Optimization for Machine Learning

Lecture 2: Gradient Descent

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Quiz Week 1

Let $f : \mathbb{R} \to \mathbb{R}$ and $g : \mathbb{R} \to \mathbb{R}$ be two convex functions. Which of the following combinations of f and g are convex:

1. $f(\mathbf{x}) + g(\mathbf{x})$
2. $f(\mathbf{x}) \cdot g(\mathbf{x})$
3. $\max\{f(\mathbf{x}), g(\mathbf{x})\}$
4. $\min\{f(\mathbf{x}), g(\mathbf{x})\}$
5. $f(g(\mathbf{x}))$
6. $e^{f(\mathbf{x})}$

Chapter 3

Gradient Descent

The Algorithm

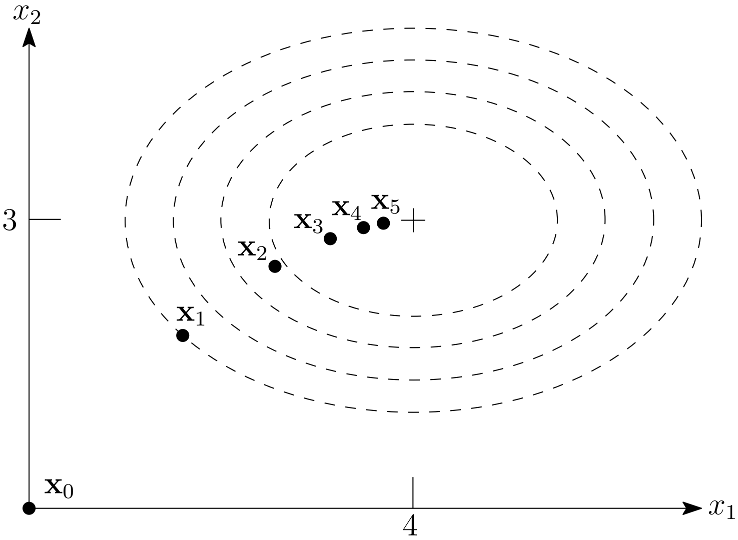
Given: Objective function $f \colon \mathbb{R}^d \to \mathbb{R}$.

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

Example



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

What does it mean to 'solve' an optimization problem?

We need to define approximate solutions:

- With respect to $\mathbf{x}^\star \in \operatorname{argmin}_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x})$:

- With respect to $\nabla f(\mathbf{x}) = \left(\frac{\partial f}{\partial x_1}(\mathbf{x}), \ldots, \frac{\partial f}{\partial x_d}(\mathbf{x}) \right)$:

How difficult is it to solve an optimization problem?

- Example 1:

- Example 2:

Summary:

Example: Lipschitz functions

A function $f\colon \mathbb{R}^d \to \mathbb{R}$ is M-Lipschitz, if

$$|f(\mathbf{x}) - f(\mathbf{y})| \leq M \|\mathbf{x} - \mathbf{y}\| \qquad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^d.$$

Problem: $$\text{minimize} \qquad f(\mathbf{x}) \qquad \text{with } \mathbf{x} \in [0,1]^d$$

A strategy to solve this problem:

Performance of Numerical Methods

- Given a problem class $\mathcal{P}$
  - (and the definition of an approximate solution)
- and a method $\mathcal{M}$
  - with oracle access to the problem instance $p \in \mathcal{P}$
- the performance of $\mathcal{M}$ on $\mathcal{P}$ is the amount of computational effort required to solve $\mathcal{P}$.

Computational effort can be measured as:

- analytic complexity (oracle calls)
- arithmetic complexity (additions, multiplications)

Gradient Descent on Smooth Functions

Smooth functions

“Not too curved”

Definition (Lecture-2).1

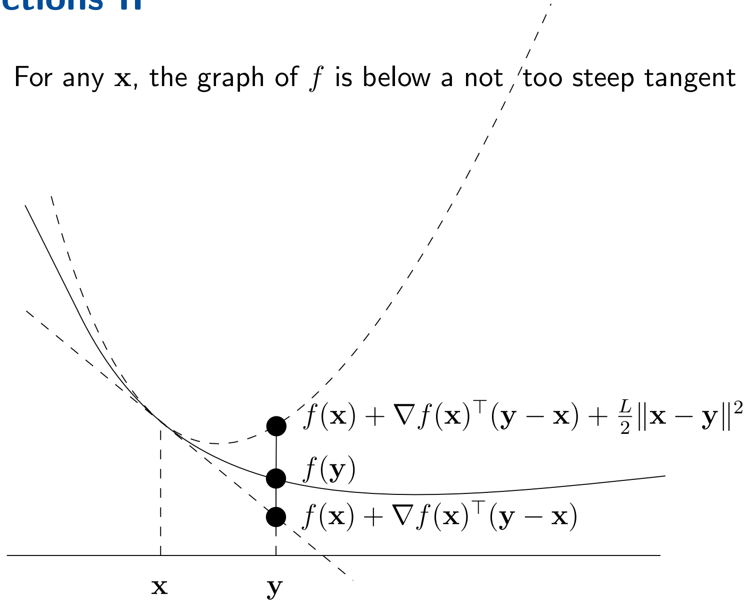
Let $f : \mathbf{dom}(f) \to \mathbb{R}$ be differentiable, $X \subseteq \mathbf{dom}(f)$, $L \in \mathbb{R}_+$. f is called smooth (with parameter L) over X if

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

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

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 19**).
- Operations that preserve smoothness (the same that preserve convexity):

Lemma (Lecture-2).2 (Exercise 22)

(i) *Let* $f_1, f_2, \ldots, f_m$ *be 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 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 is* $\|A\|$ *is the* ***spectral norm*** *of* A *(Definition 2.2).*

Smooth: Summary

- Lipschitz continuity of ∇f

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\| \leq L \|\mathbf{x} - \mathbf{y}\| \qquad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^d$$

- Quadratic upper bound:

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

- For twice differentiable functions:

$$\left\|\nabla^2 f(\mathbf{x})\right\| \leq L$$

Sufficient decrease

Lemma (Lecture-2).3

Let $f : \mathbb{R}^d \to \mathbb{R}$ 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 (Lecture-2).4

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

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

$\square$

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

Theorem (Lecture-2).5

Let $f : \mathbb{R}^d \to \mathbb{R}$ be differentiable smooth with parameter L and suppose $f^\star \leq \min f(\mathbf{x})$. With the stepsize

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

gradient descent yields

$$\min_{t \in \{0,\ldots,T-1\}} \|\nabla f(\mathbf{x}_t)\|^2 \leq \frac{2L(f(\mathbf{x}_0) - f^\star)}{T}, \quad T > 0.$$

Proof

Consider the sufficient decrease condition:

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

Equivalently:

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

By summing these equations over $t = 0, \dots, T-1$, and dividing by T:

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

Discussion

- $$\min_{t \in \{0,\ldots,T-1\}} \|\nabla f(\mathbf{x}_t)\|^2 \le \frac{2L(f(\mathbf{x}_0) - f^\star)}{T} \quad \Leftrightarrow \quad T \in \mathcal{O}\left(\frac{L(f(\mathbf{x}_0) - f^\star)}{\epsilon}\right)$$

- $\min_{t \in \{0,\ldots,T-1\}} \|\nabla f(\mathbf{x}_t)\|^2$ vs. $\|\nabla f(\mathbf{x}_T)\|^2$

- $\min_{t \in \{0,\ldots,T-1\}} \|\nabla f(\mathbf{x}_t)\|^2 \to 0$ does not imply convergence to a global (or local!) minima!

Gradient Descent on Smooth Convex Functions

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

Theorem (Lecture-2).6

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 stepsize

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

gradient descent yields

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

Proof I

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

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

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

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

And from the sufficient decrease lemma $(f(\mathbf{x}_{t+1}) \leq f(\mathbf{x}_t) - \frac{1}{2L}\|\nabla f(\mathbf{x}_t)\|^2)$:

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

Proof II

Putting everything together:

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

By summing up over $t = 0, \ldots T$

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

Using $f(\mathbf{x}_T) \geq f(\mathbf{x}^\star)$ and rewriting:

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

Where we also used that the last iterate is the best (sufficient decrease)!

Discussion

- Can we also prove convergence $\|\mathbf{x}_t - \mathbf{x}^\star\|^2 \to 0$?

- We used the stepsize $\gamma = \frac{1}{L}$. What can we do when we do not know L?

(see also **Exercise 23**)

- What is the benefit of Theorem (Lecture-2).6, if we already knew from Theorem (Lecture-2).5 that the gradient norm converges?

Can Gradient Descent Converge faster?

- Consider $f(x) := x^2$: Stepsize $\gamma := \frac{1}{4}$

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

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

  - Exponential in t !

Note that f is smooth and strongly convex **(see Exercise sheet 2)!**

Lecture 2 Recap

- We have seen two convergence criteria: suboptimality gap and distance to the optimum.
- We have seen a key proof technique: telescoping.
- We have seen (template) convergence proofs for gradient descent on smooth functions, and on convex functions.

Discussion

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