

HMWK1

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Probabilistic Graphical Models

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MLE of π

Let $(z_i)_{i \in \llbracket 1, n \rrbracket}$ iid, the log-likelihood is given by : $\ell(\pi) = \sum_{m=1}^M n_m \log \pi_m$, $n_m = \sum_{i=1}^n \mathbb{1}_{\{z_i=m\}}$

$-\ell$ being convex and as $\exists \pi \in [0, 1]^M / \pi^T \mathbf{1}_M = 1$, by Slater's constraints qualification we have strong duality and we can address its dual problem given by : $\max_{\lambda} \min_{\pi} \mathcal{L}(\lambda, \pi)$, where $\mathcal{L}(\lambda, \pi) = -\ell(\pi) + \lambda(\pi^T \mathbf{1}_M - 1)$

\mathcal{L} being convex w.r.t π we can minimize it through its gradient : $\forall m, \frac{\partial \mathcal{L}}{\partial \pi_m} = 0 \Rightarrow -\frac{n_m}{\pi_m} + \lambda = 0 \Rightarrow \pi_m = \frac{n_m}{\lambda}$

Plus, $\pi^T \mathbf{1}_M = 1 \Rightarrow \sum_{m=1}^M \frac{n_m}{\lambda} = 1 \Rightarrow \lambda = \sum_{m=1}^M n_m = n$, hence : $\forall m, \hat{\pi}_m = \frac{n_m}{n}$

MLE of Θ

Let $(x_i)_{i \in \llbracket 1, n \rrbracket}$ and $(z_i)_{i \in \llbracket 1, n \rrbracket}$ iid and $\Theta = [\theta_{mk}] \in [0, 1]^{M \times K}$. Conditional probability allow us to write the log-likelihood as : $\ell(\Theta, \pi) = \sum_{m=1}^M n_m \log \pi_m + \sum_{k=1}^K \sum_{m=1}^M n_{mk} \log \theta_{mk}$, $n_m = \sum_{i=1}^n \mathbb{1}_{\{z_i=m\}}$, $n_{mk} = \sum_{i=1}^n \mathbb{1}_{\{z_i=m, x_i=k\}}$

Similarly, $\mathcal{L}(\lambda, \Theta, \pi) = -\ell(\Theta, \pi) + (\pi^T \Theta \mathbf{1}_K - 1 - \pi^T \mathbf{1}_M - 1) \lambda$, $\lambda \in \mathbb{R}_+^2$

Derivating w.r.t π we obtain the same estimator as previously.

For Θ , the derivation goes : $\forall m, k, \frac{\partial \mathcal{L}}{\partial \theta_{mk}} = 0 \Rightarrow -\frac{n_{mk}}{\theta_{mk}} + \lambda_1 \pi_m = 0 \Rightarrow \theta_{mk} = \frac{n_{mk}}{\lambda_1 \pi_m}$

Once again, the constraints gives us $\lambda_1 = n$, hence : $\forall m, k, \hat{\theta}_{mk} = \frac{n_{mk}}{n \hat{\pi}_m} = \frac{n_{mk}}{n_m}$

LDA formulas

$$Y \sim \mathcal{B}(\pi), \quad X | \{Y = i\} \sim \mathcal{N}(\mu_i, \Sigma).$$

$$\hat{\pi} = \frac{1}{N} \sum_{i=1}^n y_i$$

$$\forall j \in \{0, 1\}, \quad \hat{\mu}_j = \frac{\sum_{i=1}^n \mathbb{1}_{\{y_i=j\}} x_i}{\sum_{i=1}^n \mathbb{1}_{\{y_i=j\}}}$$

$$\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{y_i=0\}} (x_i - \hat{\mu}_0)(x_i - \hat{\mu}_0)^T + \mathbb{1}_{\{y_i=1\}} (x_i - \hat{\mu}_1)(x_i - \hat{\mu}_1)^T$$

$$p(y = 1|x) = \frac{1}{2} \Leftrightarrow (\Sigma^{-1}(\mu_1 - \mu_0))^T x + \frac{1}{2} \mu_1^T \Sigma^{-1} \mu_1 - \frac{1}{2} \mu_0^T \Sigma^{-1} \mu_0 = \log \left(\frac{\pi}{1 - \pi} \right)$$

see page 9 for link with logistic regression

QDA formulas

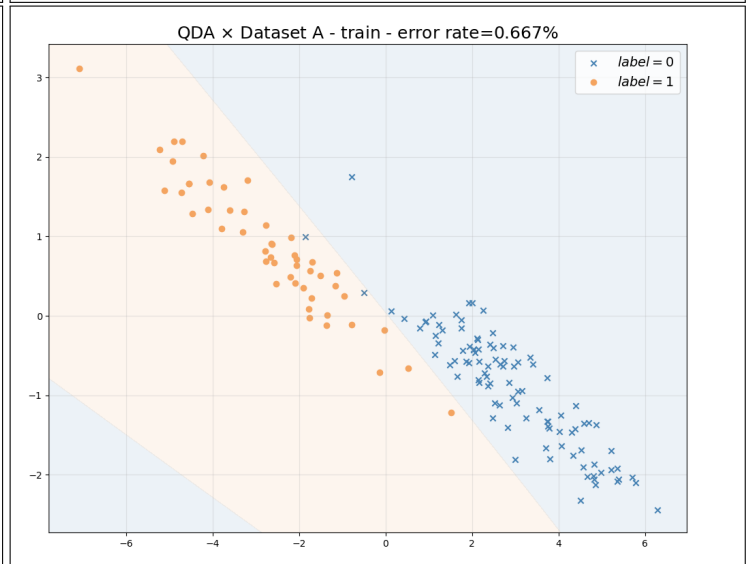
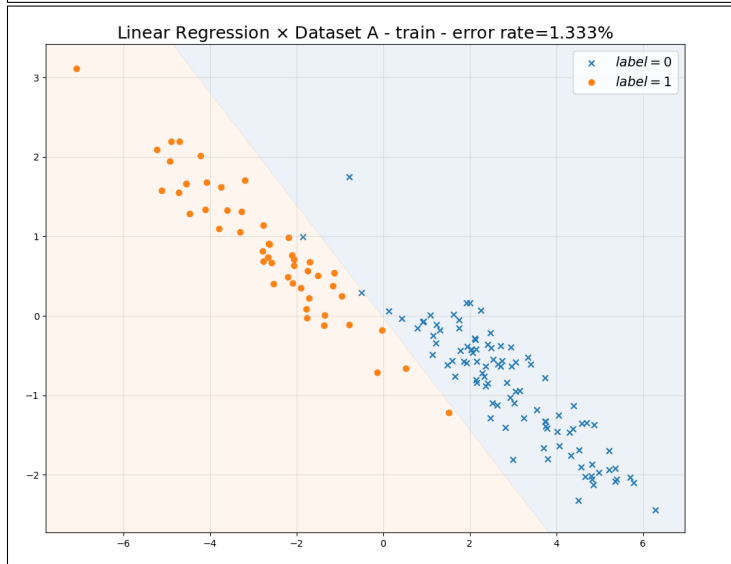
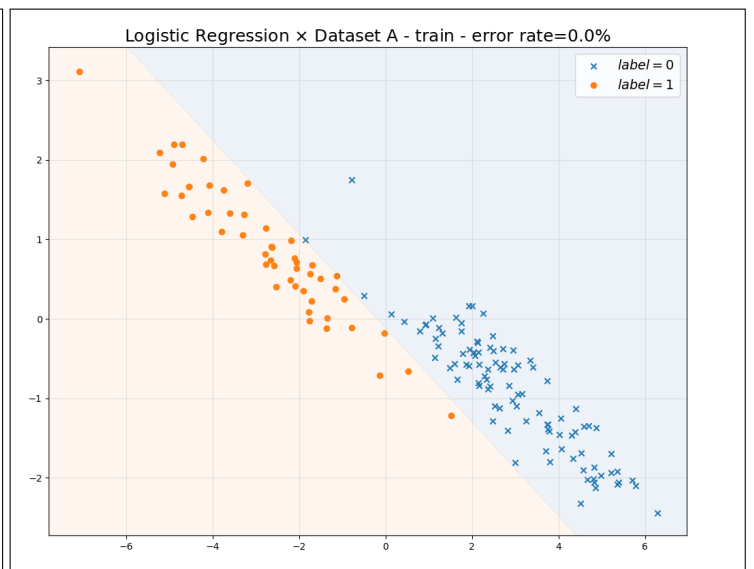
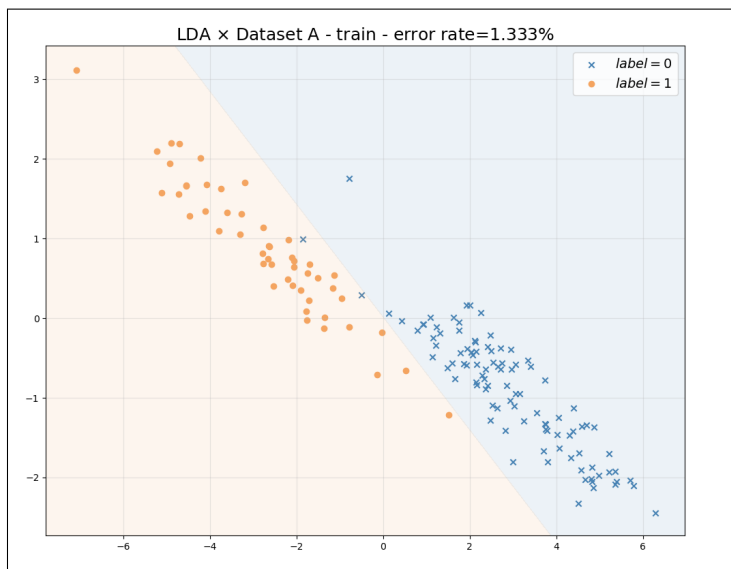
$$Y \sim \mathcal{B}(\pi), \quad X | \{Y = i\} \sim \mathcal{N}(\mu_i, \Sigma_i)$$

$$\hat{\pi} = \frac{1}{N} \sum_{i=1}^n y_i$$

$$\forall j \in \{0, 1\}, \quad \hat{\mu}_j = \frac{\sum_{i=1}^n \mathbb{1}_{\{y_i=j\}} x_i}{\sum_{i=1}^n \mathbb{1}_{\{y_i=j\}}}$$

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

$$p(y = 1|x) = \frac{1}{2} \Leftrightarrow \frac{1}{2} \log \left(\frac{\det \Sigma_1^{-1}}{\det \Sigma_0^{-1}} \right) + \frac{1}{2} [(x - \mu_1)^T \Sigma_1^{-1} (x - \mu_1) - (x - \mu_0)^T \Sigma_0^{-1} (x - \mu_0)] = \log \left(\frac{\pi}{1 - \pi} \right)$$



misclassification on Dataset A (%)

	test	train
LDA	2.000	1.333
Linear Regression	2.067	1.333
Logistic Regression	3.467	0.000
QDA	2.000	0.667

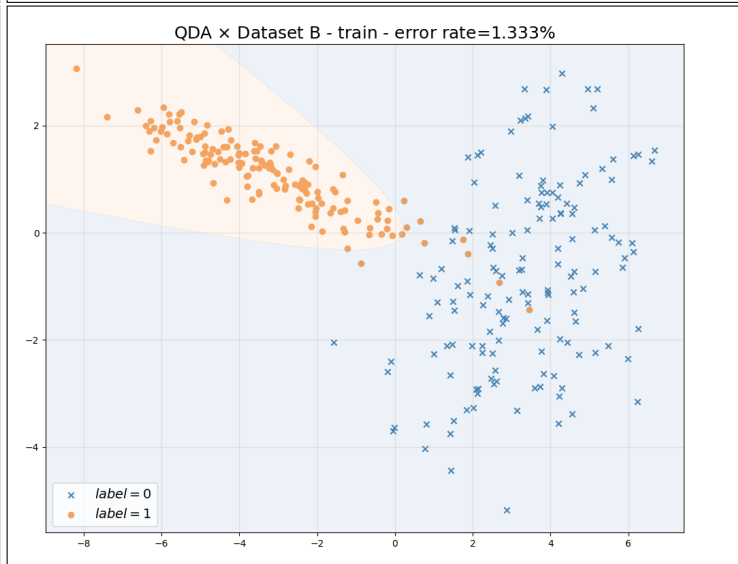
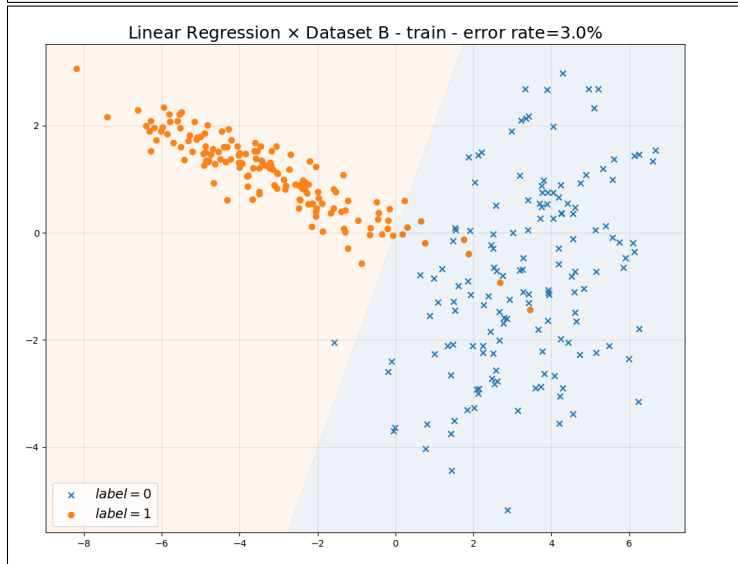
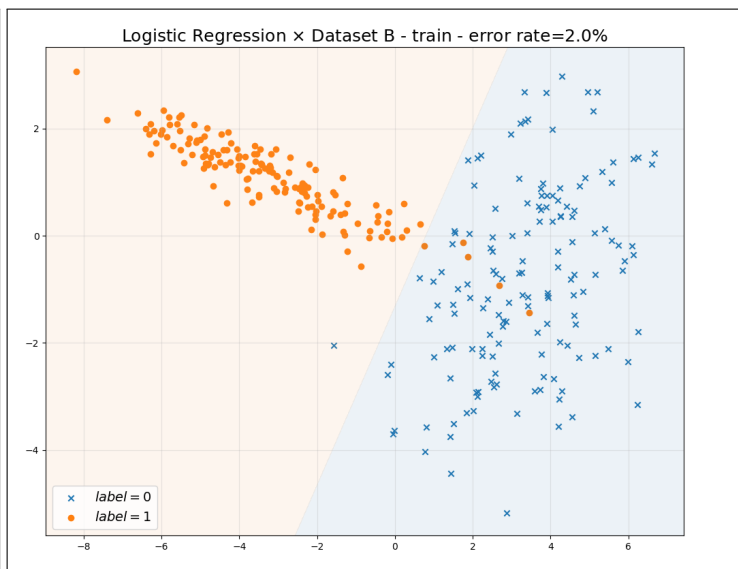
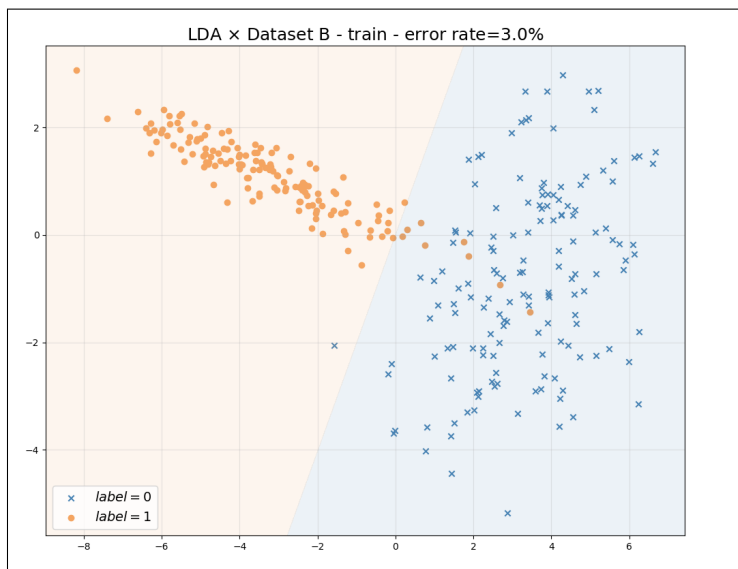
Comments:

Globally, data is linearly separable and all classifiers provide satisfying results. Logistic regression even returns a perfect score on the training set.

The best performer here is QDA, but LDA yields similar performances as the "scattering" of the two classes are similar (supporting the assumption of a unique covariance matrix).

misclassification tends to be larger on the testing set than on the training set which is an expected behavior as our classifiers learn from the train data and should hence be better at predicting from this dataset. Having a testing set 10 times larger than the training set emphasises this trend by challenging the model robustness.

For instance, Logistic Regression yields very dissimilar results, pointing out a lack of robustness.



misclassification on Dataset B (%)

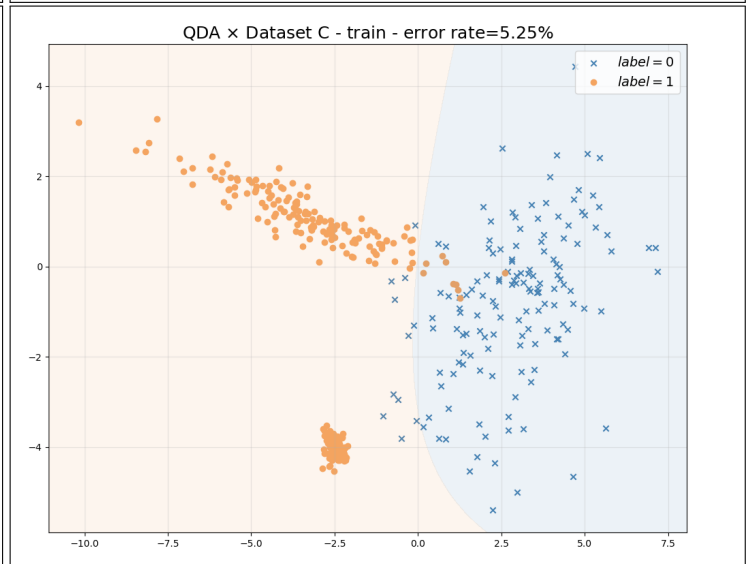
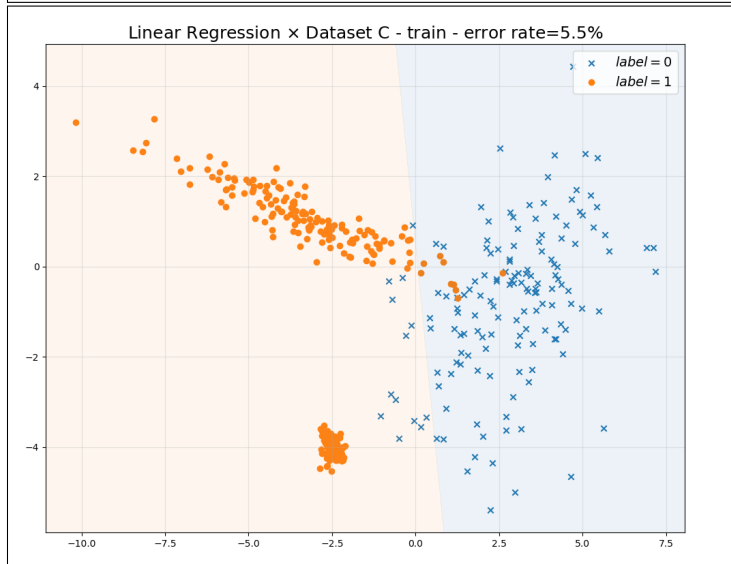
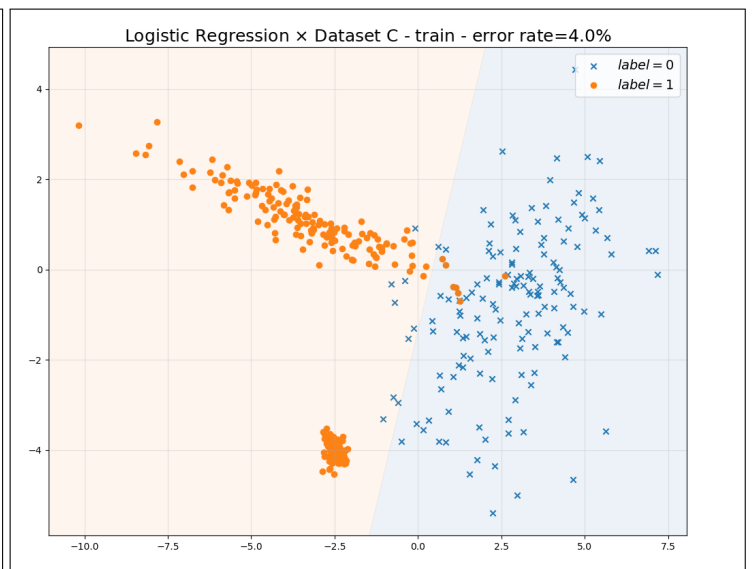
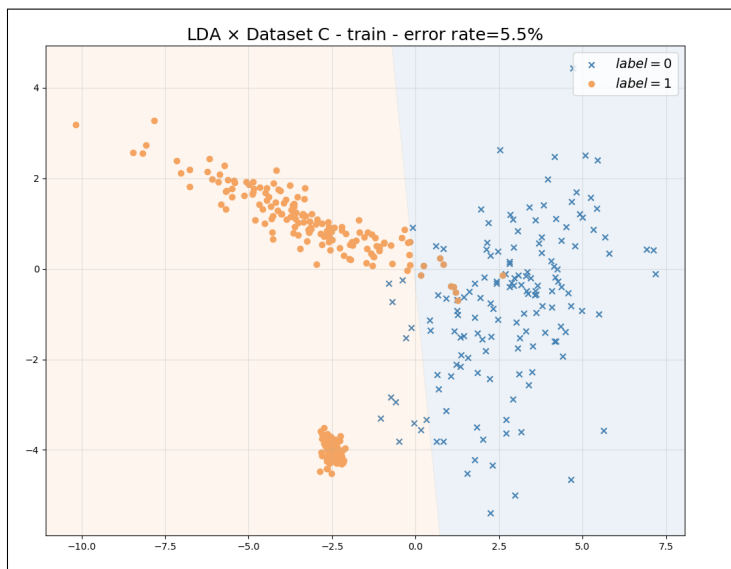
	test	train
LDA	4.15	3.000
Linear Regression	4.15	3.000
Logistic Regression	4.30	2.000
QDA	2.00	1.333

Comments:

In this dataset, there is an overlapping area between the two classes making it harder to provide a separation and even harder with a linear model. Moreover, classes "scattering" being different, we also expect QDA to provide better performances which is the case.

As classes distribution is homogeneous though, linear model still yield satisfying results.

Once again, misclassification is larger on the testing set than on the training. We note that the testing set is more than 6 times as large as the training set.



misclassification on Dataset C (%)

	test	train
LDA	4.233	5.50
Linear Regression	4.233	5.50
Logistic Regression	2.267	4.00
QDA	3.833	5.25

Comments:

This dataset presents a dense and separate cluster of 1. It is interesting to see how linear regression tries to maximize the distance between the decision boundary and this cluster even if it means misclassifying other samples. The same goes for LDA and QDA as this dense cluster tends to shift the mean estimator for class 1. Logistic Regression for one seems to give it less importance in its weighting process.

Oddly enough, classification on testing set works better than on training set. Indeed, providing more samples for classification will increase the number of samples contained in the dense cluster. Since this dense cluster is always completely well-classified, its correct classification is going to pull the misclassification rate downwards when the number of samples rises.

Learning in discrete graphic models

MLE of π

Let $(z_i)_{i \in \llbracket 1, n \rrbracket}$ iid, the log-likelihood is given by :

$$\ell(\pi) = \sum_{m=1}^M n_m \log \pi_m, \quad n_m = \sum_{i=1}^n \mathbb{1}_{\{z_i=m\}}$$

$-\ell$ being convex and as $\exists \pi \in [0, 1]^M / \pi^T 1_M = 1$, by Slater's constraints qualification we have strong duality and we can address its dual problem given by :

$$\max_{\lambda} \min_{\pi} \mathcal{L}(\lambda, \pi), \quad \text{where } \mathcal{L}(\lambda, \pi) = -\ell(\pi) + \lambda(\pi^T 1_M - 1)$$

\mathcal{L} being convex w.r.t π we can minimize it through its gradient :

$$\forall m, \frac{\partial \mathcal{L}}{\partial \pi_m} = 0 \Rightarrow -\frac{n_m}{\pi_m} + \lambda = 0 \Rightarrow \pi_m = \frac{n_m}{\lambda}$$

Plus, $\pi^T 1_M = 1 \Rightarrow \sum_{m=1}^M \frac{n_m}{\lambda} = 1 \Rightarrow \lambda = \sum_{m=1}^M n_m = n$, hence :

$$\forall m, \hat{\pi}_m = \frac{n_m}{n}$$

MLE of Θ

Let $(x_i)_{i \in \llbracket 1, n \rrbracket}$ and $(z_i)_{i \in \llbracket 1, n \rrbracket}$ iid and $\Theta = [\theta_{mk}] \in [0, 1]^{M \times K}$.

Conditional probability allows us to write the log-likelihood as :

$$\begin{aligned} \ell(\Theta, \pi) &= \sum_{i=1}^n \log(p_{\Theta}(x_i | y_i) p_{\pi}(y_i)) && \text{(Conditional probability)} \\ &= \sum_{i=1}^n \sum_{m=1}^M \log \pi_m \mathbb{1}_{\{y_i=m\}} + \sum_{i=1}^n \sum_{m=1}^M \sum_{k=1}^K \log \theta_{mk} \mathbb{1}_{\{x_i=k, y_i=m\}} \\ &= \sum_{m=1}^M n_m \log \pi_m + \sum_{k=1}^K \sum_{m=1}^M n_{mk} \log \theta_{mk} \end{aligned}$$

where,

$$n_m = \sum_{i=1}^n \mathbb{1}_{\{z_i=m\}}, \quad n_{mk} = \sum_{i=1}^n \mathbb{1}_{\{z_i=m, x_i=k\}}$$

As log is concave, and $\forall m, k \quad n_m \geq 0$ and $n_{mk} \geq 0$, $-\ell$ is convex.

Also, we can trivially find π_0 and Θ_0 satisfying the constraints given by : $\begin{cases} \pi^T \Theta 1_K = 1 \\ \pi^T 1_M = 1 \end{cases}$

By Slaters's constraints qualification, we hence have strong duality and can address its dual problem stated by :

$$\max_{\lambda \in \mathbb{R}_+^2} \min_{\Theta, \pi} \mathcal{L}(\lambda, \Theta, \pi)$$

where $\mathcal{L}(\lambda, \Theta, \pi) = -\ell(\Theta, \pi) + (\pi^T \Theta 1_K - 1 - \pi^T 1_M - 1) \lambda$

\mathcal{L} being convex w.r.t π and Θ we can minimize it through its gradient :

Derivating w.r.t π , we obtain the same estimator as previously : $\forall m, \hat{\pi}_m = \frac{n_m}{n}$

For Θ , the derivation goes :

$$\forall m, k, \frac{\partial \ell}{\partial \theta_{mk}} = \frac{n_{mk}}{\theta_{mk}}$$

$$\text{And, } \pi^T \Theta 1_K = \text{Tr}(\pi^T \Theta 1_K) = \text{Tr}(\Theta 1_K \pi^T) = \langle \Theta, \pi 1_K^T \rangle \Rightarrow \nabla_{\Theta}(\pi^T \Theta 1_K) = \pi 1_K^T$$

$$\begin{aligned} \forall m, k, \frac{\partial \mathcal{L}}{\partial \theta_{mk}} = 0 &\Rightarrow -\frac{n_{mk}}{\theta_{mk}} + \lambda_1 \pi_k = 0 \\ &\Rightarrow \theta_{mk} = \frac{n_{mk}}{\lambda_1 \pi_m} \end{aligned}$$

Once again, the constraints gives us :

$$\lambda_1 = n, \text{ hence : } \forall m, k, \hat{\theta}_{mk} = \frac{n_{mk}}{n \hat{\pi}_m} = \frac{n_{mk}}{n_m}$$

Linear classification

MLE for LDA

Hypothesis:

$$Y \sim \mathcal{B}(\pi), \quad \forall j \in \{0, 1\} \quad X | \{Y = j\} \sim \mathcal{N}(\mu_j, \Sigma)$$

MLE of π : We computed in the previous part the MLE of a Multinomial law with parameter $\pi \in [0, 1]^M$, $M \in \mathbb{N}^*$. A Bernoulli law is nothing more than a bidimensional Multinomial law, hence :

Let $(y_i)_{i \in [1, n]}$ n observations,

$$\boxed{\hat{\pi} = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{y_i=1\}} = \frac{1}{n} \sum_{i=1}^n y_i}$$

MLE of μ_j, Σ :

Let $((x_i, y_i))_{i \in [1, n]}$ a set of n iid observations

Then, if we note $\theta = (\mu_0, \mu_1, \Sigma)$

$$\begin{aligned} \ell(\theta) = \log p_{\theta}(x) &= \sum_{i=1}^n \log p_{\theta}(x_i) \\ &= \sum_{i=1}^n \log p_{\theta}(x_i | y_i) + \log p_{\theta}(y_i) \\ &= \sum_{i=1}^n y_i \left[\log \pi - \frac{1}{2} (d \log 2\pi + \log(\det \Sigma) + (x_i - \mu_1)^T \Sigma^{-1} (x_i - \mu_1)) \right] \\ &\quad + (1 - y_i) \left[\log(1 - \pi) - \frac{1}{2} (d \log 2\pi + \log(\det \Sigma) + (x_i - \mu_0)^T \Sigma^{-1} (x_i - \mu_0)) \right] \end{aligned}$$

We remind that the MLE of the multivariate Gaussian model is given by :

$$\ell_{\mathcal{N}}(\mu, \Sigma) = \sum_{i=1}^n \underbrace{-\frac{1}{2} (d \log 2\pi + \log(\det \Sigma) + (x_i - \mu)^T \Sigma^{-1} (x_i - \mu))}_{\ell_{\mathcal{N}}^{(i)}(\mu, \Sigma)}$$

and that

$$\nabla_{\mu} \ell_{\mathcal{N}}^{(i)} = \Sigma^{-1} (x_i - \mu) \quad \nabla_{\Sigma^{-1}} \ell_{\mathcal{N}}^{(i)} = \Sigma + (x_i - \mu)(x_i - \mu)^T$$

Let $j \in \{0, 1\}$, ℓ being concave and differentiable w.r.t μ_j we can maximize it by maximizing its gradient.

$$\begin{aligned} \nabla_{\mu_j} \ell(\theta) = 0 &\Rightarrow \sum_{i=1}^n \mathbb{1}_{\{y_i=j\}} \nabla_{\mu_j} \ell_{\mathcal{N}_j}^{(i)} = 0 \\ &\Rightarrow \sum_{i=1}^n \mathbb{1}_{\{y_i=j\}} \Sigma^{-1} (x_i - \mu_j) = 0 \\ &\Rightarrow \Sigma^{-1} \left(\sum_{i=1}^n \mathbb{1}_{\{y_i=j\}} (x_i - \mu_j) \right) = 0 \\ &\Rightarrow \sum_{i=1}^n \mathbb{1}_{\{y_i=j\}} (x_i - \mu_j) = 0 \quad (\Sigma^{-1} \text{ injective}) \end{aligned}$$

Thus,

$$\hat{\mu}_j = \frac{\sum_{i=1}^n \mathbb{1}_{\{y_i=j\}} x_i}{\sum_{i=1}^n \mathbb{1}_{\{y_i=j\}}}$$

Similarly,

$$\begin{aligned} \nabla_{\Sigma^{-1}} \ell(\theta) = 0 &\Rightarrow \sum_{i=1}^n y_i \nabla_{\Sigma^{-1}} \ell_{\mathcal{N}_1}^{(i)} + (1 - y_i) \nabla_{\Sigma^{-1}} \ell_{\mathcal{N}_0}^{(i)} = 0 \\ &\Rightarrow n\Sigma + \sum_{i=1}^n y_i (x_i - \mu_1)(x_i - \mu_1)^T + (1 - y_i)(x_i - \mu_0)(x_i - \mu_0)^T = 0 \end{aligned}$$

Thus,

$$\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{y_i=0\}} (x_i - \hat{\mu}_0)(x_i - \hat{\mu}_0)^T + \mathbb{1}_{\{y_i=1\}} (x_i - \hat{\mu}_1)(x_i - \hat{\mu}_1)^T$$

Decision boundary

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

with $w = \Sigma^{-1}(\mu_1 - \mu_0)$ and $b = \frac{1}{2}\mu_0^T \Sigma^{-1}\mu_0 - \frac{1}{2}\mu_1^T \Sigma^{-1}\mu_1$

The boundary decision is thus an affine boundary and we notice here that for $\pi = \frac{1}{2}$, it matches the boundary decision of a logistic regression.

MLE for QDA

Hypothesis:

$$Y \sim \mathcal{B}(\pi), \quad X | \{Y=i\} \sim \mathcal{N}(\mu_i, \Sigma_i)$$

Let $\theta = (\mu_0, \mu_1, \Sigma_0, \Sigma_1)$, keeping the notation introduced for LDA's MLE computation, the log-likelihood is given by :

$$\begin{aligned}
\ell(\theta) &= \sum_{i=1}^n y_i \left[\log \pi - \frac{1}{2} \left(d \log 2\pi + \log(\det \Sigma_1) + (x_i - \mu_1)^T \Sigma_1^{-1}(x_i - \mu_1) \right) \right] \\
&\quad + (1 - y_i) \left[\log(1 - \pi) - \frac{1}{2} \left(d \log 2\pi + \log(\det \Sigma_0) + (x_i - \mu_0)^T \Sigma_0^{-1}(x_i - \mu_0) \right) \right]
\end{aligned}$$

We can see here that this doesn't change anything for the maximisation w.r.t μ_j and the MLE would be the same. Regarding the covariance matrix, maximization goes :

$$\begin{aligned}
\forall j \in \{0, 1\} \quad \nabla_{\Sigma_j^{-1}} \ell(\theta) = 0 &\Rightarrow \sum_{i=1}^n \mathbb{1}_{\{y_i=j\}} \nabla_{\Sigma_j^{-1}} \ell_{\mathcal{N}_j}^{(i)} = 0 \\
&\Rightarrow \sum_{i=1}^n \mathbb{1}_{\{y_i=j\}} \Sigma_j + \sum_{i=1}^n \mathbb{1}_{\{y_i=j\}} (x_i - \mu_j)(x_i - \mu_j)^T = 0
\end{aligned}$$

Thus,

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

And any value in the decision boundary satisfies :

$$\begin{aligned}
p(x|y=1) = \frac{1}{2} = p(x|y=0) &\Leftrightarrow \pi \mathcal{N}(x|\mu_1, \Sigma_1) = (1 - \pi) \mathcal{N}(x|\mu_0, \Sigma_0) \\
&\Leftrightarrow \log\left(\frac{\pi}{1 - \pi}\right) = \log \mathcal{N}(x|\mu_0, \Sigma_0) - \log \mathcal{N}(x|\mu_1, \Sigma_1) \\
&\Leftrightarrow \frac{1}{2} \log\left(\frac{\det \Sigma_1^{-1}}{\det \Sigma_0^{-1}}\right) + \frac{1}{2} [(x - \mu_1)^T \Sigma_1^{-1}(x - \mu_1) - (x - \mu_0)^T \Sigma_0^{-1}(x - \mu_0)] = \log\left(\frac{\pi}{1 - \pi}\right)
\end{aligned}$$

Once developped, such relationship boils down to a conic equation that can be plotted.