Discover acceleration of gradient descent

Daniil Merkulov

Optimization methods. MIPT

Coordinate shift

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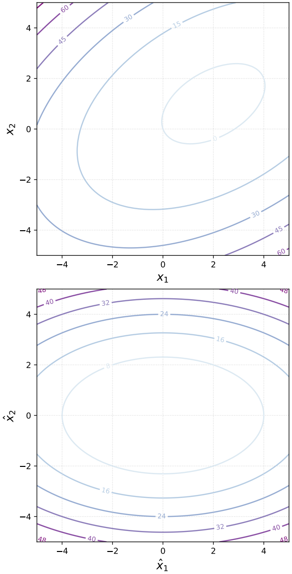

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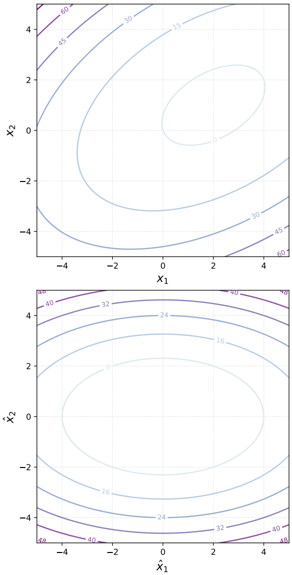
$$A = Q \Lambda Q^T$$



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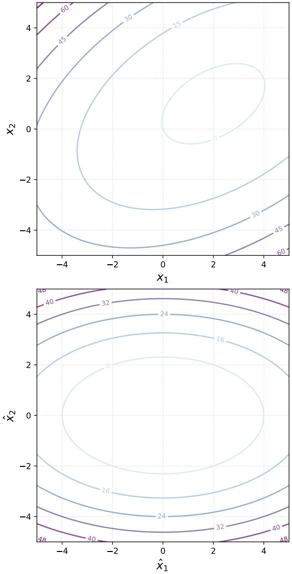
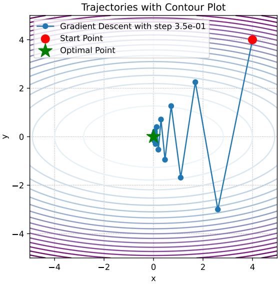
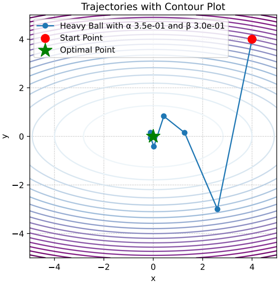
- Let's show, that we can switch coordinates in order to make an analysis a little bit easier. Let $\hat{x} = Q^T(x - x^*)$, where x^* is the minimum point of initial function, defined by $Ax^* = b$. At the same time $x = Q\hat{x} + x^*$.

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



Polyak Heavy ball method





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

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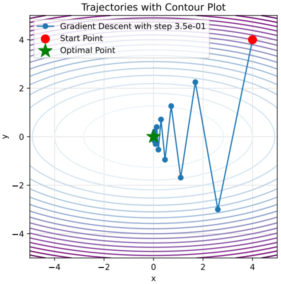

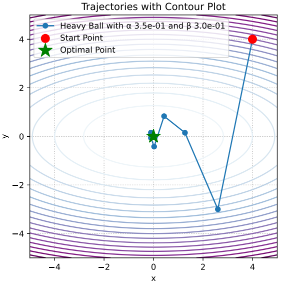

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$$\hat{x}_{k+1} = \hat{x}_k - \alpha\Lambda\hat{x}_k + \beta(\hat{x}_k - \hat{x}_{k-1}) = (I - \alpha\Lambda + \beta I)\hat{x}_k - \beta\hat{x}_{k-1}$$

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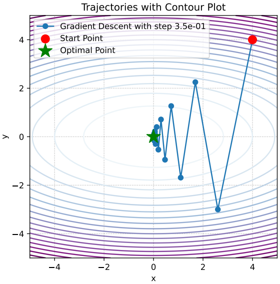

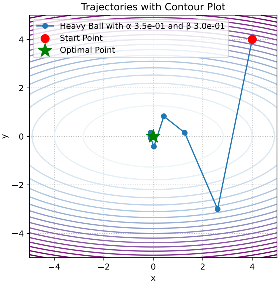

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This can be rewritten as a follows

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

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.

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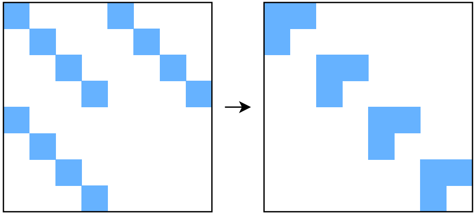

Figure 1: Illustration of matrix M rearrangement

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

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:

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

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:

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

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

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

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

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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

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

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

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