

Discover acceleration of gradient descent

Seminar

Optimization for ML. Faculty of Computer Science. HSE University

GD. Convergence rates

$$\min_{x \in \mathbb{R}^n} f(x) \quad x_{k+1} = x_k - \alpha_k \nabla f(x_k) \quad \kappa = \frac{L}{\mu}$$

	smooth & convex	smooth & strongly convex (or PL)
Upper bound	$f(x_k) - f^* \approx \mathcal{O}\left(\frac{1}{k}\right)$	$\ x_k - x^*\ ^2 \approx \mathcal{O}\left(\left(\frac{\kappa - 1}{\kappa + 1}\right)^k\right)$
Lower bound	$f(x_k) - f^* \approx \Omega\left(\frac{1}{k^2}\right)$	$\ x_k - x^*\ ^2 \approx \Omega\left(\left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^k\right)$

Three update schemes

- **Normal gradient**

$$\mathbf{x}_k - \alpha_k \nabla f(\mathbf{x}_k)$$

Move the point \mathbf{x}_k in the direction $-\nabla f(\mathbf{x}_k)$ for $\alpha_k \|\nabla f(\mathbf{x}_k)\|$ amount.

Three update schemes

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- **Polyak's Heavy Ball Method**

$$\mathbf{x}_k - \alpha_k \nabla f(\mathbf{x}_k) + \beta_k (\mathbf{x}_k - \mathbf{x}_{k-1})$$

Perform a GD, move the updated- \mathbf{x} in the direction of the previous step for $\beta_k \|\mathbf{x}_k - \mathbf{x}_{k-1}\|$ amount.

Three update schemes

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- Polyak's Heavy Ball Method

$$\mathbf{x}_k - \alpha_k \nabla f(\mathbf{x}_k) + \beta_k (\mathbf{x}_k - \mathbf{x}_{k-1})$$

Perform a GD, move the updated- \mathbf{x} in the direction of the previous step for $\beta_k \|\mathbf{x}_k - \mathbf{x}_{k-1}\|$ amount.

- Nesterov's acceleration

$$\mathbf{x}_k - \alpha_k \nabla f(\mathbf{x}_k + \beta_k (\mathbf{x}_k - \mathbf{x}_{k-1})) + \beta_k (\mathbf{x}_k - \mathbf{x}_{k-1})$$

Move the not-yet-updated- \mathbf{x} in the direction of the previous step for $\beta_k \|\mathbf{x}_k - \mathbf{x}_{k-1}\|$ amount, perform a GD on the shifted- \mathbf{x} , then move the updated- \mathbf{x} in the direction of the previous step for $\beta_k \|\mathbf{x}_k - \mathbf{x}_{k-1}\|$.

HBM for a quadratic problem

Question

Which step size strategy is used for **GD**?



Figure 1: **GD** vs. **HBM** with fixed β .

Observation: for nice f (with spherical level sets), GD is already good enough and HBM adds a little effect. However, for bad f (with elliptic level sets), HBM is better in some cases.

HBM for a quadratic problem



Figure 2: GD with $\alpha = \frac{1}{L}$ vs. HBM with fixed β .

Observation: same. If nice f (spherical lv. sets), GD is already good enough. If bad f (with elliptic lv. sets), HBM is better in some cases.

NAG as a Momentum Method

- Start by setting $k = 0, a_0 = 1, \mathbf{x}_{-1} = \mathbf{y}_0, \mathbf{y}_0$ to an arbitrary parameter setting, iterates

$$\text{Gradient update } \mathbf{x}_k = \mathbf{y}_k - \alpha_k \nabla f(\mathbf{y}_k) \quad (1)$$

$$\text{Extrapolation weight } a_{k+1} = \frac{1 + \sqrt{1 + 4a_k^2}}{2} \quad (2)$$

$$\text{Extrapolation } \mathbf{y}_{k+1} = \mathbf{x}_k + \frac{a_k - 1}{a_{k+1}} (\mathbf{x}_k - \mathbf{x}_{k+1}) \quad (3)$$

Note that here fix step-size is used: $\alpha_k = \frac{1}{L} \forall k$.

- Theorem.** If f is L -smooth and convex, the sequence $\{f(\mathbf{x}_k)\}_k$ produced by NAG converges to the optimal value f^* as the rate $\mathcal{O}(\frac{1}{k^2})$ as

$$f(\mathbf{x}_k) - f^* \leq \frac{4L \|\mathbf{x}_k - \mathbf{x}^*\|^2}{(k+2)^2}$$

- The above representation is difficult to understand, so we will rewrite these equations in a more intuitive manner.

NAG as a Momentum Method

If we define

$$\mathbf{v}_k \equiv \mathbf{x}_k - \mathbf{x}_{k-1} \quad (4)$$

$$\beta_k \equiv \frac{a_k - 1}{a_{k+1}} \quad (5)$$

then the combination of Equation 3 and Equation 5 implies:

$$\mathbf{y}_k = \mathbf{x}_{k-1} + \beta_{k-1} \mathbf{v}_{k-1}$$

which can be used to rewrite Equation 1 as follows using $\alpha_k = \alpha_{k-1}$:

$$\mathbf{x}_k = \mathbf{x}_{k-1} + \beta_{k-1} \mathbf{v}_{k-1} - \alpha_{k-1} \nabla f(\mathbf{x}_{k-1} + \beta_{k-1} \mathbf{v}_{k-1}) \quad (6)$$

$$\mathbf{v}_k = \beta_{k-1} \mathbf{v}_{k-1} - \alpha_{k-1} \nabla f(\mathbf{x}_{k-1} + \beta_{k-1} \mathbf{v}_{k-1}) \quad (7)$$

where Equation 7 is a consequence of Equation 4. Alternatively:

$$\mathbf{v}_{k+1} = \beta_k \mathbf{v}_k - \alpha_k \nabla f(\mathbf{x}_k + \beta_k \mathbf{v}_k)$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{v}_{k+1}$$

where $\alpha_k > 0$ is the **learning rate**, β_k is the **momentum coefficient**. Compare **HBM** with **NAG**.

NAG for a quadratic problem

Consider the following quadratic optimization problem:

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

Every symmetric matrix A has an eigenvalue decomposition

$$A = Q \text{diag}(\lambda_1, \dots, \lambda_n) Q^\top = Q \Lambda Q^\top, \quad Q = [q_1, \dots, q_n].$$

and, as per convention, we will assume that the λ_i 's are sorted, from smallest λ_1 to biggest λ_n . It is clear, that λ_i correspond to the **curvature** along the associated eigenvector directions.

We can reparameterize $q(x)$ by the matrix transform Q and optimize $y = Qx$ using the objective

$$p(y) \equiv q(x) = q(Q^\top y) = y^\top Q(Q^\top \Lambda Q) Q^\top y / 2 - b^\top Q^\top y = y^\top \Lambda y / 2 - c^\top y,$$

where $c = Qb$.

We can further rewrite p as

$$p(y) = \sum_{i=1}^n [p]_i ([y]_i),$$

where $[p]_i(t) = \lambda_i t^2 / 2 - [c]_i t$.

NAG for a quadratic problem

💡 Theorem 2.1 from [1].

Let $p(y) = \sum_{i=1}^n [p]_i([y]_i)$ such that $[p]_i(t) = \lambda_i t^2/2 - [c]_i t$. Let α be arbitrary and fixed. Denote by $\text{HBM}_x(\beta, p, y, v)$ and $\text{HBM}_v(\beta, p, y, v)$ the parameter vector and the velocity vector respectively, obtained by applying one step of HBM (i.e., Eq. 1 and then Eq. 2) to the function p at point y , with velocity v , momentum coefficient β , and learning rate α . Define NAG_x and NAG_v analogously. Then the following holds for $z \in \{x, v\}$:

$$\text{HBM}_z(\beta, p, y, v) = \begin{bmatrix} \text{HBM}_z(\beta, [p]_1, [y]_1, [v]_1) \\ \vdots \\ \text{HBM}_z(\beta, [p]_n, [y]_n, [v]_n) \end{bmatrix}$$

$$\text{NAG}_z(\beta, p, y, v) = \begin{bmatrix} \text{NAG}_z(\beta(1 - \alpha\lambda_1), [p]_1, [y]_1, [v]_1) \\ \vdots \\ \text{NAG}_z(\beta(1 - \alpha\lambda_n), [p]_n, [y]_n, [v]_n) \end{bmatrix}$$

NAG for a quadratic problem. Proof (1/2)

Proof:

It's easy to show that if

$$x_{i+1} = \text{HBM}_x(\beta_i, [q]_i, [x]_i, [v]_i)$$

$$v_{i+1} = \text{HBM}_v(\beta_i, [q]_i, [x]_i, [v]_i)$$

then for $y_i = Qx_i, w_i = Qv_i$

$$y_{i+1} = \text{HBM}_x(\beta_i, [p]_i, [y]_i, [w]_i)$$

$$w_{i+1} = \text{HBM}_v(\beta_i, [p]_i, [y]_i, [w]_i)$$

. Then, consider one step of HBM_v :

$$\begin{aligned}\text{HBM}_v(\beta, p, y, v) &= \beta v - \alpha \nabla p(y) \\ &= (\beta[v]_1 - \alpha \nabla_{[y]_1} p(y), \dots, \beta[v]_n - \alpha \nabla_{[y]_n} p(y)) \\ &= (\beta[v]_1 - \alpha \nabla[p]_1([y]_1), \dots, \beta[v]_n - \alpha \nabla[p]_n([y]_n)) \\ &= (\text{HBM}_v(\beta_1, [p]_1, [y]_1, [v]_1), \dots, \text{HBM}_v(\beta_i, [p]_i, [y]_i, [v]_i))\end{aligned}$$

This shows that one step of HBM_v on p is precisely equivalent to n simultaneous applications of HBM_v to the one-dimensional quadratics $[p]_i$, all with the same β and α . Similarly, for HBM_x .

NAG for a quadratic problem. Proof (2/2)

Next we show that NAG, applied to a one-dimensional quadratic with a momentum coefficient β , is equivalent to HBM applied to the same quadratic and with the same learning rate, but with a momentum coefficient $\beta(1 - \alpha\lambda)$. We show this by expanding $\text{NAG}_v(\beta, [p]_i, y, v)$ (where y and v are scalars):

$$\begin{aligned}\text{NAG}_v(\beta, [p]_i, y, v) &= \beta v - \alpha \nabla [p]_i (y + \beta v) \\ &= \beta v - \alpha (\lambda_i (y + \beta v) - c_i) \\ &= \beta v - \alpha \lambda_i \beta v - \alpha (\lambda_i y - c_i) \\ &= \beta (1 - \alpha \lambda_i) v - \alpha \nabla [p]_i (y) \\ &= \text{HBM}_v(\beta(1 - \alpha \lambda_i), [p]_i, y, v).\end{aligned}$$

QED.

Observations:

- HBM and NAG become **equivalent** when α is small (when $\alpha\lambda \ll 1$ for every eigenvalue λ of A), so NAG and HBM are distinct only when α is reasonably large.
- When α is relatively large, NAG uses smaller effective momentum for the high-curvature eigen-directions, which **prevents oscillations** (or divergence) and thus allows the use of a larger β than is possible with CM for a given α .

NAG for DL

task	$0_{(\text{SGD})}$	0.9N	0.99N	0.995N	0.999N	0.9M	0.99M	0.995M	0.999M	SGD_C	HF^\dagger	HF^*
Curves	0.48	0.16	0.096	0.091	0.074	0.15	0.10	0.10	0.10	0.16	0.058	0.11
Mnist	2.1	1.0	0.73	0.75	0.80	1.0	0.77	0.84	0.90	0.9	0.69	1.40
Faces	36.4	14.2	8.5	7.8	7.7	15.3	8.7	8.3	9.3	NA	7.5	12.0

Figure 3: The table reports the squared errors on the problems for each combination of β_{max} and a momentum type (NAG, CM). When β_{max} is 0 the choice of NAG vs CM is of no consequence so the training errors are presented in a single column. For each choice of β_{max} , the highest-performing learning rate is used. The column SGD_C lists the results of Chapelle & Erhan (2011) who used 1.7M SGD steps and tanh networks. The column HF^\dagger lists the results of HF without L2 regularization; and the column HF^* lists the results of Martens (2010).

References and Python Examples

- Figures for HBM was taken from the presentation. Visit site for more tutorials.
- Why Momentum Really Works. [Link](#).
- Run code in  Colab. The code taken from .
- On the importance of initialization and momentum in deep learning. [Link](#).