Discover acceleration of gradient descent

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Previously

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

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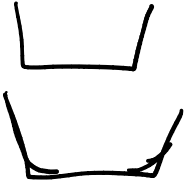

$k \sim \frac{1}{\varepsilon}$

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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

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

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$\kappa = \frac{L}{\mu} > 1$

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

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

Lower bounds

GD $\frac{1}{k}$ $\frac{1}{k^2}$?

convex (non-smooth)	smooth (non-convex)[1]	smooth & convex[2]	smooth & strongly convex (or PL)
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[1] Carmon, Duchi, Hinder, Sidford, 2017

[2] Nemirovski, 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})
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Consider a family of first-order methods, where

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

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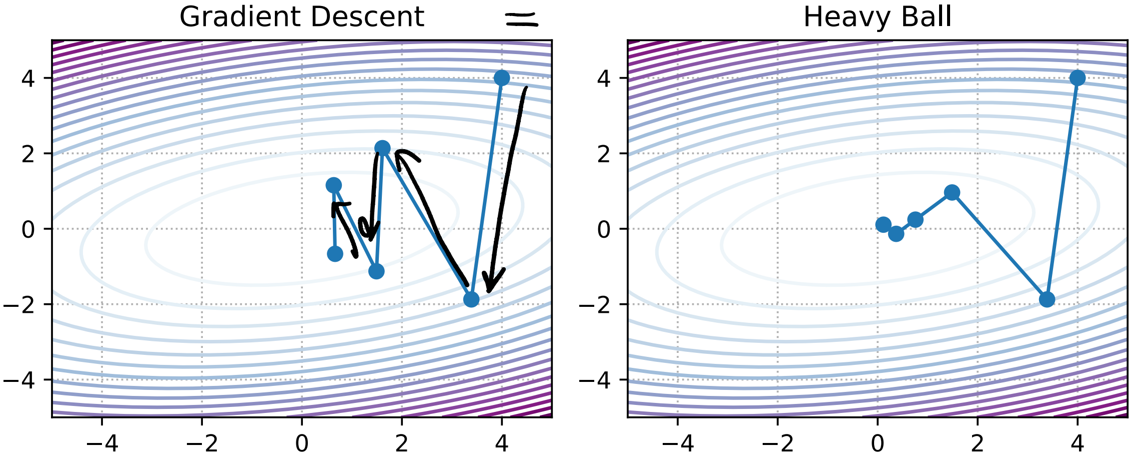
Smooth and convex case

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

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



$$f(x) = \frac{1}{2} x^T A x$$

$$\nabla f = A x$$

$$x_{k+1} = x_k - \alpha \cdot A x_k + \beta (x_k - x_{k-1}) =$$

$$x_k - x_{k-1} = -\alpha A x_{k-1} + \beta (x_{k-1} - x_{k-2})$$

$$= x_k - \alpha A x_k + \beta (-\alpha A x_{k-1} + \beta (x_{k-1} - x_{k-2}))$$

Coordinate shift

Consider the following quadratic optimization problem:

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

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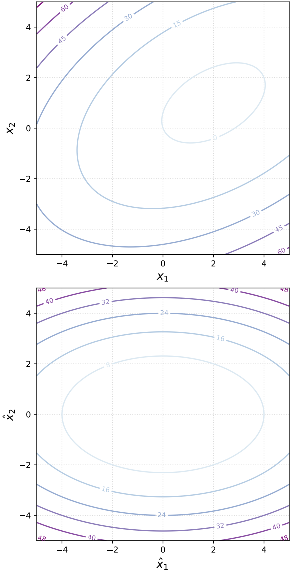

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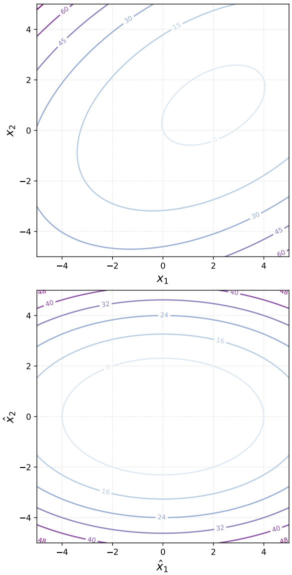
$$A = Q \Lambda Q^T$$



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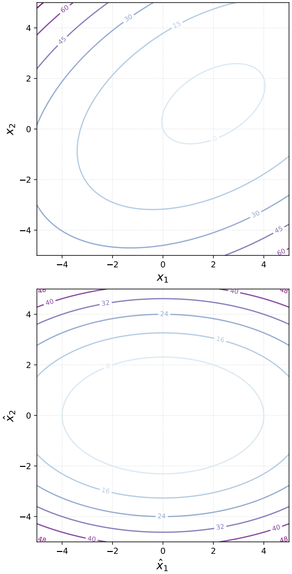
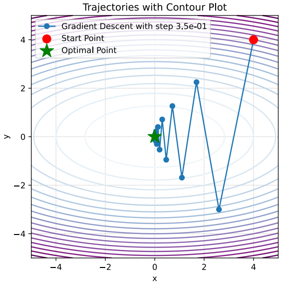
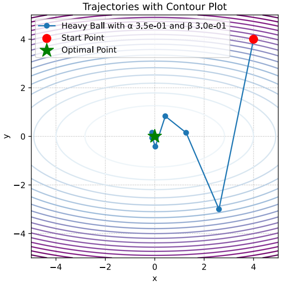
- Let's show, that we can switch coordinates in order to make an analysis a little bit easier. Let $\hat{x} = Q^T(x - x^*)$, where x^* is the minimum point of initial function, defined by $Ax^* = b$. At the same time $x = Q\hat{x} + x^*$.

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



Polyak Heavy ball method





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

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

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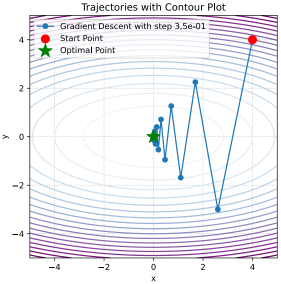

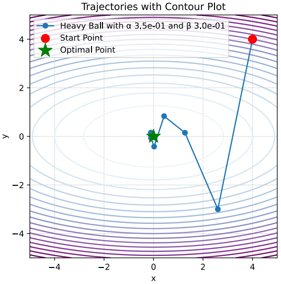

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$\nabla f = \Lambda x$

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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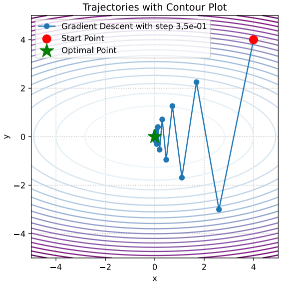

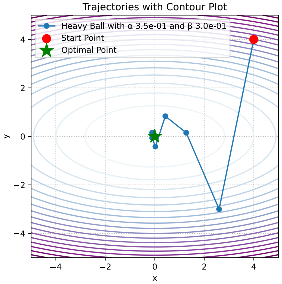

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This can be rewritten as follows

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

$Z_{k+1} = M Z_k$

$Z_k = \begin{pmatrix} x_{k+1} \\ x_k \end{pmatrix}$

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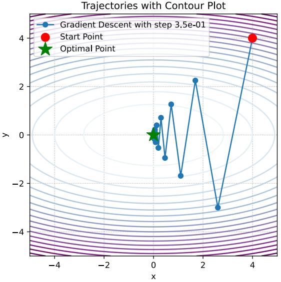

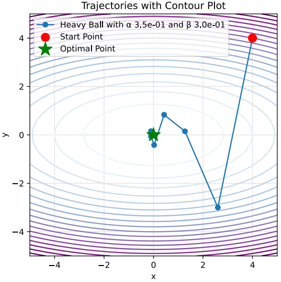

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+0 x_{k-1} 2n

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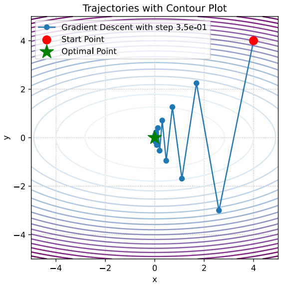

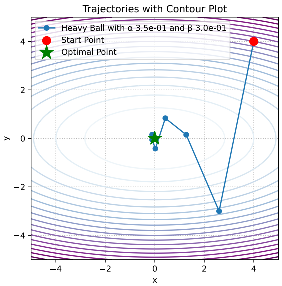

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$$M = \begin{bmatrix} I - \alpha\Lambda + \beta I & -\beta I \\ I & 0_d \end{bmatrix}.$$

Reduction to a scalar case

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

$$z_{k+1} = M z_k$$

$$\rho(M) < 1 \Leftrightarrow \text{сх-ть}$$

$$\rho(M) = \max |\lambda(M)|$$

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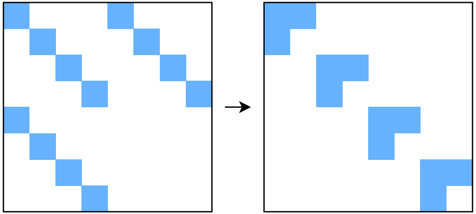

Figure 1: Illustration of matrix M rearrangement

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

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:

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

$$
\begin{pmatrix} x^{k+1}_{(i)} \\ x^{k}_{(i)} \end{pmatrix} = M_i \begin{pmatrix} x^{k}_{(i)} \\ x^{k-1}_{(i)} \end{pmatrix}
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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

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

Reduction to a scalar case

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

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It can be shown, that for such parameters the matrix M has complex eigenvalues, which forms a conjugate pair, so the distance to the optimum (in this case, $\|z_k\|$), generally, will not go to zero monotonically.

Heavy ball quadratic convergence

We can explicitly calculate the eigenvalues of M_i:

$$\lambda^M_1, \lambda^M_2 = \lambda \left(\begin{bmatrix} 1 - \alpha\lambda_i + \beta & -\beta \\ 1 & 0 \end{bmatrix} \right) = \frac{1 + \beta - \alpha\lambda_i \pm \sqrt{(1 + \beta - \alpha\lambda_i)^2 - 4\beta}}{2}.$$

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

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$$\text{Re}(\lambda^M_1) = \frac{L + \mu - 2\lambda_i}{(\sqrt{L} + \sqrt{\mu})^2}; \quad \text{Im}(\lambda^M_1) = \frac{\pm 2\sqrt{(L - \lambda_i)(\lambda_i - \mu)}}{(\sqrt{L} + \sqrt{\mu})^2}; \quad |\lambda^M_1| = \frac{L - \mu}{(\sqrt{L} + \sqrt{\mu})^2}.$$

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

Heavy Ball quadratics convergence

$L = \lambda_{max}(\nabla^2 f(x))$

$\mu = \lambda_{min}(\nabla^2 f(x)) > 0$

$\varkappa = \frac{L}{\mu} \geq 1$

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:

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

ускоренный rate

Heavy Ball Global Convergence [3]

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

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

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

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

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

Heavy Ball Global Convergence [4]

Theorem

Assume that f is smooth and strongly convex and that

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

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,

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

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

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Heavy ball method summary

- Ensures accelerated convergence for strongly convex quadratic problems

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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)

The concept of Nesterov Accelerated Gradient method

1983

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

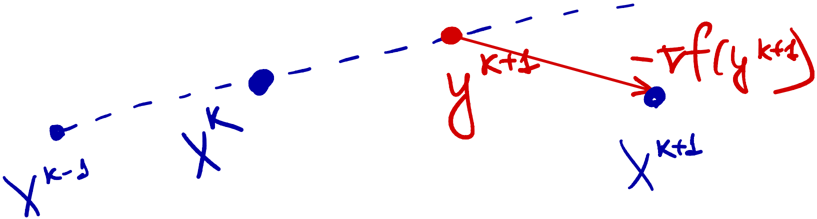
Коши GD

18...47

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

1964 HB

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



The concept of Nesterov Accelerated Gradient method

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

Let's define the following notation

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

Then we can write down:

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

NAG convergence for quadratics

General case convergence

Theorem

Let $f : \mathbb{R}^n \to \mathbb{R}$ is convex and L-smooth. The Nesterov Accelerated Gradient Descent (NAG) algorithm is designed to solve the minimization problem starting with an initial point $x_0 = y_0 \in \mathbb{R}^n$ and $\lambda_0 = 0$. The algorithm iterates the following steps:

$$
\begin{aligned}
&\textbf{Gradient update:} && y_{k+1} = x_k - \frac{1}{L}\nabla f(x_k) \\
&\textbf{Extrapolation:} && x_{k+1} = (1-\gamma_k)y_{k+1} + \gamma_k y_k \\
&\textbf{Extrapolation weight:} && \lambda_{k+1} = \frac{1+\sqrt{1+4\lambda_k^2}}{2} \\
&\textbf{Extrapolation weight:} && \gamma_k = \frac{1-\lambda_k}{\lambda_{k+1}}
\end{aligned}
$$

The sequences $\{f(y_k)\}_{k\in\mathbb{N}}$ produced by the algorithm will converge to the optimal value f^* at the rate of $\mathcal{O}\left(\frac{1}{k^2}\right)$, specifically:

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

General case convergence

Theorem

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

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:

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