

Chapter 8

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October 3, 2020

Comments and Proofs

Section 8.3.1

I found section 8.3.1 to be quite confusing, especially equation 8.5:

$$\frac{d}{d\mathbf{w}} f(\mathbf{w}) = \sum_{i=0}^N (\mu_i - y_i) \mathbf{x}_i. \quad (1)$$

In equation (1) f is the negative log likelihood and $\mu_i = p(y_i | \mathbf{x}_i, \mathbf{w}) = \sigma(\mathbf{w}^T \mathbf{x})$ where σ is the sigmoid function. We will prove equation (1), but first, some lemmas.

Lemma 1.1. *The derivative of $\sigma(z)$ is $\sigma(z)(1 - \sigma(z))$.*

Proof.

$$\begin{aligned} \frac{d\sigma}{dz} &= \frac{d}{dz} \frac{1}{1 + e^{-z}} \\ &= \frac{1 - 1 + e^{-z}}{(1 + e^{-z})^2} \\ &= \frac{1}{1 + e^{-z}} \left(1 - \frac{1}{1 + e^{-z}} \right) \\ &= \sigma(z)(1 - \sigma(z)) \end{aligned}$$

This result is not trivial, but it is quite intuitive. The whole point of the sigmoid function σ is to map the real line to $(0, 1)$ monotonically. It follows that when $\sigma(z)$ is extreme, the derivative should be close to 0, which is exactly what we see. Perhaps, it makes more sense to think of the sigmoid function as the solution to the differential equation:

$$\frac{dy}{dz} = y(y - 1).$$

Lemma 1.2. $\sigma(z) + \sigma(-z) = 1$

Proof. Since σ is symmetric about $(0, \frac{1}{2})$, $\sigma(z) = 1 - \sigma(-z)$. It follows that $\sigma(z) + \sigma(-z) = 1$.

Now we prove equation (1). Using lemmas 1.1 and 1.2, we can reduce rewrite the negative log-likelihood as

$$\begin{aligned} NLL(\mathbf{w}) &= - \sum_{i=1}^N y_i \log \mu_i + (1 - y_i) \log(1 - \mu_i) \\ &= - \sum_{i=1}^N y_i \log \sigma(\mathbf{w}^T \mathbf{x}_i) + (1 - y_i) \log \sigma(-\mathbf{w}^T \mathbf{x}_i) \end{aligned}$$

Now, we find the derivative with respect to \mathbf{w} :

$$\begin{aligned} \frac{dNLL}{d\mathbf{w}} &= - \sum_{i=1}^N y_i \frac{d}{d\mathbf{w}} \log \sigma(\mathbf{w}^T \mathbf{x}_i) + (1 - y_i) \frac{d}{d\mathbf{w}} \log \sigma(-\mathbf{w}^T \mathbf{x}_i) \\ &= \sum y_i (1 - \sigma(\mathbf{w}^T \mathbf{x}_i)) \mathbf{x}_i - (1 - y_i) \sigma(\mathbf{w}^T \mathbf{x}_i) \mathbf{x}_i \\ &= \sum (\sigma(\mathbf{w}^T \mathbf{x}_i) - y_i) \mathbf{x}_i \\ &= \sum (\mu_i - y_i) \mathbf{x}_i. \end{aligned}$$

Given lemma 1.1 and 1.2, this result comes naturally, but it is still a good exercise to do since the proof for the backpropagation algorithm is similar (but much more complicated).

Section 8.3.3

I had a lot of trouble with equation 8.15 and 8.16. I kept mixing up θ and θ_k . Also, keep in mind that the Hessian matrix \mathbf{H}_k is symmetrical due to the law of mixed partials.

If you have not had a lot of exposure to matrix calculus (like me) or always forget which vectors are transposed (also me), you can find basic matrix derivatives [here](#).

Section 8.6.2

I found this first paragraph of this section extremely confusing. Initially, I thought that \mathbf{x}_i was the i th data point and $r_i \in \{0, 1\}$ indicated whether \mathbf{x}_i was observed. I think the author means that given a data point \mathbf{x} , $r_i \in \{0, 1\}$ indicates whether the i th feature of \mathbf{x} was observed. This section would make a lot more sense if each \mathbf{x}_i was replaced with x_i .

Exercises

Exercise 3

- See section 8.3.1 above.
- See section 8.3.1 above.
- Let \mathbf{H} be the Hessian matrix of a continuous twice-differentiable function $f(\mathbf{x})$. Recall that, $H_{i,j} = \frac{\partial^2 f}{\partial x_i \partial x_j}$. By the law of mixed partials, $H_{i,j} = H_{j,i}$. In other words, \mathbf{H} is symmetric. It follows that \mathbf{H} has D eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_D$. since eigenvectors of different eigenvalues are linearly independent, there exists a orthonormal eigenbasis $\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_D$ where $\mathbf{H}\mathbf{p}_i = \lambda_i\mathbf{p}_i$. It follows that

$$\mathbf{H} = \mathbf{P}\mathbf{D}\mathbf{P}^T \quad (2)$$

where $\mathbf{D} = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_D)$ and $\mathbf{P} = [\mathbf{p}_1 \ \mathbf{p}_2 \ \dots \ \mathbf{p}_D]$.

Now we prove that all eigenvalues are positive. Following equation (2), we have

$$\mathbf{D} = \mathbf{P}^T \mathbf{H} \mathbf{P}.$$

The i th eigenvalue is the i th element of

$$\begin{aligned} \lambda_i \mathbf{e}_i &= \mathbf{D} \mathbf{e}_i \\ &= \mathbf{P}^T \mathbf{H} \mathbf{P} \mathbf{e}_i \\ &= \mathbf{P}^T \mathbf{H} \mathbf{p}_i. \end{aligned}$$

The i th eigenvalue then is given by

$$\begin{aligned} \lambda_i &= \mathbf{p}_i^T \mathbf{H} \mathbf{p}_i \\ &= \mathbf{p}_i^T \mathbf{X}^T \mathbf{S} \mathbf{X} \mathbf{p}_i \\ &= (\mathbf{X} \mathbf{p}_i)^T \mathbf{S} (\mathbf{X} \mathbf{p}_i). \end{aligned}$$

If we let $\mathbf{a}_i = \mathbf{X} \mathbf{p}_i$, we have

$$\begin{aligned} \lambda_i &= \mathbf{a}_i^T \mathbf{S} \mathbf{a}_i \\ &= \sum_{j=1}^D a_{ij}^2 \mu_j (1 - \mu_j) \\ &> 0. \end{aligned}$$

The strict inequality comes from the fact that \mathbf{X} is full rank and \mathbf{p}_i is non-zero so at least one element of $\mathbf{a}_i = \mathbf{X} \mathbf{p}_i$ is non-zero. Since \mathbf{H} is a symmetrical matrix with positive eigenvalues, it is positive definite.

Exercise 5

In this exercise we show that $\sum_{c=1}^C \hat{w}_{cj} = 0$ for any feature j when we are trying to maximize

$$f(\mathbf{W}) = \sum_{i=1}^N p(y_i|x_i, \mathbf{W}) - \sum_{c=1}^C \|\mathbf{w}_c\|_2^2.$$

Lemma 1.3. $p(y|\mathbf{x}, \mathbf{W}) = p(y|\mathbf{x}, \mathbf{W} + \mathbf{A})$ where \mathbf{A} is any matrix in the form $\mathbf{A} = [\mathbf{0} \ a_1 \mathbf{1} \ \dots \ a_D \mathbf{1}]$.

Let $\mathbf{a} = (a_1, \dots, a_D)$. It follows that

$$\begin{aligned} p(y = c|\mathbf{x}, \mathbf{W} + \mathbf{A}) &= \frac{\exp(w_{c0} + (\mathbf{w}_c + \mathbf{a})^T \mathbf{x})}{\sum_{c'=1}^C \exp(w_{c'0} + (\mathbf{w}_{c'} + \mathbf{a})^T \mathbf{x})} \\ &= \frac{\exp(w_{c0} + \mathbf{w}_c^T \mathbf{x}) \exp(\mathbf{a}^T \mathbf{x})}{\sum_{c'=1}^C \exp(w_{c'0} + \mathbf{w}_{c'}^T \mathbf{x}) \exp(\mathbf{a}^T \mathbf{x})} \\ &= \frac{\exp(w_{c0} + \mathbf{w}_c^T \mathbf{x})}{\sum_{c'=1}^C \exp(w_{c'0} + \mathbf{w}_{c'}^T \mathbf{x})} \\ &= p(y = c|\mathbf{x}, \mathbf{W}). \end{aligned}$$

Now we finish the exercise with a proof by contradiction. Say \mathbf{W} maximizes f and $\sum_{c=1}^C \hat{w}_{cj} \neq 0$ for one or more j . Let $\mathbf{W}' = \mathbf{W} - \mathbf{A}$ where $\mathbf{A} = [\mathbf{0} \ a_1 \mathbf{1} \ \dots \ a_D \mathbf{1}]$ and $a_i = \frac{1}{C} \sum_{c=1}^C w_{c,i}$. In other words, \mathbf{X}' is \mathbf{X} with centered columns (except for the zeroth column). By lemma 1.3

$$\sum_{i=0}^N p(y_i|\mathbf{x}_i, \mathbf{W}) = \sum_{i=0}^N p(y_i|\mathbf{x}_i, \mathbf{W}'). \quad (3)$$

Since \mathbf{X}' is more centered, we also have

$$\sum_{c=1}^C \|\mathbf{w}_c\|_2^2 > \sum_{c=1}^C \|\mathbf{w}'_c\|_2^2, \quad (4)$$

but equations 3 and 4 imply that $f(\mathbf{W}) < f(\mathbf{W}')$, contradicting our initial statement that \mathbf{W} maximizes f . It follows that if $\hat{\mathbf{W}}$ maximizes f , then $\sum_{c=1}^C \hat{w}_{cj} = 0$ for any $j > 0$.

Exercise 6

a. *True.* By exercise 3, \mathbf{H} , the Hessian of J , is positive definite. It follows that J is convex and has a single local optimum. This is the multivariate equivalent of a function always having a positive second derivative.

- b. *False*. Since $\frac{\partial}{\partial x_i} \|\mathbf{w}\|_2^2 = 0$ when $x_i = 0$, $\frac{\partial J}{\partial w_i}|_{w_i=0} = 0$ if and only if $\frac{\partial \ell}{\partial x_i}|_{w_i=0} = 0$ which is very unlikely.
- c. *True*. Since $\lambda = 0$, minimizing J is equivalent to maximizing ℓ . Since the data are linearly separable, there exists weights $\mathbf{w} \neq \mathbf{0}$ such that our model always makes the right prediction. In other words, $y_i \mathbf{x}_i^T \mathbf{w} > 0$. Now, consider $\ell(a\mathbf{w}, \mathcal{D})$ for some $a > 1$. Since σ is positive monotonic, $\sigma(y_i \mathbf{x}_i^T (a\mathbf{w})) > \sigma(y_i \mathbf{x}_i^T \mathbf{w})$ and $\ell(a\mathbf{w}, \mathcal{D}) > \ell(\mathbf{w}, \mathcal{D})$. It follows all the non-zero weights will become infinite.
- d. *False*. No because as λ grows, $\hat{\mathbf{w}}$ will start underfitting to the data.
- e. *False*. No because as λ grows, $\hat{\mathbf{w}}$ will start underfitting to the data.

Exercise 7

- a. The decision boundary is around $X_2 = 3(X_1 - 3)$. No errors on the training set as the data are linearly separable.
- b. The decision boundary is around $X_1 = X_2$ and the missclassification rate is $1/13$.
- c. Since we are heavily regularizing w_1 , $\hat{w}_1 = 0$ and our prediction will only be affected by X_2 . A decision boundary is $X_2 = 3$ and the missclassification rate is $2/13$.
- d. Since we are heavily regularizing w_2 , $\hat{w}_2 = 0$ and our prediction will only be affected by X_1 . A decision boundary is $X_2 = 5$ and the missclassification rate is $0/13$.