

Probabilistic Graphical Models
Homework 1

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1 Exercice 1: learning in discrete graphical model

Let z and x be two discrete random variables such that $p(z = m) = \pi_m$ and $p(x = k|z = m) = \theta_{k,m}$ with $k \in \llbracket 1, K \rrbracket$, $m \in \llbracket 1, M \rrbracket$. The maximization of the log-likelihood (see Appendix) gives :

$$\forall m \in \llbracket 1, M \rrbracket, \hat{\pi}_m = \frac{n(z)_m}{n}$$

$$\forall m \in \llbracket 1, M \rrbracket, k \in \llbracket 1, K \rrbracket, \hat{\theta}_{m,k} = \frac{n(z, x)_{m,k}}{n(z)_m}$$

where $n(z)_m = \sum_{i=1}^n \mathbb{1}_{(z^i=m)}$ and $n(z, x)_{m,k} = \sum_{i=1}^n \mathbb{1}_{(z^i=m)} \mathbb{1}_{(x^i=k)}$.

2 Exercice 2.1(a): LDA

We consider the following model:

$$y \sim \mathcal{B}(\pi) \text{ and } x|y = j \sim \mathcal{N}(\mu_j, \Sigma)$$

The maximization of the log likelihood yields :

$$\hat{\pi} = \frac{\sum_{i=1}^n \mathbb{1}_{(y_i=1)}}{n}, \quad \hat{\mu}_j = \frac{\sum_{i=1}^n \mathbb{1}_{(y_i=j)} x_i}{\sum_{i=1}^n \mathbb{1}_{(y_i=j)}} \text{ for } j = 0, 1, \quad \hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n \sum_{j=0,1} \mathbb{1}_{(y_i=j)} (x_i - \hat{\mu}_j)^T (x_i - \hat{\mu}_j)$$

Also, $p(y = 1|x)$ is analogous to a logistic regression : $p(y = 1|x) = \sigma(b^T x + a)$ with:

$$a = \log \frac{\pi}{1 - \pi} - \frac{1}{2} \left(\mu_1^T \Sigma \mu_1 - \mu_0^T \Sigma \mu_0 \right), \quad b = \Sigma^{-1T} (\mu_0 - \mu_1)$$

3 Exercice 2.5(a): QDA

We now consider different covariance matrix for each class:

$$y \sim \mathcal{B}(\pi) \text{ and } x|y = j \sim \mathcal{N}(\mu_j, \Sigma_j)$$

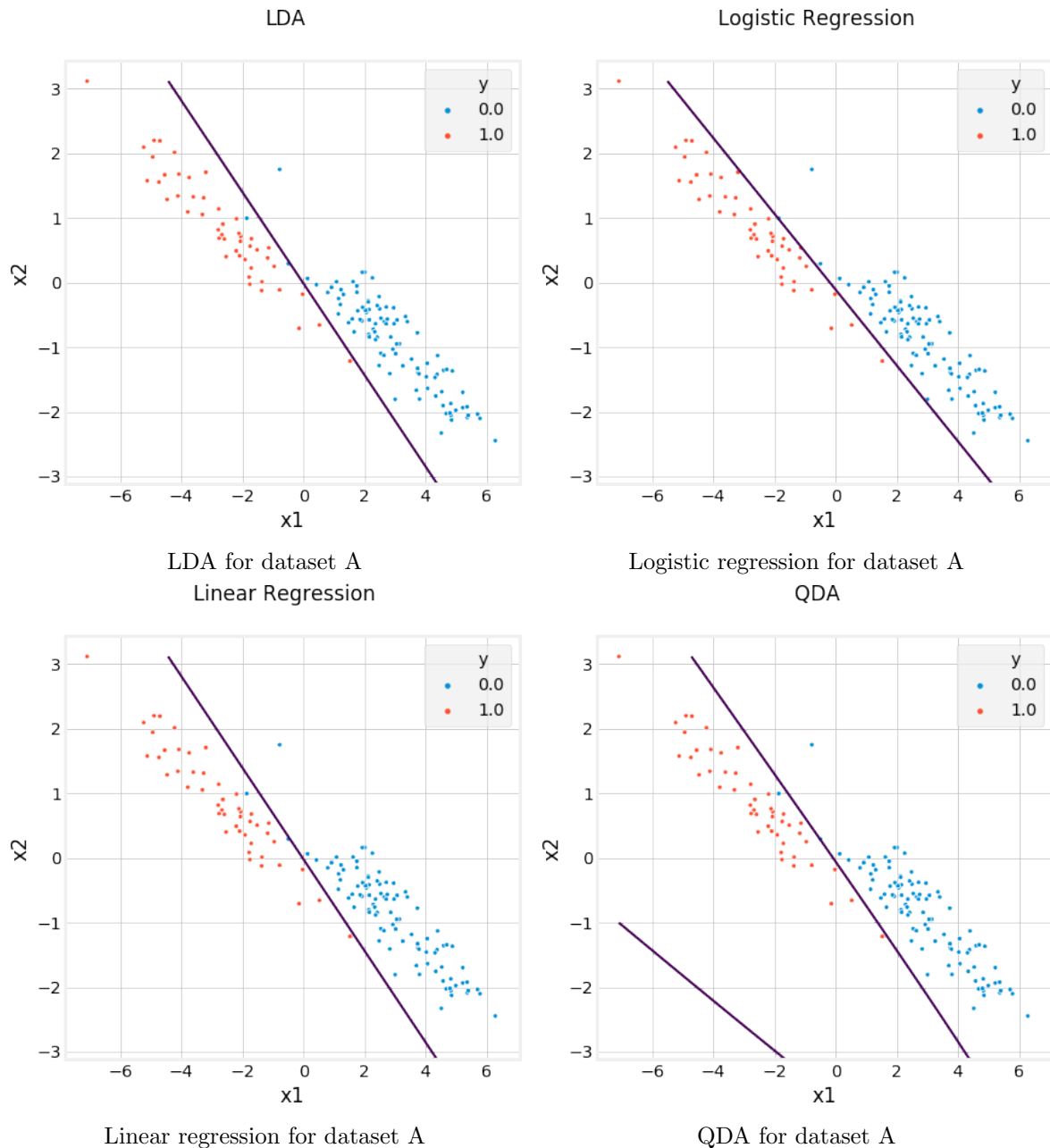
The MLE estimators are now:

$$\hat{\pi} = \frac{\sum_{i=1}^n \mathbb{1}_{(y_i=1)}}{n}, \quad \hat{\mu}_j = \frac{\sum_{i=1}^n \mathbb{1}_{(y_i=j)} x_i}{\sum_{i=1}^n \mathbb{1}_{(y_i=j)}} \text{ for } j = 0, 1, \quad \hat{\Sigma}_j = \frac{\sum_{i|y_i=j} (x_i - \hat{\mu}_j)^T (x_i - \hat{\mu}_j)}{\sum_{i=1}^n \mathbb{1}_{(y_i=j)}} \text{ for } j = 0, 1$$

Also we have $p(y = 1|x) = \sigma(-\frac{1}{2}x^T M x + b^T x + a)$ with

$$M = \Sigma_1^{-1} - \Sigma_0^{-1}, \quad b^T = \mu_1^T \Sigma_1^{-1} - \mu_0^T \Sigma_0^{-1}, \quad a = \log \frac{\pi \sqrt{\det \Sigma_0}}{(1 - \pi) \sqrt{\det \Sigma_1}} - \frac{1}{2} \left(\mu_1^T \Sigma_1^{-1} \mu_1 - \mu_0^T \Sigma_0^{-1} \mu_0 \right)$$

4 Dataset A

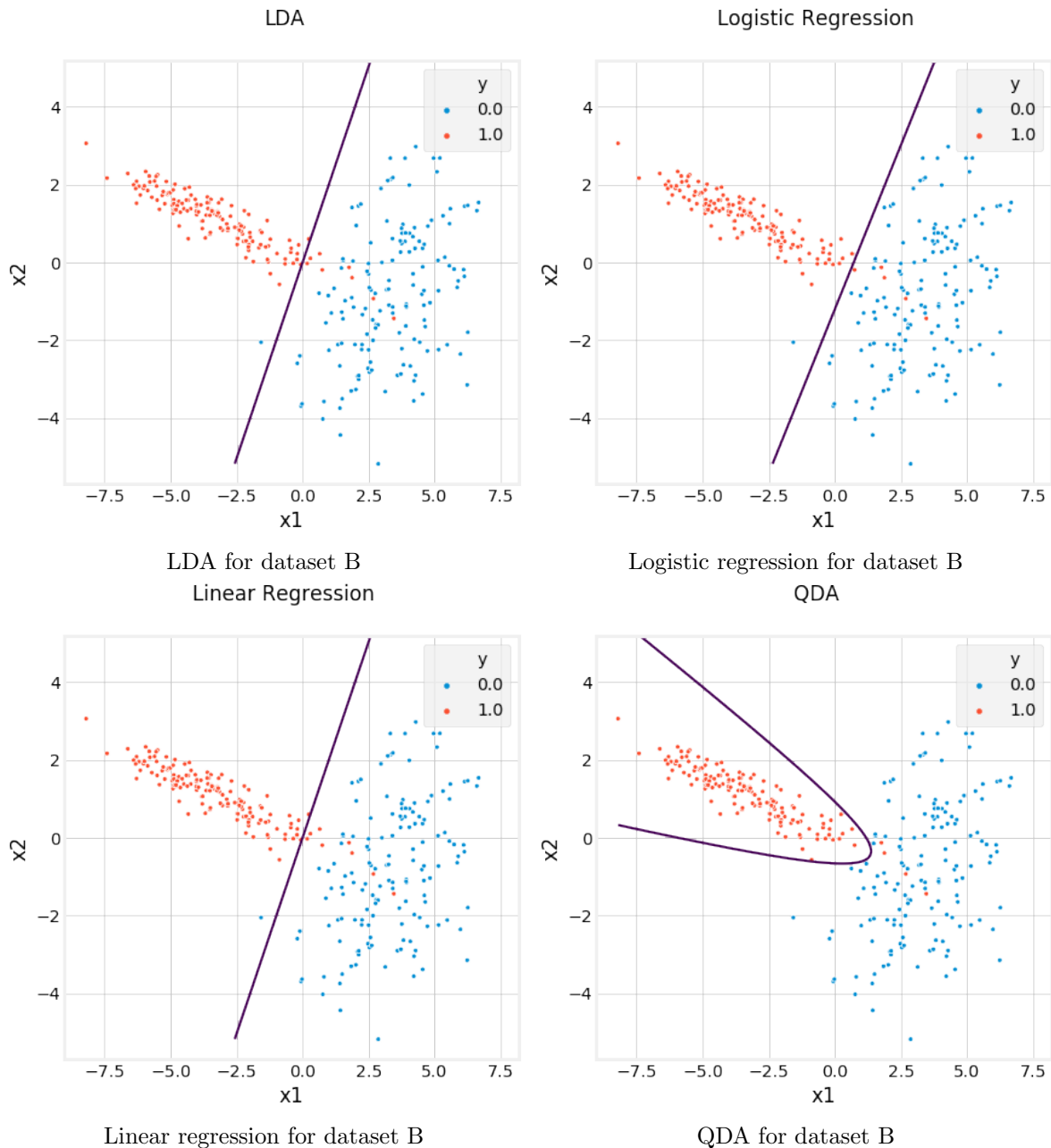


Classification error (in %)		
Model	Train	Test
LDA	1.33	2.00
Logistic reg. ^a	0.00	3.53
Linear reg.	1.33	2.07
QDA	0.67	2.00

^aThe logistic regression is computed using the IRLS algorithm with an error term $= 10^{-3}$.

- All four methods perform better on the training data than on the test data.
- The logistic regression seems to overfit the data (very low training error but relatively high test error). To avoid this we can add a regularization term.
- The QDA seems to overfit the data as well since it assumes a more complex distribution compared to the actual one.
- The LDA and linear methods have very similar performances.

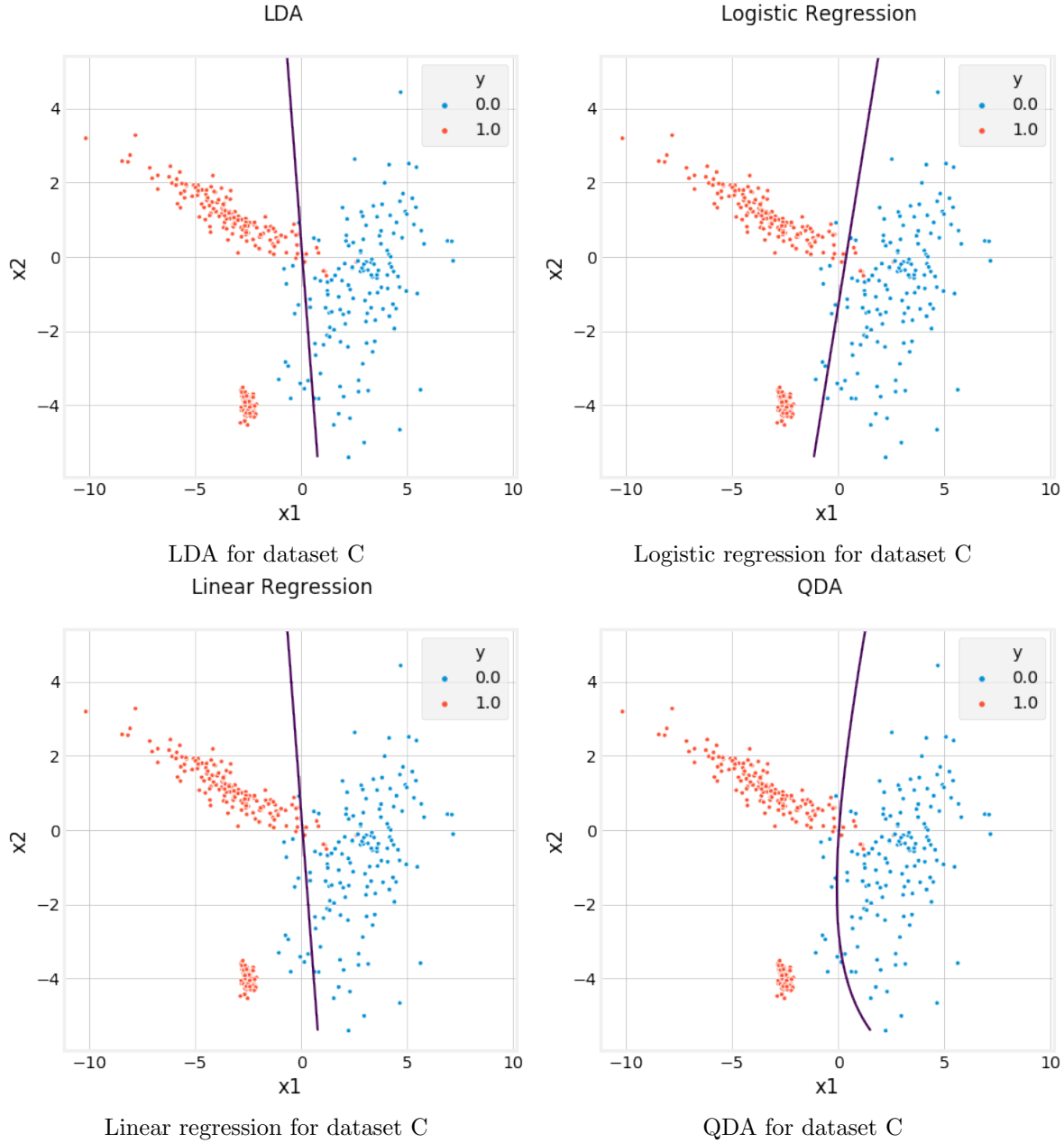
5 Dataset B



Classification error (in %)		
Model	Train	Test
LDA	3.00	4.15
Logistic reg.	2.00	4.25
Linear reg.	3.00	4.15
QDA	1.33	2.00

- Again, all four methods perform better on the training data than on the test data.
- The QDA performs better than the LDA since the hypothesis of equal variance do not hold here.
- Generative modelling with QDA outperforms the logistic regression in this context where the assumptions it makes hold and there is relatively few data to learn from.
- The LDA and Linear Regression perform similarly.

6 Dataset C



Classification error (in %)		
Model	Train	Test
LDA	5.50	4.23
Logistic reg.	4.00	2.30
Linear reg.	5.50	4.23
QDA	5.25	3.83

- Here, all four methods performs better on the test data than on the training data. While this is surprising, it is probably due to a different proportion of data points found in the small bottom cluster that are easier to classify (1/4 of data points in training data vs. 1/3 in test data).
- As for the other data sets, the LDA and Linear method have identical performances which shows the similarity in their underlying assumptions.
- The Logistic Regression performs better than the other methods since it is the only method that do not rely on a Gaussian assumption, which do not hold here.

7 Appendix

7.1 Exercise 1: Discrete model

Let z and x be two discrete random variables such that $p(z = m) = \pi_m$ and $p(x = k|z = m) = \theta_{k,m}$ with $k \in \llbracket 1, K \rrbracket$, $m \in \llbracket 1, M \rrbracket$. We also introduce the variables $(Z_m)_m$ and $(X_k)_k$ such that $Z_m = \mathbb{1}_{z=m}$ and $X_k = \mathbb{1}_{x=k}$

Given $((x_1, z_1), \dots, (x_n, z_n))$ n i.i.d observations, the likelihood of such observations is:

$$p(\pi, \theta) = \prod_{i=1}^n \mathbb{P}_\pi(z = z_i) \mathbb{P}_\theta(x = x_i | z = z_i) = \prod_{i=1}^n \prod_{m=1}^M \left(\pi^{Z_m^i} \prod_{k=1}^K \theta_{m,k}^{X_k^i Z_m^i} \right)$$

We compute the log-likelihood:

$$\begin{aligned} \log p(\pi, \theta) &= \sum_{i=1}^n \left(\sum_{m=1}^M Z_m^i \log \pi_m + \sum_{m=1}^M \sum_{k=1}^K X_k^i Z_m^i \log \theta_{m,k} \right) \\ &= \sum_{m=1}^M n(z)_m \log \pi_m + \sum_{m=1}^M \sum_{k=1}^K n(z, x)_{m,k} \log \theta_{m,k} \end{aligned}$$

where $n(z)_m = \sum_{i=1}^n \mathbb{1}_{(z^i=m)}$ and $n(z, x)_{m,k} = \sum_{i=1}^n \mathbb{1}_{(z^i=m)} \mathbb{1}_{(x^i=k)}$.

Since $\log p$ is strictly concave w.r to π_m and $\theta_{m,k}$ for all $k \in \llbracket 1, K \rrbracket$, $m \in \llbracket 1, M \rrbracket$, it has a unique global maximum on the set $\mathcal{D} = \left\{ \pi, \theta \mid \sum_{i=m}^M \pi_m = 1, \sum_{i=m}^M \sum_{k=1}^K \theta_{m,k} = 1 \right\}$

The two terms above depend only of the $(\pi_m)_m$ and the $(\theta_{m,k})_{m,k}$ respectively, so we optimize then seprately:

$$\begin{aligned} \sum_{m=1}^M n(z)_m \log \pi_m &= \sum_{m=1}^M n(z)_m \log \left(\frac{\pi_m}{n(z)_m} n \frac{n(z)_m}{n} \right) \\ &= \sum_{m=1}^M n(z)_m \log \left(\frac{\pi_m}{n(z)_m} n \right) + C \\ &\leq \sum_{m=1}^M n(z)_m \left(\frac{\pi_m}{n(z)_m} n - 1 \right) + C \end{aligned}$$

with $C = \sum_{m=1}^M n(z)_m \log \frac{n(z)_m}{n}$ a constant.

Also,

$$\sum_{m=1}^M n(z)_m \left(\frac{\pi_m}{n(z)_m} n - 1 \right) = n \underbrace{\left(\sum_{m=1}^M \pi_m \right)}_{=1} - \underbrace{\sum_{m=1}^M n(z)_m}_{=n} = 0$$

Therefore $\sum_{m=1}^M n(z)_m \log \pi_m \leq C$ with equality if $\forall m \in \llbracket 1, M \rrbracket$, $\pi_m = \hat{\pi}_m = \frac{n(z)_m}{n}$

Since $\sum_{m=1}^M n(z)_m \log \pi_m$ is strictly concave in π_m , $\hat{\pi} = (\hat{\pi}_m)_m$ is its unique global optimum.

Similarly,

$$\begin{aligned} \sum_{m=1}^M \sum_{k=1}^K n(z, x)_{m,k} \log \theta_{m,k} &= \sum_{m=1}^M \sum_{k=1}^K n(z, x)_{m,k} \log \left(\frac{\theta_{m,k}}{n(z, x)_{m,k}} n(z)_m \right) + C' \\ &\leq \sum_{m=1}^M \sum_{k=1}^K n(z, x)_{m,k} \left(\frac{\theta_{m,k}}{n(z, x)_{m,k}} n(z)_m - 1 \right) + C' \end{aligned}$$

with $C' = \sum_{m=1}^M \sum_{k=1}^K n(z, x)_{m,k} \log \left(\frac{n(z, x)_{m,k}}{n(z)_m} \right)$

Since

$$\sum_{m=1}^M \sum_{k=1}^K n(z, x)_{m,k} = n$$

and

$$\sum_{m=1}^M \sum_{k=1}^K \theta_{m,k} n(z)_m = \sum_{m=1}^M n(z)_m \underbrace{\sum_{k=1}^K \theta_{m,k}}_{=1} = \sum_{m=1}^M n(z)_m = n$$

We have $\sum_{m=1}^M \sum_{k=1}^K n(z, x)_{m,k} \left(\frac{\theta_{m,k}}{n(z, x)_{m,k}} n(z)_m - 1 \right) = 0$

Therefore,

$$\sum_{m=1}^M \sum_{k=1}^K n(z, x)_{m,k} \log \theta_{m,k} \leq C'$$

with equality if $\forall k \in \llbracket 1, K \rrbracket, \forall m \in \llbracket 1, M \rrbracket, \theta_{m,k} = \frac{n(x, z)_{m,k}}{n(z)_m}$, which is the optimal point because of the strict concavity of the objective function.

In conclusion, the MLE estimators for this model are:

$$\forall k \in \llbracket 1, K \rrbracket, \forall m \in \llbracket 1, M \rrbracket, \quad \boxed{\widehat{\pi}_m = \frac{n(z)_m}{n}}, \quad \boxed{\widehat{\theta}_{m,k} = \frac{n(x, z)_{m,k}}{n(z)_m}}$$

NB: Here we make the assumption that all classes (m, k) are found at least once in the data. If it is not the case for a given pair (m_0, k_0) , we simply consider the set $\llbracket 1, M \rrbracket \times \llbracket 1, K \rrbracket \setminus \{(m_0, k_0)\}$

7.2 Exercise 2.1: LDA model

We consider the following model:

$$y \sim \mathcal{B}(\pi) \text{ and } x|y = j \sim \mathcal{N}(\mu_j, \Sigma)$$

Given $((x_1, y_1), \dots, (x_n, y_n))$ n i.i.d observations, the log-likelihood of such observations is:

$$\log p(\pi, \mu_0, \mu_1, \Sigma) = \underbrace{\sum_{i=1}^n \left[\overbrace{y_i \log(\pi) + (1 - y_i) \log(1 - \pi)}^A - \log(\sqrt{(2\pi)^d |\Sigma|}) - \underbrace{\frac{1}{2} \sum_{j=0,1} (x_i - \mu_j)^T \Sigma^{-1} (x_i - \mu_j) \mathbb{1}_{(y_i=j)}}_B \right]}_C$$

In order to maximize with respect to π , μ and Σ , we will consider respectively A , B and C .

- $\sum_{i=1}^n y_i \log(\pi) + (1 - y_i) \log(1 - \pi)$ is strictly concave in π because of the strict concavity of the log function. Therefore, the optimization problem

$$\begin{aligned} \max_{\pi} \quad & \log p(\pi, \mu, \Sigma) \\ \text{s.t.} \quad & \pi \in]0, 1[\end{aligned}$$

can be solved by setting the gradient of the objective function to 0:

$$\frac{\partial}{\partial \pi} \log p(\pi, \mu, \Sigma) = \frac{n(y)}{\pi} + \frac{n - n(y)}{1 - \pi} = 0 \iff \boxed{\pi = \hat{\pi} = \frac{n(y)}{n}}$$

with $n(y)$ the number of y^i equal to 1.

- The optimization process in order to find μ_j is the same for $j = 0$ or $j = 1$. Let's consider $j = 0$:

$$\sum_{i=1}^n -\frac{1}{2}(x_i - \mu_0)^T \Sigma^{-1}(x_i - \mu_0) \mathbb{1}_{(y_i=0)} = -\frac{1}{2} \sum_{i=1}^n \text{Tr}(\Sigma^{-1}(x_i - \mu_0)(x_i - \mu_0)^T) \mathbb{1}_{(y_i=0)}$$

This function is differentiable and concave in μ_0 as a quadratic function with a negative leading coefficient.

Therefore, the problem

$$\begin{aligned} \max_{\mu_0} \quad & \log p(\pi, \mu_0, \mu_1, \Sigma) \\ \text{s.t.} \quad & \mu_0 \in [0, 1] \end{aligned}$$

admits a unique optimal solution $\hat{\mu}_0$ such that $\frac{\partial}{\partial \mu_0} \log p(\pi, \hat{\mu}_0, \mu_1, \Sigma) = 0$

$$\Rightarrow \sum_{i=1}^n \Sigma^{-1}(x_i - \hat{\mu}_0) \mathbb{1}_{(y_i=0)} = 0 \iff \boxed{\hat{\mu}_0 = \frac{1}{n(y)_0} \sum_{\substack{i=1 \\ y_i=0}}^n x_i}$$

Respectively for μ_1 :

$$\boxed{\hat{\mu}_1 = \frac{1}{n(y)_1} \sum_{\substack{i=1 \\ y_i=1}}^n x_i}$$

- Since the MLE estimators $\hat{\pi}$, $\hat{\mu}_0$ and $\hat{\mu}_1$ that we found so far do not depend on Σ , the MLE estimator for Σ is found by maximizing $\log p(\hat{\pi}, \hat{\mu}_0, \hat{\mu}_1, \cdot)$, which is equivalent to the following problem:

$$\begin{aligned} \max_{\Sigma} \quad & -\frac{n}{2} \log \det \Sigma - \frac{1}{2} \text{Tr}(\Sigma^{-1} \hat{M}) \\ \text{s.t.} \quad & \Sigma \in \mathcal{S}_{++}^d \end{aligned}$$

where $\hat{M} = \sum_{i=1}^n \sum_{j=0,1} \mathbb{1}_{(y_i=j)} (x_i - \hat{\mu}_j)(x_i - \hat{\mu}_j)^T$

The objective function of this optimization problem is not concave because $A \mapsto -\log \det A$ is convex. However, we introduce $\Lambda = \Sigma^{-1}$. The problem is now equivalent to

$$\begin{aligned} \max_{\Lambda} \quad & \frac{n}{2} \log \det \Lambda - \frac{1}{2} \text{Tr}(\Lambda \hat{M}) \\ \text{s.t.} \quad & \Lambda \in \mathcal{S}_{++}^d \end{aligned}$$

where the objective function is concave as the sum of a concave function and a linear function, and the feasible set is convex.

Therefore, it admits an optimal point in $\hat{\Lambda}$ such that, with $f : A \mapsto \frac{n}{2} \log \det A - \frac{1}{2} \text{Tr}(A \hat{M})$,

$$\frac{\partial}{\partial \Lambda} f(\hat{\Lambda}) = \frac{n}{2} \hat{\Lambda}^{-1} - \frac{1}{2} \hat{M} = 0 \iff \hat{\Lambda}^{-1} = \frac{1}{n} \hat{M}$$

Therefore,

$$\boxed{\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n \sum_{j=0,1} \mathbb{1}_{(y_i=j)} (x_i - \hat{\mu}_j)(x_i - \hat{\mu}_j)^T}$$

NB: here we assume that \hat{M} is invertible.

Link to logistic regression

Here we detail how, in such a model, $p(y = 1|x)$ compares to a logistic regression. We express $p(y|x)$ by keeping only the terms that depend on y :

$$\begin{aligned} p(y|x) &= p(y)p(x, y) \\ &\propto \pi^y(1-\pi)^{1-y} \exp\left(-\frac{1}{2}(x-\mu_1)^T \Sigma^{-1}(x-\mu_1)y - \frac{1}{2}(x-\mu_0)^T \Sigma^{-1}(x-\mu_0)(1-y)\right) \\ &\propto \pi^y(1-\pi)^{1-y} \exp\left(-\frac{1}{2}y(2(\mu_0-\mu_1)^T \Sigma^{-1}x + \mu_1^T \Sigma^{-1}\mu_1 - \mu_0^T \Sigma^{-1}\mu_0)\right) \\ &\propto \exp(ya + yb^T x) \end{aligned}$$

with

$$a = \log \frac{\pi}{1-\pi} - \frac{1}{2}(\mu_1 \Sigma^{-1} \mu_1 - \mu_0 \Sigma^{-1} \mu_0), \text{ and } b = -(\Sigma^{-1})^T(\mu_0 - \mu_1)$$

Finally, we obtain $p(y = 1|x)$ by normalizing (thus cancelling all the terms of the product that are constant in y):

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

7.3 Exercise 2.5: QDA model

We consider different covariance matrix for each class:

$$y \sim \mathcal{B}(\pi) \text{ and } x|y = j \sim \mathcal{N}(\mu_j, \Sigma_j)$$

Given $((x_1, y_1), \dots, (x_n, y_n))$ n i.i.d observations, the log-likelihood of such observations is:

$$\begin{aligned} \log p(\pi, \mu_0, \mu_1, \Sigma) &= \sum_{i=1}^n \left[y_i \log(\pi) + (1 - y_i) \log(1 - \pi) \right. \\ &\quad - \mathbb{1}_{(y_i=1)} \left(\log(\sqrt{(2\pi)^d |\Sigma_1|}) + \frac{1}{2}(x_i - \mu_1)^T \Sigma_1^{-1}(x_i - \mu_1) \right) \\ &\quad \left. - \mathbb{1}_{(y_i=0)} \left(\log(\sqrt{(2\pi)^d |\Sigma_0|}) + \frac{1}{2}(x_i - \mu_0)^T \Sigma_0^{-1}(x_i - \mu_0) \right) \right] \end{aligned}$$

- The optimization with respect to π is the same as in the Linear Discriminant Analysis, *i.e.*:

$$\hat{\pi} = \frac{n(y)}{n}$$

- The same goes for each μ_j :

$$\text{For } j = 0, 1, \quad \hat{\mu}_j = \frac{1}{n(y)_j} \sum_{\substack{i=1 \\ y_i=j}}^n x_i$$

- Again, the MLE estimators $\hat{\pi}$, $\hat{\mu}_0$ and $\hat{\mu}_1$ that we found so far do not depend of Σ_0 and Σ_1 , we can compute $\hat{\Sigma}_0$ (resp. $\hat{\Sigma}_1$) by maximizing $-\log p(\hat{\pi}, \hat{\mu}_0, \hat{\mu}_1, \cdot, \Sigma_1)$ (resp. $-\log p(\hat{\pi}, \hat{\mu}_0, \hat{\mu}_1, \Sigma_0, \cdot)$), under the condition that both $\hat{\Sigma}$ do not depend of each other. Because of the symmetry of the terms depending on the Σ_j in the log-likelihood function, the optimization process in order to find each $\hat{\Sigma}_j$ is the same for both $j = 0$ and $j = 1$. For $j = 0$, we have the following optimization problem:

$$\begin{aligned} \max_{\Sigma_0} \quad & -\frac{n}{2} \log \det \Sigma_0 - \frac{1}{2} \text{Tr}(\Sigma_0^{-1} \hat{M}_0) \\ \text{s.t.} \quad & \Sigma_0 \in \mathcal{S}_{++}^d \end{aligned}$$

where $\hat{M}_0 = \sum_{\substack{i=1 \\ y_i=0}}^n (x_i - \hat{\mu}_0)(x_i - \hat{\mu}_0)^T$.

Similarly to the LDA, we introduce $\Lambda_0 = \Sigma_0^{-1}$ so that the objective function $f_0 : A \mapsto \frac{n(y)_0}{2} \log \det A - \frac{1}{2} \text{Tr}(A \hat{M}_0)$ is differentiable and convex. Since the feasible set \mathcal{S}_{++}^d is also convex, we compute $\hat{\Lambda}$ the global maximum with:

$$\frac{\partial}{\partial \Lambda_0} f_0(\hat{\Lambda}_0) = \frac{n(y)_0}{2} \hat{\Lambda}_0^{-1} - \frac{1}{2} \hat{M}_0 = 0 \iff \hat{\Lambda}_0^{-1} = \frac{1}{n(y)_0} \hat{M}_0$$

Hence,

$$\boxed{\hat{\Sigma}_0 = \frac{1}{n(y)_0} \sum_{\substack{i=1 \\ y_i=0}}^n (x_i - \hat{\mu}_0)^T (x_i - \hat{\mu}_0)} \text{ and similarly } \boxed{\hat{\Sigma}_1 = \frac{1}{n(y)_1} \sum_{\substack{i=1 \\ y_i=1}}^n (x_i - \hat{\mu}_1)^T (x_i - \hat{\mu}_1)}$$

Then, we have:

$$\begin{aligned} p(y|x) &\propto \pi^y (1-\pi)^{1-y_i} \exp\left(-\frac{y}{2}(x - \mu_1)^T \Sigma_1^{-1} (x - \mu_1) - \frac{1-y}{2}(x - \mu_0)^T \Sigma_0^{-1} (x - \mu_0)\right) \\ &\quad \cdot \exp\left(-\frac{y}{2} \log \det \Sigma_1 - \frac{1-y}{2} \log \det \Sigma_0\right) \\ &\propto \pi^y (1-\pi)^{1-y_i} \exp\left(-\frac{1}{2} y x^T (\Sigma_1^{-1} - \Sigma_0^{-1}) x + y(\mu_1^T \Sigma_1^{-1} - \mu_0^T \Sigma_0^{-1}) x - \frac{1}{2} y(\mu_1^T \Sigma_1^{-1} \mu_1 - \mu_0^T \Sigma_0^{-1} \mu_0)\right) \\ &\quad \cdot \exp\left(-\frac{y}{2} \log \frac{\det \Sigma_1}{\det \Sigma_0}\right) \\ &\propto \exp\left(-\frac{1}{2} y x^T M x + y b^T x + y a\right) \end{aligned}$$

where

$$\boxed{M = \Sigma_1^{-1} - \Sigma_0^{-1}}, \quad \boxed{b^T = \mu_1^T \Sigma_1^{-1} - \mu_0^T \Sigma_0^{-1}}, \quad \boxed{a = \log \frac{\pi \sqrt{\det \Sigma_0}}{(1-\pi) \sqrt{\det \Sigma_1}} - \frac{1}{2} (\mu_1^T \Sigma_1^{-1} \mu_1 - \mu_0^T \Sigma_0^{-1} \mu_0)}$$

Finally,

$$\boxed{p(y=1|x) = \frac{\exp(-\frac{1}{2} x^T M x + b^T x + a)}{1 + \exp(-\frac{1}{2} x^T M x + b^T x + a)} = \sigma(-\frac{1}{2} x^T M x + b^T x + a)}$$