

Discover acceleration of gradient descent

Daniil Merkulov

Optimization for ML. Faculty of Computer Science. HSE University



Previously

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

Previously

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

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

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

Previously

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

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

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

Finally we have

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

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

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

Previously

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

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

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

Finally we have

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

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

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

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

Previously

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

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

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

Finally we have

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

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

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

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

Lower bounds

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

¹Carmon, Duchi, Hinder, Sidford, 2017

²Nemirovski, Yudin, 1979

Lower bounds

The iteration of gradient descent:

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

Lower bounds

The iteration of gradient descent:

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

Consider a family of first-order methods, where

$$x^{k+1} \in x^0 + \text{span} \{ \nabla f(x^0), \nabla f(x^1), \dots, \nabla f(x^k) \} \quad (1)$$

Lower bounds

The iteration of gradient descent:

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

Consider a family of first-order methods, where

$$x^{k+1} \in x^0 + \text{span} \{ \nabla f(x^0), \nabla f(x^1), \dots, \nabla f(x^k) \} \quad (1)$$

Non-smooth convex case

There exists a function f that is M -Lipschitz and convex such that any first-order method of the form 1 satisfies

$$\min_{i \in [1, k]} f(x^i) - f^* \geq \frac{M \|x^0 - x^*\|_2}{2(1 + \sqrt{k})}$$

Lower bounds

The iteration of gradient descent:

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

Consider a family of first-order methods, where

$$x^{k+1} \in x^0 + \text{span} \{ \nabla f(x^0), \nabla f(x^1), \dots, \nabla f(x^k) \} \quad (1)$$

Non-smooth convex case

There exists a function f that is M -Lipschitz and convex such that any first-order method of the form 1 satisfies

$$\min_{i \in [1, k]} f(x^i) - f^* \geq \frac{M \|x^0 - x^*\|_2}{2(1 + \sqrt{k})}$$

Smooth and convex case

There exists a function f that is L -smooth and convex such that any first-order method of the form 1 satisfies

$$\min_{i \in [1, k]} f(x^i) - f^* \geq \frac{3L \|x^0 - x^*\|_2^2}{32(1 + k)^2}$$

Oscillations and acceleration

Gradient Descent



Heavy Ball



Coordinate shift

Consider the following quadratic optimization problem:

$$\min_{x \in \mathbb{R}^d} f(x) = \min_{x \in \mathbb{R}^d} \frac{1}{2} x^\top A x - b^\top x + c, \text{ where } A \in \mathbb{S}_{++}^d.$$

Coordinate shift

Consider the following quadratic optimization problem:

$$\min_{x \in \mathbb{R}^d} f(x) = \min_{x \in \mathbb{R}^d} \frac{1}{2} x^\top A x - b^\top x + c, \text{ where } A \in \mathbb{S}_{++}^d.$$

- Firstly, without loss of generality we can set $c = 0$, which will not affect optimization process.



Coordinate shift

Consider the following quadratic optimization problem:

$$\min_{x \in \mathbb{R}^d} f(x) = \min_{x \in \mathbb{R}^d} \frac{1}{2} x^\top A x - b^\top x + c, \text{ where } A \in \mathbb{S}_{++}^d.$$

- Firstly, without loss of generality we can set $c = 0$, which will not affect optimization process.
- Secondly, we have a spectral decomposition of the matrix A :

$$A = Q \Lambda Q^\top$$



Coordinate shift

Consider the following quadratic optimization problem:

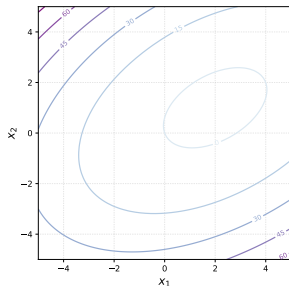
$$\min_{x \in \mathbb{R}^d} f(x) = \min_{x \in \mathbb{R}^d} \frac{1}{2} x^\top A x - b^\top x + c, \text{ where } A \in \mathbb{S}_{++}^d.$$

- Firstly, without loss of generality we can set $c = 0$, which will not affect optimization process.
- Secondly, we have a spectral decomposition of the matrix A :

$$A = Q \Lambda Q^\top$$

- Let's show, that we can switch coordinates in order to make an analysis a little bit easier. Let $\hat{x} = Q^\top(x - x^*)$, where x^* is the minimum point of initial function, defined by $Ax^* = b$. At the same time $x = Q\hat{x} + x^*$.

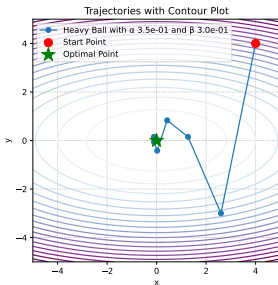
$$\begin{aligned} f(\hat{x}) &= \frac{1}{2} (Q\hat{x} + x^*)^\top A (Q\hat{x} + x^*) - b^\top (Q\hat{x} + x^*) \\ &= \frac{1}{2} \hat{x}^\top Q^\top A Q \hat{x} + (x^*)^\top A Q \hat{x} + \frac{1}{2} (x^*)^\top A (x^*) - b^\top Q \hat{x} - b^\top x^* \\ &= \frac{1}{2} \hat{x}^\top \Lambda \hat{x} \end{aligned}$$



Polyak Heavy ball method

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

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



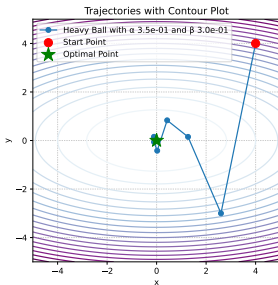
Polyak Heavy ball method

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

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

Which is in our (quadratics) case is

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



Polyak Heavy ball method

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

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

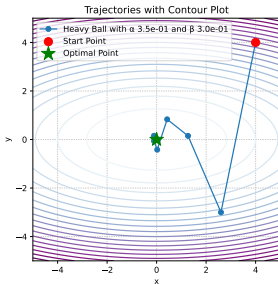
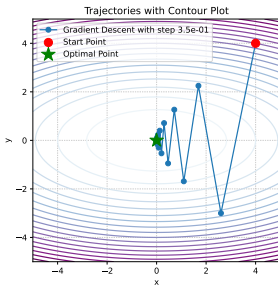
Which is in our (quadratics) case is

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

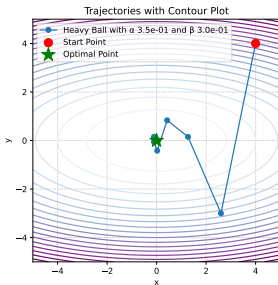
This can be rewritten as follows

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

$$\hat{x}_k = \hat{x}_k.$$



Polyak Heavy ball method



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

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

Which is in our (quadratics) case is

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

This can be rewritten as follows

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

$$\hat{x}_k = \hat{x}_k.$$

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

Polyak Heavy ball method



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

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

Which is in our (quadratics) case is

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

This can be rewritten as follows

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

$$\hat{x}_k = \hat{x}_k.$$

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:

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

Reduction to a scalar case

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

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.



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:

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

Reduction to a scalar case

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

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

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

$$\alpha^*, \beta^* = \arg \min_{\alpha, \beta} \max_{\lambda \in [\mu, L]} \rho(M) \quad \alpha^* = \frac{4}{(\sqrt{L} + \sqrt{\mu})^2}; \quad \beta^* = \left(\frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}} \right)^2.$$

Reduction to a scalar case

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

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

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

$$\alpha^*, \beta^* = \arg \min_{\alpha, \beta} \max_{\lambda \in [\mu, L]} \rho(M) \quad \alpha^* = \frac{4}{(\sqrt{L} + \sqrt{\mu})^2}; \quad \beta^* = \left(\frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}} \right)^2.$$

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 :

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

Heavy ball quadratic convergence

We can explicitly calculate the eigenvalues of M_i :

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

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

Heavy ball quadratic convergence

We can explicitly calculate the eigenvalues of M_i :

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

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 :

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

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

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

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

Heavy Ball quadratics convergence

Theorem

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

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

converges linearly:

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

Heavy Ball Global Convergence³

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

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 $q \in [0, 1)$.

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

Heavy ball method summary

- Ensures accelerated convergence for strongly convex quadratic problems

Heavy ball method summary

- Ensures accelerated convergence for strongly convex quadratic problems
- Local accelerated convergence was proved in the original paper.

Heavy ball method summary

- Ensures accelerated convergence for strongly convex quadratic problems
- Local accelerated convergence was proved in the original paper.
- Recently was proved, that there is no global accelerated convergence for the method.

Heavy ball method summary

- Ensures accelerated convergence for strongly convex quadratic problems
- Local accelerated convergence was proved in the original paper.
- Recently was proved, that there is no global accelerated convergence for the method.
- Method was not extremely popular until the ML boom

Heavy ball method summary

- Ensures accelerated convergence for strongly convex quadratic problems
- Local accelerated convergence was proved in the original paper.
- 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)

The concept of Nesterov Accelerated Gradient method

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

The concept of Nesterov Accelerated Gradient method

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

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:

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

NAG convergence for quadratics

General case convergence

Theorem

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is convex and L -smooth. The Nesterov Accelerated Gradient (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

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:

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