Acceleration of GD via Momentum

Axel Böhm

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1. Optimal methods
2. Nesterov momentum
3. Heavy ball

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

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

- GD converges with $\mathcal{O}(1/k)$
- cannot go faster ("lower bound")

Maybe gradient descent 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 the data only via an oracle which returns 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 means: 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 (no method can be faster than $\mathcal{O}(1/k^2)$).

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

- Nesterov 1983 came up with 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** $k = 0, 1, \ldots$ **do**

2: $\quad x_{k+1} = y_k - \frac{1}{L} \nabla f(y_k)$

3: $\quad z_{k+1} = z_k - \frac{k+1}{2L} \nabla f(y_k)$

4: $\quad y_{k+1} = \frac{k+1}{k+3} x_{k+1} + \frac{2}{k+3} z_{k+1}$

- 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

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

- differs from GD on in momentum/inertia term $\beta_k(x_k - x_{k-1})$
- has to 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

Theorem

Let $f : R^d \to \mathbb{R}$ be convex and L-smooth with minimum x^*, 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

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

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

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

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

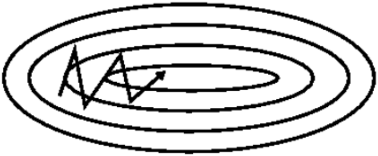

Figure: with momentum

Momentum in terms of velocity

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

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

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

In terms of iterates:

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

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

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

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 do momentum or gradient first.
- Nesterov momentum applies inertia first then gradient.

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

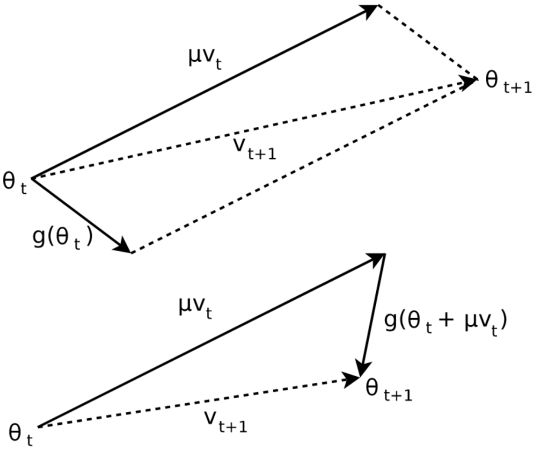

Figure: Nesterov vs Polyak momentum.

Momentum for strongly convex functions

For smooth strongly convex we know that GD obtains

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

and

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

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 momentum (and additional tricks) to

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

Improvement only in the "**transient phase**" before noise takes over.
For worst case rates, only the asymptotic phase matters.

Momentum in the nonconvex world

While it is extremely difficult to show a benefit of momentum in for nonconvex problems.
Empirical evidence (for many different problems) is strong.
Theory is mostly limited to escaping of saddle points.