.

Subgradients: global underestimators



$$f(x) \geq f(y) + \langle g, x - y \rangle$$

If one of the $g = 0$, then y a global min.

Subgradients – basic facts

- ▶ f is convex, differentiable: $\nabla f(y)$ the **unique** subgradient at y
- ▶ A vector g is a subgradient at a point y if and only if $f(y) + \langle g, x - y \rangle$ is **globally** smaller than $f(x)$.
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- ▶ Usually, **one** subgradient costs approx. as much as $f(x)$
- ▶ Determining all subgradients at a given point — **difficult**.
- ▶ Subgradient calculus—major achievement in convex analysis
- ▶ **Fenchel-Young inequality**: $f(x) + f^*(s) \geq \langle s, x \rangle$ (tight at a subgradient)

Example: computing subgradients

$$f(x) := \sup_{y \in \mathcal{Y}} h(x, y)$$

Simple way to obtain some $g \in \partial f(x)$:

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$$f(x) := \sup_{y \in \mathcal{Y}} h(x, y)$$

Simple way to obtain some $g \in \partial f(x)$:

- ▶ Pick **any** y^* for which $h(x, y^*) = f(x)$
- ▶ Pick **any** subgradient $g \in \partial h(x, y^*)$
- ▶ This $g \in \partial f(x)$

Proof:

$$h(z, y^*) \geq h(x, y^*) + g^T(z - x)$$

$$h(z, y^*) \geq f(x) + g^T(z - x)$$

$$f(z) \geq h(z, y) \quad (\text{because of sup})$$

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

Computing subgradients

Several other simple rules can be proved; see Boyd's lecture notes (or my EE227A lecture slides)

- Subgradient from max
- Subgradient from expectation
- Subgradient of composition

Subdifferential*

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- ♣ If $\partial f(x) = \{g\}$, then f is differentiable and $g = \nabla f(x)$

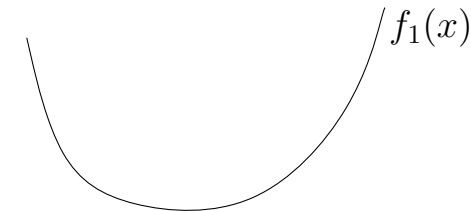
Exercise: What is $\partial f(x)$ for the *ReLU* function: $\max(0, x)$?

Subdifferential – example

$f(x) := \max(f_1(x), f_2(x));$ both f_1, f_2 convex, differentiable

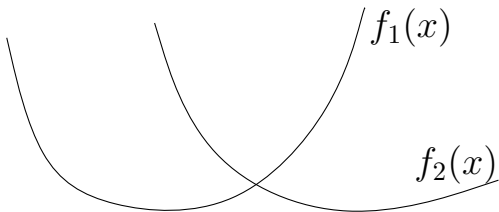
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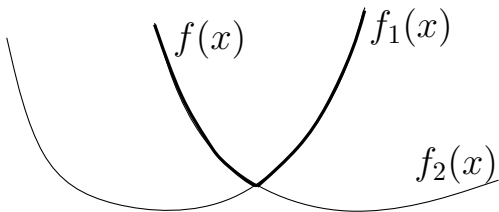
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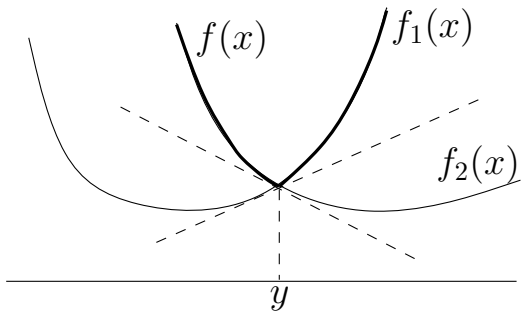
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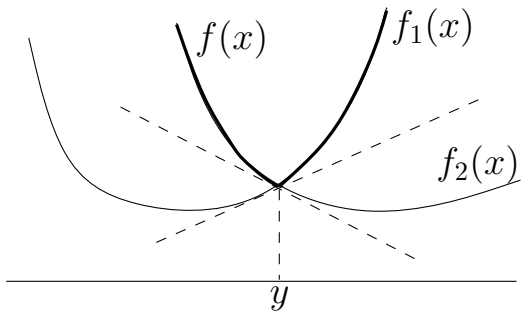
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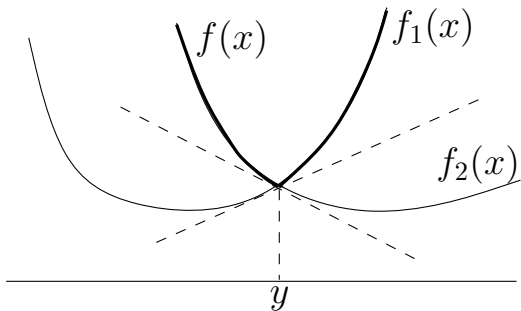
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★ $f_1(x) > f_2(x)$: unique subgradient of f is $f_1'(x)$

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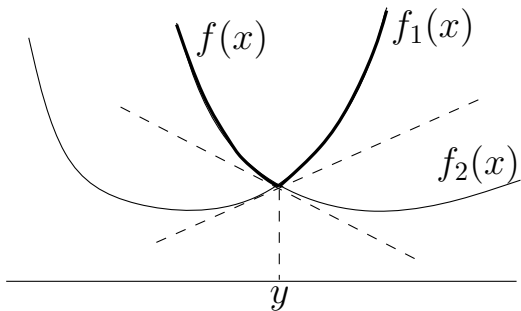
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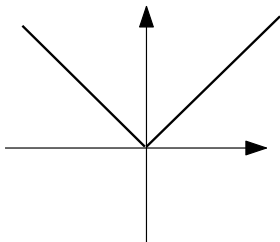
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- ★ $f_1(x) < f_2(x)$: unique subgradient of f is $f_2'(x)$
- ★ $f_1(y) = f_2(y)$: subgradients, the segment $[f_1'(y), f_2'(y)]$
(imagine all supporting lines turning about point y)

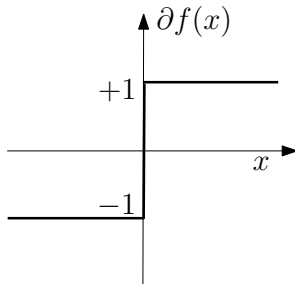
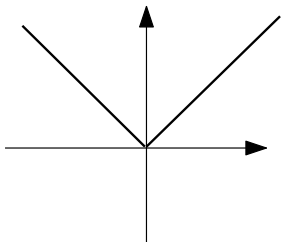
Subdifferential for abs value

$$f(x) = |x|$$



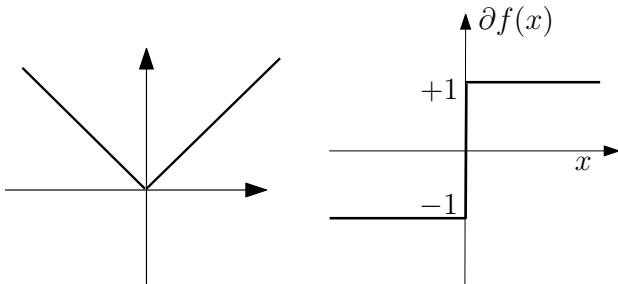
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Subdifferential for abs value

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$$\partial|x| = \begin{cases} -1 & x < 0, \\ +1 & x > 0, \\ [-1, 1] & x = 0. \end{cases}$$

Subdifferential for Euclidean norm

Example. $f(x) = \|x\|_2$. Then,

$$\partial f(x) := \begin{cases} x/\|x\|_2 & x \neq 0, \\ \{z \mid \|z\|_2 \leq 1\} & x = 0. \end{cases}$$

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Proof.

$$\begin{aligned} \|z\|_2 &\geq \|x\|_2 + \langle g, z - x \rangle \\ \|z\|_2 &\geq \langle g, z \rangle \\ \implies \|g\|_2 &\leq 1. \end{aligned}$$

Example: difficulties

Example. A convex function need not be subdifferentiable everywhere. Let

$$f(x) := \begin{cases} -(1 - \|x\|_2^2)^{1/2} & \text{if } \|x\|_2 \leq 1, \\ +\infty & \text{otherwise.} \end{cases}$$

f diff. for all x with $\|x\|_2 < 1$, but $\partial f(x) = \emptyset$ whenever $\|x\|_2 \geq 1$.

Subdifferential calculus

- ♠ Finding **one** subgradient within $\partial f(x)$
- ♠ Determining entire subdifferential $\partial f(x)$ at a point x
- ♠ Do we have the chain rule?

Subdifferential calculus

⌘ If f is differentiable, $\partial f(x) = \{\nabla f(x)\}$

⌘ **Scaling** $\alpha > 0$, $\partial(\alpha f)(x) = \alpha \partial f(x) = \{\alpha g \mid g \in \partial f(x)\}$

⌘ **Addition***: $\partial(f + k)(x) = \partial f(x) + \partial k(x)$ (set addition)

⌘ **Chain rule***: Let $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, $f : \mathbb{R}^m \rightarrow \mathbb{R}$, and $h : \mathbb{R}^n \rightarrow \mathbb{R}$ be given by $h(x) = f(Ax + b)$. Then,

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

⌘ **Chain rule***: $h(x) = f \circ k$, where $k : X \rightarrow Y$ is diff.

$$\partial h(x) = \partial f(k(x)) \circ Dk(x) = [Dk(x)]^T \partial f(k(x))$$

⌘ **Max function***: If $f(x) := \max_{1 \leq i \leq m} f_i(x)$, then

$$\partial f(x) = \text{conv} \bigcup \{ \partial f_i(x) \mid f_i(x) = f(x) \},$$

convex hull over subdifferentials of “active” functions at x

⌘ **Conjugation**: $z \in \partial f(x)$ if and only if $x \in \partial f^*(z)$

* — can fail to hold without precise assumptions.

Example: breakdown

It can happen that $\partial(f_1 + f_2) \neq \partial f_1 + \partial f_2$

Example. Define f_1 and f_2 by

$$f_1(x) := \begin{cases} -2\sqrt{x} & \text{if } x \geq 0, \\ +\infty & \text{if } x < 0, \end{cases} \quad \text{and} \quad f_2(x) := \begin{cases} +\infty & \text{if } x > 0, \\ -2\sqrt{-x} & \text{if } x \leq 0. \end{cases}$$

Then, $f = \max\{f_1, f_2\} = \mathbb{1}_{\{0\}}$, whereby $\partial f(0) = \mathbb{R}$

But $\partial f_1(0) = \partial f_2(0) = \emptyset$.

However, $\partial f_1(x) + \partial f_2(x) \subset \partial(f_1 + f_2)(x)$ always holds.

Subdifferential – example

Example. $f(x) = \|x\|_\infty$. Then,

$$\partial f(0) = \text{conv} \{ \pm e_1, \dots, \pm e_n \},$$

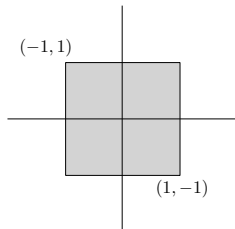
where e_i is i -th canonical basis vector.

To prove, notice that $f(x) = \max_{1 \leq i \leq n} \{ |e_i^T x| \}$

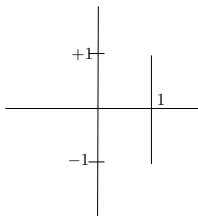
Then use, *chain rule* and *max rule* and $\partial |\cdot|$

Subdifferential - example (Boyd)

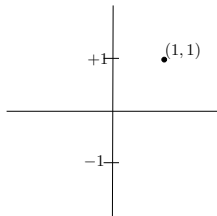
Example. Let $f(x) = \max \{s^T x \mid s_i \in \{-1, 1\}\}$ (2^n members)



∂f at $x = (0, 0)$



∂f at $x = (1, 0)$



∂f at $x = (1, 1)$

Optimality via subdifferentials

Theorem. (Fermat's rule): Let $f : \mathbb{R}^n \rightarrow (-\infty, +\infty]$. Then,

$$\operatorname{argmin} f = \operatorname{zer}(\partial f) := \{x \in \mathbb{R}^n \mid 0 \in \partial f(x)\}.$$

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Nonsmooth optimality

$$\min \quad f(x) \quad \text{s.t. } x \in \mathcal{X}$$

$$\min \quad f(x) + \mathbb{1}_{\mathcal{X}}(x).$$

Optimality via subdifferentials: application

- ▶ Minimizing x must satisfy: $0 \in \partial(f + \mathbb{1}_{\mathcal{X}})(x)$
- ▶ **(CQ)** Assuming $\text{ri}(\text{dom } f) \cap \text{ri}(\mathcal{X}) \neq \emptyset$, $0 \in \partial f(x) + \partial \mathbb{1}_{\mathcal{X}}(x)$
- ▶ Recall, $g \in \partial \mathbb{1}_{\mathcal{X}}(x)$ iff $\mathbb{1}_{\mathcal{X}}(y) \geq \mathbb{1}_{\mathcal{X}}(x) + \langle g, y - x \rangle$ for all y .
- ▶ So $g \in \partial \mathbb{1}_{\mathcal{X}}(x)$ means $x \in \mathcal{X}$ and $0 \geq \langle g, y - x \rangle \forall y \in \mathcal{X}$.
- ▶ **Normal cone:**

$$\mathcal{N}_{\mathcal{X}}(x) := \{g \in \mathbb{R}^n \mid 0 \geq \langle g, y - x \rangle \quad \forall y \in \mathcal{X}\}$$

Application. $\min f(x) \quad \text{s.t. } x \in \mathcal{X}$:

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Application. $\min f(x) \quad \text{s.t. } x \in \mathcal{X}$:

- ◇ If f is diff., we get $0 \in \nabla f(x^*) + \mathcal{N}_{\mathcal{X}}(x^*)$
- ◇ $-\nabla f(x^*) \in \mathcal{N}_{\mathcal{X}}(x^*) \iff \langle \nabla f(x^*), y - x^* \rangle \geq 0$ for all $y \in \mathcal{X}$.

Duality

$$\min_{\theta \in \mathcal{S}} f(\theta)$$

Primal problem

Let $f_i : \mathbb{R}^n \rightarrow \mathbb{R}$ ($0 \leq i \leq m$). Generic **nonlinear program**

$$\begin{aligned} \min \quad & f_0(x) \\ \text{s.t.} \quad & f_i(x) \leq 0, \quad 1 \leq i \leq m, \\ & x \in \{\text{dom } f_0 \cap \text{dom } f_1 \cdots \cap \text{dom } f_m\}. \end{aligned} \tag{P}$$

Def. Domain: The set $\mathcal{D} := \{\text{dom } f_0 \cap \text{dom } f_1 \cdots \cap \text{dom } f_m\}$

- ▶ We call (P) the **primal problem**
- ▶ The variable x is the **primal variable**
- ▶ We will attach to (P) a **dual problem**
- ▶ In our initial derivation: no restriction to convexity.

Lagrangian

To the primal problem, associate **Lagrangian** $\mathcal{L} : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}$,

$$\mathcal{L}(x, \lambda) := f_0(x) + \sum_{i=1}^m \lambda_i f_i(x).$$

♠ Variables $\lambda \in \mathbb{R}^m$ called **Lagrange multipliers**

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- ♠ Variables $\lambda \in \mathbb{R}^m$ called **Lagrange multipliers**
- ♠ Suppose x is feasible, and $\lambda \geq 0$. Then, we get the lower-bound:

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- ♠ Lagrangian helps write problem in **unconstrained form**

Lagrange dual function

Def. We define the **Lagrangian dual** as

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Observations:

- ▶ g is pointwise inf of affine functions of λ
- ▶ Thus, g is concave; it may take value $-\infty$
- ▶ Recall: $f_0(x) \geq \mathcal{L}(x, \lambda) \quad \forall x \in \mathcal{X}, \lambda \geq 0$; thus
- ▶ $\forall x \in \mathcal{X}, \quad f_0(x) \geq \inf_{x'} \mathcal{L}(x', \lambda) =: g(\lambda)$
- ▶ Now minimize over x on lhs, to obtain

$$\forall \lambda \in \mathbb{R}_+^m \quad p^* \geq g(\lambda).$$

Lagrange dual problem

$$\sup_{\lambda} g(\lambda) \quad \text{s.t. } \lambda \geq 0.$$

Lagrange dual problem

$$\sup_{\lambda} g(\lambda) \quad \text{s.t. } \lambda \geq 0.$$

- ▶ **dual feasible:** if $\lambda \geq 0$ and $g(\lambda) > -\infty$
- ▶ **dual optimal:** λ^* if sup is achieved
- ▶ Lagrange dual is **always concave**, regardless of original

Weak duality

Def. Denote **dual optimal value** by d^* , i.e.,

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Theorem. (Weak-duality): For problem (P), we have $p^* \geq d^*$.

Proof: We showed that for all $\lambda \in \mathbb{R}_+^m$, $p^* \geq g(\lambda)$.
Thus, it follows that $p^* \geq \sup g(\lambda) = d^*$.

Duality gap

$$p^* - d^* \geq 0$$

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Strong duality if duality gap is zero: $p^* = d^*$

Notice: both p^* and d^* may be $+\infty$

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Several **sufficient** conditions known, especially for convex optimization.

“Easy” necessary and sufficient conditions: **unknown**

Example: Slater's sufficient conditions

$$\begin{aligned} \min \quad & f_0(x) \\ \text{s.t.} \quad & f_i(x) \leq 0, \quad 1 \leq i \leq m, \\ & Ax = b. \end{aligned}$$

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Constraint qualification: There exists $x \in \text{ri } \mathcal{D}$ s.t.

$$f_i(x) < 0, \quad Ax = b.$$

That is, there is a **strictly feasible** point.

Theorem. Let the primal problem be convex. If there is a feasible point such that is strictly feasible for the non-affine constraints (and merely feasible for affine, linear ones), then strong duality holds. Moreover, the dual optimal is attained (i.e., $d^* > -\infty$).

Reading: Read BV §5.3.2 for a proof.

Example: failure of strong duality

$$\min_{x,y} e^{-x} \quad x^2/y \leq 0,$$

over the domain $\mathcal{D} = \{(x, y) \mid y > 0\}$.

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Dual problem

$$d^* = \max_{\lambda} 0 \quad \text{s.t. } \lambda \geq 0.$$

Thus, $d^* = 0$, and gap is $p^* - d^* = 1$.

Here, we had no strictly feasible solution.

Zero duality gap: nonconvex example

Trust region subproblem (TRS)

$$\min \quad x^T A x + 2b^T x \quad x^T x \leq 1.$$

A is symmetric but not necessarily semidefinite!

Theorem. TRS always has zero duality gap.

Remark: Above theorem extremely important result; part of a family of related results on strong duality for certain quadratic nonconvex problems.

Example: dual for Support Vector Machine

$$\begin{aligned} \min_{x, \xi} \quad & \frac{1}{2} \|x\|_2^2 + C \sum_i \xi_i \\ \text{s.t.} \quad & Ax \geq 1 - \xi, \quad \xi \geq 0. \end{aligned}$$

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$$\begin{aligned} g(\lambda, \nu) &:= \inf L(x, \xi, \lambda, \nu) \\ &= \begin{cases} \lambda^T \mathbf{1} - \frac{1}{2} \|A^T \lambda\|_2^2 & \lambda + \nu = C \mathbf{1} \\ +\infty & \text{otherwise} \end{cases} \\ d^* &= \max_{\lambda \geq 0, \nu \geq 0} g(\lambda, \nu) \end{aligned}$$

Exercise: Using $\nu \geq 0$, eliminate ν from above problem.

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Say $\|\bar{y}\|_* < 1$, such that $A^T \bar{y} \in \text{ri}(\text{dom } f^*)$, then we have strong duality (e.g., for instance $0 \in \text{ri}(\text{dom } f^*)$)

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But $\lambda_i^* \geq 0$ and $f_i(x^*) \leq 0$, so **complementary slackness**

$$\lambda_i^* f_i(x^*) = 0, \quad i = 1, \dots, m.$$

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Exercise: Prove the above sufficiency of KKT. *Hint:* Use that $\mathcal{L}(x, \lambda^*)$ is convex, and conclude from KKT conditions that $g(\lambda^*) = f_0(x^*)$, so that (x^*, λ^*) optimal primal-dual pair.