Optimization for Machine Learning
CS-439

Lecture 2: Gradient Descent

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EPFL – github.com/epfml/OptML_course

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Chapter 2

Gradient Descent

The Algorithm

Get near to a minimum $\mathbf{x}^\star$ / close to the optimal value $f(\mathbf{x}^\star)$?

(Assumptions: $f : \mathbb{R}^d \to \mathbb{R}$ convex, differentiable, has a global minimum $\mathbf{x}^\star$)

Goal: Find $\mathbf{x} \in \mathbb{R}^d$ such that

$$f(\mathbf{x}) - f(\mathbf{x}^\star) \leq \varepsilon.$$

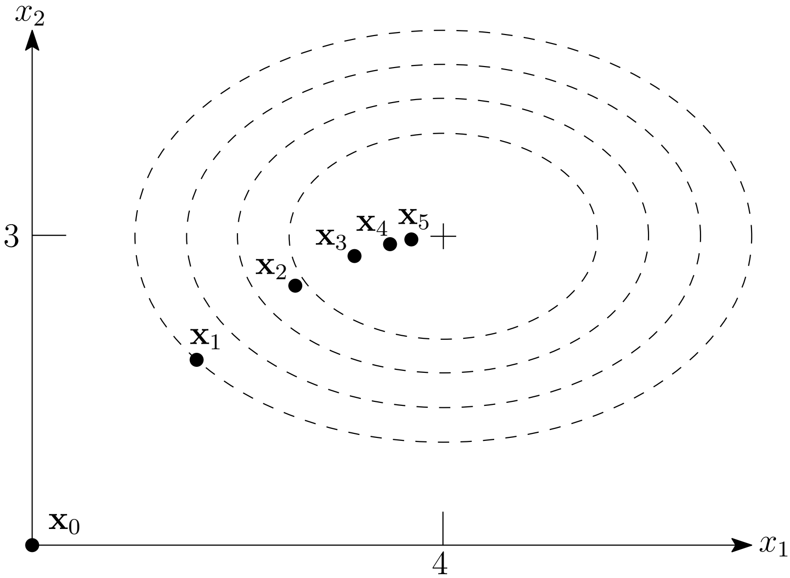
Note that there can be several minima $\mathbf{x}_1^\star \neq \mathbf{x}_2^\star$ with $f(\mathbf{x}_1^\star) = f(\mathbf{x}_2^\star)$.

Iterative Algorithm:

$$\mathbf{x}_{t+1} := \mathbf{x}_t - \gamma \nabla f(\mathbf{x}_t),$$

for **timesteps** $t = 0, 1, \ldots,$ and **stepsize** $\gamma \geq 0$.

Example



x_2
3
$\mathbf{x}_5$
$\mathbf{x}_4$
$\mathbf{x}_3$
$\mathbf{x}_2$
$\mathbf{x}_1$
$\mathbf{x}_0$
4
x_1

Vanilla analysis

How to bound $f(\mathbf{x}_t) - f(\mathbf{x}^\star)$?

- Abbreviate $\mathbf{g}_t := \nabla f(\mathbf{x}_t)$, and consider (using the definition of gradient descent)

$$\mathbf{g}_t^\top(\mathbf{x}_t - \mathbf{x}^\star) = \frac{1}{\gamma}(\mathbf{x}_t - \mathbf{x}_{t+1})^\top(\mathbf{x}_t - \mathbf{x}^\star).$$

- Apply $2\mathbf{v}^\top\mathbf{w} = \|\mathbf{v}\|^2 + \|\mathbf{w}\|^2 - \|\mathbf{v}-\mathbf{w}\|^2$ to rewrite

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

- Sum this up over the iterations t:

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

Vanilla analysis, II

- Now we invoke convexity of f with $\mathbf{x} = \mathbf{x}_t, \mathbf{y} = \mathbf{x}^\star$:

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

  giving

$$\sum_{t=0}^{T-1} \big(f(\mathbf{x}_t) - f(\mathbf{x}^\star)\big) \leq \frac{\gamma}{2} \sum_{t=0}^{T-1} \|\mathbf{g}_t\|^2 + \frac{1}{2\gamma} \|\mathbf{x}_0 - \mathbf{x}^\star\|^2,$$

  an upper bound for the average error $f(\mathbf{x}_t) - f(\mathbf{x}^\star)$ over the steps

- last iterate is not necessarily the best one
- stepsize is crucial

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

Assume that all gradients of f are bounded in norm.

- Equivalent to f being Lipschitz (**Exercise 11**).

Theorem

Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex and differentiable with a global minimum $\mathbf{x}^\star$; furthermore, suppose that $\|\mathbf{x}_0 - \mathbf{x}^\star\| \le R$ and $\|\nabla f(\mathbf{x})\| \le B$ for all $\mathbf{x}$. Choosing the stepsize

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

gradient descent yields

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

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

Proof.

$\square$

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

$$T \geq \frac{R^2 B^2}{\varepsilon^2} \quad \Rightarrow \quad \text{average error } \leq \frac{RB}{\sqrt{T}} \leq \varepsilon.$$

Advantages:

- dimension-independent!
- holds for both average, or best iterate

In Practice:

What if we don't know R and B?

$\rightarrow$ **Exercise 13**

Smooth functions

"Not too curved"

Definition

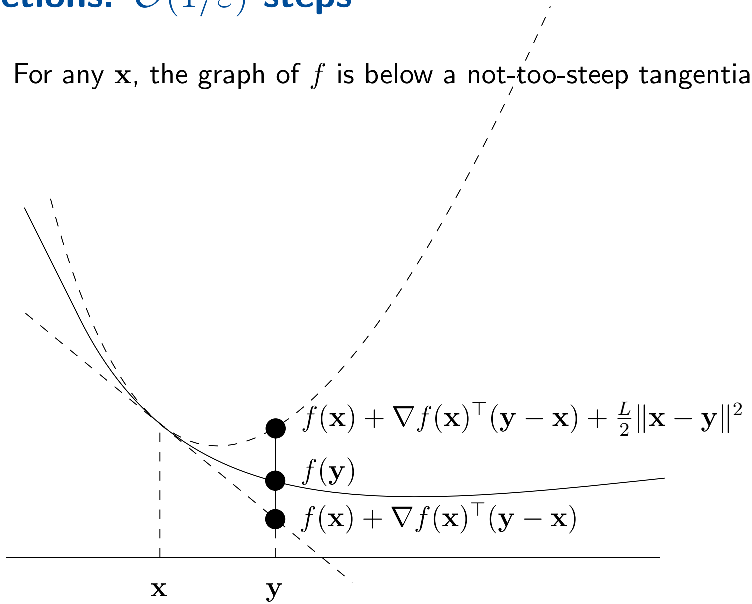
Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex and differentiable. f is called smooth (with parameter $L \geq 0$) if

$$f(\mathbf{y}) \leq f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x}) + \frac{L}{2}\|\mathbf{x} - \mathbf{y}\|^2, \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^d.$$

Definition does not require convexity (useful later)

Smooth functions: $\mathcal{O}(1/\varepsilon)$ steps

Smoothness: For any $\mathbf{x}$, the graph of f is below a not-too-steep tangential paraboloid at $(\mathbf{x}, f(\mathbf{x}))$:



Smooth functions: $\mathcal{O}(1/\varepsilon)$ steps

- Quadratic functions are smooth (**Exercise 11**)
- Operations that preserve smoothness:

Lemma (Exercise 14)

(i) *Let $f_1, f_2, \ldots, f_m$ be convex functions that are smooth with parameters $L_1, L_2, \ldots, L_m$, and let $\lambda_1, \lambda_2, \ldots, \lambda_m \in \mathbb{R}_+$. Then the convex function $f := \sum_{i=1}^m \lambda_i f_i$ is smooth with parameter $\sum_{i=1}^m \lambda_i L_i$.*

(ii) *Let f be convex and smooth with parameter L, and let $g(\mathbf{x}) = A\mathbf{x} + \mathbf{b}$, for $A \in \mathbb{R}^{d \times m}$ and $\mathbf{b} \in \mathbb{R}^d$. Then the convex function $f \circ g$ is smooth with parameter $L\|A\|^2$, where*

$$\|A\| = \max_{\mathbf{x} \neq 0} \frac{\|A\mathbf{x}\|}{\|\mathbf{x}\|}$$

*is the 2-**norm** (or spectral norm) of A.*

Smooth vs Lipschitz

- Bounded gradients $\Leftrightarrow$ Lipschitz continuity of f,
- Now: smoothness $\Leftrightarrow$ Lipschitz continuity of ∇f.

Lemma

Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex and differentiable. The following two statements are equivalent.

(i) *f is smooth with parameter L.*

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

Smooth functions: $\mathcal{O}(1/\varepsilon)$ steps

Theorem

Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex and differentiable with a global minimum $\mathbf{x}^\star$; furthermore, suppose that f is smooth with parameter L.Choosing

$$\gamma := \frac{1}{L},$$

gradient descent with arbitrary $\mathbf{x}_0$ satisfies

(i) *Function values are monotone decreasing:*

$$f(\mathbf{x}_{t+1}) \leq f(\mathbf{x}_t) - \frac{1}{2L}\|\nabla f(\mathbf{x}_t)\|^2, \quad t \geq 0.$$

(ii) *Use the fact that* $2\mathbf{v}^\top \mathbf{w} = \|\mathbf{v}\|^2 + \|\mathbf{w}\|^2 - \|\mathbf{v} - \mathbf{w}\|^2$ *to obtain*

$$f(\mathbf{x}_T) - f(\mathbf{x}^\star) \leq \frac{L}{2T}\|\mathbf{x}_0 - \mathbf{x}^\star\|^2.$$

Smooth functions: $\mathcal{O}(1/\varepsilon)$ steps. Proof

Proof. $\square$

Smooth functions: $\mathcal{O}(1/\varepsilon)$ steps

In Practice:

What if we don't know the smoothness parameter L?

$\rightarrow$ **Exercise 15**