Labs

Optimization for Machine LearningSpring 2020

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github.com/epfml/OptML_course

Problem Set 2 — Solutions (Gradient Descent)

Gradient Descent

Exercise 5. Consider the function ℓ defined in (1.11). 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 (1.10). Using Lemma 1.13 (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 therefore convex (a proof goes via the Hessian [BV04, 3.1.5]). The second summand is a linear function and therefore also convex. Hence the sum is convex by Lemma 1.13 (i).

Exercise 6. 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 (1.11) when we only have two classes.

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

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

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:

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 $-\lambda y_0(\mathbf{w}'^{\top}\mathbf{x}_0) < 0$.

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 W' be the set of all such trivial separators of P. We just showed that

$$\inf_{\mathbf{w} \in \mathbb{R}^d} \ell(\mathbf{w}) = \inf_{\mathbf{w} \perp W'} \ell(\mathbf{w}).$$

Thus without loss of generality, we can restrict ourselves to weight vectors $\mathbf{w} \perp W'$. Now define the sublevel set of $\mathbf{w}_0 = 0$ with $\ell(0) = |P| \ln(2)$:

$$\tilde{W} = \{ \mathbf{w} \perp W' : \ell(\mathbf{w}) \le |P| \ln(2) \}.$$

If we show that \tilde{W} is bounded, we can appeal to Theorem 1.24 to finish the proof that ℓ has a global minimum. To see that \tilde{W} is indeed bounded, consider any fixed $\mathbf{w} \in \tilde{W}$. Since \mathbf{w} is not a separator, there exists $(\mathbf{x}_0, y_0) \in P$ such that $y_0 \mathbf{w}^{\top} \mathbf{x}_0 < 0$. Then

$$\lim_{\lambda \to \infty} \ell(\lambda \mathbf{w}) =$$

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

$$\geq \lim_{\lambda \to \infty} \ln \left(1 + \exp \left(-\lambda y_0 \mathbf{w}^{\top} \mathbf{x}_0 \right) \right) = \infty.$$

The last equality is true since $-y_0\mathbf{w}^{\top}\mathbf{x}_0 > 0$. This shows that for a large enough λ , $\ell(\lambda\mathbf{w}) > |P|\ln(2)$ and so $\lambda\mathbf{w} \notin \tilde{W}$. Thus, the set \tilde{W} cannot be unbounded.

Exercise 9. 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 1.17,

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

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 11. Prove Lemma 2.3: 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: As the function $\mathbf{x} \mapsto \mathbf{b}^{\top} \mathbf{x} + c$ is affine and hence smooth with parameter 0, it suffices by Lemma 2.5 to restrict ourselves to the case $f(\mathbf{x}) := \mathbf{x}^{\top} Q \mathbf{x}$.

Because Q is symmetric, $\mathbf{x}^{\top}Q\mathbf{y} = \mathbf{y}^{\top}Q\mathbf{x}$ for any \mathbf{x} and \mathbf{y} . Thus, a simple calculation shows that

$$f(\mathbf{y}) = \mathbf{y}^{\top} Q \mathbf{y} = \mathbf{x}^{\top} Q \mathbf{x} + 2 \mathbf{x}^{\top} Q (\mathbf{y} - \mathbf{x}) + (\mathbf{x} - \mathbf{y})^{\top} Q (\mathbf{x} - \mathbf{y})$$
$$= f(\mathbf{x}) + 2 \mathbf{x}^{\top} Q (\mathbf{y} - \mathbf{x}) + (\mathbf{x} - \mathbf{y})^{\top} Q (\mathbf{x} - \mathbf{y}).$$

Cauchy-Schwarz for $(\mathbf{x} - \mathbf{y})^{\top} Q(\mathbf{x} - \mathbf{y}) \leq \|\mathbf{x} - \mathbf{y}\| \|Q(\mathbf{x} - \mathbf{y})\|$, and using and the definition of spectral norm for $\|Q(\mathbf{x} - \mathbf{y})\| \leq \|Q\| \|\mathbf{x} - \mathbf{y}\|$ we get

$$f(\mathbf{y}) \le f(\mathbf{x}) + 2\mathbf{x}^{\top} Q(\mathbf{y} - \mathbf{x}) + ||Q|| ||\mathbf{x} - \mathbf{y}||^2$$

Because $||x-y||^2$ vanishes as (x-y) goes to 0, differentiability of f (Definition 1.7) implies that $\nabla f(\mathbf{x})^{\top} = 2\mathbf{x}^{\top}Q$, so we further get

$$f(\mathbf{y}) \leq f(\mathbf{x}) + \nabla f(\mathbf{x})(\mathbf{y} - \mathbf{x}) + \frac{2 \|Q\|}{2} \left\|\mathbf{x} - \mathbf{y}\right\|^2,$$

That is, f is smooth with parameter $2 \|Q\|$.

References

[BV04] Stephen Boyd and Lieven Vandenberghe. *Convex Optimization*. Cambridge University Press, New York, NY, USA, 2004. https://web.stanford.edu/~boyd/cvxbook/.