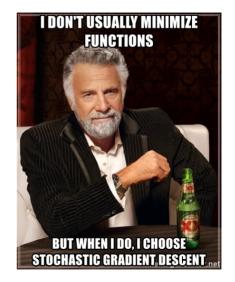
Stochastic Gradient Descent

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- Introduction
- Convergence in expectation
- High probability bounds



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Many optimization problems in Data science are sum structured:

$$f(x) = \frac{1}{n} \sum_{i=1}^{n} f_i(x).$$

- known as empirical risk (minimization)
- f_i corresponds to the loss of the i-th observation
- for example: linear regression

$$f(x) = ||Ax - b||^2 = \sum_{i=1}^{n} (a_i^T x - b_i)^2$$

 \diamond evaluating ∇f can be expensive if *n* is large

Risk minimization

In theory we would even like to minimize the population risk

$$f(x) = \mathbb{E}_{\xi}[f(x,\xi)]$$

- ⋄ Typically no access to f
- most of what follows works in this more general setting

sample
$$i \in 1, ..., n$$
 uniformly at random $x_{k+1} = x_k - \alpha \nabla f_i(x_k)$.

- ⋄ requires only **one** gradient instead of *n* per iteration.
- \diamond we call $g_k := \nabla f_i(x_k)$ a stochastic gradient (estimator)

Unbiased

Can't really use convexity as before since

$$f(x_k) - f(x^*) \le \langle \nabla f_i(x_k), x^* - x_k \rangle$$

might not hold in general.

- But holds in expectation!
- \diamond For this we need that $\nabla f_i(x)$ is unbiased estimator of $\nabla f(x)$

$$\mathbb{E}[\nabla f_i(x)] = \frac{1}{n} \sum_{i=1}^n \nabla f_i(x) = \nabla f(x)$$

Gradient inequality holds in expectation

We would like to conclude that

$$\mathbb{E}\left[\langle g_k, x^* - x_k \rangle\right] = \langle \mathbb{E}[g_k], \mathbb{E}[x^* - x_k] \rangle$$

but this is not so clear since x_k is also stochastic and in general $\mathbb{E}[XY] \neq \mathbb{E}[X]\mathbb{E}[Y]$.

 \diamond We use the **conditional Expectation** $\mathbb{E}[\cdot|x_k]$ (read as expectation of \cdot given x_k). Then

$$\mathbb{E}\left[\langle g_k, x^* - x_k \rangle | x_k \right] = \langle \mathbb{E}[g_k | x_k], x^* - x_k \rangle = \langle \nabla f(x_k), x^* - x_k \rangle.$$

⋄ Together with the tower property $\mathbb{E}[\mathbb{E}[X|Y]] = \mathbb{E}[X]$:

$$\mathbb{E}\left[\langle g_k, x^* - x_k \rangle\right] = \mathbb{E}\left[\mathbb{E}\left[\langle g_k, x^* - x_k \rangle | x_k\right]\right]$$
$$= \mathbb{E}\left[\langle \nabla f(x_k), x^* - x_k \rangle\right] \leq \mathbb{E}[f(x^*) - f(x_k)].$$

Assumptions

- \diamond f is convex and differentiable
- $||x_0 x^*|| < D$
- \diamond stochastic gradient are bounded in expectation $\mathbb{E}[\|g_k\|^2] \leq B^2$.

Theorem

With the assumptions above and stepsize

$$\alpha = \frac{D}{B\sqrt{k}}$$

yields

$$\mathbb{E}\left[f(\bar{x}_k)-f^*\right]\leq \frac{DB}{\sqrt{k}}.$$

Proof

Proof.

We start as usual $(g_k$ is a stochastic gradient)

$$||x_{k+1} - x^*||^2 \le ||x_k - \alpha g_k - x^*||^2$$

= $||x_k - x^*||^2 + 2\alpha \langle g_k, x^* - x_k \rangle + \alpha^2 ||g_k||^2$.

Now take expectation

$$\mathbb{E}\left[\|x_{k+1} - x^*\|^2\right] \le \mathbb{E}\left[\|x_k - x^*\|^2\right] + 2\alpha \mathbb{E}[f^* - f(x_k)] + \alpha^2 \mathbb{E}[\|g_k\|^2].$$

Bound gradients and telescope to finish the proof.

Comparing constants: SGD vs. GD

⋄ GD: In the bounded (sub-)gradient analysis we assumed $\|\nabla f(x)\|^2 \le B_{BG}^2$. For finite-sum this gives

$$\left\|\frac{1}{n}\sum_{i=1}^n \nabla f_i(x)\right\|^2 \leq B_{BG}^2$$

SGD: We assumed that the expected squared norm are bounded, i.e.

$$\mathbb{E}[\|\nabla f_i(x)\|^2] = \frac{1}{n} \sum_{i=1}^n \|\nabla f_i(x)\|^2 \le B_{SGD}^2$$

By convexity we have that

$$\diamond \ B_{BG}^2 \approx \left\| \frac{1}{n} \sum_{i=1}^n \nabla f_i(x) \right\|^2 \leq \frac{1}{n} \sum_{i=1}^n \| \nabla f_i(x) \|^2 \approx B_{SGD}^2$$

but usually comparable

Minibatch SGD

Instead of just using a single element f_i we can use several $S \subset \{1, \ldots, n\}$

$$g_k := \frac{1}{|S|} \sum_{j \in S} \nabla f_j(x_k)$$

Interpolates between

- $\diamond |S| = 1 \Leftrightarrow \text{(vanilla) SGD, as defined earlier}$
- $\diamond |S| = n \Leftrightarrow (batch) GD$

Benefit: Gradient computation can parallelized.

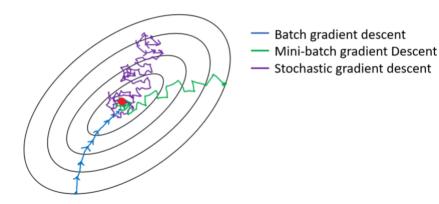
Increasing batch size reduces variance

Taking an average of independent random variables will reduce variance.

$$\begin{aligned} \mathbb{V}[g_k] &= \mathbb{E}\left[\|g_k - \nabla f(x_k)\|^2\right] = \mathbb{E}\left[\left\|\frac{1}{|S|} \sum_{j \in S} f_j(x_k) - \nabla f(x_k)\right\|^2\right] \\ &= \frac{1}{|S|} \mathbb{E}\left[\|\nabla f_i(x_k) - \nabla f(x_k)\|^2\right] \\ &= \frac{1}{|S|} \mathbb{V}[\nabla f_i(x_k)] \end{aligned}$$

However: We have to use a different analysis to make use of this.

Minibatch illustration



Stochastic Subgradient Method

If we go back to the proof: We did not use smoothness. If we choose unbiased estimate of subgradient $\mathbb{E}[g_k|x_k] \in \partial f(x_k)$ and iterate

sample
$$i \in 1, ..., n$$
 uniformly at random let $g_k \in \partial f_i(x_k)$
 $x_{k+1} = x_k - \alpha g_k$.

We can get the same $\mathcal{O}(\epsilon^{-2})$ complexity. Smoothness did not provide any benefit (in terms of rate). With a more refined analysis one can get better dependence on constants.

Projected SGD

- Previous proof can be extended (trivially) to the constrained setting
- \diamond with same complexity $\mathcal{O}(\epsilon^{-2})$
- but (of course) with an additional projection

$$x_{k+1} = \Pi_C(x_k - \alpha \nabla f_i(x_k))$$

High probability bounds

Theorem

Hoeffding's inequality Let X_i be independent random variables that satisfy

$$\diamond \mathbb{E}X_i = 0$$

$$\diamond ||X_i|| \leq M.$$

Then,

$$\mathbb{P}\left[X_1+\cdots+X_k\geq t\right]\leq e^{-\frac{t^2}{2kM^2}}$$

Azuma-Hoeffding's generalization does not require independence, only $\mathbb{E}[X_k|X_{k-1},\ldots,X_1]=0$.

Statement with high probability

Theorem

Let $\delta > 0$ and assumptions as before + iterates remain in bounded set with diameter D (for example constraint set). Then,

$$f(\bar{x}_k)-f^*\leq \frac{DB\delta}{\sqrt{k}}.$$

with probability more than $1 - e^{-\delta^2/8}$.

 \Rightarrow choose δ large for bound in higher probability.

Proof.

$$||x_{k+1} - x^*||^2$$

$$\leq ||x_k - x^*||^2 + 2\alpha \langle g_k, x^* - x_k \rangle + \alpha^2 ||g_k||^2$$

$$< ||x_k - x^*||^2 + 2\alpha \langle \nabla f(x_k), x^* - x_k \rangle + \alpha^2 ||g_k||^2 + \langle v_k, x^* - x_k \rangle$$

with $v_k = g_k - \nabla f(x_k)$. Continue as usual

$$f(\bar{x}_k) - f^* \le \frac{\|x_0 - x^*\|^2}{2\alpha k} + \alpha B^2 + \frac{1}{k} \sum_{i=1}^k X_i$$

with

$$X_k := \langle v_k, x^* - x_k \rangle < ||v_k|| ||x_k - x^*|| < 2BD$$

and $\mathbb{E}[X_k] = 0$ fulfilling Hoeffding's assumptions. Use it with $t = DB\sqrt{k}\delta$.