Mathematics of Data: From Theory to Computation

Prof. Volkan Cevher
volkan.cevher@epfl.ch

Lecture 5: Unconstrained, smooth minimization II

Laboratory for Information and Inference Systems (LIONS)
École Polytechnique Fédérale de Lausanne (EPFL)

EE-556 (Fall 2017)

License Information for Mathematics of Data Slides

Outline

- This lecture
  1. Gradient and accelerated gradient descent methods
- Next lecture
  1. The quadratic case and conjugate gradient
  2. Other optimization methods

Recommended reading

- Chapters 2, 3, 5, 6 in Nocedal, Jorge, and Wright, Stephen J., *Numerical Optimization*, Springer, 2006.
- Chapter 9 in Boyd, Stephen, and Vandenberghe, Lieven, *Convex optimization*, Cambridge university press, 2009.
- Chapter 1 in Bertsekas, Dimitris, *Nonlinear Programming*, Athena Scientific, 1999.
- Chapters 1, 2 and 4 in Nesterov, Yurii, *Introductory Lectures on Convex Optimization: A Basic Course*, Vol. 87, Springer, 2004.

Overview

Overview

This lecture covers the basics of numerical methods for *unconstrained* and *smooth* convex minimization.

Recall: convex, unconstrained, smooth minimization

Problem (**Mathematical formulation**)

$$\boxed{F^\star := \min_{\mathbf{x}\in\mathbb{R}^p} \left\{ F(\mathbf{x}) := f(\mathbf{x}) \right\}} \tag{1}$$

where f is convex and twice differentiable.
Note that (1) is unconstrained.

How de we design efficient optimization algorithms with accuracy-computation tradeoffs for this class of functions?

Basic principles of descent methods

Template for iterative descent methods

1. Let $\mathbf{x}^0 \in \mathrm{dom}(f)$ be a starting point.
2. Generate a sequence of vectors $\mathbf{x}^1, \mathbf{x}^2, \cdots \in \mathrm{dom}(f)$ so that we have descent:

$$f(\mathbf{x}^{k+1}) < f(\mathbf{x}^k), \quad \text{for all } k = 0, 1, \ldots$$

until $\mathbf{x}_k$ is ϵ-optimal.

Such a sequence $\left\{\mathbf{x}^k\right\}_{k \geq 0}$ can be generated as:

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \alpha_k \mathbf{p}^k$$

where $\mathbf{p}^k$ is a descent direction and $\alpha_k > 0$ a step-size.

Remarks

- Iterative algorithms can use various **oracle** information from the objective, such as its value, gradient, or Hessian, in different ways to obtain α_k and $\mathbf{p}^k$
- These choices determine the overall convergence rate and complexity
- The type of oracle information used becomes a defining characteristic

Basic principles of descent methods

A condition for local descent directions

The iterates are given as:

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \alpha_k \mathbf{p}^k$$

By Taylor's theorem, we have

$$f(\mathbf{x}^{k+1}) = f(\mathbf{x}^k) + \alpha_k \langle \nabla f(\mathbf{x}^k),\ \mathbf{p}^k \rangle + O(\alpha_k^2 \|\mathbf{p}\|_2^2).$$

For α_k small enough, the term $\alpha_k \langle \nabla f(\mathbf{x}^k),\ \mathbf{p}^k \rangle$ dominates $O(\alpha_k^2)$ for a fixed $\mathbf{p}^k$. Therefore, in order to have $f(\mathbf{x}^{k+1}) < f(\mathbf{x}^k)$, we require

$$\langle \nabla f(\mathbf{x}^k),\ \mathbf{p}^k \rangle < 0$$

Basic principles of descent methods

Local steepest descent direction

Since

$$\langle \nabla f(\mathbf{x}^k),\ \mathbf{p}^k \rangle = \|\nabla f(\mathbf{x}^k)\| \|\mathbf{p}^k\| \cos\theta \ ,$$

where θ is the angle between $\nabla f(\mathbf{x}^k)$ and $\mathbf{p}^k$, we have that

$$\mathbf{p}^k := -\nabla f(\mathbf{x}^k)$$

is the local *steepest descent* direction.

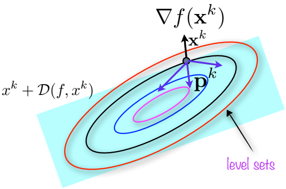


Figure: Descent directions in 2D should be an element of the cone of descent directions $\mathcal{D}(f, \cdot)$.

A reminder on notation

Important notation **used throughout the whole lecture**:

- $\mathcal{F}_L^{l,m}$: Functions that are l-times differentiable with m-th order Lipschitz property
  - In this lecture, $m = 1$, and $l \in \{1, 2, \infty\}$
- $\mathcal{F}_{L,\mu}^{l,m}$: Subset of $\mathcal{F}_L^{l,m}$ also satisfying μ-strong convexity

Gradient descent methods

Gradient descent (GD) algorithm

The gradient method we discussed before indeed use the local steepest direction:

$$\mathbf{p}^k = -\nabla f(\mathbf{x}^k)$$

so that

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k \nabla f(\mathbf{x}^k).$$

Key question: How do we choose α_k so that we are guaranteed to successfully descend? (ideally as fast as possible)

Gradient descent methods

Gradient descent (GD) algorithm

The gradient method we discussed before indeed use the local steepest direction:

$$\mathbf{p}^k = -\nabla f(\mathbf{x}^k)$$

so that

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k \nabla f(\mathbf{x}^k).$$

Key question: How do we choose α_k so that we are guaranteed to successfully descend? (ideally as fast as possible)

Answer: By exploiting the structures within the convex function

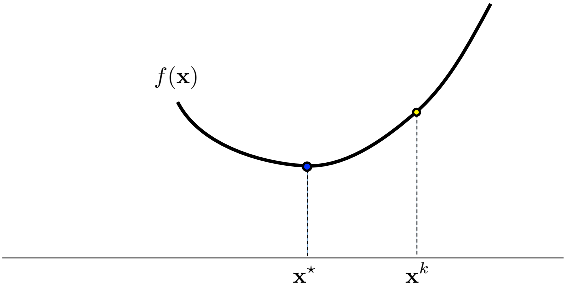
When $f \in \mathcal{F}_L^{2,1}$, we can use $\alpha_k = 1/L$ so that $\mathbf{x}^{k+1} = \mathbf{x}^k - \frac{1}{L}\nabla f(\mathbf{x}^k)$ is contractive.

- Note that the above GD method only uses the gradient information, and hence, it is called a **first-order method**.

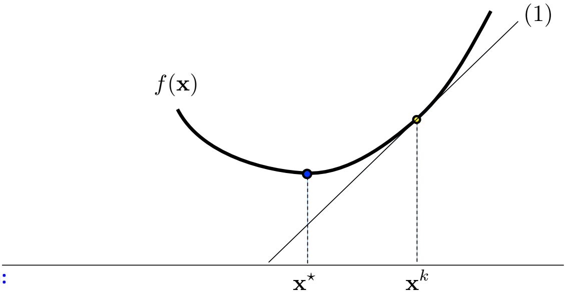
First-order methods employ only first-order oracle information about the objective, namely the value of f and ∇f at specific points.

- **Second-order methods** also use the Hessian $\nabla^2 f$.

Recall: Gradient descent methods - a geometrical intuition



Recall: Gradient descent methods - a geometrical intuition



Structure in optimization:

$$(1) \qquad f(\mathbf{x}) \geq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle$$

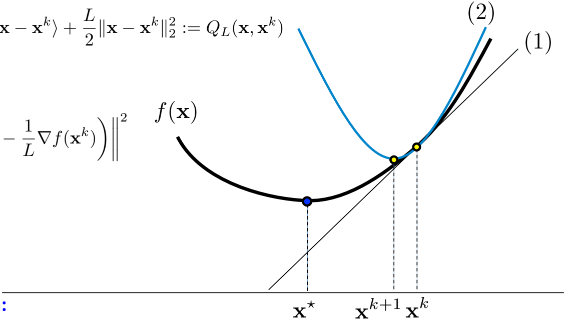
Recall: Gradient descent methods - a geometrical intuition

Majorize:

$$f(\mathbf{x}) \leq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{L}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2 := Q_L(\mathbf{x}, \mathbf{x}^k)$$

Minimize:

$$\begin{aligned}
\mathbf{x}^{k+1} &= \arg\min_{\mathbf{x}} Q_L(\mathbf{x}, \mathbf{x}^k) \\
&= \arg\min_{\mathbf{x}} \left\| \mathbf{x} - \left(\mathbf{x}^k - \frac{1}{L}\nabla f(\mathbf{x}^k) \right) \right\|^2 \\
&= \mathbf{x}^k - \frac{1}{L}\nabla f(\mathbf{x}^k)
\end{aligned}$$



Structure in optimization:

(1) $\quad f(\mathbf{x}) \geq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle$

(2) $\quad f(\mathbf{x}) \leq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{L}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2$

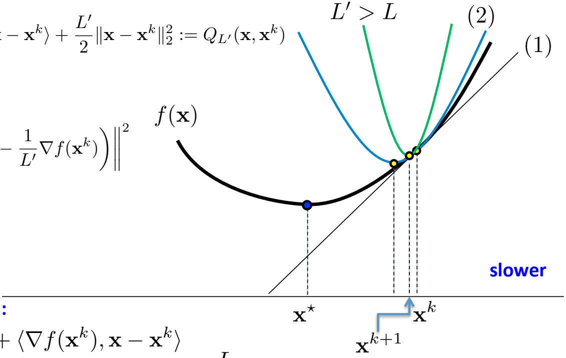
Recall: Gradient descent methods - a geometrical intuition

Majorize:

$$f(\mathbf{x}) \leq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{L'}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2 := Q_{L'}(\mathbf{x}, \mathbf{x}^k)$$

Minimize:

$$\begin{aligned} \mathbf{x}^{k+1} &= \arg\min_{\mathbf{x}} Q_{L'}(\mathbf{x}, \mathbf{x}^k) \\ &= \arg\min_{\mathbf{x}} \left\| \mathbf{x} - \left(\mathbf{x}^k - \frac{1}{L'} \nabla f(\mathbf{x}^k) \right) \right\|^2 \\ &= \mathbf{x}^k - \frac{1}{L'} \nabla f(\mathbf{x}^k) \end{aligned}$$



Structure in optimization:

(1) $\qquad f(\mathbf{x}) \geq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle$

(2) $\qquad f(\mathbf{x}) \leq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{L}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2$

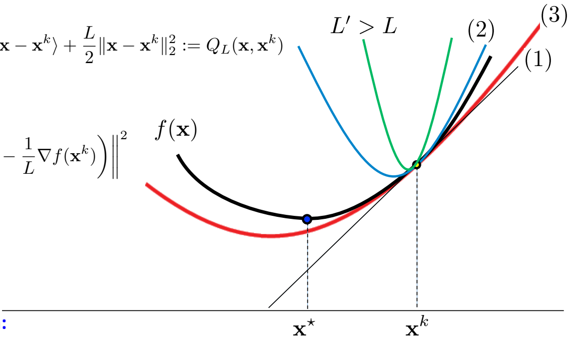
Recall: Gradient descent methods - a geometrical intuition

Majorize:

$$f(\mathbf{x}) \leq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{L}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2 := Q_L(\mathbf{x}, \mathbf{x}^k)$$

Minimize:

$$\begin{aligned}
\mathbf{x}^{k+1} &= \arg\min_{\mathbf{x}} Q_L(\mathbf{x}, \mathbf{x}^k) \\
&= \arg\min_{\mathbf{x}} \left\| \mathbf{x} - \left(\mathbf{x}^k - \frac{1}{L}\nabla f(\mathbf{x}^k) \right) \right\|^2 \\
&= \mathbf{x}^k - \frac{1}{L}\nabla f(\mathbf{x}^k)
\end{aligned}$$



Structure in optimization:

(1) $\quad f(\mathbf{x}) \geq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle$

(2) $\quad f(\mathbf{x}) \leq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{L}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2$

(3) $\quad f(\mathbf{x}) \geq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{\mu}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2$

Convergence rate of gradient descent

Theorem

Let the starting point for GD be $\mathbf{x}^0 \in dom(f)$.

- *If $f \in \mathcal{F}_L^{2,1}$, with the choice $\alpha = \frac{1}{L}$, the iterates of GD satisfy*

$$\boxed{f(\mathbf{x}^k) - f(\mathbf{x}^\star) \leq \frac{2L}{k+4}\|\mathbf{x}^0 - \mathbf{x}^\star\|_2^2}$$

- *If $f \in \mathcal{F}_{L,\mu}^{2,1}$, with the choice $\alpha = \frac{2}{L+\mu}$, the iterates of GD satisfy*

$$\boxed{\|\mathbf{x}^k - \mathbf{x}^\star\|_2 \leq \left(\frac{L-\mu}{L+\mu}\right)^k \|\mathbf{x}^0 - \mathbf{x}^\star\|_2}$$

- *If $f \in \mathcal{F}_{L,\mu}^{2,1}$, with the choice $\alpha = \frac{1}{L}$, the iterates of GD satisfy*

$$\boxed{\|\mathbf{x}^k - \mathbf{x}^\star\|_2 \leq \left(\frac{L-\mu}{L+\mu}\right)^{\frac{k}{2}} \|\mathbf{x}^0 - \mathbf{x}^\star\|_2}$$

Proof of convergence rates of gradient descent - part I (self-study)

- We first need to prove a basic result about functions in $\mathcal{F}_L^{1,1}$

Lemma

Let $f \in \mathcal{F}_L^{1,1}$. Then it holds that

$$\frac{1}{L}\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|^2 \leq \langle \nabla f(\mathbf{x}) - \nabla f(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle \tag{2}$$

Proof (Advanced material).

First, recall the following result about Lipschitz gradient functions $h \in \mathcal{F}_L^{1,1}$

$$h(\mathbf{x}) \leq h(\mathbf{y}) + \langle \nabla h(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle + \frac{L}{2}\|\mathbf{x} - \mathbf{y}\|_2^2. \tag{3}$$

To prove the result, let $\phi(\mathbf{y}) := f(\mathbf{y}) - \langle \nabla f(\mathbf{x}), \mathbf{y} \rangle$, with $\nabla \phi(\mathbf{y}) = \nabla f(\mathbf{y}) - \nabla f(\mathbf{x})$. Clearly, $\phi(\mathbf{y})$ attains its minimum value at $\mathbf{y}^\star = \mathbf{x}$. Hence, and by also applying (3) with $h = \phi$ and $\mathbf{x} = \mathbf{y} - \frac{1}{L}\nabla \phi(\mathbf{y})$, we get

$$\phi(\mathbf{x}) \leq \phi\left(\mathbf{y} - \frac{1}{L}\nabla \phi(\mathbf{y})\right) \leq \phi(\mathbf{y}) - \frac{1}{2L}\|\nabla \phi(\mathbf{y})\|_2^2.$$

Substituting the above definitions into the left and right hand sides gives

$$f(\mathbf{x}) + \langle \nabla f(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle + \frac{1}{2L}\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_2^2 \leq f(\mathbf{y}) \tag{4}$$

By adding two copies of (4) with each other, with $\mathbf{x}$ and $\mathbf{y}$ swapped, we obtain (2). □

Proof of convergence rates of gradient descent - part II (self-study)

Theorem

If $f \in \mathcal{F}_L^{2,1}$, with the choice $\alpha = \frac{1}{L}$, the iterates of GD satisfy

$$\boxed{f(\mathbf{x}^k) - f(\mathbf{x}^\star) \leq \frac{2L}{k+4}\|\mathbf{x}^0 - \mathbf{x}^\star\|_2^2} \tag{5}$$

Proof

- Consider the constant step-size iteration $\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha\nabla f(\mathbf{x}^k)$.
- Let $r_k := \|\mathbf{x}^k - \mathbf{x}^\star\|$, where $\mathbf{x}^\star$ denotes a minimizer. Show $\boxed{r_k \leq r_0}$.

$$\begin{aligned} r_{k+1}^2 &:= \|\mathbf{x}^{k+1} - \mathbf{x}^\star\|^2 = \|\mathbf{x}^k - \mathbf{x}^\star - \alpha\nabla f(\mathbf{x}^k)\|^2 \\ &= \|\mathbf{x}^k - \mathbf{x}^\star\|^2 - 2\alpha\langle\nabla f(\mathbf{x}^k) - \nabla f(\mathbf{x}^\star), \mathbf{x}^k - \mathbf{x}^\star\rangle + \alpha^2\|\nabla f(\mathbf{x}^k)\|^2 \\ &\leq r_k^2 - \alpha(2/L - \alpha)\|\nabla f(\mathbf{x}^k)\|^2 \quad \text{(by (2))} \\ &\leq r_k^2, \quad \forall\alpha < 2/L. \end{aligned}$$

  Hence, the gradient iterations are contractive when $\alpha < 2/L$ for all $k \geq 0$.

- **An auxiliary result:** Let $\Delta_k := f(\mathbf{x}^k) - f^\star$. Show $\boxed{\Delta_k \leq r_0\|\nabla f(\mathbf{x}^k)\|}$.

$$\Delta_k \leq \langle\nabla f(\mathbf{x}^k), \mathbf{x}^k - \mathbf{x}^\star\rangle \leq \|\nabla f(\mathbf{x}^k)\|\|\mathbf{x}^k - \mathbf{x}^\star\| = r_k\|\nabla f(\mathbf{x}^k)\| \leq r_0\|\nabla f(\mathbf{x}^k)\|.$$

Proof of convergence rates of gradient descent - part III (self-study)

Proof (continued)

- We can establish **convergence** along with the auxiliary result above:

$$f(\mathbf{x}^{k+1}) \leq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x}^{k+1} - \mathbf{x}^k \rangle + \frac{L}{2}\|\mathbf{x}^{k+1} - \mathbf{x}^k\|^2$$
$$= f(\mathbf{x}^k) - \omega_k \|\nabla f(\mathbf{x}^k)\|^2, \quad \omega_k := \alpha(1 - L\alpha/2).$$

Subtract f^* from both sides and apply the last inequality of the previous slide to get $\boxed{\Delta_{k+1} \leq \Delta_k - (\omega_k/r_0^2)\Delta_k^2}$. Thus, dividing by $\Delta_{k+1}\Delta_k$

$$\Delta_{k+1}^{-1} \geq \Delta_k^{-1} + (\omega_k/r_0^2)\Delta_k/\Delta_{k+1} \geq \Delta_k^{-1} + (\omega_k/r_0^2).$$

By induction, we have $\Delta_{k+1}^{-1} \geq \Delta_0^{-1} + (\omega_k/r_0^2)(k+1)$. Then, taking $(\cdot)^{-1}$ of both sides (and hence replacing $\geq$ by $\leq$) and substituting all of the definitions gives

$$f(\mathbf{x}^k) - f(\mathbf{x}^\star) \leq \frac{2(f(\mathbf{x}_0) - f(\mathbf{x}^\star))\|\mathbf{x}_0 - \mathbf{x}^\star\|_2^2}{2\|\mathbf{x}_0 - \mathbf{x}^\star\|_2^2 + k\alpha(2 - \alpha L)(f(\mathbf{x}_0) - f^\star)},$$

- In order to choose the **optimal** step-size, we maximize the function $\phi(\alpha) = \alpha(2 - \alpha L)$. Hence, the optimal step size for the gradient method for $f \in \mathcal{F}_L^{1,1}$ is given by $\alpha = \frac{1}{L}$.
- Finally, since $f(\mathbf{x}_0) \leq f^* + \nabla f(\mathbf{x}^\star)^T(\mathbf{x}_0 - \mathbf{x}^\star) + (L/2)\|\mathbf{x}_0 - \mathbf{x}^\star\|_2^2 = f^* + (L/2)r_0^2$, we obtain (5).

□

Proof of convergence rates of gradient descent - part IV (self-study)

Theorem

- *If* $f \in \mathcal{F}^{2,1}_{L,\mu}$, *with the choice* $\alpha = \frac{2}{L+\mu}$, *the iterates of GD satisfy*

$$\boxed{\|\mathbf{x}^k - \mathbf{x}^\star\|_2 \leq \left(\frac{L-\mu}{L+\mu}\right)^k \|\mathbf{x}^0 - \mathbf{x}^\star\|_2} \tag{6}$$

- *If* $f \in \mathcal{F}^{2,1}_{L,\mu}$, *with the choice* $\alpha = \frac{1}{L}$, *the iterates of GD satisfy*

$$\boxed{\|\mathbf{x}^k - \mathbf{x}^\star\|_2 \leq \left(\frac{L-\mu}{L+\mu}\right)^{\frac{k}{2}} \|\mathbf{x}^0 - \mathbf{x}^\star\|_2} \tag{7}$$

Before proving the convergence rate, we first need a result about functions in $\mathcal{F}^{1,1}_{L,\mu}$. It is proved similarly to (2).

Theorem

If $f \in \mathcal{F}^{1,1}_{L,\mu}$, *then for any* $\mathbf{x}$ *and* $\mathbf{y}$, *we have*

$$\langle \nabla f(\mathbf{x}) - \nabla f(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle \geq \frac{\mu L}{\mu + L}\|\mathbf{x} - \mathbf{y}\|^2 + \frac{1}{\mu + L}\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|^2. \tag{8}$$

Proof of convergence rates of gradient descent - part V (self-study)

Proof of (6) and (7)

- Let $r_k = \|\mathbf{x}^k - \mathbf{x}^\star\|$. Then, using (8) and the fact that $\nabla f(x^*) = 0$, we have

$$\begin{aligned} r_{k+1}^2 &= \|\mathbf{x}_{k+1} - \mathbf{x}^\star - \alpha \nabla f(\mathbf{x}^k)\|^2 \\ &= r_k^2 - 2\alpha\langle \nabla f(\mathbf{x}^k), \mathbf{x}^k - \mathbf{x}^\star\rangle + \alpha^2 \|\nabla f(\mathbf{x}^k)\|^2 \\ &\leq \left(1 - \frac{2\alpha\mu L}{\mu + L}\right) r_k^2 + \alpha\left(\alpha - \frac{2}{\mu + L}\right)\|\nabla f(\mathbf{x}^k)\|^2 \end{aligned}$$

- Since $\mu \leq L$, we have $\alpha \leq \frac{2}{\mu+L}$ in both the cases $\alpha = \frac{1}{L}$ or $\alpha = \frac{2}{\mu+L}$. So the last term in the previous inequality is negative, and hence

$$r_{k+1}^2 \leq \left(1 - \frac{2\alpha\mu L}{\mu + L}\right)^k r_0^2$$

- Plugging $\alpha = \frac{1}{L}$ and $\alpha = \frac{2}{\mu+L}$, we obtain the rates as advertised.
- For $f \in \mathcal{F}_{L,\mu}^{1,1}$, the **optimal** step-size is given by $\alpha = \frac{2}{\mu+L}$ (i.e., it optimizes the worst case bound).

□

Convergence rate of gradient descent

Convergence rate of gradient descent

$$f \in \mathcal{F}_L^{2,1}, \quad \alpha = \frac{1}{L} \qquad\qquad f(\mathbf{x}^k) - f(\mathbf{x}^\star) \leq \frac{2L}{k+4}\|\mathbf{x}^0 - \mathbf{x}^\star\|_2^2$$

$$f \in \mathcal{F}_{L,\mu}^{2,1}, \quad \alpha = \frac{2}{L+\mu} \qquad\qquad \|\mathbf{x}^k - \mathbf{x}^\star\|_2 \leq \left(\frac{L-\mu}{L+\mu}\right)^k \|\mathbf{x}^0 - \mathbf{x}^\star\|_2$$

$$f \in \mathcal{F}_{L,\mu}^{2,1}, \quad \alpha = \frac{1}{L} \qquad\qquad \|\mathbf{x}^k - \mathbf{x}^\star\|_2 \leq \left(\frac{L-\mu}{L+\mu}\right)^{\frac{k}{2}} \|\mathbf{x}^0 - \mathbf{x}^\star\|_2$$

Remarks

- Assumption: Lipschitz gradient. Result: convergence rate in **objective values**.
- Assumption: Strong convexity. Result: convergence rate in **sequence** of the iterates and in **objective values**.
- Note that the suboptimal step-size choice $\alpha = \frac{1}{L}$ **adapts** to the strongly convex case (i.e., it features a linear rate vs. the standard sublinear rate).

Example: Ridge regression

Optimization formulation

- Let $\mathbf{A} \in \mathbb{R}^{n \times p}$ and $\mathbf{b} \in \mathbb{R}^n$ given by the model $\mathbf{b} = \mathbf{A}\mathbf{x}^\natural + \mathbf{w}$, where $\mathbf{w} \in \mathbb{R}^n$ is some noise.
- We can try to estimate $\mathbf{x}^\natural$ by solving the Tikhonov regularized least squares

$$\min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x}) := \frac{1}{2}\|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2^2 + \frac{\rho}{2}\|\mathbf{x}\|_2^2.$$

where $\rho \geq 0$ is a regularization parameter.

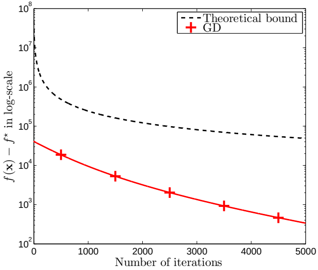
Remarks

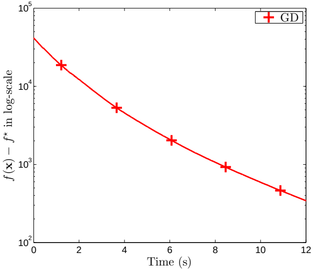
- $f \in \mathcal{F}_{L,\mu}^{2,1}$ with:
  - $L = \lambda_p(\mathbf{A}^T\mathbf{A}) + \rho$;
  - $\mu = \lambda_1(\mathbf{A}^T\mathbf{A}) + \rho$;
  - where $\lambda_1(\mathbf{A}^T\mathbf{A}) \leq \ldots \leq \lambda_p(\mathbf{A}^T\mathbf{A})$ are the eigenvalues of $\mathbf{A}^T\mathbf{A}$.
- The ratio $\frac{L}{\mu}$ decreases as ρ increases, leading to faster linear convergence.
- Note that if $n < p$ and $\rho = 0$, we have $\mu = 0$, hence $f \in \mathcal{F}_L^{2,1}$ and we can expect only $O(1/k)$ convergence from the gradient descent method.

Example: Ridge regression

Case 1:

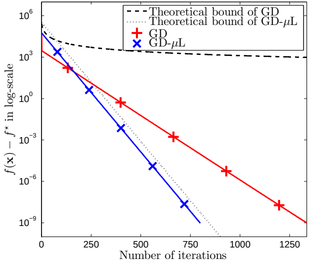
$n = 500, p = 2000, \rho = 0$

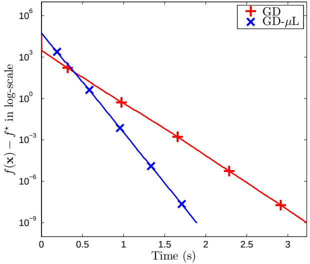




Case 2:

$n = 500, p = 2000, \rho = 0.01\lambda_p(\mathbf{A}^T\mathbf{A})$





Information theoretic lower bounds [3]

What is the **best** achievable rate for a **first-order** method (one using gradient information but not higher-order quantities)?

$f \in \mathcal{F}_L^{\infty,1}$: Smooth and Lipschitz-gradient

It is possible to construct a function in $\mathcal{F}_L^{\infty,1}$, for which **any** first order method must satisfy

$$f(\mathbf{x}^k) - f(\mathbf{x}^\star) \geq \frac{3L}{32(k+1)^2}\|\mathbf{x}^0 - \mathbf{x}^\star\|_2^2 \quad \text{for all } k \leq (p-1)/2$$

$f \in \mathcal{F}_{L,\mu}^{\infty,1}$: Smooth and strongly convex

It is possible to construct a function in $\mathcal{F}_{L,\mu}^{\infty,1}$, for which **any** first order method must satisfy

$$\|\mathbf{x}^k - \mathbf{x}^\star\|_2 \geq \left(\frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}\right)^k \|\mathbf{x}^0 - \mathbf{x}^\star\|_2$$

Gradient descent is $O(1/k)$ for $\mathcal{F}_L^{\infty,1}$ and it is slower for $\mathcal{F}_{L,\mu}^{\infty,1}$, hence it does not achieve the lower bounds!

Accelerated gradient descent algorithm

Problem

Is it possible to design optimal first-order methods with convergence rates matching the theoretical lower bounds?

Accelerated gradient descent algorithm

Problem

Is it possible to design optimal first-order methods with convergence rates matching the theoretical lower bounds?

Solution [Nesterov's accelerated scheme]

Accelerated Gradient (AG) methods achieve optimal convergence rates at a negligible increase in the computational cost.

Accelerated gradient descent algorithm

Problem

Is it possible to design optimal first-order methods with convergence rates matching the theoretical lower bounds?

Solution [Nesterov's accelerated scheme]

Accelerated Gradient (AG) methods achieve optimal convergence rates at a negligible increase in the computational cost.

Accelerated Gradient algorithm for $\mathcal{F}_L^{1,1}$ (AG-L)

1. Set $\mathbf{x}^0 = \mathbf{y}^0 \in \mathrm{dom}(f)$ and $t_0 := 1$.
2. For $k = 0, 1, \ldots,$ iterate

$$\begin{cases} \mathbf{x}^{k+1} &= \mathbf{y}^k - \frac{1}{L}\nabla f(\mathbf{y}^k) \\ t_{k+1} &= (1 + \sqrt{4t_k^2 + 1})/2 \\ \mathbf{y}^{k+1} &= \mathbf{x}^{k+1} + \frac{(t_k - 1)}{t_{k+1}}(\mathbf{x}^{k+1} - \mathbf{x}^k) \end{cases}$$

Accelerated gradient descent algorithm

Problem

Is it possible to design optimal first-order methods with convergence rates matching the theoretical lower bounds?

Solution [Nesterov's accelerated scheme]

Accelerated Gradient (AG) methods achieve optimal convergence rates at a negligible increase in the computational cost.

Accelerated Gradient algorithm for $\mathcal{F}_L^{1,1}$ (AG-L)

1. Set $\mathbf{x}^0 = \mathbf{y}^0 \in \mathrm{dom}(f)$ and $t_0 := 1$.
2. For $k = 0, 1, \ldots,$ iterate

$$\begin{cases} \mathbf{x}^{k+1} &= \mathbf{y}^k - \frac{1}{L}\nabla f(\mathbf{y}^k) \\ t_{k+1} &= (1 + \sqrt{4t_k^2 + 1})/2 \\ \mathbf{y}^{k+1} &= \mathbf{x}^{k+1} + \frac{(t_k - 1)}{t_{k+1}}(\mathbf{x}^{k+1} - \mathbf{x}^k) \end{cases}$$

Accelerated Gradient algorithm for $\mathcal{F}_{L,\mu}^{1,1}$ (AG-μL)

1. Choose $\mathbf{x}^0 = \mathbf{y}^0 \in \mathrm{dom}(f)$
2. For $k = 0, 1, \ldots,$ iterate

$$\begin{cases} \mathbf{x}^{k+1} &= \mathbf{y}^k - \frac{1}{L}\nabla f(\mathbf{y}^k) \\ \mathbf{y}^{k+1} &= \mathbf{x}^{k+1} + \gamma(\mathbf{x}^{k+1} - \mathbf{x}^k) \end{cases}$$

where $\gamma = \frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}$.

Accelerated gradient descent algorithm

Problem

Is it possible to design optimal first-order methods with convergence rates matching the theoretical lower bounds?

Solution [Nesterov's accelerated scheme]

Accelerated Gradient (AG) methods achieve optimal convergence rates at a negligible increase in the computational cost.

Accelerated Gradient algorithm for $\mathcal{F}_L^{1,1}$ (AG-L)

1. Set $\mathbf{x}^0 = \mathbf{y}^0 \in \mathrm{dom}(f)$ and $t_0 := 1$.
2. For $k = 0, 1, \ldots,$ iterate

$$\begin{cases} \mathbf{x}^{k+1} &= \mathbf{y}^k - \frac{1}{L}\nabla f(\mathbf{y}^k) \\ t_{k+1} &= (1 + \sqrt{4t_k^2 + 1})/2 \\ \mathbf{y}^{k+1} &= \mathbf{x}^{k+1} + \frac{(t_k - 1)}{t_{k+1}}(\mathbf{x}^{k+1} - \mathbf{x}^k) \end{cases}$$

Accelerated Gradient algorithm for $\mathcal{F}_{L,\mu}^{1,1}$ (AG-μL)

1. Choose $\mathbf{x}^0 = \mathbf{y}^0 \in \mathrm{dom}(f)$
2. For $k = 0, 1, \ldots,$ iterate

$$\begin{cases} \mathbf{x}^{k+1} &= \mathbf{y}^k - \frac{1}{L}\nabla f(\mathbf{y}^k) \\ \mathbf{y}^{k+1} &= \mathbf{x}^{k+1} + \gamma(\mathbf{x}^{k+1} - \mathbf{x}^k) \end{cases}$$

where $\gamma = \frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}$.

NOTE: AG is not monotone, but the cost-per-iteration is essentially the same as GD.

Global convergence of AGD [3]

Theorem (f is convex with Lipschitz gradient)

If $f \in \mathcal{F}_L^{1,1}$ or $\mathcal{F}_{L,\mu}^{1,1}$, the sequence $\{\mathbf{x}^k\}_{k\geq 0}$ generated by **AGD-L** *satisfies*

$$f(\mathbf{x}^k) - f^\star \leq \frac{4L}{(k+2)^2}\|\mathbf{x}^0 - \mathbf{x}^\star\|_2^2, \ \forall k \geq 0. \tag{9}$$

Global convergence of AGD [3]

Theorem (f is convex with Lipschitz gradient)

If $f \in \mathcal{F}_L^{1,1}$ or $\mathcal{F}_{L,\mu}^{1,1}$, the sequence $\{\mathbf{x}^k\}_{k\geq 0}$ generated by **AGD-L** *satisfies*

$$f(\mathbf{x}^k) - f^\star \leq \frac{4L}{(k+2)^2}\|\mathbf{x}^0 - \mathbf{x}^\star\|_2^2, \ \forall k \geq 0. \tag{9}$$

AGD-L is **optimal** *for $\mathcal{F}_L^{1,1}$ but NOT for $\mathcal{F}_{L,\mu}^{1,1}$!*

Theorem (f is strongly convex with Lipschitz gradient)

If $f \in \mathcal{F}_{L,\mu}^{1,1}$, the sequence $\{\mathbf{x}^k\}_{k\geq 0}$ generated by **AGD-μL** *satisfies*

$$f(\mathbf{x}^k) - f^\star \leq L\left(1 - \sqrt{\frac{\mu}{L}}\right)^k \|\mathbf{x}^0 - \mathbf{x}^\star\|_2^2, \ \forall k \geq 0 \tag{10}$$

$$\|\mathbf{x}^k - \mathbf{x}^\star\|_2 \leq \sqrt{\frac{2L}{\mu}}\left(1 - \sqrt{\frac{\mu}{L}}\right)^{\frac{k}{2}} \|\mathbf{x}^0 - \mathbf{x}^\star\|_2, \ \forall k \geq 0. \tag{11}$$

- AGD-L's iterates are not guaranteed to converge.
- AGD-L does not have a **linear** convergence rate for $\mathcal{F}_{L,\mu}^{1,1}$.
- AGD-μL does, but needs to know μ.

AGD achieves the iteration lowerbound within a constant!

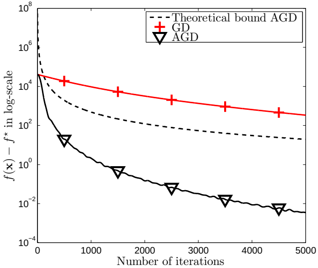
Example: Ridge regression

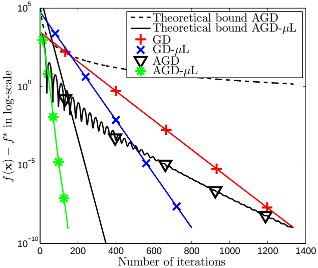
Case 1:

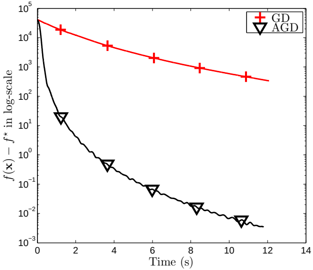
$$n = 500, p = 2000, \rho = 0$$

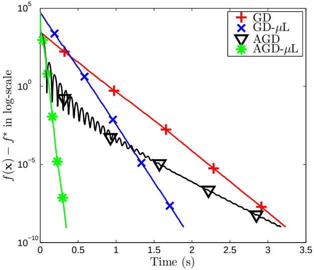
Case 2:

$$n = 500, p = 2000, \rho = 0.01\lambda_p(\mathbf{A}^T\mathbf{A})$$









Enhancements

Two enhancements

1. Line-search for estimating L for both GD and AGD.
2. Restart strategies for AGD.

Enhancements

Two enhancements

1. Line-search for estimating L for both GD and AGD.
2. Restart strategies for AGD.

When do we need a line-search procedure?

We can use a line-search procedure for both GD and AGD when

- L is **known** but it is expensive to evaluate;
- The global constant L usually does not capture the local behavior of f or it is **unknown**;

Enhancements

Two enhancements

1. Line-search for estimating L for both GD and AGD.
2. Restart strategies for AGD.

When do we need a line-search procedure?

We can use a line-search procedure for both GD and AGD when

- L is **known** but it is expensive to evaluate;
- The global constant L usually does not capture the local behavior of f or it is **unknown**;

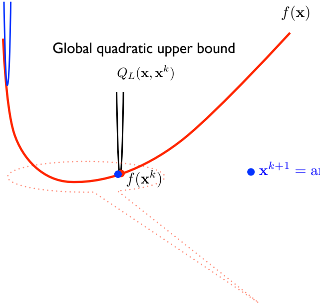
Line-search

At each iteration, we try to find a constant L_k that satisfies:

$$f(\mathbf{x}^{k+1}) \leq Q_{L_k}(\mathbf{x}^{k+1}, \mathbf{y}^k) := f(\mathbf{y}^k) + \langle \nabla f(\mathbf{y}^k), \mathbf{x}^{k+1} - \mathbf{y}^k \rangle + \frac{L_k}{2} \|\mathbf{x}^{k+1} - \mathbf{y}^k\|_2^2.$$

Here: $L_0 > 0$ is given (e.g., $L_0 := c\frac{\|\nabla f(\mathbf{x}^1) - \nabla f(\mathbf{x}^0)\|_2}{\|\mathbf{x}^1 - \mathbf{x}^0\|_2}$) for $c \in (0, 1]$.

How can we better adapt to the local geometry?

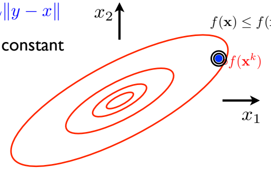


- $\mathbf{x}^{k+1} = \arg\min_{\mathbf{x}} \left\{ f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{L}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2 \right\}$

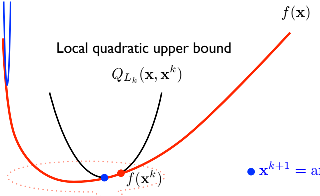
$\|\nabla f(x) - \nabla f(y)\| \leq L\|y - x\|$

L is a global worst-case constant

$$f(\mathbf{x}) \leq f(\mathbf{x}^k) + \nabla f(\mathbf{x}^k)^T(\mathbf{x} - \mathbf{x}^k) + \frac{L}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2$$



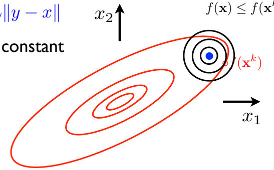
How can we better adapt to the local geometry?



- $\mathbf{x}^{k+1} = \arg\min_{\mathbf{x}} \left\{ f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{L_k}{2} \|\mathbf{x} - \mathbf{x}^k\|_2^2 \right\}$

$$\|\nabla f(x) - \nabla f(y)\| \leq L\|y - x\|$$

L is a global worst-case constant



$$f(\mathbf{x}) \leq f(\mathbf{x}^k) + \nabla f(\mathbf{x}^k)^T(\mathbf{x} - \mathbf{x}^k) + \frac{L_k}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2$$

applies only locally

Enhancements

Why do we need a restart strategy?

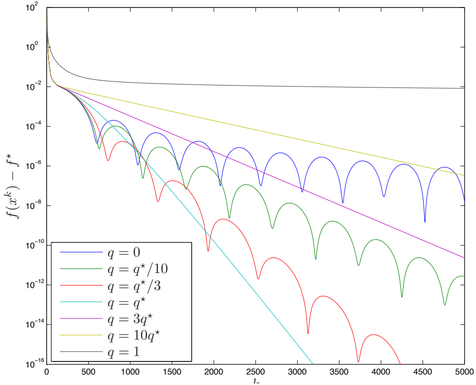
- AG-μL requires knowledge of μ and AG-L does not have optimal convergence for strongly convex f.
- AG is non-monotonic (i.e., $f(\mathbf{x}^{k+1}) \leq f(\mathbf{x}^k)$ is not always satisfied).
- AG has a periodic behavior, where the momentum depends on the local condition number $\kappa = L/\mu$.
- A **restart strategy** tries to reset this momentum whenever we observe high periodic behavior. We often use function values but other strategies are possible.

Restart strategies

1. **O'Donoghue - Candes's strategy [4]:** There are at least three options: Restart with fixed number of iterations, restart based on objective values, and restart based on a gradient condition.
2. **Giselsson-Boyd's strategy [2]:** Do not require $t_k = 1$ and do not necessary require function evaluations.
3. **Fercoq-Qu's strategy [1]:** Unconditional periodic restart for strongly convex functions. Do not require the strong convexity parameter.

Oscillatory behavior of AGD

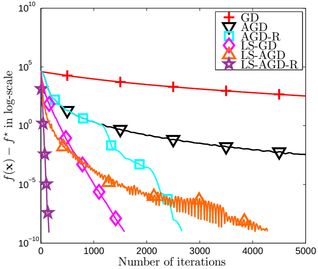
- Minimize a quadratic function $f(\mathbf{x}) = \mathbf{x}^T \boldsymbol{\Phi} \mathbf{x}$, with $p = 200$ and $\kappa(\boldsymbol{\Phi}) = L/\mu = 2.4 \times 10^4$
- Use stepsize $\alpha = 1/L$ and update $\mathbf{x}^{k+1} + \gamma_{k+1}(\mathbf{x}^{k+1} - \mathbf{x}^k)$ where
  - $\gamma_{k+1} = \theta_k(1-\theta_k)/(\theta_k^2 + \theta_{k+1})$
  - θ_{k+1} solves $\theta_{k+1}^2 = (1-\theta_{k+1})\theta_k^2 + q\theta_{k+1}$.
- The parameter q should be equal to the reciprocal of condition number $q^* = \mu/L$.
- A different choice of q might lead to oscillatory behavior.

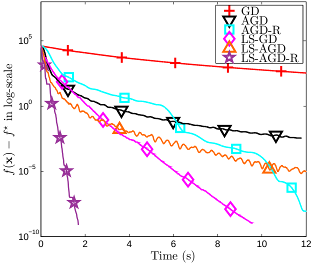


Example: Ridge regression

Case 1:

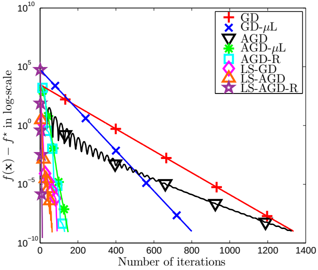
$n = 500, p = 2000, \rho = 0$

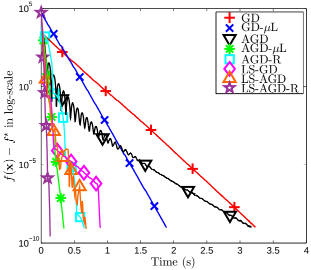




Case 2:

$n = 500, p = 2000, \rho = 0.01\lambda_p(\mathbf{A}^T\mathbf{A})$





The (special) quadratic case – Step-size

Consider the minimization of a quadratic function

$$\min_{\mathbf{x}} f(\mathbf{x}) := \frac{1}{2}\langle \mathbf{x}, \mathbf{A}\mathbf{x}\rangle - \langle \mathbf{b}, \mathbf{x}\rangle$$

where $\mathbf{A}$ is a $p \times p$ symmetric positive definite matrix, i.e., $\mathbf{A} = \mathbf{A}^T \succ 0$.

Gradient Descent

$$\alpha_k = 1/L \quad \text{with } L = \|\mathbf{A}\|$$

Steepest descent

$$\alpha_k = \frac{\|\nabla f(\mathbf{x}^k)\|^2}{\langle \nabla f(\mathbf{x}^k), \mathbf{A}\nabla f(\mathbf{x}^k)\rangle} \tag{12}$$

Barzilai-Borwein

$$\alpha_k = \frac{\|\nabla f(\mathbf{x}^{k-1})\|^2}{\langle \nabla f(\mathbf{x}^{k-1}), \mathbf{A}\nabla f(\mathbf{x}^{k-1})\rangle} \tag{13}$$

The (special) quadratic case – convergence rates

For $f(\mathbf{x}) = \frac{1}{2}\langle \mathbf{x}, \mathbf{A}\mathbf{x}\rangle - \langle \mathbf{b}, \mathbf{x}\rangle$, we have $L = \|\mathbf{A}\| = \lambda_p$ and $\mu = \lambda_1$, where $0 < \lambda_1 \leq \lambda_2 \leq \cdots \lambda_p$ are the eigenvalues of $\mathbf{A}$.

Theorem (Gradient Descent)

$$\|\mathbf{x}^k - \mathbf{x}^\star\|_2 \leq \left(1 - \frac{\lambda_1}{\lambda_p}\right)^k \|\mathbf{x}^0 - \mathbf{x}^\star\|_2$$

Theorem (Steepest Descent)

$$\|\mathbf{x}^{k+1} - \mathbf{x}^\star\|_{\mathbf{A}} \leq \left(\frac{\lambda_p - \lambda_1}{\lambda_p + \lambda_1}\right)^k \|\mathbf{x}^0 - \mathbf{x}^\star\|_{\mathbf{A}}$$

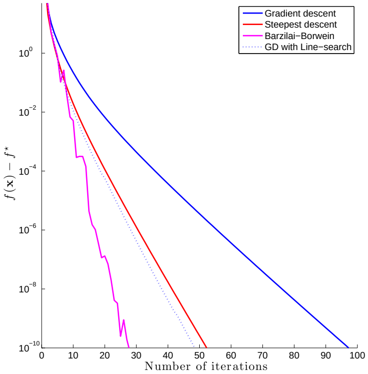
Theorem (Barzilai-Borwein)

Under the condition $\lambda_p < 2\lambda_1$

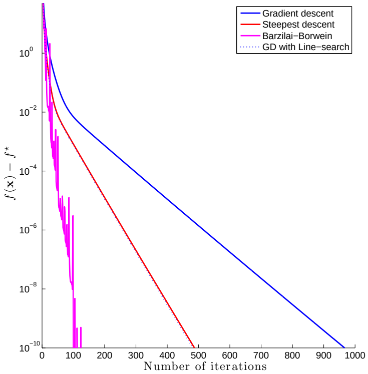
$$\|\mathbf{x}^{k+1} - \mathbf{x}^\star\|_2 \leq \left(\frac{\lambda_p - \lambda_1}{\lambda_1}\right)^k \|\mathbf{x}^0 - \mathbf{x}^\star\|_2$$

Example: Quadratic function

<u>Case 1:</u> $n = p = 100, \kappa(\mathbf{A}) = 10$



<u>Case 1:</u> $n = p = 100, \kappa(\mathbf{A}) = 100$



References I

[1] Olivier Fercoq and Zheng Qu.
Restarting accelerated gradient methods with a rough strong convexity estimate.
2016.
arXiv:16009.07358v1.

[2] Pontus Giselsson and Stephen Boyd.
Monotonicity and restart in fast gradient methods.
In *IEEE 53rd Ann. Conf. Decision and Control*, pages 5058–5063, 2014.

[3] Yu. Nesterov.
Introductory Lectures on Convex Optimization: A Basic Course.
Kluwer, Boston, MA, 2004.

[4] Brendan O'Donoghue and Emmanuel Candes.
Adaptive restart for accelerated gradient schemes.
Found. Comput. Math., 15(3):715–732, 2015.