Optimization for Machine Learning
CS-439

Lecture 4: Proximal and Subgradient Descent

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Section 3.6

Proximal Gradient Descent

Composite optimization problems

Consider objective functions composed as

$$f(\mathbf{x}) := g(\mathbf{x}) + h(\mathbf{x})$$

where g is a "nice" function, where as h is a "simple" additional term, which however doesn't satisfy the assumptions of niceness which we used in the convergence analysis so far.

In particular, an important case is when h is not differentiable.

Idea

The classical gradient step for minimizing g:

$$\mathbf{x}_{t+1} = \operatorname*{argmin}_{\mathbf{y}} \; g(\mathbf{x}_t) + \nabla g(\mathbf{x}_t)^\top (\mathbf{y} - \mathbf{x}_t) + \frac{1}{2\gamma} \|\mathbf{y} - \mathbf{x}_t\|^2 \; .$$

For the stepsize $\gamma := \frac{1}{L}$ it exactly minimizes the local quadratic model of g at our current iterate $\mathbf{x}_t$, formed by the smoothness property with parameter L.

Now for $f = g + h$, keep the same for g, and add h unmodified.

$$\begin{aligned}\mathbf{x}_{t+1} :=& \operatorname*{argmin}_{\mathbf{y}} \; g(\mathbf{x}_t) + \nabla g(\mathbf{x}_t)^\top (\mathbf{y} - \mathbf{x}_t) + \frac{1}{2\gamma} \|\mathbf{y} - \mathbf{x}_t\|^2 + h(\mathbf{y}) \\ =& \operatorname*{argmin}_{\mathbf{y}} \; \frac{1}{2\gamma} \|\mathbf{y} - (\mathbf{x}_t - \gamma \nabla g(\mathbf{x}_t))\|^2 + h(\mathbf{y}) \; ,\end{aligned}$$

the proximal gradient descent update.

The proximal gradient descent algorithm

An iteration of proximal gradient descent is defined as

$$\mathbf{x}_{t+1} := \operatorname{prox}_{h,\gamma}(\mathbf{x}_t - \gamma \nabla g(\mathbf{x}_t)) \ .$$

where the proximal mapping for a given function h, and parameter $\gamma > 0$ is defined as

$$\operatorname{prox}_{h,\gamma}(\mathbf{z}) := \operatorname*{argmin}_{\mathbf{y}} \left\{ \frac{1}{2\gamma} \|\mathbf{y} - \mathbf{z}\|^2 + h(\mathbf{y}) \right\} \ .$$

The update step can be equivalently written as

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma G_\gamma(\mathbf{x}_t)$$

for $G_{h,\gamma}(\mathbf{x}) := \frac{1}{\gamma}\Big(\mathbf{x} - \operatorname{prox}_{h,\gamma}(\mathbf{x} - \gamma \nabla g(\mathbf{x}))\Big)$ being the so called generalized gradient of f.

A generalization of gradient descent?

- $h \equiv 0$: recover gradient descent
- $h \equiv \boldsymbol{\iota}_X$: recover projected gradient descent!

  Given a closed convex set X, the indicator function of the set X is given as the convex function

$$
\begin{aligned}
\boldsymbol{\iota}_X : \mathbb{R}^d &\to \mathbb{R} \cup +\infty \\
\mathbf{x} \mapsto \boldsymbol{\iota}_X(\mathbf{x}) &:= \begin{cases} 0 & \text{if } \mathbf{x} \in X, \\ +\infty & \text{otherwise.} \end{cases}
\end{aligned}
$$

  Proximal mapping becomes

$$
\operatorname{prox}_{h,\gamma}(\mathbf{z}) := \underset{\mathbf{y}}{\operatorname{argmin}} \left\{ \frac{1}{2\gamma} \|\mathbf{y} - \mathbf{z}\|^2 + \boldsymbol{\iota}_X(\mathbf{y}) \right\} = \underset{\mathbf{y} \in X}{\operatorname{argmin}} \ \|\mathbf{y} - \mathbf{z}\|^2
$$

Convergence in $\mathcal{O}(1/\varepsilon)$ steps

Same as vanilla case for smooth functions, but now for any h for which we can compute the proximal mapping.

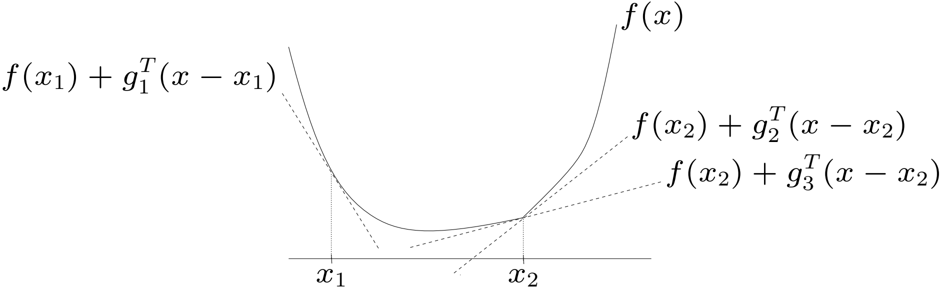
Subgradients

What if f is not differentiable?

Definition

$\mathbf{g} \in \mathbb{R}^d$ is a subgradient of f at $\mathbf{x}$ if

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \mathbf{g}^\top(\mathbf{y} - \mathbf{x}) \qquad \text{for all } \mathbf{y} \in \mathbf{dom}(f)$$


$f(x)$
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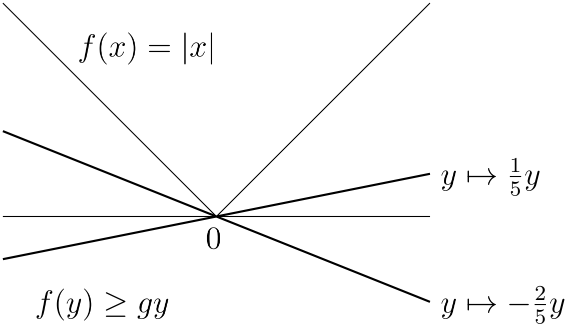
$f(x_2) + g_2^T(x - x_2)$
$f(x_2) + g_3^T(x - x_2)$
x_1
x_2

$\partial f(\mathbf{x}) \subseteq \mathbb{R}^d$ is the subdifferential, the set of subgradients of f at $\mathbf{x}$.

Subgradients II

Example:



Subgradient condition at $x = 0$: $f(y) \geq f(0) + g(y - 0) = gy$.

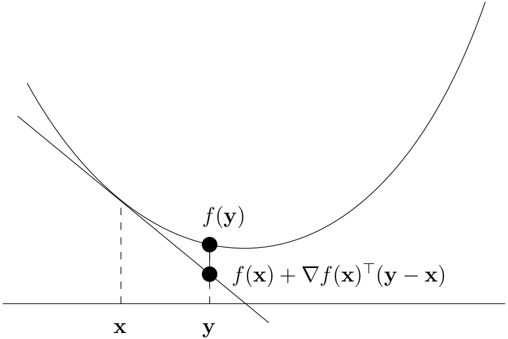
$\partial f(0) = [-1, 1]$

Subgradients III

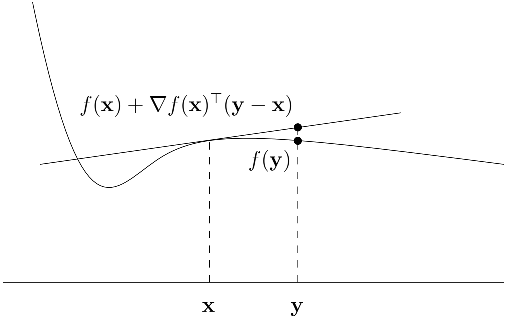
Lemma (Exercise 28)

If $f : \mathbf{dom}(f) \to \mathbb{R}$ *is differentiable at* $\mathbf{x} \in \mathbf{dom}(f)$, *then* $\partial f(\mathbf{x}) \subseteq \{\nabla f(\mathbf{x})\}$.

Either exactly one subgradient $\nabla f(\mathbf{x})$...   ...or no subgradient at all.



$f(\mathbf{y})$
$f(\mathbf{x}) + \nabla f(\mathbf{x})^\top(\mathbf{y} - \mathbf{x})$
$\mathbf{x}$
$\mathbf{y}$



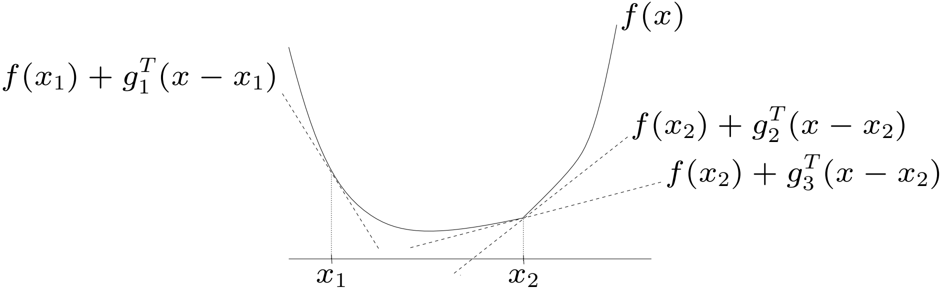
$f(\mathbf{x}) + \nabla f(\mathbf{x})^\top(\mathbf{y} - \mathbf{x})$
$f(\mathbf{y})$
$\mathbf{x}$
$\mathbf{y}$

Subgradient characterization of convexity

"convex = subgradients everywhere"

Lemma (Exercise 29)

A function $f : \mathbf{dom}(f) \to \mathbb{R}$ *is convex if and only if* $\mathbf{dom}(f)$ *is convex and* $\partial f(\mathbf{x}) \neq \emptyset$ *for all* $\mathbf{x} \in \mathbf{dom}(f)$.


$f(x)$
$f(x_1) + g_1^T(x - x_1)$
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x_1
x_2

Convex and Lipschitz = bounded subgradients

Lemma (Exercise 30)

Let $f : \mathbf{dom}(f) \to \mathbb{R}$ *be convex,* $\mathbf{dom}(f)$ *open,* $B \in \mathbb{R}_+$. *Then the following two statements are equivalent.*

(i) $\|\mathbf{g}\| \leq B$ *for all* $\mathbf{x} \in \mathbf{dom}(f)$ *and all* $\mathbf{g} \in \partial f(\mathbf{x})$.

(ii) $|f(\mathbf{x}) - f(\mathbf{y})| \leq B\|\mathbf{x} - \mathbf{y}\|$ *for all* $\mathbf{x}, \mathbf{y} \in \mathbf{dom}(f)$.

Subgradient optimality condition

Lemma

Suppose that $f : \mathbf{dom}(f) \to \mathbb{R}$ *and* $\mathbf{x} \in \mathbf{dom}(f)$*. If* $\mathbf{0} \in \partial f(\mathbf{x})$*, then* $\mathbf{x}$ *is a global minimum.*

Proof.

By definition of subgradients, $\mathbf{g} = \mathbf{0} \in \partial f(\mathbf{x})$ gives

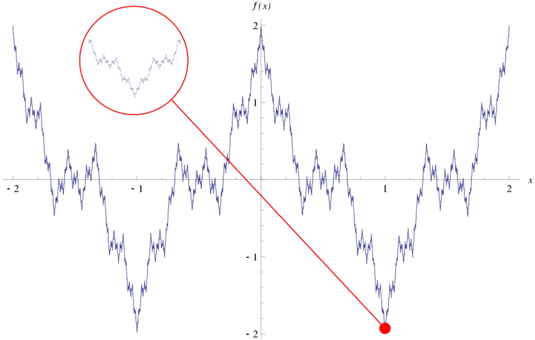
$$f(\mathbf{y}) \geq f(\mathbf{x}) + \mathbf{g}^\top(\mathbf{y} - \mathbf{x}) = f(\mathbf{x})$$

for all $\mathbf{y} \in \mathbf{dom}(f)$, so $\mathbf{x}$ is a global minimum. □

Differentiability of convex functions

How “wild” can a non-differentiable convex function be?

Weierstrass function: a function that is continuous everywhere but differentiable nowhere



https://commons.wikimedia.org/wiki/File:WeierstrassFunction.svg

Differentiability of convex functions

Theorem ([Roc97, Theorem 25.5])

A convex function $f : \mathbf{dom}(f) \to \mathbb{R}$ is differentiable almost everywhere.

In other words:

- Set of points where f is non-differentiable has measure 0 (no volume).
- For all $\mathbf{x} \in \mathbf{dom}(f)$ and all $\varepsilon > 0$, there is a point $\mathbf{x}'$ such that $\|\mathbf{x} - \mathbf{x}'\| < \varepsilon$ and f is differentiable at $\mathbf{x}'$.

The subgradient descent algorithm

Subgradient descent: choose $\mathbf{x}_0 \in \mathbb{R}^d$.

Let $\mathbf{g}_t \in \partial f(\mathbf{x}_t)$

$$\mathbf{x}_{t+1} := \mathbf{x}_t - \gamma_t \mathbf{g}_t$$

for **times** $t = 0, 1, \ldots,$ and **stepsizes** $\gamma_t \geq 0$.

Stepsize can vary with time!

This is possible in (projected) gradient descent as well, but so far, we didn't need it.

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

Theorem

Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex and B-Lipschitz continuous with a global minimum $\mathbf{x}^\star$; furthermore, suppose that $\|\mathbf{x}_0 - \mathbf{x}^\star\| \leq R$. Choosing the constant stepsize

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

subgradient descent yields

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

Proof is identical to the one of Theorem 2.1, except...

- In vanilla analyis, now use $\mathbf{g}_t \in \partial f(\mathbf{x}_t)$ instead of $\mathbf{g}_t = \nabla f(\mathbf{x}_t)$.
- Inequality $f(\mathbf{x}_t) - f(\mathbf{x}^\star) \leq \mathbf{g}_t^\top(\mathbf{x}_t - \mathbf{x}^\star)$ now follows from subgradient property instead of first-order charaterization of convexity.

Optimality of first-order methods

With all the convergence rates we have seen so far, a very natural question to ask is if these rates are best possible or not. Surprisingly, the rate can indeed not be improved in general.

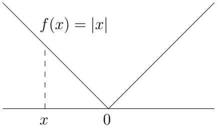
Theorem (Nesterov)

For any $T \leq d-1$ and starting point $\mathbf{x}_0$, there is a function f in the problem class of B-Lipschitz functions over $\mathbb{R}^d$, such that any (sub)gradient method has an objective error at least

$$f(\mathbf{x}_T) - f(\mathbf{x}^\star) \geq \frac{RB}{2(1+\sqrt{T+1})} \ .$$

Smooth (non-differentiable) functions?

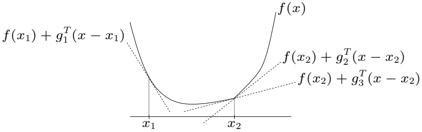
They don't exist (Exercise 31)!



At 0, graph can't be below a tangent paraboloid.

Can we still improve over $O(1/\varepsilon^2)$ steps for Lipschitz functions?

Yes, if we also require strong convexity (graph is above not too flat tangent paraboloids).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x_2

Strongly convex functions

“Not too flat”

Straightforward generalization to the non-differentiable case:

Definition

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

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

Strongly convex functions: characterization via "normal" convexity

Lemma (Exercise 33)

Let $f : \mathbf{dom}(f) \to \mathbb{R}$ *be convex,* $\mathbf{dom}(f)$ *open,* $\mu \in \mathbb{R}_+, \mu > 0$. f *is strongly convex with parameter* μ *if and only if* $f_\mu : \mathbf{dom}(f) \to \mathbb{R}$ *defined by*

$$f_\mu(\mathbf{x}) = f(\mathbf{x}) - \frac{\mu}{2} \|\mathbf{x}\|^2, \quad \mathbf{x} \in \mathbf{dom}(f)$$

is convex.

Tame strong convexity

For fast convergence, we consider additional assumptions.

Smoothness? - Not an option in the non-differentiable case (Exercise 31).

Instead: assume that all subgradients $\mathbf{g}_t$ that we encounter during the algorithm are bounded in norm.

May be realistic if. . .

- we start close to optimality
- we run projected subgradient descent over a compact set X

May also fail!

- Over $\mathbb{R}^d$, strong convexity and bounded subgradients contradict each other! (Exercise 35).

Tame strong convexity: $\mathcal{O}(1/\varepsilon)$ steps

Theorem

Let $f : \mathbb{R}^d \to \mathbb{R}$ be strongly convex with parameter $\mu > 0$ and let $\mathbf{x}^\star$ be the unique global minimum of f. With decreasing step size

$$\gamma_t := \frac{2}{\mu(t+1)}, \quad t > 0,$$

subgradient descent yields

$$f\left(\frac{2}{T(T+1)}\sum_{t=1}^{T} t \cdot \mathbf{x}_t\right) - f(\mathbf{x}^\star) \le \frac{2B^2}{\mu(T+1)},$$

where $B = \max_{t=1}^{T} \|\mathbf{g}_t\|$. ↑

convex combination of iterates

Tame strong convexity: $\mathcal{O}(1/\varepsilon)$ steps II

Proof.

Vanilla analysis ($\mathbf{g}_t \in \partial f(\mathbf{x}_t)$):

$$\mathbf{g}_t^\top(\mathbf{x}_t - \mathbf{x}^\star) = \frac{\gamma_t}{2}\|\mathbf{g}_t\|^2 + \frac{1}{2\gamma_t}\left(\|\mathbf{x}_t - \mathbf{x}^\star\|^2 - \|\mathbf{x}_{t+1} - \mathbf{x}^\star\|^2\right).$$

Lower bound from strong convexity:

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

Putting it together (with $\|\mathbf{g}_t\|^2 \leq B^2$):

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

Summing over $t = 1, \ldots, T$: we used to have telescoping ($\gamma_t = \gamma, \mu = 0$)...

Tame strong convexity: $\mathcal{O}(1/\varepsilon)$ steps III

Proof.

So far we have:

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

To get telescoping, we would need $\gamma_t^{-1} = \gamma_{t+1}^{-1} - \mu$.

Works with $\gamma_t^{-1} = \mu(1+t)$, but not $\gamma_t^{-1} = \mu(1+t)/2$ (the choice here).

Exercise 36: what happens with $\gamma_t^{-1} = \mu(1+t)$?

Now: what happens with $\gamma_t^{-1} = \mu(1+t)/2$ (the choice here)?

Tame strong convexity: $\mathcal{O}(1/\varepsilon)$ steps IV

Proof.

So far we have:

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

Plug in $\gamma_t^{-1} = \mu(1+t)/2$ and multiply with t on both sides:

$$\begin{aligned} t \cdot \big(f(\mathbf{x}_t) - f(\mathbf{x}^\star)\big) &\leq \frac{B^2 t}{\mu(t+1)} + \frac{\mu}{4}\Big(t(t-1)\left\|\mathbf{x}_t - \mathbf{x}^\star\right\|^2 - (t+1)t\left\|\mathbf{x}_{t+1} - \mathbf{x}^\star\right\|^2\Big) \\ &\leq \frac{B^2}{\mu} + \frac{\mu}{4}\Big(t(t-1)\left\|\mathbf{x}_t - \mathbf{x}^\star\right\|^2 - (t+1)t\left\|\mathbf{x}_{t+1} - \mathbf{x}^\star\right\|^2\Big). \end{aligned}$$

Tame strong convexity: $\mathcal{O}(1/\varepsilon)$ steps V

Proof.

We have

$$\begin{aligned} t \cdot \big(f(\mathbf{x}_t) - f(\mathbf{x}^\star)\big) &\leq \frac{B^2 t}{\mu(t+1)} + \frac{\mu}{4}\Big(t(t-1)\left\|\mathbf{x}_t - \mathbf{x}^\star\right\|^2 - (t+1)t\left\|\mathbf{x}_{t+1} - \mathbf{x}^\star\right\|^2\Big) \\ &\leq \frac{B^2}{\mu} + \frac{\mu}{4}\Big(t(t-1)\left\|\mathbf{x}_t - \mathbf{x}^\star\right\|^2 - (t+1)t\left\|\mathbf{x}_{t+1} - \mathbf{x}^\star\right\|^2\Big). \end{aligned}$$

Now we get telescoping. . .

$$\sum_{t=1}^{T} t \cdot \big(f(\mathbf{x}_t) - f(\mathbf{x}^\star)\big) \leq \frac{TB^2}{\mu} + \frac{\mu}{4}\Big(0 - T(T+1)\left\|\mathbf{x}_{T+1} - \mathbf{x}^\star\right\|^2\Big) \leq \frac{TB^2}{\mu}.$$

Tame strong convexity: $\mathcal{O}(1/\varepsilon)$ steps VI

Proof.

Almost done:

$$\underline{\sum_{t=1}^{T} t \cdot \left(f(\mathbf{x}_t) - f(\mathbf{x}^\star)\right)} \leq \frac{TB^2}{\mu} + \frac{\mu}{4}\left(0 - T(T+1)\left\|\mathbf{x}_{T+1} - \mathbf{x}^\star\right\|^2\right) \leq \frac{TB^2}{\mu}.$$

Since

$$\frac{2}{T(T+1)} \sum_{t=1}^{T} t = 1,$$

Jensen's inequality yields

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

□

Tame strong convexity: Discussion

$$f\left(\frac{2}{T(T+1)}\sum_{t=1}^{T} t \cdot \mathbf{x}_t\right) - f(\mathbf{x}^\star) \leq \frac{2B^2}{\mu(T+1)},$$

Weighted average of iterates achieves the bound (later iterates have more weight)

Bound is independent of initial distance $\|\mathbf{x}_0 - \mathbf{x}^\star\|\ldots$

$\ldots$but not really: B typically depends on $\|\mathbf{x}_0 - \mathbf{x}^\star\|$ (for example, $B = \mathcal{O}(\|\mathbf{x}_0 - \mathbf{x}^\star\|)$ for quadratic functions)

Recall: we can only hope that B is small (can be checked while running the algorithm)

What if we don't know the parameter μ of strong convexity?

→ **Bad luck!** In practice, try some μ's, pick best solution obtained

Bibliography

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Princeton Landmarks in Mathematics. Princeton University Press, 1997.