SGD and GD Revisited

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Terminology

Iterative Optimization Methods

Iterative Optimization (Generic Version)

1. Pick some starting point $x^{(0)} \in \mathbf{R}^d$.
2. For $k = 0, 1, \ldots$
   1. Choose a **step** or **search direction** $v^{(k)}$.
   2. Choose a **step size** $t^{(k)}$.
   3. Set $x^{(k+1)} = x^{(k)} + t^{(k)} v^{(k)}$

- Despite the names,
  - $v^{(k)}$ is **not** generally a unit vector.
  - $t^{(k)}$ is **not** $\|x^{(k+1)} - x^{(k)}\|$ (unless $\|v^{(k)}\| = 1$).

Descent Directions

Definition

A **[one-sided] directional derivative** of f at x in the direction v is

$$f'(x;v) = \lim_{h \downarrow 0} \frac{f(x+hv) - f(x)}{h}.$$

[Note: Can be $\pm\infty$, e.g. for discontinuous functions.]

Definition

v is a **descent direction** for f at x if $f'(x;v) < 0$.

Descent Directions

- If f is differentiable, then

$$f'(x,v) = \nabla f(x)^T v.$$

- So if f is differentiable, then v is a descent direction at x iff

$$\nabla f(x)^T v < 0.$$

- **Newton** step is a descent direction for strictly convex functions:

$$v_{\text{newton}} = -\left[\nabla^2 f(x)\right]^{-1} \nabla f(x)$$

  - Much faster convergence close to the optimum.
  - Computing/storing inverse Hessian is too much in high dimensions.
  - Quasi-Newton methods approximate Newton step, without Hessian (e.g. L-BFGS).

Descent Method

Definition

An iterative optimization method is a **descent method** if every step is a descent direction.

- Equivalently, we have a descent method if

$$f(x^{(k+1)}) < f(x^{(k)}),$$

  except when $x^{(k)}$ is optimal.

- Is SGD a descent method?

Stochastic Gradient Descent

Gradient Descent

Gradient Descent

- Initialize $x = 0$
- repeat
  - $x \leftarrow x - \eta \nabla f(x)$

"Noisy" Gradient Descent

"Noisy" Gradient Descent (not a standard name)

- Initialize $x = 0$
- repeat
  - $x \leftarrow x - \eta v$

Where ν is some estimate of $\nabla f(x)$

- In minibatch SGD, we have $\mathbb{E}v = \nabla f(x)$.
- With large batches, we get better estimates. ($\operatorname{Var}(v)$ decreases.)

SGD on Regularized Empirical Risk

- Our typical objective function is of the form

$$\begin{aligned} J(w) &= \lambda\Omega(w) + \frac{1}{n}\sum_{i=1}^{n} \ell(f_w(x_i), y_i) \\ &= \frac{1}{n}\sum_{i=1}^{n} h_i(w) \end{aligned}$$

  where

$$h_i(w) = \lambda\Omega(w) + \ell(f_w(x_i), y_i).$$

- SGD on $J(w)$:
  - Choose $i \in \{1, \ldots, n\}$ uniformly at random
  - Approximate approximate $\nabla J(w)$ by $\nabla h_i(w)$.
- Step is unbiased for gradient:

$$\mathbb{E}_{i \sim \text{Unif}(1,\ldots,n)} \nabla h_i(w) = \nabla J(w)$$

SGD on Risk

- Suppose $(x, y) \sim P_{\mathcal{X} \times \mathcal{Y}}$ and objective is the expected loss:

$$J(w) = \mathbb{E}\ell(f_w(x), y).$$

- SGD on $J(w)$:
  - Choose $(x, y) \sim P_{\mathcal{X} \times \mathcal{Y}}$.
  - Approximate $\nabla_w J(w)$ by $\nabla_w \ell(f_w(x), y)$.
- Step is unbiased for gradient:

$$\mathbb{E}_{(x,y) \sim P_{\mathcal{X} \times \mathcal{Y}}} \nabla_w \ell(f_w(x), y) = \nabla_w \mathbb{E}\ell(f_w(x), y)$$

- To implement this, need fresh samples from $P_{\mathcal{X} \times \mathcal{Y}}$.
- If we're resampling from training set, $(x, y) \sim \hat{P}_{\mathcal{X} \times \mathcal{Y}}$ we get back SGD.

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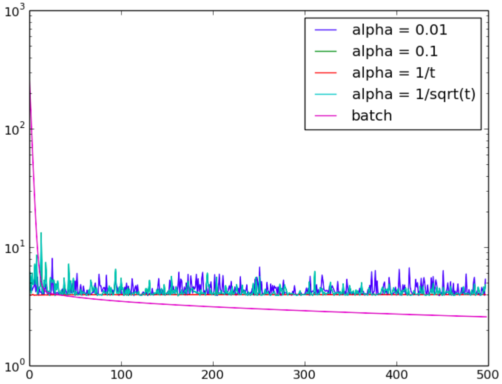
http://planetmath.org/differentiationundertheintegralsign.

Convergence Rates

Does SGD Catch Up to GD?

- Loss on ridge regression for GD and SGD with various stepsizes



- Why doesn't SGD catch up to batch GD?
- Short answer: It does, just takes a very long time.

Convergence Rates for Gradient Descent

Assume $f : \mathbf{R}^n \to \mathbf{R}$ is convex and differentiable, and

- ∇f is **Lipschitz continuous** with constant $L > 0$, that is:

$$|\nabla f(x) - \nabla f(y)| \leqslant L\|x - y\| \text{ for all } x, y$$

Theorem

Gradient descent with fixed step size $t \leqslant 1/L$ satisfies

$$f(x^{(k)}) - f(x^*) \leqslant \frac{\|x^{(0)} - x^*\|^2}{2tk}.$$

- So GD has convergence rate $O(1/k)$.
- To get $f(x^{(k)}) - f(x^*) \leqslant \varepsilon$, need $O(1/\varepsilon)$ iterations.
- Same rate with backtracking line search.

Based on `https://www.cs.cmu.edu/~ggordon/10725-F12/slides/05-gd-revisited.pdf`

Convergence Rates for GD with Strong Convexity

Definition

A differentiable function f is strongly convex if there is some $d > 0$ for which

$$f(y) \geqslant f(x) + \nabla f(x)^T (y - x) + \frac{d}{2}\|y - x\|^2 \text{ all } x, y.$$

(e.g. ridge regression because of the ℓ_2 regularization term)

Theorem

Under same Lipschitz condition as before and strong convexity, GD with fixed step size or with backtracking line search satisfies

$$f(x^{(k)}) - f(x^*) \leqslant c^k \frac{L}{2}\|x^{(0)} - x^*\|^2,$$

where $0 < c < 1$*.*

Convergence Rates for GD with Strong Convexity

Theorem

Under same Lipschitz condition as before and strong convexity, GD with fixed step size or with backtracking line search satisfies

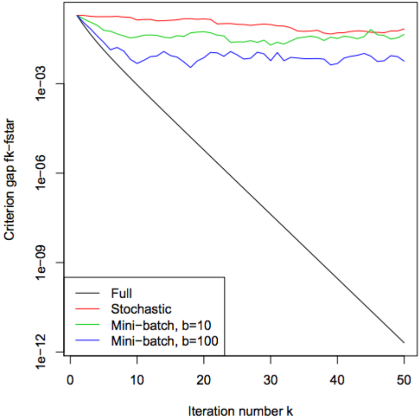
$$f(x^{(k)}) - f(x^*) \leqslant c^k \frac{L}{2} \|x^{(0)} - x^*\|^2,$$

where $0 < c < 1$.

- So with strong convexity, GD converges at rate $O(c^k)$. (exponentially fast!)
- To get $f(x^{(k)}) - f(x^*) \leqslant \varepsilon$, need $O(\log[1/\varepsilon])$ iterations.
- Called "**linear convergence**" because looks linear on semi-log plot.

Based on `https://www.cs.cmu.edu/~ggordon/10725-F12/slides/05-gd-revisited.pdf`

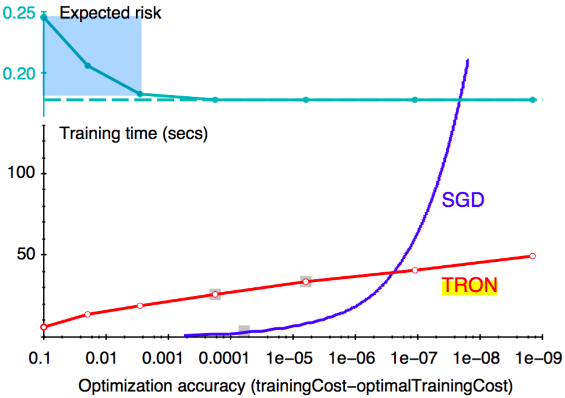
SGD vs GD on Log Scale



- Shows **linear convergence** for "Full" GD; **sublinear** for others.
- Note: logarithmic y-axis

SGD is Slow Close to the Optimum – Does it Matter?

- TRON is a 2nd order method (very fast close to the optimum)



Plots from Bottou and Bousquet's "The Tradeoffs of Large Scale Learning."