(Sub)-gradient method

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- Intro
- 2 Subgradient theory
- 3 Convergence subgradient method
- Smooth case

Spoiler: Smooth vs. nonsmooth

We consider the convex optimization problem

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

$$x_{k+1} = x_k - \alpha g_k$$

- ⋄ If f is smooth we take $g_k = \nabla f(x_k) \rightarrow$ Gradient Descent.
- stepsize can be constant 1/L (smoothness constant)
- ⋄ convergence rate $f(x_k) f^* = \mathcal{O}(1/k)$

- \diamond If not we take g_k a subgradient \to Subgradient method.
- \diamond stepsize has to be chosen small or decreasing $\approx 1/\sqrt{k}$
- ⋄ convergence rate is *worse* $f(x_k) f^* = \mathcal{O}(1/\sqrt{k})$

Intuition behind GD

- ⋄ derivative (gradient) points in the direction of steepest ascent
 → GD is also called steepest descent
- GD update is equivalent to

$$x_{k+1} = \arg\min_{\mathbf{x} \in \mathbb{R}^d} \left\{ \underbrace{f(x_k) + \langle \nabla f(x_k), \mathbf{x} - \mathbf{x}_k \rangle}_{\text{linearization of } f} + \frac{1}{2\alpha} \|\mathbf{x} - \mathbf{x}_k\|^2 \right\}$$

- ▶ solves a linear model of f
- minimizing unconstrained linear models is no good
- ▶ so we add a "proximity term"

Subgradients

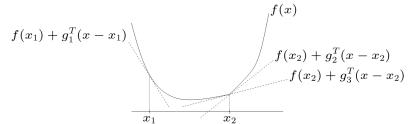
What if f is not differentiable?

Definition

 $g \in \mathbb{R}^d$ is a subgradient of f at x if

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

$$f(\mathbf{y}) \ge f(\mathbf{x}) + \mathbf{g}^{\top}(\mathbf{y} - \mathbf{x})$$
 for all $\mathbf{y} \in \mathbf{dom}(f)$

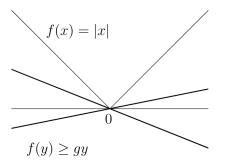


Subgradients II

Definition

The subdifferential $\partial f(x)$ is the set of all subgradients of f at x.

Example



Subgradient condition at x = 0 is $f(y) \ge f(0) + g(y - 0) = gy$.

What is $\partial f(0)$?

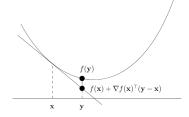


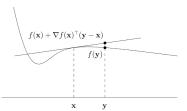
Subgradients III

Lemma

If f is differentiable at x then $\partial f(x) \subset {\nabla f(x)}$

So either one subgradient or none.





Subgradient characterization of convexity

Lemma

A function $f: \mathbb{R}^d \to \mathbb{R}$ is convex if and only if $\partial f(x)$ is not empty for all x.

$$f(\mathbf{y}) \ge f(\mathbf{x}) + \mathbf{g}^{\top}(\mathbf{y} - \mathbf{x})$$
 for all $\mathbf{y} \in \mathbf{dom}(f)$

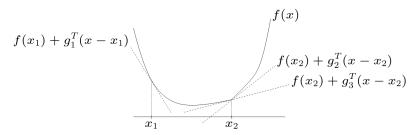


Figure: Subgradients at every point.

Lipschitz = bounded subgradients

Definition

We call f L-Lipschitz (continuous) if

$$||f(x) - f(y)|| \le L||x - y||.$$

Lemma

Let f be convex. Then the following two are equivalent.

(i) All subgradients are uniformly bounded.

$$\|g\| \le L \quad \forall x, \forall g \in \partial f(x)$$

(ii) f is L-Lipschitz

Convergence subgradient method

Subgradient optimality condition

Lemma

Let $0 \in \partial f(\bar{x})$, then \bar{x} is a global minimum.

Proof.

By the definition of subgradients, $g = 0 \in \partial f(\bar{x})$ gives

$$f(y) \ge f(\bar{x}) + g^{T}(y - \bar{x}) = f(\bar{x}).$$

Convergence statement: Subgradient method

We assume there exists minimizer x^* and we write $f^* = f(x^*)$.

Theorem

f is convex, subgradients are bounded $||g(x)|| \le G$ for all $g(x) \in \partial f(x)$. Then,

$$f(\bar{x}_k) - f^* \le \frac{\|x_0 - x^*\|^2 G}{\sqrt{k}}$$

for the **averaged** iterates $\bar{x}_k = \frac{1}{k} \sum_{i=0}^{k-1} x_i$

- ♦ Also holds for the "best" iterate.
- ⋄ Dimension independent! (no d)

Proof

$$||x_{k+1} - x^*||^2 \le ||x_k - \alpha g_k - x^*||^2$$

= $||x_k - x^*||^2 + 2\alpha \langle g_k, x^* - x_k \rangle + \alpha^2 ||g_k||^2$.

Using the subgradient inequality $\langle g_k, x^* - x_k \rangle \leq f(x^*) - f(x_k)$

$$||x_{k+1} - x^*||^2 \le ||x_k - x^*||^2 + 2\alpha(f(x^*) - f(x_k)) + \alpha^2||g_k||^2.$$

Summing up (telescoping) yields

$$2\sum_{i=0}^{k-1}\alpha(f(x_i)-f(x^*))+\|x_k-x^*\|^2\leq \|x_0-x^*\|^2+\alpha^2\sum_{i=0}^{k-1}\|g_k\|^2.$$
 (1)

Via the bounded subgradient assumption

$$2\sum_{i=0}^{k-1}\alpha(f(x_i)-f(x^*))\leq ||x_0-x^*||^2+\alpha^2kG^2.$$

Proof [contd]

We divide by 2α and k

$$\frac{1}{k} \sum_{i=0}^{k-1} f(x_i) - f^* \le \frac{1}{2\alpha k} ||x_0 - x^*||^2 + \frac{\alpha G^2}{2}$$

Using Jensens inequality (convexity with more than 2 points)

$$\sum_{i=0}^{k-1} \frac{1}{k} f(x_i) \ge \sum_i f\left(\frac{1}{k} \sum_{i=0}^{k-1} x_i\right)$$

we obtain

$$f(\bar{x}_k) - f^* \le \frac{1}{2\alpha k} ||x_0 - x^*||^2 + \frac{\alpha G^2}{2}.$$

How to choose the stepsize?

We have

$$f(\bar{x}_k) - f^* \le \frac{1}{2\alpha k} \|x_0 - x^*\|^2 + \frac{\alpha G^2}{2}.$$

Choose α such that *RHS* is minimized, i.e.

$$\alpha = \frac{\|x_0 - x^*\|}{G\sqrt{k}},$$

which gives

$$f(\bar{x}_k) - f^* \leq \frac{\|x_0 - x^*\|G}{\sqrt{k}}. \quad \Box$$

When ignoring constants (and focusing on the rate) we sometimes write

$$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$$
.

Complexity

For convex Lipschitz functions we require $\mathcal{O}(\epsilon^{-2})$ iterations. For

$$D := ||x_0 - x^*||$$

$$f(\bar{x}_k) - f^* \le \frac{DG}{\sqrt{k}}$$

Q: How many iterations to get

$$f(\bar{x}_k) - f^* \leq \epsilon$$
?

A: We get this if

$$\frac{DG}{\sqrt{k}} \le \epsilon$$

Equivalently

$$k \geq \frac{D^2G^2}{\epsilon^2}$$
.

Polyak stepsize

Let's revisit the convergence proof of the subgradient method

$$||x_{k+1} - x^*||^2 \le ||x_k - \alpha_k g_k - x^*||^2$$

$$= ||x_k - x^*||^2 + 2\alpha \langle g_k, x^* - x_k \rangle + \alpha^2 ||g_k||^2$$

$$\le ||x_k - x^*||^2 + 2\alpha (f^* - f(x_k)) + \alpha^2 ||g_k||^2.$$

Can we pick α such that the RHS is minimized?

$$\min_{\alpha} \alpha^2 ||g_k||^2 + 2\alpha (f^* - f(x_k))$$

gives

$$\alpha_k^* = \frac{f(x_k) - f^*}{\|g_k\|^2}$$

$$||x_{k+1} - x^*||^2 = ||x_k - x^*||^2 - \left(\frac{f(x_k) - f^*}{||g_k||}\right)^2$$

- Requires us to know the optimal objective function value
- can be the case in certain setting: separable data, feasibility problems
- modern deep learning interpolation setting



Figure: from openai.com

Can we do better if the function is smooth?

Definition

We call a function *I*-smooth if

$$f(y) \le f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2} ||y - x||^2.$$

Can be upper bounded by a quadratic.

Lemma

If the gradient of f is L-Lipschitz

$$\|\nabla f(x) - \nabla f(y)\| \le L\|x - y\|.$$

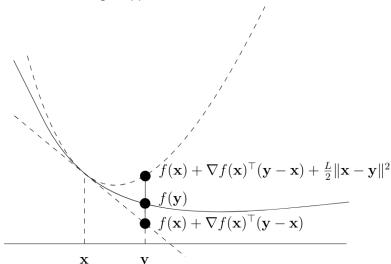
then it is also L-smooth.

Note: Definition does not require convexity.



Smoothness

If *f* is convex we get upper and lower bound:



Smooth vs. Lipschitz

- \diamond Bounded (sub)gradients \Leftrightarrow Lipschitz continuity of f
- \diamond Smoothness \Leftrightarrow Lipschitz continuity of ∇f (if convex)

Lemma

Let f be convex and differentiable, then the following are equivalent

- (i) f is smooth with parameter L
- (ii) ∇f is L-Lipschitz

Sufficient decrease

Lemma

If f is L-smooth with stepsize $\alpha = 1/L$, then gradient descent satisfies

$$f(x_{k+1}) \le f(x_k) - \frac{1}{2I} \|\nabla f(x_k)\|^2$$

Proof.

$$f(x_{k+1}) \leq f(x_k) + \langle \nabla f(x_k), x_{k+1} - x_k \rangle + \frac{L}{2} ||x_{k+1} - x_k||^2$$

$$= f(x_k) - \alpha ||\nabla f(x_k)||^2 + \frac{\alpha^2 L}{2} ||\nabla f(x_k)||^2$$

$$= f(x_k) - \left(\frac{1}{L} - \frac{1}{2L}\right) ||\nabla f(x_k)||^2$$

Smooth convex functions

Theorem

Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex and L-smooth and the stepsize $\alpha = 1/L$, then gradient descent yields

$$f(x_k) - f^* \le \frac{L}{2k} ||x_0 - x^*||^2.$$

- holds for last iterate
- \diamond independet of dimension d

Complexity of gradient method

Denote
$$D^2 := ||x_1 - x^*||^2$$

iteration:
$$k \ge \frac{D^2L}{2\epsilon} \Rightarrow \text{error} \le \frac{LD^2}{2k} \le \epsilon$$

Convergence subgradient method

Given error $\epsilon = 0.01$ results in

- \diamond 50 · D^2L iterations for *smooth* case
- \diamond 10000 \cdot D^2G^2 for nonsmooth but Lipschitz

What if we don't know L?

Proof of $\mathcal{O}(\epsilon^{-1})$ for smooth functions

Subgradient analysis gave us

$$\sum_{i=0}^{k-1} (f(x_i) - f^*) \le \frac{1}{2\alpha} ||x_0 - x^*||^2 + \frac{\alpha}{2} \sum_{i=0}^{k-1} ||g_k||^2,$$

see (1). This time we use sufficient decrease to bound gradient norm

$$\frac{1}{2L}\sum_{i=0}^{k-1}\|\nabla f(x_k)\|^2 \leq \sum_{i=0}^{k-1}(f(x_i)-f(x_{i+1}))=f(x_0)-f(x_k)$$

Combining the above two (with $\alpha = 1/L$)

$$\sum_{i=0}^{k-1} (f(x_i) - f^*) \le \frac{L}{2} \|x_0 - x^*\|^2 + \frac{1}{2L} \sum_{i=0}^{k-1} \|g_k\|^2$$

$$\le \frac{L}{2} \|x_0 - x^*\|^2 + f(x_0) - f(x_k)$$

Proof II

By rewriting:

$$\sum_{i=1}^{k} (f(x_i) - f^*) \le \frac{L}{2} ||x_0 - x^*||^2$$

As last iterate is the best (sufficient decrease):

$$f(x_k) - f^* \le \frac{1}{k} \sum_{i=1}^k f(x_i) - f^* \le \frac{L}{2k} ||x_0 - x^*||^2$$