Optimization for Machine Learning

Lecture 2: Conjugates, subdifferentials

6.881: MIT

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18 Feb, 2021

Some norms

(cont'd from last time)

Vector norms: recap

Example. The **Euclidean** or ℓ_2-norm is $\|x\|_2 = \left(\sum_i x_i^2\right)^{1/2}$

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

Exercise: Verify that $\|x\|_p$ is indeed a norm.

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

Example. (Frobenius-norm): Let $A \in \mathbb{C}^{m \times n}$. The **Frobenius** norm of A is $\|A\|_{\mathrm{F}} := \sqrt{\sum_{ij} |a_{ij}|^2}$; that is, $\|A\|_{\mathrm{F}} = \sqrt{\mathrm{Tr}(A^* A)}$.

Important example: Distance function

Claim. Let $\mathcal{Y}$ be a convex set. Let $x \in \mathbb{R}^d$ be some point. The distance of x to the set $\mathcal{Y}$ is defined as

$$\operatorname{dist}(x, \mathcal{Y}) := \inf_{y \in \mathcal{Y}} \quad \|x - y\|.$$

Proof. Observe that $\|x - y\|$ is jointly convex in (x, y) (**Why?**). Thus, the function $\operatorname{dist}(x, \mathcal{Y})$ is a convex function of x using the partial minimization rule.

Matrix Norms: induced norm

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Verify it is a norm

- Clearly, $\|A\| = 0$ iff $A = 0$ (definiteness)
- $\|\alpha A\| = |\alpha|\ \|A\|$ (homogeneity)
- $\|A + B\| = \sup \frac{\|(A+B)x\|}{\|x\|} \leq \sup \frac{\|Ax\|+\|Bx\|}{\|x\|} \leq \|A\| + \|B\|.$

Operator norm

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It can be shown that $\|A\|_2 = \sigma_{\max}(A)$, where $\sigma_{\max}$ is the largest singular value of A.

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- ***Schatten p-norm:*** ℓ_p-norm of vector of singular values.
- **Exercise:** Let $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$ be singular values of a matrix $A \in \mathbb{R}^{m \times n}$. Prove that

$$\|A\|_{(k)} := \sum_{i=1}^{k} \sigma_i(A),$$

is a norm; $1 \leq k \leq n$.

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Def. Let $\|\cdot\|$ be a norm on $\mathbb{R}^d$. Its **dual norm** is

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Exercise: Let $1/p + 1/q = 1$, where $p, q \geq 1$. Show that $\|\cdot\|_q$ is dual to $\|\cdot\|_p$. In particular, the ℓ_2-norm is self-dual.

Exercise. Verify the generalized *Hölder inequality* $u^T x \leq \|u\|\|x\|_*$ using the definition of dual norms.

Support functions and Hausdorff distance*

Def. Let $K, L \subseteq \mathbb{R}^d$ be two sets. The **Hausdorff distance** between them is defined as

$$d_H(K, L) := \inf \{\lambda \geq 0 \mid K \subseteq L + \lambda B(0,1), L \subseteq K + \lambda B(0,1)\}.$$

(See e.g., *https://en.wikipedia.org/wiki/Hausdorff_distance*)

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Lemma Let K, L be convex bodies in $\mathbb{R}^d$. Then,

$$d_H(K, L) = \sup_{\|u\|_2 \leq 1} |\sigma_K(u) - \sigma_L(u)|.$$

Explore. Support functions are important in the subject of *convex geometry*; read up on them and explore a bit!

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Theorem. Let f be a closed convex function (i.e., epi $f = \{(x,t) \mid f(x) \leq t\}$ is a closed convex set; equivalently, f is lower semi-continuous). Then, $f^{**} = f$.

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Exercise: Show that $f^* = f \iff f = \frac{1}{2}\|\cdot\|_2^2$.

Fenchel conjugate – examples

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Exercise: If $f(x) = \max(0, 1-x)$, then $\operatorname{dom} f^*$ is $[-1, 0]$, and within this domain, $f^*(z) = z$.

Fenchel conjugate of norms

Recall: Dual norm

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Proof.

- Consider two cases: (i) $\|z\|_* > 1$; (ii) $\|z\|_* \leq 1$
- (i): by def. of dual norm there is a u s.t. $\|u\| \leq 1$ and $z^T u > 1$
- $f^*(z) = \sup_x x^T z - f(x)$. Rewrite $x = \alpha u$, and let $\alpha \to \infty$
- Then, $z^T x - \|x\| = \alpha z^T u - \|\alpha u\| = \alpha(z^T u - \|u\|); \to \infty$
- Case (ii): Since $z^T x \leq \|x\| \|z\|_*$, $x^T z - \|x\| \leq \|x\|(\|z\|_* - 1) \leq 0$.
- $x = 0$ maximizes $\|x\|(\|z\|_* - 1)$, hence $f(z) = 0$.
- Thus, $f^*(z) = +\infty$ if (i), and 0 if (ii), completing the proof.

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Challenge. Recall: $f(x) = \frac{1}{2}x^TAx$ ($A \succ 0$) then $f^*(z) = \frac{1}{2}z^TA^{-1}z$. Let $f_i(x) := x^TA_ix$ for $A_i \succ 0$ and $1 \le i \le n$. Consider,

$$F(z) := \sum_i f_i^*(z) - \sum_{i<j}(f_i + f_j)^*(z) + \cdots + (-1)^{n+1}(f_1 + \cdots + f_n)^*(z).$$

Prove or disprove that F is convex.

Fenchel conjugates are special*

Let $\Gamma_0(\mathbb{R}^d)$ denote class of closed, convex functions on $\mathbb{R}^d$. The (Legendre)-Fenchel transform of $f \in \Gamma_0$ is defined as

$$\mathcal{L} : f \mapsto \quad \sup_y \langle \cdot, y \rangle - f(y)$$

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Theorem. *Let $\mathcal{T}$ be a transform that maps $\Gamma_0 \to \Gamma_0$ and satifies: (i) $\mathcal{T}(\mathcal{T}f) = f$ (closure); and (ii) $f \le g \implies \mathcal{T}f \ge \mathcal{T}g$.*
Then, $\mathcal{T}$ must "essentially" be the Fenchel transform. More precisely, there exists $c \in \mathbb{R}$, $v \in \mathbb{R}^d$ and $B \in GL_n(\mathbb{R})$ such that

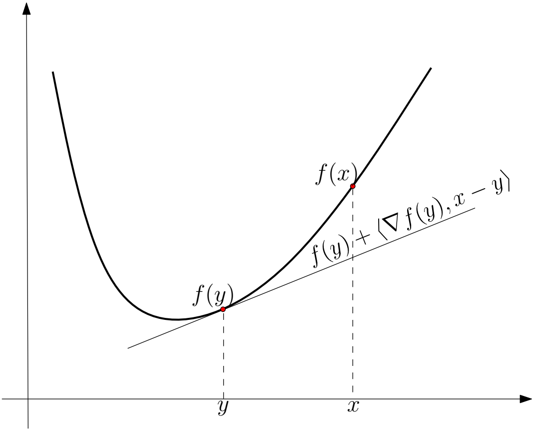
$$(\mathcal{T}f)(x) = (\mathcal{L}f)(Bx + v) + \langle v, x \rangle + c$$

Explore: Study other classes instead of $\Gamma_0(\mathbb{R}^d)$ for which similar theorems can be proved.

Subdifferentials

DO: (Read S. Boyd's EE364B notes)

First order global underestimator



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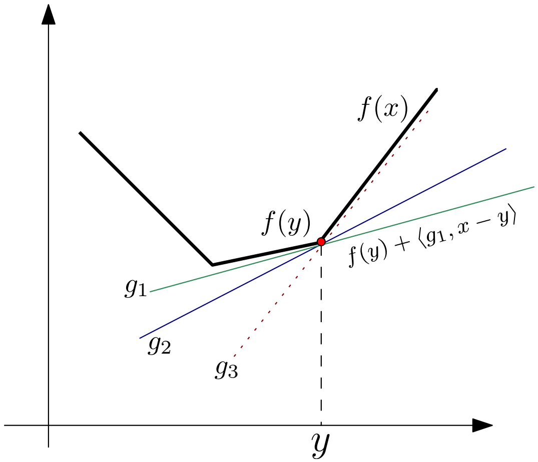

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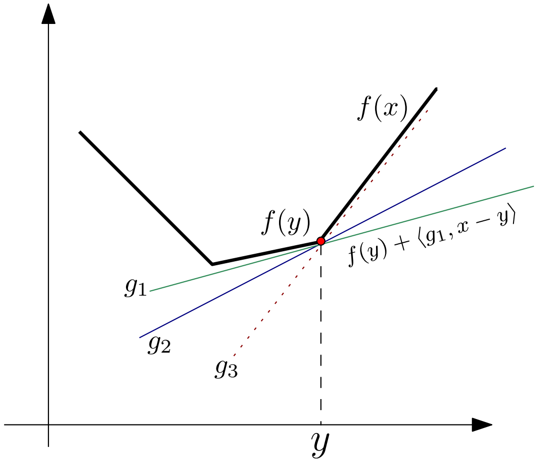
Subgradients



g_1, g_2, g_3 are subgradients at y

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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- Subgradient calculus: great achievement in convex analysis
- Without convexity, things become wild (e.g., chain rule fails!)

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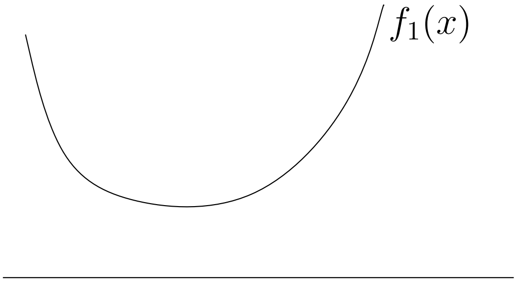

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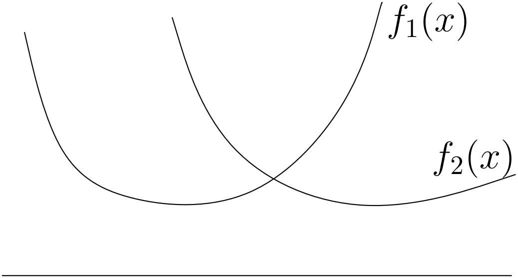

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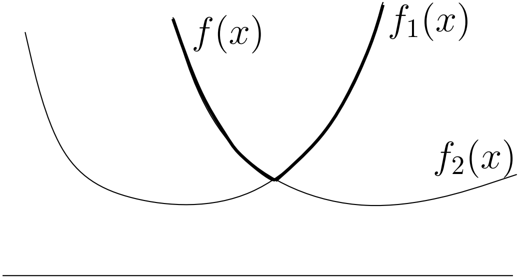

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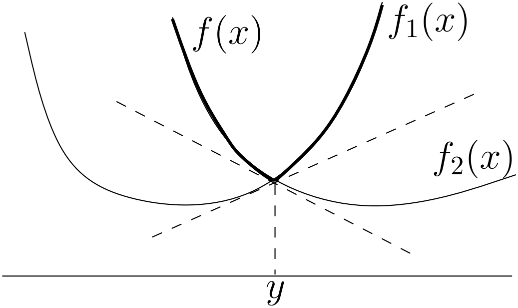

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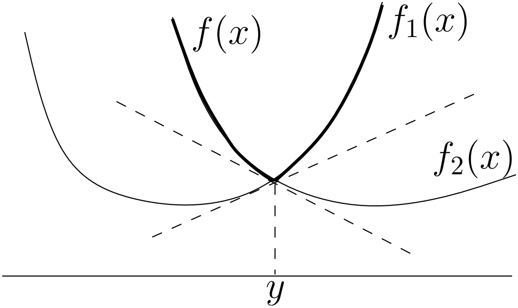

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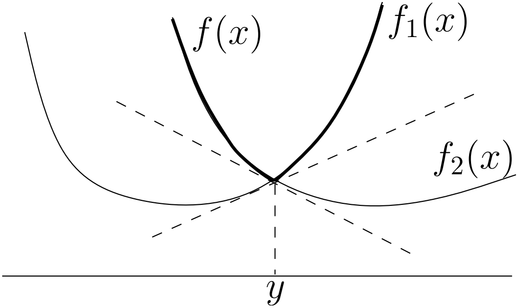

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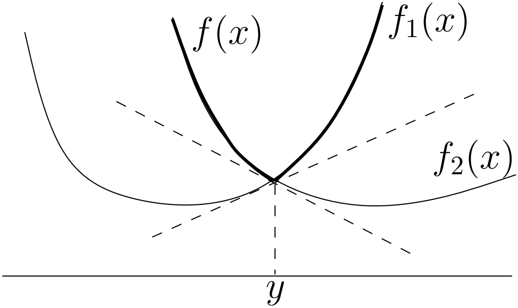

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- ⋆ $f_1(x) < f_2(x)$: unique subgradient of f is $f_2'(x)$
- ⋆ $f_1(y) = f_2(y)$: subgradients, the segment $[f_1'(y), f_2'(y)]$ (imagine all supporting lines turning about point y)

Subgradients and the Subdifferential (Set)

Def. A vector $g \in \mathbb{R}^n$ is called a **subgradient** at a point y, if for all $x \in \operatorname{dom} f$, it holds that

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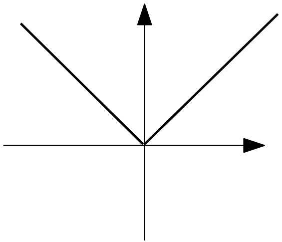
- ♣ If f differentiable at x, then $\partial f(x) = \{\nabla f(x)\}$
- ♣ If $\partial f(x) = \{g\}$, then f is differentiable and $g = \nabla f(x)$

Subdifferential – example

$$\boxed{f(x) = |x|}$$



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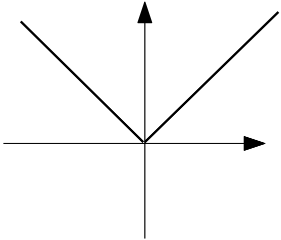

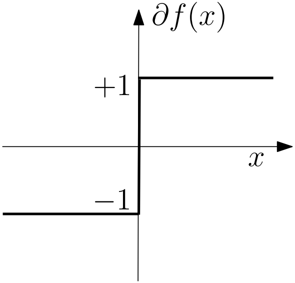

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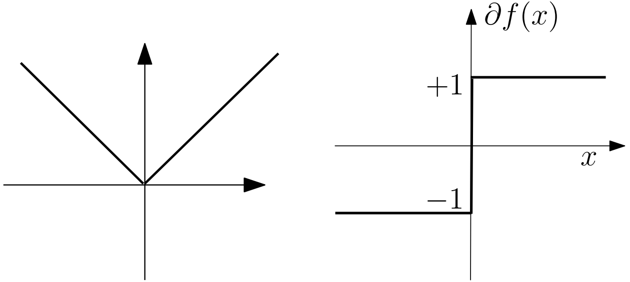

$$\partial|x| = \begin{cases} -1 & x < 0, \\ +1 & x > 0, \\ [-1, 1] & x = 0. \end{cases}$$

More examples

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

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

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Proof.

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

Calculus rules

Recall basic calculus

If f and k are differentiable, we know that

- **Addition**: $\nabla(f+k)(x) = \nabla f(x) + \nabla k(x)$
- **Scaling**: $\nabla(\alpha f(x)) = \alpha \nabla f(x)$

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Chain rule

If $f : \mathbb{R}^n \to \mathbb{R}^m$, and $k : \mathbb{R}^m \to \mathbb{R}^p$. Let $h : \mathbb{R}^n \to \mathbb{R}^p$ be the composition $h(x) = (k \circ f)(x) = k(f(x))$. Then,

$$Dh(x) = Dk(f(x))Df(x).$$

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Example. If $f : \mathbb{R}^n \to \mathbb{R}$ and $k : \mathbb{R} \to \mathbb{R}$, then using the fact that $\nabla h(x) = [Dh(x)]^T$, we obtain

$$\nabla h(x) = k'(f(x))\nabla f(x).$$

Subgradient calculus

♠ Finding one subgradient within $\partial f(x)$

Subgradient calculus

- ♠ Finding one subgradient within $\partial f(x)$
- ♠ Determining entire subdifferential $\partial f(x)$ at a point x

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- Do we have the chain rule?

Subgradient calculus

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- Determining entire subdifferential $\partial f(x)$ at a point x
- Do we have the chain rule?
- Usually not easy!

Subgradient calculus

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Subgradient calculus

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convex hull over subdifferentials of "active" functions at x
- **Conjugation:** $z \in \partial f(x)$ if and only if $x \in \partial f^*(z)$

Failure of addition rule

$$\boxed{\text{It can happen that } \partial(f_1 + f_2) \neq \partial f_1 + \partial f_2}$$

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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, $f = f_1 + f_2 = \mathbb{1}_0$, whereby $\partial f(0) = \mathbb{R}$
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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.

Exercise: Prove the above statement.

Subdifferential: two examples

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

$$\partial f(0) = \operatorname{conv}\{\pm e_1, \ldots, \pm e_n\},$$

where e_i is i-th canonical basis vector

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Example. Let $f_1, f_2, \ldots, f_m$ be differentiable and convex. Let

$$f(x) := \max(f_1(x), \ldots, f_m(x))$$

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Computing subgradients

Subgradient for pointwise sup

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

$$\boxed{\text{Getting } \partial f(x) \text{ is complicated!}}$$

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Example

Suppose $a_i \in \mathbb{R}^n$ and $b_i \in \mathbb{R}$. And

$$f(x) := \max_{1 \le i \le n} (a_i^T x + b_i).$$

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- Here $f(x; y) = f_k(x) = a_k^T x + b_k$, and $\partial f_k(x) = \{\nabla f_k(x)\}$
- Hence, $a_k \in \partial f(x)$ works!

Subgradient of expectation

Suppose $f = \mathbf{E}f(x,u)$, where f is convex in x for each u (an r.v.)

$$f(x) := \int f(x,u)p(u)du$$

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- For each u choose any $g(x,u) \in \partial_x f(x,u)$
- Then, $g = \int g(x,u)p(u)du = \mathbf{E}g(x,u) \in \partial f(x)$

Ref. D. P. Bertsekas, *"Stochastic optimization problems with nondifferentiable cost functionals."* JOTA v.12(2), 1973.

Subgradient of composition

Suppose $h : \mathbb{R}^n \to \mathbb{R}$ cvx and increasing; each f_i cvx

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Exercise: Verify $g \in \partial f(x)$ by showing $f(z) \geq f(x) + \boxed{g}^T(z - x)$