Optimization for Machine Learning
机器学习中的优化方法

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Review: gradient descent

For unconstrained convex optimization, the **gradient descent** method starts with an initial point $\mathbf{x}_0$, and iteratively computes

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \eta_t \nabla f(\mathbf{x}_t).$$

For constrained convex optimization with constraint $\mathcal{C}$, the **projected gradient descent** method starts with an initial point $\mathbf{x}_0$, and iteratively computes

$$\mathbf{x}_{t+1} = \mathcal{P}_{\mathcal{C}}(\mathbf{x}_t - \eta_t \nabla f(\mathbf{x}_t)).$$

Review: convergence rate

condition	constrained	convergence rate	iteration complexity
strongly convex & smooth	no	$O\left(\left(1-\frac{1}{\kappa}\right)^t\right)$	$O(\kappa \log \frac{1}{\varepsilon})$
strongly convex & smooth	yes	$O\left(\left(1-\frac{1}{\kappa}\right)^t\right)$	$O(\kappa \log \frac{1}{\varepsilon})$
convex & smooth	no	$O\left(\frac{1}{t}\right)$	$O\left(\frac{1}{\varepsilon}\right)$
convex & smooth	yes	$O\left(\frac{1}{t}\right)$	$O\left(\frac{1}{\varepsilon}\right)$

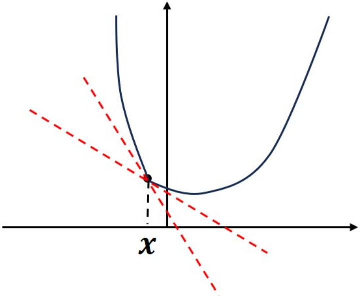
Table: Convergence Properties of GD & PGD

Can we drop the smoothness condition?

Outline

1. Subgradient descent method

Subgradient (次梯度)



We say $\mathbf{g}$ is a subgradient of f at the point $\mathbf{x}$ if

$$f(\mathbf{y}) \geq \underbrace{f(\mathbf{x}) + \langle \mathbf{g}, \mathbf{y} - \mathbf{x} \rangle}_{\text{a linear under-estimate of } f}, \qquad \forall \mathbf{y} \in \mathrm{dom}\ f$$

The set of all subgradients of f at $\mathbf{x}$ is called the subdifferential of f at $\mathbf{x}$, denoted by $\partial f(\mathbf{x})$.

Subgradient descent method (次梯度下降法)

In each iteration, the (projected) subgradient descent method computes

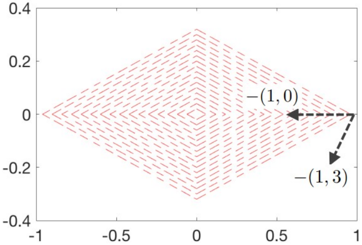
$$\mathbf{x}_{t+1} = \mathcal{P}_{\mathcal{C}}(\mathbf{x}_t - \eta_t \mathbf{g}_t),$$

where $\mathbf{g}_t$ is any subgradient of f at $\mathbf{x}_t$.

Remark: this update rule does NOT necessarily yield reduction w.r.t. the objective values.

Negative subgradients are not necessarily descent directions

Example: $f(\mathbf{x}) = |x_1| + 3|x_2|$



at $\mathbf{x} = (1, 0)$:

- $\mathbf{g}_1 = (1, 0) \in \partial f(\mathbf{x})$, $-\mathbf{g}_1$ is a descent direction;
- $\mathbf{g}_2 = (1, 3) \in \partial f(\mathbf{x})$, $-\mathbf{g}_2$ is not a descent direction.

Negative subgradients are not necessarily descent directions

Since $f(\mathbf{x}_t)$ is not necessarily monotone, we will keep track of the best point

$$f_{best,t} \triangleq \min_{1 \leq i \leq t} f(\mathbf{x}_i)$$

We denote $f^* = \min_{\mathbf{x}} f(\mathbf{x})$ the optimal objective value.

Convex and Lipschitz problems

Clearly, we cannot analyze all nonsmooth functions. Thus we start with Lipschitz continuous functions.

Remember that a function $f : \mathbb{R}^d \to \mathbb{R}$ is G-Lipschitz continuous if for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$, we have

$$|f(\mathbf{x}) - f(\mathbf{y})| \leq G \left\|\mathbf{x} - \mathbf{y}\right\|_2 .$$

f is G-Lipschitz continuous implies that all its subgradients $\mathbf{g}$ is bounded, i.e., $\left\|\mathbf{g}\right\|_2 \leq G$.

Polyak's stepsize

We'd like to optimize $\|\mathbf{x}_{t+1} - \mathbf{x}^*\|_2^2$, but don't have access to $\mathbf{x}^*$

Key idea (majorization-minimization): find another function that majorizes $\|\mathbf{x}_{t+1} - \mathbf{x}^*\|_2^2$, and optimize the majorizing function

Lemma. Projected subgradient update rule obeys

$$\|\mathbf{x}_{t+1} - \mathbf{x}^*\|_2^2 \le \underbrace{\underbrace{\|\mathbf{x}_t - \mathbf{x}^*\|_2^2}_{\textit{fixed}} - 2\eta_t(f(\mathbf{x}_t) - f^*) + \eta_t^2 \|\mathbf{g}_t\|_2^2}_{\textit{majorizing function}} \tag{1}$$

Polyak's Stepsize

The majorizing function in equation (1) suggests a stepsize (Polyak '87)

$$\eta_t = \frac{f(\mathbf{x}_t) - f^*}{\|\mathbf{g}_t\|_2^2}$$

which leads to error reduction

$$\|\mathbf{x}_{t+1} - \mathbf{x}^*\|_2^2 \leq \|\mathbf{x}_t - \mathbf{x}^*\|_2^2 - \frac{(f(\mathbf{x}_t) - f^*)^2}{\|\mathbf{g}_t\|_2^2}$$

- require to know f^*
- the estimation error is monotonically decreasing with Polyak's stepsize

Convergence rate with Polyak's stepsize

Suppose f is convex and G-Lipschitz continuous over $\mathcal{C}$. The projected subgradient descent with Polyak's stepsize obeys

$$f_{best,t} - f^* \leq \frac{G \left\| \mathbf{x}_0 - \mathbf{x}^* \right\|_2}{\sqrt{t+1}}$$

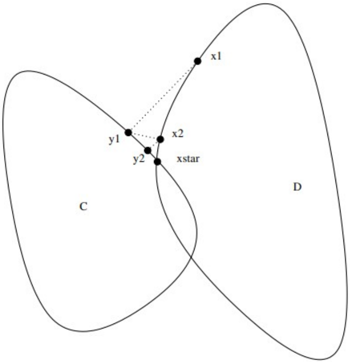
Example: projection onto intersection of convex sets

Let $\mathcal{C}_1$ and $\mathcal{C}_2$ be closed convex sets and suppose $\mathcal{C}_1 \cap \mathcal{C}_2 \neq \emptyset$. We want to find $\mathbf{x} \in \mathcal{C}_1 \cap \mathcal{C}_2$ which is the solution of

$$\min_{\mathbf{x} \in \mathcal{C}_1 \cap \mathcal{C}_2} \max\{dist_{\mathcal{C}_1}(\mathbf{x}), dist_{\mathcal{C}_2}(\mathbf{x})\},$$

where $dist_{\mathcal{C}}(\mathbf{x}) \triangleq \min_{\mathbf{y} \in \mathcal{C}} \|\mathbf{x} - \mathbf{y}\|_2$

Example: projection onto intersection of convex sets



For this problem, the subgradient method with Polyak's stepsize rule is equivalent to alternating projection

$$\mathbf{x}_{t+1} = \mathcal{P}_{\mathcal{C}_1}(\mathbf{x}_t), \qquad \mathbf{x}_{t+2} = \mathcal{P}_{\mathcal{C}_2}(\mathbf{x}_{t+1})$$

Other Stepsize

Suppose f is convex and G-Lipschitz continuous over $\mathcal{C}$. The projected subgradient descent obeys

$$f_{best,t} - f^* \leq \frac{\|\mathbf{x}_0 - \mathbf{x}^*\|_2^2 + \sum_{k=0}^{t} \eta_k^2 \|\mathbf{g}_k\|^2}{2\sum_{k=0}^{t} \eta_k}.$$

Diminishing step size: $\frac{\sum_{t=0}^{T} \eta_t^2}{\sum_{t=0}^{T} \eta_t} \to 0$ as $T \to \infty$

Other Stepsize

Suppose f is convex and G-Lipschitz continuous over $\mathcal{C}$. The projected subgradient descent obeys

$$f_{best,t} - f^* \leq \frac{\|\mathbf{x}_0 - \mathbf{x}^*\|_2^2 + \sum_{k=0}^{t} \eta_k^2 \|\mathbf{g}_k\|^2}{2\sum_{k=0}^{t} \eta_k}.$$

If we choose $\eta_t = \frac{1}{\sqrt{t+1}}$, we get

$$f_{best,t} - f^* \leq \frac{\|\mathbf{x}_0 - \mathbf{x}^*\|_2^2 + G^2(\log(t+1)+1)}{4\sqrt{t+1}}.$$

If we choose $\eta_t = \frac{1}{\sqrt{t+1}\|\mathbf{g}_t\|}$, we get

$$f_{best,t} - f^* \leq \frac{G(\|\mathbf{x}_0 - \mathbf{x}^*\|_2^2 + \log(t+1)+1)}{4\sqrt{t+1}}.$$

Without knowing $f_{best,t}$

Now we consider $\bar{\mathbf{x}}_t = \sum_{k=0}^{t} \frac{\eta_k \mathbf{x}_k}{\sum_{j=0}^{t} \eta_j}$. By Jensen's inequality, we have

$$\begin{aligned}
\sum_{k=0}^{t} \eta_k (f(\mathbf{x}_k) - f^*) &= \left(\sum_{k=0}^{t} \eta_k\right) \left(\sum_{k=0}^{t} \frac{\eta_k}{\sum_{j=0}^{t} \eta_j}\right) (f(\mathbf{x}_k) - f^*) \\
&\geq \left(\sum_{k=0}^{t} \eta_k\right) \left(f\left(\sum_{k=0}^{t} \frac{\eta_k \mathbf{x}_k}{\sum_{j=0}^{t} \eta_j}\right) - f^*\right) \\
&= \left(\sum_{k=0}^{t} \eta_k\right) (f(\bar{\mathbf{x}}_t) - f^*)
\end{aligned}$$

Optimal result

Suppose f is convex and G-Lipschitz continuous over $\mathcal{C}$. Suppose $\mathcal{C}$ is bounded and convex with diameter $D > 0$, i.e., $\|\mathbf{x} - \mathbf{y}\|_2 \geq D$ for any $\mathbf{x}, \mathbf{y} \in \mathcal{C}$. If we choose $\eta_t = \frac{D}{G\sqrt{t+1}}$, we get

$$f(\bar{\mathbf{x}}_t) - f^* \leq \frac{DG}{\sqrt{t+1}},$$

where $\bar{\mathbf{x}}_t = \sum_{k=\lceil \frac{t}{2} \rceil}^{t} \frac{\eta_k \mathbf{x}_k}{\sum_{j=\lceil \frac{t}{2} \rceil}^{t} \eta_j}$ or $\bar{\mathbf{x}}_t = \min_{\lceil \frac{t}{2} \rceil \leq i \leq t} f(\mathbf{x}_i)$.

Strongly convex and Lipschitz problems

Let f be μ-strongly convex and G-Lipschitz continuous over $\mathcal{C}$. If $\eta_t = \frac{2}{\mu(t+1)}$, then the projected subgradient descent obeys

$$f_{best,t} - f^* \leq \frac{2G^2}{\mu(t+1)}.$$

Summary

condition	stepsize	convergence rate	iteration complexity
convex & smooth	$\eta_t = \frac{1}{L}$	$O\left(\frac{1}{t}\right)$	$O\left(\frac{1}{\varepsilon}\right)$
strongly convex & smooth	$\eta_t = \frac{1}{L}$	$O\left(\left(1 - \frac{1}{\kappa}\right)^t\right)$	$O(\kappa \log \frac{1}{\varepsilon})$

Table: Convergence Properties of GD & PGD

	stepsize	convergence rate	iteration complexity
convex	$\eta_t \approx \frac{1}{\sqrt{t}}$	$O\left(\frac{1}{\sqrt{t}}\right)$	$O(\frac{1}{\varepsilon^2})$
strongly convex	$\eta_t \approx \frac{1}{t}$	$O\left(\frac{1}{t}\right)$	$O\left(\frac{1}{\varepsilon}\right)$

Table: Convergence Properties of Subgradient Descent

Questions