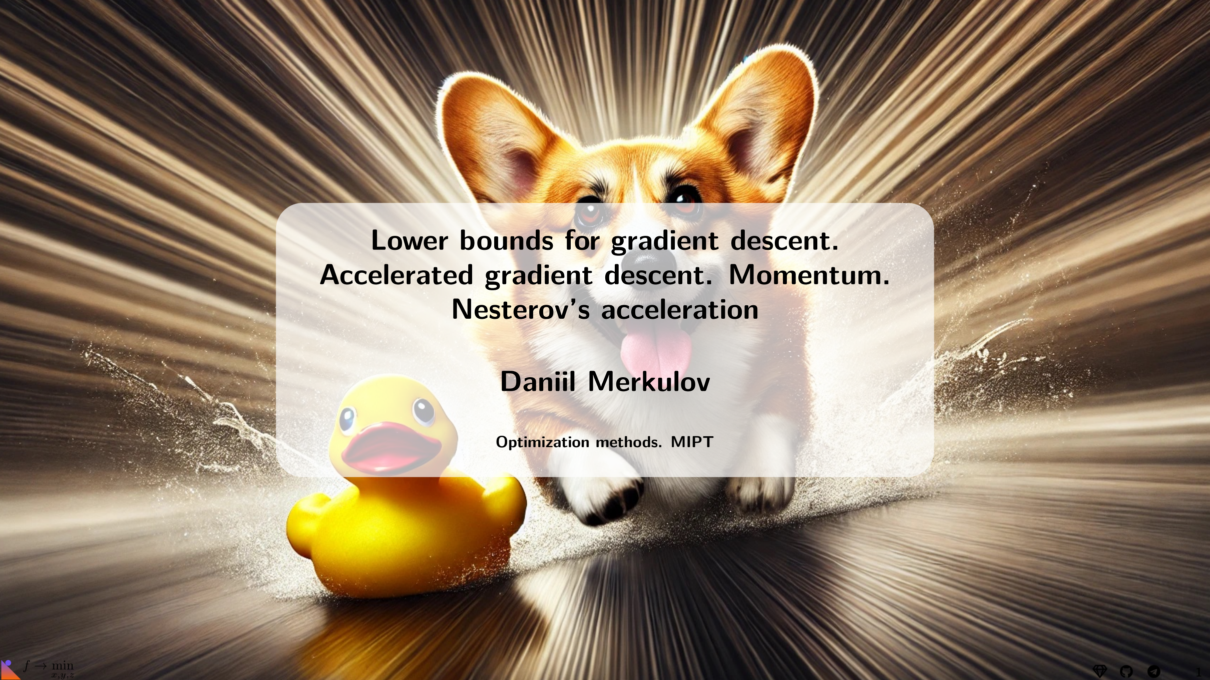

Lower bounds for gradient descent. Accelerated gradient descent. Momentum. Nesterov's acceleration

Daniil Merkulov

Optimization methods. MIPT

Recap of Gradient Descent convergence

Gradient Descent: $\min\limits_{x \in \mathbb{R}^n} f(x)$ $\qquad x^{k+1} = x^k - \alpha^k \nabla f(x^k)$

convex (non-smooth)	smooth (non-convex)	smooth & convex	smooth & strongly convex (or PL)
$f(x^k) - f^* \sim \mathcal{O}\left(\dfrac{1}{\sqrt{k}}\right)$ $k_\varepsilon \sim \mathcal{O}\left(\dfrac{1}{\varepsilon^2}\right)$	$\|\nabla f(x^k)\|^2 \sim \mathcal{O}\left(\dfrac{1}{k}\right)$ $k_\varepsilon \sim \mathcal{O}\left(\dfrac{1}{\varepsilon}\right)$	$f(x^k) - f^* \sim \mathcal{O}\left(\dfrac{1}{k}\right)$ $k_\varepsilon \sim \mathcal{O}\left(\dfrac{1}{\varepsilon}\right)$	$\|x^k - x^*\|^2 \sim \mathcal{O}\left(\left(1 - \dfrac{\mu}{L}\right)^k\right)$ $k_\varepsilon \sim \mathcal{O}\left(\varkappa \log \dfrac{1}{\varepsilon}\right)$

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For smooth strongly convex we have:

$$f(x^k) - f^* \leq \left(1 - \frac{\mu}{L}\right)^k (f(x^0) - f^*).$$

Note also, that for any x, since e^{-x} is convex and $1 - x$ is its tangent line at $x = 0$, we have:

$$1 - x \leq e^{-x}$$

Recap of Gradient Descent convergence

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Finally we have

$$\begin{aligned}
\varepsilon = f(x^{k_\varepsilon}) - f^* &\leq \left(1 - \frac{\mu}{L}\right)^{k_\varepsilon} (f(x^0) - f^*) \\
&\leq \exp\left(-k_\varepsilon \frac{\mu}{L}\right) (f(x^0) - f^*) \\
k_\varepsilon \geq \varkappa \log \frac{f(x^0) - f^*}{\varepsilon} &= \mathcal{O}\left(\varkappa \log \frac{1}{\varepsilon}\right)
\end{aligned}$$

Recap of Gradient Descent convergence

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convex (non-smooth)	smooth (non-convex)	smooth & convex	smooth & strongly convex (or PL)
$f(x^k) - f^* \sim \mathcal{O}\left(\dfrac{1}{\sqrt{k}}\right)$	$\\|\nabla f(x^k)\\|^2 \sim \mathcal{O}\left(\dfrac{1}{k}\right)$	$f(x^k) - f^* \sim \mathcal{O}\left(\dfrac{1}{k}\right)$	$\\|x^k - x^*\\|^2 \sim \mathcal{O}\left(\left(1 - \dfrac{\mu}{L}\right)^k\right)$
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Question: Can we do faster, than this using the first-order information?

Recap of Gradient Descent convergence

Gradient Descent: $\min_{x \in \mathbb{R}^n} f(x)$ $\qquad x^{k+1} = x^k - \alpha^k \nabla f(x^k)$

convex (non-smooth)	smooth (non-convex)	smooth & convex	smooth & strongly convex (or PL)
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$$

Question: Can we do faster, than this using the first-order information? **Yes, we can.**

Lower bounds

Lower bounds

convex (non-smooth)	smooth (non-convex)[1]	smooth & convex[2]	smooth & strongly convex (or PL)
$\mathcal{O}\left(\dfrac{1}{\sqrt{k}}\right)$ $k_\varepsilon \sim \mathcal{O}\left(\dfrac{1}{\varepsilon^2}\right)$	$\mathcal{O}\left(\dfrac{1}{k^2}\right)$ $k_\varepsilon \sim \mathcal{O}\left(\dfrac{1}{\sqrt{\varepsilon}}\right)$	$\mathcal{O}\left(\dfrac{1}{k^2}\right)$ $k_\varepsilon \sim \mathcal{O}\left(\dfrac{1}{\sqrt{\varepsilon}}\right)$	$\mathcal{O}\left(\left(1 - \sqrt{\dfrac{\mu}{L}}\right)^k\right)$ $k_\varepsilon \sim \mathcal{O}\left(\sqrt{\varkappa} \log \dfrac{1}{\varepsilon}\right)$

[1] Carmon, Duchi, Hinder, Sidford, 2017

[2] Nemirovski, Yudin, 1979

Black box iteration

The iteration of gradient descent:

$$
\begin{aligned}
x^{k+1} &= x^k - \alpha^k \nabla f(x^k) \\
&= x^{k-1} - \alpha^{k-1} \nabla f(x^{k-1}) - \alpha^k \nabla f(x^k) \\
&\;\vdots \\
&= x^0 - \sum_{i=0}^{k} \alpha^{k-i} \nabla f(x^{k-i})
\end{aligned}
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\end{aligned}
$$

Consider a family of first-order methods, where

$$
\begin{aligned}
x^{k+1} &\in x^0 + \text{span}\left\{\nabla f(x^0), \nabla f(x^1), \ldots, \nabla f(x^k)\right\} & f \text{ - smooth} \\
x^{k+1} &\in x^0 + \text{span}\left\{g_0, g_1, \ldots, g_k\right\}\text{, where } g_i \in \partial f(x^i) & f \text{ - non-smooth}
\end{aligned}
\tag{1}
$$

Black box iteration

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x^{k+1} &\in x^0 + \text{span}\left\{g_0, g_1, \dots, g_k\right\}, \text{ where } g_i \in \partial f(x^i) & f \text{ - non-smooth}
\end{aligned}
\tag{1}
$$

In order to construct a lower bound, we need to find a function f from corresponding class such that any method from the family 1 will work at least as slow as the lower bound.

Smooth case

Theorem

There exists a function f that is L-smooth and convex such that any method 1 satisfies for any $k : 1 \leq k \leq \frac{n-1}{2}$:

$$
f(x^k) - f^* \geq \frac{3L\|x^0 - x^*\|_2^2}{32(k+1)^2}
$$

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- No matter what gradient method you provide, there is always a function f that, when you apply your gradient method on minimizing such f, the convergence rate is lower bounded as $\mathcal{O}\left(\frac{1}{k^2}\right)$.

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- Note, that this bound $\mathcal{O}\left(\frac{1}{k^2}\right)$ does not match the rate of gradient descent $\mathcal{O}\left(\frac{1}{k}\right)$. Two options possible:
  a. The lower bound is not tight.
  b. **The gradient method is not optimal for this problem.**

Nesterov's worst function

- Let $n = 2k + 1$ and $A \in \mathbb{R}^{n \times n}$.

$$
A = \begin{bmatrix}
2 & -1 & 0 & 0 & \cdots & 0 \\
-1 & 2 & -1 & 0 & \cdots & 0 \\
0 & -1 & 2 & -1 & \cdots & 0 \\
0 & 0 & -1 & 2 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
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\end{bmatrix}
$$

- Notice, that

$$
x^T A x = x_1^2 + x_n^2 + \sum_{i=1}^{n-1} (x_i - x_{i+1})^2,
$$

Therefore, $x^T A x \geq 0$. It is also easy to see that $0 \preceq A \preceq 4I$.

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Example, when $n = 3$:

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A = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}
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A = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}
$$

Lower bound:

$$
\begin{aligned}
x^T A x &= 2x_1^2 + 2x_2^2 + 2x_3^2 - 2x_1 x_2 - 2x_2 x_3 \\
&= x_1^2 + x_1^2 - 2x_1 x_2 + x_2^2 + x_2^2 - 2x_2 x_3 + x_3^2 + x_3^2 \\
&= x_1^2 + (x_1 - x_2)^2 + (x_2 - x_3)^2 + x_3^2 \geq 0
\end{aligned}
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- Let $n = 2k+1$ and $A \in \mathbb{R}^{n \times n}$.

$$A = \begin{bmatrix} 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 \\ 0 & 0 & -1 & 2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 2 \end{bmatrix}$$

- Notice, that

$$x^T A x = x_1^2 + x_n^2 + \sum_{i=1}^{n-1} (x_i - x_{i+1})^2,$$

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Example, when $n = 3$:

$$A = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$$

Lower bound:

$$\begin{aligned} x^T A x &= 2x_1^2 + 2x_2^2 + 2x_3^2 - 2x_1x_2 - 2x_2x_3 \\ &= x_1^2 + x_1^2 - 2x_1x_2 + x_2^2 + x_2^2 - 2x_2x_3 + x_3^2 + x_3^2 \\ &= x_1^2 + (x_1 - x_2)^2 + (x_2 - x_3)^2 + x_3^2 \geq 0 \end{aligned}$$

Upper bound

$$\begin{aligned} x^T A x &= 2x_1^2 + 2x_2^2 + 2x_3^2 - 2x_1x_2 - 2x_2x_3 \\ &\leq 4(x_1^2 + x_2^2 + x_3^2) \\ 0 &\leq 2x_1^2 + 2x_2^2 + 2x_3^2 + 2x_1x_2 + 2x_2x_3 \\ 0 &\leq x_1^2 + x_1^2 + 2x_1x_2 + x_2^2 + x_2^2 + 2x_2x_3 + x_3^2 + x_3^2 \\ 0 &\leq x_1^2 + (x_1 + x_2)^2 + (x_2 + x_3)^2 + x_3^2 \end{aligned}$$

Nesterov's worst function

- Define the following L-smooth convex function: $f(x) = \frac{L}{4}\left(\frac{1}{2}x^T A x - e_1^T x\right) = \frac{L}{8}x^T A x - \frac{L}{4}e_1^T x$.

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- Define the following L-smooth convex function: $f(x) = \frac{L}{4}\left(\frac{1}{2}x^T Ax - e_1^T x\right) = \frac{L}{8}x^T Ax - \frac{L}{4}e_1^T x$.
- The optimal solution x^* satisfies $Ax^* = e_1$, and solving this system of equations gives:

$$\begin{bmatrix} 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 \\ 0 & 0 & -1 & 2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 2 \end{bmatrix} \begin{bmatrix} x_1^* \\ x_2^* \\ x_3^* \\ \vdots \\ x_n^* \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \qquad \begin{cases} 2x_1^* - x_2^* = 1 \\ -x_i^* + 2x_{i+1}^* - x_{i+2}^* = 0, \ i = 2, \ldots, n-1 \\ -x_{n-1}^* + 2x_n^* = 0 \end{cases}$$

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- The hypothesis: $x_i^* = a + bi$ (inspired by physics). Check, that the second equation is satisfied, while a and b are computed from the first and the last equations.

Nesterov's worst function

- Define the following L-smooth convex function: $f(x) = \frac{L}{4}\left(\frac{1}{2}x^TAx - e_1^Tx\right) = \frac{L}{8}x^TAx - \frac{L}{4}e_1^Tx$.
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\end{bmatrix}
\begin{bmatrix} x_1^* \\ x_2^* \\ x_3^* \\ \vdots \\ x_n^* \end{bmatrix}
=
\begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}
\qquad
\begin{cases}
2x_1^* - x_2^* = 1 \\
-x_i^* + 2x_{i+1}^* - x_{i+2}^* = 0, \; i = 2, \ldots, n-1 \\
-x_{n-1}^* + 2x_n^* = 0
\end{cases}
$$

- The hypothesis: $x_i^* = a + bi$ (inspired by physics). Check, that the second equation is satisfied, while a and b are computed from the first and the last equations.
- The solution is:

$$
x_i^* = 1 - \frac{i}{n+1},
$$

Nesterov's worst function

- Define the following L-smooth convex function: $f(x) = \frac{L}{4}\left(\frac{1}{2}x^T Ax - e_1^T x\right) = \frac{L}{8}x^T Ax - \frac{L}{4}e_1^T x$.
- The optimal solution x^* satisfies $Ax^* = e_1$, and solving this system of equations gives:

$$
\begin{bmatrix}
2 & -1 & 0 & 0 & \cdots & 0 \\
-1 & 2 & -1 & 0 & \cdots & 0 \\
0 & -1 & 2 & -1 & \cdots & 0 \\
0 & 0 & -1 & 2 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 2
\end{bmatrix}
\begin{bmatrix} x_1^* \\ x_2^* \\ x_3^* \\ \vdots \\ x_n^* \end{bmatrix}
=
\begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}
\qquad
\begin{cases}
2x_1^* - x_2^* = 1 \\
-x_i^* + 2x_{i+1}^* - x_{i+2}^* = 0, \ i = 2, \ldots, n-1 \\
-x_{n-1}^* + 2x_n^* = 0
\end{cases}
$$

- The hypothesis: $x_i^* = a + bi$ (inspired by physics). Check, that the second equation is satisfied, while a and b are computed from the first and the last equations.
- The solution is:

$$
x_i^* = 1 - \frac{i}{n+1},
$$

- And the objective value is

$$
f(x^*) = \frac{L}{8}x^{*T}Ax^* - \frac{L}{4}\langle x^*, e_1\rangle = -\frac{L}{8}\langle x^*, e_1\rangle = -\frac{L}{8}\left(1 - \frac{1}{n+1}\right).
$$

Smooth case (proof)

- Suppose, we start from $x^0 = 0$. Asking the oracle for the gradient, we get $g_0 = -e_1$. Then, x^1 must lie on the line generated by e_1. At this point all the components of x^1 are zero except the first one, so

$$x^1 = \begin{bmatrix} \bullet \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

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- At the second iteration we ask the oracle again and get $g_1 = Ax^1 - e_1$. Then, x^2 must lie on the line generated by e_1 and $Ax^1 - e_1$. All the components of x^2 are zero except the first two, so

$$\begin{bmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ 0 & -1 & 2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 2 \end{bmatrix} \begin{bmatrix} \bullet \\ 0 \\ \vdots \\ 0 \end{bmatrix} \Rightarrow x^2 = \begin{bmatrix} \bullet \\ \bullet \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

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- Due to the structure of the matrix A one can show using induction that after k iterations we have all the last $n - k$ components of x^k to be zero.

$$x^{(k)} = \begin{array}{c} \begin{bmatrix} \bullet \\ \bullet \\ \vdots \\ \bullet \\ 0 \\ \vdots \\ 0 \end{bmatrix} \end{array} \begin{array}{l} 1 \\ 2 \\ \vdots \\ k \\ k+1 \\ \vdots \\ n \end{array}$$

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- However, since every iterate x^k produced by our method lies in $S_k = \text{span}\{e_1, e_2, \dots, e_k\}$ (i.e. has zeros in the coordinates $k+1, \dots, n$), it cannot "reach" the full optimal vector x^*. In other words, even if one were to choose the best possible vector from S_k, denoted by

$$\tilde{x}^k = \arg\min_{x \in S_k} f(x),$$

Smooth case (proof)

- Because $x^k \in S_k = \text{span}\{e_1, e_2, \ldots, e_k\}$ and $\tilde{x}^k$ is the best possible approximation to x^* within S_k, we have

$$f(x^k) \geq f(\tilde{x}^k).$$

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$$
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&\overset{n=2k+1}{=} \frac{L}{16(k+1)}
\end{aligned} \tag{2}$$

Smooth case (proof)

- Now we bound $R = \|x^0 - x^*\|_2$:

$$\|x^0 - x^*\|_2^2 = \|0 - x^*\|_2^2 = \|x^*\|_2^2 = \sum_{i=1}^{n} \left(1 - \frac{i}{n+1}\right)^2$$

We observe, that

$$\sum_{i=1}^{n} i = \frac{n(n+1)}{2}$$

$$\sum_{i=1}^{n} i^2 = \frac{n(n+1)(2n+1)}{6}$$

$$\leq \frac{(n+1)^3}{3}$$

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\end{aligned}
$$

- Thus,

$$
k+1 \geq \frac{3}{2}\|x^0 - x^*\|_2^2. = \frac{3}{2}R^2 \tag{3}
$$

We observe, that

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\sum_{i=1}^{n} i = \frac{n(n+1)}{2}
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Smooth case (proof)

Finally, using (2) and (3), we get:

$$
\begin{aligned}
f(x^k) - f(x^*) &\geq \frac{L}{16(k+1)} = \frac{L(k+1)}{16(k+1)^2} \\
&\geq \frac{L}{16(k+1)^2} \frac{3}{2} R^2 \\
&= \frac{3LR^2}{32(k+1)^2}
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Which concludes the proof with the desired $\mathcal{O}\left(\frac{1}{k^2}\right)$ rate.

Smooth case lower bound theorems

Smooth convex case

There exists a function f that is L-smooth and convex such that any method 1 satisfies for any $k : 1 \leq k \leq \frac{n-1}{2}$:

$$
f(x^k) - f^* \geq \frac{3L\|x^0 - x^*\|_2^2}{32(k+1)^2}
$$

Smooth strongly convex case

For any x^0 and any $\mu > 0, \varkappa = \frac{L}{\mu} > 1$, there exists a function f that is L-smooth and μ-strongly convex such that for any method of the form 1 holds:

$$
\|x^k - x^*\|_2^2 \geq \left(\frac{\sqrt{\varkappa} - 1}{\sqrt{\varkappa} + 1} \right)^{2k} \|x^0 - x^*\|_2^2
$$

$$
f(x^k) - f^* \geq \frac{\mu}{2} \left(\frac{\sqrt{\varkappa} - 1}{\sqrt{\varkappa} + 1} \right)^{2k} \|x^0 - x^*\|_2^2
$$

Acceleration for quadratics

Convergence result for quadratics

Suppose, we have a strongly convex quadratic function minimization problem solved by the gradient descent method:

$$
f(x) = \frac{1}{2}x^T A x - b^T x \qquad x^{k+1} = x^k - \alpha_k \nabla f(x^k).
$$

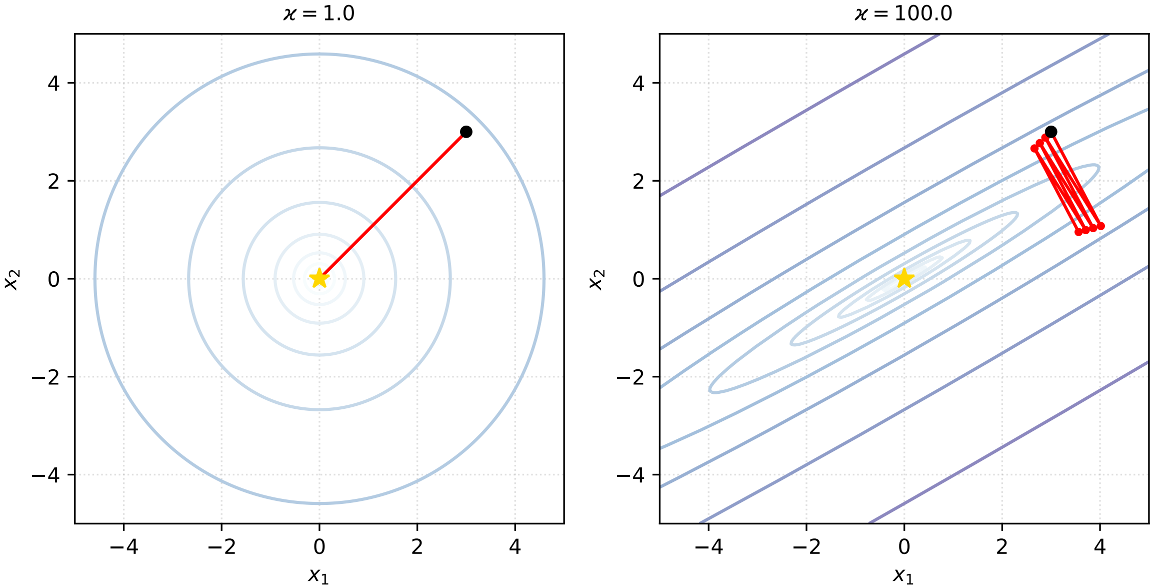
Theorem

The gradient descent method with the learning rate $\alpha_k = \frac{2}{\mu + L}$ converges to the optimal solution x^* with the following guarantee:

$$
\|x^{k+1} - x^*\|_2 = \left(\frac{\varkappa - 1}{\varkappa + 1} \right)^k \|x^0 - x^*\|_2 \qquad f(x^{k+1}) - f(x^*) = \left(\frac{\varkappa - 1}{\varkappa + 1} \right)^{2k} \left(f(x^0) - f(x^*) \right)
$$

where $\varkappa = \frac{L}{\mu}$ is the condition number of A.

Condition number $\varkappa$



Convergence from the first principles

$$f(x) = \frac{1}{2}x^T Ax - b^T x \qquad x_{k+1} = x_k - \alpha_k \nabla f(x_k).$$

Let x^* be the unique solution of the linear system $Ax = b$ and put $e_k = \|x_k - x^*\|$, where $x_{k+1} = x_k - \alpha_k(Ax_k - b)$ is defined recursively starting from some x_0, and α_k is a step size we'll determine shortly.

$$e_{k+1} = (I - \alpha_k A)e_k.$$

Polynomials

The above calculation gives us $e_k = p_k(A)e_0$,
where p_k is the polynomial

$$p_k(a) = \prod_{i=1}^{k}(1 - \alpha_k a).$$

We can upper bound the norm of the error term as

$$\|e_k\| \leq \|p_k(A)\| \cdot \|e_0\|.$$

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We can upper bound the norm of the error term as

$$\|e_k\| \leq \|p_k(A)\| \cdot \|e_0\| \, .$$

Since A is a symmetric matrix with eigenvalues in $[\mu, L]$,:

$$\|p_k(A)\| \leq \max_{\mu \leq a \leq L} |p_k(a)| \, .$$

This leads to an interesting problem: Among all polynomials that satisfy $p_k(0) = 1$ we're looking for a polynomial whose magnitude is as small as possible in the interval $[\mu, L]$.

Naive polynomial solution

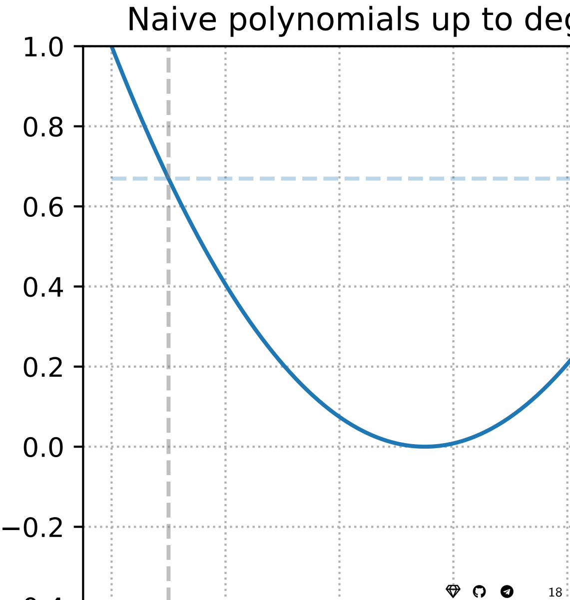
A naive solution is to choose a uniform step size $\alpha_k = \frac{2}{\mu+L}$ in the expression. This choise makes $|p_k(\mu)| = |p_k(L)|$.

$$
\|e_k\| \leq \left(1 - \frac{1}{\varkappa}\right)^k \|e_0\|
$$

This is exactly the rate we proved in the previous lecture for any smooth and strongly convex function.

Let's look at this polynomial a bit closer. On the right figure we choose $\alpha = 1$ and $\beta = 10$ so that $\kappa = 10$. The relevant interval is therefore $[1, 10]$.

Can we do better? The answer is yes.



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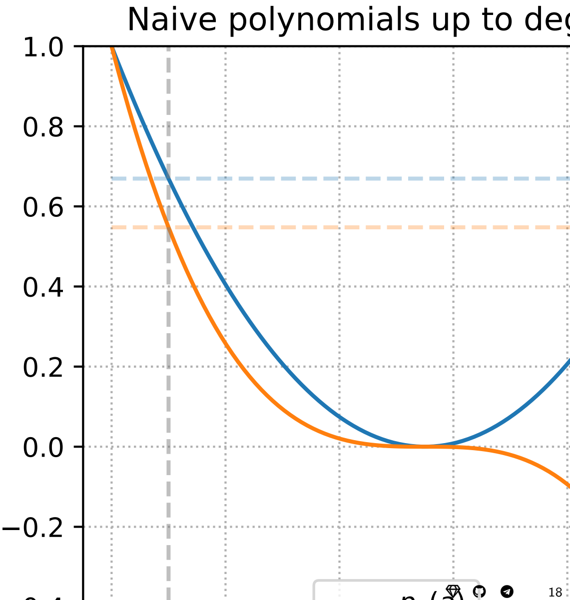

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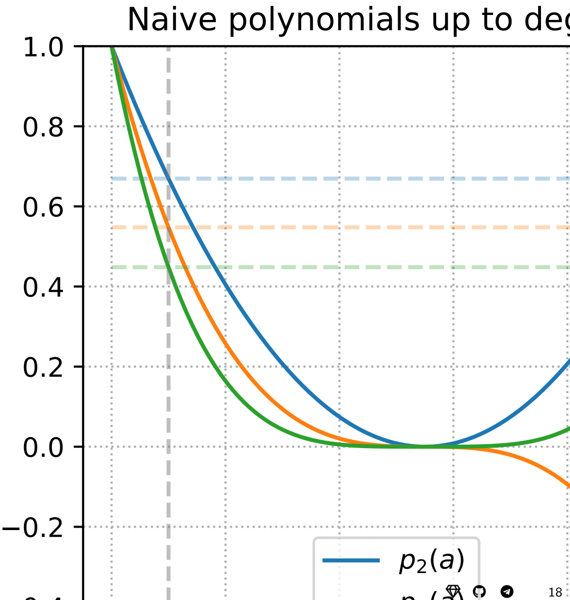

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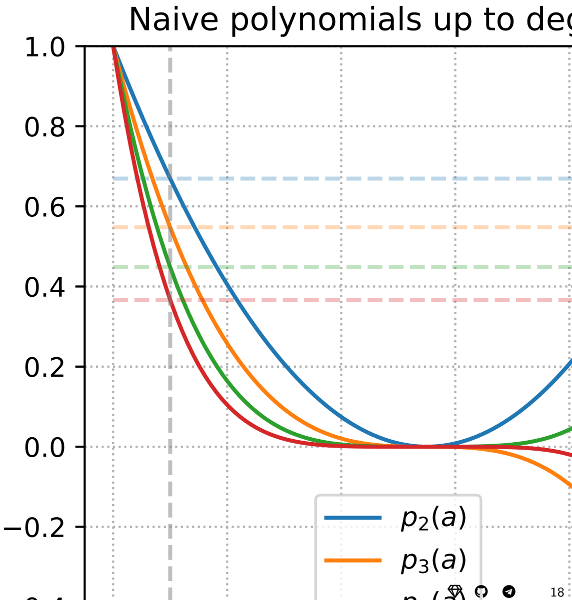

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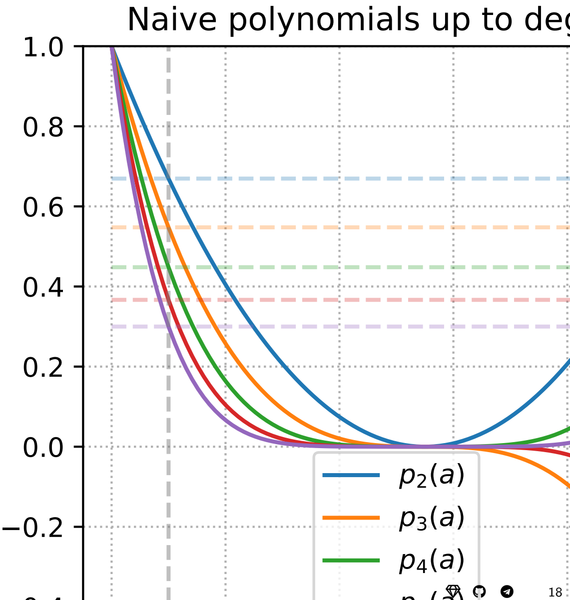

Chebyshev polynomials

Chebyshev polynomials turn out to give an optimal answer to the question that we asked. Suitably rescaled, they minimize the absolute value in a desired interval $[\mu, L]$ while satisfying the normalization constraint of having value 1 at the origin.

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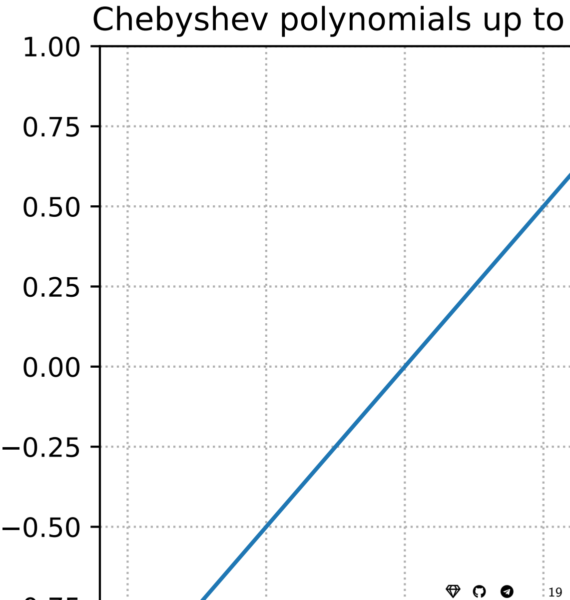
Let's plot the standard Chebyshev polynomials (without rescaling):



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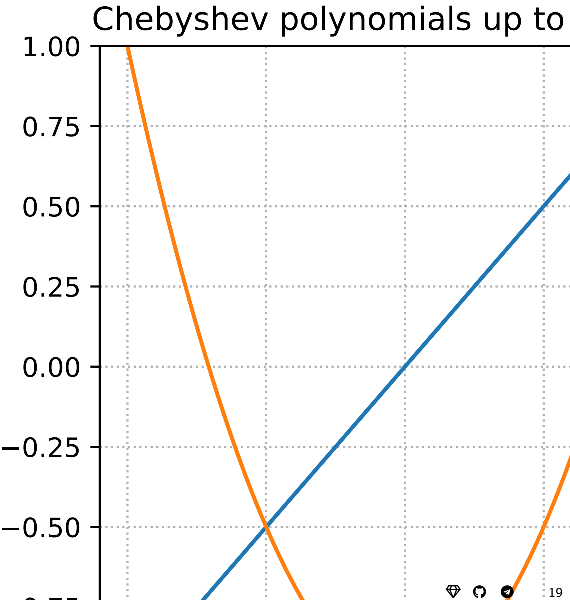

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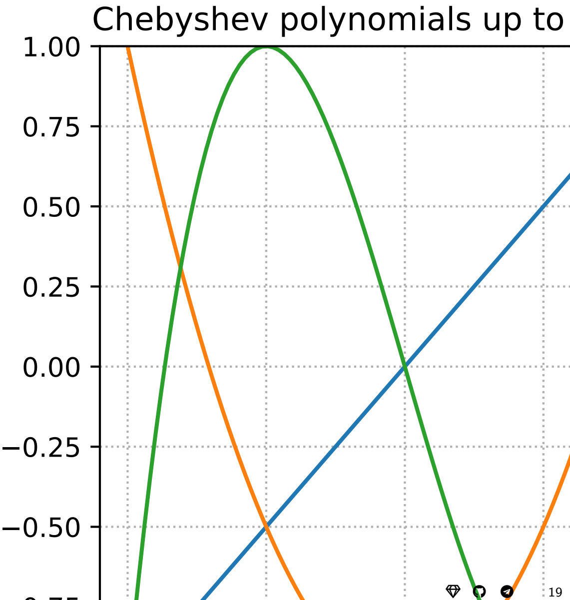

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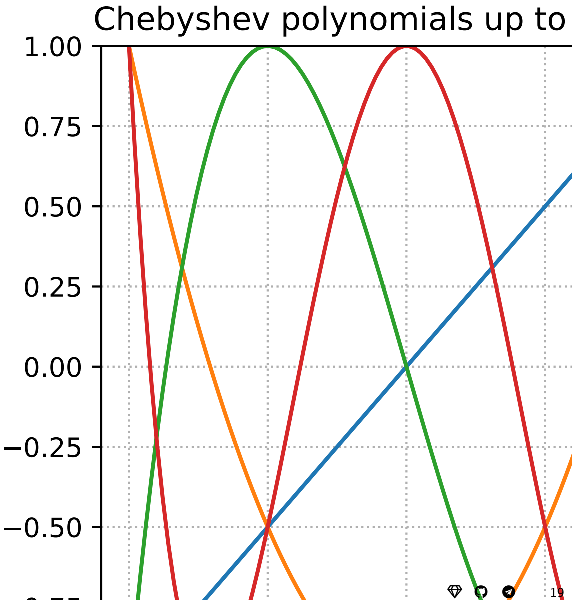

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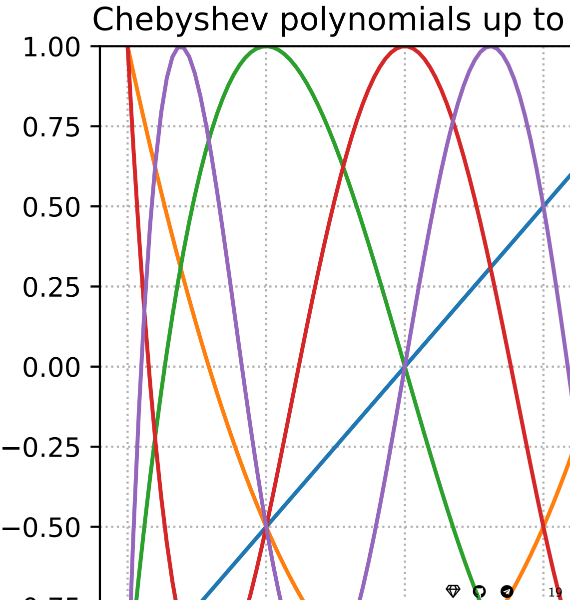

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Note, that $x = 1$ corresponds to $a = \mu$, $x = -1$ corresponds to $a = L$ and $x = 0$ corresponds to $a = \frac{\mu+L}{2}$. This transformation ensures that the behavior of the Chebyshev polynomial on $[-1, 1]$ is reflected on the interval $[\mu, L]$

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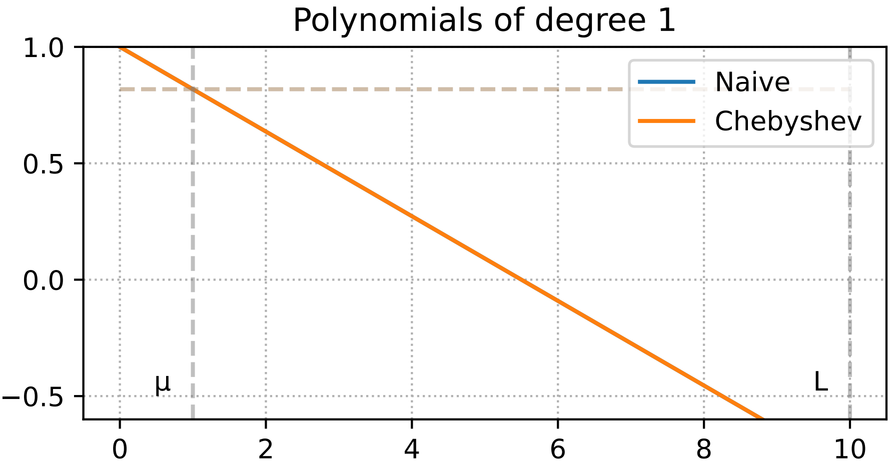
$$P_k(a) = T_k\left(\frac{L + \mu - 2a}{L - \mu}\right) \cdot T_k\left(\frac{L + \mu}{L - \mu}\right)^{-1}$$

and observe, that they are much better behaved than the naive polynomials in terms of the magnitude in the interval $[\mu, L]$.

Rescaled Chebyshev polynomials



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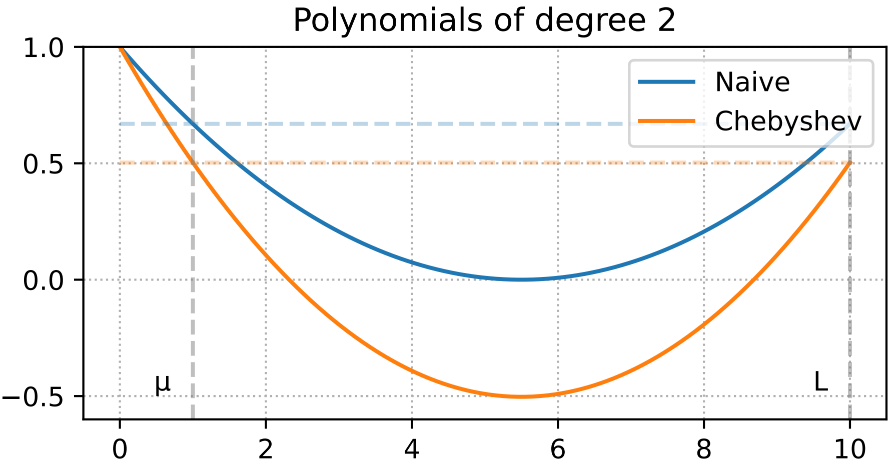

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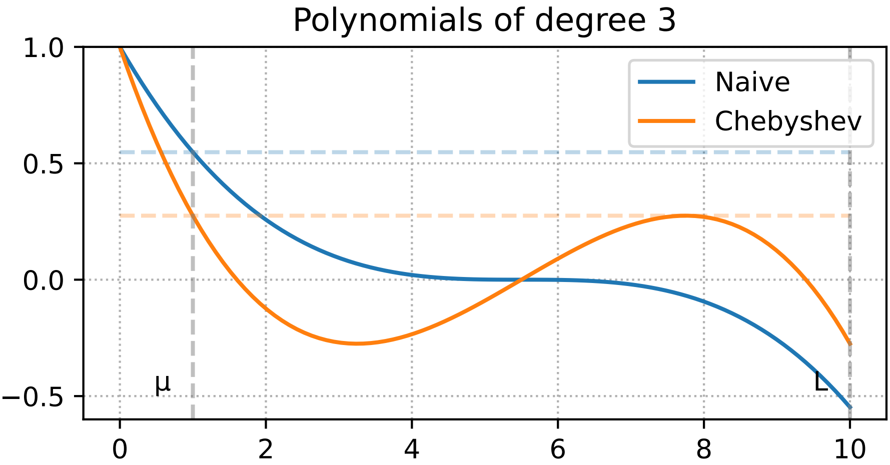

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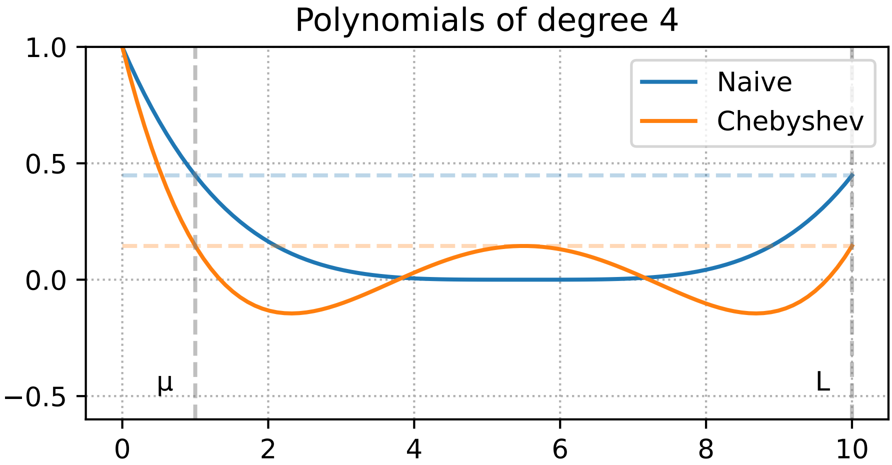

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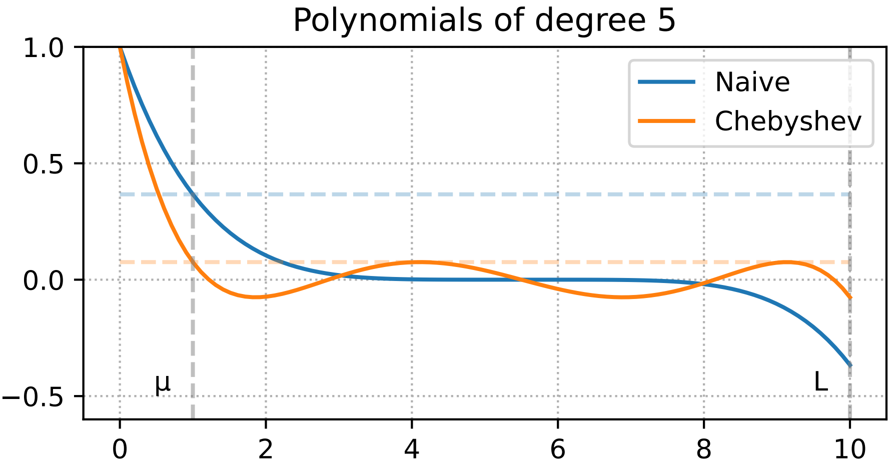

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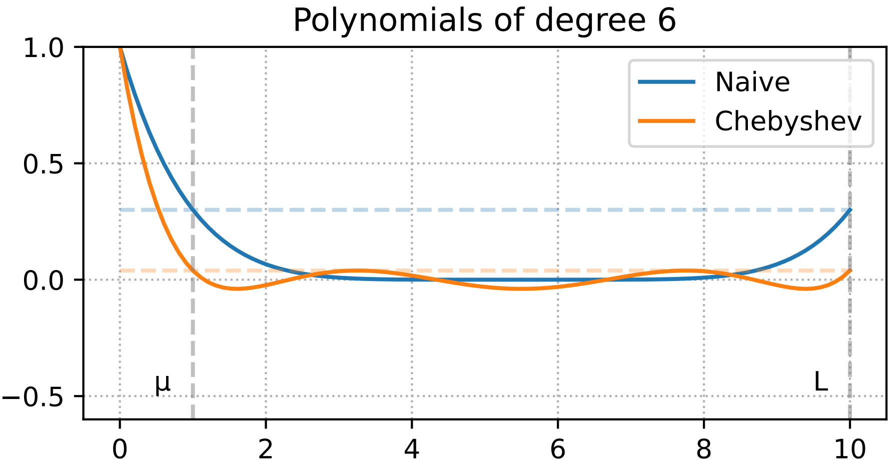

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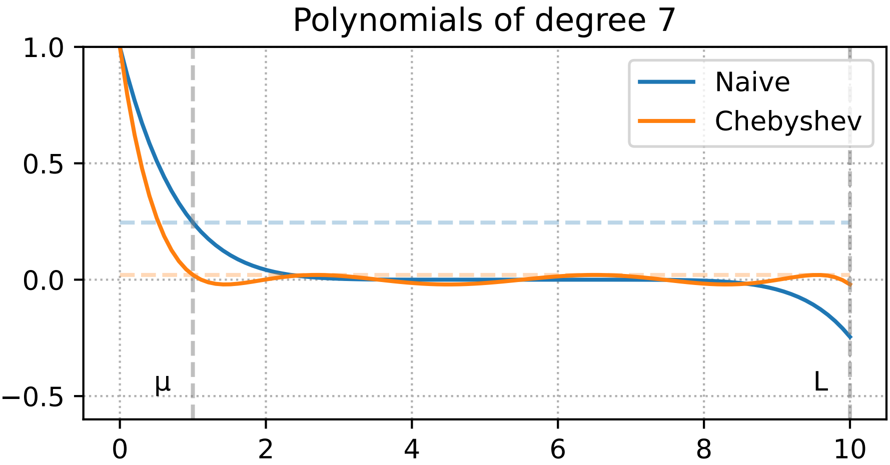

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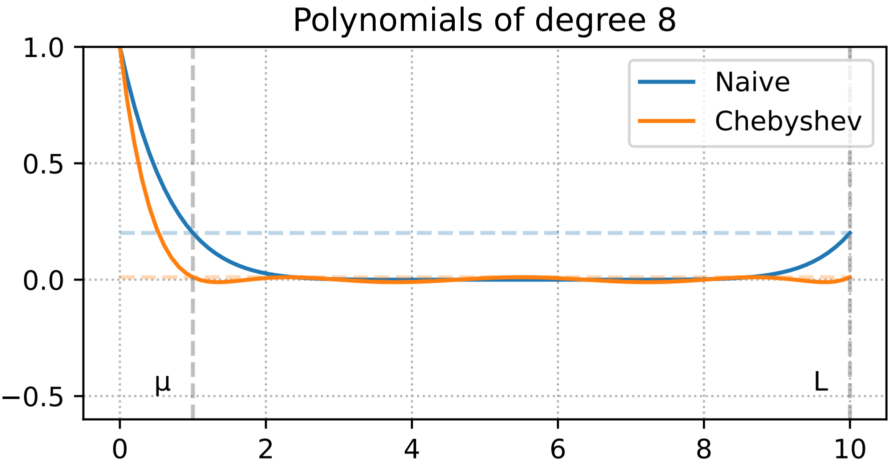

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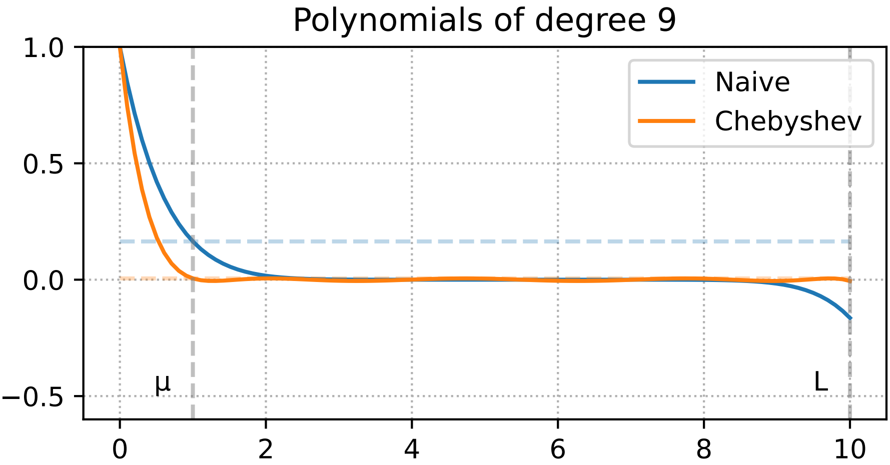

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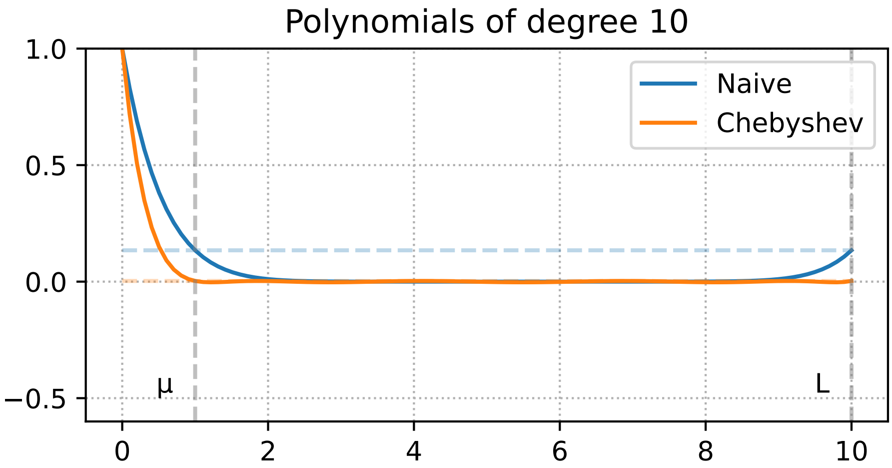

Chebyshev polynomials upper bound

We can see, that the maximum value of the Chebyshev polynomial on the interval $[\mu, L]$ is achieved at the point $a = \mu$. Therefore, we can use the following upper bound:

$$\|P_k(A)\|_2 \leq P_k(\mu) = T_k\left(\frac{L+\mu-2\mu}{L-\mu}\right) \cdot T_k\left(\frac{L+\mu}{L-\mu}\right)^{-1} = T_k\left(1\right) \cdot T_k\left(\frac{L+\mu}{L-\mu}\right)^{-1} = T_k\left(\frac{L+\mu}{L-\mu}\right)^{-1}$$

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Using the definition of condition number $\varkappa = \frac{L}{\mu}$, we get:

$$\|P_k(A)\|_2 \leq T_k\left(\frac{\varkappa+1}{\varkappa-1}\right)^{-1} = T_k\left(1 + \frac{2}{\varkappa-1}\right)^{-1} = T_k\left(1+\epsilon\right)^{-1}, \quad \epsilon = \frac{2}{\varkappa-1}.$$

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Therefore, we only need to understand the value of T_k at $1+\epsilon$. This is where the acceleration comes from. We will bound this value with $\mathcal{O}\left(\frac{1}{\sqrt{\epsilon}}\right)$.

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T_k(x) &= \cosh\left(k \operatorname{arccosh}(x)\right) \\
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5. Finally, we get:
$$\begin{aligned}
\|e_k\| \leq \|P_k(A)\| \|e_0\| &\leq \frac{2}{\left(1+\sqrt{\epsilon}\right)^k} \|e_0\| \\
&\leq 2\left(1 + \sqrt{\frac{2}{\varkappa - 1}}\right)^{-k} \|e_0\| \\
&\leq 2\exp\left(-\sqrt{\frac{2}{\varkappa-1}}k\right) \|e_0\|
\end{aligned}$$

Accelerated method [1/2]

Due to the recursive definition of the Chebyshev polynomials, we directly obtain an iterative acceleration scheme. Reformulating the recurrence in terms of our rescaled Chebyshev polynomials, we obtain:

$$T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x)$$

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Since we have $P_{k+1}(0) = P_k(0) = P_{k-1}(0) = 1$, we can find the method in the following form:

$$P_{k+1}(a) = (1 - \alpha_k a)P_k(a) + \beta_k\left(P_k(a) - P_{k-1}(a)\right).$$

Accelerated method [2/2]

Rearranging the terms, we get:

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P_{k+1}(a) &= (1+\beta_k)P_k(a) - \alpha_k a P_k(a) - \beta_k P_{k-1}(a), \\
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We are almost done :) We remember, that $e_{k+1} = P_{k+1}(A)e_0$. Note also, that we work with the quadratic problem, so we can assume $x^* = 0$ without loss of generality. In this case, $e_0 = x_0$ and $e_{k+1} = x_{k+1}$.

$$\begin{aligned} x_{k+1} &= P_{k+1}(A)x_0 = (I - \alpha_k A)P_k(A)x_0 + \beta_k \left(P_k(A) - P_{k-1}(A)\right) x_0 \\ &= (I - \alpha_k A)x_k + \beta_k \left(x_k - x_{k-1}\right) \end{aligned}$$

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$$P_{k+1}(a) = 2\frac{L+\mu}{L-\mu}\frac{t_k}{t_{k+1}}P_k(a) - \frac{4a}{L-\mu}\frac{t_k}{t_{k+1}}P_k(a) - \frac{t_{k-1}}{t_{k+1}}P_{k-1}(a)$$

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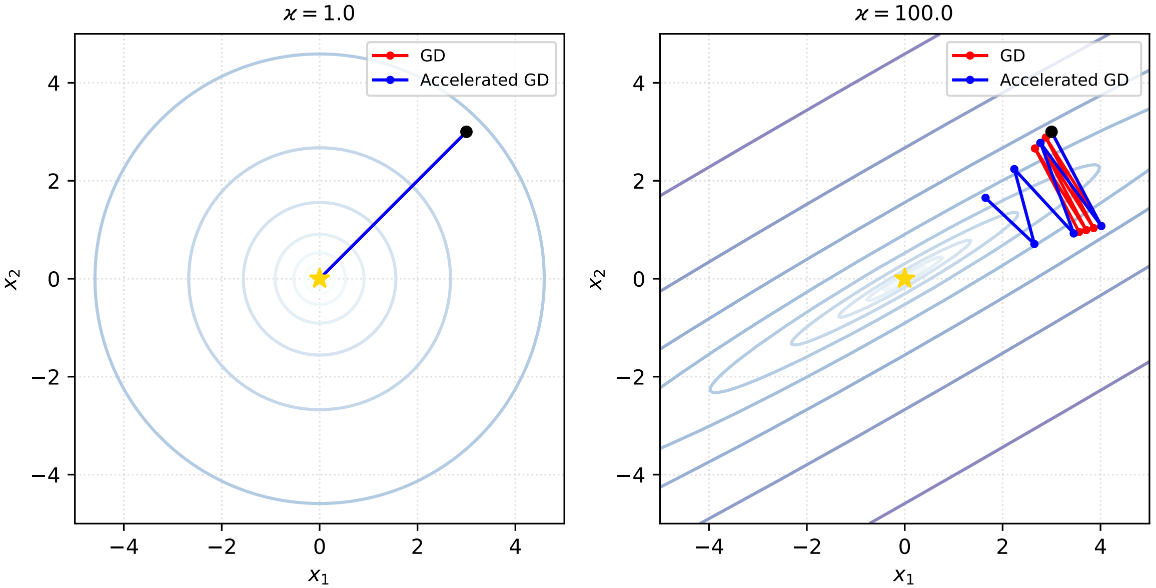
We are almost done :) We remember, that $e_{k+1} = P_{k+1}(A)e_0$. Note also, that we work with the quadratic problem, so we can assume $x^* = 0$ without loss of generality. In this case, $e_0 = x_0$ and $e_{k+1} = x_{k+1}$.

$$\begin{aligned} x_{k+1} &= P_{k+1}(A)x_0 = (I - \alpha_k A)P_k(A)x_0 + \beta_k\left(P_k(A) - P_{k-1}(A)\right)x_0 \\ &= (I - \alpha_k A)x_k + \beta_k\left(x_k - x_{k-1}\right) \end{aligned}$$

For quadratic problem, we have $\nabla f(x_k) = Ax_k$, so we can rewrite the update as:

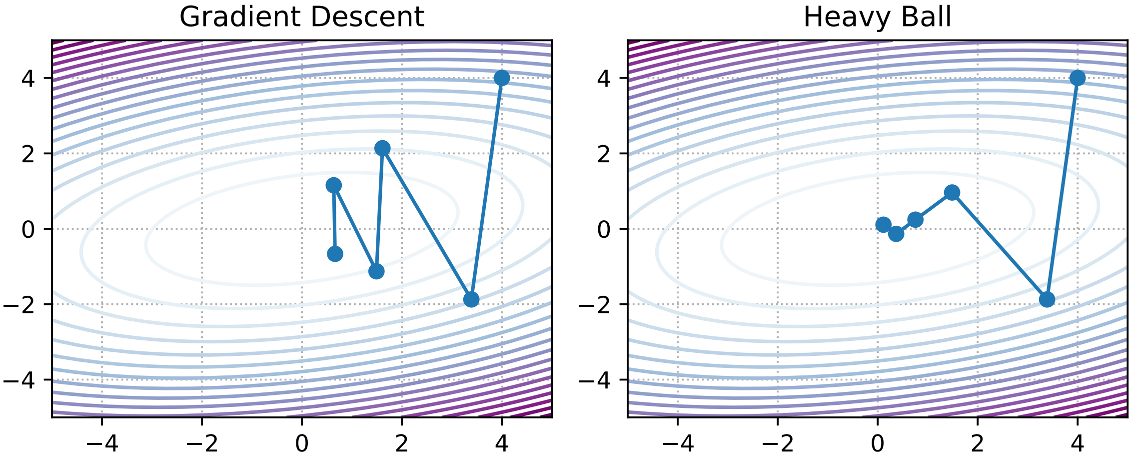
$$\boxed{x_{k+1} = x_k - \alpha_k \nabla f(x_k) + \beta_k\left(x_k - x_{k-1}\right)}$$

Acceleration from the first principles

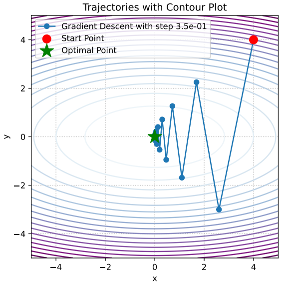


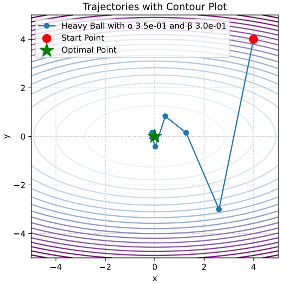
Heavy ball

Oscillations and acceleration



Polyak Heavy ball method





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

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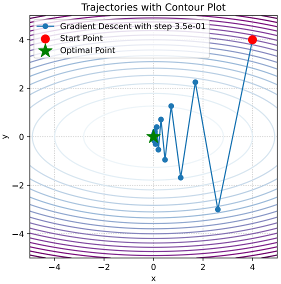

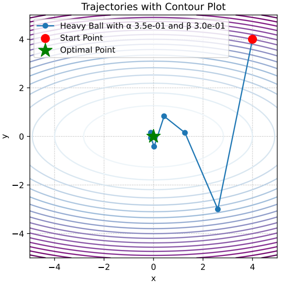

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Which is in our (quadratics) case is

$$\hat{x}_{k+1} = \hat{x}_k - \alpha \Lambda \hat{x}_k + \beta(\hat{x}_k - \hat{x}_{k-1}) = (I - \alpha\Lambda + \beta I)\hat{x}_k - \beta \hat{x}_{k-1}$$

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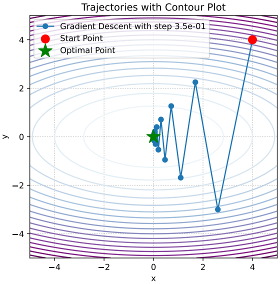

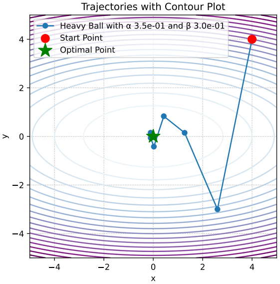

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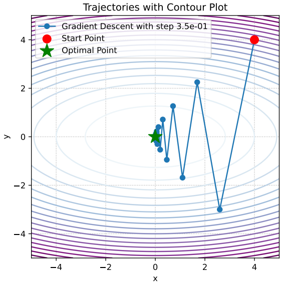

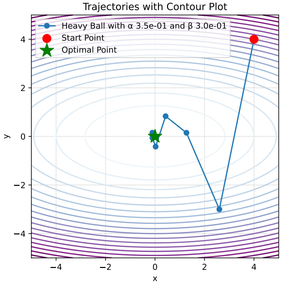

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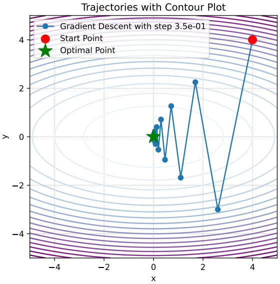
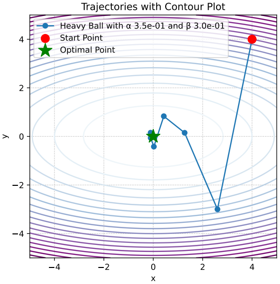
$$\begin{aligned} \hat{x}_{k+1} &= (I - \alpha\Lambda + \beta I)\hat{x}_k - \beta \hat{x}_{k-1}, \\ \hat{x}_k &= \hat{x}_k. \end{aligned}$$

Let's use the following notation $\hat{z}_k = \begin{bmatrix} \hat{x}_{k+1} \\ \hat{x}_k \end{bmatrix}$. Therefore $\hat{z}_{k+1} = M \hat{z}_k$, where the iteration matrix M is:

Polyak Heavy ball method





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$$M = \begin{bmatrix} I - \alpha\Lambda + \beta I & -\beta I \\ I & 0_d \end{bmatrix}.$$

Reduction to a scalar case

Note, that M is $2d \times 2d$ matrix with 4 block-diagonal matrices of size $d \times d$ inside. It means, that we can rearrange the order of coordinates to make M block-diagonal in the following form. Note that in the equation below, the matrix M denotes the same as in the notation above, except for the described permutation of rows and columns. We use this slight abuse of notation for the sake of clarity.

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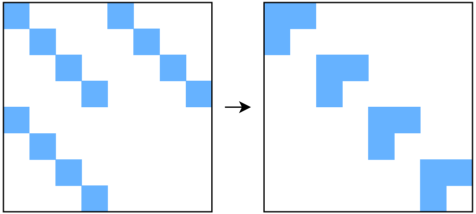

Figure 1: Illustration of matrix M rearrangement

$$
\begin{bmatrix} \hat{x}_k^{(1)} \\ \vdots \\ \hat{x}_k^{(d)} \\ \hat{x}_{k-1}^{(1)} \\ \vdots \\ \hat{x}_{k-1}^{(d)} \end{bmatrix} \to \begin{bmatrix} \hat{x}_k^{(1)} \\ \hat{x}_{k-1}^{(1)} \\ \vdots \\ \hat{x}_k^{(d)} \\ \hat{x}_{k-1}^{(d)} \end{bmatrix} \quad M = \begin{bmatrix} M_1 & & & \\ & M_2 & & \\ & & \ldots & \\ & & & M_d \end{bmatrix}
$$

where $\hat{x}_k^{(i)}$ is i-th coordinate of vector $\hat{x}_k \in \mathbb{R}^d$ and M_i stands for 2×2 matrix. This rearrangement allows us to study the dynamics of the method independently for each dimension. One may observe, that the asymptotic convergence rate of the $2d$-dimensional vector sequence of $\hat{z}_k$ is defined by the worst convergence rate among its block of coordinates. Thus, it is enough to study the optimization in a one-dimensional case.

Reduction to a scalar case

For i-th coordinate with λ_i as an i-th eigenvalue of matrix W we have:

$$M_i = \begin{bmatrix} 1 - \alpha\lambda_i + \beta & -\beta \\ 1 & 0 \end{bmatrix}.$$

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$$M_i = \begin{bmatrix} 1 - \alpha\lambda_i + \beta & -\beta \\ 1 & 0 \end{bmatrix}.$$

The method will be convergent if $\rho(M) < 1$, and the optimal parameters can be computed by optimizing the spectral radius

$$\alpha^*, \beta^* = \arg\min_{\alpha,\beta} \max_i \rho(M_i) \quad \alpha^* = \frac{4}{(\sqrt{L} + \sqrt{\mu})^2}; \quad \beta^* = \left(\frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}\right)^2.$$

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It can be shown, that for such parameters the matrix M has complex eigenvalues, which forms a conjugate pair, so the distance to the optimum (in this case, $\|z_k\|$), generally, will not go to zero monotonically.

Heavy ball quadratic convergence

We can explicitly calculate the eigenvalues of M_i:

$$\lambda^M_1, \lambda^M_2 = \lambda \left(\begin{bmatrix} 1 - \alpha\lambda_i + \beta & -\beta \\ 1 & 0 \end{bmatrix} \right) = \frac{1 + \beta - \alpha\lambda_i \pm \sqrt{(1 + \beta - \alpha\lambda_i)^2 - 4\beta}}{2}.$$

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When α and β are optimal (α^*, β^*), the eigenvalues are complex-conjugated pair $(1 + \beta - \alpha\lambda_i)^2 - 4\beta \leq 0$, i.e. $\beta \geq (1 - \sqrt{\alpha\lambda_i})^2$.

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$$\text{Re}(\lambda^M_1) = \frac{L + \mu - 2\lambda_i}{(\sqrt{L} + \sqrt{\mu})^2}; \quad \text{Im}(\lambda^M_1) = \frac{\pm 2\sqrt{(L - \lambda_i)(\lambda_i - \mu)}}{(\sqrt{L} + \sqrt{\mu})^2}; \quad |\lambda^M_1| = \frac{L - \mu}{(\sqrt{L} + \sqrt{\mu})^2}.$$

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We can explicitly calculate the eigenvalues of M_i:

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And the convergence rate does not depend on the stepsize and equals to $\sqrt{\beta^*}$.

Heavy Ball quadratics convergence

Theorem

Assume that f is quadratic μ-strongly convex L-smooth quadratics, then Heavy Ball method with parameters

$$\alpha = \frac{4}{(\sqrt{L} + \sqrt{\mu})^2}, \beta = \frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}$$

converges linearly:

$$\|x_k - x^*\|_2 \leq \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right) \|x_0 - x^*\|$$

Heavy Ball Global Convergence [3]

Theorem

Assume that f is smooth and convex and that

$$\beta \in [0,1), \quad \alpha \in \left(0, \dfrac{2(1-\beta)}{L}\right).$$

Then, the sequence $\{x_k\}$ generated by Heavy-ball iteration satisfies

$$f(\overline{x}_T) - f^\star \leq \begin{cases} \frac{\|x_0 - x^\star\|^2}{2(T+1)}\left(\frac{L\beta}{1-\beta} + \frac{1-\beta}{\alpha}\right), & \text{if } \alpha \in \left(0, \dfrac{1-\beta}{L}\right], \\ \frac{\|x_0 - x^\star\|^2}{2(T+1)(2(1-\beta)-\alpha L)}\left(L\beta + \frac{(1-\beta)^2}{\alpha}\right), & \text{if } \alpha \in \left[\dfrac{1-\beta}{L}, \dfrac{2(1-\beta)}{L}\right), \end{cases}$$

where $\overline{x}_T$ is the Cesaro average of the iterates, i.e.,

$$\overline{x}_T = \frac{1}{T+1}\sum_{k=0}^{T} x_k.$$

[3] Global convergence of the Heavy-ball method for convex optimization, Euhanna Ghadimi et.al.

Heavy Ball Global Convergence [4]

Theorem

Assume that f is smooth and strongly convex and that

$$\alpha \in (0, \frac{2}{L}), \quad 0 \leq \beta < \frac{1}{2}\left(\frac{\mu\alpha}{2} + \sqrt{\frac{\mu^2\alpha^2}{4} + 4(1 - \frac{\alpha L}{2})}\right).$$

where $\alpha_0 \in (0, 1/L]$. Then, the sequence $\{x_k\}$ generated by Heavy-ball iteration converges linearly to a unique optimizer $x^\star$. In particular,

$$f(x_k) - f^\star \leq q^k(f(x_0) - f^\star),$$

where $q \in [0, 1)$.

[4] Global convergence of the Heavy-ball method for convex optimization, Euhanna Ghadimi et.al.

Heavy ball method summary

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- Recently was proved, that there is no global accelerated convergence for the method.
- Method was not extremely popular until the ML boom
- Nowadays, it is de-facto standard for practical acceleration of gradient methods, even for the non-convex problems (neural network training)

Nesterov accelerated gradient

The concept of Nesterov Accelerated Gradient method

$$x_{k+1} = x_k - \alpha \nabla f(x_k)$$

$$x_{k+1} = x_k - \alpha \nabla f(x_k) + \beta (x_k - x_{k-1})$$

$$\begin{cases} y_{k+1} = x_k + \beta (x_k - x_{k-1}) \\ x_{k+1} = y_{k+1} - \alpha \nabla f(y_{k+1}) \end{cases}$$

The concept of Nesterov Accelerated Gradient method

$$x_{k+1} = x_k - \alpha \nabla f(x_k) \qquad x_{k+1} = x_k - \alpha \nabla f(x_k) + \beta(x_k - x_{k-1}) \qquad \begin{cases} y_{k+1} = x_k + \beta(x_k - x_{k-1}) \\ x_{k+1} = y_{k+1} - \alpha \nabla f(y_{k+1}) \end{cases}$$

Let's define the following notation

$$x^+ = x - \alpha \nabla f(x) \qquad \text{Gradient step}$$

$$d_k = \beta_k(x_k - x_{k-1}) \qquad \text{Momentum term}$$

Then we can write down:

$$x_{k+1} = x_k^+ \qquad \text{Gradient Descent}$$

$$x_{k+1} = x_k^+ + d_k \qquad \text{Heavy Ball}$$

$$x_{k+1} = (x_k + d_k)^+ \qquad \text{Nesterov accelerated gradient}$$

General case convergence

Theorem

Let $f : \mathbb{R}^n \to \mathbb{R}$ is convex and L-smooth. The Nesterov Accelerated Gradient Descent (NAG) algorithm is designed to solve the minimization problem starting with an initial point $x_0 = y_0 \in \mathbb{R}^n$ and $\lambda_0 = 0$. The algorithm iterates the following steps:

$$
\begin{aligned}
&\textbf{Gradient update:} && y_{k+1} = x_k - \frac{1}{L}\nabla f(x_k) \\
&\textbf{Extrapolation:} && x_{k+1} = (1-\gamma_k)y_{k+1} + \gamma_k y_k \\
&\textbf{Extrapolation weight:} && \lambda_{k+1} = \frac{1+\sqrt{1+4\lambda_k^2}}{2} \\
&\textbf{Extrapolation weight:} && \gamma_k = \frac{1-\lambda_k}{\lambda_{k+1}}
\end{aligned}
$$

The sequences $\{f(y_k)\}_{k\in\mathbb{N}}$ produced by the algorithm will converge to the optimal value f^* at the rate of $\mathcal{O}\left(\frac{1}{k^2}\right)$, specifically:

$$
f(y_k) - f^* \leq \frac{2L\|x_0 - x^*\|^2}{k^2}
$$

General case convergence

Theorem

Let $f : \mathbb{R}^n \to \mathbb{R}$ is μ-strongly convex and L-smooth. The Nesterov Accelerated Gradient Descent (NAG) algorithm is designed to solve the minimization problem starting with an initial point $x_0 = y_0 \in \mathbb{R}^n$ and $\lambda_0 = 0$. The algorithm iterates the following steps:

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\end{aligned}
$$

The sequences $\{f(y_k)\}_{k\in\mathbb{N}}$ produced by the algorithm will converge to the optimal value f^* linearly:

$$
f(y_k) - f^* \leq \frac{\mu + L}{2}\|x_0 - x^*\|_2^2 \exp\left(-\frac{k}{\sqrt{\kappa}}\right)
$$