

Probabilistic Graphical Models : Homework 1

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1 Formulas

1.1 Exercise 1

We have N samples (x_i, y_i) $\boldsymbol{\pi} = (\pi_1, \dots, \pi_M)$, $\boldsymbol{\theta} = (\theta_{1,1}, \dots, \theta_{M,K})$
 $a_m = |\{i \mid z_i = m, \forall i \in [1, N]\}|$, $b_{m,k} = |\{i \mid z_i = m \text{ and } x_i = k, \forall i \in [1, N]\}|$

$$\tilde{\pi}_m = \frac{a_m}{N}$$
$$\tilde{\theta}_{m,k} = \frac{b_{m,k}}{N}$$

Moreover $p(y = 1 \mid x)$ have the same form of logistic regression.

1.2 Exercise 2

1.2.1 LDA

$$\tilde{\omega} = \frac{n}{N}$$
$$\tilde{\mu}_0 = \frac{1}{n} \sum_{\substack{i=1, \\ y_i=0}}^N x_i$$
$$\tilde{\mu}_1 = \frac{1}{N-n} \sum_{\substack{i=1, \\ y_i=1}}^N x_i$$
$$\tilde{\Sigma} = \frac{1}{N} \left(\sum_{\substack{i=1, \\ y_i=0}}^N (x_i - \mu_0)^T (x_i - \mu_0) + \sum_{\substack{i=1, \\ y_i=1}}^N (x_i - \mu_1)^T (x_i - \mu_1) \right)$$

1.2.2 QDA

We have N samples and $n = |\{i, y_i = 0, \forall i \in [1, N]\}|$

$$\tilde{\omega} = \frac{n}{N}$$
$$\tilde{\mu}_0 = \frac{1}{n} \sum_{\substack{i=1, \\ y_i=0}}^N x_i$$
$$\tilde{\mu}_1 = \frac{1}{N-n} \sum_{\substack{i=1, \\ y_i=1}}^N x_i$$
$$\tilde{\Sigma}_0 = \frac{1}{n} \sum_{\substack{i=1, \\ y_i=0}}^N (x_i - \mu_0)^T (x_i - \mu_0)$$
$$\tilde{\Sigma}_1 = \frac{1}{N-n} \sum_{\substack{i=1, \\ y_i=1}}^N (x_i - \mu_1)^T (x_i - \mu_1)$$

2 Dataset A

Figure 1: LDA

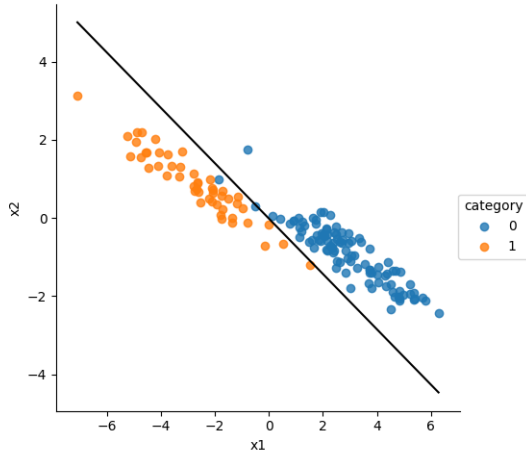


Figure 2: IRLS

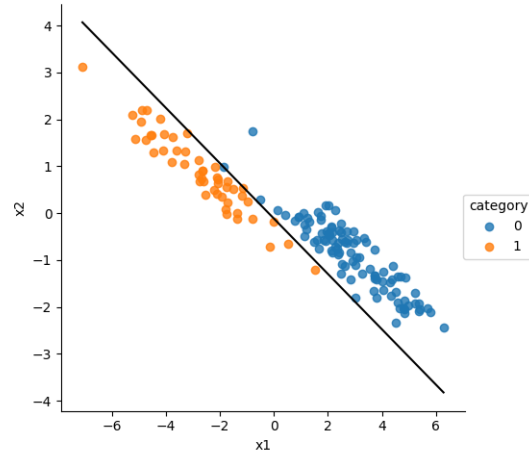


Figure 3: Linear Regression

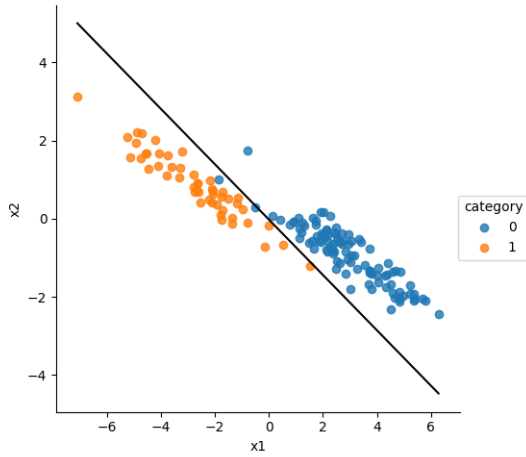
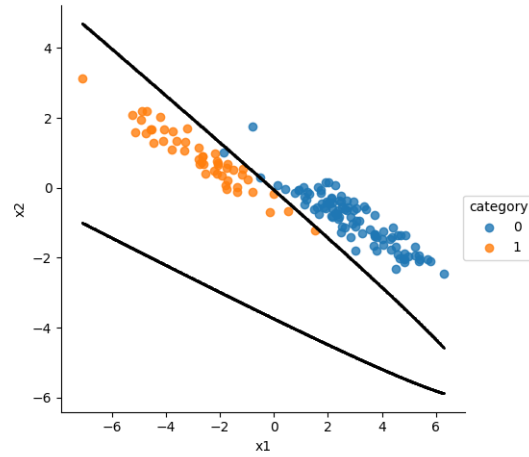


Figure 4: QDA



Results

	Train	Test
LDA	98.7	98.0
IRLS	100	96.5
LR	98.7	97.9
QDA	99.3	98.0

First we see that the model is linearly separable. IRLS scores perfectly on the training set outperforming the other models. However the situation is reversed on the test data. This means that the model overfitted the training data. LDA and Logistic Regression have the same performance which is not a surprise considering that we have proven that the LDA performs in reality a logistic regression. Finally QDA has the worst performance on the training set, but outperforms IRLS on the test data. It is the only model to have improve its test score over its training score which is great.

3 Dataset B

Figure 5: LDA

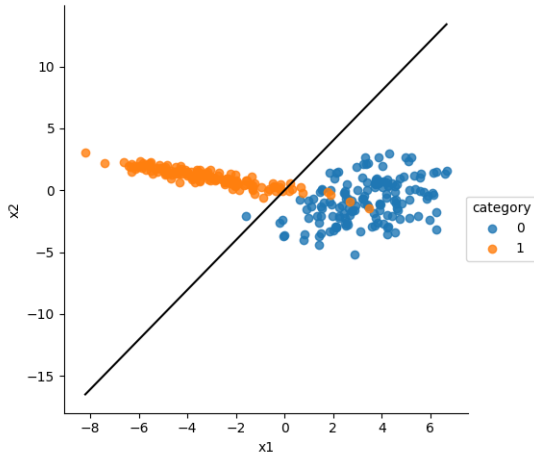


Figure 6: IRLS

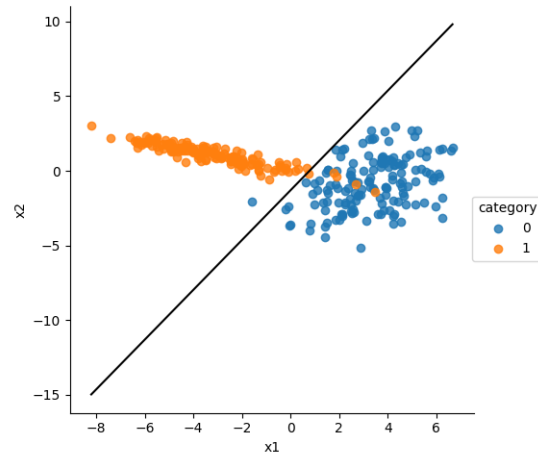


Figure 7: Linear Regression

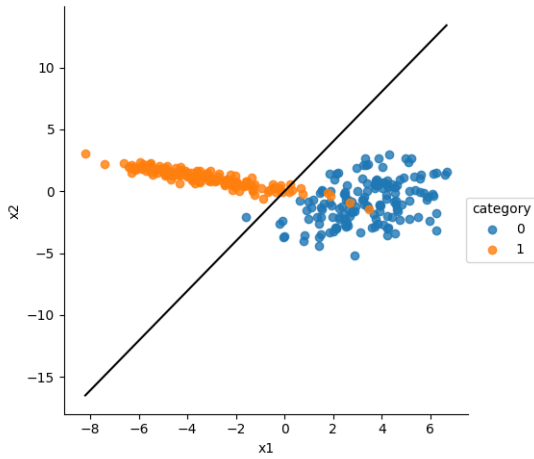
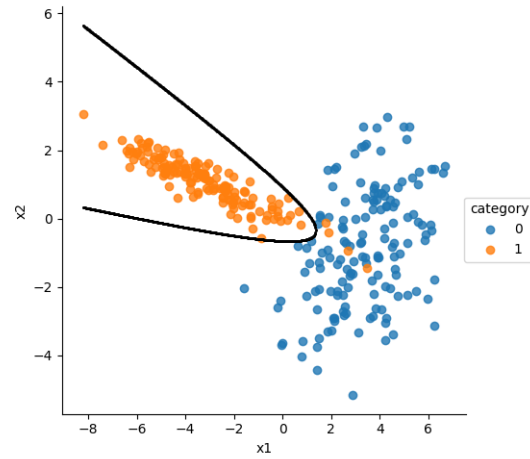


Figure 8: QDA



Results

	Train	Test
LDA	97.0	95.9
IRLS	98.0	95.7
LR	97.0	95.9
QDA	98.7	98.0

First we see that the model is linearly separable. IRLS scores perfectly on the training set outperforming the other models. However the situation is reversed on the test data. This means that the model overfitted the training data. LDA and Logistic Regression have the same performance which is not a surprise considering that we have proven that the LDA performs in reality a logistic regression. Finally QDA has the worst performance on the training set, but outperforms IRLS on the test data. It is the only model to have improve its test score over its training score which is great.

4 Dataset C

Figure 9: LDA

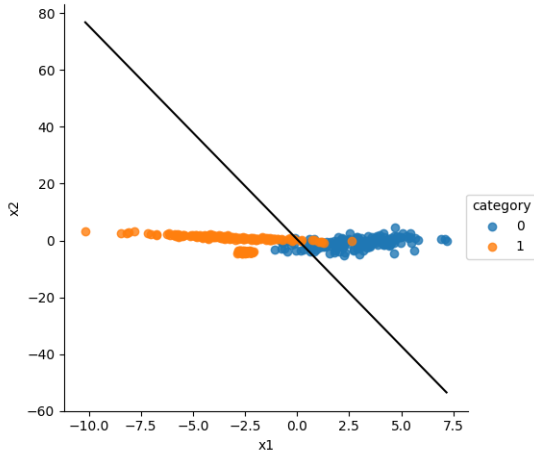


Figure 10: IRLS

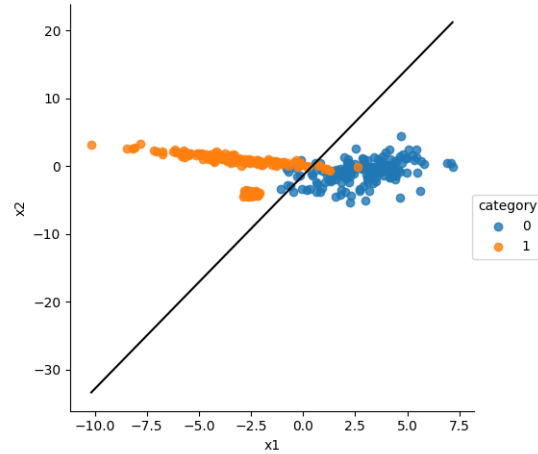


Figure 11: Linear Regression

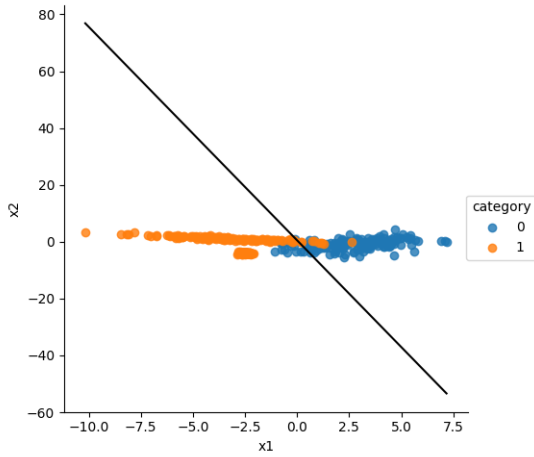
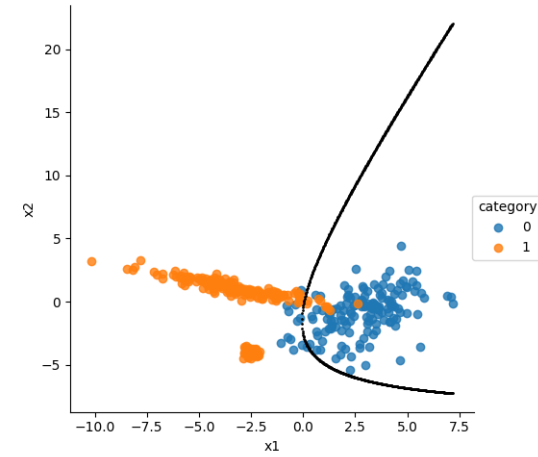


Figure 12: QDA



Results

	Train	Test
LDA	94.5	95.8
IRLS	96.0	97.7
LR	94.5	95.8
QDA	94.8	96.2

First we see that the model is linearly separable. IRLS scores perfectly on the training set outperforming the other models. However the situation is reversed on the test data. This means that the model overfitted the training data. LDA and Logistic Regression have the same performance which is not a surprise considering that we have proven that the LDA performs in reality a logistic regression. Finally QDA has the worst performance on the training set, but outperforms IRLS on the test data. It is the only model to have improve its test score over its training score which is great.

5 Comments on the models

6 Proof

6.1 Exercise 1

We have N samples (x_i, y_i) $\boldsymbol{\pi} = (\pi_1, \dots, \pi_M)$, $\boldsymbol{\theta} = (\theta_{1,1}, \dots, \theta_{M,K})$
 $a_m = |\{i \mid z_i = m, \forall i \in [1, N]\}|$, $b_{m,k} = |\{i \mid z_i = m \text{ and } x_i = k, \forall i \in [1, N]\}|$

$$\begin{aligned} l(\boldsymbol{\pi}, \boldsymbol{\theta}) &= \sum_{i=0}^n \log(p(x_i, z_i)) \\ &= \sum_{i=0}^n \log(p(x_i \mid z_i)p(z_i)) \\ &= \sum_{i=0}^n (\log(\theta_{z_i, x_i}) + \log(\pi_{x_i})) \end{aligned}$$

$l(\boldsymbol{\pi}, \boldsymbol{\theta})$ is concave. We want to minimize $-l(\boldsymbol{\pi}, \boldsymbol{\theta})$ subjected to $\sum_{k=1}^K \pi_k = 1$ and $\sum_{k=1}^K \sum_{m=1}^M \theta_{m,k} = 1$ Lets introduce the langrangian.

$$L(\boldsymbol{\pi}, \boldsymbol{\theta}, \lambda_1, \lambda_2) = -\left(\sum_{i=0}^n (\log(\theta_{z_i, x_i}) + \log(\pi_{x_i}))\right) + \lambda_1 \left(\sum_{k=1}^K \pi_k - 1\right) + \lambda_2 \left(\sum_{k=1}^K \sum_{m=1}^M \theta_{m,k} - 1\right)$$

The Slaters constraint qualification are trivially verified and therefore the problem has strong duality property. Therefore we have

$$\min_{\boldsymbol{\pi}, \boldsymbol{\theta}} -l(\boldsymbol{\pi}, \boldsymbol{\theta}) = \max_{\lambda_1, \lambda_2} L(\boldsymbol{\pi}, \boldsymbol{\theta}, \lambda_1, \lambda_2)$$

Moreover the lagrangian is convex with respect to $\boldsymbol{\pi}$ and $\boldsymbol{\theta}$

$$\begin{aligned} \frac{\partial L}{\partial \pi_m} &= 0 \Rightarrow \tilde{\pi}_m = \frac{a_m}{\lambda_1} \\ \frac{\partial L}{\partial \theta_{m,k}} &= 0 \Rightarrow \tilde{\theta}_{m,k} = \frac{b_{m,k}}{\lambda_2} \end{aligned}$$

Using the constrains we can calculate λ_1, λ_2 .

$$\begin{aligned} \tilde{\pi}_m &= \frac{a_m}{N} \\ \tilde{\theta}_{m,k} &= \frac{b_{m,k}}{N} \end{aligned}$$

6.2 Exercise 2

6.2.1 Generative model LDA

We have N samples and $n = |\{i, y_i = 0, \forall i \in [1, N]\}|$

$$\begin{aligned} l(\omega, \Sigma, \mu_0, \mu_1) &= \sum_{i=1}^N \log(p(x_i, y_i)) \\ &= \sum_{i=1}^N \log(p(x_i \mid y_i)p(y_i)) \\ &= \sum_{\substack{i=1, \\ y_i=0}}^N \log(p(x_i \mid y_i = 0)) + n \log(\omega) + \sum_{\substack{i=1, \\ y_i=0}}^N \log(p(x_i \mid y_i = 1)) + (N - n) \log(1 - \omega) \\ &= -\frac{Nd}{2} \log(2\pi) + \frac{N}{2} \log(|\Sigma^{-1}|) - \sum_{\substack{i=1, \\ y_i=0}}^N \frac{1}{2} (x_i - \mu_0)^T \Sigma^{-1} (x_i - \mu_0) \\ &\quad - \sum_{\substack{i=1, \\ y_i=1}}^N \frac{1}{2} (x_i - \mu_1)^T \Sigma^{-1} (x_i - \mu_1) + n \log(\omega) + (N - n) \log(1 - \omega) \end{aligned}$$

This log likelihood is not concave in $(\omega, \Sigma, \mu_0, \mu_1)$. It is concave in (ω, μ_0, μ_1) with Σ fixed.

$$\nabla_{\omega} l = \frac{n}{\omega} - \frac{N-n}{1-\omega}$$

$\nabla_{\omega} l = 0$ gives us :

$$\tilde{\omega} = \frac{n}{N}$$

Calculating the gradient in μ_0, μ_1 and equalating it to 0 gives us.

$$\begin{aligned}\tilde{\mu}_0 &= \frac{1}{n} \sum_{\substack{i=1, \\ y_i=0}}^N x_i \\ \tilde{\mu}_1 &= \frac{1}{N-n} \sum_{\substack{i=1, \\ y_i=1}}^N x_i\end{aligned}$$

Let us now differentiate l w.r.t. Σ^{-1} .

Let $A = \Sigma^{-1}$, $\Sigma_0 = \frac{1}{n} \sum_{\substack{i=1, \\ y_i=0}}^N (x_i - \mu_0)^T (x_i - \mu_0)$,

$\Sigma_1 = \frac{1}{N-n} \sum_{\substack{i=1, \\ y_i=1}}^N (x_i - \mu_1)^T (x_i - \mu_1)$

We have :

$$\begin{aligned}l(\omega, \Sigma, \mu_0, \mu_1) &= -\frac{Nd}{2} \log(2\pi) + \frac{N}{2} \log(|\Sigma^{-1}|) - \frac{1}{2} \text{Trace}(A(n\Sigma_0 + (N-n)\Sigma_1)) \\ &\quad + n \log(\omega) + (N-n) \log(1-\omega) \\ \nabla_A l &= \frac{N}{2} A^{-1} - \frac{1}{2} (n\Sigma_0 + (N-n)\Sigma_1)\end{aligned}$$

Which leads to

$$\tilde{\Sigma} = \frac{n}{N} \Sigma_0 + \frac{N-n}{N} \Sigma_1$$

We have found a unique stationnary point for the likelihood. To be sure it is a maximum we would have to calculate the Hessian.

Now we will calculate the $p(y = 1 | x)$.

$$p(y = 1 | x) = \frac{p(x | y = 1)p(y = 1)}{p(x)}$$

$$\begin{aligned}\log\left(\frac{p(y = 1 | x)}{p(y = 0 | x)}\right) &= \log\left(\frac{1-\omega}{\omega}\right) - \frac{1}{2}(x - \mu_1)\Sigma^{-1}(x - \mu_1) + \frac{1}{2}(x - \mu_0)\Sigma^{-1}(x - \mu_0) \\ \log\left(\frac{p(y = 1 | x)}{p(y = 0 | x)}\right) &= \log\left(\frac{1-\omega}{\omega}\right) + \frac{1}{2}(\mu_0^T \Sigma^{-1} \mu_0 - \mu_1^T \Sigma^{-1} \mu_1) + x^T \Sigma^{-1}(\mu_1 - \mu_0) \\ p(y = 1 | x) &= \frac{1}{1 + \frac{\omega}{1-\omega} \exp\left(\frac{1}{2}(\mu_1^T \Sigma^{-1} \mu_1 - \mu_0^T \Sigma^{-1} \mu_0)\right) \exp(-x^T \Sigma^{-1}(\mu_1 - \mu_0))}\end{aligned}$$

It is of the form

$$p(y = 1 | x) = \frac{1}{1 + \exp(-(x^T a + \alpha))}$$

It is the formula of logistic regression

6.2.2 QDA model

We have N samples and $n = |\{i, y_i = 0, \forall i \in [1, N]\}|$

$$\begin{aligned}
l(\omega, \Sigma_0, \Sigma_1, \mu_0, \mu_1) &= \sum_{i=1}^N \log(p(x_i, y_i)) \\
&= \sum_{i=1}^N \log(p(x_i | y_i)p(y_i)) \\
&= \sum_{\substack{i=1, \\ y_i=0}}^N \log(p(x_i | y_i = 0)) + n \log(\omega) + \sum_{\substack{i=1, \\ y_i=1}}^N \log(p(x_i | y_i = 1)) + (N - n) \log(1 - \omega) \\
&= n \log(\omega) - \frac{Nd}{2} \log(2\pi) + \frac{n}{2} \log(|\Sigma_0^{-1}|) - \sum_{\substack{i=1, \\ y_i=0}}^N \frac{1}{2} (x_i - \mu_0)^T \Sigma_0^{-1} (x_i - \mu_0) \\
&\quad + (N - n) \log(1 - \omega) + \frac{N - n}{2} \log(|\Sigma_1^{-1}|) - \sum_{\substack{i=1, \\ y_i=1}}^N \frac{1}{2} (x_i - \mu_1)^T \Sigma_1^{-1} (x_i - \mu_1)
\end{aligned}$$

This log likelihood is not concave in $(\omega, \Sigma_0, \Sigma_1, \mu_0, \mu_1)$. It is concave in (ω, μ_0, μ_1) with Σ_0 and Σ_1 fixed. We obtain like in the previous questions.

$$\begin{aligned}
\tilde{\omega} &= \frac{n}{N} \\
\tilde{\mu}_0 &= \frac{1}{n} \sum_{\substack{i=1, \\ y_i=0}}^N x_i \\
\tilde{\mu}_1 &= \frac{1}{N - n} \sum_{\substack{i=1, \\ y_i=1}}^N x_i
\end{aligned}$$

Differentiating l w.r.t. Σ_0^{-1} with the rest fixed and equalizing to 0 (and then doing the same with Σ_1^{-1}) gives us.

$$\begin{aligned}
\tilde{\Sigma}_0 &= \frac{1}{n} \sum_{\substack{i=1, \\ y_i=0}}^N (x_i - \mu_0)^T (x_i - \mu_0) \\
\tilde{\Sigma}_1 &= \frac{1}{N - n} \sum_{\substack{i=1, \\ y_i=1}}^N (x_i - \mu_1)^T (x_i - \mu_1)
\end{aligned}$$

We did not provide the calculations because it is almost the same as above.