Optimization for Machine Learning
CS-439

Lecture 2: Gradient Descent

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EPFL – github.com/epfml/OptML_course

March 2, 2018

Recap

Convexity

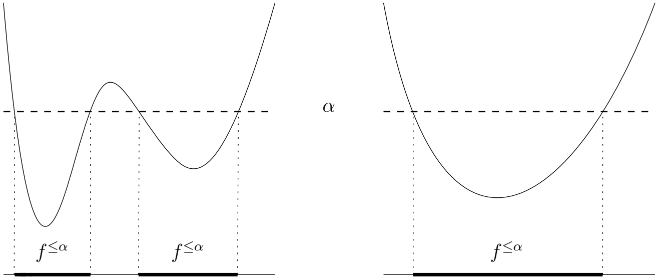
recap,
and short addition before we get to gradient descent...

Existence of a minimizer

Sublevel sets: Let $f : \mathbf{dom}(f) \to \mathbb{R}$, $\alpha \in \mathbb{R}$. The set

$$f^{\leq \alpha} := \{\mathbf{x} \in \mathbf{dom}(f) : f(\mathbf{x}) \leq \alpha\}$$

is the α-sublevel set of f;



Weierstrass Theorem

Theorem

Let $f : \mathbf{dom}(f) \to \mathbb{R}$ *be a convex function,* $\mathbf{dom}(f)$ *open, and suppose there is a nonempty and bounded sublevel set* $f^{\leq \alpha}$*. Then* f *has a global minimum.*

Proof.

$\square$

Chapter 2

Gradient Descent

The Algorithm

How to get near to a minimum $\mathbf{x}^\star$?

(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

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

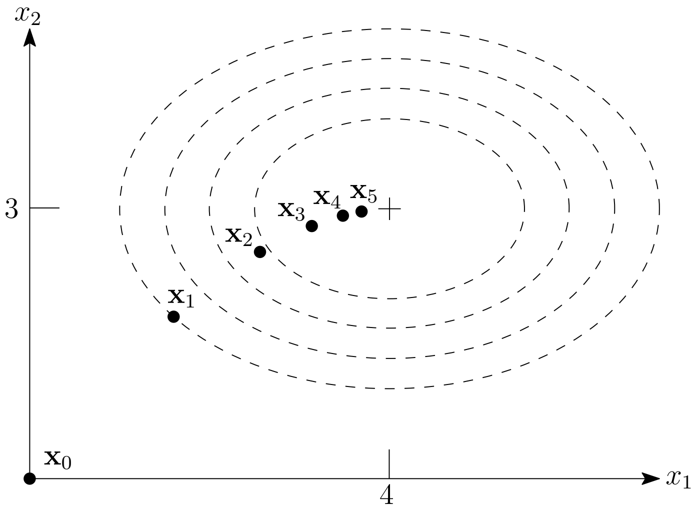
Note that there can be several minima $\mathbf{x}_1^\star \neq \mathbf{x}_2^\star$ with $f(\mathbf{x}_1^\star) = f(\mathbf{x}_2^\star)$.

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

- Convexity of f, for $\mathbf{x} = \mathbf{x}_t, \mathbf{y} = \mathbf{x}^\star$, gives

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

- Apply the definition of the iteration, $\nabla f(\mathbf{x}_t) = (\mathbf{x}_t - \mathbf{x}_{t+1})/\gamma$:

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

- Now we apply $2\mathbf{v}^\top \mathbf{w} = \|\mathbf{v}\|^2 + \|\mathbf{w}\|^2 - \|\mathbf{v} - \mathbf{w}\|^2$

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

again by the definition of gradient descent

Vanilla analysis, cont.

sum this over steps $t = 0, \ldots, T-1$:

$$
\begin{aligned}
&\sum_{t=0}^{T-1} \big(f(\mathbf{x}_t) - f(\mathbf{x}^\star)\big) \\
&\quad \leq \; \frac{\gamma}{2} \sum_{t=0}^{T-1} \|\nabla f(\mathbf{x}_t)\|^2 + \frac{1}{2\gamma} \left(\|\mathbf{x}_0 - \mathbf{x}^\star\|^2 - \|\mathbf{x}_T - \mathbf{x}^\star\|^2\right) \\
&\quad \leq \; \frac{\gamma}{2} \sum_{t=0}^{T-1} \|\nabla f(\mathbf{x}_t)\|^2 + \frac{1}{2\gamma} \|\mathbf{x}_0 - \mathbf{x}^\star\|^2
\end{aligned}
$$

an upper bound for the average error $f(\mathbf{x}_t) - f(\mathbf{x}^\star)$, $t = 0 \ldots T-1$

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

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

Assume that all gradients of f are bounded in norm.

Theorem

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

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

gradient descent yields

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

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

Proof.

$\square$

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

Advantages:

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

In Practice:

What if we don't know R and L?

$\rightarrow$ Exercise 13

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

Convex, but not too convex?

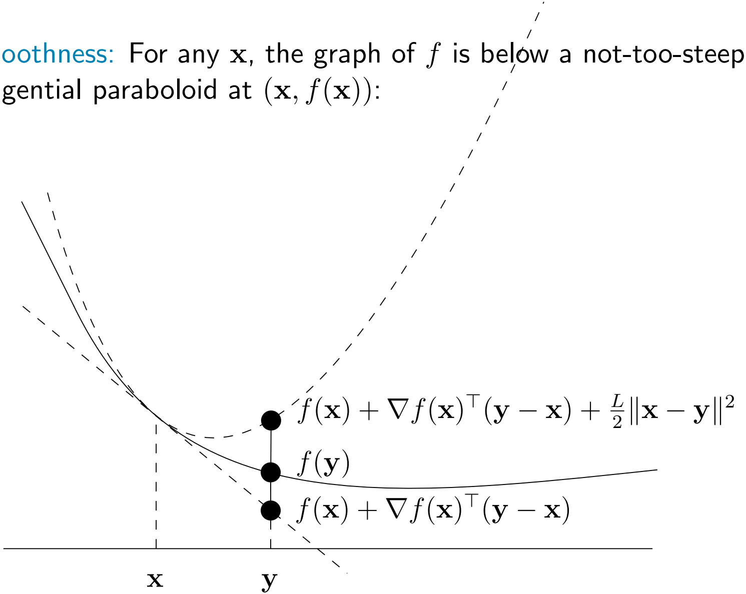
Definition

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

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

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
- Operations that preserve smoothness:

Lemma (Exercise 15)

(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*

$$\|A\| = \max_{\|\mathbf{x}\|=1} \frac{\|A\mathbf{x}\|}{\|\mathbf{x}\|}$$

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

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)

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

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

Proof.

$\square$

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

- Do we need to know L?
  No. Exercise 16.

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

- 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 $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$.*

Can we go even faster?

So far: Error decreases with $1/\sqrt{T}$, or $1/T$...

Could it decrease exponentially in T?

Can we go even faster?

- On $f(x) := x^2$: Stepsize $\gamma := \frac{1}{2}$ (f is $L = 2$ - smooth)

$$x_{t+1} = x_t - \frac{1}{2}\nabla f(x_t) = x_t - x_t = 0,$$

  - converged in one step!

- Same $f(x) := x^2$: Stepsize $\gamma := \frac{1}{4}$ (f is $L = 4$ - smooth)

$$x_{t+1} = x_t - \frac{1}{4}\nabla f(x_t) = x_t - \frac{x_t}{2} = \frac{x_t}{2},$$

  so $f(x_t) = f\left(\frac{x_0}{2^t}\right) = \frac{1}{2^{2t}}x_0^2$.

  - Exponential in t !

Strong convexity

So far: Error decreases with $1/\sqrt{T}$, or $1/T$...

Could it decrease exponentially in T?

Strong convexity: $\mathcal{O}(\log(1/\varepsilon))$ steps

Not too curved and not too flat

Definition

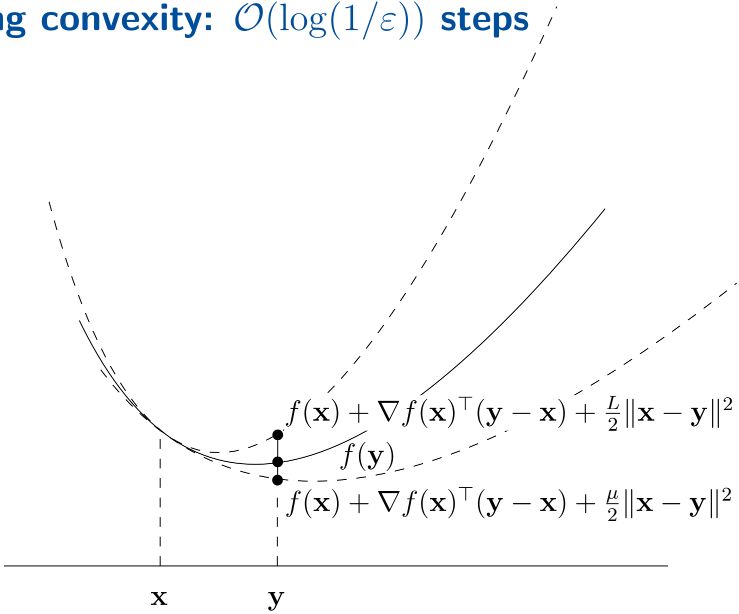
Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex and differentiable, $\mu \in \mathbb{R}_+, \mu > 0$. f is called strongly convex (with parameter μ) if

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

Lemma (Exercise 18)

If f is strongly convex with parameter $\mu > 0$, then f is strictly convex and has a unique global minimum.

Strong convexity: $\mathcal{O}(\log(1/\varepsilon))$ steps



A smooth and strongly convex function

Strong convexity: $\mathcal{O}(\log(1/\varepsilon))$ steps

Can we show $\lim_{t\to\infty} \mathbf{x}_t = \mathbf{x}^\star$?

From the vanilla analysis, we know

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

Using that f is strongly convex, we obtain

$$\leq \frac{1}{2\gamma}\left(\gamma^2\|\nabla f(\mathbf{x}_t)\|^2 + \|\mathbf{x}_t - \mathbf{x}^\star\|^2 - \|\mathbf{x}_{t+1} - \mathbf{x}^\star\|^2\right) - \frac{\mu}{2}\|\mathbf{x}_t - \mathbf{x}^\star\|^2.$$

Can bound on $\|\mathbf{x}_{t+1} - \mathbf{x}^\star\|^2$ in terms of $\|\mathbf{x}_t - \mathbf{x}^\star\|^2$, along with some "noise":

$$\|\mathbf{x}_{t+1}-\mathbf{x}^\star\|^2 \leq 2\gamma(f(\mathbf{x}^\star)-f(\mathbf{x}_t))+\gamma^2\|\nabla f(\mathbf{x}_t)\|^2+(1-\mu\gamma)\|\mathbf{x}_t-\mathbf{x}^\star\|^2 \tag{S}$$

Strong convexity: $\mathcal{O}(\log(1/\varepsilon))$ steps

Theorem

Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex, differentiable, and smooth with parameter L, and strongly convex with parameter $\mu > 0$. Choosing

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

gradient descent with arbitrary $\mathbf{x}_0$ satisfies the following two properties.

(i) *Squared distances to $\mathbf{x}^\star$ are geometrically decreasing:*

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

(ii)

$$f(\mathbf{x}_t) - f(\mathbf{x}^\star) \leq \frac{L}{2} \left(1 - \frac{\mu}{L}\right)^t \|\mathbf{x}_0 - \mathbf{x}^\star\|^2.$$

Strong convexity: $\mathcal{O}(\log(1/\varepsilon))$ steps

Proof.

For (i), we show that the noise in (S) disappears. From the above "smooth" Theorem (i), we know that

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

and hence the noise can be bounded as follows:

$$\begin{aligned}
& 2\gamma(f(\mathbf{x}^\star) - f(\mathbf{x}_t)) + \gamma^2\|\nabla f(\mathbf{x}_t)\|^2 \\
= \; & \frac{2}{L}(f(\mathbf{x}^\star) - f(\mathbf{x}_t)) + \frac{1}{L^2}\|\nabla f(\mathbf{x}_t)\|^2 \\
\le \; & -\frac{1}{L^2}\|\nabla f(\mathbf{x}_t)\|^2 + \frac{1}{L^2}\|\nabla f(\mathbf{x}_t)\|^2 = 0.
\end{aligned}$$

So, (S) actually yields

$$\|\mathbf{x}_{t+1} - \mathbf{x}^\star\|^2 \le (1-\mu\gamma)\|\mathbf{x}_t - \mathbf{x}^\star\|^2 = \left(1 - \frac{\mu}{L}\right)\|\mathbf{x}_t - \mathbf{x}^\star\|^2.$$

Strong convexity: $\mathcal{O}(\log(1/\varepsilon))$ steps

Proof.

The bound in (ii) follows from smoothness, using $\nabla f(\mathbf{x}^\star) = \mathbf{0}$:

$$f(\mathbf{x}_t) - f(\mathbf{x}^\star) \leq \nabla f(\mathbf{x}^\star)^\top (\mathbf{x}_t - \mathbf{x}^\star) + \frac{L}{2}\|\mathbf{x}^\star - \mathbf{x}_t\|^2 = \frac{L}{2}\|\mathbf{x}^\star - \mathbf{x}_t\|^2.$$

$\square$

Conclusion: To reach absolute error at most ε, we only need $\mathcal{O}(\log \frac{1}{\varepsilon})$ iterations, where the constant behind the big-$\mathcal{O}$ is roughly L/μ.