

# 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

- **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.

- **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

- 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.

- 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  $\beta$ .

**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  $\beta$ .

**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**,  $\beta_k$  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  $\lambda_i$ 's are sorted, from smallest  $\lambda_1$  to biggest  $\lambda_n$ . It is clear, that  $\lambda_i$  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  $\alpha$  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  $\beta$ , and learning rate  $\alpha$ . Define  $\text{NAG}_x$  and  $\text{NAG}_v$  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  $\text{HBM}_v$ :

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

This shows that one step of  $\text{HBM}_v$  on  $p$  is precisely equivalent to  $n$  simultaneous applications of  $\text{HBM}_v$  to the one-dimensional quadratics  $[p]_i$ , all with the same  $\beta$  and  $\alpha$ . Similarly, for  $\text{HBM}_x$ .

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

Next we show that NAG, applied to a one-dimensional quadratic with a momentum coefficient  $\beta$ , 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  $\alpha$  is small (when  $\alpha\lambda \ll 1$  for every eigenvalue  $\lambda$  of  $A$ ), so NAG and HBM are distinct only when  $\alpha$  is reasonably large.
- When  $\alpha$  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  $\beta$  than is possible with CM for a given  $\alpha$ .

# NAG for DL

task	$0_{(\text{SGD})}$	0.9N	0.99N	0.995N	0.999N	0.9M	0.99M	0.995M	0.999M	$\text{SGD}_C$	$\text{HF}^\dagger$	$\text{HF}^*$
Curves	0.48	0.16	0.096	0.091	<b>0.074</b>	0.15	0.10	0.10	0.10	0.16	0.058	0.11
Mnist	2.1	1.0	<b>0.73</b>	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	<b>7.7</b>	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  $\beta_{max}$  and a momentum type (NAG, CM). When  $\beta_{max}$  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  $\beta_{max}$ , the highest-performing learning rate is used. The column  $\text{SGD}_C$  lists the results of Chapelle & Erhan (2011) who used 1.7M SGD steps and tanh networks. The column  $\text{HF}^\dagger$  lists the results of HF without L2 regularization; and the column  $\text{HF}^*$  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](#).