

Canonical result in gradient descent convergence analysis

- if you have a function that has a Lipschitz continuous gradient
- take a step size $\leq 1/\text{Lipschitz constant}$
- then after k iterations, the criterion value is improved by a factor of k

What if we have non-convex $f(x)$?

What about nonconvex functions?

Assume f is differentiable with Lipschitz gradient as before, but now **nonconvex**. Asking for optimality is too much. So we'll settle for x such that $\|\nabla f(x)\|_2 \leq \epsilon$, called **ϵ -stationarity**.

Theorem: Gradient descent with fixed step size $t \leq 1/L$ satisfies

$$\min_{i=0,\dots,k} \|\nabla f(x^{(i)})\|_2 \leq \sqrt{\frac{2f(x^{(0)}) - f^*}{t(k+1)}}$$

Thus gradient descent has rate $O(1/\sqrt{k})$, or $O(1/\epsilon^2)$, even in the nonconvex case for finding stationary points

This rate **cannot be improved** (over class of differentiable functions with Lipschitz gradients) by any deterministic algorithm¹

¹Carmon et al. (2017), "Lower bounds for finding stationary points I"

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Proof

Key steps:

- ∇f Lipschitz with constant L means

$$f(y) \leq f(x) + \nabla f(x)^T(y - x) + \frac{L}{2}\|y - x\|_2^2 \quad \text{all } x, y$$

- Plugging in $y = x^+ = x - t\nabla f(x)$,

$$f(x^+) \leq f(x) - \left(1 - \frac{Lt}{2}\right)t\|\nabla f(x)\|_2^2$$

- Taking $0 < t \leq 1/L$, and rearranging,

$$\|\nabla f(x)\|_2^2 \leq \frac{2}{t}(f(x) - f(x^+))$$

- Summing over iterations

$$\sum_{i=0}^k \|\nabla f(x^{(i)})\|_2^2 \leq \frac{2}{t}(f(x^{(0)}) - f(x^{(k+1)})) \leq \frac{2}{t}(f(x^{(0)}) - f^*)$$

- Lower bound sum by $(k+1) \min_{i=0,\dots,k} \|\nabla f(x^{(i)})\|_2^2$, conclude

□

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In the non convex case, we can't ask for optimality - so we settle for x st $\|\nabla f(x)\|_2 \leq \epsilon$, called ϵ -stationarity.

Theorem: $\min_{i=0,\dots,k} \|\nabla f(x^{(i)})\|_2 \leq \sqrt{\frac{2(f(x^{(0)}) - f^*)}{t(k+1)}}$

- the minimum L2 norm across all the gradients you observe across k iterates of the gradient descent is upper bounded by the original criterion value weighted by a factor of $1/\sqrt{k+1}$

- So gradient descent has a rate $O(1/\sqrt{k})$

For ϵ - stationarity, you want $\|\nabla f(x)\|_2 \leq \epsilon$

- So the number of steps k it will take to guarantee this result will be

$$\epsilon = \sqrt{\frac{2(f(x^{(0)}) - f^*)}{t(k+1)}} \implies \epsilon^2 = c/k \implies k = c/\epsilon^2$$

- so gradient descent has a rate

For a small ϵ this can be quite large.

Also, this does not guarantee that you end up a local minima! Could be a saddle point or a max - any ϵ - stationary point

- however recent research suggests you are more likely to end up in minima than other stationary points

Anatomy of a convergence rate proof

1. Write down the function and all assumptions being made
2. Start with some quadratic upper or lower bound on $f(y)$ around $f(x)$ (where x is the current iterate)
eg: if gradient is Lipschitz with constant L : upper bound on $f(y)$
strong convexity: lower bound on $f(y)$
3. Establish some 'sufficient descent' property between $f(x^+)$ (the next iterate) and the current iterate

With strong convexity, typically this bound is on the iterates themselves i.e. it takes the form $\|x^+ - x^*\|_2^2 \leq \dots$

Without strong convexity, typically get a bound in terms of the criterion function evaluations,

i.e. something of the form $f(x^+) \leq f(x) - \frac{t}{2} \|\nabla f(x)\|_2^2$

4. Iterate/recurse the property to get a global statement about $f(x^{(k)})$ or $x^{(k)}$

Gradient Boosting

Idea:

- do GD on a loss fn - eg classification or regression - supervised learning task
 - smooth loss function, as in GD
- The trick is you replace gradient with the closest approximation you can make using a tree
 - map gradients to a vector of predictions given by a tree (or any other simple

method) - "weak learner"

- constrained problem: force the gradients to be part of the constraint set.

Example: find the best linear combo of trees to minimize classification error

- but this is too hard to parameterize
 - for example, the space of all $d=5$ trees is enormous
- So ignore that you want trees
- compute the gradient - if you could fit anything to the data, what is the fastest descent you can get on the criterion
- then find a tree that comes close to the gradient in its predictions, and add that to our collection
- repeat until you get some collection of trees
- https://en.wikipedia.org/wiki/Gradient_boosting#:~:text=Gradient%20boosting%20is%20a%20machine

A. Subgradients

A1. Motivation:

Recall that for a convex function $f(y) \geq f(x) + \nabla f(x)^T(y - x)$, that is, the linear approximation always underestimates f

A subgradient of f at point x is g such that the same property holds ie

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

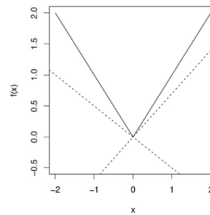
- for a convex function, a subgradient always exists on the relative interior of $\text{dom}(f)$
 - relative interior = if the domain is not full dim, then it is the interior wrt some subspace where the domain lies
 - * these are points far away from where the function is infinite
 - Proof: comes from supporting hyperplane theorem
- if a gradient exists, then it is the only subgradient
- the same definition is true for non convex f , however g may not exist

Example 1: Absolute value

- $f: \mathbb{R} \rightarrow \mathbb{R}, f(x) = |x|$
- this is a convex function
- not differentiable everywhere
 - at $x = 0$ it is not
- for $x \neq 0$, unique subgradient $g = \text{gradient} = \text{sign}(x)$
- for $x = 0$, subgradient is any element of $[-1, 1]$
 - you will underestimate $f(0)$ with a line of any slope between -1 and 1!
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Examples of subgradients

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



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

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Example 2: L2 norm

for $x \neq 0$, unique subgradient $g = x / \|x\|_2$

for $x = 0$, subgradient g is any element of $\{z : \|z\|_2 \leq 1\}$

- unit ball!

Working it out, we need some g st

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

at $x = 0$

$$\|y\|_2 \geq g^T y$$

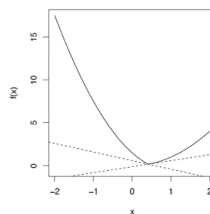
From cauchy-schwartz (?) this is true for any $g : \|g\|_2 \leq 1$

Example 3: L1 norm

- not differentiable on any of the coordinate axes
- when $x_i \neq 0$, $g = \text{gradient} = \text{sign}(x_i)$
- when $x_i = 0$, subgradient is any element of $[-1, 1]$

Example 4: max of convex functions

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

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B. Subdifferentials

- set of all subgradients of convex f is the subdifferential
- $\partial f(x) = \{g \in \mathbb{R}^n : g \text{ is a subgradient of } f \text{ at } x\}$

B1. Properties

- nonempty for convex f
- $\partial f(x)$ is closed and convex, even for non convex f
- to prove that a convex function is smooth
 - characterize the subdifferential
 - if the set has one element then it must be the gradient and the fn is differentiable

B2. Connection to convex geometry

Remember the indicator function $I_C : \mathbb{R}^n \rightarrow \mathbb{R}$

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

For $x \in C$, $\partial I_C(x) = N_C(x)$, the normal cone of C at x

Recall that $N_C(x) = \{g \in \mathbb{R}^n : g^T x \geq g^T y \text{ for any } y \in C\}$

Why?

By definition of subgradient g ,

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

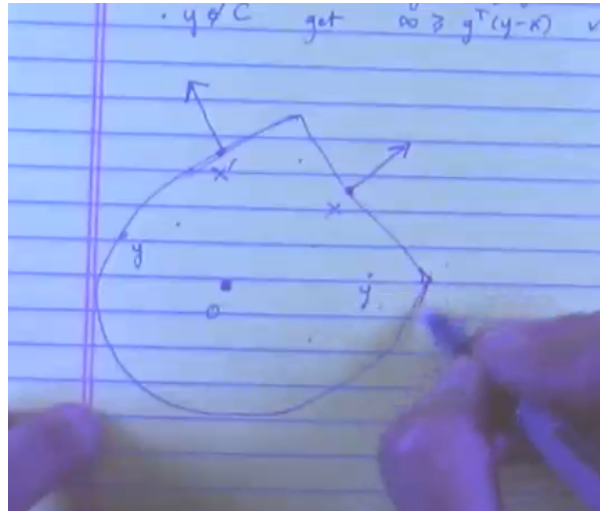
But we know:

$$\text{if } y \notin C, I_C(y) = \infty$$

$$\text{if } y \in C, I_C(y) = 0$$

so then $0 \geq g^T(y - x) \implies g^T x \geq g^T y$, which is the definition of the normal cone for x

Intuition for normal cones:



For a given point x on the boundary, the normal cone will consist of multiples of the vector that is aligned in its direction

In the interior, the normal cone is $\{0\}$ - can always find a point on the boundary more aligned with the vector you have chosen

B3: Subgradient calculus

Basic rules for convex functions

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

$$\partial f(x) = \text{conv} \left(\bigcup_{i: f_i(x) = f(x)} \partial f_i(x) \right)$$

convex hull of union of subdifferentials of active functions at x

- **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

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

And

$$\partial f(x) = \text{argmax}_{\|z\|_q \leq 1} z^T x$$

The dual representation of the L_p norm:

$$\|x\|_p = \left(\sum |x_i|^p \right)^{1/p}$$

for $p \geq 1$, $\exists q$ st $1/q + 1/p = 1$

Fact: $\|x\|_p = \max_{y: \|y\|_q \leq 1} y^T x$

Working through this myself:

For $p = 2 \Rightarrow q = 2$

Then $\|x\|_2 = \sqrt{x^T x} = y^T x \rightarrow \text{solve for } y$

Why subgradients?

1. convex analysis: relationship to duality
2. convex opt: you can minimize any convex function if you can compute a subgradient

B4. Subgradient Optimality Condition

For any f convex or not, $f(x^*) = \min f(x) \implies 0 \in \partial f(x^*)$

i.e. x^* is a minimizer iff 0 is a subgradient of f at x^* .

Why? if $g = 0$ is a subgradient, then for all y

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

B5. Derivation of first-order optimality

Example of the power of subgradients

Recall that

$\min_x f(x)$ subject to $x \in C$ is solved at x , for f convex and differentiable, iff

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

Intuitively, says the gradient increases as we move away from x .

How to prove this?

1. Recast the problem as $\min_x f(x) + I_C(x)$

2. Now apply subg optimality: $0 \in \partial(f(x) + I_C(x))$ at the solutions to this problem

$$0 \in \partial(f(x) + I_C(x))$$

$$\implies 0 \in \{\nabla f(x)\} + N_C(x) \text{ (from subg calculus - additive rule)}$$

$$\implies \text{which means } -\nabla f(x) \in N_C(x)$$

3. *by definition of normal cone, this means*

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

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

Note that the condition $0 \in \partial f(x) + N_C(x)$ is a fully general condition for optimality in convex problems

- you can express any convex problem as being some objective function + indicator function on x being in some convex set C
 - incorporate all the constraints in the construction of the set C

However, this condition is not always easy to work with - KKT conditions helpful here

Example: lasso optimality conditions

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

for some $\lambda \geq 0$.

Subgradient optimality:

$$0 \in \partial \left(\frac{1}{2} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1 \right) \text{ at } x^*$$

The first term is a convex, diff function with gradient $-X^T y + X^T X \beta$

The second term is a convex non diff function, but we know its subgradient form

So

$$\implies 0 \in -X^T(y - X\beta) + \lambda \partial \beta$$

$$\implies X^T(y - X\beta) = \lambda \partial \beta$$

$$\implies X^T(y - X\beta) = \lambda v$$

for some $v \in \partial \beta$

which means

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

Write the columns of X out as X_1, X_2, \dots, X_p . then the condition reads

$$X_i^T(y - X\beta) = \lambda \cdot \text{sign}(\beta_i) \text{ if } \beta_i \neq 0,$$

$$|X_i^T(y - X\beta)| \leq \lambda \text{ if } \beta_i = 0$$

This doesn't tell give you a closed form solution to the lasso problem. But it does give you conditions for lasso optimality!

You can check a priori if a given column will have a corresponding beta value or not by just checking if $|X_i^T(y - X\beta)| \leq \lambda$ or not!

- This can be used to screen variables even before solve - i.e. drop some variables from the model
- Also, we can check solutions using these optimality conditions

One intuitive interpretation of these optimality conditions is:

If X_i is used in the regression, then its correlation with the residual will be maximal (λ or $-\lambda$)

If it is not, then its correlation with the residual will be less

Example 2: soft-thresholding

Example: soft-thresholding

Simplified 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**:

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

Check: from last slide, subgradient optimality conditions are

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

$$\beta_i = S_\lambda(y_i)$$

$$\text{check: } \begin{array}{ll} y_i - \beta_i = \lambda \cdot \text{sign}(\beta_i) & \text{if } \beta_i \neq 0 \\ |y_i - \beta_i| \leq \lambda & \text{if } \beta_i = 0 \end{array}$$

$$\bullet y_i > \lambda \quad \beta_i = y_i - \lambda > 0$$

$$y_i - \beta_i = \lambda = \lambda \cdot \text{sign}(\beta_i) \quad \checkmark$$

$$\bullet y_i < -\lambda \quad \text{similar}$$

$$\bullet y_i \in [-\lambda, \lambda] \quad \beta_i = 0$$

$$|y_i| \leq \lambda \quad \checkmark$$