

Stochastic Gradient Descent

Axel Böhm

January 17, 2022

- 1 Introduction
- 2 Convergence in expectation
- 3 High probability bounds



Finite sum structure

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

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

- ◇ 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

(vanilla) Stochastic gradient descent

sample $i \in 1, \dots, n$ uniformly at random

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

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

Unbiased

- ◇ Can't really use convexity as before since

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

might **not hold** in general.

- ◇ But holds **in expectation**!
- ◇ 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

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

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

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

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

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

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

Convergence statement: $\mathcal{O}(\epsilon^{-2})$ steps

Assumptions

- ◇ f is convex and differentiable
- ◇ $\|x_0 - x^*\| \leq D$
- ◇ 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

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

Proof

Proof.

We start as usual (g_k is a stochastic gradient)

$$\begin{aligned}\|x_{k+1} - x^*\|^2 &\leq \|x_k - \alpha g_k - x^*\|^2 \\ &= \|x_k - x^*\|^2 + 2\alpha \langle g_k, x^* - x_k \rangle + \alpha^2 \|g_k\|^2.\end{aligned}$$

Now take expectation

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

Bound gradients and telescope to finish the proof. □

Comparing constants: SGD vs. GD

- ◇ **GD:** In the bounded (sub-)gradient analysis we assumed $\|\nabla f(x)\|^2 \leq B_{BG}^2$. 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.

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

By convexity we have that

- ◇ $B_{GD}^2 \approx \left\| \frac{1}{n} \sum_{i=1}^n \nabla f_i(x) \right\|^2 \leq \frac{1}{n} \sum_{i=1}^n \|\nabla f_i(x)\|^2 \approx B_{SGD}^2$
- ◇ but usually comparable

Minibatch SGD

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

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

Interpolates between

- ◇ $|S| = 1 \Leftrightarrow$ (vanilla) SGD, as defined earlier
- ◇ $|S| = n \Leftrightarrow$ (batch) GD

Benefit: Gradient computation can be parallelized.

Increasing batch size reduces variance

Taking an average of independent random variables will reduce variance.

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

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

Minibatch illustration



- Batch gradient descent
- Mini-batch gradient Descent
- Stochastic gradient descent

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 $i \in 1, \dots, n$ 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 provide any benefit (in terms of rate).

Projected SGD

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

High probability bounds

Theorem

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

- ◇ $\mathbb{E}X_i = 0$
- ◇ $\|X_i\| \leq M$.

Then,

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

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

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.

$$\begin{aligned}\|x_{k+1} - x^*\|^2 &\leq \|x_k - x^*\|^2 + 2\alpha \langle g_k, x^* - x_k \rangle + \alpha^2 \|g_k\|^2 \\ &\leq \|x_k - x^*\|^2 + 2\alpha \langle \nabla f(x_k), x^* - x_k \rangle + \alpha^2 \|g_k\|^2 + \langle v_k, x^* - x_k \rangle\end{aligned}$$

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

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

with

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

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