

# Optimization for Machine Learning

## CS-439

Lecture 2: Gradient Descent

**Martin Jaggi**

EPFL – [github.com/epfml/OptML\\_course](https://github.com/epfml/OptML_course)

March 5, 2021

# Chapter 2

## Gradient Descent

# The Algorithm

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

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

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

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

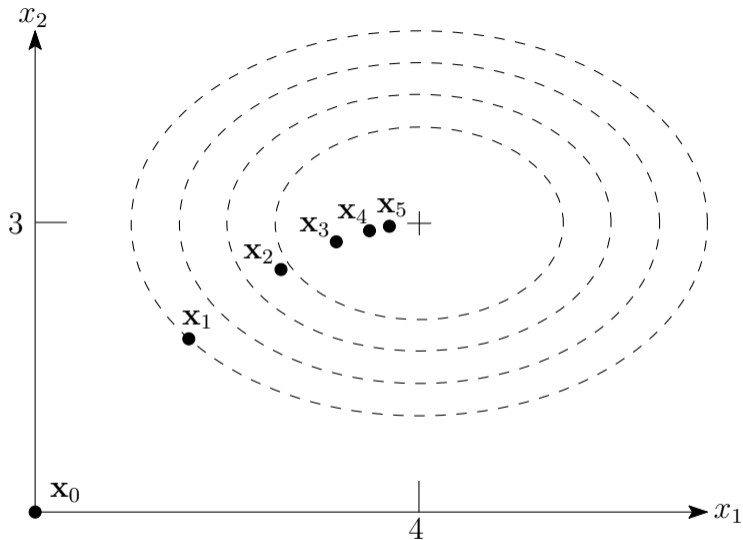
Note that there can be several global minima  $\mathbf{x}_1^* \neq \mathbf{x}_2^*$  with  $f(\mathbf{x}_1^*) = f(\mathbf{x}_2^*)$ .

**Iterative Algorithm:** choose  $\mathbf{x}_0 \in \mathbb{R}^d$ .

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

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

## Example



$$f(x_1, x_2) := 2(x_1 - 4)^2 + 3(x_2 - 3)^2, \mathbf{x}_0 := (0, 0), \gamma := 0.1$$

## Vanilla analysis

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

- ▶ Abbreviate  $\mathbf{g}_t := \nabla f(\mathbf{x}_t)$  (gradient descent:  $\mathbf{g}_t = (\mathbf{x}_t - \mathbf{x}_{t+1})/\gamma$ ).

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

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

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

- ▶ Sum this up over the first  $T$  iterations:

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

## Vanilla analysis II

Use first-order characterization of convexity:  $f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x}), \forall \mathbf{x}, \mathbf{y}$

- ▶ with  $\mathbf{x} = \mathbf{x}_t, \mathbf{y} = \mathbf{x}^*$ :

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

giving

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

an upper bound for the **average error**  $f(\mathbf{x}_t) - f(\mathbf{x}^*)$  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 (Theorem 1.9; **Exercise 12**).
- ▶ Rules out many interesting functions (for example, the “supermodel”  $f(x) = x^2$ )

### Theorem

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

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

*gradient descent yields*

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

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

Proof.

- ▶ Plug  $\|\mathbf{x}_0 - \mathbf{x}^*\| \leq R$  and  $\|\mathbf{g}_t\| \leq B$  into Vanilla Analysis II:

$$\sum_{t=0}^{T-1} (f(\mathbf{x}_t) - f(\mathbf{x}^*)) \leq \frac{\gamma}{2} \sum_{t=0}^{T-1} \|\mathbf{g}_t\|^2 + \frac{1}{2\gamma} \|\mathbf{x}_0 - \mathbf{x}^*\|^2 \leq \frac{\gamma}{2} B^2 T + \frac{1}{2\gamma} R^2.$$

- ▶ choose  $\gamma$  such that

$$q(\gamma) = \frac{\gamma}{2} B^2 T + \frac{R^2}{2\gamma}$$

is minimized.

- ▶ Solving  $q'(\gamma) = 0$  yields the minimum  $\gamma = \frac{R}{B\sqrt{T}}$ , and  $q(R/(B\sqrt{T})) = RB\sqrt{T}$ .
- ▶ Dividing by  $T$ , the result follows.





## 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 (no  $d$  in the bound)!
- ▶ holds for both average, or best iterate

### In Practice:

What if we don't know  $R$  and  $B$ ?  $\rightarrow$  **Exercise 15** (having to know  $R$  can't be avoided)

# Smooth functions

## “Not too curved”

### Definition

Let  $f : \mathbf{dom}(f) \rightarrow \mathbb{R}$  be differentiable,  $X \subseteq \mathbf{dom}(f)$ ,  $L \in \mathbb{R}_+$ .  $f$  is called **smooth** (with parameter  $L$ ) over  $X$  if

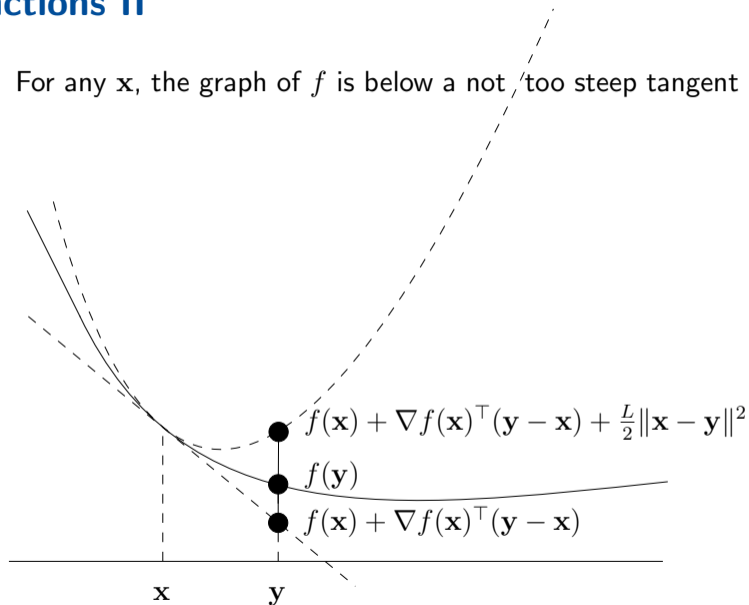
$$f(\mathbf{y}) \leq f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x}) + \frac{L}{2} \|\mathbf{x} - \mathbf{y}\|^2, \quad \forall \mathbf{x}, \mathbf{y} \in X.$$

$f$  smooth  $:\Leftrightarrow f$  smooth over  $\mathbb{R}^d$ .

Definition does not require convexity (useful later)

## Smooth functions II

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



## Smooth functions III

- ▶ In general: quadratic functions are smooth (**Exercise 13**).
- ▶ Operations that preserve smoothness (the same that preserve convexity):

### Lemma (Exercise 16)

- (i) *Let  $f_1, f_2, \dots, f_m$  be functions that are smooth with parameters  $L_1, L_2, \dots, L_m$ , and let  $\lambda_1, \lambda_2, \dots, \lambda_m \in \mathbb{R}_+$ . Then the 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 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 function  $f \circ g$  is smooth with parameter  $L\|A\|^2$ , where  $\|A\|$  is the **spectral norm** of  $A$  (Definition 1.2).*

# Smooth vs Lipschitz

- ▶ Bounded gradients  $\Leftrightarrow$  Lipschitz continuity of  $f$
- ▶ Smoothness  $\Leftrightarrow$  Lipschitz continuity of  $\nabla f$  (in the convex case).

## Lemma

Let  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  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  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ .

Proof in lecture slides of L. Vandenbergh, <http://www.seas.ucla.edu/~vandenbe/236C/lectures/gradient.pdf>.

# Sufficient decrease

## Lemma

Let  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  be differentiable and smooth with parameter  $L$ . With stepsize

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

gradient descent satisfies

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

## Remark

More specifically, this already holds if  $f$  is smooth with parameter  $L$  over the line segment connecting  $\mathbf{x}_t$  and  $\mathbf{x}_{t+1}$ .

## Sufficient decrease II

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

Proof.

Use smoothness and definition of gradient descent ( $\mathbf{x}_{t+1} - \mathbf{x}_t = -\nabla f(\mathbf{x}_t)/L$ ):

$$\begin{aligned} f(\mathbf{x}_{t+1}) &\leq f(\mathbf{x}_t) + \nabla f(\mathbf{x}_t)^\top (\mathbf{x}_{t+1} - \mathbf{x}_t) + \frac{L}{2} \|\mathbf{x}_t - \mathbf{x}_{t+1}\|^2 \\ &= f(\mathbf{x}_t) - \frac{1}{L} \|\nabla f(\mathbf{x}_t)\|^2 + \frac{1}{2L} \|\nabla f(\mathbf{x}_t)\|^2 \\ &= f(\mathbf{x}_t) - \frac{1}{2L} \|\nabla f(\mathbf{x}_t)\|^2. \end{aligned}$$

□

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

### Theorem

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

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

*gradient descent yields*

$$f(\mathbf{x}_T) - f(\mathbf{x}^*) \leq \frac{L}{2T} \|\mathbf{x}_0 - \mathbf{x}^*\|^2, \quad T > 0.$$



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

$$f(\mathbf{x}_T) - f(\mathbf{x}^*) \leq \frac{L}{2T} \|\mathbf{x}_0 - \mathbf{x}^*\|^2, \quad T > 0.$$

Proof.

Vanilla Analysis II:

$$\sum_{t=0}^{T-1} (f(\mathbf{x}_t) - f(\mathbf{x}^*)) \leq \frac{\gamma}{2} \sum_{t=0}^{T-1} \|\nabla f(\mathbf{x}_t)\|^2 + \frac{1}{2\gamma} \|\mathbf{x}_0 - \mathbf{x}^*\|^2.$$

This time, we can bound the squared gradients by sufficient decrease:

$$\frac{1}{2L} \sum_{t=0}^{T-1} \|\nabla f(\mathbf{x}_t)\|^2 \leq \sum_{t=0}^{T-1} (f(\mathbf{x}_t) - f(\mathbf{x}_{t+1})) = f(\mathbf{x}_0) - f(\mathbf{x}_T).$$



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

Putting it together with  $\gamma = 1/L$ :

$$\begin{aligned}\sum_{t=0}^{T-1} (f(\mathbf{x}_t) - f(\mathbf{x}^*)) &\leq \frac{1}{2L} \sum_{t=0}^{T-1} \|\nabla f(\mathbf{x}_t)\|^2 + \frac{L}{2} \|\mathbf{x}_0 - \mathbf{x}^*\|^2 \\ &\leq f(\mathbf{x}_0) - f(\mathbf{x}_T) + \frac{L}{2} \|\mathbf{x}_0 - \mathbf{x}^*\|^2.\end{aligned}$$

Rewriting:

$$\sum_{t=1}^T (f(\mathbf{x}_t) - f(\mathbf{x}^*)) \leq \frac{L}{2} \|\mathbf{x}_0 - \mathbf{x}^*\|^2.$$

As last iterate is the best (sufficient decrease!):

$$f(\mathbf{x}_T) - f(\mathbf{x}^*) \leq \frac{1}{T} \left( \sum_{t=1}^T (f(\mathbf{x}_t) - f(\mathbf{x}^*)) \right) \leq \frac{L}{2T} \|\mathbf{x}_0 - \mathbf{x}^*\|^2.$$

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

$$R^2 := \|\mathbf{x}_0 - \mathbf{x}^*\|^2.$$

$$T \geq \frac{R^2 L}{2\varepsilon} \quad \Rightarrow \quad \text{error} \leq \frac{L}{2T} R^2 \leq \varepsilon.$$

- ▶  $50 \cdot R^2 L$  iterations for error 0.01 ...
- ▶ ... as opposed to  $10,000 \cdot R^2 B^2$  in the Lipschitz case

In Practice:

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

→ **Exercise 17**