Subgradients

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Last time: gradient descent

Consider the problem

$$\min_x f(x)$$

for f convex and differentiable, $\mathrm{dom}(f) = \mathbb{R}^n$.

Gradient descent: choose initial $x^{(0)} \in \mathbb{R}^n$, repeat

$$x^{(k)} = x^{(k-1)} - t_k \cdot \nabla f(x^{(k-1)}), \quad k = 1, 2, 3, \ldots$$

Step sizes t_k chosen to be fixed and small, or by backtracking line search

If ∇f Lipschitz, gradient descent has convergence rate $O(1/\varepsilon)$

Downsides:

- Requires f differentiable
- Can be slow to converge

Outline

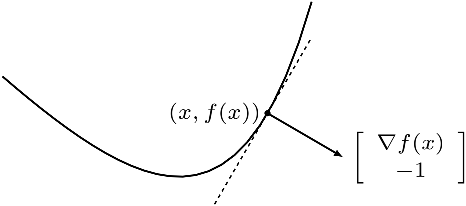
Today:

- Subgradients
- Examples
- Properties
- Optimality characterizations

Basic inequality

Recall that for convex and differentiable f,

$$f(y) \geq f(x) + \nabla f(x)^T (y - x), \ \forall x, y \in \text{dom}(f).$$



- The first-order approximation of f at x is a global lower bound.
- ∇f defines a non-vertical supporting hyperplane to epi(f) at $(x, f(x))$

$$\begin{pmatrix} \nabla f & -1 \end{pmatrix} \left(\begin{pmatrix} y \\ t \end{pmatrix} - \begin{pmatrix} x \\ f(x) \end{pmatrix} \right) \leq 0, \ \forall (y, t) \in \text{epi}(f).$$

Subgradients

A subgradient of a convex function f at x is any $g \in \mathbb{R}^n$ such that

$$f(y) \geq f(x) + g^T(y - x), \ \forall y \in \text{dom}(f).$$

- Always exists (on the relative interior of dom(f))
- If f differentiable at x, then $g = \nabla f(x)$ uniquely
- Same definition works for nonconvex f (however, subgradients need not exist).

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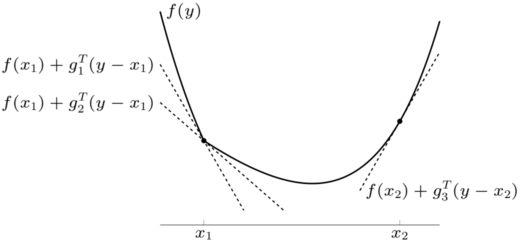
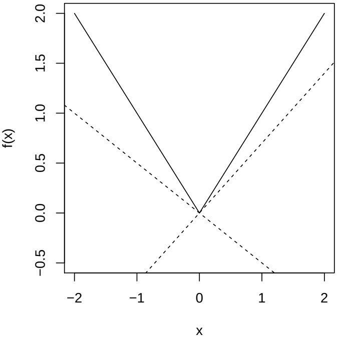


g_1 and g_2 are subgradients at x_1, g_3 is subgradient at x_2.

Examples of subgradients

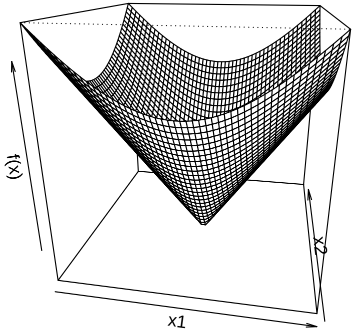
Consider $f : \mathbb{R} \to \mathbb{R}, f(x) = |x|$



- For $x \neq 0$, unique subgradient $g = \text{sign}(x)$
- For $x = 0$, subgradient g is any element of $[-1, 1]$.

Examples of subgradients

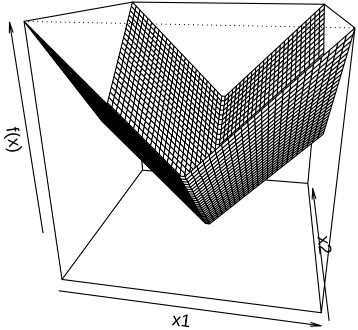
Consider $f : \mathbb{R}^n \to \mathbb{R}, f(x) = \|x\|_2$



- For $x \neq 0$, unique subgradient $g = \dfrac{x}{\|x\|_2}$
- For $x = 0$, subgradient g is any element of $\{z : \|z\|_2 \leq 1\}$.

Examples of subgradients

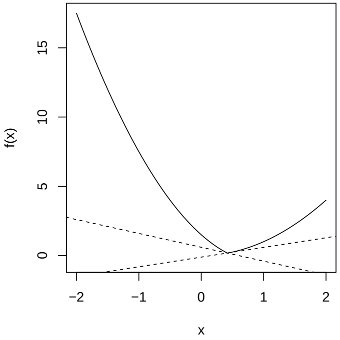
Consider $f : \mathbb{R}^n \to \mathbb{R}, f(x) = \|x\|_1$



- For $x_i \neq 0$, unique ith component $g_i = \text{sign}(x_i)$
- For $x_i = 0$, ith component g_i is any element of $[-1, 1]$.

Examples of subgradients

Consider $f(x) = \max\{f_1(x), f_2(x)\}$, for $f_1, f_2 \colon \mathbb{R}^n \to \mathbb{R}$ convex, differentiable



- For $f_1(x) > f_2(x)$, unique subgradient $g = \nabla f_1(x)$
- For $f_2(x) > f_1(x)$, unique subgradient $g = \nabla f_2(x)$
- For $f_1(x) = f_2(x)$, subgradient g is any point on line segment between $\nabla f_1(x)$ and $\nabla f_2(x)$.

Subdifferential

Set of all subgradients of convex f is called the subdifferential:

$$\partial f(x) = \{g \in \mathbb{R}^n : g \text{ is a subgradient of } f \text{ at } x\}.$$

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Properties:

- Nonempty for convex f at $x \in \text{int}(\text{dom} f)$
- $\partial f(x)$ is closed and convex (even for nonconvex f)
- If f is differentiable at x, then $\partial f(x) = \{\nabla f(x)\}$
- If $\partial f(x) = \{g\}$, then f is differentiable at x and $\nabla f(x) = g$.

Proof: See `http://www.seas.ucla.edu/~vandenbe/236C/lectures/subgradients.pdf`

Theorem

The subdifferential of a convex function f is a monotone operator

$$(u-v)^T(x-y) \geq 0,\ \forall u \in \partial f(x), v \in \partial f(y).$$

Chứng minh.

By definition we have

$$f(y) \geq f(x) + u^T(y-x) \quad \text{and} \quad f(x) \geq f(y) + v^T(x-y).$$

Combining them get shows monotonicity. $\square$

Monotonicity

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Question: Monotonicity for differentiable convex function?

$$(\nabla f(x) - \nabla f(y))^T(x-y) \geq 0,$$

which follows directly from the first order characterization of convex functions.

Examples of non-subdifferentiable functions

The following functions are not subdifferentiable at $x = 0$

- $f : \mathbb{R} \to \mathbb{R}$, $\mathrm{dom}(f) = \mathbb{R}_+$
$$f(x) = \begin{cases} 1 & \text{if } x = 0 \\ 0 & \text{if } x > 0. \end{cases}$$
- $f : \mathbb{R} \to \mathbb{R}$, $\mathrm{dom}(f) = \mathbb{R}_+$
$$f(x) = -\sqrt{x}.$$

The only supporting hyperplane to $\mathrm{epi}(f)$ at $(0, f(0))$ is vertical.

Connection to convex geometry

Convex set $C \subseteq \mathbb{R}^n$, consider indicator function $I_C : \mathbb{R}^n \to \mathbb{R}$,

$$I_C(x) = I\{x \in C\} = \begin{cases} 0 & \text{if } x \in C \\ \infty & \text{if } x \notin C. \end{cases}$$

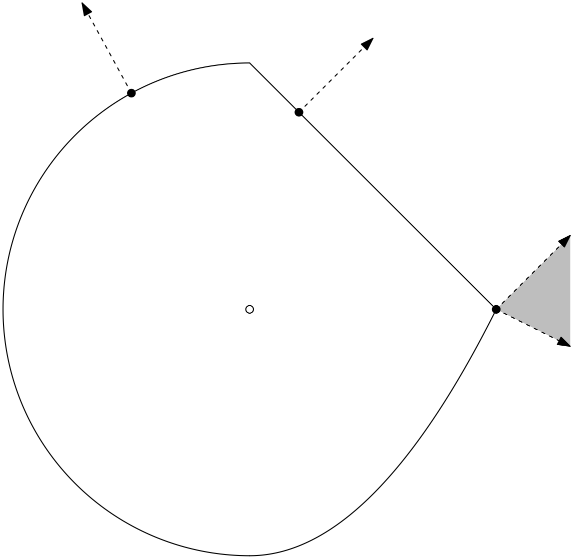
For $x \in C, \partial I_C(x) = \mathcal{N}_C(x)$, the normal cone of C at x is, recall

$$\mathcal{N}_C = \{g \in \mathbb{R}^n : g^T x \geq g^T y \text{ for any } y \in C\}.$$

Why? By definition of subgradient g,

$$I_C(y) \geq I_C(x) + g^T(y - x) \quad \text{for all } y.$$

- For $y \notin C, I_C(y) = \infty$
- For $y \in C$, this means $0 \geq g^T(y - x)$.



Subgradient calculus

Basic rules for convex functions:

- Scaling: $\partial(af) = a \cdot \partial f$ provided $a > 0$.
- Addition: $\partial(f_1 + f_2) = \partial f_1 + \partial f_2$.
- Affine composition: if $g(x) = f(Ax + b)$, then
$$\partial g(x) = A^T \partial f(Ax + b).$$
- Finite pointwise maximum: if $f(x) = \max_{i=1,\ldots m} f_i(x)$, then
$$\partial f(x) = \text{conv}\left(\bigcup_{i: f_i(x) = f(x)} \partial f_i(x) \right)$$
convex hull of union of subdifferentials of active functions at x.

Subgradient calculus

- General pointwise maximum: if $f(x) = \max_{s \in S} f_s(x)$, then
$$\partial f(x) \supseteq \text{cl}\left\{\text{conv}\left(\bigcup_{s: f_s(x) = f(x)} \partial f_s(x)\right)\right\}.$$
Under some regularity conditions (on S, f_s), we get equality.
- Norms: important special case, $f(x) = \|x\|_p$. Let q be such that $1/p + 1/q = 1$, then
$$\|x\|_p = \max_{\|z\|_q \le 1} z^T x.$$
And
$$\partial f(x) = \text{argmax}_{\|z\|_q \le 1} z^T x.$$

Why subgradients?

Subgradients are important for two reasons:

- Convex analysis: optimality characterization via subgradients, monotonicity, relationship to duality.
- Convex optimization: if you can compute subgradients, then you can minimize any convex function.

Optimality condition

Subgradient optimality condition: For any f (convex or not),

$$f(x^*) = \min_x f(x) \iff 0 \in \partial f(x^*),$$

i.e., x^* is a minimizer if and only if 0 is a subgradient of f at x^*.

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Subgradient optimality condition: For any f (convex or not),

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i.e., x^* is a minimizer if and only if 0 is a subgradient of f at x^*.

Why? Easy: $g = 0$ being a subgradient means that for all y

$$f(y) \geq f(x^*) + 0^T(y - x^*) = f(x^*).$$

Note the implication for a convex and differentiable function f with $\partial f(x) = \{\nabla f(x)\}$.

Derivation of first-order optimality

Example of the power of subgradients: we can use what we have learned so far to derive the first-order optimality condition.

Theorem

For f convex and differentiable and C convex

$$\min_x f(x) \text{ subject to } x \in C$$

is solved at x if and only if

$$\nabla f(x)^T (y - x) \geq 0 \quad \text{for all } y \in C.^a$$

[a] Direct proof see, e.g., `http://www.princeton.edu/~amirali/Public/Teaching/ORF523/S16/ORF523_S16_Lec7_gh.pdf`. Proof using subgradient next slide.

Intuitively: says that gradient increases as we move away from x.

Note that for $C = \mathbb{R}^n$ (unconstrained case) it reduces to $\nabla f = 0$.

Derivation of first-order optimality

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First recast problem as

$$\min_x f(x) + I_C(x).$$

Now apply subgradient optimality: $0 \in \partial(f(x) + I_C(x))$.

Observe

$$\begin{aligned} 0 \in \partial(f(x) + I_C(x)) &\Leftrightarrow 0 \in \{\nabla f(x)\} + \mathcal{N}_C(x) \\ &\Leftrightarrow -\nabla f(x) \in \mathcal{N}_C(x) \\ &\Leftrightarrow -\nabla f(x)^T x \geq -\nabla f(x)^T y \text{ for all } y \in C \\ &\Leftrightarrow \nabla f(x)^T (y - x) \geq 0 \text{ for all } y \in C \end{aligned}$$

as desired. □

Note: the condition $0 \in \partial f(x) + \mathcal{N}_C(x)$ is a fully general condition for optimality in convex problems. But it's not always easy to work with (KKT conditions, later, are easier).

Example: lasso optimality conditions

Given $y \in \mathbb{R}^n, X \in \mathbb{R}^{n \times p}$, lasso problem can be parametrized as

$$\min_\beta \frac{1}{2} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1$$

where $\lambda \geq 0$.

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$$\min_{\beta} \frac{1}{2} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1$$

where $\lambda \geq 0$. Subgradient optimality

$$\begin{aligned} 0 \in \partial \left(\frac{1}{2} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1 \right) &\Leftrightarrow 0 \in -X^T(y - X\beta) + \lambda \partial \|\beta\|_1 \\ &\Leftrightarrow X^T(y - X\beta) = \lambda v \end{aligned}$$

for some $v \in \partial \|\beta\|_1$, i.e.,

$$v_i \in \begin{cases} \{1\} & \text{if } \beta_i > 0 \\ \{-1\} & \text{if } \beta_i < 0, \\ [-1, 1] & \text{if } \beta_i = 0 \end{cases} \quad i = 1, \ldots, p.$$

Example: lasso optimality conditions

Write $X_1, \ldots, X_p$ for columns of X. Then our condition reads

$$\begin{cases} X_i^T(y - X\beta) = \lambda \cdot \mathrm{sign}(\beta_i) & \text{if } \beta_i \neq 0 \\ |X_i^T(y - X\beta)| \leq \lambda & \text{if } \beta_i = 0. \end{cases}$$

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Note: subgradient optimality conditions don't lead to closed-form expression for a lasso solution. However they do provide a way to check lasso optimality.

They are also helpful in understanding the lasso estimator; e.g., if $|X_i^T(y - X\beta)| < \lambda$, then $\beta_i = 0$ (used by screening rules, later?).

Example: soft-thresholding

Simplfied lasso problem with $X = I$:

$$\min_{\beta} \frac{1}{2} \|y - \beta\|_2^2 + \lambda \|\beta\|_1 .$$

This we can solve directly using subgradient optimality. Solution is $\beta = S_\lambda(y)$, where S_λ is the soft-thresholding operator

$$[S_\lambda(y)]_i = \begin{cases} y_i - \lambda & \text{if } y_i > \lambda \\ 0 & \text{if } -\lambda \le y_i \le \lambda, \\ y_i + \lambda & \text{if } y_i < -\lambda \end{cases} \quad i = 1, \ldots, n.$$

Check: from last slide, subgradient optimality conditions are

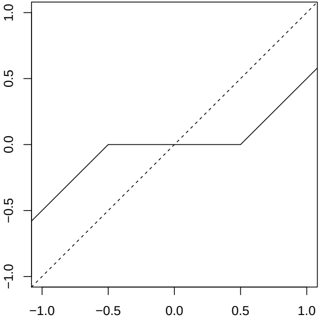
$$\begin{cases} y_i - \beta_i = \lambda \cdot \mathrm{sign}(\beta_i) & \text{if } \beta_i \neq 0 \\ |y_i - \beta_i| \le \lambda & \text{if } \beta_i = 0. \end{cases}$$

Example: soft-thresholding

Now plug in $\beta = S_\lambda(y)$ and check these are satisfied:

- When $y_i > \lambda, \beta_i = y_i - \lambda > 0$, so $y_i - \beta_i = \lambda = \lambda \cdot 1$.
- When $y_i < -\lambda$, argument is similar.
- When $|y_i| \leq \lambda, \beta_i = 0$, and $|y_i - \beta_i| = |y_i| \leq \lambda$.

Soft-thresholding in one variable



Example: distance to a convex set

Recall the distance function to a closed, convex set C

$$\operatorname{dist}(x, C) = \min_{y \in C} \|y - x\|_2 \, .$$

This is a convex function. What are its subgradients?

Example: distance to a convex set

Recall the distance function to a closed, convex set C

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Write $\mathrm{dist}(x, C) = \|x - P_C(x)\|_2$, where $P_C(x)$ is the projection of x onto C. It turns out that when $\mathrm{dist}(x, C) > 0$,

$$\partial\, \mathrm{dist}(x, C) = \left\{ \frac{x - P_C(x)}{\|x - P_C(x)\|_2} \right\}$$

only has one element, so in fact $\mathrm{dist}(x, C)$ is differentiable and this is its gradient.

Example: distance to a convex set

We will only show one direction, i.e., that

$$\frac{x - P_C(x)}{\|x - P_C(x)\|_2} \in \partial\,\mathrm{dist}(x, C).$$

Write $u = P_C(x)$. Then by first-order optimality conditions for a projection,

$$(x - u)^T(y - u) \leq 0 \quad \text{for all } y \in C.$$

Hence

$$C \subseteq H = \{y : (x - u)^T(y - u) \leq 0\}.$$

Claim

$$\mathrm{dist}(y, C) \geq \frac{(x - u)^T(y - u)}{\|x - u\|_2} \quad \text{for all } y.$$

Check: first, for $y \in H$, the right-hand side is ≤ 0.

Example: distance to a convex set

Now for $y \notin H$, we have $(x-u)^T(y-u) = \|x-u\|_2 \, \|y-u\|_2 \cos\theta$ where θ is the angle between $x-u$ and $y-u$. Thus

$$\frac{(x-u)^T(y-u)}{\|x-u\|_2} = \|y-u\|_2 \cos\theta = \mathrm{dist}(y,H) \le \mathrm{dist}(y,C)$$

as desired.

Using the claim, we have for any y

$$\begin{aligned}\mathrm{dist}(y,C) &\ge \frac{(x-u)^T(y-x+x-u)}{\|x-u\|_2} \\ &= \|x-u\|_2 + \left(\frac{x-u}{\|x-u\|_2}\right)^T (y-x)\end{aligned}$$

Hence $g = (x-u)/\|x-u\|_2$ is a subgradient of $\mathrm{dist}(x,C)$ at x.

References and further reading

- S. Boyd, *Lecture notes for EE 264B*, Stanford University, Spring 2010-2011
- R. T. Rockafellar (1970), *Convex analysis*, Chapters 23–25
- L. Vandenberghe, *Lecture notes for EE 236C*, UCLA, Spring 2011-2012