

Gradient Descent:

 $\min_{x \in \mathbb{R}^n} f(x) \hspace{1cm} x^{k+1} = x^k - \alpha^k \nabla f(x^k)$

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

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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:

$$1 - x < e^{-x}$$

Gradient Descent:

 $x^{k+1} = x^k - \alpha^k \nabla f(x^k)$ $\min_{x \in \mathbb{D}^n} f(x)$

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

convex (non-smooth)

$$(-f^*)$$
.

 $\varepsilon = f(x^{k_{\varepsilon}}) - f^* \le \left(1 - \frac{\mu}{L}\right)^{k_{\varepsilon}} \left(f(x^0) - f^*\right)$

$$(0) - f^*)$$

smooth (non-convex)

smooth & strongly convex (or PL)

 $\leq \exp\left(-k_{\varepsilon}\frac{\mu}{I}\right)(f(x^0)-f^*)$

 $k_{\varepsilon} \geq \varkappa \log \frac{f(x^0) - f^*}{\varepsilon} = \mathcal{O}\left(\varkappa \log \frac{1}{\varepsilon}\right)$

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smooth & convex

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

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

smooth (non-convex)

Finally we have

 $\leq \exp\left(-k_{\varepsilon}\frac{\mu}{L}\right)(f(x^0) - f^*)$

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smooth & strongly convex (or PL)

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 $\|\nabla f(x^k)\|^2 \sim \mathcal{O}\left(\frac{1}{k}\right)$

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smooth & strongly convex (or PL)

 $\|x^k - x^*\|^2 \sim \mathcal{O}\left(\left(1 - \frac{\mu}{L}\right)^k\right)$

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 $f(x^k) - f^* \sim \mathcal{O}\left(\frac{1}{h}\right)$

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





Lower bounds

$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right) \qquad \mathcal{O}\left(\frac{1}{k^2}\right) \qquad \mathcal{O}\left(\frac{1}{k^2}\right) \qquad \mathcal{O}\left(\left(1-\sqrt{\frac{\mu}{L}}\right)^k\right) \\ k_s \sim \mathcal{O}\left(\frac{1}{s}\right) \qquad k_s \sim \mathcal{O}\left(\frac{1}{s}\right) \qquad k_s \sim \mathcal{O}\left(\sqrt{\kappa}\log\frac{1}{s}\right)$	convex (non-smooth)	smooth (non-convex) ¹	smooth & convex ²	smooth & strongly convex (or PL)
$\varepsilon = (\varepsilon^2)$ $\varepsilon = (\sqrt{\varepsilon})$ $\varepsilon = (\sqrt{\varepsilon})$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ $k_{\varepsilon} \sim \mathcal{O}\left(\frac{1}{\varepsilon^2}\right)$	$\mathcal{O}\left(\frac{1}{k^2}\right)$ $k_{\varepsilon} \sim \mathcal{O}\left(\frac{1}{\sqrt{\varepsilon}}\right)$	$\mathcal{O}\left(\frac{1}{k^2}\right)$ $k_{\varepsilon} \sim \mathcal{O}\left(\frac{1}{\sqrt{\varepsilon}}\right)$	$\mathcal{O}\left(\left(1-\sqrt{\frac{\mu}{L}} ight)^k ight) \ k_arepsilon \sim \mathcal{O}\left(\sqrt{arkappa}\lograc{1}{arepsilon} ight)$

¹Carmon, Duchi, Hinder, Sidford, 2017 ²Nemirovski, Yudin, 1979

Black box iteration

The iteration of gradient descent:

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

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Consider a family of first-order methods, where

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

(1)

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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.

i Theorem

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

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

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 $f \to \min_{x,y}$

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- Note, that this bound $\mathcal{O}\left(\frac{1}{L^2}\right)$ does not match the rate of gradient descent $\mathcal{O}\left(\frac{1}{L}\right)$. Two options possible:
 - a. The lower bound is not tight.
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• Let n=2k+1 and $A\in\mathbb{R}^{n\times n}$.

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

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Notice, that

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

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

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

Example, when n = 3:

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

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Therefore, $x^TAx \ge 0$. It is also easy to see that $0 \le A \le 4I$.

Example, when n=3:

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

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

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Notice, that

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Therefore, $x^T Ax > 0$. It is also easy to see that $0 \prec A \prec 4I$.

Example, when n=3:

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

Lower bound:

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$$x^T A x = 2x_1^2 + 2x_2^2 + 2x_2^2 - 2x_1x_2 - 2x_2x_2$$

$$+(x_1$$

Upper bound

$$c_2^2 + c_2^2$$

 $0 < 2x_1^2 + 2x_2^2 + 2x_2^2 + 2x_1x_2 + 2x_2x_2$

 $0 < x_1^2 + (x_1 + x_2)^2 + (x_2 + x_2)^2 + x_2^2$

$$x^TAx = 2x_1^2 + 2x_2^2 + 2x_3^2 - 2x_1x_2 - 2x_2x_3$$

$$x_1^2 + 2$$

$$-2x^{2}$$

 $<4(x_1^2+x_2^2+x_3^2)$

$$= x_1 + x_1 - 2x_1x_2 + x_2 + x_2 - 2x_2x_3 + x_1$$

$$= x_1^2 + (x_1 - x_2)^2 + (x_2 - x_3)^2 + x_3^2 \ge 0$$

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$$-1$$

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

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

... Lower bounds

- 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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• 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.

 $f \to \min_{x,y,}$

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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:

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

 $f \to \min_{x,y,z}$

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

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

- 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

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

• 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

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

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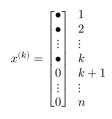
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$$x^{(k)} = \begin{bmatrix} \bullet \\ \bullet \\ \vdots \\ \vdots \\ k \\ 0 \\ k+1 \\ \vdots \\ 0 \end{bmatrix}$$

• However, since every iterate x^k produced by our method lies in $S_k = \mathrm{span}\{e_1, e_2, \dots, e_k\}$ (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

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

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

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

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$$= \frac{L}{8} \left(\frac{1}{k+1} - \frac{1}{n+1} \right) = \frac{L}{8} \left(\frac{n-k}{(k+1)(n+1)} \right)$$

 $f \to \min_{x,y,z}$ Lower

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 $\stackrel{n=2k+1}{=} \frac{L}{16(k+1)}$

 $f \to \min_{x,y,z}$

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• Now we bound $R = ||x^0 - x^*||_2$:

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

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

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

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

We observe, that

(3)

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

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

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 $f o \min_{x,y,z}$ Lower bounds

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

$$\begin{split} f(x^k) - f(x^*) &\geq \frac{L}{16(k+1)} = \frac{L(k+1)}{16(k+1)^2} \\ &\geq \frac{L}{16(k+1)^2} \frac{3}{2} R^2 \\ &= \frac{3LR^2}{32(k+1)^2} \end{split}$$



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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

i Smooth convex case

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

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

i 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:

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

Acceleration for quadratics





Convergence result for quadratics

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

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

i Theorem

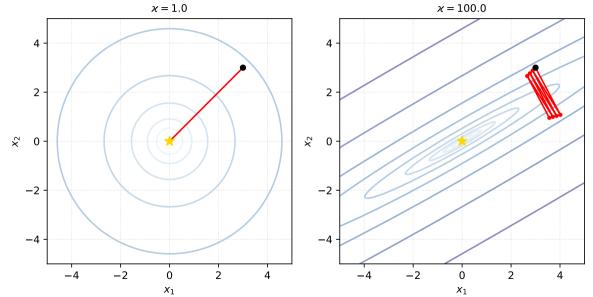
The gradient descent method with the learning rate $lpha_k=rac{2}{u+L}$ converges to the optimal solution x^* with the following guarantee:

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

where $\varkappa = \frac{L}{u}$ 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 $[\mu, L]$,:

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

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 $[\mu, L]$.

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.

relevant interval is therefore [1, 10].

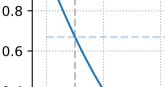
Can we do better? The answer is yes.

figure we choose $\alpha=1$ and $\beta=10$ so that $\kappa=10$. The

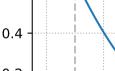
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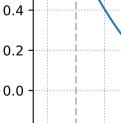
-0.2

1.0



Naive polynomials up to de







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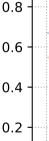
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Let's look at this polynomial a bit closer. On the right figure we choose
$$\alpha = 1$$
 and $\beta = 10$ so that $\kappa = 10$. The

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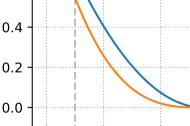
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-0.2

1.0





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Naive polynomials up to de 1.0 0.8 0.6

0.4

0.2

0.0

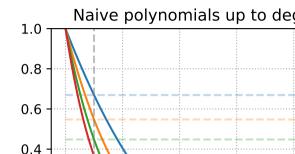
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 $p_2(a)$

0.2

0.0

-0.2



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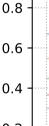
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This is exactly the rate we proved in the previous lecture for any smooth and strongly convex function. Let's look at this polynomial a bit closer. On the right

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.

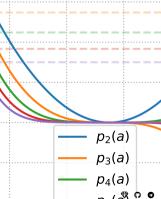
Naive polynomials up to de 1.0



0.0

-0.2

0.2



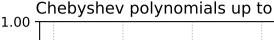


Chebyshev polynomials turn out to give an optimal answer to the guestion that we asked. Suitably rescaled, they minimize the absolute value in a desired interval $[\mu, L]$ while satisfying the normalization constraint of having value 1 at the origin.

$$T_1(x)=x$$

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





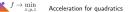


0.00

-0.25







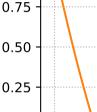
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0.00

-0.25







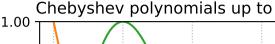
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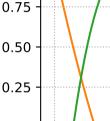
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-0.25

-0.50



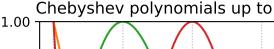




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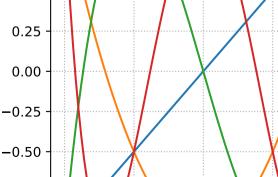
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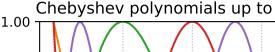


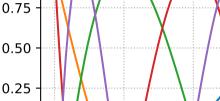
 $f \to \min_{x,y,z}$ Acceleration for quadratics

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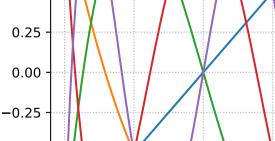
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Acceleration for quadratics

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We will use the following affine transformation:

$$x = \frac{L + \mu - 2a}{L - \mu}, \quad a \in [\mu, L], \quad x \in [-1, 1].$$

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

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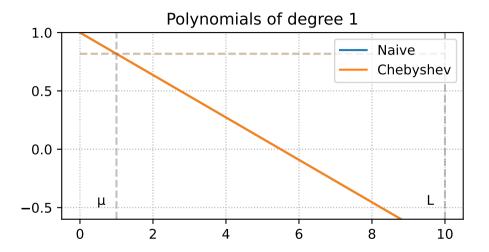
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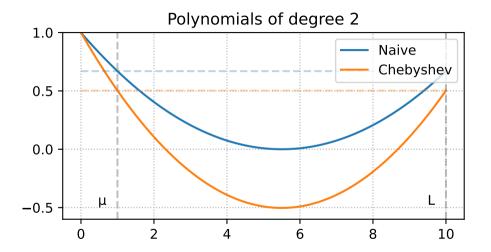
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 $P_k(a) = T_k \left(\frac{L + \mu - 2a}{L - \mu}\right) \cdot T_k \left(\frac{L + \mu}{L - \mu}\right)^{-1}$

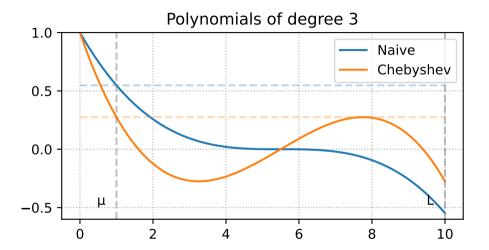
and observe, that they are much better behaved than the naive polynomials in terms of the magnitude in the interval $[\mu, L]$.





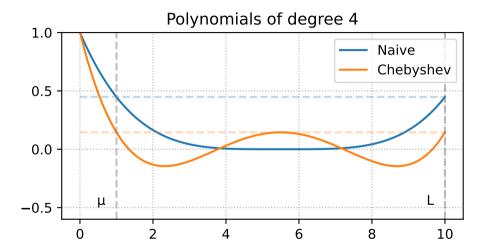






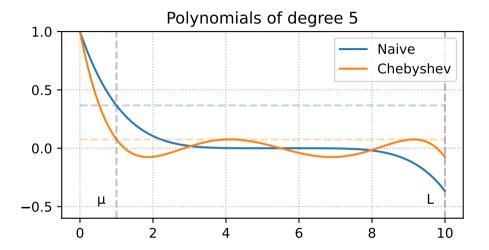




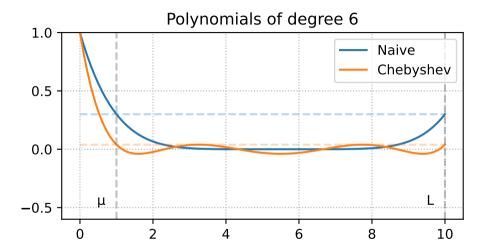




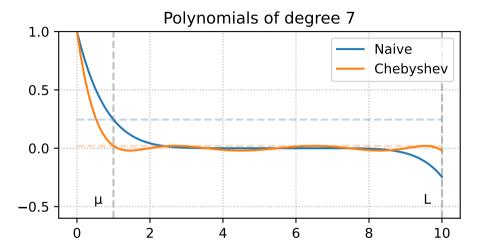




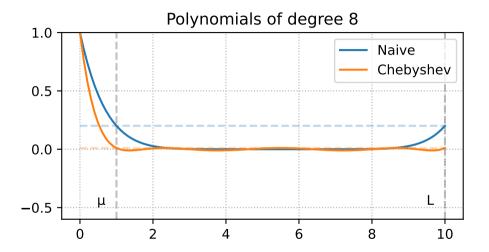






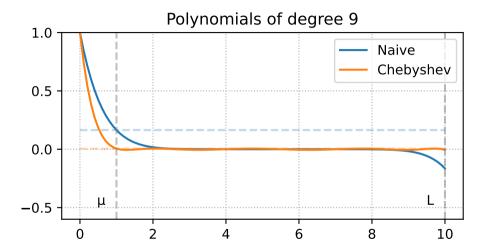






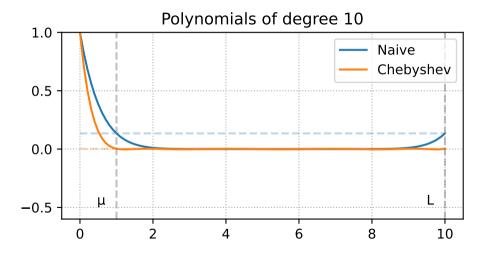














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We can see, that the maximum value of the Chebyshev polynomial on the interval $[\mu, L]$ is achieved at the point $a = \mu$. Therefore, we can use the following upper bound:

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



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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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1. For any $x \geq 1$, the Chebyshev polynomial of the first kind can be written as

$$\begin{split} T_k(x) &= \cosh\left(k \operatorname{arccosh}(x)\right) \\ T_k(1+\epsilon) &= \cosh\left(k \operatorname{arccosh}(1+\epsilon)\right). \end{split}$$

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4. Therefore.

$$\begin{split} T_k(1+\epsilon) &= \cosh\left(k \operatorname{arccosh}(1+\epsilon)\right) \\ &= \cosh\left(k\phi\right) \\ &= \frac{e^{k\phi} + e^{-k\phi}}{2} \geq \frac{e^{k\phi}}{2} \\ &= \frac{\left(1+\sqrt{\epsilon}\right)^k}{2}. \end{split}$$

Acceleration for quadratics

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 $\|e_k\| \le \|P_k(A)\| \|e_0\| \le \frac{2}{(1+\sqrt{\epsilon})^k} \|e_0\|$

 $\leq 2\left(1+\sqrt{\frac{2}{\varkappa-1}}\right)^{-k}\|e_0\|$

 $\leq 2\exp\left(-\sqrt{\frac{2}{\varkappa-1}}k\right)\|e_0\|$

 $=\frac{e^{k\phi}+e^{-k\phi}}{2}\geq \frac{e^{k\phi}}{2}$

 $=\cosh(k\phi)$

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:

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

Given the fact, that $x = \frac{L + \mu - 2a}{L - \mu}$, and:

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$$L+\mu-2a \qquad (L+\mu)$$

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$$\begin{split} P_{k+1}(a)t_{k+1} &= 2\frac{L+\mu-2a}{L-\mu}P_k(a)t_k - P_{k-1}(a)t_{k-1} \text{, where } t_k = T_k\left(\frac{L+\mu}{L-\mu}\right) \\ P_{k+1}(a) &= 2\frac{L+\mu-2a}{L-\mu}P_k(a)\frac{t_k}{t_{k+1}} - P_{k-1}(a)\frac{t_{k-1}}{t_{k+1}} \end{split}$$

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

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

Acceleration for quadratics

Rearranging the terms, we get:

$$\begin{split} P_{k+1}(a) &= (1+\beta_k)P_k(a) - \alpha_k a P_k(a) - \beta_k P_{k-1}(a), \\ P_{k+1}(a) &= 2\frac{L+\mu}{L-\mu}\frac{t_k}{t_{k+1}}P_k(a) - \frac{4a}{L-\mu}\frac{t_k}{t_{k+1}}P_k(a) - \frac{t_{k-1}}{t_{k+1}}P_{k-1}(a) \end{split}$$

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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 $e_{k+1} = x_{k+1}$.

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

$$\begin{aligned} &\text{Rearranging the terms, we get:} \\ &P_{k+1}(a) = (1+\beta_k)P_k(a) - \alpha_k a P_k(a) - \beta_k P_{k-1}(a), \\ &P_{k+1}(a) = 2\frac{L+\mu}{L-\mu}\frac{t_k}{t_{k+1}}P_k(a) - \frac{4a}{L-\mu}\frac{t_k}{t_{k+1}}P_k(a) - \frac{t_{k-1}}{t_{k+1}}P_{k-1}(a) \end{aligned} \qquad \begin{cases} \beta_k = \frac{t_{k-1}}{t_{k+1}}, \\ \alpha_k = \frac{4}{L-\mu}\frac{t_k}{t_{k+1}}, \\ 1+\beta_k = 2\frac{L+\mu}{L-\mu}\frac{t_k}{t_{k+1}}, \\ 1+\beta_k = 2\frac{L+\mu}{L-\mu}\frac{t_k}{t_{k+1}}, \end{cases}$$

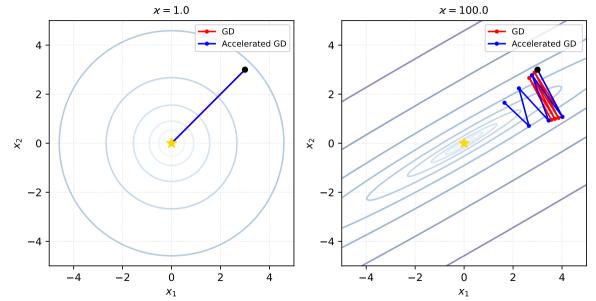
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For quadratic problem, we have $\nabla f(x_k) = Ax_k$, so we can rewrite the update as:

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

Acceleration from the first principles



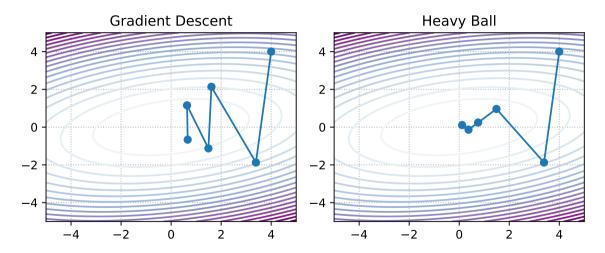
Heavy ball



Heavy ball

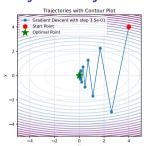


Oscillations and acceleration



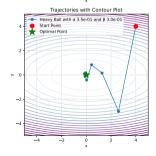


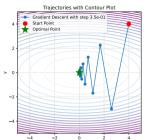




Let's introduce the idea of momentum, proposed by Polyak in 1964. Recall that the momentum update is

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



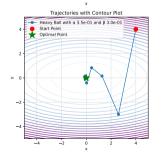


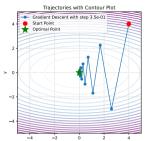
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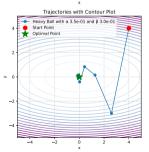
$$x^{k+1} = x^k - \alpha \nabla f(x^k) + \beta (x^k - x^{k-1}).$$

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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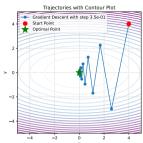
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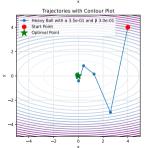
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This can be rewritten as follows

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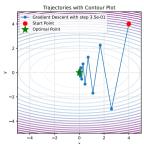
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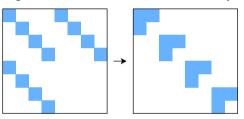
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$$M = \begin{bmatrix} I - \alpha \Lambda + \beta I & -\beta I \\ I & 0_d \end{bmatrix}.$$

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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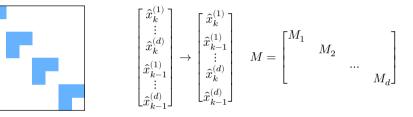


Рисунок 1: Illustration of matrix ${\cal M}$ rearrangement

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.

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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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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 ${\cal M}_i$:

$$\lambda_1^M, \lambda_2^M = \lambda \left(\begin{bmatrix} 1 - \alpha \lambda_i + \beta & -\beta \\ 1 & 0 \end{bmatrix} \right) = \frac{1 + \beta - \alpha \lambda_i \pm \sqrt{(1 + \beta - \alpha \lambda_i)^2 - 4\beta}}{2}.$$

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

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

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

 $f \to \min_{x,y,z}$ Heavy ball

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Heavy Ball quadratics convergence

i 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:

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





Heavy Ball Global Convergence ³

i Theorem

Assume that f is smooth and convex and that

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

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

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

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

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

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

Heavy Ball Global Convergence 4

i Theorem

Assume that f is smooth and strongly convex and that

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

Then, the sequence $\{x_k\}$ generated by Heavy-ball iteration converges linearly to a unique optimizer x^\star . In particular,

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

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

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

• Ensures accelerated convergence for strongly convex quadratic problems



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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)







Nesterov accelerated gradient





The concept of Nesterov Accelerated Gradient method

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

The concept of Nesterov Accelerated Gradient method

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

Let's define the following notation

$$x^+ = x - \alpha \nabla f(x) \hspace{1cm} \text{Gradient step}$$

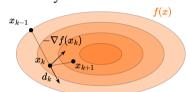
$$d_k = \beta_k (x_k - x_{k-1}) \hspace{1cm} \text{Momentum term}$$

Then we can write down:

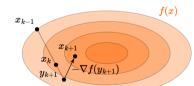
$$\begin{array}{ll} x_{k+1} = x_k^+ & \text{Gradient Descent} \\ x_{k+1} = x_k^+ + d_k & \text{Heavy Ball} \\ x_{k+1} = (x_k + d_k)^+ & \text{Nesterov accelerated gradient} \end{array}$$

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

Polyak momentum



Nesterov momentum



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General case convergence

i 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:

Extrapolation: $x_{k+1} = (1-\gamma_k)y_{k+1} + \gamma_k y_k$

 $y_{k+1} = x_k - \frac{1}{L} \nabla f(x_k)$

Extrapolation weight:
$$\lambda_{k+1} = \frac{1+\sqrt{1+4\lambda_k^2}}{2}$$

$$1-\lambda_k$$

Extrapolation weight: $\gamma_k = \frac{1-\lambda_k}{\lambda_{k+1}}$

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:

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

Nesterov accelerated gradient

General case convergence

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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:

Gradient update:
$$y_{k+1} = x_k - \frac{1}{L} \nabla f(x_k)$$

Extrapolation:
$$x_{k+1} = (1+\gamma_k)y_{k+1} - \gamma_k y_k$$

Extrapolation weight:
$$\gamma_k = \frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}$$

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

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

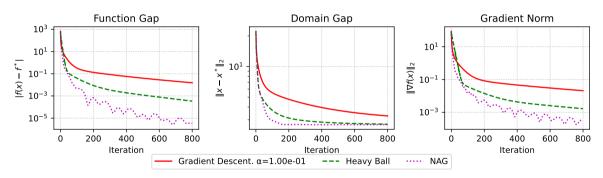
 $f \to \min_{x,y,z}$ Nesterov accelerated gradient

Numerical experiments



Convex quadratics (aka linear regression)

Convex quadratics: n=60, random matrix, μ =0, L=10

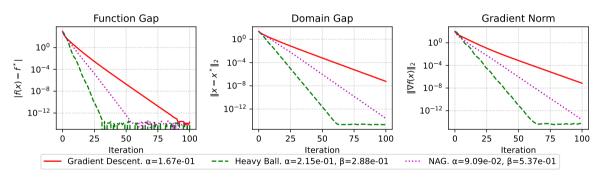






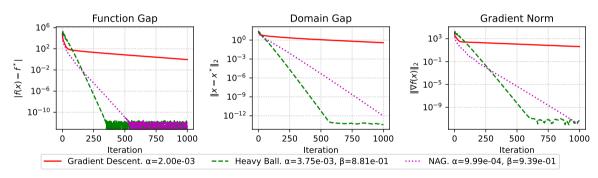
Strongly convex quadratics (aka regularized linear regression)

Strongly convex quadratics: n=60, random matrix, $\mu=1$, L=10



Strongly convex quadratics (aka regularized linear regression)

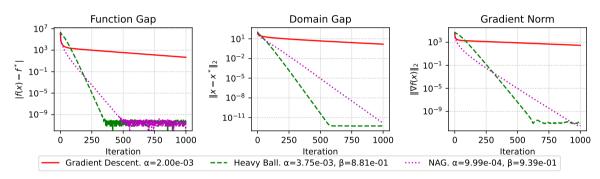
Strongly convex quadratics: n=60, random matrix, $\mu=1$, L=1000



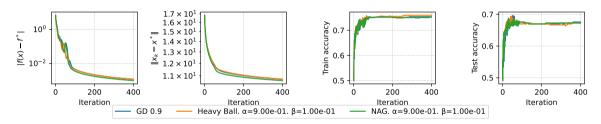


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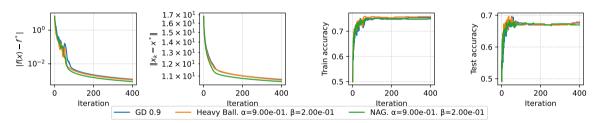
Strongly convex quadratics: n=1000, random matrix, μ =1, L=1000





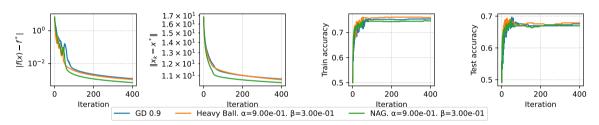






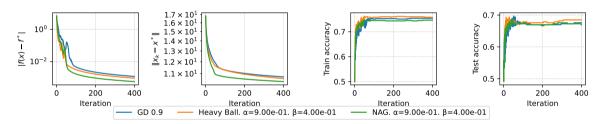






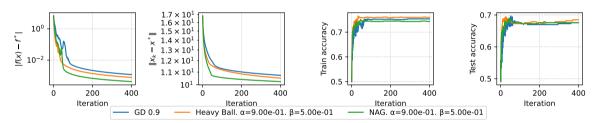






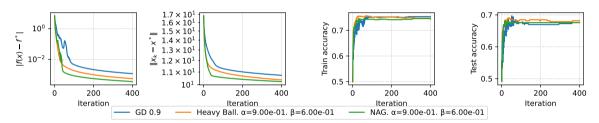






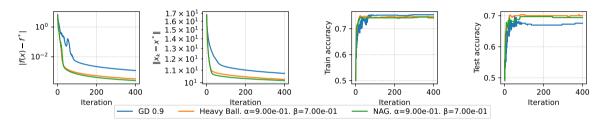




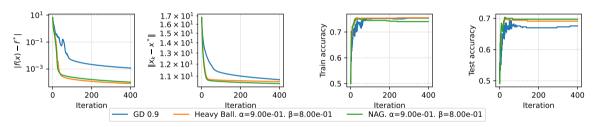






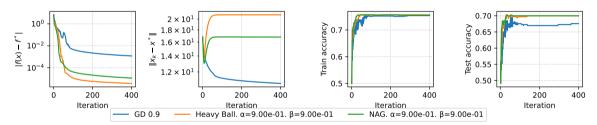








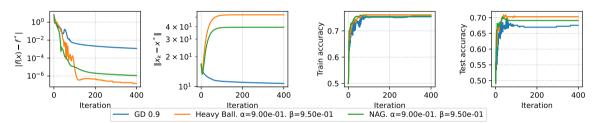








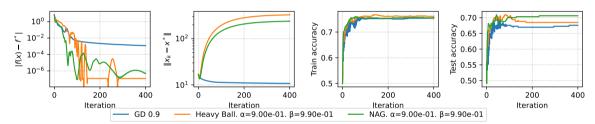








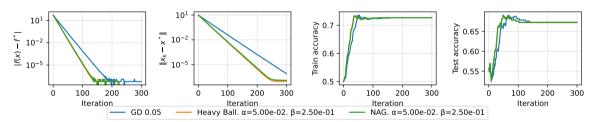








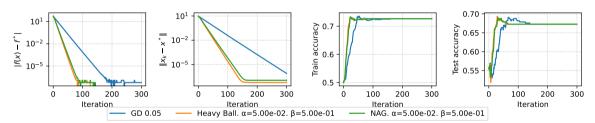








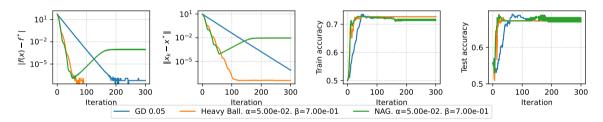








Strongly convex binary logistic regression. mu=1.







Strongly convex binary logistic regression. mu=1.

