Optimization for Machine Learning CS-439

Lecture 4: Proximal and Subgradient Descent

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Section 3.6

Proximal Gradient Descent

Composite optimization problems

Consider objective functions composed as

$$f(\mathbf{x}) := g(\mathbf{x}) + h(\mathbf{x})$$

where g is a "nice" function, where as h is a "simple" additional term, which however doesn't satisfy the assumptions of niceness which we used in the convergence analysis so far.

In particular, an important case is when h is not differentiable.

Idea

The classical gradient step for minimizing g:

$$\mathbf{x}_{t+1} = \underset{\mathbf{y}}{\operatorname{argmin}} \ g(\mathbf{x}_t) + \nabla g(\mathbf{x}_t)^{\top} (\mathbf{y} - \mathbf{x}_t) + \frac{1}{2\gamma} ||\mathbf{y} - \mathbf{x}_t||^2 .$$

For the stepsize $\gamma := \frac{1}{L}$ it exactly minimizes the local quadratic model of g at our current iterate \mathbf{x}_t , formed by the smoothness property with parameter L.

Now for f = g + h, keep the same for g, and add h unmodified.

$$\mathbf{x}_{t+1} := \underset{\mathbf{y}}{\operatorname{argmin}} \ g(\mathbf{x}_t) + \nabla g(\mathbf{x}_t)^{\top} (\mathbf{y} - \mathbf{x}_t) + \frac{1}{2\gamma} \|\mathbf{y} - \mathbf{x}_t\|^2 + h(\mathbf{y})$$
$$= \underset{\mathbf{y}}{\operatorname{argmin}} \ \frac{1}{2\gamma} \|\mathbf{y} - (\mathbf{x}_t - \gamma \nabla g(\mathbf{x}_t))\|^2 + h(\mathbf{y}) ,$$

the proximal gradient descent update.

The proximal gradient descent algorithm

An iteration of proximal gradient descent is defined as

$$\mathbf{x}_{t+1} := \operatorname{prox}_{h,\gamma}(\mathbf{x}_t - \gamma \nabla g(\mathbf{x}_t))$$
.

where the proximal mapping for a given function h, and parameter $\gamma > 0$ is defined as

$$\operatorname{prox}_{h,\gamma}(\mathbf{z}) := \underset{\mathbf{y}}{\operatorname{argmin}} \left\{ \frac{1}{2\gamma} \|\mathbf{y} - \mathbf{z}\|^2 + h(\mathbf{y}) \right\}.$$

The update step can be equivalently written as

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma G_{\gamma}(\mathbf{x}_t)$$

for $G_{h,\gamma}(\mathbf{x}) := \frac{1}{\gamma} \Big(\mathbf{x} - \mathrm{prox}_{h,\gamma}(\mathbf{x} - \gamma \nabla g(\mathbf{x})) \Big)$ being the so called generalized gradient of f.

A generalization of gradient descent?

- ▶ $h \equiv 0$: recover gradient descent
- ▶ $h \equiv \iota_X$: recover projected gradient descent!

Given a closed convex set X, the indicator function of the set X is given as the convex function

$$oldsymbol{\iota}_X: \mathbb{R}^d o \mathbb{R} \cup +\infty$$

$$\mathbf{x} \mapsto oldsymbol{\iota}_X(\mathbf{x}) := egin{cases} 0 & ext{if } \mathbf{x} \in X, \\ +\infty & ext{otherwise}. \end{cases}$$

Proximal mapping becomes

$$\operatorname{prox}_{h,\gamma}(\mathbf{z}) := \underset{\mathbf{y}}{\operatorname{argmin}} \left\{ \frac{1}{2\gamma} \|\mathbf{y} - \mathbf{z}\|^2 + \iota_X(\mathbf{y}) \right\} = \underset{\mathbf{y} \in X}{\operatorname{argmin}} \|\mathbf{y} - \mathbf{z}\|^2$$

Convergence in $\mathcal{O}(1/\varepsilon)$ steps

Same as vanilla case for smooth functions, but now for any h for which we can compute the proximal mapping.

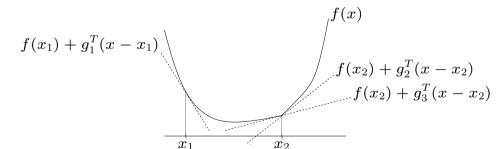
Subgradients

What if f is not differentiable?

Definition

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

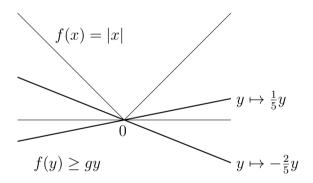
$$f(\mathbf{y}) \ge f(\mathbf{x}) + \mathbf{g}^{\top}(\mathbf{y} - \mathbf{x})$$
 for all $\mathbf{y} \in \mathbf{dom}(f)$



 $\partial f(\mathbf{x}) \subseteq \mathbb{R}^d$ is the subdifferential, the set of subgradients of f at \mathbf{x} .

Subgradients II

Example:



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

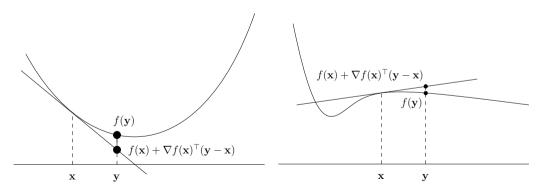
$$\partial f(0) = [-1, 1]$$

Subgradients III

Lemma (Exercise 26)

If $f : \mathbf{dom}(f) \to \mathbb{R}$ is differentiable at $\mathbf{x} \in \mathbf{dom}(f)$, then $\partial f(\mathbf{x}) \subseteq {\nabla f(\mathbf{x})}$.

Either exactly one subgradient $\nabla f(\mathbf{x})$... or no subgradient at all.

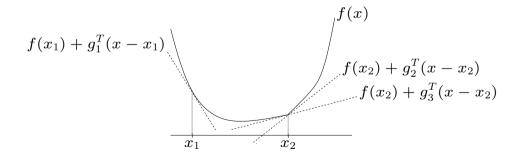


Subgradient characterization of convexity

"convex = subgradients everywhere"

Lemma (Exercise 27)

A function $f : \mathbf{dom}(f) \to \mathbb{R}$ is convex if and only if $\mathbf{dom}(f)$ is convex and $\partial f(\mathbf{x}) \neq \emptyset$ for all $\mathbf{x} \in \mathbf{dom}(f)$.



Convex and Lipschitz = bounded subgradients

Lemma (Exercise 28)

Let $f : \mathbf{dom}(f) \to \mathbb{R}$ be convex, $\mathbf{dom}(f)$ open, $B \in \mathbb{R}_+$. Then the following two statements are equivalent.

- (i) $\|\mathbf{g}\| \leq B$ for all $\mathbf{x} \in \mathbf{dom}(f)$ and all $\mathbf{g} \in \partial f(\mathbf{x})$.
- (ii) $|f(\mathbf{x}) f(\mathbf{y})| \le B ||\mathbf{x} \mathbf{y}||$ for all $\mathbf{x}, \mathbf{y} \in \mathbf{dom}(f)$.

Subgradient optimality condition

Lemma

Suppose that $f : \mathbf{dom}(f) \to \mathbb{R}$ and $\mathbf{x} \in \mathbf{dom}(f)$. If $\mathbf{0} \in \partial f(\mathbf{x})$, then \mathbf{x} is a global minimum.

Proof.

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

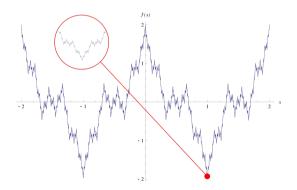
$$f(\mathbf{y}) \ge f(\mathbf{x}) + \mathbf{g}^{\top}(\mathbf{y} - \mathbf{x}) = f(\mathbf{x})$$

for all $y \in \mathbf{dom}(f)$, so x is a global minimum.

Differentiability of convex functions

How "wild" can a non-differentiable convex function be?

Weierstrass function: a function that is continuous everywhere but differentiable nowhere



https://commons.wikimedia.org/wiki/File:WeierstrassFunction.svg

Differentiability of convex functions

Theorem ([Roc97, Theorem 25.5])

A convex function $f : \mathbf{dom}(f) \to \mathbb{R}$ is differentiable almost everywhere.

In other words:

- \triangleright Set of points where f is non-differentiable has measure 0 (no volume).
- ▶ For all $\mathbf{x} \in \mathbf{dom}(f)$ and all $\varepsilon > 0$, there is a point \mathbf{x}' such that $\|\mathbf{x} \mathbf{x}'\| < \varepsilon$ and f is differentiable at \mathbf{x}' .

The subgradient descent algorithm

Subgradient descent: choose $\mathbf{x}_0 \in \mathbb{R}^d$.

Let
$$\mathbf{g}_t \in \partial f(\mathbf{x}_t)$$

 $\mathbf{x}_{t+1} := \mathbf{x}_t - \gamma_t \mathbf{g}_t$

for times $t = 0, 1, \ldots$, and stepsizes $\gamma_t \ge 0$.

Stepsize can vary with time!

This is possible in (projected) gradient descent as well, but so far, we didn't need it.

Lipschitz convex functions: $\mathcal{O}(1/\varepsilon^2)$ **steps**

Theorem

Let $f: \mathbb{R}^d \to \mathbb{R}$ be convex and B-Lipschitz continuous with a global minimum \mathbf{x}^{\star} ; furthermore, suppose that $\|\mathbf{x}_0 - \mathbf{x}^{\star}\| \leq R$. Choosing the constant stepsize

$$\gamma := \frac{R}{B\sqrt{T}},$$

subgradient descent yields

$$\frac{1}{T} \sum_{t=0}^{T-1} f(\mathbf{x}_t) - f(\mathbf{x}^*) \le \frac{RB}{\sqrt{T}}.$$

Proof is identical to the one of Theorem 2.1, except...

- ▶ In vanilla analyis, now use $\mathbf{g}_t \in \partial f(\mathbf{x}_t)$ instead of $\mathbf{g}_t = \nabla f(\mathbf{x}_t)$.
- ▶ Inequality $f(\mathbf{x}_t) f(\mathbf{x}^*) \leq \mathbf{g}_t^\top (\mathbf{x}_t \mathbf{x}^*)$ now follows from subgradient property instead of first-order characterization of convexity.

Optimality of first-order methods

With all the convergence rates we have seen so far, a very natural question to ask is if these rates are best possible or not. Surprisingly, the rate can indeed not be improved in general.

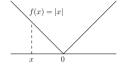
Theorem (Nesterov)

For any $T \leq d-1$ and starting point \mathbf{x}_0 , there is a function f in the problem class of B-Lipschitz functions over \mathbb{R}^d , such that any (sub)gradient method has an objective error at least

$$f(\mathbf{x}_T) - f(\mathbf{x}^*) \ge \frac{RB}{2(1+\sqrt{T+1})}$$
.

Smooth (non-differentiable) functions?

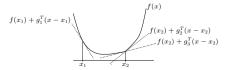
They don't exist (Exercise 29)!



At 0, graph can't be below a tangent paraboloid.

Can we still improve over $O(1/\varepsilon^2)$ steps for Lipschitz functions?

Yes, if we also require strong convexity (graph is above not too flat tangent paraboloids).



Strongly convex functions

"Not too flat"

Straightforward generalization to the non-differentiable case:

Definition

Let $f : \mathbf{dom}(f) \to \mathbb{R}$ be convex, $\mu \in \mathbb{R}_+, \mu > 0$. Function f is called strongly convex (with parameter μ) if

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \mathbf{g}^{\top}(\mathbf{y} - \mathbf{x}) + \frac{\mu}{2} \|\mathbf{x} - \mathbf{y}\|^2, \quad \forall \mathbf{x}, \mathbf{y} \in \mathbf{dom}(f), \ \forall \mathbf{g} \in \partial f(\mathbf{x}).$$

Strongly convex functions: characterization via "normal" convexity

Lemma (Exercise 31)

Let $f: \mathbf{dom}(f) \to \mathbb{R}$ be convex, $\mathbf{dom}(f)$ open, $\mu \in \mathbb{R}_+, \mu > 0$. f is strongly convex with parameter μ if and only if $f_{\mu}: \mathbf{dom}(f) \to \mathbb{R}$ defined by

$$f_{\mu}(\mathbf{x}) = f(\mathbf{x}) - \frac{\mu}{2} \|\mathbf{x}\|^2, \quad \mathbf{x} \in \mathbf{dom}(f)$$

is convex.

Tame strong convexity

For fast convergence, we consider additional assumptions.

Smoothness? - Not an option in the non-differentiable case (Exercise 29).

Instead: assume that all subgradients \mathbf{g}_t that we encounter during the algorithm are bounded in norm.

May be realistic if...

- we start close to optimality
- ightharpoonup we run projected subgradient descent over a compact set X

May also fail!

ightharpoonup Over \mathbb{R}^d , strong convexity and bounded subgradients contradict each other! (Exercise 33).

Tame strong convexity: $\mathcal{O}(1/\varepsilon)$ steps

Theorem

Let $f: \mathbb{R}^d \to \mathbb{R}$ be strongly convex with parameter $\mu > 0$ and let \mathbf{x}^* be the unique global minimum of f. With decreasing step size

$$\gamma_t := \frac{2}{\mu(t+1)}, \quad t > 0,$$

subgradient descent yields

$$f\left(\frac{2}{T(T+1)}\sum_{t=1}^{T}t\cdot\mathbf{x}_{t}\right)-f(\mathbf{x}^{\star})\leq\frac{2B^{2}}{\mu(T+1)},$$

where
$$B = \max_{t=1}^{T} \|\mathbf{g}_t\|$$
. \uparrow convex combination of iterates

Tame strong convexity: $\mathcal{O}(1/\varepsilon)$ steps II

Proof.

Vanilla analysis $(\mathbf{g}_t \in \partial f(\mathbf{x}_t))$:

$$\mathbf{g}_t^{\top}(\mathbf{x}_t - \mathbf{x}^{\star}) = \frac{\gamma_t}{2} \|\mathbf{g}_t\|^2 + \frac{1}{2\gamma_t} \left(\|\mathbf{x}_t - \mathbf{x}^{\star}\|^2 - \|\mathbf{x}_{t+1} - \mathbf{x}^{\star}\|^2 \right).$$

Lower bound from strong convexity:

$$\mathbf{g}_t^{\top}(\mathbf{x}_t - \mathbf{x}^{\star}) \ge f(\mathbf{x}_t) - f(\mathbf{x}^{\star}) + \frac{\mu}{2} \|\mathbf{x}_t - \mathbf{x}^{\star}\|^2.$$

Putting it together (with $\|\mathbf{g}_t\|^2 \leq B^2$):

$$f(\mathbf{x}_t) - f(\mathbf{x}^*) \le \frac{B^2 \gamma_t}{2} + \frac{(\gamma_t^{-1} - \mu)}{2} \|\mathbf{x}_t - \mathbf{x}^*\|^2 - \frac{\gamma_t^{-1}}{2} \|\mathbf{x}_{t+1} - \mathbf{x}^*\|^2.$$

Summing over $t=1,\ldots,T$: we used to have telescoping $(\gamma_t=\gamma,\mu=0)\ldots$

Tame strong convexity: $\mathcal{O}(1/\varepsilon)$ steps III

Proof.

So far we have:

$$f(\mathbf{x}_t) - f(\mathbf{x}^*) \le \frac{B^2 \gamma_t}{2} + \frac{(\gamma_t^{-1} - \mu)}{2} \|\mathbf{x}_t - \mathbf{x}^*\|^2 - \frac{\gamma_t^{-1}}{2} \|\mathbf{x}_{t+1} - \mathbf{x}^*\|^2.$$

To get telescoping, we would need $\gamma_t^{-1} = \gamma_{t+1}^{-1} - \mu$.

Works with $\gamma_t^{-1} = \mu(1+t)$, but not $\gamma_t^{-1} = \mu(1+t)/2$ (the choice here).

Exercise 34: what happens with $\gamma_t^{-1} = \mu(1+t)$?

Now: what happens with $\gamma_t^{-1} = \mu(1+t)/2$ (the choice here)?

Tame strong convexity: $\mathcal{O}(1/\varepsilon)$ steps IV

Proof.

So far we have:

$$f(\mathbf{x}_t) - f(\mathbf{x}^*) \le \frac{B^2 \gamma_t}{2} + \frac{(\gamma_t^{-1} - \mu)}{2} \|\mathbf{x}_t - \mathbf{x}^*\|^2 - \frac{\gamma_t^{-1}}{2} \|\mathbf{x}_{t+1} - \mathbf{x}^*\|^2.$$

Plug in $\gamma_t^{-1} = \mu(1+t)/2$ and multiply with t on both sides:

$$t \cdot (f(\mathbf{x}_{t}) - f(\mathbf{x}^{*})) \leq \frac{B^{2}t}{\mu(t+1)} + \frac{\mu}{4} (t(t-1) \|\mathbf{x}_{t} - \mathbf{x}^{*}\|^{2} - (t+1)t \|\mathbf{x}_{t+1} - \mathbf{x}^{*}\|^{2})$$
$$\leq \frac{B^{2}}{\mu} + \frac{\mu}{4} (t(t-1) \|\mathbf{x}_{t} - \mathbf{x}^{*}\|^{2} - (t+1)t \|\mathbf{x}_{t+1} - \mathbf{x}^{*}\|^{2}).$$

Tame strong convexity: $\mathcal{O}(1/\varepsilon)$ steps **V**

Proof.

We have

$$t \cdot (f(\mathbf{x}_{t}) - f(\mathbf{x}^{*})) \leq \frac{B^{2}t}{\mu(t+1)} + \frac{\mu}{4} (t(t-1) \|\mathbf{x}_{t} - \mathbf{x}^{*}\|^{2} - (t+1)t \|\mathbf{x}_{t+1} - \mathbf{x}^{*}\|^{2})$$
$$\leq \frac{B^{2}}{\mu} + \frac{\mu}{4} (t(t-1) \|\mathbf{x}_{t} - \mathbf{x}^{*}\|^{2} - (t+1)t \|\mathbf{x}_{t+1} - \mathbf{x}^{*}\|^{2}).$$

Now we get telescoping...

$$\sum_{t=1}^{T} t \cdot \left(f(\mathbf{x}_{t}) - f(\mathbf{x}^{\star}) \right) \leq \frac{TB^{2}}{\mu} + \frac{\mu}{4} \left(0 - T(T+1) \|\mathbf{x}_{T+1} - \mathbf{x}^{\star}\|^{2} \right) \leq \frac{TB^{2}}{\mu}.$$

Tame strong convexity: $\mathcal{O}(1/\varepsilon)$ steps VI

Proof.

Almost done:

$$\sum_{t=1}^{T} t \cdot \left(f(\mathbf{x}_{t}) - f(\mathbf{x}^{*}) \right) \leq \frac{TB^{2}}{\mu} + \frac{\mu}{4} \left(0 - T(T+1) \|\mathbf{x}_{T+1} - \mathbf{x}^{*}\|^{2} \right) \leq \frac{TB^{2}}{\mu}.$$

Since

$$\frac{2}{T(T+1)} \sum_{t=1}^{T} t = 1,$$

Jensen's inequality yields

$$f\left(\frac{2}{T(T+1)}\sum_{t=1}^{T}t\cdot\mathbf{x}_{t}\right)-f(\mathbf{x}^{\star})\leq\frac{2}{T(T+1)}\sum_{t=1}^{T}t\cdot\left(f(\mathbf{x}_{t})-f(\mathbf{x}^{\star})\right).$$



Tame strong convexity: Discussion

$$f\left(\frac{2}{T(T+1)}\sum_{t=1}^{T}t\cdot\mathbf{x}_{t}\right)-f(\mathbf{x}^{\star})\leq\frac{2B^{2}}{\mu(T+1)},$$

Weighted average of iterates achieves the bound (later iterates have more weight)

Bound is independent of initial distance $\|\mathbf{x}_0 - \mathbf{x}^{\star}\|$...

... but not really: B typically depends on $\|\mathbf{x}_0 - \mathbf{x}^*\|$ (for example, $B = \mathcal{O}(\|\mathbf{x}_0 - \mathbf{x}^*\|)$ for quadratic functions)

Recall: we can only hope that B is small (can be checked while running the algorithm)

What if we don't know the parameter μ of strong convexity?

ightarrow Bad luck! In practice, try some μ 's, pick best solution obtained

Bibliography



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