Labs

Optimization for Machine LearningSpring 2022

EPFL

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github.com/epfml/OptML_course

Problem Set 2 — Solutions (Gradient Descent)

Gradient Descent

Exercise 6. Consider the function ℓ defined in (1.13). Prove that ℓ is convex!

Solution: It suffices to show that the function $-\ln z_j(\mathbf{y})$ is convex for all j, with z_j as in (1.12). Using Lemma 1.18 (i) and (ii), it then follows that ℓ is convex. We compute

$$-\ln z_i(\mathbf{y}) = \ln (e^{y_0} + \dots + e^{y_9}) - y_i.$$

The first summand is a *log-sum-exp* function and is convex (a proof goes via the Hessian [?, 3.1.5]). The second summand is a linear function and therefore also convex. Hence the sum is convex by Lemma 1.18 (i).

Exercise 7. Consider the logistic regression problem with two classes. Given a training set P consisting of datapoint and label pairs (\mathbf{x},y) where $\mathbf{x} \in \mathbb{R}^d$ and $y \in \{-1,+1\}$, we define our loss ℓ for weight vector $\mathbf{w} \in \mathbb{R}^d$ to be

$$\ell(\mathbf{w}) = \sum_{(\mathbf{x}, y) \in P} -\ln \left(z(y\mathbf{w}^{\top}\mathbf{x}) \right) ,$$

where $z(s) = 1/(1 + \exp(-s))$. This loss function is in fact a simplification of (1.13) when we only have two classes.

We say that the weight vector \mathbf{w} is a separator for P if for all $(\mathbf{x}, y) \in P$,

$$y(\mathbf{w}^{\top}\mathbf{x}) > 0$$
.

A separator is said to be trivial if for all $(\mathbf{x}, y) \in P$,

$$y(\mathbf{w}^{\top}\mathbf{x}) = 0$$
.

For example $\mathbf{w}=0$ is a trivial separator. Depending on the data P, there may be other trivial separators. Prove the following statement: the function ℓ has a global minimum if and only if all separators are trivial.

Solution:

Left to right implication. First we show that if \mathbf{w}' is a nontrivial separator, then for every \mathbf{w} , $\ell(\mathbf{w} + \lambda \mathbf{w}') < \ell(\mathbf{w})$ for all $\lambda > 0$. So if there exists a nontrivial separator, we can always decrease the value of ℓ and hence ℓ cannot have a global minimum.

Fix some $\mathbf{w} \in \mathbb{R}^d$, some number $\lambda > 0$ and some nontrivial separator \mathbf{w}' . By definition of a nontrivial separator, there exists some $(\mathbf{x}_0, y_0) \in P$ such that $y_0(\mathbf{w}'^\top \mathbf{x}_0) > 0$ and $(\mathbf{w}'^\top \mathbf{x})y \geq 0$ for all $(\mathbf{x}, y) \in P$. We get:

$$\ell(\mathbf{w} + \lambda \mathbf{w}') =$$

$$= \sum_{(\mathbf{x}, y) \in P} \ln \left(1 + \exp \left(-y \left(\mathbf{w} + \lambda \mathbf{w}' \right)^{\top} \mathbf{x} \right) \right)$$

$$= \sum_{(\mathbf{x}, y) \in P} \ln \left(1 + \exp \left(-y \mathbf{w}^{\top} \mathbf{x} - \lambda y \mathbf{w}'^{\top} \mathbf{x} \right) \right)$$

$$= \sum_{(\mathbf{x}, y) \in P} \ln \left(1 + \exp \left(-y \mathbf{w}^{\top} \mathbf{x} \right) \exp \left(-\lambda y \mathbf{w}'^{\top} \mathbf{x} \right) \right)$$

$$< \sum_{(\mathbf{x}, y) \in P} \ln \left(1 + \exp \left(-y \mathbf{w}^{\top} \mathbf{x} \right) = \ell(\mathbf{w}).$$

To see why the last inequality is true, observe that $-y(\mathbf{w}'^{\top}\mathbf{x}) \leq 0$ and that both \exp and \ln are increasing functions. The inequality is strict for $\lambda > 0$ because there exists a term in the summation such that $-\lambda y_0(\mathbf{w}'^{\top}\mathbf{x}_0) < 0$.

Right to left implication. Now let us prove that if all separators are trivial, then ℓ has a global minimum. Note that a separator $\mathbf{w}' \neq 0$ is trivial only if \mathbf{w}' is orthogonal to all datapoints \mathbf{x} . For any such trivial separator \mathbf{w}' , $\mathbf{w} \in \mathbb{R}^d$ and $\lambda \in \mathbb{R}$, the loss value $\ell(\mathbf{w} + \lambda \mathbf{w}') = \ell(\mathbf{w})$:

$$\ell(\mathbf{w} + \lambda \mathbf{w}') =$$

$$= \sum_{(\mathbf{x}, y) \in P} \ln \left(1 + \exp \left(-y \left(\mathbf{w} + \lambda \mathbf{w}' \right)^{\top} \mathbf{x} \right) \right)$$

$$= \sum_{(\mathbf{x}, y) \in P} \ln \left(1 + \exp \left(-y \mathbf{w}^{\top} \mathbf{x} - \lambda y \mathbf{w}'^{\top} \mathbf{x} \right) \right)$$

$$= \sum_{(\mathbf{x}, y) \in P} \ln \left(1 + \exp \left(-y \mathbf{w}^{\top} \mathbf{x} \right) \right) = \ell(\mathbf{w}).$$

Let $V = \operatorname{span}(x_1, \dots, x_n)$ be the linear span of the datapoints. We therefore have that V^{\perp} is exactly the set of trivial separators of P. Since every vector $\mathbf{w} \in \mathbb{R}^d$ can be decomposed as $\mathbf{w} = \mathbf{v} + \mathbf{u}$, where $\mathbf{v} \in V$, $\mathbf{u} \in V^{\perp}$, the previously proved property means that $\ell(\mathbf{w}) = \ell(\mathbf{v} + \mathbf{u}) = \ell(\mathbf{v})$ and this means that

$$\inf_{\mathbf{w} \in \mathbb{R}^d} \ell(\mathbf{w}) = \inf_{\mathbf{w} \in \operatorname{span}(x_1, \dots, x_n)} \ell(\mathbf{w}).$$

Thus without loss of generality, we can restrict ourselves to weight vectors in V. Now we define the following sublevel set A:

$$A = \{ \mathbf{w} \in V : \ell(\mathbf{w}) \le |P| \ln(2) \}.$$

A is non-empty since $\ell(0) = |P| \ln(2)$. Hence if we show that A is bounded, then we can use Theorem 1.29 to finish the proof and show that ℓ has a global minimum on V and hence on \mathbb{R}^d .

To see that A is indeed bounded we proceed by contradiction. Assume that A is not bounded, then we can construct a sequence of points $(w_n)_{n\geq 0}\in A$ such that $\|w_n\|\to\infty$. Note that the sequence $\frac{w_n}{\|w_n\|}$ lives in the compact (closed and bounded in finite dimension) set $S=\{v\in V:\|v\|=1\}$, hence there exists a subsequence such that $\frac{w_{\phi(n)}}{\|w_{\phi(n)}\|}\underset{n\to+\infty}{\longrightarrow} d$ where $d\in S$. Since $d\in \mathrm{span}(x_1,\ldots,x_n)$ and is not 0,d cannot be a trivial separator, by assumption it therefore cannot be a separator. Hence there must exist $(\mathbf{x}_0,y_0)\in P$ such that $y_0d^{\top}\mathbf{x}_0=-a<0$, where a>0. Therefore $y_0\frac{1}{\|w_{\phi(n)}\|}w_{\phi(n)}^{\top}\mathbf{x}_0\underset{n\to+\infty}{\longrightarrow} -a$ and for n big enough, $y_0w_{\phi(n)}^{\top}\mathbf{x}_0<-\frac{a}{2}\|w_{\phi(n)}\|$ and:

$$\ell(\mathbf{w}_{\phi(n)}) = \sum_{(\mathbf{x}, y) \in P} \ln\left(1 + \exp\left(-y\mathbf{w}_{\phi(n)}^{\top}\mathbf{x}\right)\right)$$

$$\geq \ln\left(1 + \exp\left(-y_0\mathbf{w}_{\phi(n)}^{\top}\mathbf{x}_0\right)\right)$$

$$\geq \ln\left(1 + \exp\left(\frac{a}{2}\|w_{\phi(n)}\|\right)\right) \underset{n \to \infty}{\longrightarrow} +\infty$$

This is contradictory because the w_n 's are in A and the $\ell(w_n)$'s must therefore be bounded. Thus, the set A cannot be unbounded and this concludes the proof.

Exercise 11. Suppose that we have centered observations (\mathbf{x}_i, y_i) such that $\sum_{i=1}^n \mathbf{x}_i = \mathbf{0}, \sum_{i=1}^n y_i = 0$. Let $w_0^{\star}, \mathbf{w}^{\star}$ be the global minimum of the least squares objective

$$f(w_0, \mathbf{w}) = \sum_{i=1}^n (w_0 + \mathbf{w}^T \mathbf{x}_i - y_i)^2.$$

Prove that $w_0^{\star} = 0$. Also, suppose \mathbf{x}_i' and y_i' are such that for all i, $\mathbf{x}_i' = \mathbf{x}_i + \mathbf{q}$, $y_i' = y_i + r$. Show that (w_0, \mathbf{w}) minimizes f if and only if $(w_0 - \mathbf{w}^{\top} \mathbf{q} + r, \mathbf{w})$ minimizes

$$f'(w_o, \mathbf{w}) = \sum_{i=1}^n (w_0 + \mathbf{w}^T \mathbf{x}_i' - y_i')^2.$$

Solution: We compute

$$\frac{\partial f(w_0, \mathbf{w})}{\partial w_0} = 2 \sum_{i=1}^n (w_0 + \mathbf{w}^\top \mathbf{x}_i - y_i) = 2 \sum_{i=1}^n w_0 = 2nw_0.$$

since the observations are centered. Also, by the first-order characterization of optimality as by Lemma 1.22,

$$0 = \frac{\partial f(w_0, \mathbf{w})}{\partial w_0} \Big|_{w_0 = w_0^{\star}, \mathbf{w} = \mathbf{w}^{\star}} = 2nw_0^{\star}.$$

The second part follows from

$$f'(w_o - \mathbf{w}^{\top} \mathbf{q} + r, \mathbf{w}) = \sum_{i=1}^{n} (w_0 - \mathbf{w}^{\top} \mathbf{q} + r + \mathbf{w}^{T} \mathbf{x}_i' - y_i')^2$$

$$= \sum_{i=1}^{n} (w_0 - \mathbf{w}^{\top} \mathbf{q} + r + \mathbf{w}^{T} (\mathbf{x}_i + \mathbf{q}) - (y_i + r))^2$$

$$= \sum_{i=1}^{n} (w_0 + \mathbf{w}^{T} \mathbf{x}_i - y_i)^2 = f(w_0, \mathbf{w}).$$

Exercise 14. Prove Lemma 2.4: The quadratic function $f(\mathbf{x}) = \mathbf{x}^{\top} Q \mathbf{x} + \mathbf{b}^{\top} \mathbf{x} + c$ is smooth with parameter $2 \|Q\|$.

Solution: Note that we do not assume that Q is a positive matrix, hence f is not necessarily convex (note that the notion of smoothness is valid for any differentiable function). Straightforward computations lead to $\nabla^2 f(x) = 2Q$ for all $x \in \mathbb{R}^d$. Hence, trivially, $\|\nabla^2 f(x)\| \le 2\|Q\|$ for all $x \in \mathbb{R}^d$. Hence using Theorem 1.9, we have that ∇f is $2\|Q\|$ -Lipschitz. To conclude we use implication (ii) \Rightarrow (i) in Lemma 2.5 (note that, as explained in the lecture notes, we do not need any convexity assumption for this implication). This shows that f is smooth with parameter $2\|Q\|$.