

Gradient Descent:

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

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

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For smooth strongly convex we have:

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

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:

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

 $\min_{x \in \mathbb{R}^n} f(x)$

smooth & convex smooth & strongly convex (or PL) $||x^k - x^*||^2 \sim \mathcal{O}\left(\left(1 - \frac{\mu}{L}\right)^k\right)$ $f(x^k) - f^* \sim \mathcal{O}\left(\frac{1}{h}\right)$ $k_{arepsilon} \sim \mathcal{O}\left(arkappa \log rac{1}{arepsilon}
ight)$ $k_{\varepsilon} \sim \mathcal{O}\left(\frac{1}{\varepsilon}\right)$

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

$$k_{\varepsilon} \sim \mathcal{O}\left(\frac{1}{\varepsilon^2}\right) \qquad \qquad k_{\varepsilon} \sim \mathcal{O}\left(\frac{1}{\varepsilon}\right)$$

its tangent line at x=0, we have:

convex (non-smooth)

For smooth strongly convex we have: Finally we have
$$f(x^k)-f^*\leq \left(1-\frac{\mu}{I}\right)^k(f(x^0)-f^*).$$
 $\varepsilon=f(x^k)$

smooth (non-convex)

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

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

 $k_{\varepsilon} \ge \varkappa \log \frac{f(x^0) - f^*}{2} = \mathcal{O}\left(\varkappa \log \frac{1}{2}\right)$

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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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Finally we have

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

 $k_{\varepsilon} \sim \mathcal{O}\left(\frac{1}{\varepsilon}\right)$

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 $k_{\varepsilon} \sim \mathcal{O}\left(\frac{1}{c^2}\right)^{V}$

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$$\leq \exp\left(-k_\varepsilon \frac{\mu}{L}\right) (f(x^0) - f^*)$$
 its tangent line at $x = 0$, we have:

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

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

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

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$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right) \qquad \mathcal{O}\left(\frac{1}{k^2}\right) \qquad \mathcal{O}\left(\frac{1}{k^2}\right) \qquad \mathcal{O}\left(\left(1 - \sqrt{\frac{\mu}{L}}\right)^k\right)$ $k_2 \approx \mathcal{O}\left(\frac{1}{k^2}\right) \qquad k_3 \approx \mathcal{O}\left(\frac{1}{k^2}\right) \qquad k_4 \approx \mathcal{O}\left(\sqrt{k}\log\frac{1}{k^2}\right)$	convex (non-smooth)	smooth (non-convex) ¹	smooth & convex ²	smooth & strongly convex (or PL)
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¹Carmon, Duchi, Hinder, Sidford, 2017

²Nemirovski, Yudin, 1979 $f \to \min_{x,y,z}$ Lower bounds

Black box iteration

The iteration of gradient descent:

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

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

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$$= x^0 - \sum_{i=0}^k \alpha^{k-i} \nabla f(x^{k-i})$$

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Consider a family of first-order methods, where

$$x^{k+1} \in x^0 + \operatorname{span}\left\{\nabla f(x^0), \nabla f(x^1), \dots, \nabla f(x^k)\right\}$$
 f - smooth $x^{k+1} \in x^0 + \operatorname{span}\left\{q_0, q_1, \dots, q_k\right\}$, where $q_i \in \partial f(x^i)$ f - 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.

(1)

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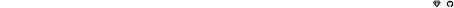
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• Let n = 2k + 1 and $A \in \mathbb{R}^{n \times n}$.

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

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

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Example, when n = 3:

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

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Lower bound:

$$x^{T}Ax = 2x_{1}^{2} + 2x_{2}^{2} + 2x_{3}^{2} - 2x_{1}x_{2} - 2x_{2}x_{3}$$

$$= x_{1}^{2} + x_{1}^{2} - 2x_{1}x_{2} + x_{2}^{2} + x_{2}^{2} - 2x_{2}x_{3} + x_{3}^{2} + x_{3}^{2}$$

$$= x_{1}^{2} + (x_{1} - x_{2})^{2} + (x_{2} - x_{3})^{2} + x_{3}^{2} \ge 0$$

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

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Notice, that

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Therefore, $x^T A x \ge 0$. 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:

$$x^{T}Ax = 2x_{1}^{2} + 2x_{2}^{2} + 2x_{3}^{2} - 2x_{1}x_{2} - 2x_{2}x_{3}$$

Upper bound

 $x^{T}Ax = 2x_{1}^{2} + 2x_{2}^{2} + 2x_{2}^{2} - 2x_{1}x_{2} - 2x_{2}x_{2}$

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

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

 $0 \le x_1^2 + x_1^2 + 2x_1x_2 + x_2^2 + x_2^2 + 2x_2x_3 + x_2^2 + x_2^2$

 $=x_1^2+x_1^2-2x_1x_2+x_2^2+x_2^2-2x_2x_2+x_2^2+x_2^2$

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

 $0 \le x_1^2 + (x_1 + x_2)^2 + (x_2 + x_2)^2 + x_2^2$

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

 $J \rightarrow \lim_{x,y,z}$ Lower bounds

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

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

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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:

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

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

Lower bounds

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

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

- 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:

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

And the objective value is

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

Smooth case (proof)
• Suppose, we start from $x^0 = 0$. Asking the oracle for the gradient, we get $q_0 = -e_1$. 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

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

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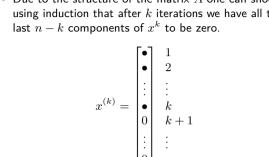
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$$x^{(k)} = \begin{bmatrix} \bullet \\ \bullet \\ \vdots \\ \vdots \\ \vdots \\ k \\ k+1 \\ \vdots \\ 0 \end{bmatrix}$$

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



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

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

A A A

• 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

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

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

$$\leq \frac{(n+1)^3}{2}$$

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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)

$$\sum_{i=1}^{n} i = \frac{n(n+1)}{2}$$
$$\sum_{i=1}^{n} i^{2} = \frac{n(n+1)(2n+1)}{6}$$
$$\leq \frac{(n+1)^{3}}{2}$$

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

$$f(x^k) - f(x^*) \ge \frac{L}{16(k+1)} = \frac{L(k+1)}{16(k+1)^2}$$
$$\ge \frac{L}{16(k+1)^2} \frac{3}{2} R^2$$
$$= \frac{3LR^2}{32(k+1)^2}$$



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Which concludes the proof with the desired $\mathcal{O}\left(\frac{1}{k^2}\right)$ rate.

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

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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:

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

Acceleration for quadratics





Convergence result for quadratics

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

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

i Theorem

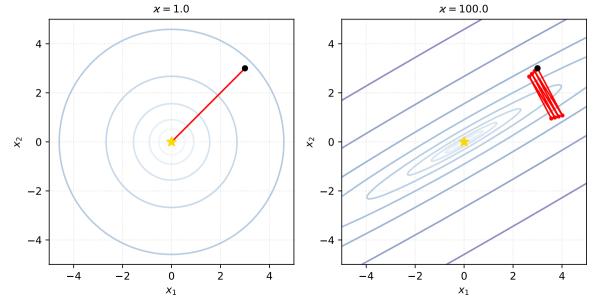
The gradient descent method with the learning rate $\alpha_k=rac{2}{\mu+L}$ converges to the optimal solution x^* with the following guarantee:

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

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



Condition number ×



Convergence from the first principles

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

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 x_0 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

$$p_k(a) = \prod^k (1 - \alpha_k a).$$

We can upper bound the norm of the error term as

$$||e_k|| < ||p_k(A)|| \cdot ||e_0||$$
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We can upper bound the norm of the error term as

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

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

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

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 $[\mu, L]$.



relevant interval is therefore [1, 10].

Can we do better? The answer is yes.

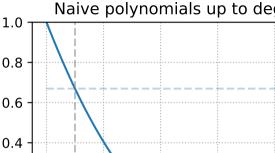
 $\alpha_k = \frac{2}{\mu + L}$ in the expression. This choise makes $|p_k(\mu)| = |p_k(L)|$.

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

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

0.2 0.0

-0.2





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Naive polynomials up to de 1.0 0.8 0.6

relevant interval is therefore [1, 10]. Can we do better? The answer is yes.

0.40.2 0.0 -0.2





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

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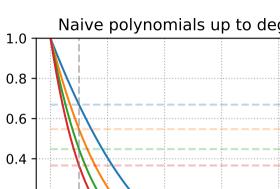


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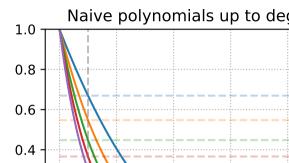


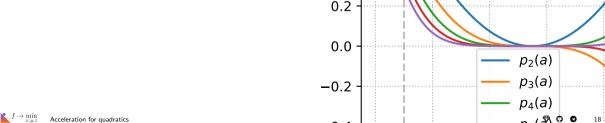
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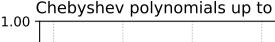


to the question that we asked. Suitably rescaled, they minimize the absolute value in a desired interval $[\mu, L]$ while satisfying the normalization constraint of having value 1 at the origin.

$$T_1(x) = x$$

 $T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x), \qquad k \ge 2.$

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







0.00

-0.25

-0.50











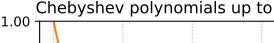
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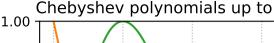


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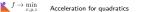
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Let's plot the standard Chebyshev polynomials (without rescaling):









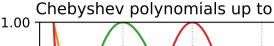
Chebyshev polynomials

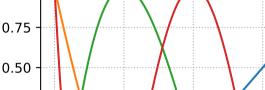
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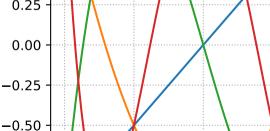
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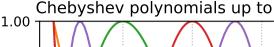


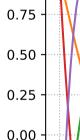
Acceleration for quadratics

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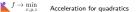




-0.25

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We will use the following affine transformation:

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

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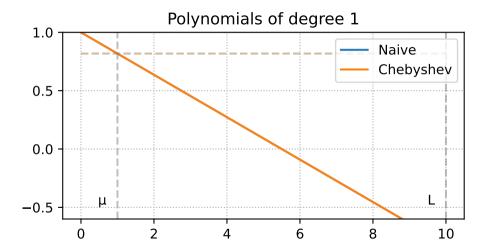
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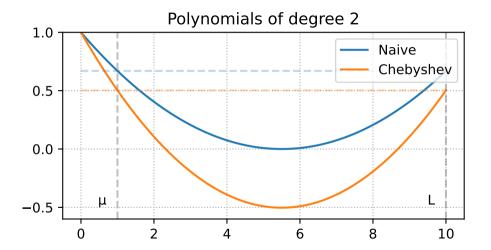
Let's plot the rescaled Chebyshev polynomials $P_k(a)=T_k\left(\frac{L+\mu-2a}{L-\mu}\right)\cdot T_k\left(\frac{L+\mu}{L-\mu}\right)^{-1}$

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



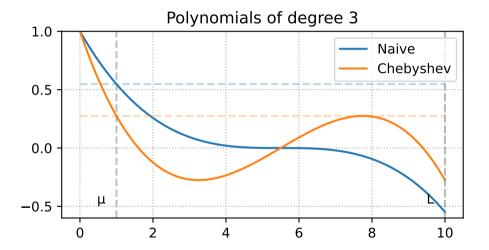






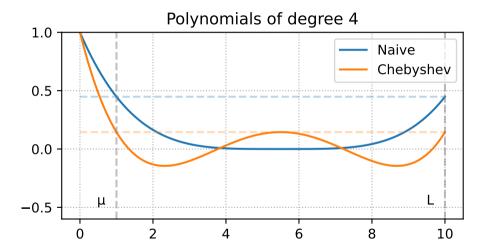


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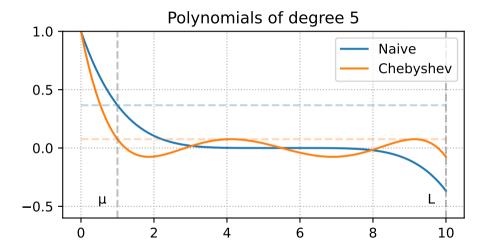


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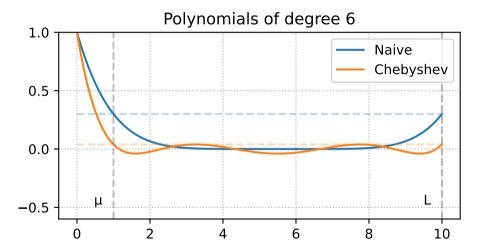


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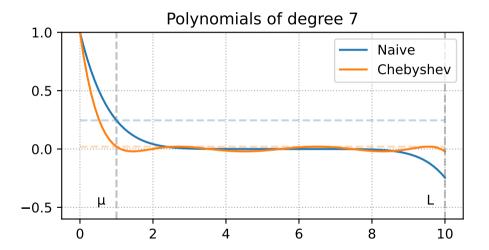






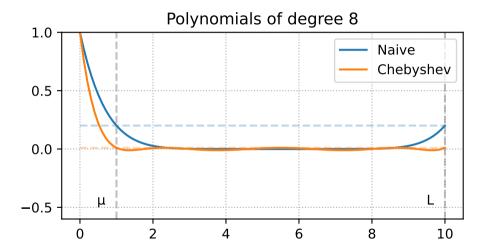






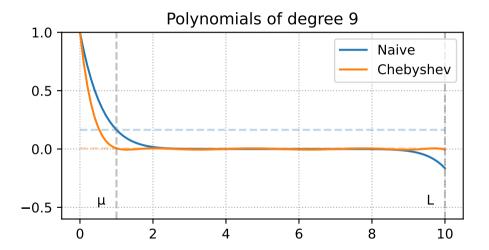






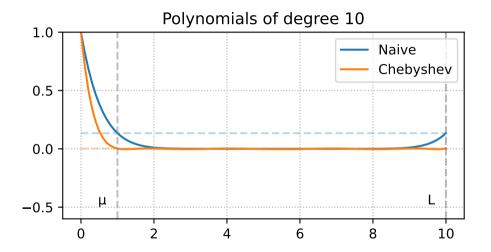














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We can see, that the maximum value of the Chebyshev polynomial on the interval $[\mu, L]$ is achieved at the point $a = \mu$. Therefore, we can use the following upper bound:

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



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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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Acceleration for quadratics



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- 5. Finally, we get:

 $T_k(1+\epsilon) = \cosh(k \operatorname{arccosh}(1+\epsilon))$

 $=\cosh(k\phi)$

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

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

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

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







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

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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:

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



Rearranging the terms, we get:

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

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

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

$$x_{k+1} = P_{k+1}(A)x_0 = (I - \alpha_k A)P_k(A)x_0 + \beta_k (P_k(A) - P_{k-1}(A))x_0$$
$$= (I - \alpha_k A)x_k + \beta_k (x_k - x_{k-1})$$

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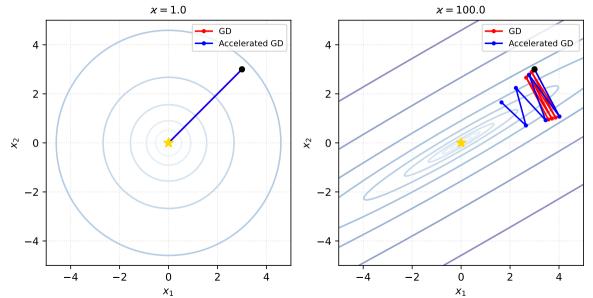
= $(I - \alpha_k A)x_k + \beta_k (x_k - x_{k-1})$

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

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



Acceleration from the first principles





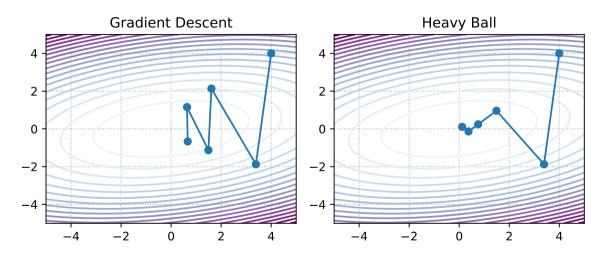
Heavy ball



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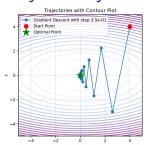


Oscillations and acceleration



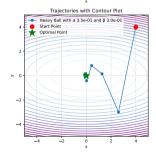


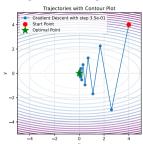




Let's introduce the idea of momentum, proposed by Polyak in 1964. Recall that the momentum update is

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



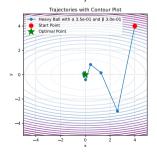


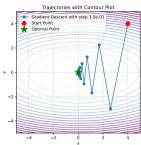
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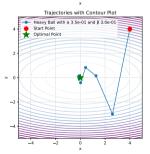
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$$\hat{x}_{k+1} = \hat{x}_k - \alpha \Lambda \hat{x}_k + \beta (\hat{x}_k - \hat{x}_{k-1}) = (I - \alpha \Lambda + \beta I)\hat{x}_k - \beta \hat{x}_{k-1}$$







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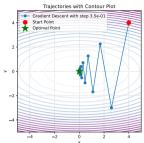
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Trajectories with Contour Plot

Heavy Bail with a 3.5e 01 and β 3.0e 01

Start Point

Optimal Point

2

-2

-2

-3

-4

-2

-2

-4

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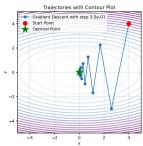
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Let's use the following notation $\hat{z}_k = \begin{bmatrix} \hat{x}_{k+1} \\ \hat{x}_k \end{bmatrix}$. Therefore $\hat{z}_{k+1} = M\hat{z}_k$, where the iteration matrix M is:



Trajectories with Contour Plot

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A Star Point

Optimal Point

2 0 2 4

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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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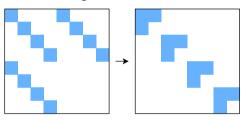


Figure 1: Illustration of matrix M rearrangement

$$\begin{bmatrix} \hat{x}_{k}^{(1)} \\ \vdots \\ \hat{x}_{k}^{(d)} \\ \hat{x}_{k-1}^{(1)} \\ \vdots \\ \hat{x}_{k-1}^{(d)} \end{bmatrix} \rightarrow \begin{bmatrix} \hat{x}_{k}^{(1)} \\ \hat{x}_{k-1}^{(1)} \\ \vdots \\ \hat{x}_{k}^{(d)} \\ \hat{x}_{k-1}^{(d)} \end{bmatrix} \quad M = \begin{bmatrix} M_{1} & & & \\ & M_{2} & & \\ & & & M_{d} \end{bmatrix}$$

where $\hat{x}_{i}^{(i)}$ 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.

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

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

Y x,y,z Heavy ball

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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.

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

Heavy ball quadratic convergence

We can explicitly calculate the eigenvalues of 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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$$\operatorname{Re}(\lambda_1^M) = \frac{L + \mu - 2\lambda_i}{(\sqrt{L} + \sqrt{\mu})^2}; \quad \operatorname{Im}(\lambda_1^M) = \frac{\pm 2\sqrt{(L - \lambda_i)(\lambda_i - \mu)}}{(\sqrt{L} + \sqrt{\mu})^2}; \quad |\lambda_1^M| = \frac{L - \mu}{(\sqrt{L} + \sqrt{\mu})^2}.$$

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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

Heavy Ball quadratics convergence

i Theorem

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

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

converges linearly:

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



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

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

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

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

 $^{^3\}mbox{Global}$ convergence of the Heavy-ball method for convex optimization, Euhanna Ghadimi et.al.

Heavy Ball Global Convergence 4

1 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,

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

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

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



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Let's define the following notation

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

Then we can write down:

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



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:

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

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 $\mathcal{O}\left(\frac{1}{L^2}\right)$, specifically:

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

Nesterov accelerated gradient

General case convergence

i 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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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:

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

Nesterov accelerated gradient