Subgradients

Ryan Tibshirani Convex Optimization 10-725

Last time: gradient descent

Consider the problem

 $\min_x f(x)$

for f convex and differentiable, $dom(f) = \mathbb{R}^n$. Gradient descent: choose initial $x^{(0)} \in \mathbb{R}^n$, repeat

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

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

If ∇f is Lipschitz, gradient descent has convergence rate $O(1/\epsilon)$. Downsides:

- Requires *f* differentiable
- Can be slow to converge

Outline

Today: crucial mathematical underpinnings!

- Subgradients
- Examples
- Properties
- Optimality characterizations

Subgradients

Recall that for convex and differentiable f,

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

That is, linear approximation always underestimates \boldsymbol{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 exists¹
- If f differentiable at x, then $g=\nabla f(x)$ uniquely
- Same definition works for nonconvex *f* (however, subgradients need not exist)

¹On the relative interior of dom(f)

Examples of subgradients

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



- For $x \neq 0$, unique subgradient $g = \operatorname{sign}(x)$
- 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 $\{z : ||z||_2 \le 1\}$

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



• For $x_i \neq 0$, unique *i*th component $g_i = \operatorname{sign}(x_i)$

• For $x_i = 0$, *i*th component g_i is any element of [-1, 1]

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

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

- Nonempty (only for convex *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 $\nabla f(x) = g$

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

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

Why? By definition of subgradient g,

$$I_C(y) \ge I_C(x) + g^T(y-x)$$
 for all y

• For
$$y \notin C$$
, $I_C(y) = \infty$

• For $y \in C$, this means $0 \ge g^T(y-x)$



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 $f(x) = \max_{i=1,\dots,m} f_i(x)$, then

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

convex hull of union of subdifferentials of active functions at \boldsymbol{x}

• General composition: if

$$f(x) = h(g(x)) = h(g_1(x), \dots, g_k(x))$$

where $g : \mathbb{R}^n \to \mathbb{R}^k$, $h : \mathbb{R}^k \to \mathbb{R}$, $f : \mathbb{R}^n \to \mathbb{R}$, h is convex and nondecreasing in each argument, g is convex, then

$$\partial f(x) \subseteq \left\{ p_1 q_1 + \dots + p_k q_k : \\ p \in \partial h(g(x)), \ q_i \in \partial g_i(x), \ i = 1, \dots, k \right\}$$

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

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

Under some regularity conditions (on S, f_s), we get equality

 Norms: important special case. To each norm || · ||, there is a dual norm || · ||_∗ such that

$$||x|| = \max_{||z||_* \le 1} z^T x$$

(For example, $\|\cdot\|_p$ and $\|\cdot\|_q$ are dual when 1/p + 1/q = 1.) In fact, for $f(x) = \|x\|$ (and $f_z(x) = z^T x$), we get equality:

$$\partial f(x) = \operatorname{cl}\left\{\operatorname{conv}\left(\bigcup_{z:f_z(x)=f(x)}\partial f_z(x)\right)\right\}$$

Note that $\partial f_z(x) = z$. And if z_1, z_2 each achieve the max at x, which means that $z_1^T x = z_2^T x = ||x||$, then by linearity, so will $tz_1 + (1-t)z_2$ for any $t \in [0,1]$. Thus

$$\partial f(x) = \underset{\|z\|_* \le 1}{\operatorname{argmax}} \ z^T x$$

Optimality condition

For any f (convex or not),

$$f(x^{\star}) = \min_{x} f(x) \iff 0 \in \partial f(x^{\star})$$

That is, x^* is a minimizer if and only if 0 is a subgradient of f at x^* . This is called the subgradient optimality condition

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

$$f(y) \ge f(x^{\star}) + 0^T (y - x^{\star}) = f(x^{\star})$$

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

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

is solved at x, for f convex and differentiable, if and only if

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

Intuitively: says that gradient increases as we move away from x. How to prove it? First recast problem as

$$\min_{x} f(x) + I_C(x)$$

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

Observe

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

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 $\lambda \geq 0$. Subgradient optimality:

$$0 \in \partial \left(\frac{1}{2} \|y - X\beta\|_{2}^{2} + \lambda \|\beta\|_{1}\right)$$

$$\iff 0 \in -X^{T}(y - X\beta) + \lambda \partial \|\beta\|_{1}$$

$$\iff X^{T}(y - X\beta) = \lambda v$$

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

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

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

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

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:

$$[S_{\lambda}(y)]_{i} = \begin{cases} y_{i} - \lambda & \text{if } y_{i} > \lambda \\ 0 & \text{if } -\lambda \leq y_{i} \leq \lambda \\ y_{i} + \lambda & \text{if } y_{i} < -\lambda \end{cases}$$

Check: from last slide, subgradient optimality conditions are

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

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 closed, convex set C:

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

This is a convex function. What are its subgradients?

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

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

Only has one element, so in fact dist(x, C) is differentiable and this is its gradient

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

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

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

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

Hence

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

Claim:

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

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

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

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

as desired

Using the claim, we have for any y

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

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