Chapter 4

Statistical learning

LDA (QDA)
logit
SVM.

References:

- The Elements of Statistical Learning [13] [1]
- Probabilistic Machine Learning: An Introduction [25] [2]
- Pattern Recognition and Machine Learning [3] [3]
- Mathematics of Machine Learning by Prof. Philippe Rigollet (lecture note) [4]
- Statistical Methods for Machine Learning by Larry Wasserman (lecture note) [5]
- An Introduction to Statistical Learning: with Applications in R [15][6]

4.1 Linear Methods for Classification

As explained in [15, Section 4.2] (Why Not Linear Regression?), there are at least two reasons not to perform classification using a regression method:

- a regression method cannot accommodate a qualitative response with more than two classes;
- a regression method will not provide meaningful estimates of $\mathbb{P}(Y|X)$, even with just two classes.

4.1.1 LDA and QDA

Theorem 4.1.1. The true error rate of a classifier h is given by

$$L(h) := \mathbb{P}(h(X) \neq Y).$$

Consider the special case where $Y \in \mathcal{Y} = \{0, 1\}$. Let $\underline{r(x) = \mathbb{P}(Y = 1|X = x)}$. In this case the Bayes classification rule h^* is given by

$$h^*(x) = \begin{cases} 1, & r(x) > \frac{1}{2} \\ 0, & r(x) \leq \frac{1}{2}. \end{cases}$$

Prove that the Bayes classification rule is optimal, that is, if h is any other classification rule then $L(h^*) \leq L(h)$.

Proof.

[1] https://web.stanford.edu/~hastie/ElemStatLearn/printings/ESLII_print12.pdf
[2] https://probml.github.io/pml-book/book1.html
[3] https://cds.cern.ch/record/998831/files/9780387310732_TOC.pdf
[4] https://ocw.mit.edu/courses/mathematics/18-657-mathematics-of-machine-learning-fall-2015/lecture-notes/MIT18_657F15_LecNote.pdf
[5] https://www.stat.cmu.edu/~larry/=sml/
[6] https://www.statlearning.com/

$\{(x_i, y_i)\}_{i=1}^{n}$, $x_i = \begin{bmatrix} x_{i1} \\ \vdots \\ x_{id} \end{bmatrix} \in \mathcal{X}$ $\mathbb{R}^{d \times 1}$

classification rule is a function $h: \mathcal{X} \to \mathcal{Y}$.
Given a new x, predict y to be $h(x)$.

Error rate: The true error rate of a h is

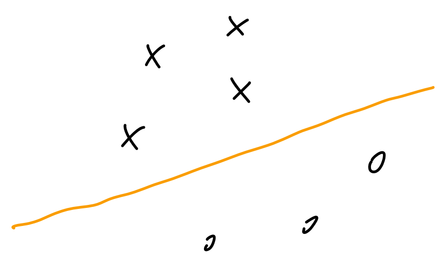
$$L(h) := \mathbb{P}(h(x) \neq y)$$

Empirical error rate (training error) is

$$\mathbb{E}\, \hat{L}_n := \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}\{h(x_i) \neq y_i\}$$

Bayes classifier.

$\mathcal{Y} = \{0, 1\}$



Decision Boundary:

$$D(h) := \{x : \mathbb{P}(Y=1 \mid X=x) = \mathbb{P}(Y=0 \mid X=x)\}.$$

$$r(x) = \frac{\mathbb{P}(X=x \mid Y=1)\, \mathbb{P}(Y=1)}{\mathbb{P}(X=x \mid Y=1)\, \mathbb{P}(Y=1) + \mathbb{P}(X=x \mid Y=0)\, \mathbb{P}(Y=0)}$$

Density estimation:

$$\mathbb{P}(Y=1) = \frac{1}{n}\sum y_i.$$

$$h(x) = \begin{cases} 1, & \text{if } \hat{r}(x) > \frac{1}{2} \\ 0, & \text{if } \hat{r}(x) < \frac{1}{2}. \end{cases}$$

$\mathcal{Y} = \{1, 2, \cdots, k\}$, optimal rule is

$$h^*(x) = \arg\max_k \mathbb{P}(y=k \mid X=x)$$

$$f_k(x) = \mathbb{P}(X=x \mid y=k), \quad \pi_k = \mathbb{P}(y=k)$$

$$\mathbb{P}(y=k \mid X=x) = \boxed{\frac{f_k(x)\,\pi_k}{\sum f_k(x)\,\pi_k}.}$$

LDA: ① Assume $f_k(x) \sim N(\mu_k, \Sigma_k)$

k, l

$\{0, 1\}$

$$\underline{f_1(x)\pi_1} \sim f_0(x)\pi_0 \quad (*)$$

$$f_k(x) = \frac{1}{(2\pi)^{d/2}|\Sigma_k|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(x-\mu_k)^T \underline{\Sigma_k}^{-1}(x-\mu_k)\right)$$

② $\Sigma_1 = \Sigma_0 = \Sigma.$

k, l

$\mu_k - \mu_l$

$$\log \frac{f_1(x)\pi_1}{f_0(x)\pi_0} = x^T \Sigma^{-1} (\underline{\mu_1 - \mu_0}) - \frac{1}{2}(\mu_1+\mu_0)^T \Sigma^{-1}(\mu_1 - \mu_0) + \log\left(\frac{\pi_1}{\pi_0}\right)$$

$$= a^T x + b$$

QDA: $\Sigma_1 \neq \Sigma_0$

$$\boxed{x^T A x + b^T x + c = 0}$$

$$\underline{\delta_k(x)} = x^T \Sigma^{-1}\mu_k - \frac{1}{2}\mu_k^T \Sigma^{-1}\mu_k + \log \pi_k$$

$$h^*(x) = \arg\max_k \delta_k(x)$$

QDA:

$$\delta_k = -\frac{1}{2}\log|\Sigma_k| - \frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k) + \log\pi_k$$

$$\{x : \delta_i(x) = \delta_j(x)\} \quad \forall\, i, j$$

- $\hat{\pi}_k = \dfrac{n_k}{n}$, $\quad n_k$: # class k
- $\hat{\mu}_k = \displaystyle\sum_{y_i = k} \frac{x_i}{n_k}$
- $\hat{\Sigma} = \dfrac{1}{n-k}\displaystyle\sum_{j=1}^{k}\sum_{y_i = j}(x_i - \hat{\mu}_j)(x_i - \hat{\mu}_j)^T$

In LDA,

$$\hat{\Sigma} = \frac{\sum_{r=1}^{k}(n_r\Sigma_r)}{\sum_{r=1}^{k} n_r}$$

Case 1: $\Sigma_k = Id.$

$$\delta_k = -\frac{1}{2}(x-\mu_k)^T(x-\mu_k) + \log\pi_k.$$

Case 2: $\exists \; U_k U_k^T = Id$, $\quad \Sigma_k = U_k \Lambda_k U_k^T$.

$$\delta_k = (x-\mu_k)^T (U_k \Lambda_k U_k^T)^{-1} (x-\mu_k)$$
$$= (\Lambda_k^{-\frac{1}{2}} U_k^T x - \Lambda_k^{-\frac{1}{2}} U_k^T \mu_k)^T (\Lambda_k^{-\frac{1}{2}} U_k^T x - \Lambda_k^{-\frac{1}{2}} U_k^T \mu_k)$$

Let $A_k = U_k \Lambda_k^{-\frac{1}{2}}$

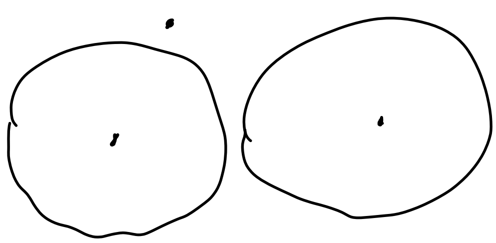
$$\delta_k = (A_k^T x - A_k^T \mu_k)^T (A_k^T x - A_k^T \mu_k).$$

LDA:

① sphere the data w.r.t. $\hat{\Sigma}$

$$\underline{X}^* \leftarrow \Lambda^{-\frac{1}{2}} U_k^T \underline{X}$$

②



$$\hat{\Sigma}_k(\alpha) = \alpha \hat{\Sigma}_k + (1-\alpha) \hat{\Sigma}.$$

For a classifier h, we rewrite the true error rate $L(h)$ by

$$\begin{aligned} L(h) &= \mathbb{P}(h(X) \neq Y) = \mathbb{P}(h(X) = 1, Y = 0) + \mathbb{P}(h(X) = 0, Y = 1) \\ &= \mathbb{E}(\mathbb{E}(\mathbf{1}_{\{h(X)=1,Y=0\}}|X)) + \mathbb{E}(\mathbb{E}(\mathbf{1}_{\{h(X)=0,Y=1\}}|X)) \end{aligned}$$

where $\mathbf{1}_A$ is the indicator function over a set A and we write $\mathbb{P}(h(X) = 1, Y = 0) = \mathbb{E}\mathbf{1}_{\{h(X)=1,Y=0\}}$, the second equality is from the disjoint of two events, and the third equality is from the law of total expectation conditioning on X.

Since $h(X)$ is measurable w.r.t X, then we take it away from the inner expectation. So the above equation becomes

$$\begin{aligned} L(h) &= \mathbb{E}(\mathbf{1}_{\{h(X)=0\}}\mathbb{E}(\mathbf{1}_{\{Y=1\}}|X)) + \mathbb{E}(\mathbf{1}_{\{h(X)=1\}}\mathbb{E}(\mathbf{1}_{\{Y=0\}}|X)) \\ &= \mathbb{E}(\mathbf{1}_{\{h(X)=0\}}r(X)) + \mathbb{E}(\mathbf{1}_{\{h(X)=1\}}(1 - r(X))) \\ &= \mathbb{E}(\mathbf{1}_{\{h(X)=0\}}r(X) + \mathbf{1}_{\{h(X)=1\}}(1 - r(X))) \end{aligned} \tag{4.1}$$

where we rewrite $\mathbb{E}(\mathbf{1}_{\{Y=1\}}|X) = \mathbb{P}(Y = 1|X)$ and replace it by $r(X)$ in the second equality.

For a classifier h and the Bayes classifier h^*, using the equality (4.1) we obtain

$$\begin{aligned} L(h) - L(h^*) &= \mathbb{E}(\mathbf{1}_{\{h(X)=0\}}r(X) + \mathbf{1}_{\{h(X)=1\}}(1 - r(X))) - \mathbb{E}(\mathbf{1}_{\{h^*(X)=0\}}r(X) + \mathbf{1}_{\{h^*(X)=1\}}(1 - r(X))) \\ &= \mathbb{E}[(\mathbf{1}_{\{h(X)=0\}} - \mathbf{1}_{\{h^*(X)=0\}})r(X) + (\mathbf{1}_{\{h(X)=1\}} - \mathbf{1}_{\{h^*(X)=1\}})(1 - r(X))] \\ &= \mathbb{E}[(\mathbf{1}_{\{h(X)=0\}} - \mathbf{1}_{\{h^*(X)=0\}})(2r(X) - 1)] \end{aligned}$$

where we use identity $\mathbf{1}_{\{h(X)=1\}} = 1 - \mathbf{1}_{\{h(X)=0\}}$ in the third equality.

There are three cases for the last equality. For $h(X) = h^*(X)$, $L(h) - L(h^*) = 0$. For $h(X) = 1, h^*(X) = 0$, $L(h) - L(h^*) = -\mathbb{E}(2r(X) - 1) = \mathbb{E}(|2r(X) - 1|)$ since $r(X) \leq \frac{1}{2}$. For $h(X) = 0, h^*(X) = 1$, $L(h) - L(h^*) = \mathbb{E}(2r(X) - 1)$. Hence, from the above discussion and definition of h^* we have

$$L(h) - L(h^*) = \mathbb{E}[\mathbf{1}_{\{h(X) \neq h^*(X)\}}|2r(X) - 1|] \geqslant 0$$

which implies $L(h^*) \leq L(h)$. This gives the desired result. □

Theorem 4.1.2. Suppose that $Y \in \{1, \dots, k\}$ and $\mathbb{P}(X = x|Y = k)$ is Gaussian $N(\mu_k, \Sigma_k)$.

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- If $\Sigma_k \neq \Sigma_l$ for any k, l, then the Bayes classifier is

  $$h^*(x) = \operatorname*{argmax}_k \delta_k(x)^{(1)}$$

  provided by

  $$\delta_k^{(1)}(x) = -\frac{1}{2}\log|\Sigma_k| - \frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1}(x - \mu_k) + \log(\pi_k).$$
- If $\Sigma_k = \Sigma_l$ for any k, l, then the Bayes classifier is

  $$h^*(x) = \operatorname*{argmax}_k \delta_k^{(2)}(x)$$

  provided by

  $$\delta_k^{(2)}(x) = x^T \Sigma^{-1}\mu_k - \frac{1}{2}\mu_k^T \Sigma_k^{-1}\mu_k + \log(\pi_k).$$

Exercise 1. If $X|Y = 0 \sim N(\mu_0, \Sigma_0)$ and $X|Y = 1 \sim N(\mu_1, \Sigma_1)$, then the Bayes rule is

$$h(x) = \begin{cases} 1 & \text{if } r_1^2 < r_2^2 + 2\log\frac{\pi_1}{\pi_0} + \log\frac{|\Sigma_0|}{|\Sigma_1|} \\ 0 & \text{otherwise} \end{cases} \tag{4.2}$$

where $r_i^2 = (x - \mu_i)^T \Sigma_i^{-1}(x - \mu_i), i = 0, 1$.

Proof. Let $\mathbb{P}(X = x|Y = k) = f_k(x)$ and $\mathbb{P}(Y = k) = \pi_k$ for $k = 0, 1$. From the Bayes' theorem, we have

$$\mathbb{P}(Y = i|X = x) = \frac{f_i(x)\pi_i(x)}{\sum_{k=0}^{1} f_k(x)\pi_k}, \quad \text{for } i = 0, 1.$$

Since the Bayes rule is $h^*(x) = \mathbf{1}_{\{\mathbb{P}(Y=1|X=x) > \mathbb{P}(Y=0|X=x)\}}$, we need to simplify $\mathbb{P}(Y = 1|X = x) > \mathbb{P}(Y =$

$0|X = x)$ which is

$$\frac{f_1(x)\pi_1(x)}{\sum_k f_k(x)\pi_k} > \frac{f_0(x)\pi_0(x)}{\sum_k f_k(x)\pi_k}.$$

Note that the denominator can be canceled. Then we have

$$f_1(x)\pi_1(x) > f_0(x)\pi_0(x).$$

Since $X|Y = i \sim \mathcal{N}(\mu_i, \Sigma_i)$ for $i = 0, 1$, the above inequality yields (here we cancel the same term $(2\pi)^{-d/2}$ for both side)

$$|\Sigma_1|^{-1/2} \exp\left(-r_1^2/2\right) > |\Sigma_0|^{-1/2} \exp\left(-r_0^2/2\right)$$

where let $r_i^2 = (x-\mu_i)^T \Sigma_i^{-1}(x-\mu_i), i = 0, 1$.

We take logarithm for both side to get

$$-\frac{1}{2}\log|\Sigma_1| - \frac{1}{2}r_1^2 + \log\pi_1 > -\frac{1}{2}\log|\Sigma_0| - \frac{1}{2}r_0^2 + \log\pi_0.$$

This is just

$$r_1^2 < r_0^2 + \log\frac{|\Sigma_0|}{|\Sigma_1|} + 2\log\frac{\pi_1}{\pi_0}.$$

Hence,

$$h^*(x) = \begin{cases} 1, & \text{if } r_1^2 < r_0^2 + \log\frac{|\Sigma_0|}{|\Sigma_1|} + 2\log\frac{\pi_1}{\pi_0}, \\ 0, & \text{otherwise} \end{cases}$$

where let $r_i^2 = (x-\mu_i)^T \Sigma_i^{-1}(x-\mu_i), i = 0, 1$. □

Exercise 2. Consider a classifier with class conditional densities of the form $N(x|\mu_c, \Sigma_c)$. In LDA, we assume $\Sigma_c = \Sigma$ and in QDA, each Σ_c is arbitrary. Assume that $\Sigma_1 = k\Sigma_2$ for $k > 1$. That is, the Gaussian ellipsoids have the same"shape", but the one for class 1 is "wider". Derive an expression for the decision boundary.

Proof. Here we consider two classes that $Y \in \{1, 2\}$ and We use same notations as class. Let $f_k(x) := \mathbb{P}(X = x|Y = k)$ for $k = 1, 2$. Since class conditional densities of $f_k(x)$ are of the form $\mathcal{N}(x|\mu_c, \Sigma_c)$, which are given by

$$f_k(x) = \frac{1}{(2\pi)^{d/2}|\Sigma_k|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_k)^T \Sigma^{-1}(x-\mu_k)\right), \, k = 1, 2.$$

In this question, we consider the decision boundary

$$D(h) = \{x : \mathbb{P}(Y = 1|X = x) = \mathbb{P}(Y = 2|X = x)\}.$$

From the Bayes' theorem, we have

$$\mathbb{P}(Y = i|X = x) = \frac{f_i(x)\pi_i(x)}{\sum_{k=1}^2 f_k(x)\pi_k}, \text{ for } i = 1, 2.$$

Using the above equation, the conditional probability equation in decision boundary becomes

$$f_1(x)\pi_1 = f_2(x)\pi_2. \tag{4.3}$$

Plug class conditional densities of $f_k(x)$ into (4.3) and take logarithm for both side, we obtain

$$-\frac{1}{2}\log|\Sigma_1| - \frac{1}{2}(x-\mu_1)^T\Sigma_1^{-1}(x-\mu_1) + \log\pi_1 = -\frac{1}{2}\log|\Sigma_2| - \frac{1}{2}(x-\mu_2)^T\Sigma_2^{-1}(x-\mu_2) + \log\pi_2.$$

Since we know that $\Sigma_1 = k\Sigma_2$ for $k > 1$, the above equation becomes

$$\log\frac{|k\Sigma_2|}{|\Sigma_2|} + (x-\mu_1)^T(k\Sigma_2)^{-1}(x-\mu_1) - (x-\mu_2)^T\Sigma_2^{-1}(x-\mu_2) + 2\log\frac{\pi_2}{\pi_1} = 0.$$

Using $|k\Sigma_2| = k^d|\Sigma_2|$ and expanding the above bracket, we get

$$(\frac{1}{k} - 1)x^T\Sigma_2^{-1}x + (2\mu_2^T - \frac{2}{k}\mu_1^T)\Sigma_2^{-1}x + \frac{1}{k}\mu_1^T\Sigma_2^{-1}\mu_1 - \mu_2^T\Sigma_2^{-1}\mu_2 + d\log k + 2\log\frac{\pi_2}{\pi_1} = 0.$$

□

Exercise 3. Ex 4.2 in [13].

Proof.
part (a)

We follow the same notations as class. Since there are two classes, assume that $Y \in \{1, 2\}$. In LDA, let $\mathbb{P}(X = x|Y = k) = f_k(x)$ and $\mathbb{P}(Y = k) = \pi_k$ for $k = 1, 2$. We need to compare $\mathbb{P}(Y = 1|X = x)$ and $\mathbb{P}(Y = 2|X = x)$ in LDA. From the Bayes' theorem, we have

$$\mathbb{P}(Y = i|X = x) = \frac{f_i(x)\pi_i(x)}{\sum_{k=1}^{2} f_k(x)\pi_k}, \quad \text{for } i = 1, 2.$$

To compare $\mathbb{P}(Y = 2|X = x) > \mathbb{P}(Y = 1|X = x)$ is equivalent to

$$\frac{f_2(x)\pi_2(x)}{\sum_k f_k(x)\pi_k} > \frac{f_1(x)\pi_1(x)}{\sum_k f_k(x)\pi_k}.$$

Note that the denominator can be canceled. Then we have

$$f_2(x)\pi_2(x) > f_1(x)\pi_1(x). \tag{4.4}$$

Since each class density $f_k(x)$ is multivariate Gaussian, then

$$f_k(x) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x - \mu_k)^T \Sigma^{-1}(x - \mu_k)\Big), \; k = 1, 2$$

where two classes have same covariance matrix Σ.

We plug densities of f_k into (4.4) and take logarithm for both side to get

$$-\frac{1}{2}(x - \mu_1)^T \Sigma^{-1}(x - \mu_1) + \log \pi_1 > -\frac{1}{2}(x - \mu_2)^T \Sigma^{-1}(x - \mu_2) + \log \pi_2.$$

We expand the above and cancel $x^T \Sigma^{-1} x$, then the above inequality yields

$$-\frac{1}{2}\mu_2^T \Sigma^{-1}\mu_2 + \frac{1}{2}\mu_1^T \Sigma^{-1}\mu_1 + (\mu_2 - \mu_1)^T \Sigma^{-1} x + \log \pi_2 - \log \pi_1 > 0$$

Note that we estimate $\pi_1 = \frac{n_1}{n}$ and $\pi_2 = \frac{n_2}{n}$ since the size of class 1 and class 2 are n_1 and n_2 respectively. Using this estimate, we obtain

$$-\frac{1}{2}\mu_2^T \Sigma^{-1}\mu_2 + \frac{1}{2}\mu_1^T \Sigma^{-1}\mu_1 + (\mu_2 - \mu_1)^T \Sigma^{-1} x + \log\Big(\frac{n_2}{n}\Big) - \log\Big(\frac{n_1}{n}\Big) > 0$$

Hence,

$$x^T \Sigma^{-1}(\mu_2 - \mu_1) > \frac{1}{2}\mu_2^T \Sigma^{-1}\mu_2 - \frac{1}{2}\mu_1^T \Sigma^{-1}\mu_1 + \log\Big(\frac{n_1}{n}\Big) - \log\Big(\frac{n_2}{n}\Big). \tag{4.5}$$

part (b) We label class 1 as C_1 of size n_1 and class 1 as C_2 of size n_2. To minimize the least squares $\sum_{i=1}^{n}(y_i - \beta_0 - \beta^T x_i)^2$, it suffices to take the derivatives with respect to β_0 and β to zero. We obtain

$$\sum_{i=1}^{n}(y_i - \beta_0 - \beta^T x_i) = 0 \tag{4.6}$$

and

$$\sum_{i=1}^{n}(y_i - \beta_0 - \beta^T x_i)x_i = 0 \tag{4.7}$$

So we just need to solve β_0 and β from above equations.

Note that the target coded of y_i as $-n/n_1$ for class 1 and n/n_2 for class 2, we have

$$\sum_{i=1}^{n} y_i = -n_1\frac{n}{n_1} + n_2\frac{n}{n_2} = 0. \tag{4.8}$$

Plug (4.8) into (4.6), we obtain

$$n\beta_0 + \beta^T \sum_{i=1}^{n} x_i = 0 \tag{4.9}$$

Note that

$$\frac{1}{n}\sum_{i=1}^{n} x_i = \frac{1}{n}(n_1\widehat{\mu}_1 + n_2\widehat{\mu}_2). \tag{4.10}$$

Using (4.10), the equation (4.9) becomes

$$\beta_0 = (-\frac{n_1}{n}\widehat{\mu}_1^T - \frac{n_2}{n}\widehat{\mu}_2^T)\beta. \tag{4.11}$$

Next, we try to solve β from equation (4.7). Before that, we need some preparation. Since there are two classes, we estimate the mean as in [13, Chapter 4.3] given by

$$\widehat{\mu}_1 = \frac{\sum_{i\in C_1} x_i}{n_1},\ \widehat{\mu}_2 = \frac{\sum_{i\in C_2} x_i}{n_2}.$$

where $i \in C_1$ means that y_i is labeled in the first class coded as $-n/n_1$ and $i \in C_2$ means that y_i is labeled in the second class coded as n/n_2.

Then We have

$$\sum_i x_i = \sum_{i\in C_1} x_i + \sum_{i\in C_2} x_i = n_1\widehat{\mu}_1 + n_2\widehat{\mu}_2. \tag{4.12}$$

Also, We estimate the covariance matrix from our training data as in [13, Chapter 4.3]

$$\widehat{\Sigma} = \frac{1}{n-2}\left[\sum_{i\in C_1}(x_i-\widehat{\mu}_1)(x_i-\widehat{\mu}_1)^T + \sum_{i\in C_2}(x_i-\widehat{\mu}_2)(x_i-\widehat{\mu}_2)^T\right] = \frac{1}{n-2}\left[\sum_{i=1}^n x_i x_i^T - n_1\widehat{\mu}_1\widehat{\mu}_1^T - n_2\widehat{\mu}_2\widehat{\mu}_2^T\right]. \tag{4.13}$$

So

$$\sum_{i=1}^n x_i x_i^T = (n-2)\widehat{\Sigma} + n_1\widehat{\mu}_1\widehat{\mu}_1^T + n_2\widehat{\mu}_2\widehat{\mu}_2^T. \tag{4.14}$$

Moreover, we use the target coded of y_i again to get

$$\sum_{i=1}^n x_i y_i = \sum_{i\in C_1} x_i y_i + \sum_{i\in C_2} x_i y_i = -\frac{n}{n_1}\sum_{i\in C_1} x_i + \frac{n}{n_2}\sum_{i\in C_2} x_i = -n\widehat{\mu}_1 + n\widehat{\mu}_2. \tag{4.15}$$

Now we plug (4.11) into equation (4.7) and use equations (4.12), (4.14), and (4.15) for equation (4.7). Thus, we have

$$(n_1\widehat{\mu}_1 + n_2\widehat{\mu}_2)(-\frac{n_1}{n}\widehat{\mu}_1^T - \frac{n_2}{n}\widehat{\mu}_2^T)\beta + ((n-2)\widehat{\Sigma} + n_1\widehat{\mu}_1\widehat{\mu}_1^T + n_2\widehat{\mu}_2\widehat{\mu}_2^T)\beta = n(\widehat{\mu}_2 - \widehat{\mu}_1). \tag{4.16}$$

After some algebra for LHS of (4.16), note that

$$\begin{aligned}(n_1\widehat{\mu}_1 + n_2\widehat{\mu}_2)(-\frac{n_1}{n}\widehat{\mu}_1^T - \frac{n_2}{n}\widehat{\mu}_2^T) + n_1\widehat{\mu}_1\widehat{\mu}_1^T + n_2\widehat{\mu}_2\widehat{\mu}_2^T &= \frac{n_1n_2}{n}\widehat{\mu}_1\widehat{\mu}_1^T + \frac{n_1n_2}{n}\widehat{\mu}_2\widehat{\mu}_2^T - 2\frac{n_1n_2}{n}\widehat{\mu}_1\widehat{\mu}_2^T \\ &= \frac{n_1n_2}{n}(\widehat{\mu}_1\widehat{\mu}_1^T - 2\widehat{\mu}_1\widehat{\mu}_2^T + \widehat{\mu}_2\widehat{\mu}_2^T) \\ &= \frac{n_1n_2}{n}(\widehat{\mu}_1 - \widehat{\mu}_2)(\widehat{\mu}_1 - \widehat{\mu}_2)^T.\end{aligned}$$

Hence, equation (4.16) becomes

$$(\frac{n_1n_2}{n}(\widehat{\mu}_1 - \widehat{\mu}_2)(\widehat{\mu}_1 - \widehat{\mu}_2)^T + (n-2)\widehat{\Sigma})\beta = n(\widehat{\mu}_2 - \widehat{\mu}_1).$$

Hence,

$$(\frac{n_1n_2}{n}\widehat{\Sigma}_B + (n-2)\widehat{\Sigma})\beta = n(\widehat{\mu}_2 - \widehat{\mu}_1) \tag{4.17}$$

where $\widehat{\Sigma}_B = (\widehat{\mu}_2 - \widehat{\mu}_1)(\widehat{\mu}_2 - \widehat{\mu}_1)^T$. This gives the desired result.

part (c) Since $\widehat{\Sigma}_B\beta = (\widehat{\mu}_2 - \widehat{\mu}_1)(\widehat{\mu}_2 - \widehat{\mu}_1)^T\beta$ and $(\widehat{\mu}_2 - \widehat{\mu}_1)^T\beta$ is a scalar, then $\widehat{\Sigma}_B\beta$ is in the direction of $(\widehat{\mu}_2 - \widehat{\mu}_1)$. Note that equation (4.17) can be rewritten as

$$(n-2)\widehat{\Sigma}\beta = n(\widehat{\mu}_2 - \widehat{\mu}_1) - \frac{n_1n_2}{n}\widehat{\Sigma}_B\beta. \tag{4.18}$$

Since terms $\frac{n_1n_2}{n}\widehat{\Sigma}_B\beta$ and $n(\widehat{\mu}_2 - \widehat{\mu}_1)$ are in the direction of $(\widehat{\mu}_2 - \widehat{\mu}_1)$, then the RHS of (4.18) is also in the direction of $(\widehat{\mu}_2 - \widehat{\mu}_1)$. Thus, β is proportional to $\widehat{\Sigma}^{-1}(\widehat{\mu}_2 - \widehat{\mu}_1)$. From equation (4.5), the least squares regression coefficient is identical to the LDA coefficient up to a scalar multiple.

□

Exercise 4. Show that the Naive Bayes Classifier is equivalent to a linear classification rule.

Proof. See https://www.cs.cornell.edu/courses/cs4780/2018fa/lectures/lecturenote05.html.

□

$$\mathbb{P}(Y=1 \mid X=x) = \frac{1}{1+e^{-\beta^T x}} = \frac{e^{\beta \cdot x}}{1+e^{\beta^T x}}$$

$$\mathbb{P}(Y=0 \mid X=x) = \frac{1}{1+e^{\beta^T x}}$$

$$\theta = \underset{i}{\arg\max}\ L(x_i;\theta)$$

$$\frac{\partial l}{\partial \beta} = 0$$

$$\beta^{new} = \beta^{old} - \left(\frac{\partial^2 l(\beta)}{\partial \beta \, \partial \beta^T}\right)^{-1} \frac{\partial l(\beta)}{\partial \beta}.$$

4.1.2 Logistic regression

Exercise 5. Ex 4.4 in [13] for the multi-class logistic regression model.

Proof. For multi-classes logistic regression model, assume that we have K classes and N labels. The response y_{il} is given by that if the data point x_i is from class l where $1 \leq l \leq K-1$, then the $l-$th element of y_i is one and others are zero, and if x_i is from class K, then all elements of y_i are zero. So response y_{il} form a target matrix corresponding to sample $1 \leq n \leq N$ and class $1 \leq k \leq K$. That is

$$y_i = \mathbf{1}_{\{x \text{ is from class } l \text{ and } i = l\}}.$$

From textbook [13, Section 4.4], we know that the posterior probability that x_i comes from class k are given by

$$\mathbb{P}(y = k|X = x) = \frac{\exp\big(\beta_{k0} + \beta_k^T x\big)}{1 + \sum_{l=1}^{K-1} \exp\big(\beta_{l0} + \beta_l^T x\big)}, \; k = 1, 2, \ldots, K-1,$$
$$\mathbb{P}(y = K|X = x) = \frac{1}{1 + \sum_{l=1}^{K-1} \exp\big(\beta_{l0} + \beta_l^T x\big)}.$$

Let

$$h_k(x) = \mathbb{P}(y = k|X = x), \; k = 1, 2, \ldots, K$$

The likelihood function for a data point x is given by

$$L(\beta; x) = h_1(x)^{y_1} h_2(x)^{y_2} \cdots h_{K-1}(x)^{y_{K-1}} (h_K(x))^{1-\sum_{l=1}^{K-1} y_l} \tag{4.19}$$

From the posterior probability $\mathbb{P}(y = k|X = x)$, we have the log-likelihold function for a data point x

$$\ell(\beta; x) = y_1(\beta_{10} + \beta_1^T x) + y_2(\beta_{20} + \beta_2^T x) + \cdots + y_{K-1}(\beta_{(K-1)0} + \beta_{K-1}^T x) + \log(h_K) \tag{4.20}$$

Then sum over the equation (4.20) for all data points x_i, we get the log-likelihood of parameter β, that is,

$$\begin{aligned}
\ell(\beta) &= \sum_{i=1}^{N} \sum_{l=1}^{K-1} [y_{il} \beta_l^T x_i + \log(h_K)] \\
&= \sum_{i=1}^{N} \sum_{l=1}^{K-1} [y_{il} \beta_l^T x_i - \log\left(1 + \sum_{l=1}^{K-1} \exp\big(\beta_{l0} + \beta_l^T x_i\big)\right)]
\end{aligned}$$

where x_i is the $i-$th sample, β_l is a vector of coefficients for the $l-$th class with size $(p+1)$, $\beta = [\beta_1, \beta_2, \ldots, \beta_{K-1}]^T$ is of size $(K-1)(p+1)$.

Next, we compute the derivative of $\ell(\beta)$.

$$\begin{aligned}
\frac{\partial \ell(\beta)}{\partial \beta_k} &= \sum_{i=1}^{N} \left[y_{ik} x_i^T - \frac{\exp\big(\beta_{k0} + \beta_k^T x_i\big)}{1 + \sum_{l=1}^{K-1} \exp\big(\beta_{l0} + \beta_l^T x_i\big)} x_i^T \right] \\
&= \sum_{i=1}^{N} (y_{ik} - \mathbb{P}(y = k|X = x_i)) x_i^T \\
&= (y_{ik} - h_k(x_i)) x_i^T.
\end{aligned}$$

Let $y_l = [y_{1l}, y_{2l}, \ldots, y_{Nl}]^T$ and $p_l = [h_l(x_1), h_l(x_2), \ldots, h_l(x_N)]^T$. Then we have

$$\frac{\partial \ell(\beta)}{\partial \beta} = \begin{bmatrix} X^T(y_1 - h_1) \\ X^T(y_2 - h_2) \\ \vdots \\ X^T(y_{K-1} - h_{k-1}) \end{bmatrix}$$

where X is the $N \times (p+1)$ matrix of x_i values.

The Hessian matrix of $\ell(\beta)$ is given by

$$\frac{\partial^2 \ell(\beta)}{\partial \beta_k \partial \beta_k'^T} = -\sum_{i=1}^{N} h_k(x_i) h_{k'}(x_i) x_i x_i^T, \; \text{ for } k \neq k'$$

and for $k = k'$ we have

$$\begin{aligned}
\frac{\partial^2 \ell(\beta)}{\partial \beta_k \partial \beta_k^T} &= -\sum_{i=1}^{N} \left[\frac{\exp\left(\beta_{k0} + \beta_k^T x_i\right) x_i (1 + \sum_{l=1}^{K-1} \exp\left(\beta_{l0} + \beta_l^T x_i\right)) - \exp\left(\beta_{k0} + \beta_k^T x_i\right)^2 x_i}{(1 + \sum_{l=1}^{K-1} \exp\left(\beta_{l0} + \beta_l^T x_i\right))^2} x_i^T \right] \\
&= -\sum_{i=1}^{N} [(h_k(x_i) x_i - h_k(x_i)^2 x_i) x_i^T] \\
&= -\sum_{i=1}^{N} [h_k(x_i)(1 - h_k(x_i)) x_i x_i^T].
\end{aligned}$$

Write above second order derivative in form of matrix. Let H_k be $N \times N$ diagonal matrices for $k = 1, 2, \ldots, K-1$ with diagonal elements $h_k(x_i)(1 - h_k(x_i)$, $i = 1, 2, \ldots, N$. Then we rewrite the second derivative of $\ell(\beta)$ as $k = k'$

$$\frac{\partial^2 \ell(\beta)}{\partial \beta_k \partial \beta_k^T} = -X^T H_k X.$$

Let T_k be $N \times N$ diagonal matrices for $k = 1, 2, \ldots, K-1$ with diagonal elements $h_k(x_i)$, $i = 1, 2, \ldots, N$. Then we rewrite the second derivative of $\ell(\beta)$ as $k \neq k'$

$$\frac{\partial^2 \ell(\beta)}{\partial \beta_k \partial \beta_k'^T} = -X^T T_k T_{k'} X.$$

Hence, the Hessian matrix of $\ell(\beta)$ is given by

$$\begin{aligned}
\frac{\partial^2 \ell(\beta)}{\partial \beta \partial \beta^T} &= \begin{bmatrix} -X^T H_1 X & -X^T T_1 T_2 X & \cdots & -X^T T_1 T_{K-1} X \\ -X^T T_2 T_1 X & -X^T H_2 X & \cdots & -X^T T_2 T_{K-1} X \\ \vdots & & \ddots & \vdots \\ -X^T T_{K-1} T_1 X & -X^T T_{K-1} T_2 X & \cdots & -X^T H_{K-1} X \end{bmatrix} \\
&= -\widehat{X}^T W \widehat{X}
\end{aligned}$$

where $\widehat{X} = X \cdot \mathrm{Id}_{K-1}$, Id_{K-1} is a $(K-1) \times (K-1)$ identity matrix, $\widehat{X}$ is a $(K-1) \times (K-1)$ matrix with each block matrix of size $(p+1) \times (p+1)$, and

$$W = \begin{bmatrix} H_1 & T_1 T_2 & \cdots & T_1 T_{K-1} \\ T_2 T_1 & H_2 & \cdots & T_2 T_{K-1} \\ \vdots & & \ddots & \vdots \\ T_{K-1} T_1 & T_{K-1} T_2 & \cdots & H_{K-1} \end{bmatrix}$$

Now our Newton-Raphson algorithm for maximizing the log-likelihood is given by

$$\beta^{new} = \beta^{old} + (\widehat{X}^T W \widehat{X})^{-1} \widehat{X}^T \begin{bmatrix} (y_1 - h_1) \\ (y_2 - h_2) \\ \vdots \\ (y_{K-1} - h_{k-1}) \end{bmatrix}$$

Let

$$y - h = \begin{bmatrix} (y_1 - h_1) \\ (y_2 - h_2) \\ \vdots \\ (y_{K-1} - h_{k-1}) \end{bmatrix}$$

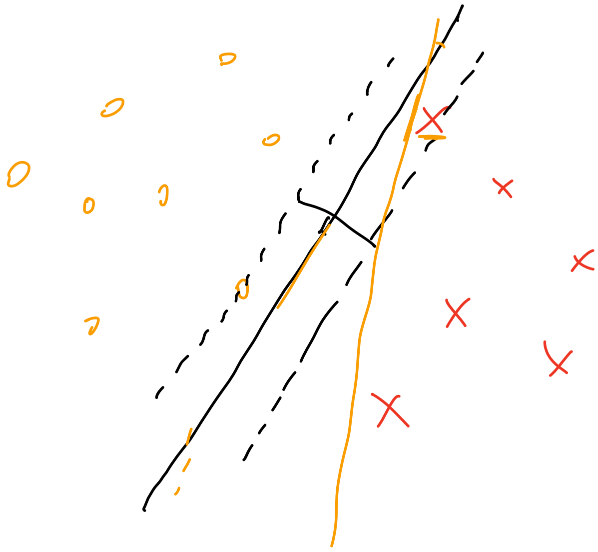
Hence, the algorithm can be expressed as

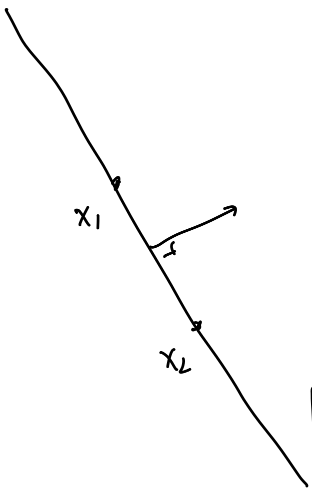
$$\beta^{new} \leftarrow (\widehat{X}^T W \widehat{X})^{-1} \widehat{X}^T W (\widehat{X} \beta^{old} + W^{-1}(y - h))$$

So β^{new} is the solution of a non-diagonal weighted least squares problem with a response $(\widehat{X}\beta^{old} + W^{-1}(y - h))$. We can still use the Netwon algorithm as an iteratively reweighted least squares algorithm. Let $z = (\widehat{X}\beta^{old} + W^{-1}(y - h))$. The iteratively reweighted least squares algorithm is as follows. Set $\beta^0 = 0$, update β^{new} by

$$\beta^{new} \leftarrow \underset{\beta}{\operatorname{argmin}} (z - \widehat{X}\beta) W (z - \widehat{X}\beta)$$

$\{(x_i, y_i)\}_{i=1}^{N}$, $y_i = \pm 1$,





$L : \beta^T x + \beta_0 = 0$

① $\forall\ x_1, x_2 \in L$, $\quad \beta^T (x_1 - x_2) = 0$

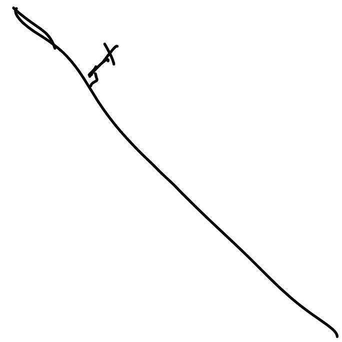
$$\beta^* = \frac{\beta}{\|\beta\|} \perp L$$

② $\forall\ x_0 \in L$, $\quad \beta^T x_0 = -\beta_0$

③ $$\text{dist}(x, L) = \beta^{*T}(x - x_0)$$

$$= \boxed{\frac{|\beta^T x + \beta_0|}{\|\beta\|}} \left(= \frac{f(x)}{\|f'(x)\|} \right)$$

P. L. A.



$y_i = -1$, $x_i^T \beta + \beta_0 < 0$

$$\min \quad D(\beta, \beta_0) = -\sum_{i \in M} y_i (x_i^T \beta + \beta_0)$$

$$\frac{\partial D}{\partial \beta} = -\sum_{i \in M} y_i x_i$$

$$\frac{\partial D}{\partial \beta_0} = -\sum_{i \in M} y_i$$

SGD.

$$\begin{bmatrix} \beta \\ \beta_0 \end{bmatrix} \leftarrow \begin{bmatrix} \beta \\ \beta_0 \end{bmatrix} + \rho \begin{bmatrix} y_i x_i \\ y_i \end{bmatrix}$$

Ex 4.6.

$\exists \ \beta_{sep}$ s.t. $y_i \beta_{sep}^T z_i \geq 1$

$$\| \underbrace{\beta_{new} - \beta_{sep}}_{\downarrow} \|^2 \leq \| \underbrace{\beta_{old} - \beta_{sep}}_{\downarrow 0} \|^2 - 1$$

Hard margin SVM.

$$\text{margin}(\beta, \beta_0) = \min \text{dist}(X, L)$$

$$= \min_{\substack{\beta, \beta_0 \\ x_i}} \frac{|\beta^T x_i + \beta_0|}{\|\beta\|}$$

$$\begin{cases} \max_{\beta, \beta_0} \min \frac{1}{\|\beta\|} \boxed{(\beta^T x_i + \beta_0) y_i} \\ \text{s.t.} \quad y_i (\beta^T x_i + \beta_0) \underline{\geq 0} \end{cases}$$

$$\exists C, \quad y_i(\beta^T x_i + \beta_0) \geq C \Rightarrow y_i \left(\frac{\beta^T}{C} x_i + \frac{\beta_0}{C}\right) \geq 1$$

$$\Rightarrow y_i(\beta'^T x_i + \beta_0') \geq 1$$

$$\Leftrightarrow \begin{cases} \max_{\beta, \beta_0} \frac{1}{\|\beta\|} \\ \text{s.t.} \quad y_i(\beta^T x_i + \beta_0) \geq 1 \end{cases}$$

$$\Leftrightarrow \begin{cases} \min_{\beta, \beta_0} \underline{\frac{1}{2}\|\beta\|^2} \\ \text{s.t.} \quad \underline{y_i(x_i^T \beta + \beta_0) \geq 1.} \quad \text{for } i = 1, \cdots, N. \end{cases}$$

$$L_P = \underbrace{\frac{1}{2}\|\beta\|^2}_{\beta^T \beta} - \sum_{i=1}^{N} \alpha_i [\underline{y_i (x_i^T \beta + \beta_0) - 1}]$$

$$\begin{cases} \beta = \sum \alpha_i y_i x_i & (1) \\ 0 = \sum \alpha_i y_i & (2) \end{cases}$$

Dual:

$$L_D = \frac{1}{2} \beta^T \sum \alpha_i y_i x_i - \beta^T \sum \alpha_i y_i x_i + \sum \alpha_i$$

$$= -\frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j x_i^T x_j + \sum \alpha_i , \quad \alpha_i \geq 0$$

KKT.

$$\begin{cases} \min & f(x) \\ \text{s.t.} & g_i(x) \geq 0 \end{cases}$$

(1) $\frac{\partial L_P}{\partial x}(x^*) = 0$

(2) $g_i(x^*) \geq 0$

(3) $\alpha_i \geq 0$

(4) $\alpha_i g_i(x^*) = 0$

$\boxed{\text{If } \alpha_i > 0, \text{ then } y_i(x_i^T \beta + \beta_0) = 1.}$

$$\boxed{\beta^*} = \sum \alpha_i y_i x_i$$

Solve $\beta_0 = y_i - \beta^T x_i = y_i - \sum \alpha_i y_i x_i^T x_i$

$$f(x) = \text{sign}(\beta^{*T} x + \beta_0^*)$$

However, the Hessian maybe not negative definite, Newton-Raphson update cannot perform effective.

Here we implement a improved Newton-Raphson algorithm from paper [11]. Given an intial value β^0, let λ_1 be the largest eigenvalue of Hessian matrix of $\ell(\beta)$ at β^0 defined by $H(\ell(\beta^0))$. Let ε be the step size and let $\alpha = \lambda_1 + \varepsilon \|\frac{\partial \ell(\beta^0)}{\partial \beta}\|_2$. Define the controlling of Hessian matrix H by

$$H_\alpha(\ell(\beta^0)) = \begin{cases} H(\ell(\beta^0)) - \alpha \cdot \mathrm{Id}, & \text{if } \alpha > 0, \\ H(\ell(\beta^0)), & \text{otherwise} \end{cases}$$

where $H_\alpha(\ell(\beta^0))$ is always negative definite.

Update β^{new} by

$$\beta^{new} = \beta^{old} - H_\alpha^{-1}(\ell(\beta^{old}))\frac{\partial \ell(\beta^{old})}{\partial \beta}$$

where we have computed the Hessian and gradient of $\ell(\beta)$ in form of matrix as before. □

4.1.3 SVM

Exercise 6. Show that if their convex hulls intersect, the two sets of points cannot be linearly separable.

Proof. See Bishop 3.4 in https://www.cise.ufl.edu/~anand/fa05/hw1sol_fall05.pdf. □

Exercise 7 (Exercise in [3])**.** In the maximum-margin hyperplane problem, let's τ denotes the value of the margin. Show that

$$\frac{1}{\tau^2} = 2\sum \alpha - \sum_{k=1}^{n}\sum_{j=1}^{n} \alpha_k \alpha_j y_k y_j x_k^T x_j.$$

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