Theory problems
Machine Learning Course
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Problem Set 7, Nov 2, 2017 (Solutions to Theory Questions)

1 Convexity

1. We need to check that

$$f(\theta x + (1-\theta)y) \leq \theta f(x) + (1-\theta)f(y)$$

for all $x, y \in \mathbb{R}$ and $\theta \in [0,1]$. Since the function is linear, we get an equality and the expression is equal to

$$a(\theta x + (1-\theta)y) = b.$$

2. For any elements x, y in the common fixed domain we have that

$$\begin{aligned} g(\theta x + (1-\theta)y)) &= \sum_i f_i(\theta x + (1-\theta)y) \\ &\leq \sum_i [\theta f_i(x) + (1-\theta)f_i(y)] \\ &= \theta \sum_i f_i(x) + (1-\theta)\sum_i f_i(y) \\ &= \theta g(x) + (1-\theta)g(y). \end{aligned}$$

3. Recall: In one dimension, a function is convex if and only if its second derivative is non-negative.
Let $h(x) = g(f(x))$. We have that

$$\begin{aligned} h'(x) &= g'(f(x))f'(x), \\ h''(x) &= g''(f(x))(f'(x))^2 + g'(f(x))f''(x). \end{aligned}$$

   - Since g is convex, $g'' \geq 0$.
   - Since g is increasing, $g' \geq 0$.
   - Since f is convex, $f'' \geq 0$.

   Combining these three observations, we see that $h'' \geq 0$, i.e., h is convex.

4. Let $\boldsymbol{x}$ and $\boldsymbol{y}$ be two elements in the domain. Let $x = \boldsymbol{w}^\top \boldsymbol{x} + b$ and $y = \boldsymbol{w}^\top \boldsymbol{y} + b$. Let $\theta \in [0,1]$. We need to show that

$$f(\theta x + (1-\theta)y) \leq \theta f(x) + (1-\theta)f(y),$$

which follows since by assumption f was convex.

5. Also we can check the convexity by second derivative: for a twice differentiable function of a single variable, if the second derivative is greater than or equal to zero for its entire domain, then the function is convex.

6. Assume that it has two global minima at $x^\star$ and $y^\star$. Let $z^\star = (x^\star + y^\star)/2$. Then, since f is strictly convex, we have $f(z^\star) < \frac{1}{2}(f(x^\star) + f(y^\star)) = f(x^\star) = f(y^\star)$, which means neither points $x^\star$ and $y^\star$ are global minima. This contradicts the initial assumption and proves that a strictly convex function has a unique global minimizer.

2 Extension of Logistic Regression to Multi-Class Classification

1. We will use $\mathbf{W} = \mathbf{w}_1, ..., \mathbf{w}_K$ to avoid heavy notation. We have that

$$\log \mathbb{P}[\hat{\mathbf{y}} = \mathbf{y}|\mathbf{X}, \mathbf{W}] = \log \prod_{n=1}^{N} \mathbb{P}[\hat{y}_n = y_n|\mathbf{x}_n, \mathbf{W}]$$

Where $\hat{\mathbf{y}}$ are our predictions and $\mathbf{y}$ represent the ground truth for our samples. We can rewrite the equation as follow, dividing the samples in groups based on their class.

$$\log \mathbb{P}[\hat{\mathbf{y}} = \mathbf{y}|\mathbf{X}, \mathbf{W}] = \log \prod_{n:y_n=1} \mathbb{P}[\hat{y}_n = 1|\mathbf{x}_n, \mathbf{W}] ... \prod_{n:y_n=K} \mathbb{P}[\hat{y}_n = K|\mathbf{x}_n, \mathbf{W}]$$

We introduce the following notation to simplify the expression. Let $1_{y_n=k}$ be the indicator function for $y_n = k$, i.e., it is equal to one if $y_n = k$ and 0 otherwise. Notice that we can write that

$$\mathbb{P}[\hat{y}_n = k|\mathbf{x}_n, \mathbf{W}] = \prod_{j=1}^{K} \mathbb{P}[\hat{y}_n = j|\mathbf{x}_n, \mathbf{W}]^{1_{y_n=j}},$$

as $\mathbb{P}[\hat{y}_n = j|\mathbf{x}_n, \mathbf{W}]^{1_{y_n=j}}$ is 1 when $j \neq k$ (elevating to 0), whereas $\mathbb{P}[\hat{y}_n = k|\mathbf{x}_n, \mathbf{W}]$ is left unchanged.

$$\begin{aligned}
\log \mathbb{P}[\hat{\mathbf{y}} = \mathbf{y}|\mathbf{X}, \mathbf{W}] &= \log \prod_{k=1}^{K} \prod_{n=1}^{N} \mathbb{P}[y_n = k|\mathbf{x}_n, \mathbf{W}]^{1_{y_n=k}} \\
&= \sum_{n=1}^{N} \sum_{k=1}^{K} 1_{y_n=k} \log \mathbb{P}[y_n = k|\mathbf{x}_n, \mathbf{W}] \\
&= \sum_{n=1}^{N} \sum_{k=1}^{K} 1_{y_n=k} \left[\mathbf{w}_k^\top \mathbf{x}_n - \log \sum_{j=1}^{K} \exp(\mathbf{w}_j^\top \mathbf{x}_n) \right] \\
&= \sum_{n=1}^{N} \sum_{k=1}^{K} 1_{y_n=k} \mathbf{w}_k^\top \mathbf{x}_n - \sum_{n=1}^{N} \sum_{k=1}^{K} 1_{y_n=k} \log \sum_{j=1}^{K} \exp(\mathbf{w}_j^\top \mathbf{x}_n) \\
&= \sum_{n=1}^{N} \sum_{k=1}^{K} 1_{y_n=k} \mathbf{w}_k^\top \mathbf{x}_n - \sum_{n=1}^{N} \log \sum_{k=1}^{k} \exp(\mathbf{w}_k^\top \mathbf{x}_n).
\end{aligned}$$

The last step is obtained by $\sum_{k=1}^{K} 1_{y_n=k} = 1$.

2. We get

$$\frac{\partial \log \mathbb{P}[\mathbf{y}|\mathbf{X}, \mathbf{W}]}{\partial \mathbf{w}_k} = \sum_{n=1}^{N} 1_{y_n=k} \mathbf{x}_n - \sum_{n=1}^{N} \text{softmax}(\eta, k) \mathbf{x}_n.$$

Where $\text{softmax}(\eta, k) = \frac{\exp(\eta_k)}{\sum_{i=1}^{K} \exp(\eta_i)}$.

3. The negative of the log-likelihood is

$$-\sum_{n=1}^{N} \sum_{k=1}^{K} 1_{y_n=k} \mathbf{w}_k \mathbf{x}_n + \sum_{n=1}^{N} \log \sum_{k=1}^{K} \exp(\mathbf{w}_k^\top \mathbf{x}_n).$$

We have already shown that a sum of convex functions is convex, so we only need to show that the following is convex.

$$-\sum_{k=1}^{K} 1_{y_n=k} \mathbf{w}_k \mathbf{x}_n + \log \sum_{k=1}^{K} \exp(\mathbf{w}_k^\top \mathbf{x}_n).$$

The first part is a linear function, which is convex. We only need to prove that the following is convex.

$$\log \sum_{k=1}^{K} \exp(\mathbf{w}_k^\top \mathbf{x}_n)$$

This form is know as a log-sum-exp, and you may know that it is convex. It would be perfectly fine to use this as a fact, but we will prove it using the definition of convexity for the sake of completeness.

To prove: We want to show that for all sets of weights $\mathbf{A} = \mathbf{a}_1, ..., \mathbf{a}_k, \mathbf{B} = \mathbf{b}_1, ..., \mathbf{b}_k$, we have that

$$\lambda \log \left(\sum_k e^{\mathbf{a}_k^\top \mathbf{x}} \right) + (1-\lambda) \log \left(\sum_k e^{\mathbf{b}_k^\top \mathbf{x}} \right) \geq \log \left(\sum_k e^{\lambda \mathbf{a}_k^\top \mathbf{x}} e^{(1-\lambda) \mathbf{b}_k^\top \mathbf{x}} \right).$$

Simplifying the expression: First, we use the following properties of the $\log$, $y \log x = \log x^y$ and $\log x + \log y = \log xy$, to get to the following expression

$$\log \left(\left(\sum_k e^{\mathbf{a}_k^\top \mathbf{x}} \right)^{\lambda} \left(\sum_k e^{\mathbf{b}_k^\top \mathbf{x}} \right)^{(1-\lambda)} \right) \geq \log \left(\sum_k e^{\lambda \mathbf{a}_k^\top \mathbf{x}} e^{(1-\lambda) \mathbf{b}_k^\top \mathbf{x}} \right).$$

We will now prove this

$$\left(\sum_k e^{\mathbf{a}_k^\top \mathbf{x}} \right)^{\lambda} \left(\sum_k e^{\mathbf{b}_k^\top \mathbf{x}} \right)^{(1-\lambda)} \geq \sum_k e^{\lambda \mathbf{a}_k^\top \mathbf{x}} e^{(1-\lambda) \mathbf{b}_k^\top \mathbf{x}}.$$

Notice that in $\left(\sum_k e^{\mathbf{a}_k^\top \mathbf{x}} \right)^{\lambda}$, we are summing over positive numbers due to the exponential. In general, we have that $(\sum_i x_i)^y \geq \sum_i x_i^y$ if all the x_i and y are non negative. Applying this to the left hand side, we have

$$\left(\sum_k e^{\mathbf{a}_k^\top \mathbf{x}} \right)^{\lambda} \left(\sum_k e^{\mathbf{b}_k^\top \mathbf{x}} \right)^{(1-\lambda)} \geq \left(\sum_k e^{\lambda \mathbf{a}_k^\top \mathbf{x}} \right) \left(\sum_k e^{(1-\lambda) \mathbf{b}_k^\top \mathbf{x}} \right)$$

Now, we will rewrite the sum by applying the following transformation: $(\sum_i x_i)(\sum_i y_i) = \sum_i x_i y_i + \sum_i \sum_{j \neq i} x_i y_j$. This gets us

$$\left(\sum_k e^{\mathbf{a}_k^\top \mathbf{x}} \right)^{\lambda} \left(\sum_k e^{\mathbf{b}_k^\top \mathbf{x}} \right)^{(1-\lambda)} \geq \sum_k e^{\lambda \mathbf{a}_k^\top \mathbf{x}} e^{(1-\lambda) \mathbf{b}_k^\top \mathbf{x}} + \sum_i \sum_{j \neq i} e^{\lambda \mathbf{a}_i^\top \mathbf{x}} e^{(1-\lambda) \mathbf{b}_j^\top \mathbf{x}}$$

Notice that in the last term, we are summing over non negative numbers, so it is at least 0 and we have another lower bound,

$$\left(\sum_k e^{\mathbf{a}_k^\top \mathbf{x}} \right)^{\lambda} \left(\sum_k e^{\mathbf{b}_k^\top \mathbf{x}} \right)^{(1-\lambda)} \geq \sum_k e^{\lambda \mathbf{a}_k^\top \mathbf{x}} e^{(1-\lambda) \mathbf{b}_k^\top \mathbf{x}} + \sum_i \sum_{j \neq i} e^{\lambda \mathbf{a}_i^\top \mathbf{x}} e^{(1-\lambda) \mathbf{b}_j^\top \mathbf{x}} \geq \sum_k e^{\lambda \mathbf{a}_k^\top \mathbf{x}} e^{(1-\lambda) \mathbf{b}_k^\top \mathbf{x}}$$

Which concludes the proof.