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

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Review of Gradient Descent

Consider an unconstrained convex optimization problem

$$\min_{\mathbf{x}\in\mathbb{R}^d} \; f(\mathbf{x}).$$

The **gradient descent** method starts with an initial point $\mathbf{x}_0$, and iteratively computes

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

Review of Gradient Descent

	stepsize	convergence rate	iteration complexity
strongly convex & smooth	$\eta_t = \frac{1}{L}$ or $\eta_t = \frac{2}{\mu+L}$	$O\left(\left(1-\frac{1}{\kappa}\right)^t\right)$	$O(\kappa \log \frac{1}{\varepsilon})$
locally strongly convex & smooth	$\eta_t = \frac{1}{L}$	$O\left(\left(1-\frac{1}{\kappa}\right)^t\right)$	$O(\kappa \log \frac{1}{\varepsilon})$
PL condition & smooth	$\eta_t = \frac{1}{L}$	$O\left(\left(1-\frac{1}{\kappa}\right)^t\right)$	$O(\kappa \log \frac{1}{\varepsilon})$
convex & smooth	$\eta_t = \frac{1}{L}$	$O\left(\frac{1}{t}\right)$	$O\left(\frac{1}{\varepsilon}\right)$

Table: Convergence Property of GD

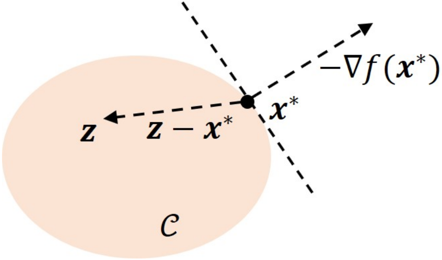
Outline

Constrained convex optimization

Suppose f is a convex function and $\mathcal{C} \in \mathbb{R}^d$ is a closed and convex set. The constrained convex optimization problem is:

$$\min_{\mathbf{x}} \ f(\mathbf{x})$$
$$\text{s.t. } \mathbf{x} \in \mathcal{C}$$

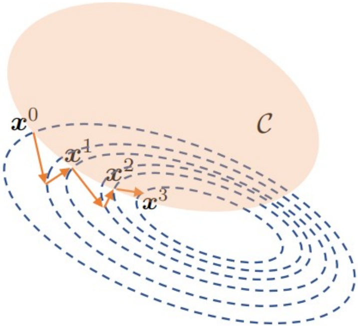
Optimality condition



Suppose f is convex and differentiable, $\mathcal{C}$ is close and convex. Then

$$\mathbf{x}^* \in \arg\min_{\mathbf{x}\in\mathcal{C}} f(\mathbf{x}) \iff \langle -\nabla f(\mathbf{x}^*), \mathbf{z} - \mathbf{x}^* \rangle \leq 0, \ \forall\ \mathbf{z} \in \mathcal{C}$$

Projected gradient descent (投影梯度下降法)



Idea: project onto $\mathcal{C}$ after every gradient descent step:

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

where $\mathcal{P}_{\mathcal{C}}(\mathbf{x}) \triangleq \arg\min_{\mathbf{z}\in\mathcal{C}} \|\mathbf{z} - \mathbf{x}\|_2^2$ is Euclidean projection onto $\mathcal{C}$.

Question

Suppose f is a convex function and $\mathcal{C}$ is a closed convex set. Let

$$\hat{\mathbf{x}} = \arg\min_{\mathbf{x}\in\mathbb{R}^d} \ f(\mathbf{x}) \quad \text{and} \quad \mathbf{x}^* = \arg\min_{\mathbf{x}\in\mathcal{C}} \ f(\mathbf{x})$$

Is it true that

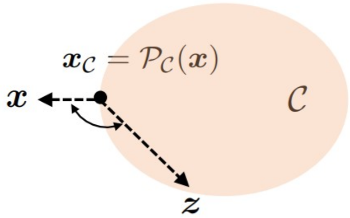
$$\mathbf{x}^* = \mathcal{P}_{\mathcal{C}}(\hat{\mathbf{x}})?$$

The answer is NO!

Counterexample: $f(\mathbf{x}) = x_1^2 + 5x_2^2$, $\mathcal{C} = \{\mathbf{x} | x_1 + x_2 = 1\}$.

We have $\hat{\mathbf{x}} = (0, 0)$, $\mathbf{x}^* = (0.5, 0.5)$, but $f(\hat{\mathbf{x}}) = 1 < f(\mathbf{x}^*) = 1.5$.

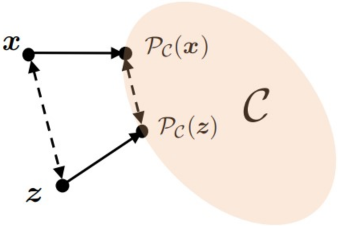
Properties of projection



Let $\mathcal{C} \in \mathbb{R}^d$ be closed and convex, $\mathbf{z} \in \mathcal{C}$, $\mathbf{x} \in \mathbb{R}^d$. Then

- $\langle \mathbf{x} - \mathcal{P}_{\mathcal{C}}(\mathbf{x}), \mathbf{z} - \mathcal{P}_{\mathcal{C}}(\mathbf{x}) \rangle \leq 0$.
- $\|\mathbf{x} - \mathcal{P}_{\mathcal{C}}(\mathbf{x})\|_2^2 + \|\mathbf{z} - \mathcal{P}_{\mathcal{C}}(\mathbf{x})\|_2^2 \leq \|\mathbf{x} - \mathbf{z}\|_2^2$.

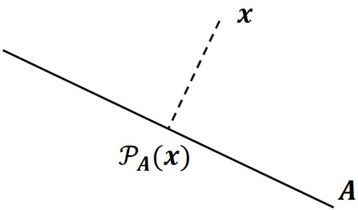
Properties of projection: nonexpansivness



Let $\mathcal{C} \in \mathbb{R}^d$ be closed and convex. For any $\mathbf{x}, \mathbf{z} \in \mathbb{R}^d$, we have

$$\|\mathcal{P}_{\mathcal{C}}(\mathbf{x}) - \mathcal{P}_{\mathcal{C}}(\mathbf{z})\|_2 \leq \|\mathbf{x} - \mathbf{z}\|_2 .$$

Example: affine subspace

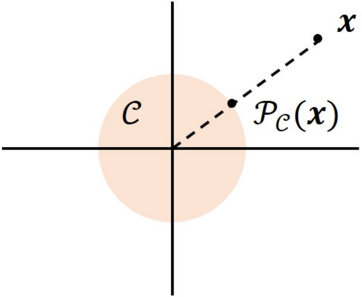


Projecting onto an affine subspace:

$$\mathbf{y} = \arg\min_{\mathbf{z}} \|\mathbf{A}\mathbf{z} - \mathbf{x}\|_2 = (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top \mathbf{x}$$

$$\mathcal{P}_{\mathbf{A}}(\mathbf{x}) = \mathbf{A}\mathbf{y} = \mathbf{A}(\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top \mathbf{x}$$

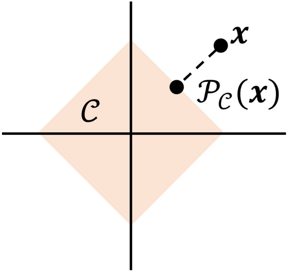
Example: unit Euclidean ball



Projecting onto a unit Euclidean ball (ℓ_2 ball):

$$\mathcal{P}_{\mathcal{C}}(\mathbf{x}) = \arg\min_{\|\mathbf{z}\|_2 \leq 1} \|\mathbf{x} - \mathbf{z}\|_2 = \frac{\mathbf{x}}{\max\{1, \|\mathbf{x}\|_2\}}$$

Example: unit ℓ_1 ball*



Projecting onto a unit ℓ_1 ball:

$$\mathbf{y} = \mathcal{P}_{\mathcal{C}}(\mathbf{x}) = \arg\min_{\|\mathbf{z}\|_1 \leq 1} \|\mathbf{x} - \mathbf{z}\|_2$$

If $\|\mathbf{x}\|_1 \leq 1$ then $\mathcal{P}_{\mathcal{C}}(\mathbf{x}) = \mathbf{x}$. Otherwise,

$$y_i = sign(x_i)(|x_i| - \lambda)_+$$

where $(\cdot)_+ = \max\{\cdot, 0\}$ and λ is the root of $\sum_{i=1}^{n}(|x_i| - \lambda)_+ = 1$.

Smooth and strongly convex constrained problems

$$\min_{\mathbf{x}} \; f(\mathbf{x})$$
$$\text{s.t. } \mathbf{x} \in \mathcal{C}$$

- f: L-smooth and μ-strongly convex
- $\mathcal{C} \in \mathbb{R}^d$: closed and convex

Smooth and strongly convex constrained problems

Let f be L-smooth and μ-strongly convex. If $\eta_t = \eta = \frac{2}{\mu+L}$, then PGD obeys

$$\left\|\mathbf{x}_t - \mathbf{x}^*\right\|_2 \leq \left(\frac{\kappa - 1}{\kappa + 1}\right)^t \left\|\mathbf{x}_0 - \mathbf{x}^*\right\|_2 .$$

the same convergence rate as for the unconstrained case!

Contraction Mapping (压缩映射)

Contraction mapping in Euclidean space: If a function $f : \mathcal{X} \to \mathcal{X}$ satisfies

$$\|f(x) - f(y)\|_2 \leq \gamma \|x - y\|_2 \,, \; \forall \; x, y \in \mathcal{X}$$

for some $\gamma \in (0, 1)$, then we call f is a contraction mapping.

The contraction mapping f has a unique fixed point $\hat{x}$, i.e., $f(\hat{x}) = \hat{x}$.

Convergence analysis

Remember that we have the following inequality

$$\langle \nabla f(\mathbf{x}) - \nabla f(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle \geq \frac{\mu L}{\mu + L} \|\mathbf{x} - \mathbf{y}\|_2^2 + \frac{1}{\mu + L} \|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_2^2.$$

We can show that $h(\mathbf{x}) = \mathcal{P}_{\mathcal{C}}(\mathbf{x} - \eta \nabla f(\mathbf{x}))$ is a contraction mapping with fix point $\hat{\mathbf{x}} = \mathbf{x}^*$ if $\eta = \frac{2}{\mu + L}$.

Smooth and convex constrained problems

$$\min_{\mathbf{x}} \; f(\mathbf{x})$$
$$\text{s.t. } \mathbf{x} \in \mathcal{C}$$

- f: convex and L-smooth
- $\mathcal{C} \in \mathbb{R}^d$: closed and convex

Smooth and convex constrained problems

Let f be convex and L-smooth. If $\eta_t = \eta = \frac{1}{L}$, then PGD obeys

$$f(\mathbf{x}_t) - f(\mathbf{x}^*) \leq \frac{L\|\mathbf{x}_0 - \mathbf{x}^*\|^2}{2t}$$

the same convergence rate as for the unconstrained case

Convergence analysis

Recall the main steps when handling the unconstrained case:

- **Step 1:** show improvement

$$f(\mathbf{x}_{t+1}) \le f(\mathbf{x}_t) - \frac{1}{2L} \|\nabla f(\mathbf{x}_t)\|_2^2 \quad \text{not true for constrained case}$$

- **Step 2:** by convexity,

$$\begin{aligned} f(\mathbf{x}_{t+1}) \le & f(\mathbf{x}^*) - \langle \nabla f(\mathbf{x}_t), \mathbf{x}^* - \mathbf{x}_t \rangle - \frac{1}{2L} \|\nabla f(\mathbf{x}_t)\|_2^2 \\ = & f(\mathbf{x}^*) + \frac{L}{2} \{ \|\mathbf{x}_t - \mathbf{x}^*\|_2^2 - \|\mathbf{x}_{t+1} - \mathbf{x}^*\|_2 \} \end{aligned}$$

- **Step 3:** telescoping

$$f(\mathbf{x}_T) - f(\mathbf{x}^*) \le \frac{1}{T} \sum_{t=0}^{T-1} (f(\mathbf{x}_{t+1}) - f(\mathbf{x}^*)) \le \frac{L}{2T} \|\mathbf{x}_0 - \mathbf{x}^*\|^2$$

Convergence analysis

For the constrained case, we aim to replace $\nabla f(\mathbf{x})$ by

$$g_{\mathcal{C}}(\mathbf{x}) = L(\mathbf{x} - T(\mathbf{x})), \text{ where } T(\mathbf{x}) = \mathcal{P}_{\mathcal{C}}(\mathbf{x} - \frac{1}{L}\nabla f(\mathbf{x})).$$

Then we have $g_{\mathcal{C}}(\mathbf{x}_t) = L(\mathbf{x}_t - \mathbf{x}_{t+1})$.

- **Step 1:** descent guarantee

$$f(\mathbf{x}_{t+1}) \leq f(\mathbf{x}_t) - \frac{1}{2L}\|g_{\mathcal{C}}(\mathbf{x}_t)\|_2^2$$

- **Step 2:**

$$\begin{aligned} f(\mathbf{x}_{t+1}) \leq & f(\mathbf{x}^*) - \langle g_{\mathcal{C}}(\mathbf{x}_t), \mathbf{x}^* - \mathbf{x}_t\rangle - \frac{1}{2L}\|g_{\mathcal{C}}(\mathbf{x}_t)\|_2^2 \\ = & f(\mathbf{x}^*) + \frac{L}{2}\{\|\mathbf{x}_t - \mathbf{x}^*\|_2^2 - \|\mathbf{x}_{t+1} - \mathbf{x}^*\|_2\} \end{aligned}$$

- **Step 3:** telescoping

$$f(\mathbf{x}_T) - f(\mathbf{x}^*) \leq \frac{1}{T}\sum_{t=0}^{T-1}(f(\mathbf{x}_{t+1}) - f(\mathbf{x}^*)) \leq \frac{L}{2T}\|\mathbf{x}_0 - \mathbf{x}^*\|^2$$

Convergence analysis

Lemma. For any $\mathbf{u}, \mathbf{v} \in \mathcal{C}$, we have

$$f(T(\mathbf{u})) - f(\mathbf{v}) \leq \langle g_{\mathcal{C}}(\mathbf{u}), \mathbf{u} - \mathbf{v} \rangle - \frac{1}{2L} \|g_{\mathcal{C}}(\mathbf{u})\|_2^2 .$$

If we choose $\mathbf{u} = \mathbf{v} = \mathbf{x}_t$, we can obtain

$$f(T(\mathbf{x}_t)) - f(\mathbf{x}_t) = f(\mathbf{x}_{t+1}) - f(\mathbf{x}_t) \leq -\frac{1}{2L} \|g_{\mathcal{C}}(\mathbf{x}_t)\|_2^2 .$$

If we choose $\mathbf{u} = \mathbf{x}_t$, $\mathbf{v} = \mathbf{x}^*$, we can obtain

$$\begin{aligned} f(T(\mathbf{x}_t)) - f(\mathbf{x}^*) \leq & \langle g_{\mathcal{C}}(\mathbf{x}_t), \mathbf{x}_t - \mathbf{x}^* \rangle - \frac{1}{2L} \|g_{\mathcal{C}}(\mathbf{x}_t)\|_2^2 \\ = & \frac{L}{2} \left\{ \|\mathbf{x}_t - \mathbf{x}^*\|_2^2 - \|\mathbf{x}_{t+1} - \mathbf{x}^*\|_2^2 \right\} . \end{aligned}$$

Outline

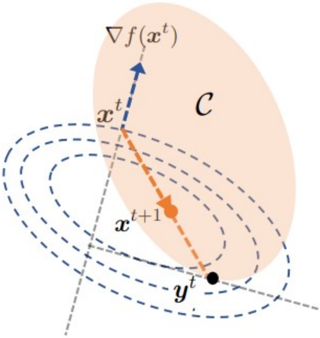
Frank-Wolfe Algorithm

Consider following problem:

$$\min_{\mathbf{x}} \; f(\mathbf{x})$$
$$\text{s.t. } \mathbf{A}\mathbf{x} \leq \mathbf{b}$$

Computing projection is very expensive!

Frank-Wolfe Algorithm



Algorithm 1 Frank-Wolfe (a.k.a. conditional gradient) Algorithm

for $t = 1, 2, \ldots$ **do**

$\mathbf{y}_t = \arg\min_{\mathbf{x}\in\mathcal{C}} \langle \nabla f(\mathbf{x}_t), \mathbf{x} \rangle$ //direction finding

$\mathbf{x}_{t+1} = (1 - \eta_t)\mathbf{x}_t + \eta_t \mathbf{y}_t$ //line search and update

Frank-Wolfe Algorithm

Algorithm 2 Frank-Wolfe (a.k.a. conditional gradient) Algorithm

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for $t = 1, 2, \ldots$ **do**

$\mathbf{y}_t = \arg\min_{\mathbf{x} \in \mathcal{C}} \langle \nabla f(\mathbf{x}_t), \mathbf{x} \rangle$ //direction finding

$\mathbf{x}_{t+1} = (1 - \eta_t)\mathbf{x}_t + \eta_t \mathbf{y}_t$ //line search and update

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- main step: linearization of the objective function
- appealing when linear optimization is much cheaper than projection
- stepsize: $\eta_t = \frac{2}{t+2}$

Frank-Wolfe Algorithm

Let f be convex and L-smooth. If $\eta_t = \frac{2}{t+2}$, one has

$$f(\mathbf{x}_t) - f(\mathbf{x}^*) \leq \frac{2LD^2}{t+2}$$

where $D = \sup_{\mathbf{x},\mathbf{y}\in\mathcal{C}} \|\mathbf{x} - \mathbf{y}\|_2$

For compact constraint sets, Frank-Wolfe attains ε-accuracy with $O(\frac{1}{\varepsilon})$ iterations.

Question

Can we expect to improve convergence guarantees of Frank-Wolfe in the presence of **strong convexity**?

- in general, the answer is NO
- maybe improvable under additional conditions, such as strongly convex feasible set

Summary

Table: Convergence Property of Projected GD

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

Table: Convergence Property of FW

	stepsize	convergence rate	iteration complexity
convex & smooth	$\eta_t = \frac{1}{t}$	$O\left(\frac{1}{t}\right)$	$O\left(\frac{1}{\epsilon}\right)$