L02 Subgradients and Stochastic Gradient Descent

50.579 Optimization for Machine Learning Ioannis Panageas ISTD, SUTD

Definitions

Definition (Subgradients). Let $f(x) : \mathcal{X} \to \mathbb{R}$ be a function, with $\mathcal{X} \subset \mathbb{R}^d$. $g_x \in \mathbb{R}^d$ is called a subgradient of f at x if for all $y \in \mathcal{X}$ we have

$$f(y) - f(x) \ge g_x^\top (y - x).$$

You can define the set of subgradients at x, we denote it by $\partial f(x)$.

Definitions

Definition (Subgradients). Let $f(x) : \mathcal{X} \to \mathbb{R}$ be a function $g_x \in \mathbb{R}^d$ is called a subgradient of f at x if for all $y \in \mathcal{X}$ we have

$$f(y) - f(x) \ge g_x^\top (y - x).$$

Example: |x|

You can define the set of subgradients at x, we denote it by $\partial f(x)$.

Lemma (Existence and convexity). Let $f : \mathcal{X} \to \mathbb{R}$ be a function such that $\partial f(x) \neq \emptyset$ for all x. It holds that f is convex.

Proof. It holds that there exists a vector g such that

$$f(ty + (1 - t)x) - f(x) \le g^{\top}t(y - x),$$

$$f(ty + (1 - t)x) - f(y) \le g^{\top}(1 - t)(x - y)$$

$$f(ty + (1-t)x) - f(x) \le g^{\top} t(y-x) \quad (1),$$

$$f(ty + (1-t)x) - f(y) \le g^{\top} (1-t)(x-y) \quad (2).$$

$$f(ty + (1-t)x) \le (1-t)f(x) + tf(y).$$

Converse is also true! Application of Supporting Hyperplane Theorem...

$$f(ty + (1-t)x) - f(x) \le g^{\top} t(y-x) \quad (1),$$

$$f(ty + (1-t)x) - f(y) \le g^{\top} (1-t)(x-y) \quad (2).$$

$$f(ty + (1 - t)x) \le (1 - t)f(x) + tf(y).$$

Converse is also true! Application of Supporting Hyperplane Theorem...

Lemma (Local minima are global minima). Let $f : \mathcal{X} \to \mathbb{R}$ be a convex *function. If* x *is a local minimum then it is a global minimum. This happens if and only if* $\mathbf{0} \in \partial f(x)$.

Proof. It is a global minimum if and only if $\mathbf{0} \in \partial f(x)$.

Moreover, for t > 0 small enough,

Hence $f(x) \leq f(y)$.

$$f(x) \le f(tx + (1-t)y) \le tf(x) + (1-t)f(y).$$

Optimization for Machine Learning

Definitions

Definition (Revisited Gradient Descent). Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex function *not necessarily differentiable in some convex set* \mathcal{X} . *GD is defined iteratively:*

 $x_{k+1} = x_k - \alpha g_{x_k}.$

Remarks

- $g_{x_k} \in \partial f(x_k)$ is the subgradient computed at x_k .
- Same guarantees as classic and projected GD.

Theorem (Gradient Descent). Let $f : \mathbb{R}^d \to \mathbb{R}$ be differentiable, convex (want to minimize) and L-Lipschitz. Let $R = ||x_1 - x^*||_2$, the distance between the initial point x_0 and minimizer x^* . It holds for $T = \frac{R^2 L^2}{\epsilon^2}$

$$f\left(\frac{1}{T}\sum_{t=1}^{T}x_t\right) - f(x^*) \leq \epsilon,$$

with appropriately choosing $\alpha = \frac{\epsilon}{L^2}$.

Proof. It holds that

 $f(x_t) - f(x^*) \le g_{x_t}^\top (x_t - x^*)$ def. subgradient,

Proof. It holds that

 $f(x_t) - f(x^*) \le g_{x_t}^\top (x_t - x^*) \text{ def. subgradient,}$ $= \frac{1}{\alpha} (x_t - x_{t+1})^\top (x_t - x^*) \text{ definition of GD,}$

Proof. It holds that

$$f(x_t) - f(x^*) \le g_{x_t}^\top (x_t - x^*) \text{ def. subgradient,} = \frac{1}{\alpha} (x_t - x_{t+1})^\top (x_t - x^*) \text{ definition of GD,} = \frac{1}{2\alpha} \left(\|x_t - x^*\|_2^2 + \|x_t - x_{t+1}\|_2^2 - \|x_{t+1} - x^*\|_2^2 \right) \text{ law of Cosines,}$$

Proof. It holds that

$$f(x_t) - f(x^*) \le g_{x_t}^\top (x_t - x^*) \text{ def. subgradient,}$$

= $\frac{1}{\alpha} (x_t - x_{t+1})^\top (x_t - x^*) \text{ definition of GD,}$
= $\frac{1}{2\alpha} \left(\|x_t - x^*\|_2^2 + \|x_t - x_{t+1}\|_2^2 - \|x_{t+1} - x^*\|_2^2 \right) \text{ law of Cosines,}$
= $\frac{1}{2\alpha} \left(\|x_t - x^*\|_2^2 - \|x_{t+1} - x^*\|_2^2 \right) + \frac{\alpha}{2} \|g_{x_t}\|_2^2 \text{ Def. of GD,}$

Proof. It holds that

 $f(x_{t}) - f(x^{*}) \leq g_{x_{t}}^{\top}(x_{t} - x^{*}) \text{ def. subgradient,}$ $= \frac{1}{\alpha}(x_{t} - x_{t+1})^{\top}(x_{t} - x^{*}) \text{ definition of GD,}$ $= \frac{1}{2\alpha}\left(\|x_{t} - x^{*}\|_{2}^{2} + \|x_{t} - x_{t+1}\|_{2}^{2} - \|x_{t+1} - x^{*}\|_{2}^{2}\right) \text{ law of Cosines,}$ $= \frac{1}{2\alpha}\left(\|x_{t} - x^{*}\|_{2}^{2} - \|x_{t+1} - x^{*}\|_{2}^{2}\right) + \frac{\alpha}{2}\|g_{x_{t}}\|_{2}^{2} \text{ Def. of GD,}$ $\leq \frac{1}{2\alpha}\left(\|x_{t} - x^{*}\|_{2}^{2} - \|x_{t+1} - x^{*}\|_{2}^{2}\right) + \frac{\alpha L^{2}}{2} \text{ Exercise 3.}$

Exercise 3 (General case). Suppose f(x) is L-Lipschitz continous and $\partial f(x) \neq \emptyset$. Then $\forall x \in dom(f)$

$$\|g_x\|_2 \leq L$$
 where $g_x \in \partial f(x)$.

Optimization for Machine Learning

Proof cont. Since

$$f(x_t) - f(x^*) \leq \frac{1}{2\alpha} \left(\|x_t - x^*\|_2^2 - \|x_{t+1} - x^*\|_2^2 \right) + \frac{\alpha L^2}{2},$$

taking the telescopic sum we have

$$\frac{1}{T} \sum_{t=1}^{T} f(x_t) - f(x^*) \le \frac{1}{2\alpha T} (\|x_1 - x^*\|_2^2 - \|x_{t+1} - x^*\|_2^2) + \frac{\alpha L^2}{2}.$$
$$\le \frac{R^2}{2\alpha T} + \frac{\alpha L^2}{2} = \epsilon \text{ by choosing appropriately } \alpha, T.$$

The claim follows by convexity since $\frac{1}{T} \sum_{t=1}^{T} f(x_t) \ge f\left(\frac{1}{T} \sum_{t=1}^{T} f(x_t)\right)$ (Jensen's inequality).

Stochastic Gradient Descent (SGD)

Definition (Stochastic Gradient Descent). Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex (want to minimize). The algorithm below is called stochastic gradient descent

$$x_{k+1} = x_k - \alpha_k v_k,$$

where $\mathbb{E}[v_k|x_k] \in \partial f(x_k)$.

Remarks

- α_k is called the stepsize. Intuitively the smaller, the slower the algorithm.
- α_k must depend on k (vanishing to talk about convergence).
- v_k and moreover x_k are random vectors!

Theorem (Stochastic Gradient Descent). Let $f : \mathbb{R}^d \to \mathbb{R}$ be μ -strongly convex (want to minimize). Moreover assume that $\mathbb{E}[||v_k||^2] \leq \rho^2$. Let x^* be a minimizer. It holds for $\alpha_k = \frac{1}{\mu k}$,

$$\mathbb{E}\left[f\left(\frac{1}{T}\sum_{t}x_{t}\right)\right] - f(x^{*}) \leq \frac{\rho^{2}}{2\mu T}(1 + \log T).$$

Remarks

- α_k scales as $\frac{1}{k}$ and is vanishing to talk about convergence.
- For $T = \Theta\left(\frac{1}{\epsilon}\log\frac{1}{\epsilon}\right)$ we get error ϵ .
- Rakhlin, Shamir & Sridharan (2012) derived a convergence rate in which the log *T* is eliminated for a variant.
- Shamir & Zhang (2013) shown theorem above for last iterate x_T !

Proof of Theorem. Set $\nabla^t = \mathbb{E}[v_t|x_t]$.

From strong convexity we get

$$(x_t - x^*)^\top \nabla^t \ge f(x_t) - f(x^*) + \frac{\mu}{2} ||x_t - x^*||_2^2.$$

Proof of Theorem. Set $\nabla^t = \mathbb{E}[v_t|x_t]$.

From strong convexity we get

$$\mathbb{E}\left[(x_t - x^*)^\top \nabla^t\right] \ge \mathbb{E}\left[f(x_t) - f(x^*) + \frac{\mu}{2} \|x_t - x^*\|_2^2\right].$$

Claim.

$$\mathbb{E}[(x_t - x^*)^\top \nabla^t] \le \frac{\mathbb{E}[\|x_t - x^*\|_2^2 - \|x_{t+1} - x^*\|_2^2]}{2\alpha_t} + \frac{\alpha_t}{2}\rho^2.$$

Proof of Claim. Law of Cosines gives

$$\|x_t - x^*\|_2^2 - \|x_{t+1} - x^*\|_2^2 \ge 2\alpha_t (x_t - x^*)^\top v_t - a_t^2 \|v_t\|_2^2$$

Law of total expectation ... Tower property!

Optimization for Machine Learning

Proof of Cont.

Combining the two above we get (lin. expectation)

$$\mathbb{E}\left[f(x_t) - f(x^*)\right] \le \frac{\mathbb{E}\left[\|x_t - x^*\|_2^2 \left(1 - \alpha_t \mu\right) - \|x_{t+1} - x^*\|_2^2\right]}{2\alpha_t} + \frac{\alpha_t}{2}\rho^2.$$

Proof of Cont.

Combining the two above we get (lin. expectation)

$$\mathbb{E}\left[f(x_t) - f(x^*)\right] \le \frac{\mathbb{E}\left[\|x_t - x^*\|_2^2 \left(1 - \alpha_t \mu\right) - \|x_{t+1} - x^*\|_2^2\right]}{2\alpha_t} + \frac{\alpha_t}{2}\rho^2.$$

Therefore (lin. expectation), recall $a_t = \frac{1}{t\mu}$,

$$\mathbb{E}\left[\frac{1}{T}\sum_{t}f(x_{t})\right] - f(x^{*}) \leq \mathbb{E}\left[-\mu T \left\|x_{T} - x^{*}\right\|_{2}^{2}\right] + \frac{\rho^{2}}{2\mu}\frac{1}{T}\sum_{t}\frac{1}{t}$$

Proof of Cont.

Combining the two above we get (lin. expectation)

$$\mathbb{E}\left[f(x_t) - f(x^*)\right] \le \frac{\mathbb{E}\left[\|x_t - x^*\|_2^2 \left(1 - \alpha_t \mu\right) - \|x_{t+1} - x^*\|_2^2\right]}{2\alpha_t} + \frac{\alpha_t}{2}\rho^2.$$

Therefore (lin. expectation), recall $a_t = \frac{1}{t\mu}$,

$$\mathbb{E}\left[\frac{1}{T}\sum_{t}f(x_{t})\right] - f(x^{*}) \leq \mathbb{E}\left[-\mu T \|x_{T} - x^{*}\|_{2}^{2}\right] + \frac{\rho^{2}}{2\mu}\frac{1}{T}\sum_{t}\frac{1}{t}$$
$$\leq \frac{\rho^{2}}{2\mu}\left(\frac{1 + \log T}{T}\right).$$

Theorem (Stochastic Gradient Descent). Let $f : \mathbb{R}^d \to \mathbb{R}$ be a convex function (want to minimize). Moreover assume that $||v_k||_2 \leq \rho$ with probability one. Let x^* be a minimizer. It holds for $\alpha = \frac{R}{\rho\sqrt{k}}$,

$$\mathbb{E}\left[f\left(\frac{1}{T}\sum_{t}x_{t}\right)\right] - f(x^{*}) \leq \frac{R\rho}{\sqrt{T}}$$

Remarks

- a scales as $\sqrt{\frac{1}{k}}$ and is vanishing to talk about convergence but fixed!
- For $T = \Theta\left(\frac{1}{\epsilon^2}\right)$ we get error ϵ .

Proof. (Recall and add expectation)

 $\mathbb{E}_{1:T} \left[f(x_t) - f(x^*) \right] \le \mathbb{E}_{1:T} \left[(x_t - x^*)^\top \nabla^t \right]$ $= \mathbb{E}_{1:t-1} \left[\mathbb{E}_{1:T} \left[(x_t - x^*)^\top \nabla^t | v_1, ..., v_{t-1} \right] \right]$

Proof. (Recall and add expectation)

$$\begin{split} \mathbb{E}_{1:T} \left[f(x_t) - f(x^*) \right] &\leq \mathbb{E}_{1:T} [(x_t - x^*)^\top \nabla^t] \\ &= \mathbb{E}_{1:t-1} [\mathbb{E}_{1:T} [(x_t - x^*)^\top \nabla^t | v_1, ..., v_{t-1}]] \\ &= \mathbb{E}_{1:T} [(x_t - x^*)]^\top \mathbb{E}_{1:t-1} [\nabla^t | v_1, ..., v_{t-1}] \\ &= \mathbb{E}_{1:T} [(x_t - x^*)]^\top v_t \end{split}$$

Proof. (Recall and add expectation)

$$\begin{split} \mathbb{E}_{1:T} \left[f(x_t) - f(x^*) \right] &\leq \mathbb{E}_{1:T} [(x_t - x^*)^\top \nabla^t] \\ &= \mathbb{E}_{1:t-1} [\mathbb{E}_{1:T} [(x_t - x^*)^\top \nabla^t | v_1, ..., v_{t-1}]] \\ &= \mathbb{E}_{1:T} [(x_t - x^*)]^\top \mathbb{E}_{1:t-1} [\nabla^t | v_1, ..., v_{t-1}] \\ &= \mathbb{E}_{1:T} [(x_t - x^*)]^\top v_t \quad \frac{\operatorname{Recall} \left| |v_t| \right| \leq \rho!}{\operatorname{Recall} \left| |v_t| \right| \leq \rho!} \\ &\leq \mathbb{E}_{1:T} \left[\frac{1}{2\alpha} \left(||x_t - x^*||_2^2 - ||x_{t+1} - x^*||_2^2 \right) \right] + \frac{\alpha \rho^2}{2}. \end{split}$$

Proof. (Recall and add expectation)

$$\begin{split} \mathbb{E}_{1:T} \left[f(x_t) - f(x^*) \right] &\leq \mathbb{E}_{1:T} \left[(x_t - x^*)^\top \nabla^t \right] \\ &= \mathbb{E}_{1:t-1} \left[\mathbb{E}_{1:T} \left[(x_t - x^*)^\top \nabla^t | v_1, ..., v_{t-1} \right] \right] \\ &= \mathbb{E}_{1:T} \left[(x_t - x^*) \right]^\top \mathbb{E}_{1:t-1} \left[\nabla^t | v_1, ..., v_{t-1} \right] \\ &= \mathbb{E}_{1:T} \left[(x_t - x^*) \right]^\top v_t \quad \frac{\operatorname{Recall} \left| |v_t| \right| \leq \rho!}{\leq \mathbb{E}_{1:T} \left[\frac{1}{2\alpha} \left(\|x_t - x^*\|_2^2 - \|x_{t+1} - x^*\|_2^2 \right) \right] + \frac{\alpha \rho^2}{2}. \end{split}$$

Taking the telescopic sum we have

$$\mathbb{E}_{1:T}\left[\frac{1}{T}\sum_{t=1}^{T}f(x_t)-f(x^*)\right] \leq \frac{R^2}{2\alpha T}+\frac{\alpha\rho^2}{2}.$$

Optimization for Machine Learning

Example: Coordinate Descent

Definition (Coordinate Descent). Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex differentiable function in some convex set \mathcal{X} . CD is defined iteratively:

Choose coordinate $i \in [d]$ and update $x_{k+1} = x_k - \alpha_k \frac{\partial f(x_k)}{\partial x_i} \cdot e_i$.

Remarks

- Similar guarantees with GD as long as each coordinate is taken often.
- If coordinate *i* is chosen uniformly at random, then instantiation of ?.

Conclusion

- Introduction to Subgradients and SGD.
 - Same guarantees as for differentiable functions.
 - SGD has rate of convergence $O\left(\frac{1}{\epsilon}\ln\frac{1}{\epsilon}\right)$ for
 - μ -convex.
 - Next Lecture we will see examples related to MLE.
- Next week we will talk about online learning/optimization!