1. Gaussian Discriminant Analysis

First of all, the Bayes' Formula:

$$p(y=c|x,\theta) = \frac{p(x|y=c;\theta)p(y=c;\theta)}{\sum_{\theta'} p(x|y=c';\theta)p(y=c';\theta)}$$
(0)

where c is one of the class.

1.1 class conditional density

We **assume** that the class conditional density is as follows:

$$p(\mathbf{x}|y=c,\theta) = N(\mathbf{x}|\mu_c, \Sigma_c) \tag{1.1}$$

To be more clear, it's a multivariable gaussian distribution and \mathbf{x} is a vector. In the following, I'll use x to replace the bold \mathbf{x} , for my own convenience.

So,

$$N(\mathbf{x}|\mu_c,\Sigma_c) = rac{1}{\sqrt{2\pi\Sigma_c}}e^{-rac{1}{2}(x-\mu_c)^T\Sigma_c^{-1}(x-\mu_c)}$$

1.2 Posterior

From, formula 0, we can know that

$$p(y = c|x, \theta) \propto \Pi_c N(x|\mu_c, \Sigma_c)$$
(1.2)

where Π_c is the prior probability of class c, p(y=c).

So, the right hand is just the upper part of formula 0. It's because the lower part is on x, which is a fixed parameter.

1.3 Log posterior

Since we're focusing on the difference between those classes, the constant is irrelevant.

$$log \ p(y=c|x; heta) = log(\Pi_c) - rac{1}{2}log|2\pi\Sigma_c| - rac{1}{2}(x-\mu_c)^T\Sigma_c^{-1}(x-\mu_c) + constant$$
 (1.3)

1.4 Quadratic decision boundaries

There's only one higher order of x, and it's $x^T \Sigma_c^{-1} x$.

If each $\boldsymbol{\Sigma}_c$ is different, it's a quadratic decision boundary.

1.5 Linear decision boundaries

On the other hand, if Σ_c is independent of c, then there's no more higher order of x. Thus, it's a linear decision boundary.

In fact, there is. But we focus on the difference between those classes. So, it's a linear one.

For some intuition, think about $y=x^3$ and $y=x^3+1$

$$egin{aligned} log \ p(y=c|x; heta) &= log(\Pi_c) - rac{1}{2}log|2\pi\Sigma| - rac{1}{2}(x-\mu_c)^T\Sigma^{-1}(x-\mu_c) + constant \ &= (log(\Pi_c) - rac{1}{2}\mu_c^T\Sigma^{-1}\mu_c) \ + \ (rac{1}{2}x^T\Sigma^{-1}\mu_c + rac{1}{2}\mu_c^T\Sigma^{-1}x) \ - \ (rac{1}{2}x^T\Sigma^{-1}x + const) \end{aligned}$$

$$= (log(\Pi_c) - \frac{1}{2}\mu_c^T \Sigma^{-1}\mu_c) + x^T \Sigma^{-1}\mu_c - (\frac{1}{2}x^T \Sigma^{-1}x + const)$$
the right most part is independent of class c
$$= r_c + x^T \beta_c + k \tag{1.4}$$

Now, it's more clear that it's a linear function of x.

1.6 LDA VS Logistic regression

The formula 1.4, though we have $p(y=c|x;\theta)$ as its left hand, is actually $p(x|y=c;\theta)p(y=c;\theta)$, the upper part of Bayes Formula, as I mentioned in 1.2.

We can notice that, the lower part of Bayes Formula is the sum of class c' in the same form as the upper part, class c.

So, we can get that

$$p(y = c | x; \theta) = \frac{e^{\beta_c^T x + r_c}}{\sum_{c'} e^{\beta_{c'}^T x + r_{c'}}} = \frac{e^{W_c^T[1, x]}}{\sum_{c'} e^{W_{c'}^T[1, x]}}$$

$$where \ W_c = [r_c, \beta_c]$$
(1.5)

That's exactly what logistic regression will get.

1.7 Binary case

To get more intuition with the relationship of LDA and Logistic regression, let's take a binary case as an example.

$$egin{aligned} p(y=1|x; heta) &= rac{e^{eta_1^Tx + r_1}}{e^{eta_1^Tx + r_1} + e^{eta_0^Tx + r_0}} \ &= rac{1}{1 + e^{(eta_0 - eta_1)^Tx + (r_0 - r_1)}} \ &= \sigma((eta_1 - eta_0)^Tx + (r_1 - r_0)) \end{aligned}$$

To get the form like $\sigma(W^T(x-x_0))$, we can set

$$W = \beta_1 - \beta_0 = \Sigma^{-1}(\mu_1 - \mu_0) \tag{1.6}$$

What we need to do is find a x_0 , which meet $W^Tx_0=-(r_1-r_0)$,

Then, we can easily get that

$$x_0 = \frac{1}{2}(\mu_1 + \mu_0) - (\mu_1 - \mu_0) \frac{\log(\frac{\pi_1}{\pi_0})}{(\mu_1 - \mu_0)^T \Sigma^{-1}(\mu_1 - \mu_0)}$$
(1.7)

With this W and x_0 , we have

$$p(y=1|x;\theta) = \sigma(W^T(x-x_0))$$
(1.8)

And it's equal to

$$\hat{y}(x) = 1$$
 iff $W^T x > c$, where $c = W^T x_0$

GEO intuition

We knew that $W = \Sigma^{-1}(\mu_1 - \mu_0)$,

if
$$\Sigma = \sigma^2 I$$
 .

then $W=\sigma^2(\mu_1-\mu_0)$, is parallel to a line joining to the two centroids of these two classes.

And the product of x and W is to project x to this line, and find whether it's close to class 1 or class 0.

1.8 Model fitting

We are here focusing on mathematical solutions, not gradient descent.

The likelihood of the dataset is

$$p(D|theta) = \prod_{n=1}^{N} M(y_n|\Pi) \ \prod_{c=1}^{C} N(x_n|\mu_c, \Sigma_c)^{I(y_n=c)}$$

The log likelihood of the dataset would be

$$log \ p(D|\theta) = \left[\sum_{n=1}^{N} \sum_{c=1}^{C} I(y_{n=c}) log \Pi_{c}\right] + \sum_{c=1}^{C} \left[\sum_{n: y_{n}=c} log N(x_{n}|\mu_{c}, \Sigma_{c})\right] \tag{1.9}$$

So, we can optimize Π and (μ_c, Σ_c) seperately.

The result is as follows:

$$\hat{\Pi}_{c} = \frac{N_{c}}{N}$$

$$\hat{\mu}_{c} = \frac{1}{N_{c}} \sum_{n:y_{n}=c} x_{n}$$

$$\hat{\Sigma}_{c} = \frac{1}{N_{c}} \sum_{n:y_{n}=c} (x_{n} - \hat{\mu}_{c})(x_{n} - \hat{\mu}_{c})^{T}$$

$$\text{If } \Sigma_{c} = \Sigma, \text{ then}$$

$$\hat{\Sigma} = \frac{1}{N} \sum_{c=1}^{C} \sum_{n:y_{n}=c} (x_{n} - \hat{\mu}_{c})(x_{n} - \hat{\mu}_{c})^{T}$$

$$(1.10)$$

The deduction is in Chapter 2.

2. Deduction of Log likelihood

2.1 Optimization of $\hat{\Pi}_c$

When focusing on Π_{c} , the LL can be written as

$$LL = \sum_{c=1}^{C} N_c log(\Pi_c)$$

And the constraint is

$$\sum_{c=1}^{C} \Pi_c = 1$$

Then, the Lagrangian is as follows:

$$L := \sum_{c=1}^{C} N_c log(\Pi_c) - \lambda (\sum_{c=1}^{C} \Pi_c - 1)$$
 (2.1)

Taking derivatives with respect to λ , we get

$$\frac{\partial L}{\partial \lambda} = \sum_{c=1}^{C} \Pi_c - 1 = 0$$

And the derivation with respect to Π_c is:

$$\frac{\partial L}{\partial \Pi_c} = \frac{N_c}{\Pi_c} - \lambda = 0$$
$$\Pi_c = \frac{N_c}{\lambda}$$

To get rid of λ , we can make use of the sum of Π_c :

$$\sum_c\Pi_c=\sum_crac{N_c}{\lambda}=rac{N}{\lambda}$$
 We knew that $\sum_c\Pi_c=1,$ so $rac{N}{\lambda}=1,$ $N=\lambda$

As a result,

$$\Pi_c = rac{N_c}{N}$$

2.2 Optimization of μ_c

First of all, the derivation of μ_c will remove all the parameters that's not of class c.

The log likelihood with respect to class c is:

$$LL_c = \sum_{n=1}^{N_c} log N(x_n | \mu_c, \Sigma)$$

$$= \frac{N_c}{2} log |\Lambda| - \frac{1}{2} \sum_{n=1}^{N_c} (x_n - \mu_c)^T \Lambda(x_n - \mu_c), \text{ ignore the constant and } \Lambda = \lambda^{-1}$$
(2.2)

Let $z_n=x_n-\mu_c$, then

$$egin{aligned} rac{\partial LL_c}{\partial \mu_c} &= -rac{1}{2} \sum_{n=1}^{N_c} rac{\partial z_n^T \Lambda z_n}{\partial z_n} rac{\partial z_n}{\partial \mu_c} \ &= -rac{1}{2} \sum_{n=1}^{N_c} (\Lambda + \Lambda^T) z_n (-I) \end{aligned}$$

 Λ is a diagnal matrix, $\Lambda^T = \Lambda$

$$=\sum_{n=1}^{N_c}\Lambda z_n=0$$

So we get,

$$\sum_{n=1}^{N_c} \Lambda z_n = 0$$

$$\sum_{n=1}^{N_c} (x_n - \mu_c) = 0$$

$$\mu_c = \overline{x_n}$$
(2.3)

2.3 Optimization of Σ

Here we need

$$tr(scalar) = scalar$$

 $tr(ABC) = tr(BCA) = tr(CAB)$
 $\frac{\partial tr(AB)}{\partial B} = A^{T}$
 $\frac{\partial log|A|}{\partial A} = (A^{-1})^{T}$

Reference: derivation for det

Then, we're good to go,

$$egin{aligned} rac{LL_c}{\Lambda} &= rac{\partial rac{N_c}{2}log|\Lambda| - rac{1}{2}\sum_{n=1}^{N_c}(x_n - \mu_c)^T\Lambda(x_n - \mu_c)}{\partial \Lambda} \ &= rac{\partial rac{N_c}{2}log|\Lambda| - rac{1}{2}\sum_{n=1}^{N_c}tr((x_n - \mu_c)^T\Lambda(x_n - \mu_c))}{\partial \Lambda} \ &= rac{\partial rac{N_c}{2}log|\Lambda| - rac{1}{2}\sum_{n=1}^{N_c}tr((x_n - \mu_c)(x_n - \mu_c)^T\Lambda)}{\partial \Lambda} \ &= rac{N_c}{2}\Lambda^{-1} - rac{1}{2}\sum_{n=1}^{N_c}(x_n - \mu_c)(x_n - \mu_c)^T = 0 \end{aligned}$$

So, we can get

$$egin{aligned} \Lambda^{-1} &= \Sigma_c \ &= rac{1}{N_c} \sum_{n=1}^{N_c} (x_n - \mu) (x_n - \mu)^T \end{aligned}$$

Most part are based on Murphy's book, Probabilistic Machine Learning.

And part 2.3 is based on this blog.