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

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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)
$f(x^k) - f^* \sim \mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$	$\|\nabla f(x^k)\|^2 \sim \mathcal{O}\left(\frac{1}{k}\right)$	$f(x^k) - f^* \sim \mathcal{O}\left(\frac{1}{k}\right)$	$\|x^k - x^*\|^2 \sim \mathcal{O}\left(\left(1 - \frac{\mu}{L}\right)^k\right)$
$k_\varepsilon \sim \mathcal{O}\left(\frac{1}{\varepsilon^2}\right)$	$k_\varepsilon \sim \mathcal{O}\left(\frac{1}{\varepsilon}\right)$	$k_\varepsilon \sim \mathcal{O}\left(\frac{1}{\varepsilon}\right)$	$k_\varepsilon \sim \mathcal{O}\left(\varkappa \log \frac{1}{\varepsilon}\right)$

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For smooth strongly convex we have:

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f(x^k) - f^* \leq \left(1 - \frac{\mu}{L}\right)^k (f(x^0) - f^*).
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Note also, that for any x, since e^{-x} is convex and $1 - x$ is its tangent line at $x = 0$, we have:

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1 - x \leq e^{-x}
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\begin{aligned}
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k_\varepsilon \geq \varkappa \log \frac{f(x^0) - f^*}{\varepsilon} &= \mathcal{O}\left(\varkappa \log \frac{1}{\varepsilon}\right)
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Question: Can we do faster, than this using the first-order information?

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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)
$\mathcal{O}\left(\dfrac{1}{\sqrt{k}}\right)$	$\mathcal{O}\left(\dfrac{1}{k^2}\right)$	$\mathcal{O}\left(\dfrac{1}{k^2}\right)$	$\mathcal{O}\left(\left(1-\sqrt{\dfrac{\mu}{L}}\right)^k\right)$
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[1] Carmon, Duchi, Hinder, Sidford, 2017
[2] Nemirovski, Yudin, 1979

Black box iteration

The iteration of gradient descent:

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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) \\
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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}
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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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    b. The gradient method is not optimal for this problem.

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

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Lower bound:

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

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

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- The optimal solution x^* satisfies $Ax^* = e_1$, and solving this system of equations gives:

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\begin{bmatrix}
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\end{bmatrix}
=
\begin{bmatrix}
1 \\ 0 \\ 0 \\ \vdots \\ 0
\end{bmatrix}
\qquad
\begin{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.

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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.
- 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 $S_k = \text{span}\{e_1, e_2, \ldots, e_k\}$ (i.e. has zeros in the coordinates $k+1, \ldots, n$), 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

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

its objective value $f(\tilde{x}^k)$ will be strictly worse than $f(x^*)$.

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

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

- Thus,

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

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:

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

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

Acceleration for quadratics

Convergence result for quadratics

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

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

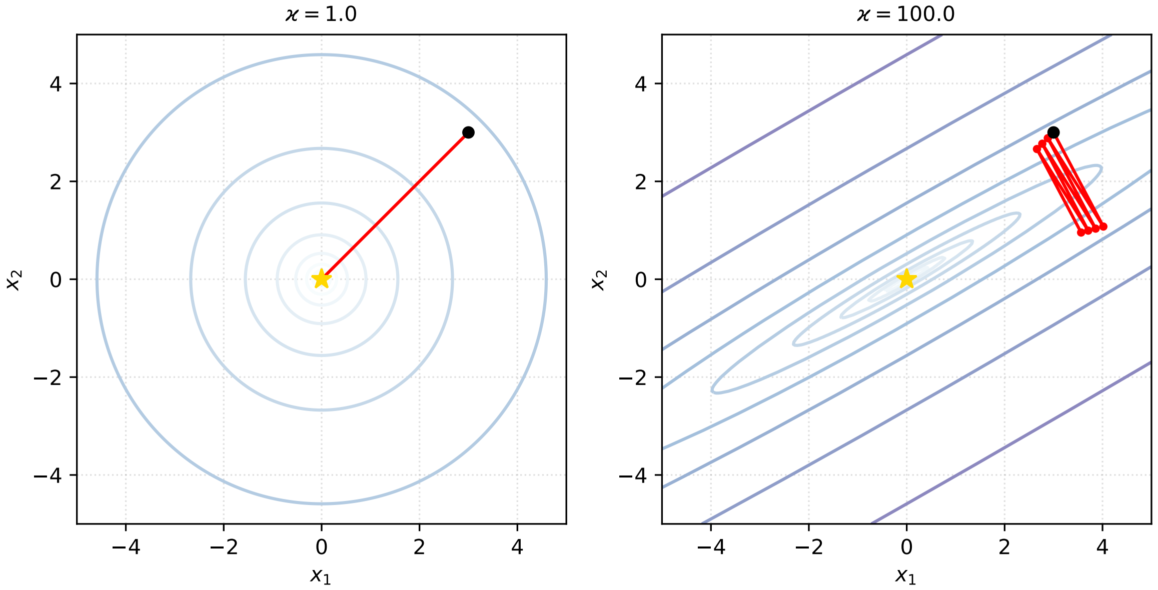
Theorem

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

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

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

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

We can upper bound the norm of the error term as

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

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

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

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

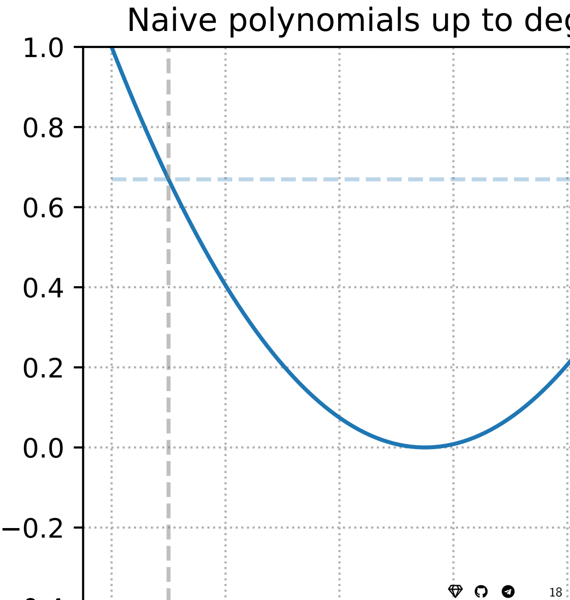
This leads to an interesting problem: Among all polynomials that satisfy $p_k(0) = 1$ we're looking for a polynomial whose magnitude is as small as possible in the interval $[\mu, L]$.

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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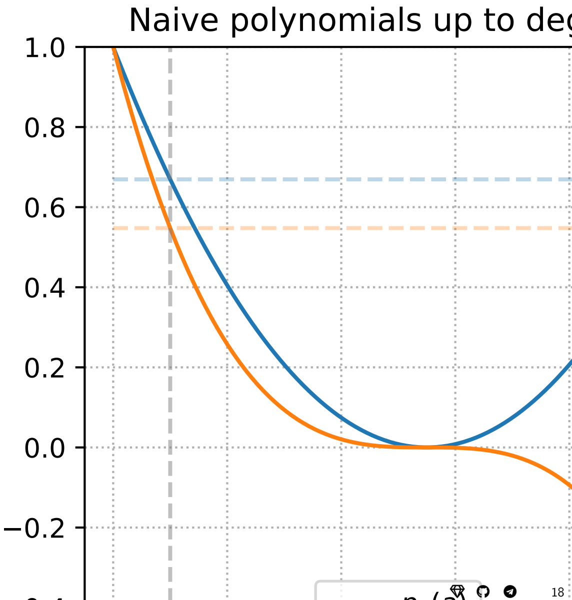

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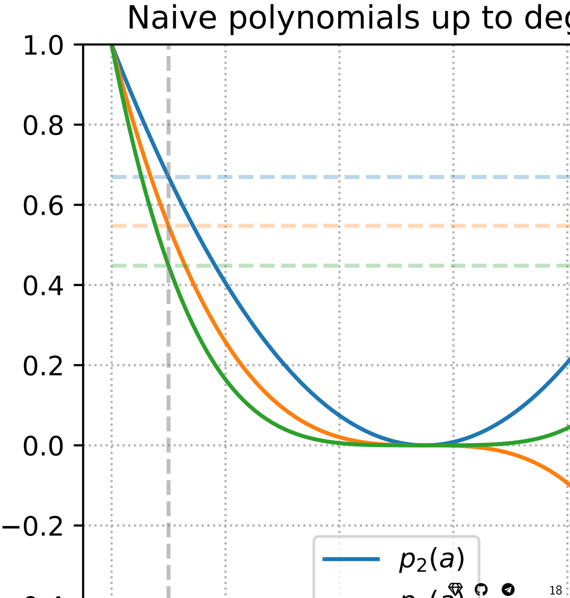

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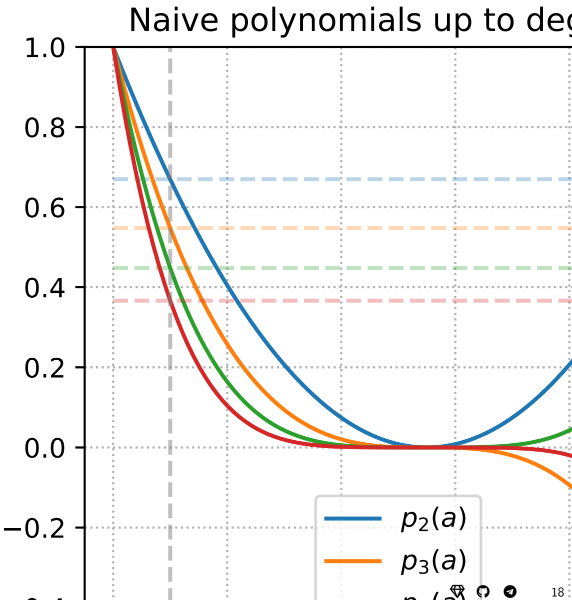

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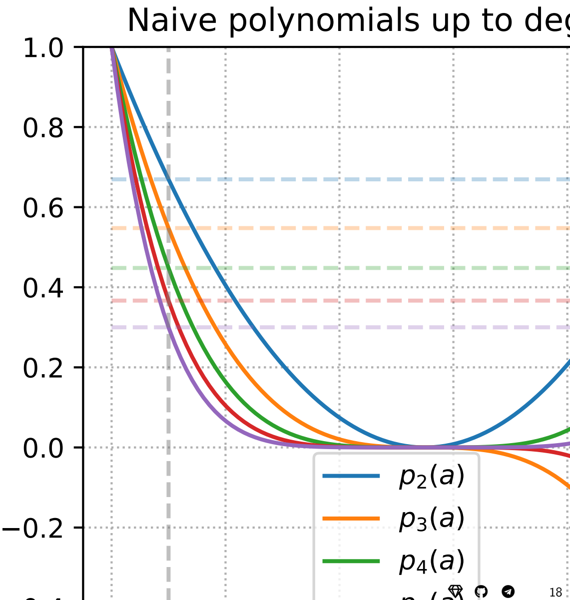

Chebyshev polynomials

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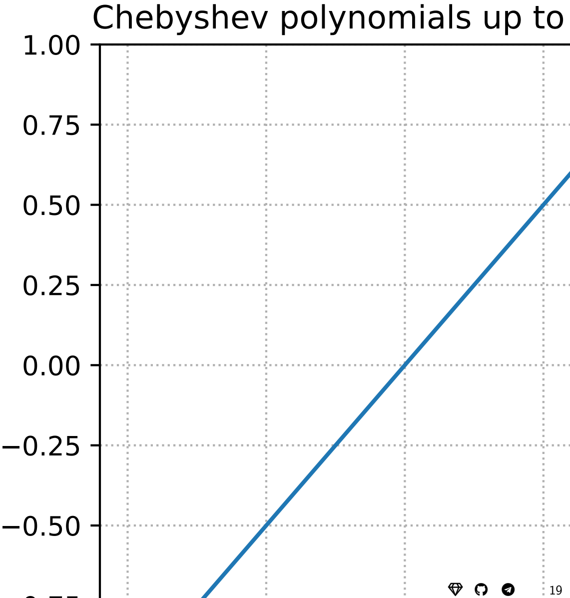

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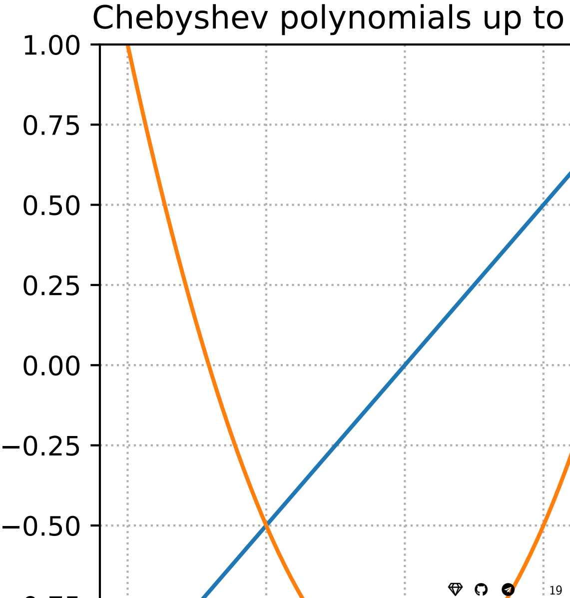

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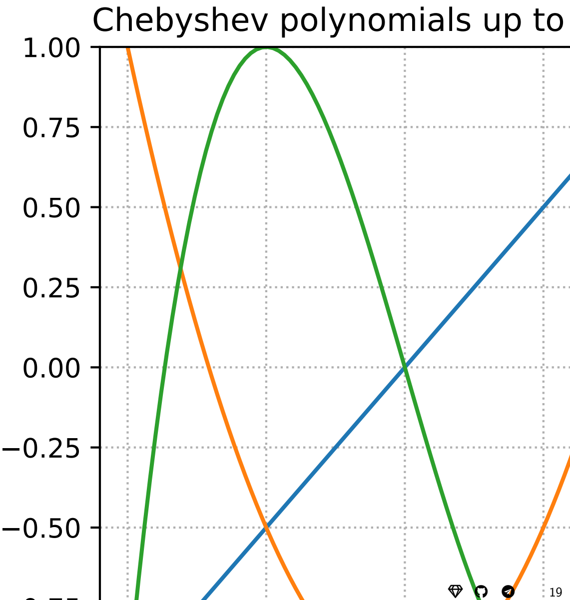

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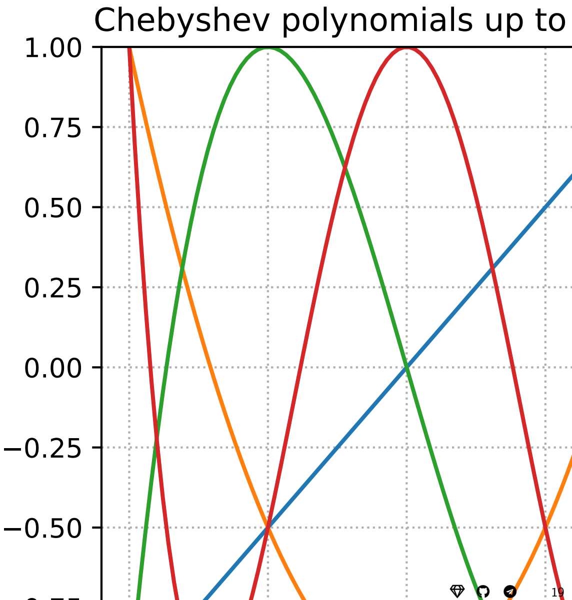

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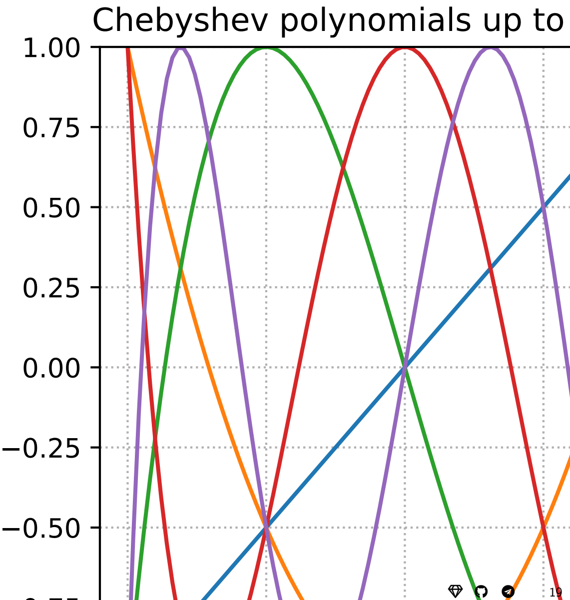

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Note, that $x = 1$ corresponds to $a = \mu$, $x = -1$ corresponds to $a = L$ and $x = 0$ corresponds to $a = \frac{\mu+L}{2}$. This transformation ensures that the behavior of the Chebyshev polynomial on $[-1, 1]$ is reflected on the interval $[\mu,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

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In our error analysis, we require that the polynomial equals 1 at 0 (i.e., $p_k(0) = 1$). After applying the transformation, the value T_k takes at the point corresponding to $a = 0$ might not be 1. Thus, we multiply by the inverse of T_k evaluated at

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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 $[\mu, L]$.

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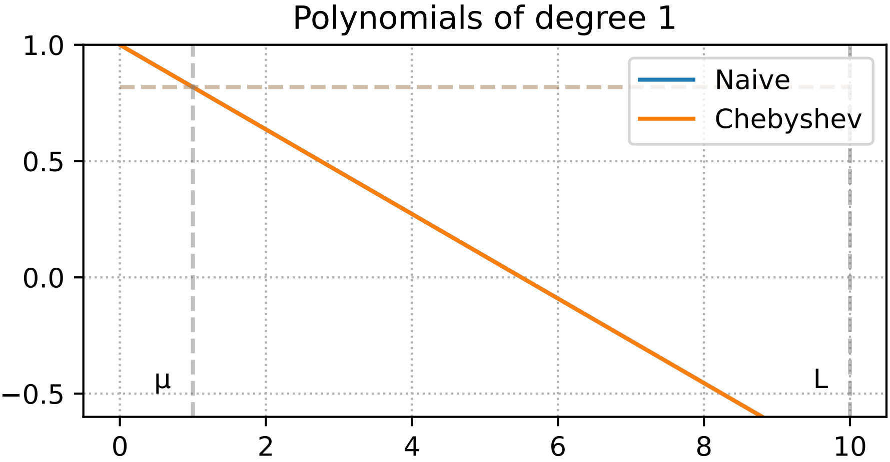

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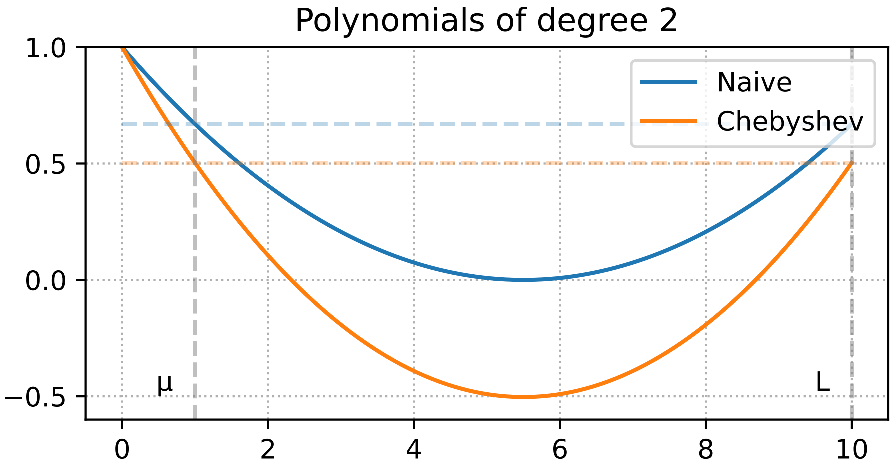

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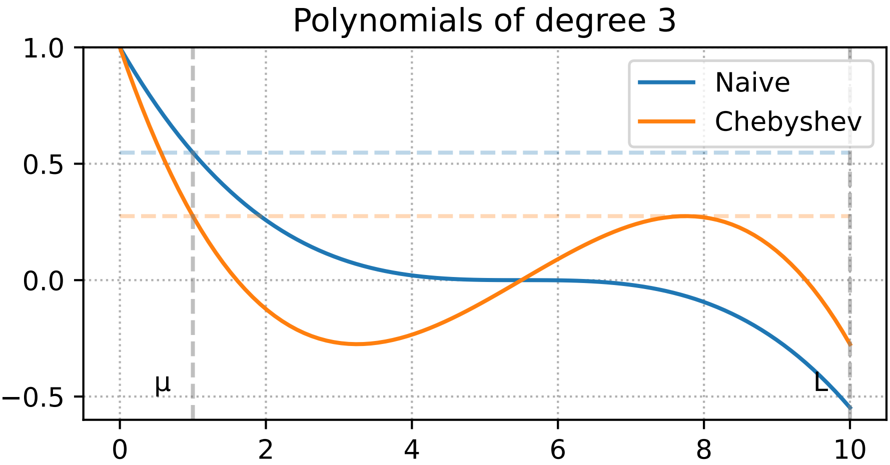

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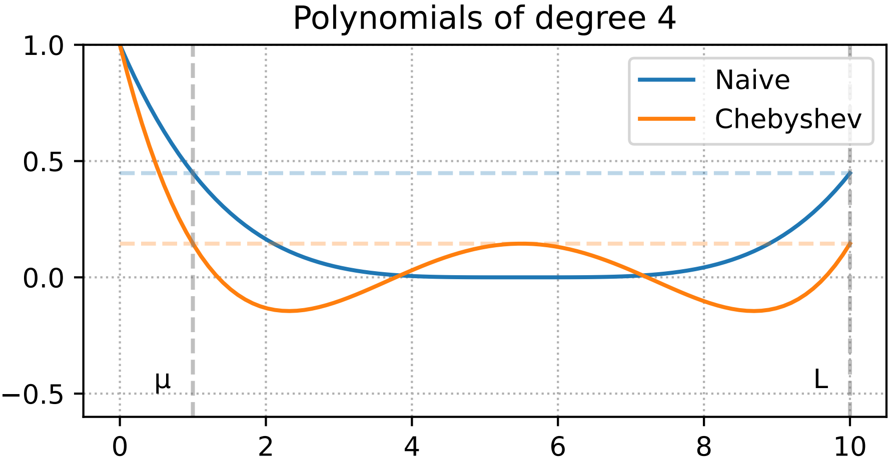

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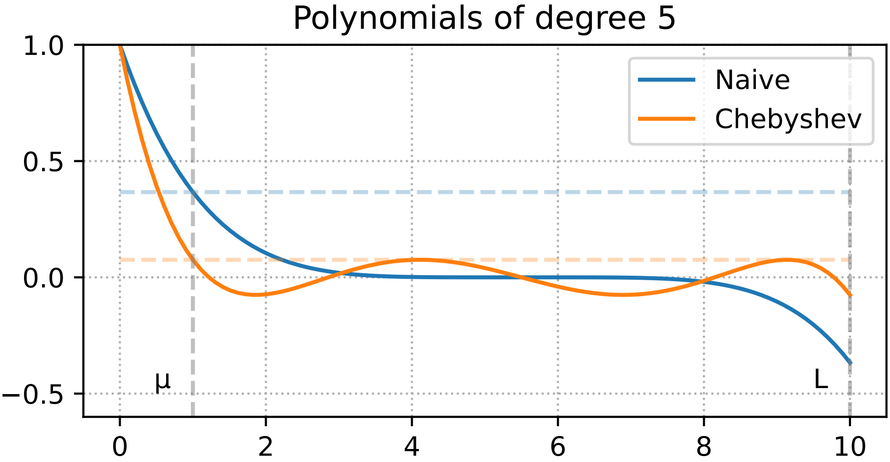

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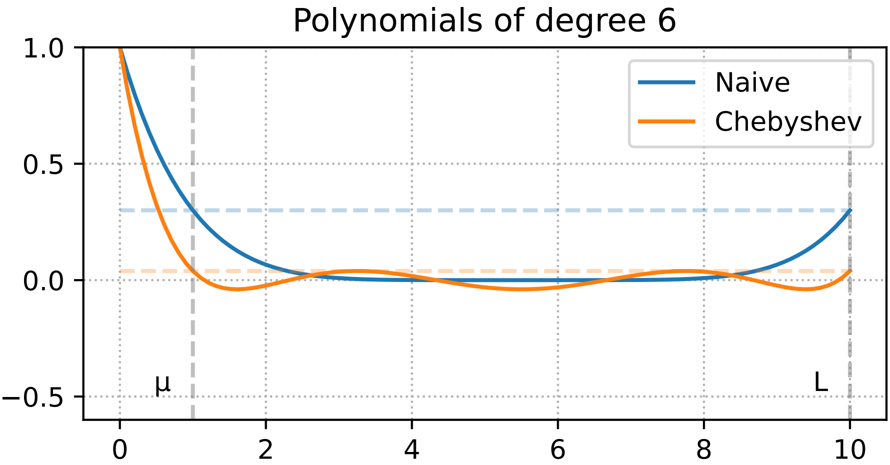

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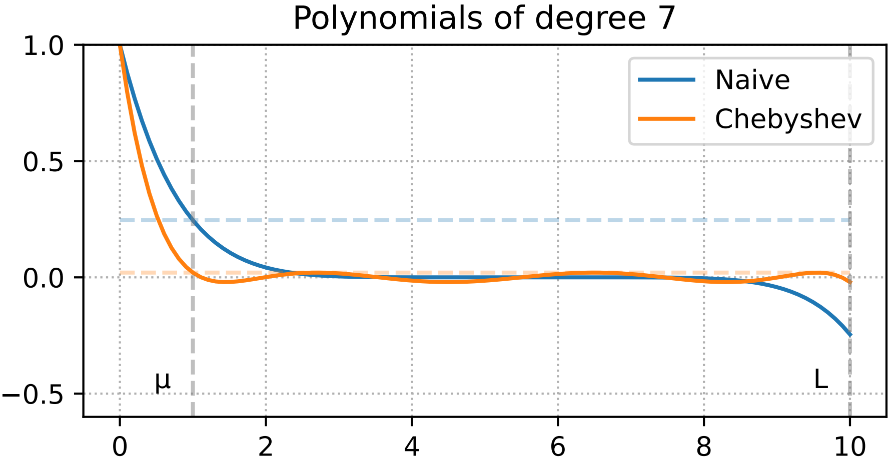

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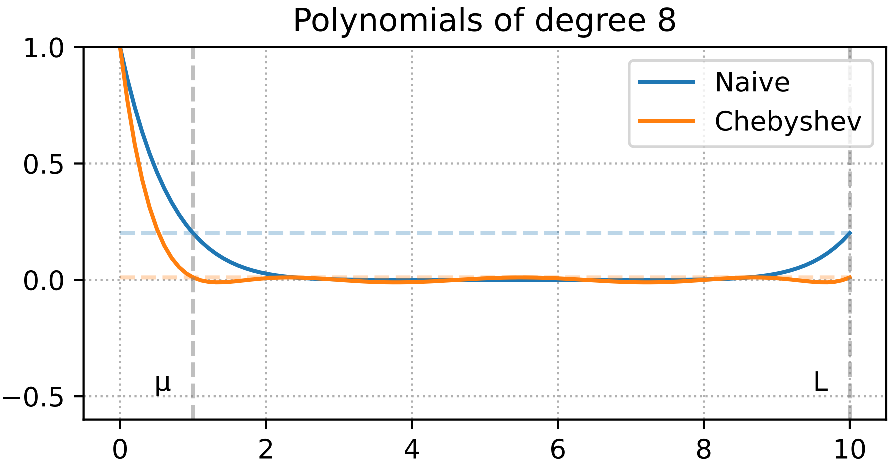

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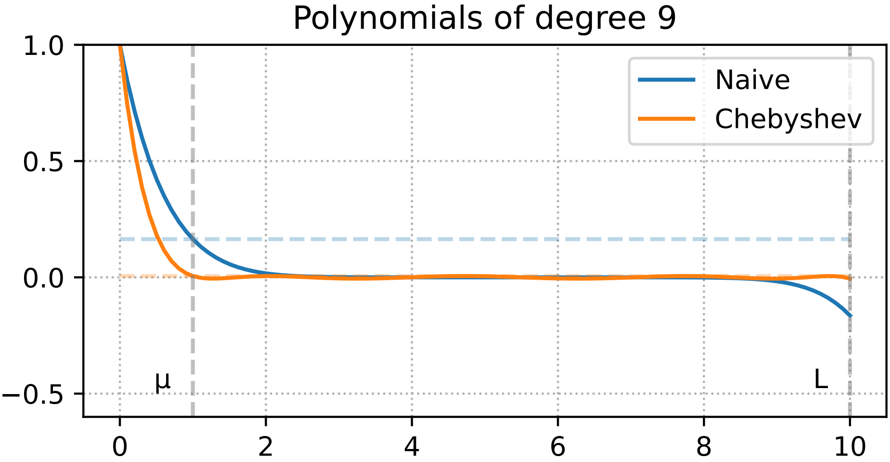

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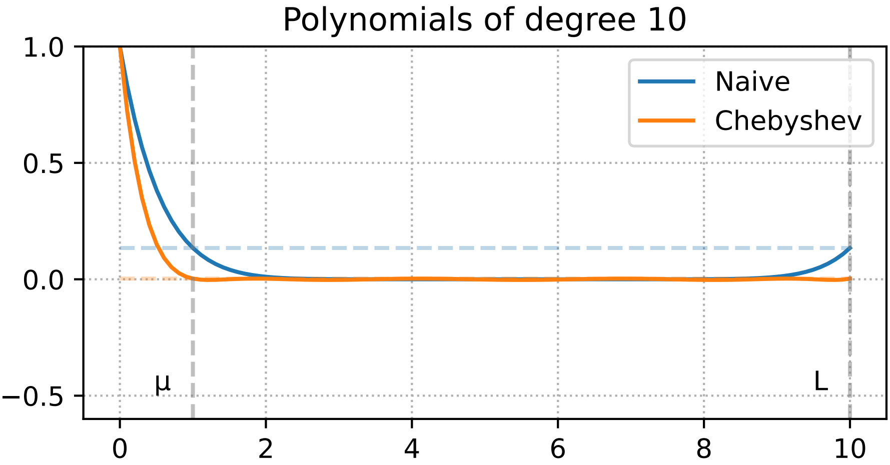

Chebyshev polynomials upper bound

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:

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\|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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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}
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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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\begin{aligned}
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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\beta_k = \dfrac{t_{k-1}}{t_{k+1}}, \\
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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)
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Rearranging the terms, we get:

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

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

$$\begin{cases} \beta_k = \dfrac{t_{k-1}}{t_{k+1}}, \\ \alpha_k = \dfrac{4}{L-\mu}\dfrac{t_k}{t_{k+1}}, \\ 1+\beta_k = 2\dfrac{L+\mu}{L-\mu}\dfrac{t_k}{t_{k+1}} \end{cases}$$

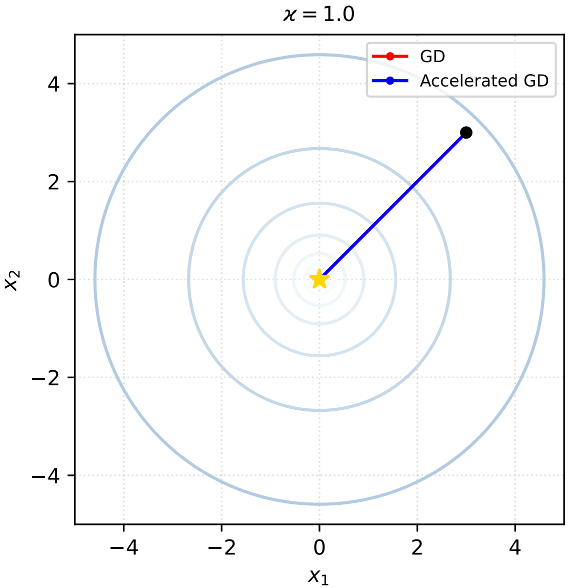
We are almost done :) We remember, that $e_{k+1} = P_{k+1}(A)e_0$. Note also, that we work with the quadratic problem, so we can assume $x^* = 0$ without loss of generality. In this case, $e_0 = x_0$ and $e_{k+1} = x_{k+1}$.

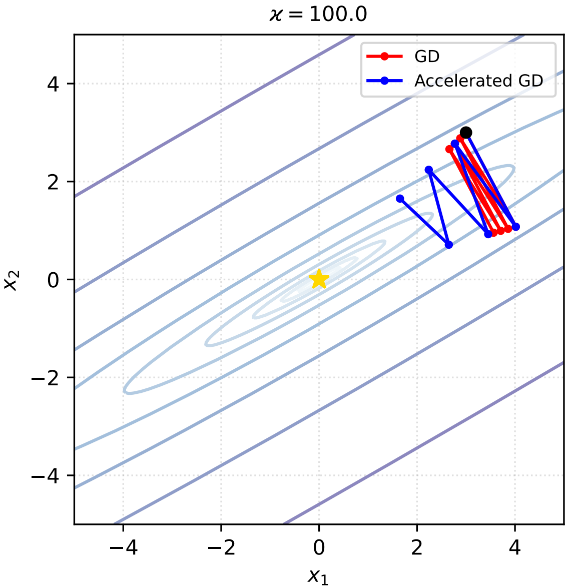
$$\begin{aligned} x_{k+1} &= P_{k+1}(A)x_0 = (I - \alpha_k A)P_k(A)x_0 + \beta_k \left(P_k(A) - P_{k-1}(A)\right) x_0 \\ &= (I - \alpha_k A)x_k + \beta_k \left(x_k - x_{k-1}\right) \end{aligned}$$

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

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

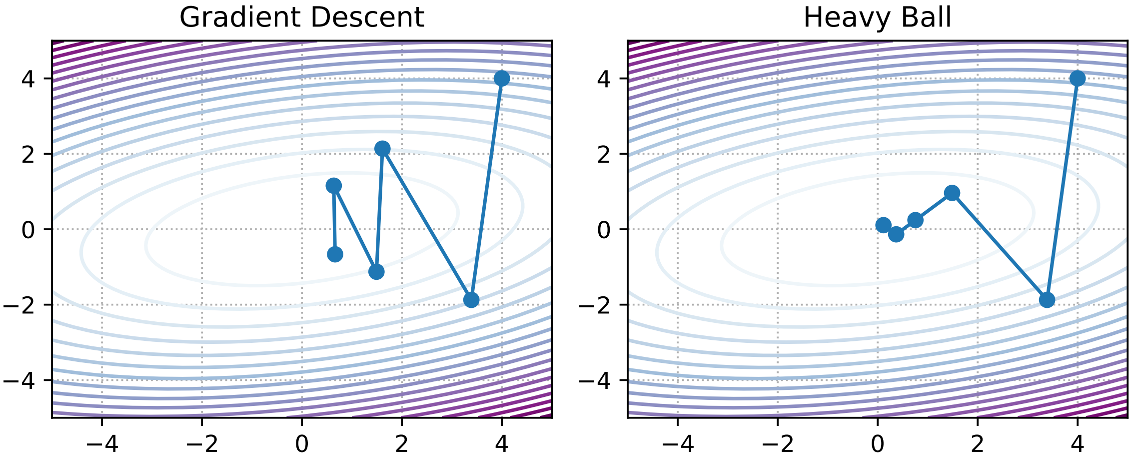
Acceleration from the first principles



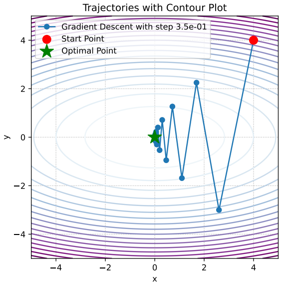


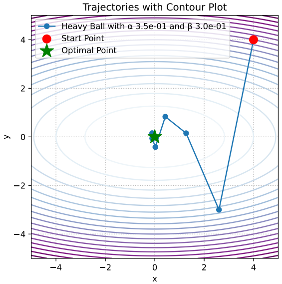
Heavy ball

Oscillations and acceleration



Polyak Heavy ball method





Let's introduce the idea of momentum, proposed by Polyak in 1964. Recall that the momentum update is

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

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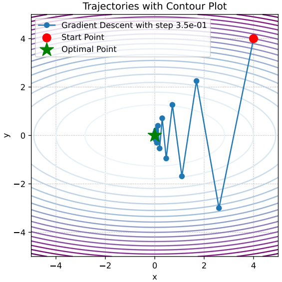

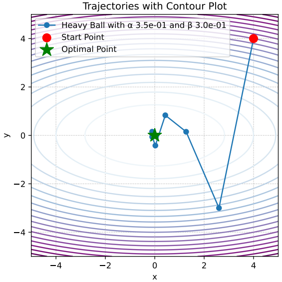

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Which is in our (quadratics) case is

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

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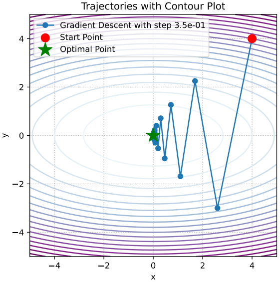

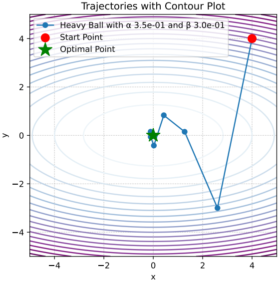

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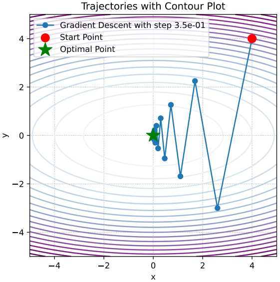

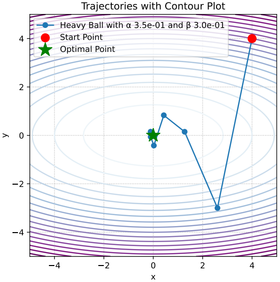

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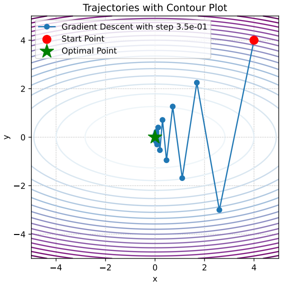

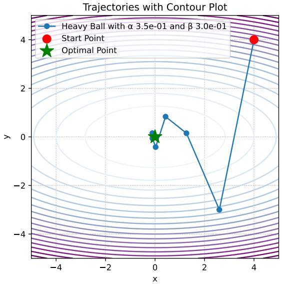

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$$M = \begin{bmatrix} I - \alpha\Lambda + \beta I & -\beta I \\ I & 0_d \end{bmatrix}.$$

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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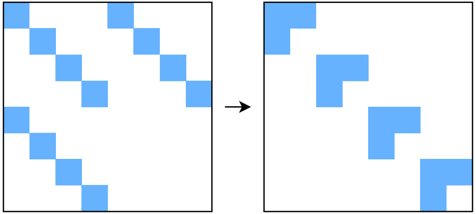

$$
\begin{bmatrix} \hat{x}_k^{(1)} \\ \vdots \\ \hat{x}_k^{(d)} \\ \hat{x}_{k-1}^{(1)} \\ \vdots \\ \hat{x}_{k-1}^{(d)} \end{bmatrix} \to \begin{bmatrix} \hat{x}_k^{(1)} \\ \hat{x}_{k-1}^{(1)} \\ \vdots \\ \hat{x}_k^{(d)} \\ \hat{x}_{k-1}^{(d)} \end{bmatrix} \quad M = \begin{bmatrix} M_1 & & & \\ & M_2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

Рисунок 1: Illustration of matrix M rearrangement

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

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

converges linearly:

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

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

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

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

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

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 $q \in [0, 1)$.

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- 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)

[5] Provable non-accelerations of the heavy-ball method

Nesterov accelerated gradient

The concept of Nesterov Accelerated Gradient method

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

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

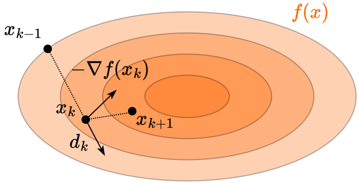
Let's define the following notation

$$x^+ = x - \alpha \nabla f(x) \qquad \text{Gradient step}$$
$$d_k = \beta_k (x_k - x_{k-1}) \qquad \text{Momentum term}$$

Then we can write down:

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

Polyak momentum



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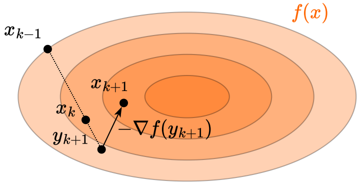

General case convergence

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}
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General case convergence

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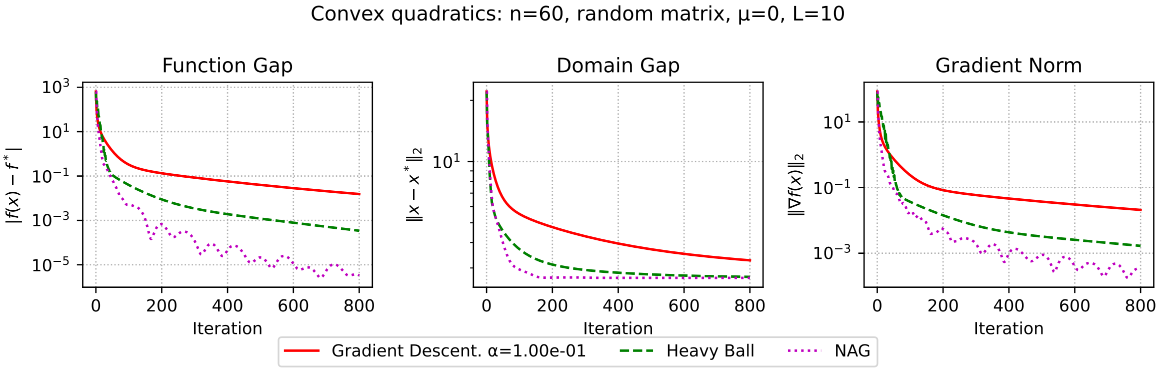
\end{aligned}
$$

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

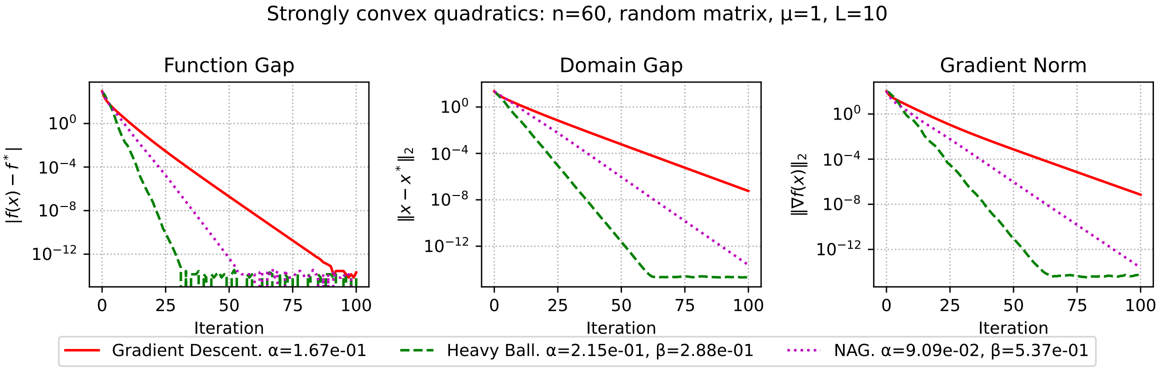
$$
f(y_k) - f^* \leq \frac{\mu + L}{2}\|x_0 - x^*\|_2^2 \exp\left(-\frac{k}{\sqrt{\kappa}}\right)
$$

Numerical experiments

Convex quadratics (aka linear regression)



Strongly convex quadratics (aka regularized linear regression)



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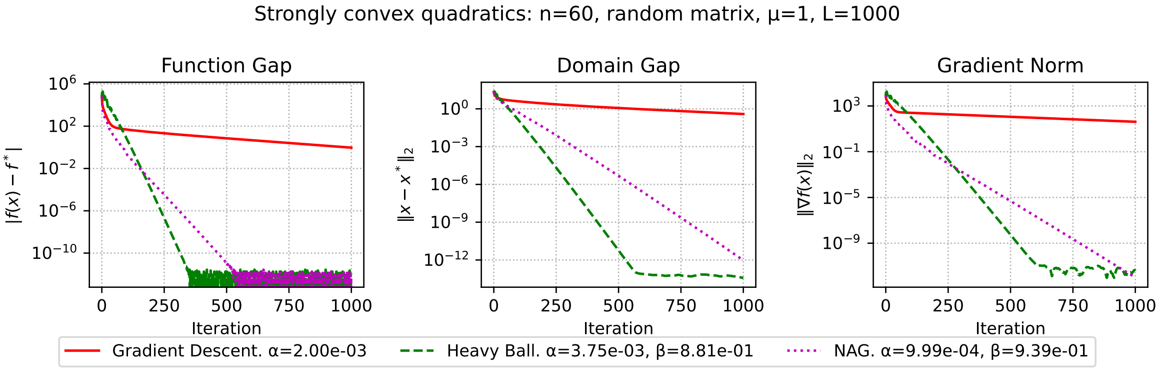

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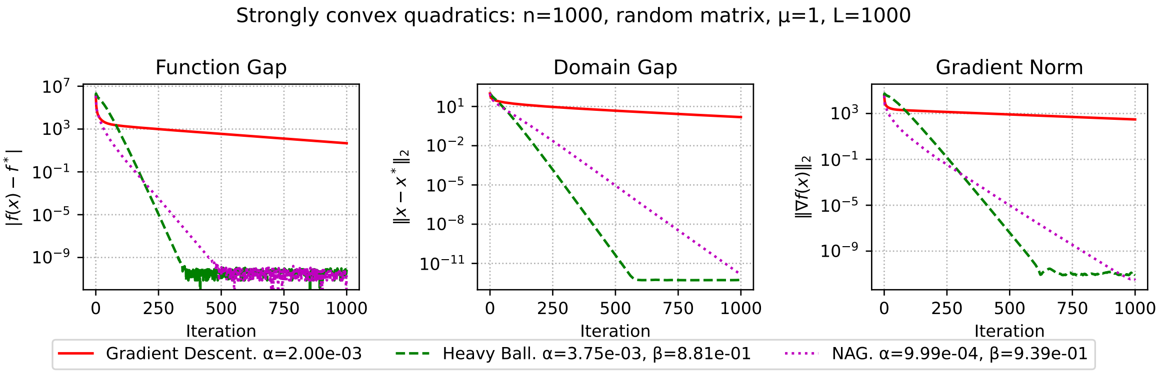
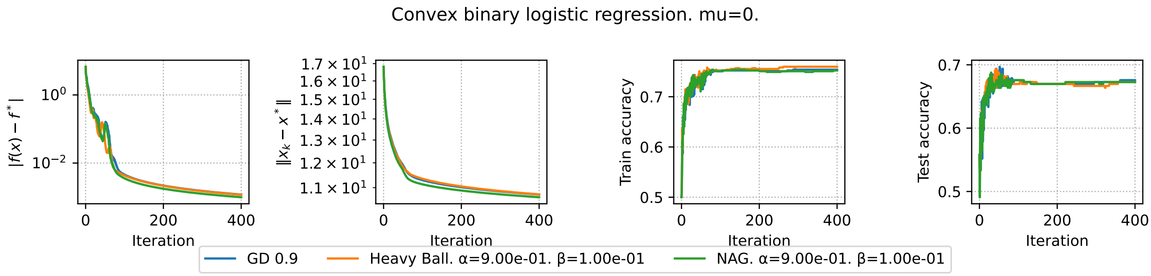


Convex binary logistic regression



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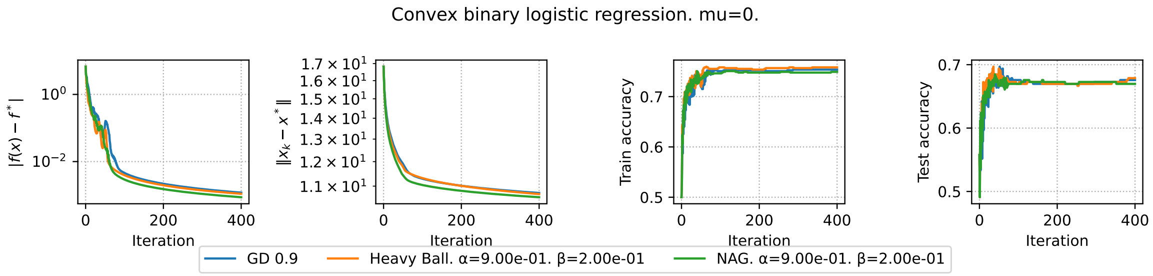

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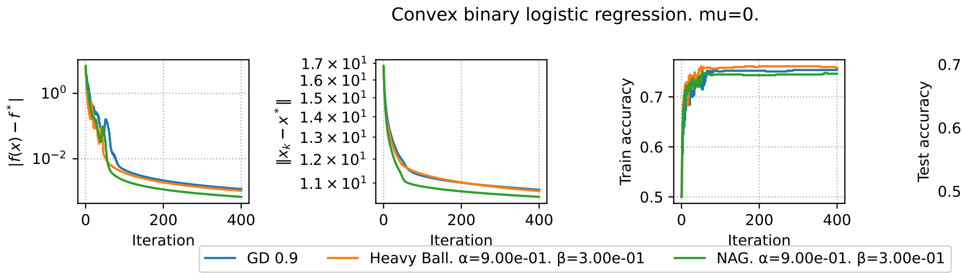
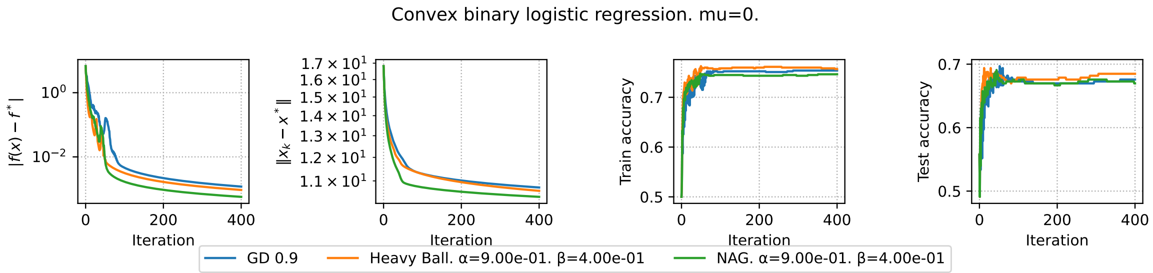


Convex binary logistic regression



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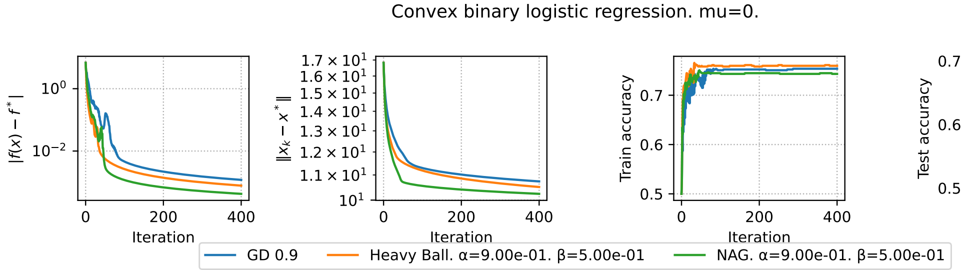

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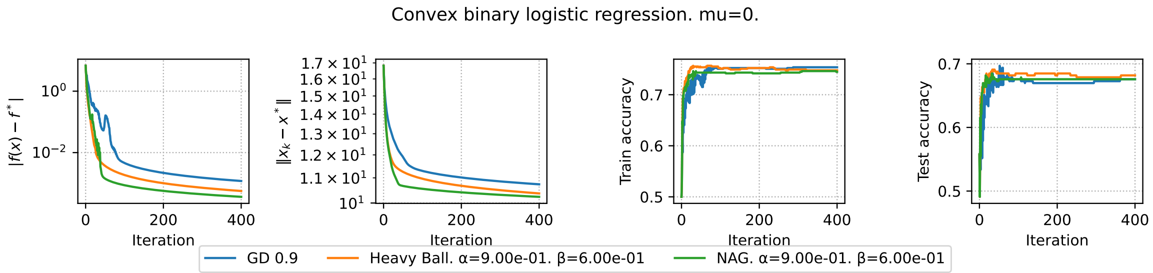

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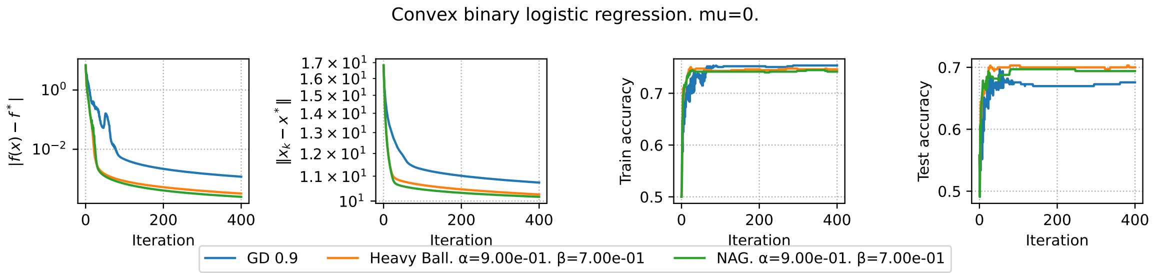

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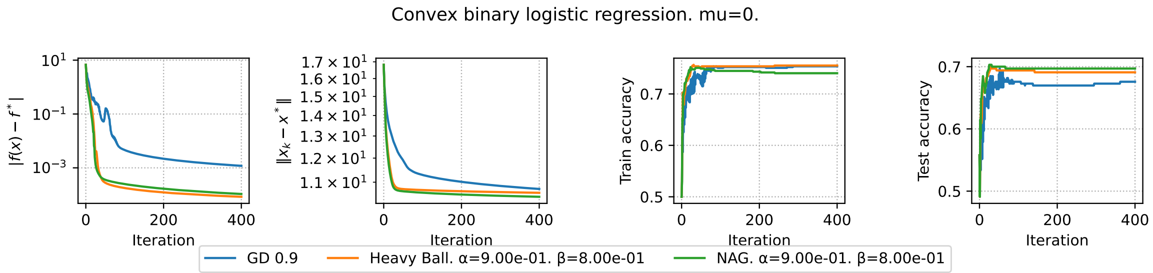

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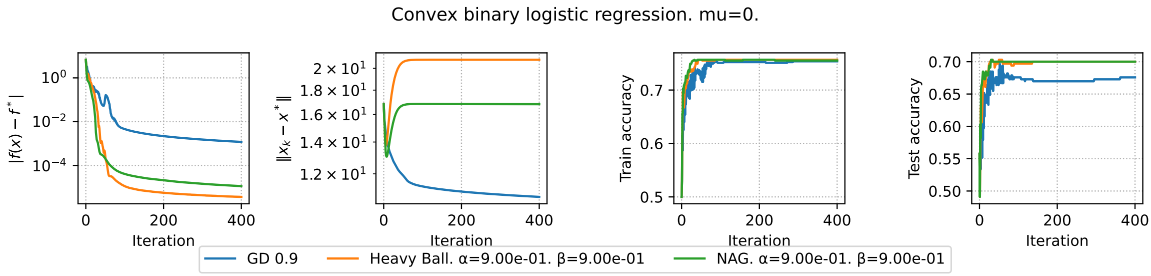

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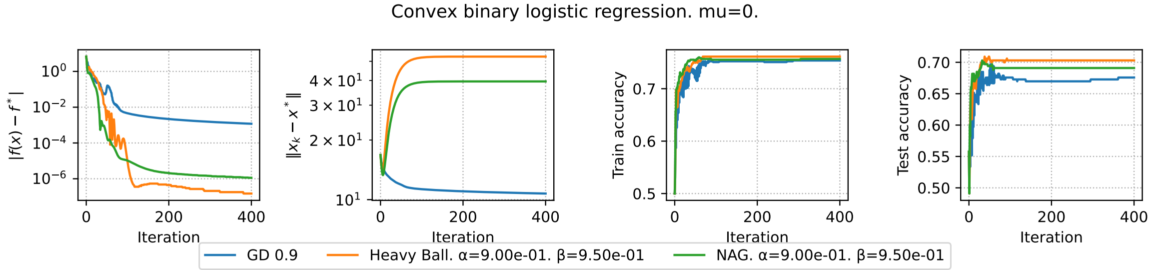

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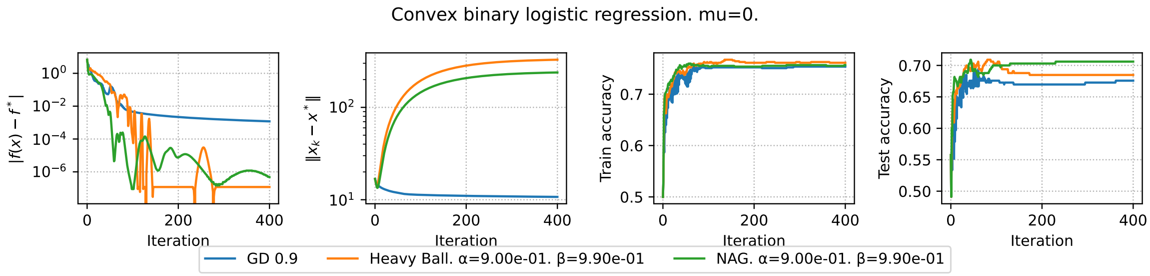

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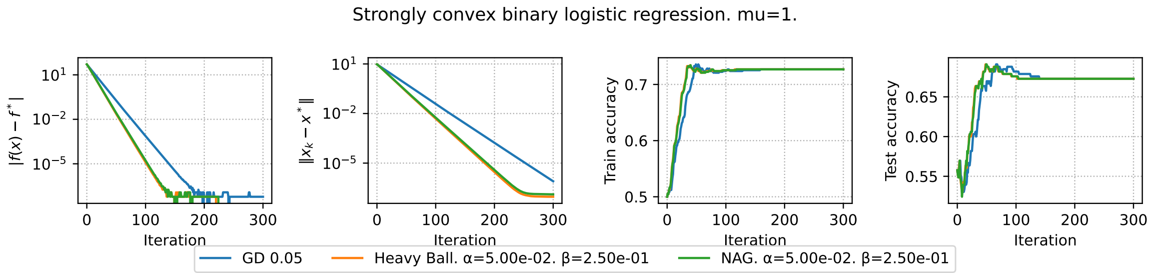
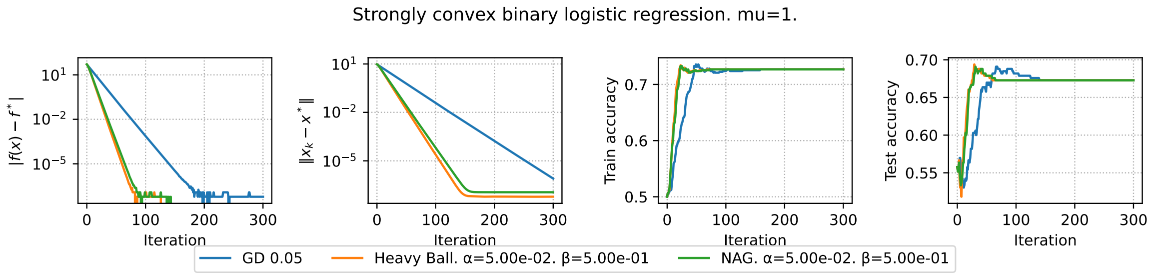
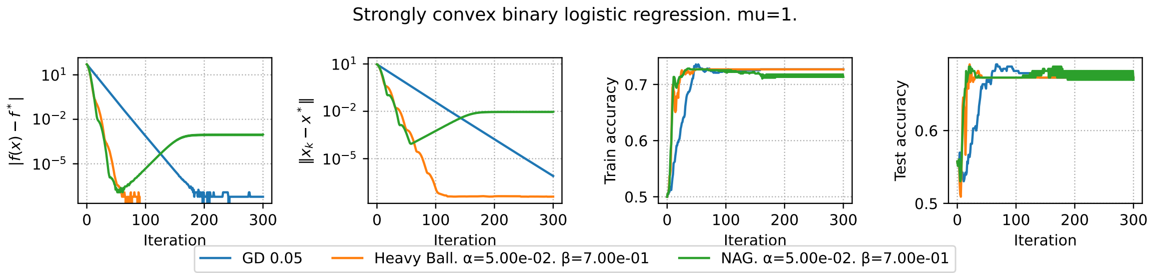


Strongly convex binary logistic regression



Strongly convex binary logistic regression



Strongly convex binary logistic regression