Chapter 8: Optimization for Data Science
Projected Gradient Descent

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Constrained Optimization Problems

Constrained minimization problem

$$\min_{x \in \mathcal{X}} f(x) = f(x^*)$$

- $\mathcal{X} \subseteq \mathbb{R}^n$ closed and convex.
- $f : \mathbb{R}^n \to \mathbb{R}$ convex and differentiable

Goal: Find a approximate solution $\in \mathbb{R}^n$ such that

$$f(\tilde{x}) - f(x^*) < \varepsilon$$

- Compute iteratively via projected gradient descent.

Projected Gradient Descent Algorithm

We choose an arbitrary $x_0 \in \mathcal{X}$ and for $t > 0$ define

Projected gradient descent:

$$
\begin{aligned}
y_{t+1} &= x_t - \gamma \nabla f(x_t) \\
x_{t+1} &= \Pi_{\mathcal{X}}(y_{t+1}) = \arg\min_{x \in \mathcal{X}} ||x - y_{t+1}||^2
\end{aligned}
$$

- Projection onto $\mathcal{X}$ ensures $x_t \in \mathcal{X}$ for all $t > 0$.
- Projection is well-defined as $||x - y||^2$ is strongly convex in x.
- Computing $\Pi_{\mathcal{X}}(y_{t+1})$ means to solve an auxiliary convex constrained minimization problem in each step.

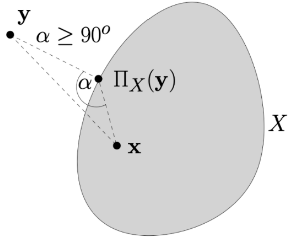
Auxiliary Results on the Projection

Facts: For every $x \in \mathcal{X}, y \in \mathbb{R}^n$

(i) $(x - \Pi_{\mathcal{X}}(y))^T(y - \Pi_{\mathcal{X}}(y)) \leq 0$

(ii) $||x - \Pi_{\mathcal{X}}(y)||^2 + ||y - \Pi_{\mathcal{X}}(y)||^2 \leq ||x - y||^2$

Proof: To show (i), recall that optimization conditions for convex problems state that $\nabla f(x^*)^T(x - x^*) \geq 0, \forall x \in \mathcal{X}$. We now consider $f(x) = ||x - y||^2$ and let $x^* = \min_{x \in \mathcal{X}} f(x) = \Pi_{\mathcal{X}}(y)$. Then (i) follows directly. Assertion (ii) follows from (i) via the equation $2v^T w = ||v||^2 + ||w||^2 - ||v - w||^2$, which holds for any $v, w \in \mathbb{R}^n$.



Bounded Gradients

Theorem (Projected gradient descent for Lipschitz functions:)
Let $f : \mathbb{R}^n \to \mathbb{R}$ be convex, differentiable and $\mathcal{X} \subset \mathbb{R}^n$ closed, convex with global minimum $x^* \in \mathcal{X}$. Suppose that $||x_0 - x^*|| \leq R$ and $||\nabla f(x)|| \leq B, \forall x \in \mathbb{R}^n$. Choosing the step size $\gamma = R/B\sqrt{T}$, the projected gradient descent for $x_0 \in \mathcal{X}$ yields

$$\frac{1}{T}\sum_{t=0}^{T-1}(f(x_t) - f(x^*)) \leq \frac{RB}{\sqrt{T}}$$

Smooth Convex Functions

Lemma (Sufficient decrease): Let $f : \mathbb{R}^n \to \mathbb{R}$ be convex, differentiable, L-smooth and $\mathcal{X} \subset \mathbb{R}^n$ be closed, convex. For $\gamma = 1/L$, projected gradient descent with any $x_0 \in \mathcal{X}$ yields

$$f(x_{t+1}) \leq f(x_t) - \frac{1}{2L}||\nabla f(x_t)||^2 + \frac{L}{2}||y_{t+1} - x_{t+1}||^2, t \geq 0$$

Theorem (Projected gradient descent for smooth functions): Let $f : \mathbb{R}^n \to \mathbb{R}$ be convex, differentiable, L-smooth and $\mathcal{X} \in \mathbb{R}^n$ be closed, convex with global minimum x^*. For $\gamma = 1/L$ and any $x - 0 \in \mathcal{X}$ projected gradient descent yields

$$f(x_T) - f(x^*) \leq \frac{L}{2T}||x_0 - x^*||^2, T > 0$$

Smooth and Strongly Convex Functions

Theorem (Smooth and Strongly Convex Function): Let $f : \mathbb{R}^n \to \mathbb{R}$ be μ-strongly convex, differentiable, L-smooth and $\mathcal{X} \subset \mathbb{R}^n$ be closed, convex with global minimum x^*. For a step size $\gamma = 1/L$ and any $x_0 \in \mathcal{X}$, projected gradient descent yields

(i) $||x_{t+1} - x^*||^2 \leq (1 - \frac{\mu}{L})||x_t - x^*||^2, t \geq 0.$

(ii) $$f(x_T) - f(x^*) \leq ||\nabla f(x^*)||(1 - \tfrac{\mu}{L})^{T/2}||x_0 - x^*||^2 + \frac{L}{2}(1 - \tfrac{\mu}{L})^T||x_0 - x^*||^2, T > 0$$

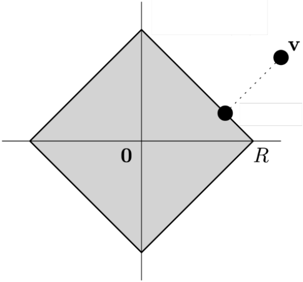
- Recall that $\nabla f(x^*)$ does not necessarily vanish in the constrained case.
- Given again an iteration complexity of $\mathcal{O}(\log(1/\varepsilon))$

Projecting onto l_1 balls

Goal: Compute $\Pi_{\mathcal{X}}(v)$

$$\mathcal{X} = \underbrace{\left\{ x \in \mathbb{R}^n : ||x||_1 = \sum_{i=1}^{d} |x_i| \leq R \right\}}_{=\mathbb{B}_1(R)}$$

- $\mathcal{X}$ is a polytope with 2^n many facets.
- Problem can be simplified in several steps



Fact 1: We can assume without loss of generality that (i) $R = 1$, (ii) $v_i \geq 0$ for all i and (iii) $\sum_{i=1}^{n} v_i > 1$.

Proof of Fact 1

(i) If we project v/R onto $\mathbb{B}_1(1)$, we obtain $\Pi_{\mathcal{X}}(v)/R$, so we can restrict to $R = 1$.

(ii) Observe that simultaneously flipping the signs of a fixed subset of coordinates in both v and $x \in \mathcal{X}$ yields vectors v' and $x' \in \mathcal{X}$ such that $||x - v|| = ||x' - v'||$; thus x minimizes the distance to v if and only if x' minimizes the distance to v'. Hence, it suffices to compute $\Pi_{\mathcal{X}}(v)$ for vectors with nonnegative entries.

(iii) If $\sum_{i=1}^{n} v_i \leq 1$, then $\Pi_{\mathcal{X}}(v) = v$ and there is nothing to compute, so the interesting case is $\sum_{i=1}^{n} v_i > 1$

Projecting onto l_1 balls Cont'd

Fact 2: Under the assumptions of Fact 1, $x = \Pi_{\mathcal{X}}(v)$ satisfies (i) $x_i \geq 0$ for all i and (ii) $\sum_{i=1}^{n} x_i = 1$.

Proof:

(i) Consider $x = \Pi_{\mathcal{X}}(v)$ and suppose $x_i < 0$ for some i. We show this leads to a contradiction and hence $x_i \geq 0$. Suppose $x_i < 0$ for some i, then $(-x_i - v_i) \leq (x_i - v_i)^2$, since $v_i \geq 0$. Therefore, flipping the sign of the $i-$th component of x would yield another vector in $\mathcal{X}$ at least as close to v as x. Since $x = \Pi_{\mathcal{X}}(v)$ and the 2-norm is strictly convex, this is impossible.

(ii) Suppose for the sake of contradiction that $\sum_{i=1}^{n} x_i < 1$, then considering $x' = x + \lambda(v - x) \in \mathcal{X}$ for some small $\lambda > 0$, but then $||x' - v|| = (1 - \lambda)||x - v|| < ||x - v||$, which contradicts the optimality of x. Hence, $x = \Pi_{\mathcal{X}}(v) = \arg\min_{x \in \Delta_n} ||x - v||^2$

Projecting onto l_1 balls Cont'd

Fact 3: We assume without loss of generality that $v_1 \geq \cdots \geq v_n$.

Lemma 1: Let $x^* = \arg\min_{x \in \Delta_n} ||x - v||^2$. Under assumption of Fact 3, there exists a unique $p \in \{1, ..., n\}$ such that

$$\begin{cases} x_i^* > 0, & i \leq p \\ x_i^* = 0, & i > p \end{cases}$$

Proof: We consider the convex function $d_v(z) = ||z - v||^2$ and by the optimality criterion

$$\nabla d_v(x^*)(x - x^*) = 2(x^* - v)^T(x - x^*) \geq 0, x \in \Delta_n \qquad (1)$$

Projecting onto l_1 balls cont'd

Lemma 2: Let $x^* = \arg\min_{x \in \Delta_n} ||x - v||^2$. Under assumption of Fact 3 and with p as in Lemma 1

$$x_i^* = v_i - \theta_p, i \leq p, \quad \text{where} \quad \theta_p = \frac{1}{p}(\sum_{i=1}^{p} v_i - 1)$$

Proof: We argue by contradiction. If not all $x_i^* - v_i$ for $i \leq p$ have the same value $-\theta_p$, then we have $x_i^* - v_i < x_j^* - v_j$ for some $i, j \leq p$. We can decrease x_j^* by some small $\varepsilon > 0$ and simultaneously increase x_i^* by ε to obtain $x \in \Delta_n$ such that

$$(x^* - v)^T(x - x^*) = (0 - v_i)\varepsilon - (x_{i+1}^* - v_{i+1})\varepsilon = \varepsilon(\underbrace{v_{i+1} - v_i}_{\leq 0} - \underbrace{x_{i+1}^*}_{>0}) < 0$$

which contradicts (1). The expression for θ_p is obtained from (con'd next page)

Projecting onto l_1 balls cont'd

$$1 = \sum_{i=1}^{p} x_i^* = \sum_{i=1}^{p} (v_i - \theta_p) = \sum_{i=1}^{p} v_i - p\theta_p \qquad (2)$$

What we have found so far: we have n candidates for x^*, namely the vectors

$$x^*(p) = (v_1 - \theta_p, ..., v_p - \theta_p, 0, ..., 0), \;\; p \in \{1, ..., n\}$$

But which p should we select?

- By Lemma 1, $v_p - \theta_p > 0$
- We could just simply choose p that $||x^*(p) - v||^2$ is minimal
- But there is an even simpler criterion

Projecting onto l_1 balls cont'd

Lemma 3: Under assumption of Fact 3 with $x^*(p)$ as in (2) and

$$p^* = \max\{p \in \{1, ..., n\} : v_p - \frac{1}{p}\left(\sum_{i=1}^{p} v_i - 1\right) > 0$$

it holds that

$$\arg\min_{x \in \Delta_n} ||x - v||^2 = x^*(p^*).$$

This can be computed in $\mathcal{O}(n \log n)$