HMWK1

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Master M2 MVA 2018/2019
Probabilistic Graphical Models

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MLE of π

Let $(z_i)_{i\in[\![1,n]\!]}$ *iid*, the log-likelighood 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 $\exists \pi \in [0,1]^M / \pi^T 1_M = 1$, 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 $\mathcal{L}(\lambda,\pi) = -\ell(\pi) + \lambda(\pi^T 1_M - 1)$

$\mathcal{L}$ being convex w.r.t to 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 $(x_i)_{i\in[\![1,n]\!]}$ and $(z_i)_{i\in[\![1,n]\!]}$ *iid* and $\Theta = [\theta_{mk}] \in [0,1]^{M\times K}$. Conditional probability allow us to write the log-likelihood as : $\ell(\Theta,\pi) = \sum_{m=1}^{M} n_m \log \pi_m + \sum_{k=1}^{K}\sum_{m=1}^{M} n_{mk} \log \theta_{mk}\,,\;\; n_m = \sum_{i=1}^{n} \mathbb{1}_{\{z_i=m\}}\,,\;\; n_{mk} = \sum_{i=1}^{n} \mathbb{1}_{\{z_i=m, x_i=k\}}$

Samely, $\mathcal{L}(\lambda,\Theta,\pi) = -\ell(\Theta,\pi) + \begin{pmatrix}\pi^T\Theta 1_K - 1 & \pi^T 1_M - 1\end{pmatrix}\lambda\,,\;\; \lambda \in \mathbb{R}_+^2$

Derivating w.r.t to π we obtain the same estimtor 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

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

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

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

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

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

QDA formulas

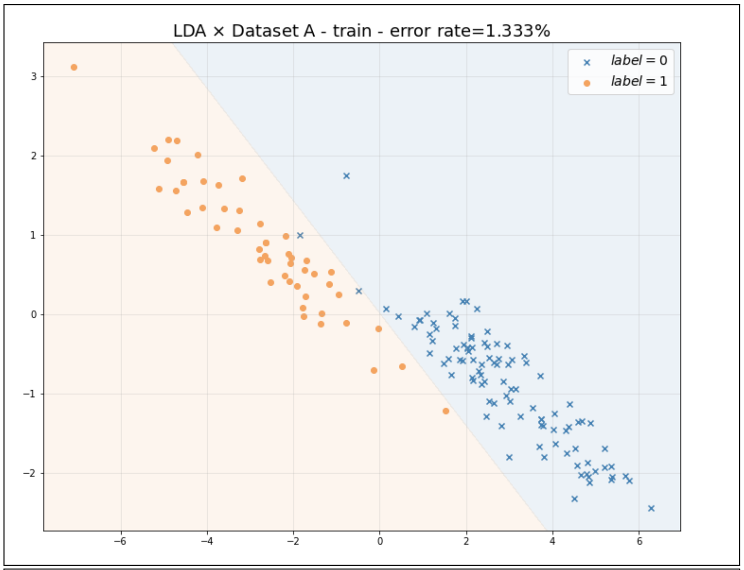
$$Y \sim \mathcal{B}(\pi),\;\; X \,|\, \{Y\!=\!i\} \sim \mathcal{N}\left(\mu_i, \Sigma_i\right)$$

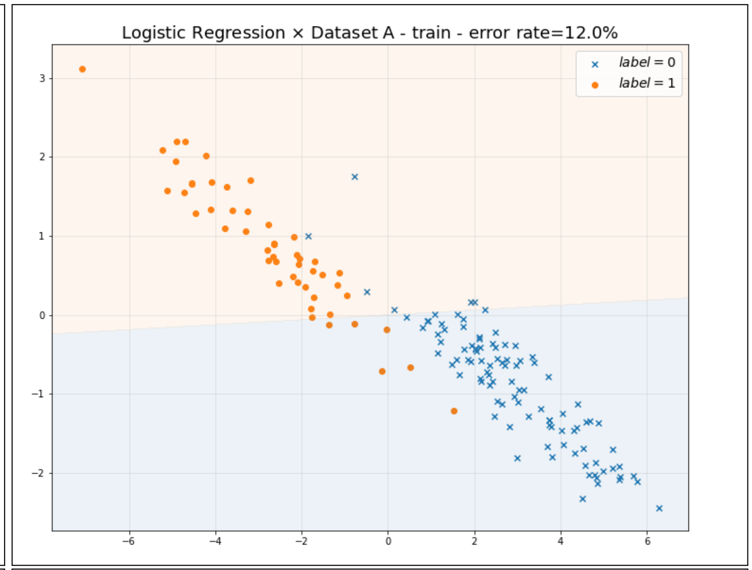
$$\hat{\pi} = \frac{1}{N}\sum_{i=1}^{n} y_i$$

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

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

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


LDA × Dataset A - train - error rate=1.333%
label = 0
label = 1


Logistic Regression × Dataset A - train - error rate=12.0%
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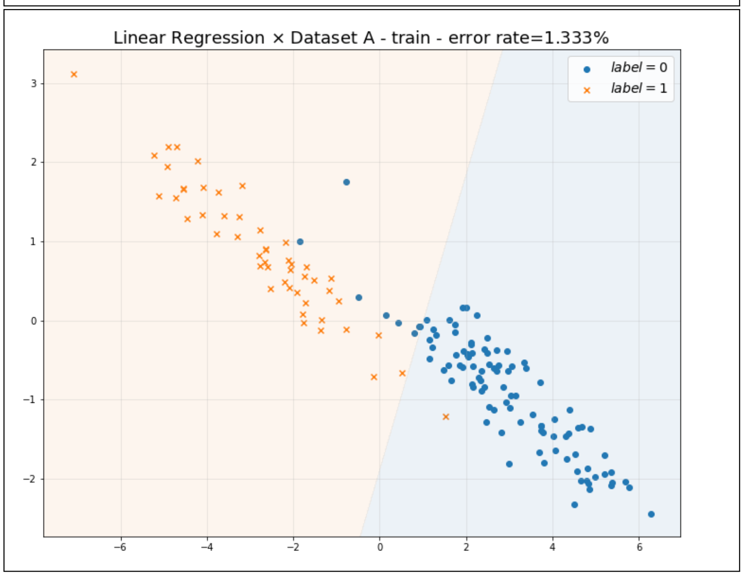
Linear Regression × Dataset A - train - error rate=1.333%
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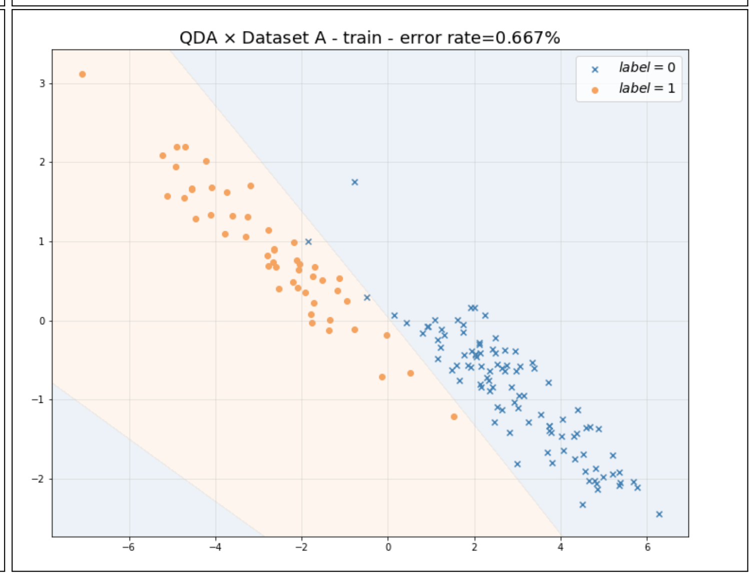
QDA × Dataset A - train - error rate=0.667%
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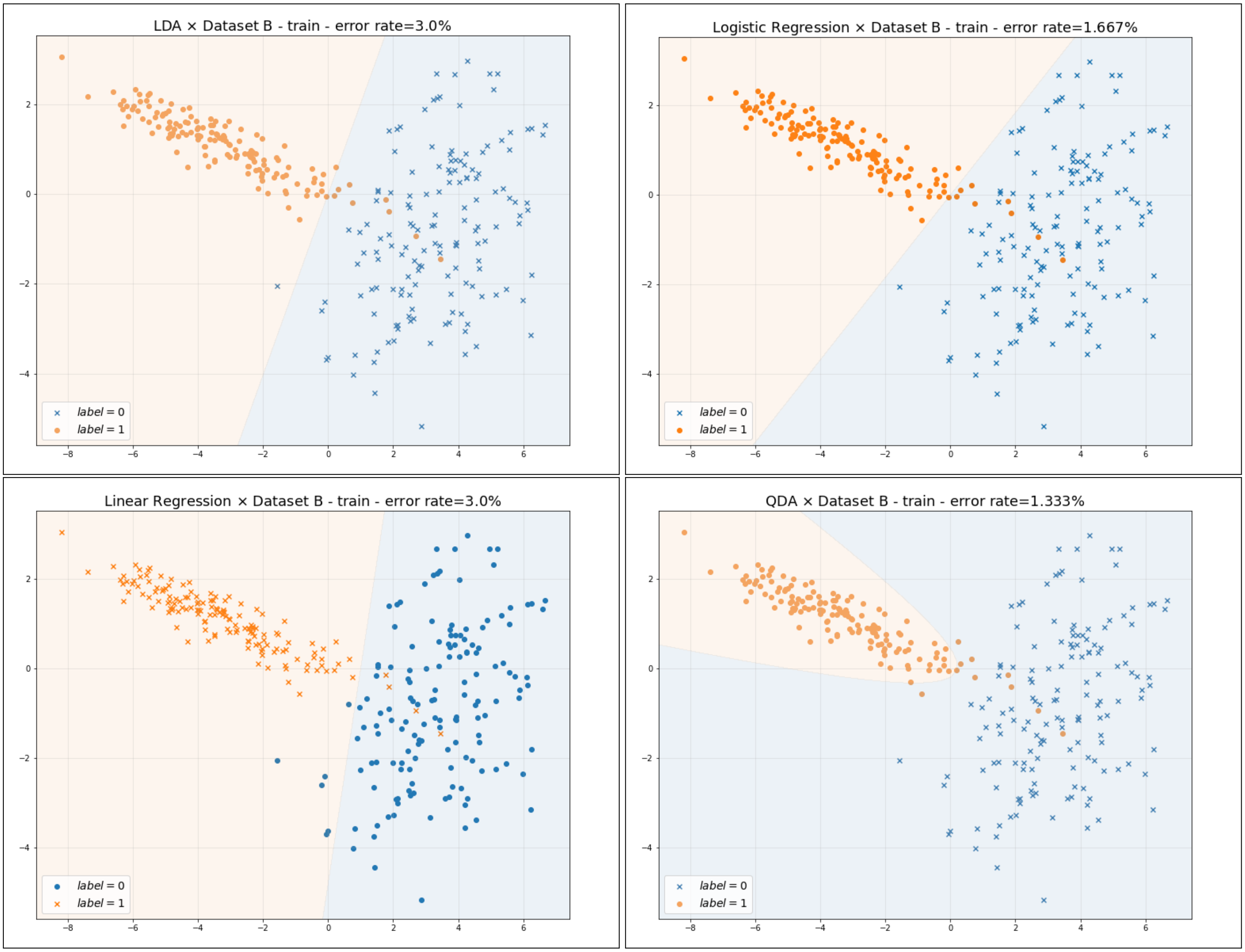
LDA × Dataset B - train - error rate=3.0%
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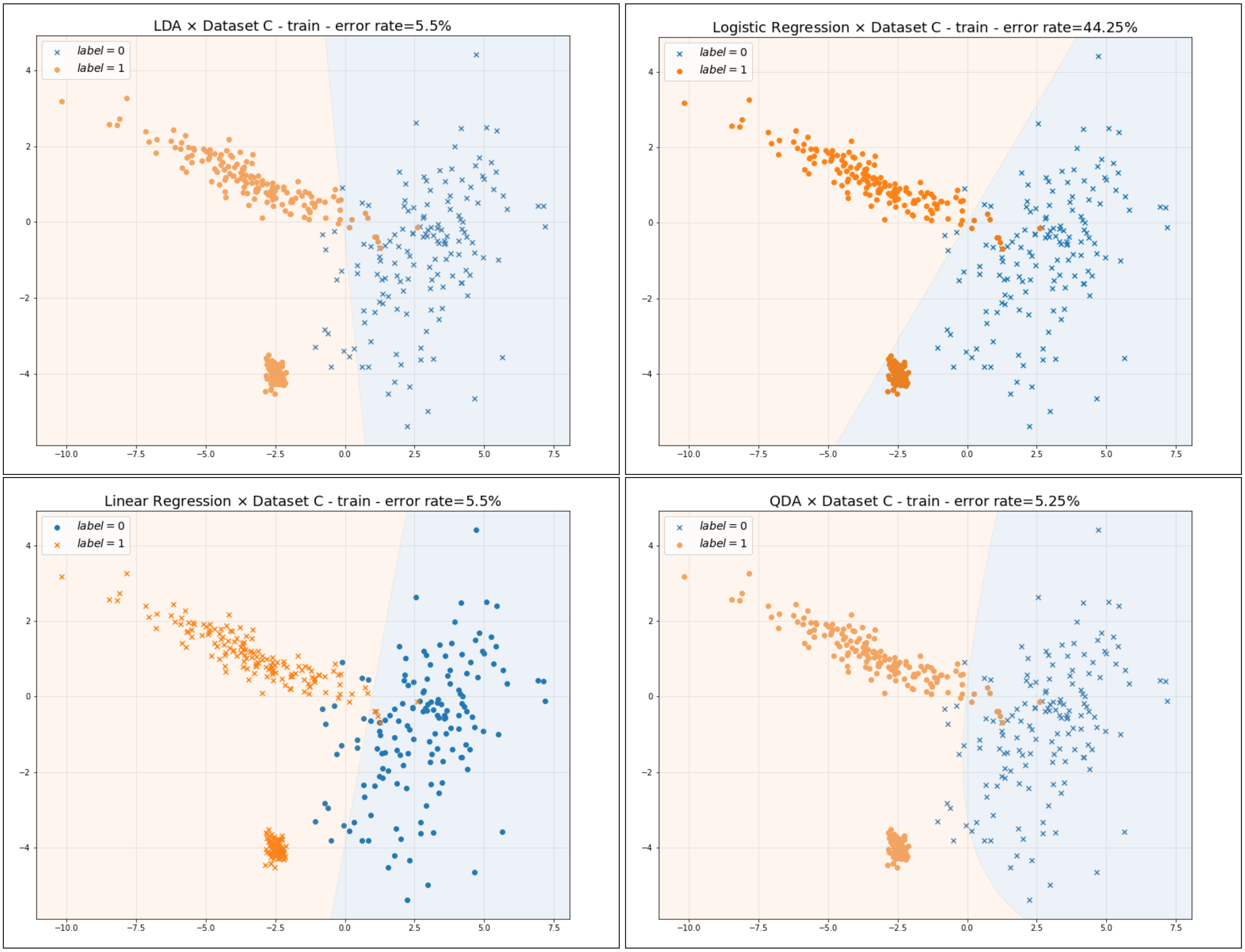
label = 1
Logistic Regression × Dataset B - train - error rate=1.667%
label = 0
label = 1
Linear Regression × Dataset B - train - error rate=3.0%
label = 0
label = 1
QDA × Dataset B - train - error rate=1.333%
label = 0
label = 1


LDA × Dataset C - train - error rate=5.5%
label = 0
label = 1
Logistic Regression × Dataset C - train - error rate=44.25%
label = 0
label = 1
Linear Regression × Dataset C - train - error rate=5.5%
label = 0
label = 1
QDA × Dataset C - train - error rate=5.25%
label = 0
label = 1
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
4
2
0
−2
−4

Learning in discrete graphic models

MLE of π

Let $(z_i)_{i\in[\![1,n]\!]}$ *iid*, the log-likelighood 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 $\exists \pi \in [0,1]^M / \pi^T 1_M = 1$, by Slater's constraints qualification we have strong duality and we can address its dual problem given by :

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

$\mathcal{L}$ being convex w.r.t to 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 $(x_i)_{i\in[\![1,n]\!]}$ and $(z_i)_{i\in[\![1,n]\!]}$ *iid* and $\Theta = [\theta_{mk}] \in [0,1]^{M\times K}$.

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

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

where,

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

As log is concave, and $\forall m,k \;\; n_m \geq 0$ 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 $\mathcal{L}(\lambda, \Theta, \pi) = -\ell(\Theta, \pi) + \begin{pmatrix} \pi^T \Theta 1_K - 1 & \pi^T 1_M - 1 \end{pmatrix} \lambda$

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

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

For Θ, the derivation goes :

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

And, $\pi^T \Theta 1_K = \text{Tr}\left(\pi^T \Theta 1_K\right) = \text{Tr}\left(\Theta 1_K \pi^T\right) =< \Theta, \pi 1_K^T > \Rightarrow \nabla_\Theta \left(\pi^T \Theta 1_K\right) = \pi 1_K^T$

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

Once again, the constraints gives us :
$\lambda_1 = n$, 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:

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

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 $\theta = (\mu_0, \mu_1, \Sigma)$

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

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

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

and that

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

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

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

Thus,

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

Samely,

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

Thus,

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

Decision boundary

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

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.

Logitic Regression regularisation

By adding a ridge penalty in the logisitc regression, we get :

$$\mathcal{L}(\beta,w)=\ell(w)+\frac{\beta}{2}\|w\|^2$$

$$\nabla\mathcal{L}(\beta,w)=\nabla\ell(w)+\beta w$$

$$H\mathcal{L}(\beta,w)=H\ell(w)+\beta I$$

MLE for QDA

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 :

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

We can see here that this doesn't change anything for the maximisation w.r.t to μ_j and the MLE would be the same.
Regarding the covariance matrix, maximization goes :
$\forall j\in\{0,1\}$,

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

Thus,

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

And any value in the decision boundary satisfies :

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

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

	Train data			Test Data		
	A	B	C	A	B	C
LDA error	1,3	3	5,5	2	4,15	4,23
LogReg error	12	1,6	44,25	18,23	4,6	39,46
LinReg error	1,3	3	5,5	2	4,15	4,23
QDA error	0,6	1,3	5,25	2	2	3,83