annotated version

# Optimization for Machine Learning CS-439

## Lecture 5: Subgradient and Stochastic Gradient Descent


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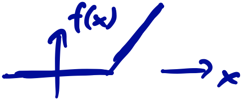
# Chapter 4

## Subgradient Descent

# Subgradients



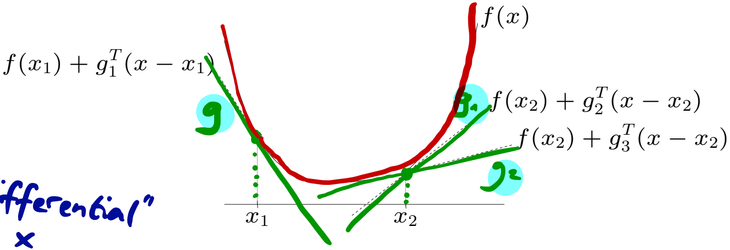

· Hinge loss
· ReLU

What if $f$ is not differentiable?

## Definition

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

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




„Subdifferential" at x

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

# What are subgradients good for?

**Convexity**

Lemma (Exercise 23)

*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 $\mathbf{x} \in \mathbf{dom}(f)$.*

**Lipschitz Continuity**

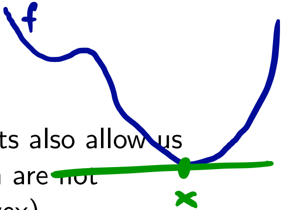
Lemma (Exercise 24)

*Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex, $B \in \mathbb{R}_+$. Then the following two statements are equivalent.*

(i) $\|\mathbf{g}\| \leq B$ *for all* $\mathbf{x} \in \mathbb{R}^d$ *and all* $\mathbf{g} \in \partial f(\mathbf{x})$.

(ii) $|f(\mathbf{x}) - f(\mathbf{y})| \leq B\|\mathbf{x} - \mathbf{y}\|$ *for all* $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$.

# What are subgradients good for?




**Subgradient Optimality Condition.** Subgradients also allow us to describe cases of optimality for functions which are not necessarily differentiable (and not necessarily convex)

## Lemma

*Suppose that $f$ is any function over $\mathbf{dom}(f)$, and $\mathbf{x} \in \mathbf{dom}(f)$. If $\mathbf{0} \in \partial f(\mathbf{x})$, then $\mathbf{x}$ is a global minimum.*

Proof. $g = 0$ subgrad $\iff$

$$f(y) \geq \underbrace{f(x) + \underbrace{g^T(y-x)}_{=0}}_{=f(x)} \quad \forall y$$

$\square$

# The subgradient descent algorithm

An iteration of subgradient descent is defined as

$$
\text{Let } \mathbf{g}_t \in \partial f(\mathbf{x}_t)
$$
$$
\mathbf{x}_{t+1} := \mathbf{x}_t - \gamma \mathbf{g}_t.
$$

# Bounded subgradients: $\mathcal{O}(1/\varepsilon^2)$ steps

The following result gives the convergence for Subgradient Descent. It is identical to Theorem 2.1, up to relaxing the requirement of differentiability.

### Theorem

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

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

Same

*subgradient descent yields*

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

Same

# Bounded subgradients: $\mathcal{O}(1/\varepsilon^2)$ steps

Proof.

Identical to vanilla analysis.

At the start:
use subgradient property

□

# 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*

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

## Chapter 5

# Stochastic Gradient Descent

SGD

# Sum structured objective functions

Consider sum structured objective functions:

$$f(\mathbf{x}) := \frac{1}{n} \sum_{i=1}^{n} f_i(\mathbf{x}).$$

Here $f_i$ is typically the cost function of the $i$-th datapoint, taken from a training set of $n$ elements in total.

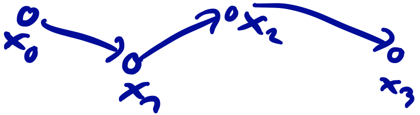
# The SGD algorithm

$f = \frac{1}{n} \sum f_i$

An iteration of stochastic gradient descent (SGD) is defined as

$$\begin{aligned}&\text{sample } i \in [n] \text{ uniformly at random}\\ &\mathbf{x}_{t+1} := \mathbf{x}_t - \gamma_t \boxed{\nabla f_i(\mathbf{x}_t)}.\end{aligned}$$

The vector $\boxed{\mathbf{g}_t} := \nabla f_i(\mathbf{x}_t)$ is called a stochastic gradient.



# Unbiasedness of a stochastic gradient

**Why uniform sampling?**
In expectation over the random choice of $i$, $\mathbf{g}_t$ does coincide with the full gradient of $f$:

$$\mathbb{E}[\mathbf{g}_t | \mathbf{x}_t] = \nabla f(\mathbf{x}_t).$$

- $\mathbf{g}_t$ is an unbiased stochastic gradient.

**Why SGD?**
$n$ times **cheaper**! (gradient computation)

# Stochastic vanilla analysis

stochastic gradient

Idea: follow the vanilla analysis with $\nabla f(\mathbf{x}_t)$ replaced by $\mathbf{g}_t$..

NO!!!

$$f(\mathbf{x}_t) - f(\mathbf{x}^\star) \cancel{\leq} \mathbf{g}_t^\top(\mathbf{x}_t - \mathbf{x}^\star).$$

$f(.) - f(.) \leq \nabla f^\top (x - x^*)$ (full gradient)

but

$$\begin{aligned}
\mathbf{g}_t^\top(\mathbf{x}_t - \mathbf{x}^\star) &= \frac{1}{\gamma}(\mathbf{x}_t - \mathbf{x}_{t+1})^\top(\mathbf{x}_t - \mathbf{x}^\star). \\
&= \frac{1}{2\gamma}\left(\|\mathbf{x}_t - \mathbf{x}_{t+1}\|^2 + \|\mathbf{x}_t - \mathbf{x}^\star\|^2 - \|\mathbf{x}_{t+1} - \mathbf{x}^\star\|^2\right) \\
&= \frac{1}{2\gamma}\left(\gamma^2\|\mathbf{g}_t\|^2 + \|\mathbf{x}_t - \mathbf{x}^\star\|^2 - \|\mathbf{x}_{t+1} - \mathbf{x}^\star\|^2\right),
\end{aligned}$$

$2a^\top b = \|a\|^2 + \|b\|^2 - \|a-b\|^2$

using the definition SGD again. Finally, the telescoping sum:

$$\sum_{t=0}^{T-1} \left(\mathbf{g}_t^\top(\mathbf{x}_t - \mathbf{x}^\star)\right) \leq \frac{\gamma}{2}\sum_{t=0}^{T-1}\|\mathbf{g}_t\|^2 + \frac{1}{2\gamma}\|\mathbf{x}_0 - \mathbf{x}^\star\|^2.$$

(*)

will use later

# Bounded stochastic gradients: $\mathcal{O}(1/\varepsilon^2)$ steps

**Classic GD:** For vanilla analysis, we assumed that $\|\nabla f(\mathbf{x})\|^2 \leq B_{\mathsf{GD}}^2$ for all $\mathbf{x} \in \mathbb{R}^d$, where $B_{\mathsf{GD}}$ was a constant. So for sum-objective:

$$\Big\|\frac{1}{n}\sum_i \nabla f_i(\mathbf{x})\Big\|^2 \leq B_{\mathsf{GD}}^2 \qquad \forall \mathbf{x}$$

Jensen $\geq$

**SGD:** Assuming same for the expected squared norms of our stochastic gradients, now called $B_{\mathsf{SGD}}^2$.

can be equal!

$$\frac{1}{n}\sum_i \|\nabla f_i(\mathbf{x})\|^2 \leq B_{\mathsf{SGD}}^2 \qquad \forall \mathbf{x}$$

$\mathbb{E}[\qquad]$

- get same convergence result, now for expected objective $f$...

but <u>much</u> cheaper iterations

# Bounded stochastic gradients: $\mathcal{O}(1/\varepsilon^2)$ steps

Theorem

*Let* $f : \mathbb{R}^d \to \mathbb{R}$ *be convex and differentiable,* $\mathbf{x}^\star$ *a global minimum; furthermore, suppose that* $\|\mathbf{x}_0 - \mathbf{x}^\star\| \leq R$*, and that* $\mathbb{E}\big[\|\mathbf{g}_t\|^2\big] \leq B^2$ *for all* $t$*. Choosing the constant stepsize*

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

*stochastic gradient descent yields*

$$\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}\big[f(\mathbf{x}_t)\big] - f(\mathbf{x}^\star) \leq \frac{RB}{\sqrt{T}}.$$

# Bounded stochastic gradients: $\mathcal{O}(1/\varepsilon^2)$ steps

**Proof.** Using convexity and unbiasedness of $\mathbf{g}_t$, we compute

$$
\begin{aligned}
\mathbb{E}\big[f(\mathbf{x}_t)\big] - f(\mathbf{x}^\star) &= \mathbb{E}\big[f(\mathbf{x}_t) - f(\mathbf{x}^\star)\big] \\
&\leq \mathbb{E}\big[\nabla f(\mathbf{x}_t)^\top(\mathbf{x}_t - \mathbf{x}^\star)\big] \qquad \text{convexity of } f \\
&= \mathbb{E}\big[\mathbb{E}\big[\mathbf{g}_t|\mathbf{x}_t\big]^\top(\mathbf{x}_t - \mathbf{x}^\star)\big] \\
&= \mathbb{E}\big[\mathbb{E}\big[\mathbf{g}_t^\top(\mathbf{x}_t - \mathbf{x}^\star)\underbrace{|\mathbf{x}_t}\big]\big] \qquad \text{linear. } \mathbb{E} \\
&= \mathbb{E}\big[\mathbf{g}_t^\top(\mathbf{x}_t - \mathbf{x}^\star)\big],
\end{aligned}
$$

where the second-to-last step uses linearity of (conditional) expectations, while the last step is known as the tower rule; see Exercise 25.

$$\mathbb{E}\big(\mathbb{E}[x|y]\big) = \mathbb{E}[x]$$

# Bounded stochastic gradients: $\mathcal{O}(1/\varepsilon^2)$ steps

Now we can again use linearity of expectation and then (*). We get

slide 14

$$
\begin{aligned}
\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}\big[f(\mathbf{x}_t)\big]-f(\mathbf{x}^\star) &\leq \frac{1}{T}\mathbb{E}\Big[\sum_{t=0}^{T-1}\mathbf{g}_t^\top(\mathbf{x}_t-\mathbf{x}^\star)\Big] \\
&= \frac{1}{T}\mathbb{E}\Big[\frac{\gamma}{2}\sum_{t=0}^{T-1}\|\mathbf{g}_t\|^2+\frac{1}{2\gamma}\|\mathbf{x}_0-\mathbf{x}^\star\|^2\Big] \\
&= \frac{1}{T}\left(\frac{\gamma}{2}\sum_{t=0}^{T-1}\mathbb{E}\big[\|\mathbf{g}_t\|^2\big]+\frac{1}{2\gamma}\|\mathbf{x}_0-\mathbf{x}^\star\|^2\right) \\
&\leq \frac{RB}{\sqrt{T}},
\end{aligned}
$$

after plugging in our value of $\gamma$ and the assumption on $\mathbb{E}\big[\|\mathbf{g}_t\|^2\big] \leq B$ and $\|\mathbf{x}_0-\mathbf{x}^\star\|$.

Bounded stochastic gradients $\square$