Acceleration of GD via Momentum

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Optimal methods

Nesterov momentum

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

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

- \diamond 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:

- \diamond 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

- \diamond 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, ... **do**
- 2: $x_{k+1} = y_k \frac{1}{L} \nabla f(y_k)$
- 3: $z_{k+1} = z_k \frac{t+1}{2L} \nabla f(y_k)$
- 4: $y_{k+1} = \frac{t+1}{t+3} x_{k+1} + \frac{2}{t+3} z_{k+1}$
 - \diamond perform "smooth step" from y_k to x_{k+1}
 - \diamond 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

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

- \diamond differs from GD on in momentum/inertia term $\beta_k(x_k x_{k-1})$
- \diamond has to chosen carefully $\beta_k = \frac{k-1}{k+2}$
- \diamond 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

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

Recall that the gradient descent bound was

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

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

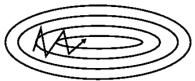


Figure: with momentum

Momentum in terms of velocity

Consider a ball rolling down a slope. Its velocity is

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

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

- \diamond 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

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

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.

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

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

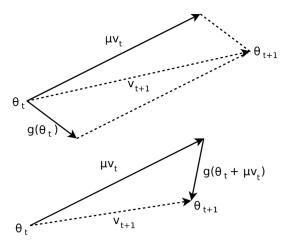


Figure: Nesterov vs Polyak momentum.

Momentum for strongly convex functions

For smooth strongly convex we know that GD obtains

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

and

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

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

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

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