

SGD

Def

A function $R: \mathbb{R}^d \rightarrow \mathbb{R}$ is convex if $\forall \theta, \theta' \in \mathbb{R}^d$, $R(t\theta + (1-t)\theta') \leq tR(\theta) + (1-t)R(\theta')$ $\forall t \in [0, 1]$.

Lemma

Let $R: \mathbb{R}^d \rightarrow \mathbb{R}$ be differentiable on the interior of its domain. R is convex iff $\forall \theta, \theta' \in \mathbb{R}^d$ $(\theta')^\top R'(\theta) \geq R(\theta) + (\theta')^\top R(\theta)$. ← 1st order approx is a global minimization

pf) \Rightarrow From def of convexity, $R(\theta + t(\theta' - \theta)) \leq R(\theta) + t(R(\theta') - R(\theta))$. $\therefore R(\theta) - R(\theta) \geq \frac{1}{t}(R(\theta + t(\theta' - \theta)) - R(\theta))$. Send $t \rightarrow 0$.
 \Leftarrow Define $\theta_t = t\theta + (1-t)\theta'$. Combining $R(\theta) \geq R(\theta_t) + (\theta_t)^\top R(\theta_t)$, $R(\theta') \geq R(\theta_t) + (\theta_t)^\top R(\theta')$, $tR(\theta) + (1-t)R(\theta') \geq R(\theta_t) + (\theta_t)^\top (t\theta + (1-t)\theta' - \theta_t)$ $\forall t \in [0, 1]$. □

Rmk The latter def of convexity motivates generalization of gradients to nonsmooth, convex functions.

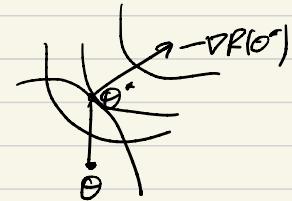
Optimality

Consider $\min_{\theta \in \Theta} R(\theta)$, for $R: \mathbb{R}^d \rightarrow \mathbb{R}$ diff; convex.

Lemma $\theta^* = \arg\min_{\theta \in \Theta} R(\theta)$ iff $D\theta(\theta^*)^\top (\theta - \theta^*) \geq 0 \quad \forall \theta \in \Theta$

pf) \Leftarrow From prev lemma, $R(\theta) - R(\theta^*) \geq D\theta(\theta^*)^\top (\theta - \theta^*) \geq 0 \quad \forall \theta \in \Theta$.

$\Rightarrow D\theta(\theta^*)^\top (\theta - \theta^*) = \lim_{t \downarrow 0} \frac{1}{t}(R(\theta^* + t(\theta - \theta^*)) - R(\theta^*)) \geq 0 \quad \forall \theta \in \Theta$. □



Cor Let Θ be a closed convex set in \mathbb{R}^d . Define the projection operator $\Pi_\Theta(\theta) := \arg\min_{\theta' \in \Theta} \|\theta - \theta'\|_2$.

Then, $\|\Pi_\Theta(\theta) - \theta\|_2 \leq \|\theta - \theta'\|_2 \quad \forall \theta' \in \Theta \quad \forall \theta \in \mathbb{R}^d$.

pf) From first order conditions for $\min_{\theta \in \Theta} \|\theta - \theta'\|_2^2$, $0 \leq (\Pi_\Theta(\theta) - \theta)^\top (\theta' - \Pi_\Theta(\theta)) = (\Pi_\Theta(\theta) - \theta)^\top (\theta' - \theta) + (\theta - \theta)^\top (\theta' - \Pi_\Theta(\theta)) = -\|\theta - \Pi_\Theta(\theta)\|_2^2 + (\theta - \theta)^\top (\theta' - \Pi_\Theta(\theta))$.

From Cauchy-Schwarz, $\|\theta - \Pi_\Theta(\theta)\|_2^2 \leq \|\theta - \theta\| \|\theta' - \Pi_\Theta(\theta)\|_2$. □

Stochastic gradients A stochastic gradient $G(\theta)$ is a RV st. $\mathbb{E} G(\theta) = \nabla R(\theta)$.

We study first-order optimization methods based on stoch. gradients.

minimize $\theta \in \mathbb{R}^d \left\{ \mathbb{E} l(\theta; z) = R(\theta) \right\}$

If $\theta \mapsto l(\theta; z)$ is differentiable, then $\nabla_\theta l(\theta; z)$ is a stochastic gradient if $\mathbb{E}, \mathbb{V}_\theta$ can be interchanged.

SGD Iden: Go in the direction of stoch. gradient, then project to Θ .

Algo: let $G_k(\theta)$ be a stoch. gradient of $R(\theta)$.

At each iteration k , $\theta_{k+1} = \Pi_\Theta(\theta_k - \alpha_k G_k(\theta_k))$ for some stepsize $\alpha_k > 0$.

We're implicitly assuming that projections are efficient to compute.

Rmk

We can't even evaluate $\mathbb{E} l(\theta; z)$. So SGD takes samples. In its simplest form, draw $z_k \sim P$, then take $G(\theta_k) := \nabla_\theta l(\theta_k; z_k)$. We could take multiple samples and average over them.

Rmk 2

We could consider ERM $\min_{\theta \in \Theta} \frac{1}{n} \sum_i l(\theta; z_i)$, and think of $\nabla_\theta l(\theta; z_i)$ as a stoch. gradient of the empirical loss. Our following convergence results still apply in this case.

The rationale for SGD wrt. empirical loss is purely computational:

instead of incurring $O(n)$ to evaluate each gradient, I want to compute an approximate gradient in $O(1)$.

Convergence Assume $\theta^* \in \arg\min_{\theta \in \Theta} R(\theta) > -\infty$ exists.

Theorem Let Θ be compact. Assume $\exists R > 0$ s.t. $\sup_{\theta \in \Theta} \|\theta - \theta^*\|_2 \leq R$, $\exists M > 0$ s.t. $\mathbb{E} \|G(\theta)\|_2^2 \leq M^2 \forall \theta \in \Theta$. Let α_k be dec. pos. step sizes, and $\bar{\theta}_k = \frac{1}{k} \sum_{i=1}^k \theta_i$. Then,

$$\mathbb{E}[R(\bar{\theta}_K) - R(\theta^*)] \leq \frac{D^2}{2K\alpha_K} + \frac{1}{2K} \sum_{i=1}^K \alpha_i M^2.$$

Pf) We expand on the error $\|\theta_{k+1} - \theta^*\|_2^2$.

$$\begin{aligned} \frac{1}{2} \|\theta_{k+1} - \theta^*\|_2^2 &= \frac{1}{2} \|\Pi_\Theta(\theta_k - \alpha_k G(\theta_k)) - \theta^*\|_2^2 \\ &\leq \frac{1}{2} \|\theta_k - \alpha_k G(\theta_k) - \theta^*\|_2^2 \quad \text{by non-expansiveness of } \Pi_\Theta \\ &= \frac{1}{2} \|\theta_k - \theta^*\|_2^2 - \alpha_k \langle G(\theta_k), \theta_k - \theta^* \rangle + \frac{\alpha_k^2}{2} \|G(\theta_k)\|_2^2. \end{aligned}$$

Add & subtract $\alpha_k \langle \nabla R(\theta_k), \theta_k - \theta^* \rangle$ to get

$$\begin{aligned} &= \frac{1}{2} \|\theta_k - \theta^*\|_2^2 - \alpha_k \langle \nabla R(\theta_k), \theta_k - \theta^* \rangle + \frac{\alpha_k^2}{2} \|G(\theta_k)\|_2^2 - \alpha_k \langle G(\theta_k) - \nabla R(\theta_k), \theta_k - \theta^* \rangle \\ &\leq \frac{1}{2} \|\theta_k - \theta^*\|_2^2 - \alpha_k (R(\theta_k) - R(\theta^*)) + \frac{\alpha_k^2}{2} \|G(\theta_k)\|_2^2 - \alpha_k \langle G(\theta_k) - \nabla R(\theta_k), \theta_k - \theta^* \rangle \quad \text{by convexity} \end{aligned}$$

Divide each side by α_k , and rearrange

$$R(\theta_k) - R(\theta^*) \leq \frac{1}{2\alpha_k} (\|\theta_k - \theta^*\|_2^2 - \|\theta_{k+1} - \theta^*\|_2^2) + \frac{\alpha_k}{2} \|G(\theta_k)\|_2^2 - \langle G(\theta_k) - \nabla R(\theta_k), \theta_k - \theta^* \rangle \quad \cdots (*)$$

$$\begin{aligned} \text{Now, note that } \sum_{k=1}^K \frac{1}{2\alpha_k} (\|\theta_k - \theta^*\|_2^2 - \|\theta_{k+1} - \theta^*\|_2^2) &= \frac{1}{2\alpha_1} \|\theta_1 - \theta^*\|_2^2 - \frac{1}{2\alpha_K} \|\theta_K - \theta^*\|_2^2 + \sum_{k=2}^K \left(\frac{1}{2\alpha_k} - \frac{1}{2\alpha_{k-1}} \right) \|\theta_k - \theta^*\|_2^2 \\ &\leq \frac{D^2}{2\alpha_1} + \frac{D^2}{2} \sum_{k=2}^K \left(\frac{1}{\alpha_k} - \frac{1}{\alpha_{k-1}} \right) = \frac{D^2}{2\alpha_K}. \end{aligned}$$

So summing both sides of (*),

$$\mathbb{E} \sum R(\theta_k) - R(\theta^*) \leq \frac{D^2}{2\alpha_K} + \frac{1}{2} \sum \alpha_k M^2 - \sum_{k=1}^K \mathbb{E} \langle G(\theta_k) - \nabla R(\theta_k), \theta_k - \theta^* \rangle.$$

Taking expectations on both sides and noting

$$\begin{aligned} \mathbb{E} \langle G(\theta_k) - \nabla R(\theta_k), \theta_k - \theta^* \rangle &= \mathbb{E} \left[\mathbb{E} \left[\langle G(\theta_k) - \nabla R(\theta_k), \theta_k - \theta^* \rangle \mid \theta_k \right] \right] \\ &= \mathbb{E} \left[\langle \mathbb{E} [G(\theta_k) \mid \theta_k] - \nabla R(\theta_k), \theta_k - \theta^* \rangle \right] = 0, \end{aligned}$$

we get $\sum R(\theta_k) - R(\theta^*) \leq \frac{D^2}{2\alpha_K} + \frac{1}{2} \sum \alpha_k M^2$. Noting $R(\bar{\theta}_K) \leq \frac{1}{K} \sum R(\theta_k)$, we get the result. \blacksquare

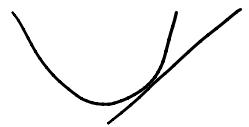
Cor For $\alpha_k = \frac{D}{M\sqrt{k}}$, $\mathbb{E} R(\bar{\theta}_K) - R(\theta^*) \leq \frac{3DM}{2\sqrt{K}}$.

Pf) Noting $\sum_{i=1}^K \frac{1}{\sqrt{i}} \leq \int_1^K \frac{1}{\sqrt{t}} dt = 2\sqrt{K}$, RHS $\leq \frac{DM}{2\sqrt{K}} + \frac{DM}{\sqrt{K}}$. \blacksquare .

Rmk Think of K as # access to gradient oracle. If $G(\theta) = \nabla_\theta l(\theta; z_i)$, then $K = \# \text{ samples}$.

Rmk Often, we iterate through data C times. This gives gains on empirical loss. But population loss-wise, theory doesn't give gains as C grows. In fact, we can't do better. We show this next class.

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R is convex iff $R(\theta') \geq R(\theta) + \nabla R(\theta)^T(\theta' - \theta)$, $\forall \theta, \theta' \in \mathbb{R}^d$

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1st order approx is a global majorization

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Ques

Let Θ be a closed convex set in \mathbb{R}^d .

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(canonical)
problem

$$\text{minimize}_{\theta \in \mathbb{H}} \left\{ \mathbb{E} l(\theta; z) =: R(\theta) \right\}$$

- SGD Iden: Go in the direction of stoch. gradient, then project to \mathbb{H} .
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At each iteration k ,

$$\theta_{k+1} = \Pi_{\mathbb{H}} (\theta_k - \alpha_k G_k(\theta_k)) \quad \text{for some stepsize } \alpha_k > 0.$$

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$$\mathbb{E}[R(\bar{\theta}_k) - R(\theta^*)] \leq \frac{D^2}{2k\alpha_k} + \frac{1}{2k} \sum_1^k \alpha_n M^2.$$

Cor For $\alpha_k = \frac{D}{M\sqrt{k}}$, $\mathbb{E}R(\bar{\theta}_k) - R(\theta^*) \leq \frac{3DM}{2\sqrt{k}}$.

Pf) Noting $\sum_{j=1}^k \frac{1}{j\sqrt{k}} \leq \int_0^k \frac{1}{t\sqrt{k}} dt = 2\sqrt{k}$, RHS $\leq \frac{DM}{2\sqrt{k}} + \frac{DM}{\sqrt{k}}$.