



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

Daniil Merkulov

Optimization methods. MIPT

Recap of Gradient Descent convergence

Gradient Descent:

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

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

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

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For smooth strongly convex we have:

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

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

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

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Finally we have

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

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

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

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

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Lower bounds

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¹Carmon, Duchi, Hinder, Sidford, 2017

²Nemirovski, Yudin, 1979

Black box iteration

The iteration of gradient descent:

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

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Consider a family of first-order methods, where

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

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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.

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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 - b. **The gradient method is not optimal for this problem.**

Nesterov's worst function

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

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

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- Notice, that

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

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

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Upper bound

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

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

- And the objective value is

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

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.

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

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

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

Smooth case (proof)

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

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

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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

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

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- Thus,

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

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

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

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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 $k : 1 \leq k \leq \frac{n-1}{2}$:

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

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:

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

Acceleration for quadratics

Convergence result for quadratics

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

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

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:

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

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

Condition number κ

$\kappa = 1.0$



$\kappa = 100.0$



Convergence from the first principles

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

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 choice makes $|p_k(\mu)| = |p_k(L)|$.

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

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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Chebyshev polynomials

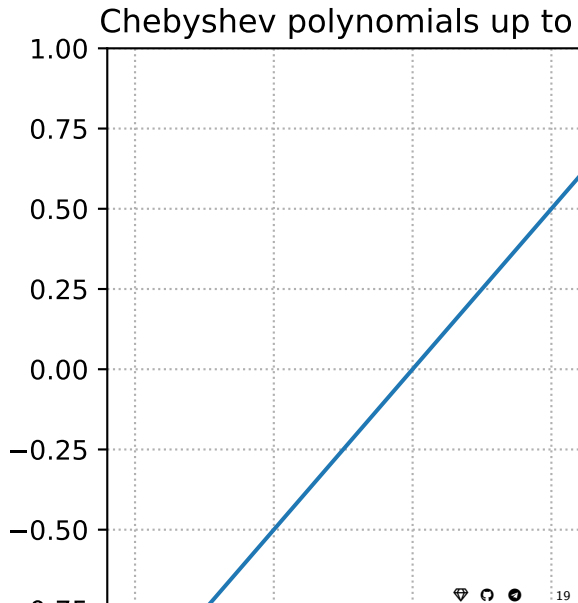
Chebyshev polynomials turn out to give an optimal answer to the question that we asked. Suitably rescaled, they minimize the absolute value in a desired interval $[\mu, L]$ while satisfying the normalization constraint of having value 1 at the origin.

$$T_0(x) = 1$$

$$T_1(x) = x$$

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

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



Chebyshev polynomials

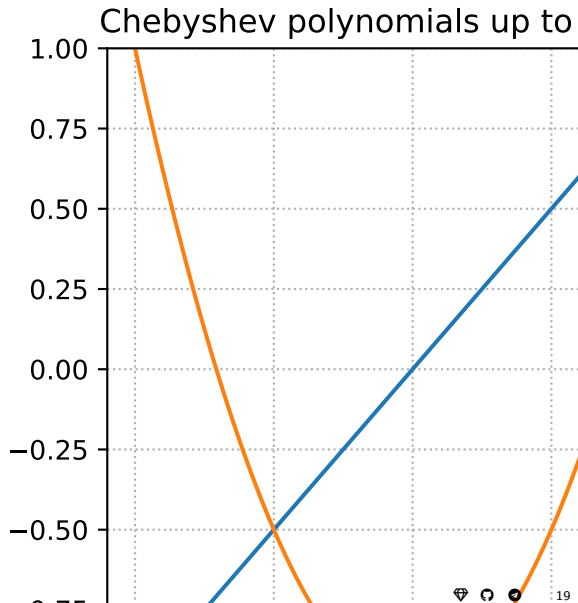
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We will use the following affine transformation:

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

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 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

$$\frac{L + \mu}{L - \mu}, \quad \text{ensuring that} \quad P_k(0) = T_k\left(\frac{L + \mu - 0}{L - \mu}\right) \cdot T_k\left(\frac{L + \mu}{L - \mu}\right)^{-1} = 1.$$

Rescaled Chebyshev polynomials

Original Chebyshev polynomials are defined on the interval $[-1, 1]$. To use them for our purposes, we need to rescale them to the interval $[\mu, L]$.

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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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 $[\mu, L]$.

Rescaled Chebyshev polynomials



Rescaled Chebyshev polynomials



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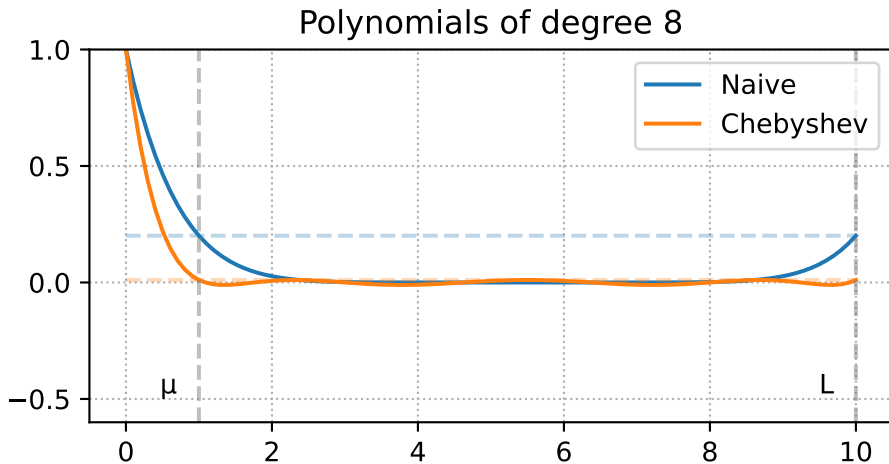
Rescaled Chebyshev polynomials



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Chebyshev polynomials upper bound

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

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

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

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

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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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To upper bound $|P_k|$, we need to lower bound $|T_k(1 + \epsilon)|$.

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$$T_k(x) = \cosh(k \operatorname{arccosh}(x))$$

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5. Finally, we get:

$$\begin{aligned}\|e_k\| &\leq \|P_k(A)\| \|e_0\| \leq \frac{2}{(1 + \sqrt{\epsilon})^k} \|e_0\| \\&\leq 2 \left(1 + \sqrt{\frac{2}{\kappa - 1}}\right)^{-k} \|e_0\| \\&\leq 2 \exp\left(-\sqrt{\frac{2}{\kappa - 1}} k\right) \|e_0\|\end{aligned}$$

Accelerated method [1/2]

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

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

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

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

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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:

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

Accelerated method [2/2]

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

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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

$\kappa = 1.0$



$\kappa = 100.0$



Heavy ball

Oscillations and acceleration

Gradient Descent



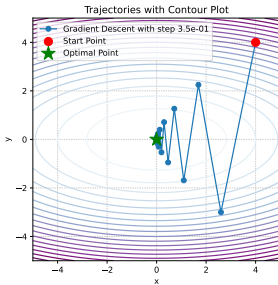
Heavy Ball



Polyak Heavy ball method

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

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Reduction to a scalar case

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

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Figure 1: Illustration of matrix M rearrangement

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

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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 :

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

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

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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. $\beta \geq (1 - \sqrt{\alpha\lambda_i})^2$.

$$\operatorname{Re}(\lambda_1^M) = \frac{L + \mu - 2\lambda_i}{(\sqrt{L} + \sqrt{\mu})^2}; \quad \operatorname{Im}(\lambda_1^M) = \frac{\pm 2\sqrt{(L - \lambda_i)(\lambda_i - \mu)}}{(\sqrt{L} + \sqrt{\mu})^2}; \quad |\lambda_1^M| = \frac{L - \mu}{(\sqrt{L} + \sqrt{\mu})^2}.$$

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

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:

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

Heavy Ball Global Convergence³

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

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

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

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

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

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

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

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

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

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Heavy ball method summary

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

Nesterov accelerated gradient

The concept of Nesterov Accelerated Gradient method

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

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Let's define the following notation

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

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

Then we can write down:

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

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

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

General case convergence

i Theorem

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ 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 $\mathcal{O}\left(\frac{1}{k^2}\right)$, specifically:

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

General case convergence

i Theorem

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ 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:

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