Optimization for Machine Learning

Lecture 1b: Gradient Descent

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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

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

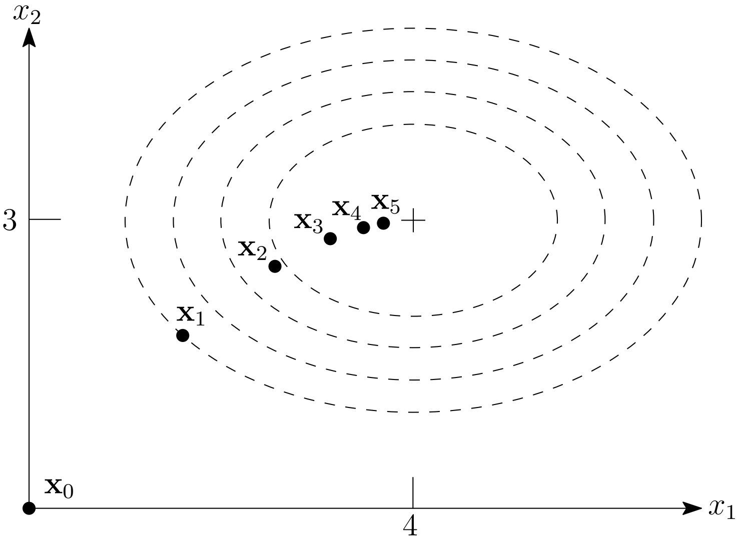
Note that there can be several global minima $\mathbf{x}_1^\star \neq \mathbf{x}_2^\star$ with $f(\mathbf{x}_1^\star) = f(\mathbf{x}_2^\star)$.

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



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

Vanilla analysis

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

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

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

- 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 first T iterations:

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

Vanilla analysis II

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 $\mathbf{x} = \mathbf{x}_t, \mathbf{y} = \mathbf{x}^\star$:
$$f(\mathbf{x}_t) - f(\mathbf{x}^\star) \leq \mathbf{g}_t^\top(\mathbf{x}_t - \mathbf{x}^\star)$$
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 (Theorem 1.10; **Exercise 12**).
- Rules out many interesting functions (for example, the "supermodel" $f(x) = x^2$)

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 $\|\nabla f(\mathbf{x})\| \leq B$ for all $\mathbf{x}$. Choosing the stepsize

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

gradient descent yields

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

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

Proof.

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

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

- choose γ 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.

$\square$

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 (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 16** (having to know R can't be avoided)

Smooth functions

"Not too curved"

Definition

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

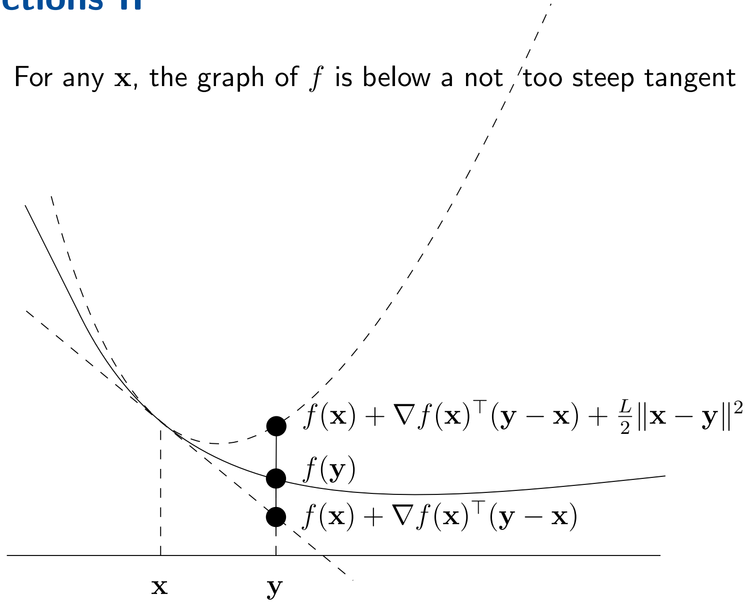
$$f(\mathbf{y}) \leq f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x}) + \frac{L}{2}\|\mathbf{x} - \mathbf{y}\|^2, \quad \forall \mathbf{x}, \mathbf{y} \in X.$$

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

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 14**).
- Operations that preserve smoothness (the same that preserve convexity):

Lemma (Exercise 17)

(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 1.2).*

Smooth vs Lipschitz

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

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

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

Sufficient decrease

Lemma

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

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

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

Proof.

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

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

□

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

Theorem

Let $f : \mathbb{R}^d \to \mathbb{R}$ 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

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

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

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

Proof.

Vanilla Analysis II:

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

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

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

□

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

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

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

Rewriting:

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

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

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

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

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

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

- $50 \cdot R^2 L$ 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?

$\rightarrow$ **Exercise 18**

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 !

Strongly convex functions

"Not too flat"

Definition

Let $f : \mathbf{dom}(f) \to \mathbb{R}$ be a differentiable function, $X \subseteq \mathbf{dom}(f)$ convex and $\mu \in \mathbb{R}_+, \mu > 0$. Function f is called strongly convex (with parameter μ) over X if

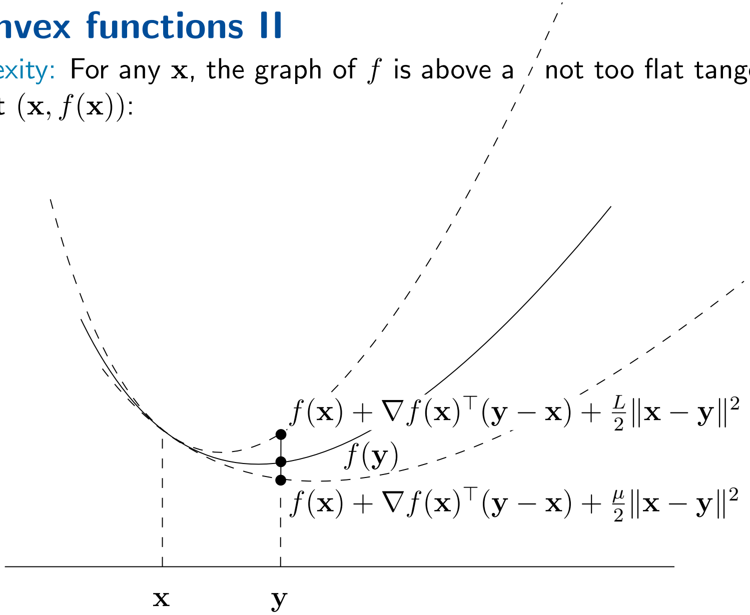
$$f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x}) + \frac{\mu}{2} \|\mathbf{x} - \mathbf{y}\|^2, \quad \forall \mathbf{x}, \mathbf{y} \in X.$$

Lemma (Exercise 21)

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

Strongly convex functions II

Strong convexity: For any $\mathbf{x}$, the graph of f is above a not too flat tangential paraboloid at $(\mathbf{x}, f(\mathbf{x}))$:



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

Want to show: $\lim_{t\to\infty} \mathbf{x}_t = \mathbf{x}^\star$

Vanilla Analysis:

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

Now use stronger lower bound on left hand side, coming from strong convexity:

$$\nabla f(\mathbf{x}_t)^\top(\mathbf{x}_t - \mathbf{x}^\star) \geq f(\mathbf{x}_t) - f(\mathbf{x}^\star) + \frac{\mu}{2}\|\mathbf{x}_t - \mathbf{x}^\star\|^2$$

Putting it together:

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

Rewriting:

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

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

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

Squared distance to $\mathbf{x}^\star$ goes down by a constant factor, up to some "noise".

Theorem

Let $f : \mathbb{R}^d \to \mathbb{R}$ be differentiable with a global minimum $\mathbf{x}^\star$; suppose that f is 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) *The absolute error after T iterations is exponentially small in T:*

$$f(\mathbf{x}_T)-f(\mathbf{x}^\star) \leq \frac{L}{2}\left(1-\frac{\mu}{L}\right)^T\|\mathbf{x}_0-\mathbf{x}^\star\|^2, \quad T > 0.$$

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

$$\underline{\|\mathbf{x}_{t+1} - \mathbf{x}^\star\|^2} \le 2\gamma(f(\mathbf{x}^\star) - f(\mathbf{x}_t)) + \gamma^2\|\nabla f(\mathbf{x}_t)\|^2 + \underline{(1-\mu\gamma)\|\mathbf{x}_t - \mathbf{x}^\star\|^2}.$$

Proof of (i).

Bounding the noise: $\gamma = 1/L$, sufficient decrease

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

Hence, the noise is nonpositive, and we get (i):

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

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

Proof of (ii).

From (i):

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

Smoothness together with $\nabla f(\mathbf{x}^\star) = \mathbf{0}$:

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

Putting it together:

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

$\square$

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

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

$$T \geq \frac{L}{\mu} \ln\left(\frac{R^2 L}{2\varepsilon}\right) \quad \Rightarrow \quad \text{error} \ \leq \frac{L}{2}\left(1 - \frac{\mu}{L}\right)^T R^2 \leq \varepsilon.$$

Conclusion: To reach absolute error at most ε, we only need $\mathcal{O}(\log \frac{1}{\varepsilon})$ iterations, e.g.

- $\frac{L}{\mu} \ln(50 \cdot R^2 L)$ iterations for error 0.01 ...
- ... as opposed to $50 \cdot R^2 L$ in the smooth case

In Practice:

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

$\rightarrow$ (similar to) **Exercise 15**