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

- This work is released under a [Creative Commons License](#) with the following terms:
  - **Attribution**
    - The licensor permits others to copy, distribute, display, and perform the work. In return, licensees must give the original authors credit.
  - **Non-Commercial**
    - The licensor permits others to copy, distribute, display, and perform the work. In return, licensees may not use the work for commercial purposes – unless they get the licensor’s permission.
  - **Share Alike**
    - The licensor permits others to distribute derivative works only under a license identical to the one that governs the licensor’s work.
  - [Full Text of the License](#)
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

## Overview

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

Problem (Mathematical formulation)

\[
F^* := \min_{x \in \mathbb{R}^p} \{ F(x) := f(x) \}
\]  \hspace{1cm} (1)

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

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

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

until $x_k$ is $\epsilon$-optimal.

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

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

where $p^k$ 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 $\alpha_k$ and $p^k$.
- 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:

\[ x^{k+1} = x^k + \alpha_k p^k \]

By Taylor’s theorem, we have

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

For \( \alpha_k \) small enough, the term \( \alpha_k \langle \nabla f(x^k), p^k \rangle \) dominates \( O(\alpha_k^2) \) for a fixed \( p^k \).

Therefore, in order to have \( f(x^{k+1}) < f(x^k) \), we require

\[ \langle \nabla f(x^k), p^k \rangle < 0 \]
Basic principles of descent methods

Local steepest descent direction

Since

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

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

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

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 $\mu$-strong convexity
Gradient descent methods

Gradient descent (GD) algorithm

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

\[ p^k = -\nabla f(x^k) \]

so that

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

**Key question:** How do we choose \( \alpha_k \) 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:

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

so that

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

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

**Answer**: By exploiting the structures within the convex function

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

- **Second-order methods** also use the Hessian \( \nabla^2 f \).
Recall: Gradient descent methods - a geometrical intuition

\[ f(x) \]

\[ x^* \quad x^k \]
Recall: Gradient descent methods - a geometrical intuition

Structure in optimization:

\[(1) \quad f(x) \geq f(x^k) + \langle \nabla f(x^k), x - x^k \rangle \]
Recall: Gradient descent methods - a geometrical intuition

Majorize:
\[ f(x) \leq f(x^k) + \langle \nabla f(x^k), x - x^k \rangle + \frac{L}{2} \| x - x^k \|^2 := Q_L(x, x^k) \]

Minimize:
\[ x^{k+1} = \arg \min_x Q_L(x, x^k) \]
\[ = \arg \min_x \left\| x - \left( x^k - \frac{1}{L} \nabla f(x^k) \right) \right\|^2 \]
\[ = x^k - \frac{1}{L} \nabla f(x^k) \]

Structure in optimization:
(1) \[ f(x) \geq f(x^k) + \langle \nabla f(x^k), x - x^k \rangle \]
(2) \[ f(x) \leq f(x^k) + \langle \nabla f(x^k), x - x^k \rangle + \frac{L}{2} \| x - x^k \|^2 \]
Recall: Gradient descent methods - a geometrical intuition

Majorize:

\[ f(x) \leq f(x^k) + \langle \nabla f(x^k), x - x^k \rangle + \frac{L'}{2} \| x - x^k \|^2 := Q_L'(x, x^k) \]

Minimize:

\[ x^{k+1} = \arg\min_x Q_L'(x, x^k) \]

\[ = \arg\min_x \left\| x - \left( x^k - \frac{1}{L'} \nabla f(x^k) \right) \right\|^2 \]

\[ = x^k - \frac{1}{L'} \nabla f(x^k) \]

Structure in optimization:

(1) \[ f(x) \geq f(x^k) + \langle \nabla f(x^k), x - x^k \rangle \]

(2) \[ f(x) \leq f(x^k) + \langle \nabla f(x^k), x - x^k \rangle + \frac{L}{2} \| x - x^k \|^2 \]
Recall: Gradient descent methods - a geometrical intuition

**Majorize:**
\[
f(x) \leq f(x^k) + \langle \nabla f(x^k), x - x^k \rangle + \frac{L}{2} \| x - x^k \|^2 := Q_L(x, x^k)
\]

**Minimize:**
\[
x^{k+1} = \arg\min_x Q_L(x, x^k)
\]
\[
= \arg\min_x \left\| x - \left( x^k - \frac{1}{L} \nabla f(x^k) \right) \right\|^2
\]
\[
= x^k - \frac{1}{L} \nabla f(x^k)
\]

**Structure in optimization:**

1. \[
f(x) \geq f(x^k) + \langle \nabla f(x^k), x - x^k \rangle
\]
2. \[
f(x) \leq f(x^k) + \langle \nabla f(x^k), x - x^k \rangle + \frac{L}{2} \| x - x^k \|^2
\]
3. \[
f(x) \geq f(x^k) + \langle \nabla f(x^k), x - x^k \rangle + \frac{\mu}{2} \| x - x^k \|^2
\]
Convergence rate of gradient descent

Theorem

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

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

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

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

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

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

$$\|x^k - x^*\|_2 \leq \left( \frac{L - \mu}{L + \mu} \right)^{\frac{k}{2}} \|x^0 - x^*\|_2$$
Proof of convergence rates of gradient descent

- 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

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

**Proof (Advanced material).**

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

$$h(x) \leq h(y) + \langle \nabla h(y), x - y \rangle + \frac{L}{2} \|x - y\|^2.$$  \hspace{1cm} (3)

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

$$\phi(x) \leq \phi \left( y - \frac{1}{L} \nabla \phi(y) \right) \leq \phi(y) - \frac{1}{2L} \|\nabla \phi(y)\|^2.$$  \hspace{1cm} (4)

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

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

By adding two copies of (4) with each other, with $x$ and $y$ swapped, we obtain (2).
The proof of convergence rates - part I

**Theorem**

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

\[
f(x^k) - f(x^*) \leq \frac{2L}{k+4} \|x^0 - x^*\|_2^2
\]  

(5)

**Proof - part I**

- Consider the constant step-size iteration \( x^{k+1} = x^k - \alpha \nabla f(x^k) \).

- Let \( r_k := \|x^k - x^*\| \), where \( x^* \) denotes a minimizer. Show \( r_k \leq r_0 \).

\[
r_{k+1}^2 := \|x^{k+1} - x^*\|^2 = \|x^k - x^* - \alpha \nabla f(x^k)\|^2
\]

\[
= \|x^k - x^*\|^2 - 2\alpha \langle \nabla f(x^k) - \nabla f(x^*), x^k - x^* \rangle + \alpha^2 \|\nabla f(x^k)\|^2
\]

\[
\leq r_k^2 - \alpha(2/L - \alpha)\|\nabla f(x^k)\|^2 \quad \text{(by (2))}
\]

\[
\leq r_k^2, \quad \forall \alpha < 2/L.
\]

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

- An auxiliary result: Let \( \Delta_k := f(x^k) - f^* \). Show \( \Delta_k \leq r_0 \|\nabla f(x^k)\| \).

\[
\Delta_k \leq \langle \nabla f(x^k), x^k - x^* \rangle \leq \|\nabla f(x^k)\| \|x^k - x^*\| = r_k \|\nabla f(x^k)\| \leq r_0 \|\nabla f(x^k)\|.
\]
We can establish convergence along with the auxiliary result above:

\[
f(x^{k+1}) \leq f(x^k) + \langle \nabla f(x^k), x^{k+1} - x^k \rangle + \frac{L}{2} \|x^{k+1} - x^k\|^2
\]

\[
= f(x^k) - \omega_k \|\nabla f(x^k)\|^2, \quad \omega_k := \alpha (1 - L\alpha/2).
\]

Subtract \( f^* \) from both sides and apply the last inequality of the previous slide to get

\[
\Delta_{k+1} \leq \Delta_k - \left( \omega_k / r_0^2 \right) \Delta_k^2.
\]

Thus, dividing by \( \Delta_{k+1} \Delta_k \)

\[
\Delta_{k+1}^{-1} \geq \Delta_k^{-1} + \left( \omega_k / r_0^2 \right) \Delta_k / \Delta_{k+1} \geq \Delta_k^{-1} + \left( \omega_k / r_0^2 \right).
\]

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

\[
f(x^k) - f(x^*) \leq \frac{2(f(x_0) - f(x^*))\|x_0 - x^*\|^2}{2\|x_0 - x^*\|^2 + k\alpha(2 - \alpha L)(f(x_0) - f^*)},
\]

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 \( f \in \mathcal{F}^{1,1}_L \) is given by \( \alpha = \frac{1}{L} \).

Finally, since \( f(x_0) \leq f^* + \nabla f(x^*)^T (x_0 - x^*) + (L/2)\|x_0 - x^*\|^2 = f^* + (L/2)r_0^2 \), we obtain (5).
The proof of convergence rates - part III

**Theorem**

- If $f \in \mathcal{F}_{L,\mu}^{2,1}$, with the choice $\alpha = \frac{2}{L+\mu}$, the iterates of GD satisfy
  \[ \|x^k - x^*\|_2 \leq \left( \frac{L - \mu}{L + \mu} \right)^k \|x^0 - x^*\|_2 \]  
  \[ (6) \]

- If $f \in \mathcal{F}_{L,\mu}^{2,1}$, with the choice $\alpha = \frac{1}{L}$, the iterates of GD satisfy
  \[ \|x^k - x^*\|_2 \leq \left( \frac{L - \mu}{L + \mu} \right)^{\frac{k}{2}} \|x^0 - x^*\|_2 \]  
  \[ (7) \]

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

**Theorem**

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

\[ \langle \nabla f(x) - \nabla f(y), x - y \rangle \geq \frac{\mu L}{\mu + L} \|x - y\|^2 + \frac{1}{\mu + L} \|\nabla f(x) - \nabla f(y)\|^2. \]  
[8]
The proof of convergence rates - part III

Proof of (6) and (7)

- Let $r_k = \|x^k - x^*\|$. Then, using (8) and the fact that $\nabla f(x^*) = 0$, we have
  \[
  r_{k+1}^2 = \|x_{k+1} - x^* - \alpha \nabla f(x^k)\|^2 \\
  = r_k^2 - 2\alpha \langle \nabla f(x^k), x^k - x^* \rangle + \alpha^2 \|\nabla f(x^k)\|^2 \\
  \leq \left(1 - \frac{2\alpha \mu L}{\mu + L}\right) r_k^2 + \alpha \left(\alpha - \frac{2}{\mu + L}\right) \|\nabla f(x^k)\|^2
  \]

- 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
  \[
  r_{k+1}^2 \leq \left(1 - \frac{2\alpha \mu L}{\mu + L}\right) r_k^2 
  \]

- 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).

\[\square\]
## Convergence rate of gradient descent

### Convergence rate of gradient descent

\[
f \in \mathcal{F}^2_1, \quad \alpha = \frac{1}{L} \quad \Rightarrow \quad f(x^k) - f(x^*) \leq \frac{2L}{k+4} \|x^0 - x^*\|^2_2
\]

\[
f \in \mathcal{F}^2_{L,\mu}, \quad \alpha = \frac{2}{L + \mu} \quad \Rightarrow \quad \|x^k - x^*\|^2_2 \leq \left(\frac{L - \mu}{L + \mu}\right)^k \|x^0 - x^*\|^2_2
\]

\[
f \in \mathcal{F}^2_{L,\mu}, \quad \alpha = \frac{1}{L} \quad \Rightarrow \quad \|x^k - x^*\|^2_2 \leq \left(\frac{L - \mu}{L + \mu}\right)^{k/2} \|x^0 - x^*\|^2_2
\]

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

\[
\min_{x \in \mathbb{R}^p} f(x) := \frac{1}{2} \left\| b - Ax \right\|_2^2 + \frac{\rho}{2} \left\| x \right\|_2^2.
\]

where \( \rho \geq 0 \) is a regularization parameter.

Remarks

- \( f \in \mathcal{F}_{L,\mu}^{2,1} \) with:
  - \( L = \lambda_p (A^T A) + \rho; \)
  - \( \mu = \lambda_1 (A^T A) + \rho; \)
  - where \( \lambda_1 (A^T A) \leq \ldots \leq \lambda_p (A^T A) \) are the eigenvalues of \( A^T A \).
- The ratio \( \frac{L}{\mu} \) decreases as \( \rho \) 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:**

\( n = 500, \, p = 2000, \, \rho = 0.01 \lambda_p (A^T A) \)
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)?

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

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

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

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

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

\[
\|x^k - x^*\|_2 \geq \left( \frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}} \right)^k \|x^0 - x^*\|_2
\]

Gradient descent is \( O(1/k) \) for \( \mathcal{F}^{\infty,1}_L \) and it is slower for \( \mathcal{F}^{\infty,1}_{L,\mu} \), 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?

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 $F_{1,1L}$ ($AG-L$)

1. Set $x_0 = y_0 \in \text{dom}(f)$ and $t_0 = 1$.

2. For $k = 0, 1, \ldots$, iterate

$$
\begin{align*}
    x_{k+1} &= y_k - \frac{1}{L} \nabla f(y_k) \\
    t_{k+1} &= \frac{1 + \sqrt{4t_k^2 + 1}}{2} \\
    y_{k+1} &= x_{k+1} + \frac{t_k - 1}{t_k + 1} (x_{k+1} - x_k)
\end{align*}
$$

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

<table>
<thead>
<tr>
<th>Problem</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Is it possible to design optimal first-order methods with convergence rates matching the theoretical lower bounds?</em></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Solution [Nesterov’s accelerated scheme]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Accelerated Gradient (AG) methods achieve optimal convergence rates at a negligible increase in the computational cost.</td>
</tr>
</tbody>
</table>
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 $\mathcal{F}_{L,\mu}^{1,1}$ (AG-L)

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

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

NOTE: AG is not monotone, but the cost-per-iteration is essentially the same as GD.
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 $\mathcal{F}_{L,1}^{1,1}$ (AG-L)

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

\[
\begin{align*}
    x^{k+1} &= y^k - \frac{1}{L} \nabla f(y^k) \\
    t_{k+1} &= (1 + \sqrt{4t_k^2 + 1})/2 \\
    y^{k+1} &= x^{k+1} + \frac{(t_k - 1)}{t_{k+1}} (x^{k+1} - x^k)
\end{align*}
\]

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

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

\[
\begin{align*}
    x^{k+1} &= y^k - \frac{1}{L} \nabla f(y^k) \\
    y^{k+1} &= x^{k+1} + \gamma (x^{k+1} - x^k)
\end{align*}
\]

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.
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 $\mathcal{F}_{L,1}^{1,1}$ (AG-L)

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

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

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

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

   \[
   \begin{align*}
   \mathbf{x}^{k+1} &= \mathbf{y}^k - \frac{1}{L} \nabla f(\mathbf{y}^k) \\
   \mathbf{y}^{k+1} &= \mathbf{x}^{k+1} + \gamma (\mathbf{x}^{k+1} - \mathbf{x}^k)
   \end{align*}
   \]

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

\[
    f(x^k) - f^* \leq \frac{4L}{(k + 2)^2} \|x^0 - x^*\|_2^2, \quad \forall k \geq 0.
\]  

(9)
Global convergence of AGD [3]

**Theorem (f is convex with Lipschitz gradient)**

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

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

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

**Theorem (f is strongly convex with Lipschitz gradient)**

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

\[
\begin{align*}
f(x^k) - f^* & \leq L \left(1 - \sqrt{\frac{\mu}{L}}\right)^k \|x^0 - x^*\|_2^2, \ \forall k \geq 0 \tag{10} \\
\|x^k - x^*\|_2 & \leq \frac{2L}{\mu} \left(1 - \sqrt{\frac{\mu}{L}}\right)^{k/2} \|x^0 - x^*\|_2, \ \forall k \geq 0. \tag{11}
\end{align*}
\]

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

**AGD achieves the iteration lowerbound within a constant!**
Example: Ridge regression

Case 1:
\[ n = 500, p = 2000, \rho = 0 \]

Case 2:
\[ n = 500, p = 2000, \rho = 0.01\lambda_p (A^T A) \]
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:

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

Here: $L_0 > 0$ is given (e.g., $L_0 := c \frac{\| \nabla f(x^1) - \nabla f(x^0) \|_2}{\| x^1 - x^0 \|_2}$) for $c \in (0, 1]$. 
How can we better adapt to the local geometry?

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

\[ \| \nabla f(x) - \nabla f(y) \| \leq L \| y - x \| \]

L is a global worst-case constant.

Global quadratic upper bound:

\[ Q_L(x, x^k) \]
How can we better adapt to the local geometry?

$$f(x)$$

Local quadratic upper bound

$$Q_{L_k}(x, x^k)$$

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

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

$L$ is a global worst-case constant

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

Why do we need a restart strategy?

- AG-$\mu L$ requires knowledge of $\mu$ and AG-$L$ does not have optimal convergence for strongly convex $f$.
- AG is non-monotonic (i.e., $f(x^{k+1}) \leq f(x^k)$ 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 - Candès’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 \( f(x) = x^T \Phi x \), with \( p = 200 \) and \( \kappa(\Phi) = L/\mu = 2.4 \times 10^4 \)
- Use stepsize \( \alpha = 1/L \) and update \( x^{k+1} + \gamma_{k+1}(x^{k+1} - x^k) \) where
  - \( \gamma_{k+1} = \theta_k (1 - \theta_k)/(\theta_k^2 + \theta_{k+1}) \)
  - \( \theta_{k+1} \) 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.

![Figure 1: Convergence of Algorithm 1 with different estimates of \( q \).](image)
Example: Ridge regression

**Case 1:**
\[ n = 500, \ p = 2000, \ \rho = 0 \]

**Case 2:**
\[ n = 500, \ p = 2000, \ \rho = 0.01 \lambda_p (A^T A) \]
The (special) quadratic case – Step-size

Consider the minimization of a quadratic function

\[
\min_x f(x) := \frac{1}{2} \langle x, Ax \rangle - \langle b, x \rangle
\]

where \( A \) is a \( p \times p \) symmetric positive definite matrix, i.e., \( A = A^T > 0 \).

**Gradient Descent**

\[
\alpha_k = 1/L \quad \text{with} \quad L = \|A\|
\]

**Steepest descent**

\[
\alpha_k = \frac{\|\nabla f(x^k)\|^2}{\langle \nabla f(x^k), A \nabla f(x^k) \rangle} \quad (12)
\]

**Barzilai-Borwein**

\[
\alpha_k = \frac{\|\nabla f(x^{k-1})\|^2}{\langle \nabla f(x^{k-1}), A \nabla f(x^{k-1}) \rangle} \quad (13)
\]
The (special) quadratic case – convergence rates

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

**Theorem (Gradient Descent)**

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

**Theorem (Steepest Descent)**

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

**Theorem (Barzilai-Borwein)**

Under the condition $\lambda_p < 2\lambda_1$

$$\|x^{k+1} - x^*\|_2 \leq \left(\frac{\lambda_p - \lambda_1}{\lambda_1}\right)^k \|x^0 - x^*\|_2$$
Example: Quadratic function

**Case 1:** \( n = p = 100, \kappa(A) = 10 \)

**Case 1:** \( n = p = 100, \kappa(A) = 100 \)
References I

Restarting accelerated gradient methods with a rough strong convexity estimate.
2016.

Monotonicity and restart in fast gradient methods.

Introductory Lectures on Convex Optimization: A Basic Course.

Adaptive restart for accelerated gradient schemes.