annotated version

Optimization for Machine Learning
CS-439

Lecture 2: Gradient Descent

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EPFL – `github.com/epfml/OptML_course`

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Recap

Convexity

recap,

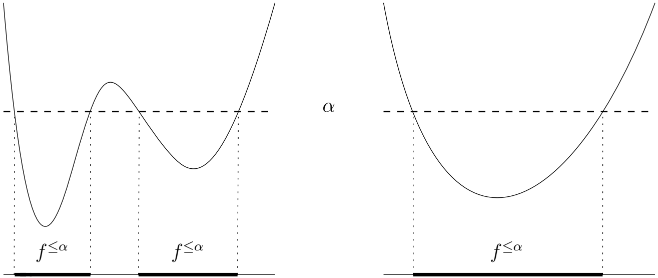
and short addition before we get to gradient descent...

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.

□

github.com/epfml/...

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

$\varepsilon > 0$ accuracy

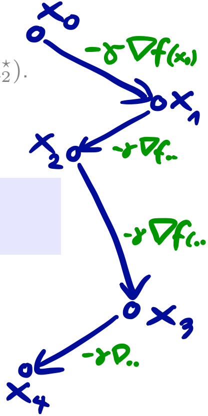
$$f(\mathbf{x}) - f(\mathbf{x}^\star) \leq \varepsilon.$$

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:

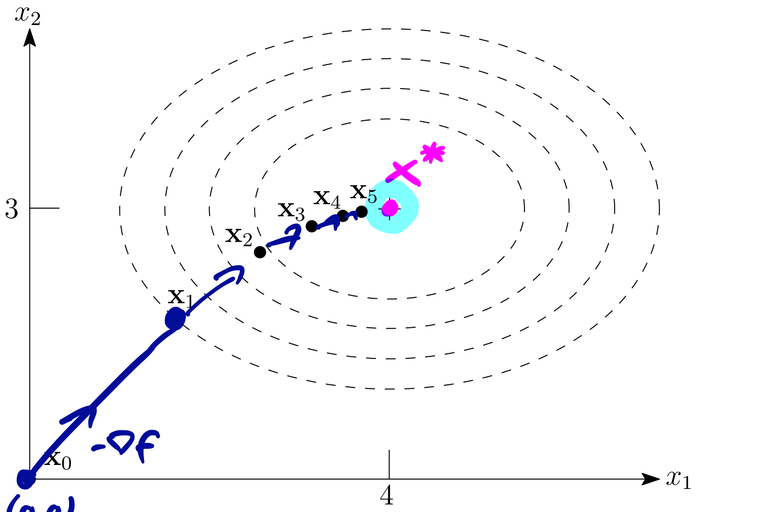
$$\mathbf{x}_{t+1} := \mathbf{x}_t - \gamma \nabla f(\mathbf{x}_t),$$

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



Example

$d=2$

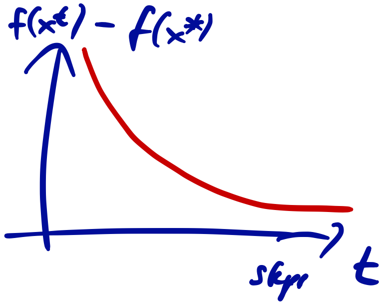


$x_0 = (0,0)$

$f(x) = \text{quadratic}$
$= 2(x^1-4)^2 + 3(x^2-3)^2$

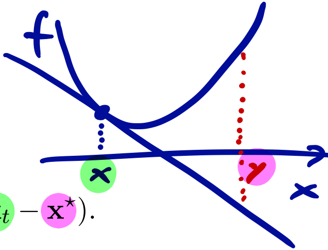
Vanilla analysis

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



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

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

$$f(y) \geq f(x) + \nabla f(x)(y - x)$$

$$x_{t+1} := x_t - \gamma \nabla f(x_t)$$

$$-(x_{t+1} - x_t) = \gamma \nabla f(x_t) \qquad \text{GD}$$

Vanilla analysis

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

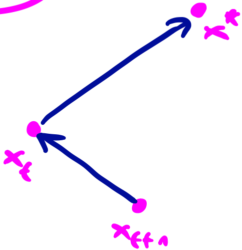
- Convexity of f, for $\mathbf{x} = \mathbf{x}_t, \mathbf{y} = \mathbf{x}^\star$, gives

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

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

$\Leftrightarrow$

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



Vanilla analysis

$f(x^*) \geq f(x_t) + \nabla f(x_t)(x - x^*) + \mu \| \cdot \|^2$

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

$$f(\mathbf{x}_t) - f(\mathbf{x}^\star) \leq \nabla f(\mathbf{x}_t)^\top (\mathbf{x}_t - \mathbf{x}^\star). - \mu \|x_t - x^*\|^2$$

- 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 $2\mathbf{v}^\top \mathbf{w} = \|\mathbf{v}\|^2 + \|\mathbf{w}\|^2 - \boxed{\|\mathbf{v} - \mathbf{w}\|^2}$

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

again by the definition gradient descent

Vanilla analysis, cont.

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

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

≥ 0

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 $\|\mathbf{x}_0 - \mathbf{x}^\star\| \le R$ and $\boxed{\|\nabla f(\mathbf{x})\| \le L}$ for all $\mathbf{x}$. Choosing the stepsize

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

$\Updownarrow$ *gradient descent yields*

?

$$\frac{1}{T}\sum_{t=0}^{T-1}\left(f(\mathbf{x}_t) - f(\mathbf{x}^\star)\right) \le \frac{RL}{\sqrt{T}}. \in \mathcal{O}\left(\frac{1}{\sqrt{T}}\right)$$

f being Lipschitz continuous with constant L

$f(y) - f(x) \le L \cdot \|x - y\|$

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

Proof. use (*) !

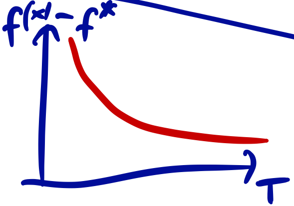
$$\sum_{t=0}^{T-1} f(x_t) - f^* \le \underbrace{\overbrace{\frac{\gamma}{2} T L^2}^{\sum \|\nabla_{..}\|} + \frac{1}{2\gamma} \overbrace{R^2}^{\|x_0 - x^*\|^2}}_{= T \frac{LR}{\sqrt{T}}}$$

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

$$= T \frac{LR}{\sqrt{T}}$$

□

divide by T



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

Advantages:

- dimension-independent! $d \gg 0$
- holds for both average, or best iterate

In Practice:

What if we don't know R and L?

$\rightarrow$ Exercise 13

$\Leftrightarrow$ „ $1/\varepsilon^2$ steps"

$$f(x_t) - f^* \leq \mathcal{O}\left(\frac{1}{\sqrt{T}}\right) \leq \varepsilon$$

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

Convex, but not too convex?

Definition

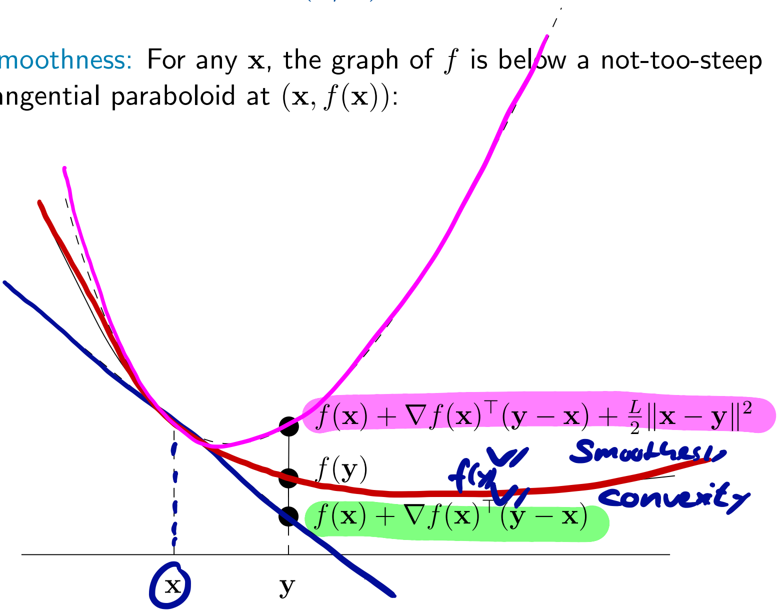
Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex and differentiable, $L \in \mathbb{R}_+$. f is called smooth (with parameter L) if

Smoothness

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

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 $f(x) := \|x\|^2$
- Operations that preserve smoothness:

Lemma (Exercise 15)

(i) *Let $f_1, f_2, \dots, f_m$ be convex 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 convex function $f := \sum_{i=1}^m \lambda_i f_i$ is smooth with parameter $\sum_{i=1}^n \lambda_i L_i$.*

(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*

$$\|A\| = \overset{x\neq 0}{\max_{\text{[redacted]}}} \frac{\|A\mathbf{x}\|}{\|\mathbf{x}\|} = \max_{\|x\|=1} \|Ax\|$$

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

operator norm

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

Convergence proof: See next lecture