

Acceleration of GD via Momentum

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Smooth convex functions: less than $\mathcal{O}(\epsilon^{-1})$ steps?

Given L and $D = \|x_0 - x^*\|$ we know that **gradient descent**

- ◇ converges with $\mathcal{O}(1/k)$
- ◇ cannot go faster (“lower bound”)

Maybe GD is not the best possible algorithm?

After all, it is arguably the simplest possible method using the gradient.

Smooth convex functions: less than $\mathcal{O}(\epsilon^{-1})$ steps?

So let's look at the following classes of methods:

First-order method:

- ◇ Access to data only via an **oracle** returning f and ∇f at given points.
- ◇ Clearly, GD is a first order method.

Q: What is the **best** first-order method for smooth convex functions.

best: smallest upper bound on the number of oracle calls *in the worst case*.

- ◇ Nemirovski and Yudin 1979 proved that

every first-order method needs at least $\Omega(1/\sqrt{\epsilon})$ iterations
to find a point \bar{x} with $f(\bar{x}) - f^* \leq \epsilon$.

\Rightarrow no method can be faster than $\mathcal{O}(1/k^2)$

Acceleration to $\mathcal{O}(1/\sqrt{\epsilon})$ steps

- ◇ Nesterov 1983 proposed a method that needs only $\mathcal{O}(1/\sqrt{\epsilon})$ iterations (and is therefore the *best one*).
- ◇ Known as **Nesterov's accelerated gradient** method.
- ◇ By now multiple similar algorithms with same complexity exist.
- ◇ Proofs are generally not really instructive (some are computer assisted).

Nesterov's accelerated gradient method

Algorithm Nesterov's accelerated gradient method (NAG)

```
1: for  $k = 0, 1, \dots$  do
2:    $x_{k+1} = y_k - \frac{1}{L} \nabla f(y_k)$ 
3:    $z_{k+1} = z_k - \frac{k+1}{2L} \nabla f(y_k)$ 
4:    $y_{k+1} = \frac{k+1}{k+3} x_{k+1} + \frac{2}{k+3} z_{k+1}$ 
```

- ◇ perform “**smooth step**” from y_k to x_{k+1}
- ◇ perform **aggressive step** from z_k to z_{k+1}
- ◇ form **weighted average** of the two
compensate for the aggressive step by giving less weight

Nesterov's algorithm as a momentum method

A different way to write the method is via **momentum**

$$\begin{aligned}y_k &= x_k + \beta_k(x_k - x_{k-1}) \\x_{k+1} &= y_k - \frac{1}{L}\nabla f(y_k).\end{aligned}$$

- ◇ differs from GD only in momentum/inertia term $\beta_k(x_k - x_{k-1})$
- ◇ has to be chosen carefully $\beta_k = \frac{k-1}{k+2}$
- ◇ coefficient approaches $\frac{k-1}{k+2} \approx 1 - \frac{3}{k}$

Nesterov's accelerated gradient method: convergence

Minimum is obtained for x^* .

Theorem

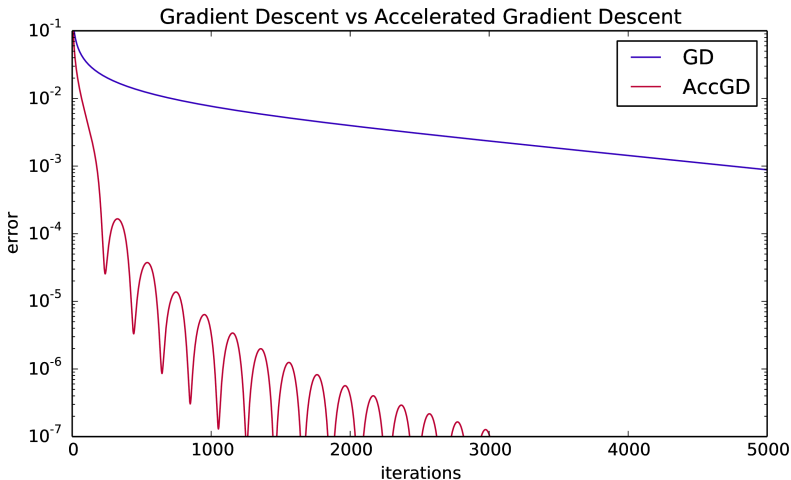
Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ be convex and L -smooth, then **NAG** yields

$$f(x_k) - f(x^*) \leq \frac{2L\|x_0 - x^*\|^2}{k(k+1)}$$

Recall that the gradient descent bound was

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

$\mathcal{O}(1/k^2)$ vs $\mathcal{O}(1/k)$ in practice



Proof idea

Potential function Φ that decreases along trajectory (standard technique).
Out of the blue: Use

$$\Phi(k) := k(k+1)(f(x_k) - f^*) + 2L\|z_k - x^*\|^2.$$

Then show that

$$\Phi(k+1) \leq \Phi(k).$$

Results in

$$\Phi(k+1) \leq \Phi(k) \leq \dots \leq \Phi(0)$$

and therefore

$$k(k+1)(f(x_k) - f^*) \leq 2L\|z_0 - x^*\|^2.$$

Why momentum?

- ◇ GD has problems with **ravines**, i.e. areas where the surface curves much more steeply in one dimension than in another.
- ◇ Results in zig-zagging.



Figure: no momentum

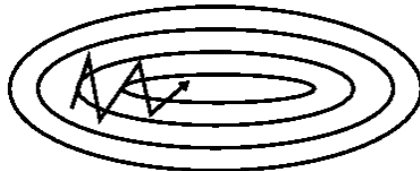
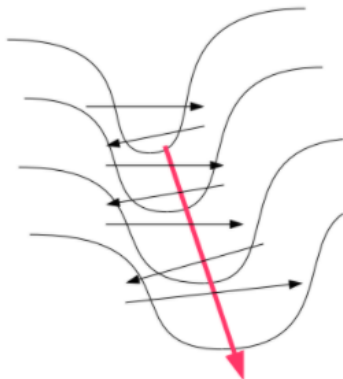
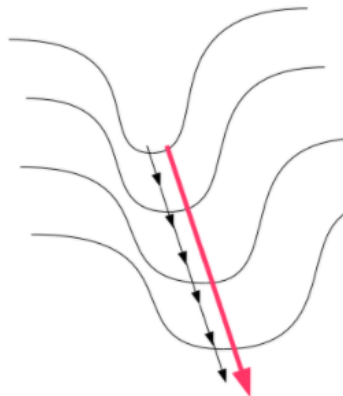


Figure: with momentum

Momentum and ravines



SGD bounces back and forth from one side of the valley to the other



Using Momentum the zig-zag cancels out, while the direction along the valley is reinforced

Momentum in terms of velocity

Consider a ball rolling down a slope. Its **velocity** is

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

$$x_{k+1} = x_k - v_k$$

- ◇ a fraction β of the **previous velocity** (friction)
- ◇ plus, steepness of the **slope**

In terms of iterates:

$$x_{k+1} = x_k - v_k$$

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

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

Heavy ball: Polyak 1964

We derived

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

while Nesterov's method was

$$\begin{aligned} y_k &= x_k + \beta_k(x_k - x_{k-1}) \\ x_{k+1} &= y_k - \frac{1}{L} \nabla f(y_k). \end{aligned}$$

However, **Polyak's** momentum provides no speedup over $\mathcal{O}(1/k)$ (for smooth convex function).

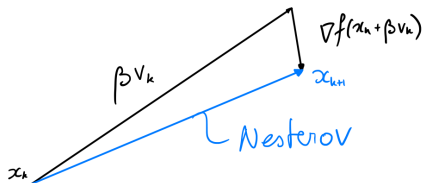
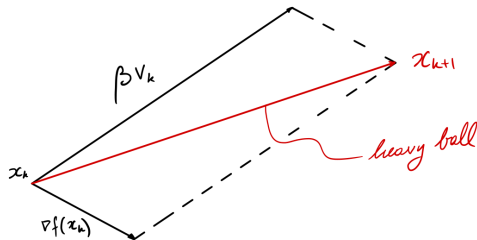
What's the difference?

- ◇ Both types of momentum seem so similar.
- ◇ Heavy ball does not care if momentum or gradient first.
- ◇ Nesterov momentum applies **inertia first**, then gradient:

$$\begin{aligned}v_k &= \beta v_{k-1} + \alpha \nabla f(x_k + \beta v_{k-1}) \\x_{k+1} &= x_k - v_k.\end{aligned}$$

Provides stabilization if inertia overshoots.

Nesterov vs. Polyak momentum.



Momentum for strongly convex functions

For L -smooth μ -strongly convex we know that GD obtains

$$\|x_{k+1} - x^*\|^2 \leq \left(1 - \frac{1}{\kappa}\right) \|x_k - x^*\|^2$$

and

$$f(x_k) - f^* \leq \left(1 - \frac{1}{\kappa}\right)^k \frac{L\|x_0 - x^*\|^2}{2}.$$

Performance depends heavily on the **condition number** $\kappa := L/\mu$

Contraction coefficient is $(1 - 1/\kappa)$.

Nesterov and Polyak momentum improve this to $(1 - 1/\sqrt{\kappa})$

Momentum for stochastic methods

SGD analysis can be extended to **smooth** functions with rate

$$\mathcal{O}\left(\frac{L}{k} + \frac{\sigma^2}{\sqrt{k}}\right),$$

where $\sigma^2 := \mathbb{E}[\|\nabla f(x) - g(x)\|^2]$ is the **variance** of the gradient estimator.

This can be improved by Nesterov momentum (and additional tricks) to

$$\mathcal{O}\left(\frac{L}{k^{\textcolor{red}{2}}} + \frac{\sigma^2}{\sqrt{k}}\right).$$

Improvement only in the “**early phase**” before noise takes over.

For worst case rates, only the asymptotic (“late”) phase matters.

Momentum and nonsmoothness

- ◇ If f is not differentiable and we have to use subgradients:
no way to improve the $\mathcal{O}(1/\sqrt{k})$ rate.
- ◇ Works objective is **structured**: $f + g$ (smooth+nonsmooth)

$$\text{FISTA: } \begin{cases} y_k &= x_k + \beta_k(x_k - x_{k-1}) \\ x_{k+1} &= \text{prox}_{\alpha g}(y_k - \alpha \nabla f(y_k)). \end{cases}$$

Accelerates from $\mathcal{O}(1/k)$ of proximal-gradient method to $\mathcal{O}(1/k^2)$.

- ◇ In particular, also works in the **constrained setting**.

Momentum in the nonconvex world

- ◇ In theory: difficult to show benefit of momentum for nonconvex problems.
 - ▶ some statements under additional smoothness assumptions
- ◇ Strong empirical evidence of usefulness.
 - ▶ especially in deep learning.
- ◇ Theory is mostly limited to escaping of saddle points.

Docs > torch.optim > SGD

SGD

```
CLASS torch.optim.SGD(params, lr=<required parameter>, momentum=0, dampening=0,  

weight_decay=0, nesterov=False) [SOURCE]
```

Implements stochastic gradient descent (optionally with momentum).

input : γ (lr), θ_0 (params), $f(\theta)$ (objective), λ (weight decay),
 μ (momentum), τ (dampening), *nesterov*

for $t = 1$ **to** ... **do**

$g_t \leftarrow \nabla_{\theta} f_t(\theta_{t-1})$

if $\lambda \neq 0$

$g_t \leftarrow g_t + \lambda \theta_{t-1}$

if $\mu \neq 0$

if $t > 1$

$\mathbf{b}_t \leftarrow \mu \mathbf{b}_{t-1} + (1 - \tau) g_t$

else

$\mathbf{b}_t \leftarrow g_t$

if *nesterov*

$g_t \leftarrow g_{t-1} + \mu \mathbf{b}_t$

else

$g_t \leftarrow \mathbf{b}_t$

$\theta_t \leftarrow \theta_{t-1} - \gamma g_t$

return θ_t

Momentum in DL: