annotated version

Optimization for Machine Learning
CS-439

Lecture 4: Projected and Proximal Gradient Descent

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Smooth constrained minimization: $\mathcal{O}(1/\varepsilon)$ steps

Theorem

Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex and differentiable. Let $X \subseteq \mathbb{R}^d$ be a closed convex set, and assume that there is a minimizer $\mathbf{x}^\star$ of f over X; furthermore, suppose that f is L-smooth over X. When choosing the stepsize

$$\gamma := \frac{1}{L},$$

projected gradient descent with $\mathbf{x}_0 \in X$ satisfies:

(i) *Function values are monotone decreasing:* ⇐ Exercise 19

$$f(\mathbf{x}_{t+1}) \leq f(\mathbf{x}_t) - \frac{1}{2L}\|\nabla f(\mathbf{x}_t)\|^2 + \frac{L}{2}\|\mathbf{y}_{t+1} - \mathbf{x}_{t+1}\|^2, \quad t \geq 0.$$

(ii)

$$f(\mathbf{x}_T) - f(\mathbf{x}^\star) \leq \frac{L}{2T}\|\mathbf{x}_0 - \mathbf{x}^\star\|^2, \quad T > 0.$$

Smooth constrained minimization: $\mathcal{O}(1/\varepsilon)$ steps

Notation $x^+ := x_{t+1}$, $x := x_t$

Proof. use smoothness:

$$f(x^+) \le f(x) + \nabla f(x)^\top (x^+ - x) + \frac{L}{2}\|x^+ - x\|^2$$

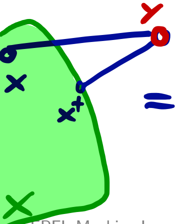
$\gamma = 1/L$

$$= f(x) - L(y - x)^\top (x^+ - x) + \frac{L}{2}\|x^+ - x\|^2$$

$2u^\top v = \|u\|^2 + \|v\|^2 - \|u - v\|^2$

$$= f(x) - \frac{L}{2}\Big(\underbrace{\|y - x\|^2}_{=\|\frac{1}{L}\nabla f(x)\|^2} + \cancel{\|x^+ - x\|^2} - \|y - x^+\|^2\Big) + \cancel{\frac{L}{2}\|x^+ - x\|^2}$$

$$= f(x) - \frac{1}{2L}\|\nabla f(x)\|^2 + \frac{L}{2}\|y - x^+\|^2 \qquad \Rightarrow i)$$



□

For ii): Mimic smooth unconstrained ...

Strongly convex constrained minimization: $\mathcal{O}(\log(1/\varepsilon))$ steps

Theorem

Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex and differentiable. Let $X \subseteq \mathbb{R}^d$ be a closed and convex set and suppose that f is smooth over X with parameter L and strongly convex over X with parameter $\mu > 0$. Choosing

$$\gamma := \frac{1}{L},$$

projected gradient descent with arbitrary $\mathbf{x}_0$ satisfies

(i)

$$\|\mathbf{x}_{t+1} - \mathbf{x}^\star\|^2 \leq \left(1 - \frac{\mu}{L}\right) \|\mathbf{x}_t - \mathbf{x}^\star\|^2, \quad t \geq 0.$$

(ii)

$$f(\mathbf{x}_t) - f(\mathbf{x}^\star) \leq \frac{L}{2} \left(1 - \frac{\mu}{L}\right)^t \|\mathbf{x}_0 - \mathbf{x}^\star\|^2.$$

same as unconstrained

Strongly convex constrained minimization: $\mathcal{O}(\log(1/\varepsilon))$ steps

$y^+ = x - \gamma \nabla f(x)$

Proof.

Strengthen the "constrained" vanilla bound

$f(x^+) - f(x^*) \leq$

$$\frac{1}{2\gamma}\left(\gamma^2\|\nabla f(\mathbf{x}_t)\|^2 + \|\mathbf{x}_t - \mathbf{x}^\star\|^2 - \|\mathbf{x}^+ - \mathbf{x}^\star\|^2 - \|\mathbf{y}^+ - \mathbf{x}^+\|^2\right)$$

to

$$\frac{1}{2\gamma}\left(\gamma^2\|\nabla f(\mathbf{x}_t)\|^2 + \|\mathbf{x}_t - \mathbf{x}^\star\|^2 - \|\mathbf{x}^+ - \mathbf{x}^\star\|^2 - \|\mathbf{y}^+ - \mathbf{x}^+\|^2\right)$$

$$-\frac{\mu}{2}\|\mathbf{x}_t - \mathbf{x}^\star\|^2$$

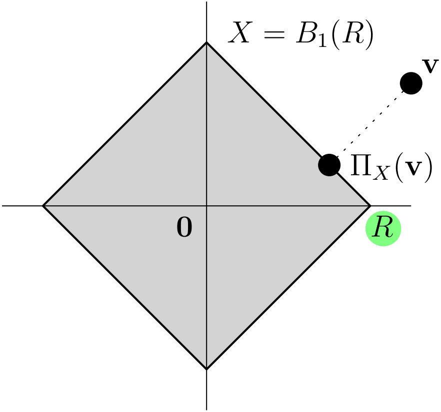
using strong convexity.

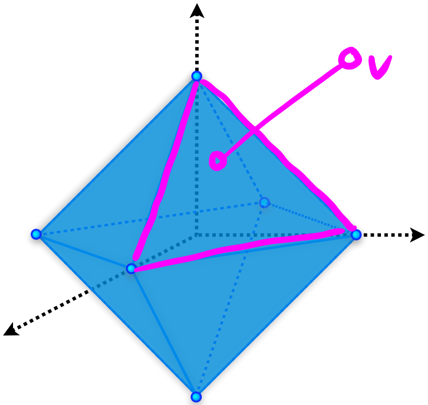
Then proceed as in the unconstrained theorem. □

continue ... use property of projection

Projecting onto ℓ_1-balls

$$X = B_1(R) := \left\{ \mathbf{x} \in \mathbb{R}^d : \|\mathbf{x}\|_1 = \sum_{i=1}^{d} |x_i| \le R \right\}$$





2^d facets!

Projecting onto ℓ_1-balls

→ project onto simplex

$\boxed{\text{w.l.o.g.}}$

- $R = 1$, ✓
- $v_i \geq 0$ for all i, ✓
- $\sum_{i=1}^{d} v_i > 1$. ✓

(*)

And using this,

corollary

$$\mathbf{x} = \Pi_X(\mathbf{v}) \text{ satisfies } \underbrace{x_i \geq 0 \text{ for all } i \text{ and } \sum_{i=1}^{d} x_i = 1}_{\text{simplex, see next}}.$$

proof: $x_i < 0$? No!

could flip sign $x_i \leftarrow -x_i$ (Exercise)

Projecting onto ℓ_1-balls

Corollary

Under our assumption (*),

$$\Pi_X(\mathbf{v}) = \operatorname*{argmin}_{\mathbf{x} \in \Delta_d} \|\mathbf{x} - \mathbf{v}\|^2,$$

where

$$\Delta_d := \left\{ \mathbf{x} \in \mathbb{R}^d : \sum_{i=1}^{d} x_i = 1, x_i \geq 0 \ \forall i \right\}$$

is the standard simplex.

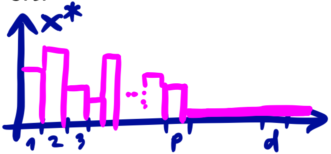
Also, w.l.o.g. assume that v is ordered decreasingly, $v_1 \geq v_2 \geq \cdots \geq v_d$. ≥ 0

Projecting onto ℓ_1-balls

Lemma

Let $\mathbf{x}^\star := \operatorname{argmin}_{\mathbf{x}\in\Delta_d} \|\mathbf{x}-\mathbf{v}\|^2$, *and* $\mathbf{v}$ *ordered decreasingly.*
There exists (a unique) index $p \in \{1,\dots,d\}$ *s.t.*

$$\boxed{\begin{array}{cccl} x_i^\star & > & 0, & i \le p, \\ x_i^\star & = & 0, & i > p. \end{array}}$$

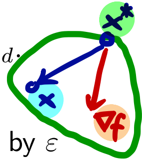


Proof.

$d_{\mathbf{v}}(\mathbf{x}) := \|\mathbf{x}-\mathbf{v}\|^2$

Optimality criterion for constrained optimization:

$$\nabla d_{\mathbf{v}}(\mathbf{x}^\star)^\top(\mathbf{x}-\mathbf{x}^\star) = 2(\mathbf{x}^\star-\mathbf{v})^\top(\mathbf{x}-\mathbf{x}^\star) \ge 0, \quad \forall \mathbf{x} \in \Delta_d.$$

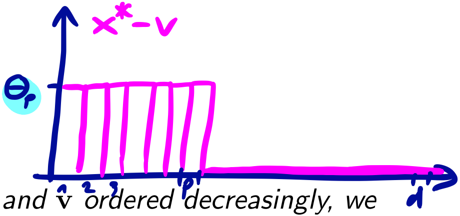


$\exists$ a positive entry in $\mathbf{x}^\star$ (because $\sum_{i=1}^d x_i^\star = 1$).
Why not $x_i^\star = 0$ and $x_{i+1}^\star > 0$? If so, we could decrease $x_{i+1}^\star$ by ε and increase $x_i^\star$ to ε to obtain $\mathbf{x} \in \Delta_d$ s.t.

$$(\mathbf{x}^\star-\mathbf{v})^\top(\mathbf{x}-\mathbf{x}^\star) = (0-v_i)\varepsilon-(x_{i+1}^\star-v_{i+1})\varepsilon = \varepsilon(\underbrace{v_{i+1}-v_i}_{\le 0} - \underbrace{x_{i+1}^\star}_{>0}) < 0,$$

contradicting the optimality. □

Projecting onto ℓ_1-balls



Can say more about $\mathbf{x}^\star$:

Lemma

With p as in the above Lemma, and $\mathbf{v}$ ordered decreasingly, we have

$$x_i^\star = v_i - \Theta_p, \quad i \le p,$$

constant!

where

$$\Theta_p = \frac{1}{p}\Big(\sum_{i=1}^{p} v_i - 1\Big).$$

Proof.

Assume there is $i, j \le p$ with $x_i^\star - v_i \overset{\neq}{<} x_j^\star - v_j$. As before, we could decrease $x_j^\star > 0$ by ε and increase $x_i^\star$ by ε to get $\mathbf{x} \in \Delta_d$ s.t.

$$\underbrace{(\mathbf{x}^\star - \mathbf{v})}_{\nabla d_{\mathbf{v}}}{}^\top(\mathbf{x} - \mathbf{x}^\star) = (x_i^\star - v_i)\varepsilon - (x_j^\star - v_j)\varepsilon = \varepsilon\underbrace{\big((x_i^\star - v_i) - (x_j^\star - v_j)\big)}_{<0} < 0,$$

again contradicting optimality of $\mathbf{x}^\star$. □

Projecting onto ℓ_1-balls

Summary: have d candidates for $\mathbf{x}^\star$, namely

$$\mathbf{x}^\star(p) := (v_1 - \Theta_p, \ldots, v_p - \Theta_p, 0, \ldots, 0), \quad p \in \{1, \ldots, d\},$$

Need to find the right one. In order for candidate $\mathbf{x}^\star(p)$ to comply with our first Lemma, we must have

$$\boxed{v_p - \Theta_p > 0,}$$

and this actually ensures $\mathbf{x}^\star(p)_i > 0$ for all $i \le p$ (because $\mathbf{v}$ is ordered) and therefore $\mathbf{x}^\star(p) \in \Delta_d$.

But there could still be several choices for p. Among them, we simply pick the one for which $\mathbf{x}^\star(p)$ minimizes the distance to $\mathbf{v}$.

In time $\mathcal{O}(d \log d)$, by first sorting v and checking incrementally.

Projecting onto ℓ_1-balls

Theorem

Let $\mathbf{v} \in \mathbb{R}^d$, $R \in \mathbb{R}_+$, $X = B_1(R)$ the ℓ_1-ball around $\mathbf{0}$ of radius R. The projection

$$\Pi_X(\mathbf{v}) = \operatorname*{argmin}_{\mathbf{x} \in X} \|\mathbf{x} - \mathbf{v}\|^2$$

of $\mathbf{v}$ onto $B_1(R)$ can be computed in time $\mathcal{O}(d \log d)$.

This can be improved to time $\mathcal{O}(d)$ by avoiding sorting.

Section 3.6

Proximal Gradient Descent

Composite optimization problems

„composite objective function"

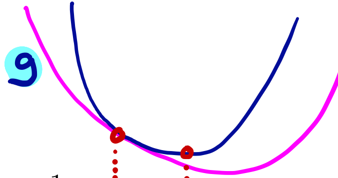
Consider objective functions composed as

$$f(\mathbf{x}) := g(\mathbf{x}) + h(\mathbf{x})$$

where g is a "nice" function, where as h is a "simple" additional term, which however doesn't satisfy the assumptions of niceness which we used in the convergence analysis so far.

In particular, an important case is when h is not differentiable.

Idea



From unconstrained minimization

The classical gradient step for minimizing g:

$$\mathbf{x}_{t+1} = \underset{\mathbf{y}}{\operatorname{argmin}}\ g(\mathbf{x}_t) + \nabla g(\mathbf{x}_t)^\top(\mathbf{y} - \mathbf{x}_t) + \frac{1}{2\gamma}\|\mathbf{y} - \mathbf{x}_t\|^2 .$$

For the stepsize $\gamma := \frac{1}{L}$ it exactly minimizes the local quadratic model of g at our current iterate $\mathbf{x}_t$, formed by the smoothness property with parameter L.

Now for $f = g + h$, keep the same for g, and add h unmodified.

$$\begin{aligned}\mathbf{x}_{t+1} &:= \underset{\mathbf{y}}{\operatorname{argmin}}\ g(\mathbf{x}_t) + \nabla g(\mathbf{x}_t)^\top(\mathbf{y} - \mathbf{x}_t) + \frac{1}{2\gamma}\|\mathbf{y} - \mathbf{x}_t\|^2 + h(\mathbf{y}) \\ &= \underset{\mathbf{y}}{\operatorname{argmin}}\ \frac{1}{2\gamma}\|\mathbf{y} - (\mathbf{x}_t - \gamma\nabla g(\mathbf{x}_t))\|^2 + h(\mathbf{y}) ,\end{aligned}$$

the proximal gradient descent update.

The proximal gradient descent algorithm

An iteration of proximal gradient descent is defined as

$$\mathbf{x}_{t+1} := \mathrm{prox}_{h,\gamma}(\mathbf{x}_t - \gamma \nabla g(\mathbf{x}_t)) \ .$$

where the proximal mapping for a given function h, and parameter $\gamma > 0$ is defined as

$$\mathrm{prox}_{h,\gamma}(\mathbf{z}) := \underset{\mathbf{y}}{\operatorname{argmin}} \left\{ \frac{1}{2\gamma} \|\mathbf{y} - \mathbf{z}\|^2 + h(\mathbf{y}) \right\} \ .$$

The update step can be equivalently written as

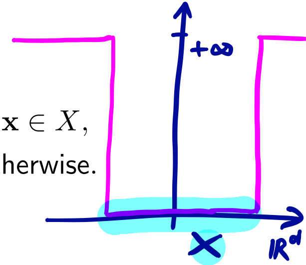
$$\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma G_\gamma(\mathbf{x}_t)$$

for $G_{h,\gamma}(\mathbf{x}) := \frac{1}{\gamma}\Big(\mathbf{x} - \mathrm{prox}_{h,\gamma}(\mathbf{x} - \gamma \nabla g(\mathbf{x}))\Big)$ being the so called generalized gradient of f.

A generalization of gradient descent?

- $h \equiv 0$: recover gradient descent
- $h \equiv \iota_X$: recover projected gradient descent!

  Given a closed convex set X, the indicator function of the set X is given as the convex function



$$\iota_X : \mathbb{R}^d \to \mathbb{R} \cup +\infty$$

$$\mathbf{x} \mapsto \iota_X(\mathbf{x}) := \begin{cases} 0 & \text{if } \mathbf{x} \in X, \\ +\infty & \text{otherwise.} \end{cases}$$

  Proximal mapping becomes

$$\operatorname{prox}_{h,\gamma}(\mathbf{z}) := \operatorname*{argmin}_{\mathbf{y}} \left\{ \frac{1}{2\gamma} \|\mathbf{y}-\mathbf{z}\|^2 + \iota_X(\mathbf{y}) \right\} = \operatorname*{argmin}_{\mathbf{y} \in X} \|\mathbf{y}-\mathbf{z}\|^2$$

projection! $= \Pi_X(z)$

Convergence in $\mathcal{O}(1/\varepsilon)$ steps

Same as vanilla case for smooth functions, but now for any h for which we can compute the proximal mapping.

<u>Examples</u>:

- $h(x) = \lambda \|x\|_1$
  prox is soft-thresholding operator.
- $h(x) = \mathbb{1}_{B_1(R)}$
  prox is projection onto ℓ_1-ball.