Subgradients

Ryan Tibshirani
Convex Optimization 10-725/36-725

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 $O(1/\epsilon)$

Downsides:

- Requires f differentiable $\leftarrow$ next lecture
- Can be slow to converge $\leftarrow$ two lectures from now

Outline

Today: crucial mathematical underpinnings!

- Subgradients
- Examples
- Subgradient rules
- Optimality characterizations

Subgradients

Remember that for convex and differentiable f,

$$f(y) \geq f(x) + \nabla f(x)^T (y - x) \quad \text{for all } x, y$$

I.e., linear approximation always underestimates f

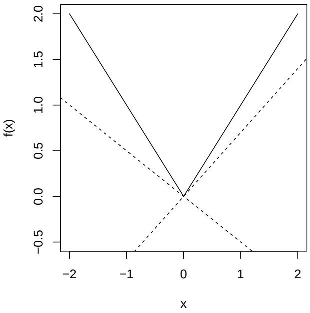
A subgradient of a convex function f at x is any $g \in \mathbb{R}^n$ such that

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

- Always exists
- If f differentiable at x, then $g = \nabla f(x)$ uniquely
- Actually, same definition works for nonconvex f (however, subgradients need not exist)

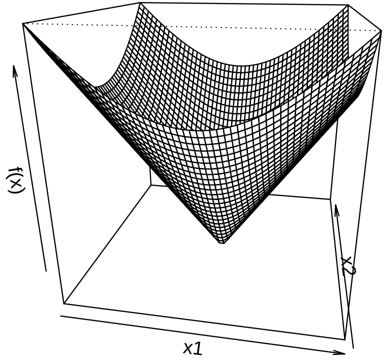
Examples of subgradients

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



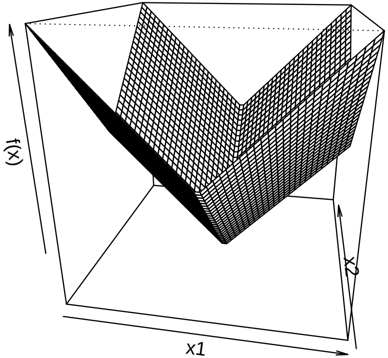
- For $x \neq 0$, unique subgradient $g = \mathrm{sign}(x)$
- For $x = 0$, subgradient g is any element of $[-1, 1]$

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



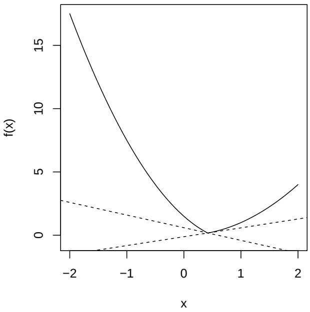
- For $x \neq 0$, unique subgradient $g = x/\|x\|_2$
- For $x = 0$, subgradient g is any element of $\{z : \|z\|_2 \leq 1\}$

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 $[-1, 1]$

Let $f_1, f_2 : \mathbb{R}^n \to \mathbb{R}$ be convex and differentiable, and consider $f(x) = \max\{f_1(x), f_2(x)\}$



- 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 the line segment between $\nabla f_1(x)$ and $\nabla f_2(x)$

Subdifferential

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

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

- $\partial f(x)$ is closed and convex (even for nonconvex f)
- Nonempty (can be empty 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 $\nabla f(x) = g$

Connection to convex geometry

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

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

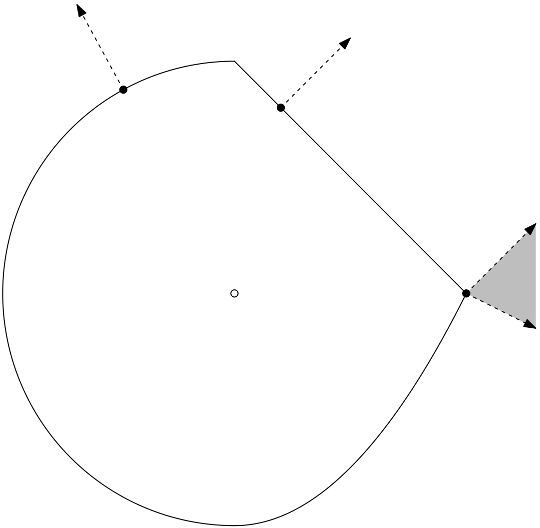
For $x \in C$, $\partial I_C(x) = \mathcal{N}_C(x)$, the normal cone of C at x, recall

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

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

$$\partial f(x) = \operatorname{conv}\Bigg(\bigcup_{i: f_i(x) = f(x)} \partial f_i(x) \Bigg)$$

  the convex hull of union of subdifferentials of all active functions at x

- General pointwise maximum: if $f(x) = \max_{s \in S} f_s(x)$, then

$$\partial f(x) \supseteq \mathrm{cl}\left\{\mathrm{conv}\left(\bigcup_{s: f_s(x) = f(x)} \partial f_s(x)\right)\right\}$$

and under some regularity conditions (on S, f_s), we get an equality above

- Norms: important special case, $f(x) = \|x\|_p$. Let q be such that $1/p + 1/q = 1$, then

$$\|x\|_p = \max_{\|z\|_q \leq 1} z^T x$$

Hence

$$\partial f(x) = \underset{\|z\|_q \leq 1}{\mathrm{argmax}} \; z^T x$$

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 (almost) any convex function

Optimality condition

For any f (convex or not),

$$f(x^\star) = \min_x \; f(x) \quad \Longleftrightarrow \quad 0 \in \partial f(x^\star)$$

I.e., $x^\star$ is a minimizer if and only if 0 is a subgradient of f at $x^\star$. This is called the subgradient optimality condition

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

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

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. Recall that for f convex and differentiable, the problem

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

is solved at x if and only if

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

Intuitively says that gradient increases as we move away from x. How to see this? First recast problem as

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

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

But

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

as desired

Note: the condition $0 \in \partial f(x) + \mathcal{N}_C(x)$ is a fully general condition for optimality in a convex problem. But this is 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:

$$\min_{\beta \in \mathbb{R}^p} \; \frac{1}{2}\|y - X\beta\|_2^2 + \lambda\|\beta\|_1$$

where $\lambda \geq 0$. Subgradient optimality:

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

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

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

Write $X_1, \ldots X_p$ for columns of X. Then subgradient optimality reads:

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

Note: the subgradient optimality conditions do not directly lead to an 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 $\beta_i = 0$

Example: soft-thresholding

Simplfied lasso problem with $X = I$:

$$\min_{\beta \in \mathbb{R}^n} \frac{1}{2}\|y - \beta\|_2^2 + \lambda \|\beta\|_1$$

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

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

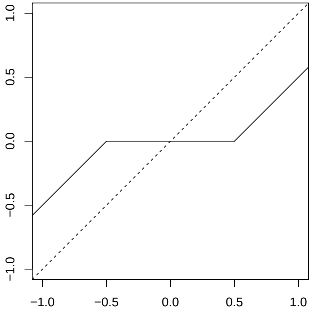
Check: from last slide, subgradient optimality conditions are

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

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 convex set C:

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

This is a convex function. What are its subgradients?

Write $\mathrm{dist}(x, C) = \|x - P_C(x)\|_2$, where $P_C(x)$ is the projection of x onto C. Then 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

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,

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

Hence

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

Claim: for any y,

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

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

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

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

as desired

Using the claim, we have for any y

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

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