Probabilistic Graphical Models MVA 2018/2019 HWK1

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Exercise 1: Learning in discrete graphical models

Let $(z_i, x_i)_{i=1,...,n}$ an i.i.d. sample of observations. Let $\boxed{n_{k,m} = \sum_{i=1}^{n} 1_{z_i=m, x_i=k}}$ and $\boxed{n_m = \sum_{i=1}^{n} 1_{z_i=m}}$ for $m \in \{1, ..., M\}$ and $k \in \{1, ..., K\}$.

The maximum likelihood estimator of π and θ are found by respectively considering the distribution of z and $x|z$:

$$\boxed{\hat{\pi_m} = \frac{n_m}{n}}, \boxed{\hat{\theta_{k,m}} = \frac{n_{k,m}}{n}}$$

Exercise 2.1.(a): LDA formulas

Let $(x_i, y_i)_{i=1,...,n}$ an i.i.d. sample of observations. For estimating π, we consider the distribution of $y \sim Bernoulli(p)$, for Σ, μ_1 and μ_0, we consider the negative log-likelihood of $x|y$ distribution knowing that $p(X|Y = j) = Normal(\mu_j, \Sigma)$ for $j \in \{0, 1\}$. Let $\boxed{n_j = \sum_{i=1}^{n} 1_{y_i=j}}$, $\boxed{\widetilde{\Sigma_j} = \frac{\sum_i^n 1_{y_i=j}(x_i - \mu_j)(x_i - \mu_j)^T}{n_j}}$ for $j \in \{0, 1\}$.
The maximum likelihood estimators are :

$$\boxed{\hat{\pi} = \frac{\sum_{i=1}^{n} y_i}{n}}, \boxed{\hat{\mu_j} = \frac{\sum_i^n x_i 1_{y_i=j}}{n_j}}, \boxed{\hat{\Sigma} = \frac{n_1\widetilde{\Sigma_1} + n_0\widetilde{\Sigma_0}}{n}}$$

With Bayes formula, we have $p(y = 1|x) = \frac{\pi p(x|y=1)}{\pi p(x|y=1)+(1-\pi)p(x|y=0)} = \frac{1}{1+\frac{1-\pi}{\pi}\frac{p(x|y=0)}{p(x|y=1)}} = \sigma(\omega^T x + C)$ with $\omega = \Sigma^{-1}(\mu_0 - \mu_1)$, C a constant wrt to x and σ the sigmoid function. We recognize here the logistic regression model.

Exercise 2.5.(a): QDA formulas

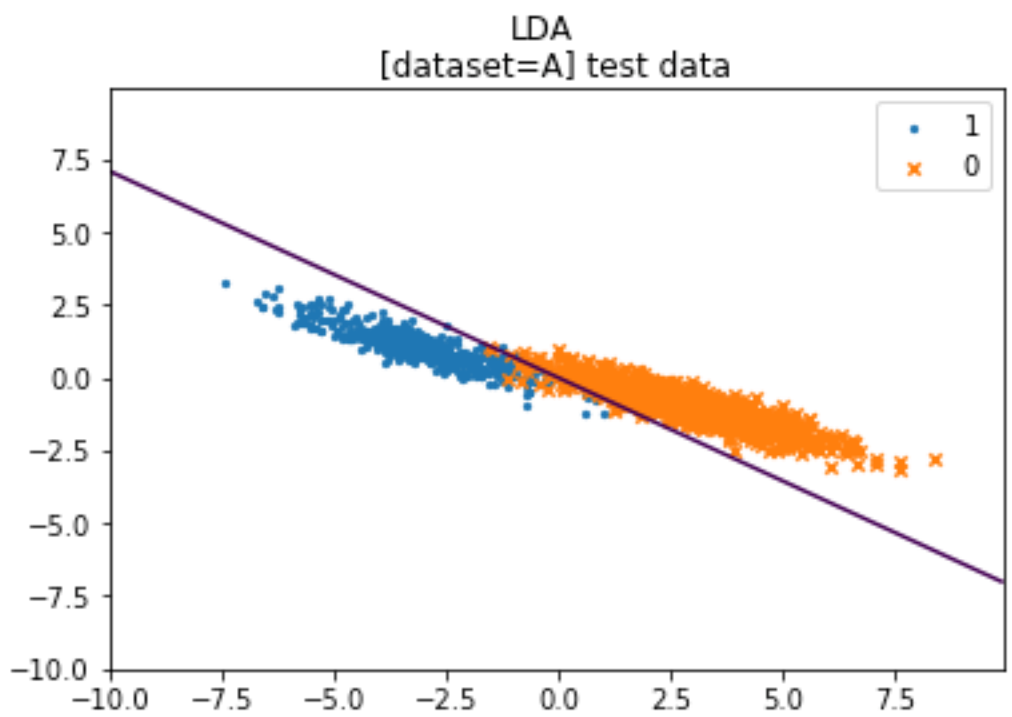
We will keep the same notations as for 2.1.(a). For estimating π, we consider the distribution of $y \sim Bernoulli(p)$, for Σ_1, Σ_0, μ_1 and μ_0, we consider the negative log-likelihood of $x|y$ distribution knowing that $p(X|Y = j) = Normal(\mu_j, \Sigma_j)$ for $j \in \{0, 1\}$.

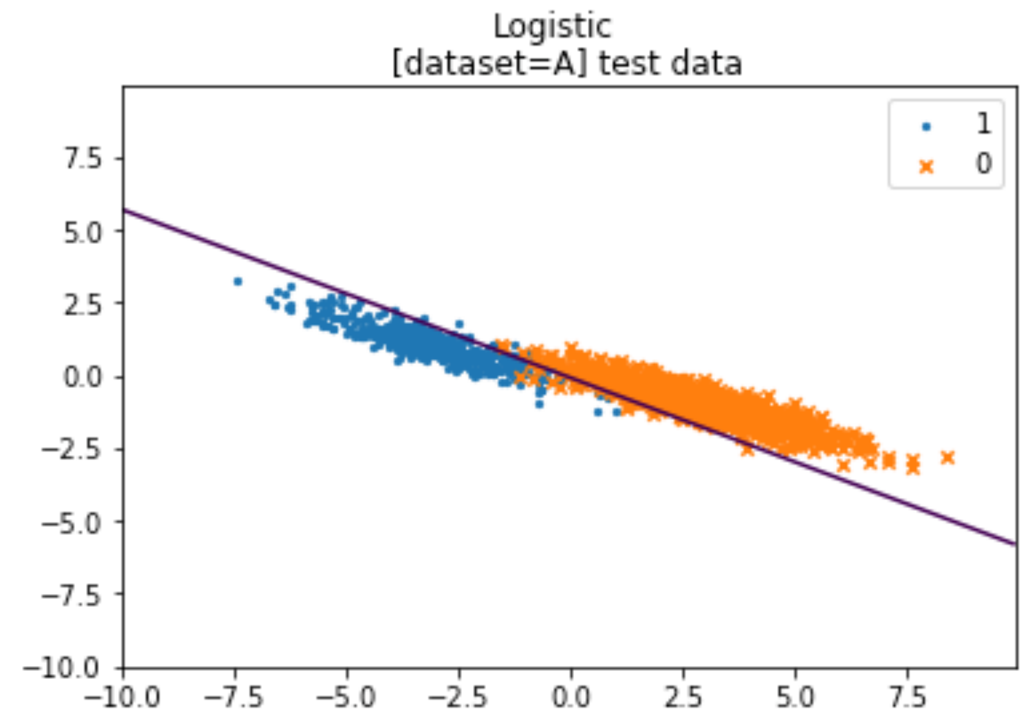
The maximum likelihood estimator of π, Σ_1, Σ_0, μ_1 and μ_0 are :

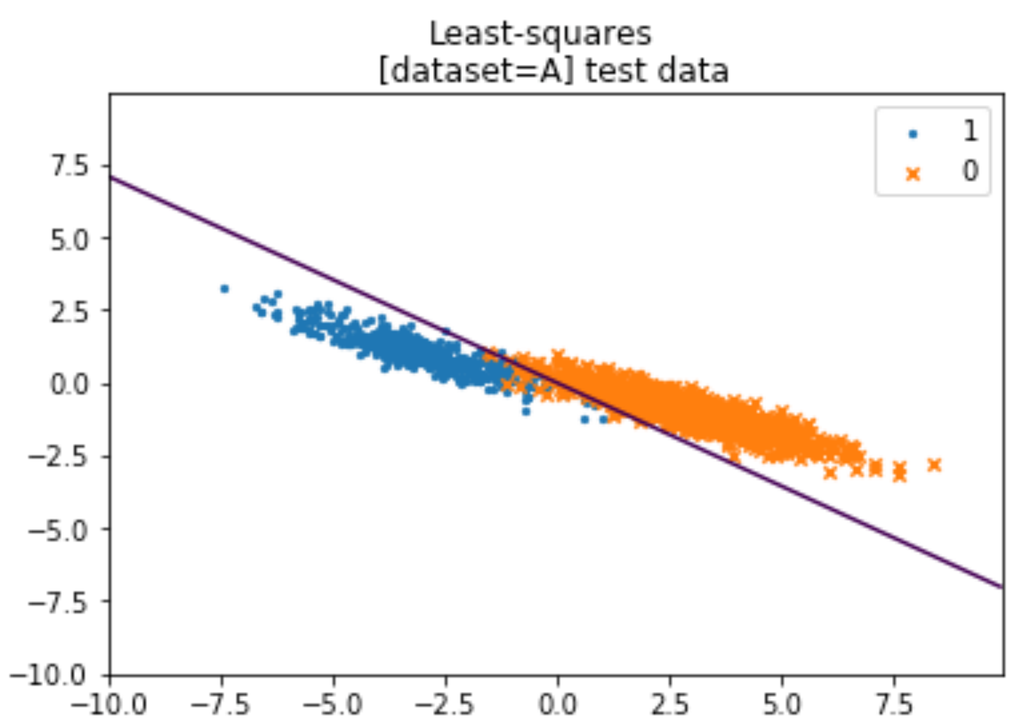
$$\boxed{\hat{\pi} = \frac{\sum_{i=1}^{n} y_i}{n}}, \boxed{\hat{\mu_j} = \frac{\sum_{i=1}^{n} x_i 1_{y_i=j}}{n_j}}, \boxed{\hat{\Sigma_j} = \widetilde{\Sigma_j}}$$

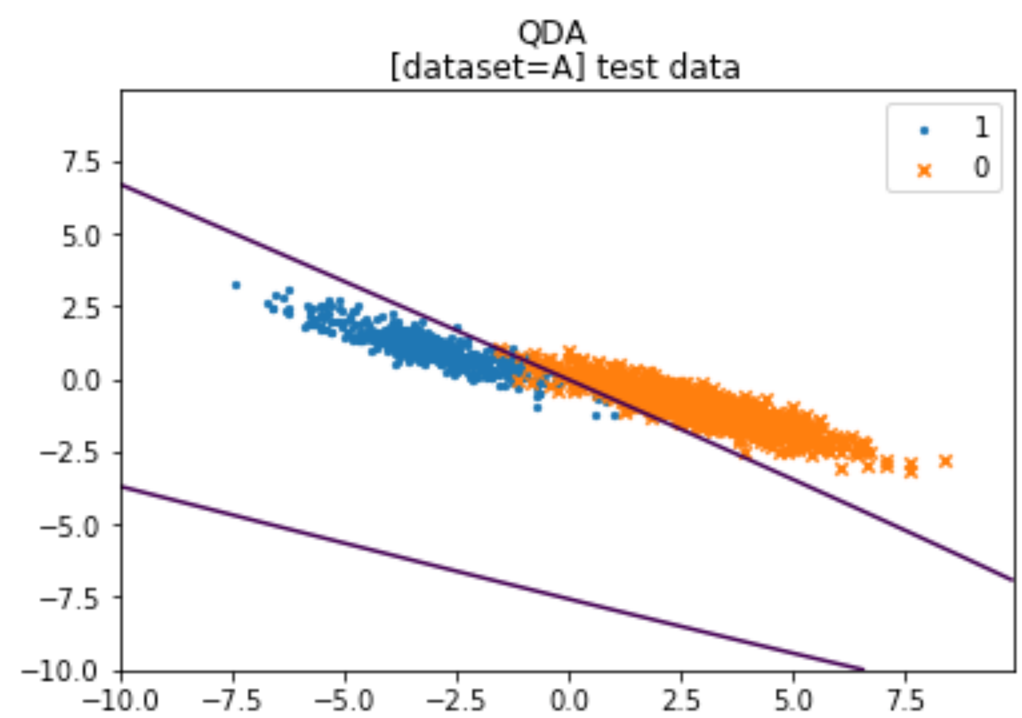
More detailed proves on page 5.

Dataset A









Misclassification error

MODEL	TRAIN	TEST
LDA	1.33%	2.00%
Logistic	0.00%	3.40%
Least-squares	1.33%	2.07%
QDA	1.33%	2.07%

Comments

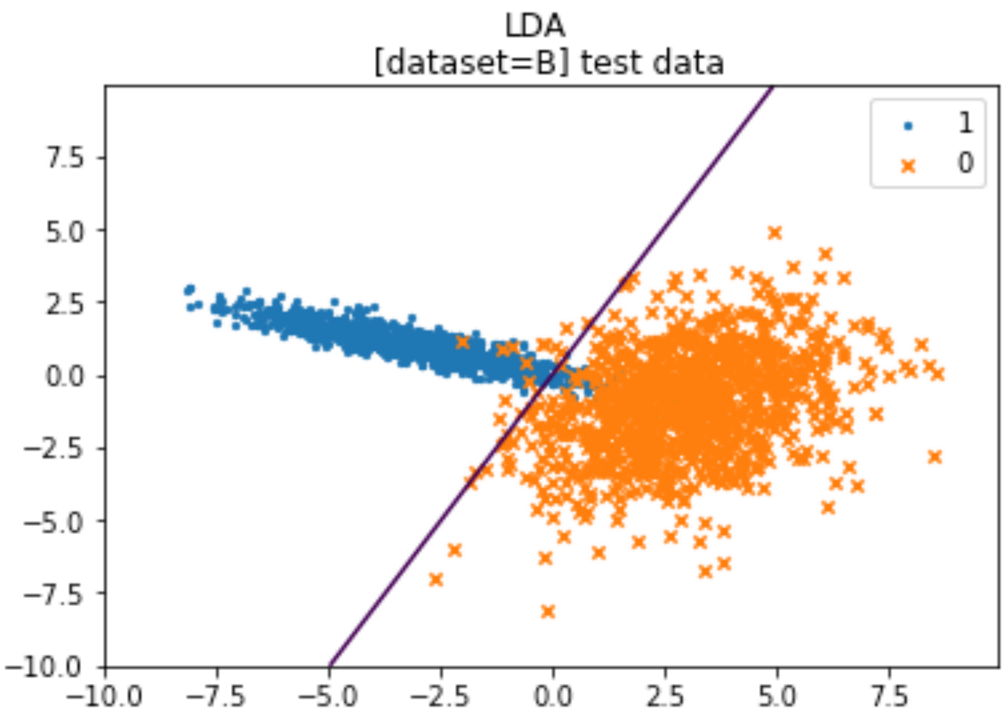
- The data is linearly separable in the training set as the **logistic regression** shows 0% misclassification error. The error rates are higher in the test set due to generalization error and the fact that data isn't separable in test set.

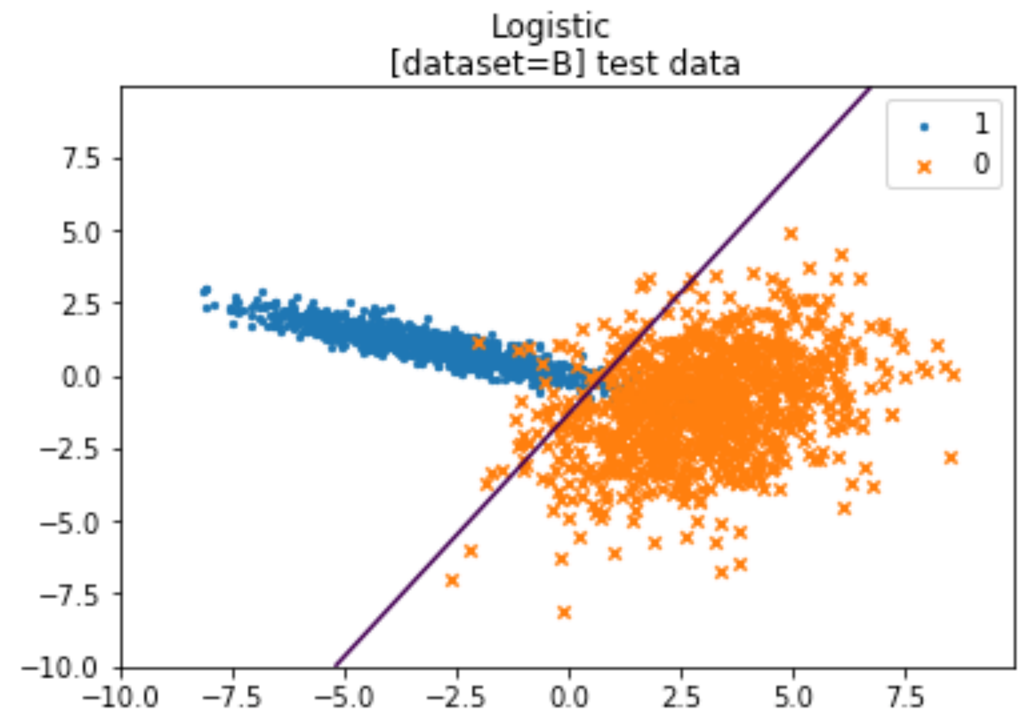
- Similarly, **LDA** and **Least-squares** model yield good results as their decision boundary is also linear. In particular, the covariance of normal distributions X|Y=0 and X|Y=1 seem very similar, which is an assumption used by LDA model.

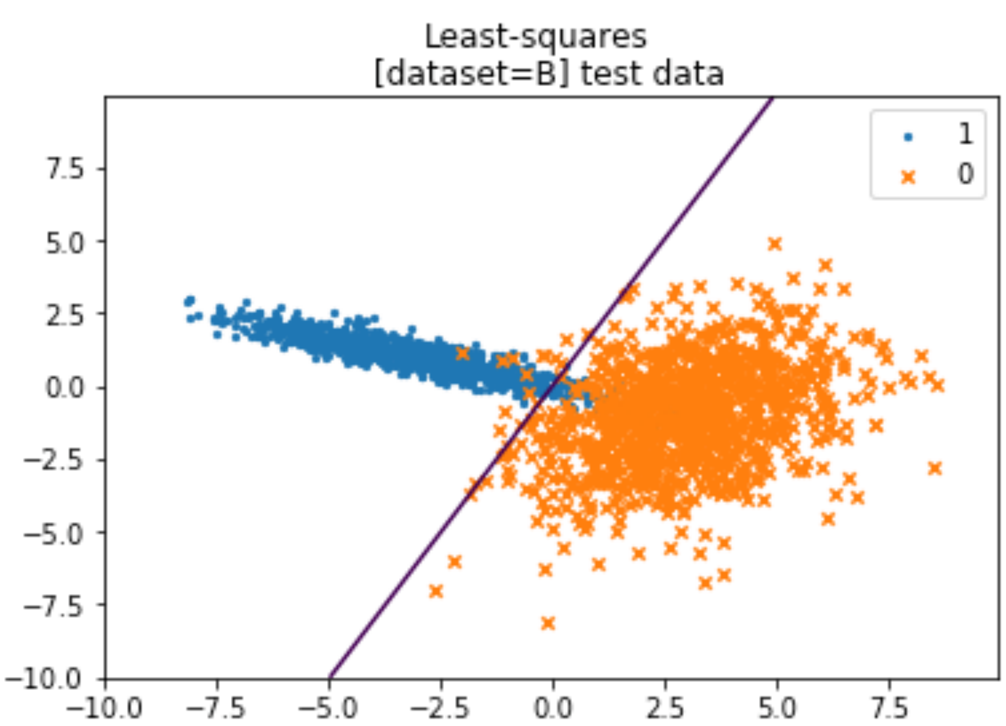
- **QDA** does not yield better results because data are almost linearly separable.

- **Logistic regression** : we can notice that the model has slightly overfitted, the test result is the worst among the different models. This may be because of unstable estimators: in the optimization process we invert the Hessian of the loss function, which is propotionial to the empirical covariance matrix. But its columns are highly colinear (correlation coefficient of -0.92 between the features x1 and x2) thus bringing numerical instabilities. It can be noticed when decreasing the tolerance stopping criteria of the optimization: when set to 10^{-6} the loss function has an infinite value towards the end of the optimization.

Dataset B







Misclassification error

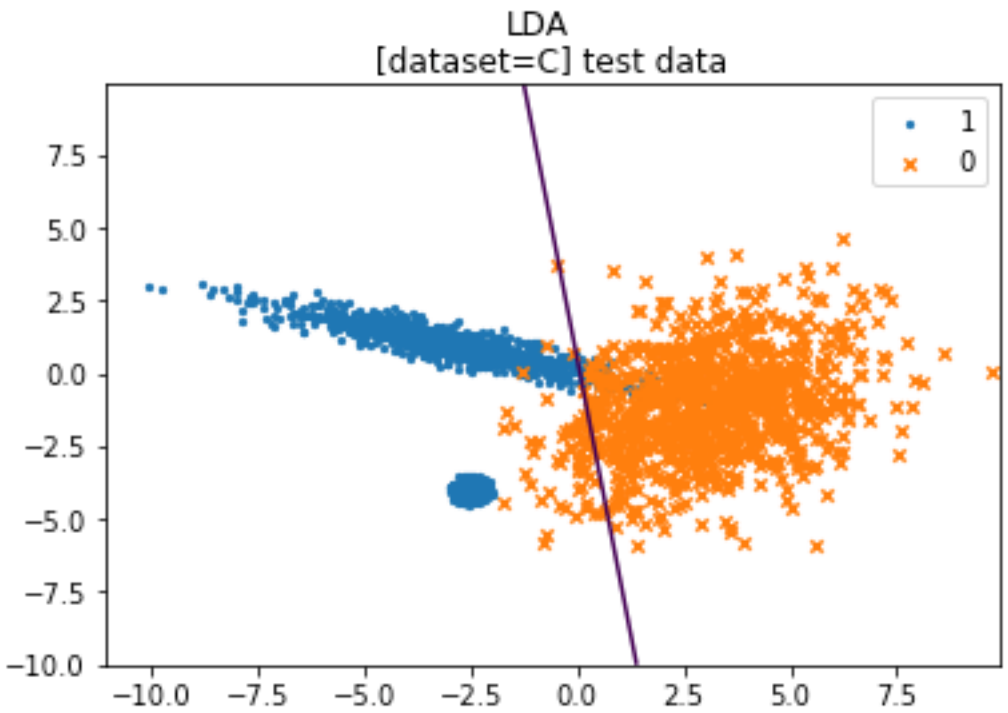
MODEL	TRAIN	TEST
LDA	3.00%	4.15%
Logistic	2.00%	4.30%
Least-squares	3.00%	4.15%
QDA	2.00%	2.80%

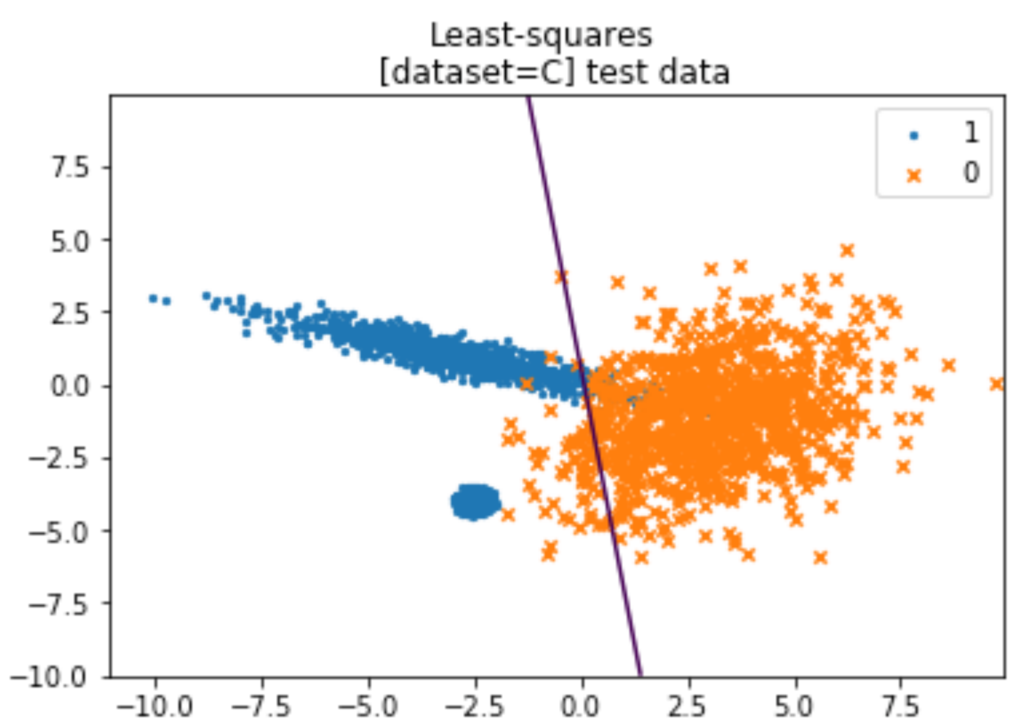
Comments

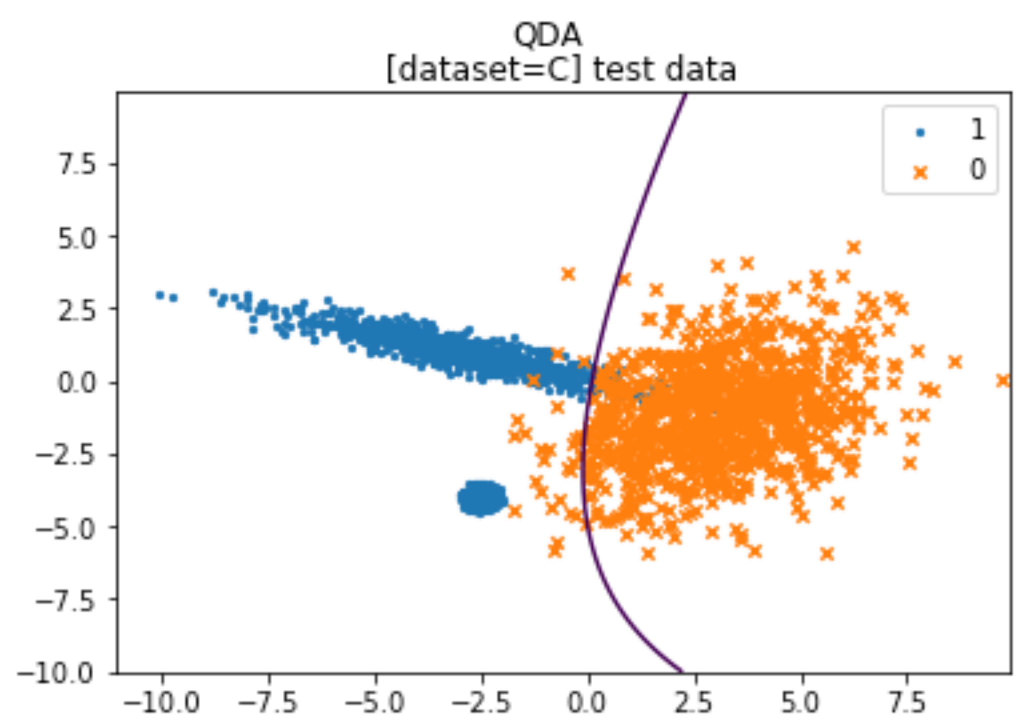
- Compared to the dataset A, X|y=0 distribution has been changed and its covariance structure is quite different from X|y=1 one. Hence **QDA**, which does not assume identical covariances between X|y=0 and X|y=1, performs better than **LDA**.

- As the data is not linearly separable, **Logistic** and **Least-squares** models perform less well. If the underlying distribution were to be known, one should compute the Bayes error rate as a benchmark for our similarly-performing results.

Dataset C







Misclassification error

MODEL	TRAIN	TEST
LDA	5.50%	4.23%
Logistic	4.00%	2.27%
Least-squares	5.50%	4.23%
QDA	4.75%	3.13%

Comments

- Compared to the dataset B, a concentration of points of the class 1 were added on the bottom left part. They do not follow the same distribution as the previous points of class 1. They can be seen as outliers with important weights and allow us to test the robustness of our models. Linear classifiers sure cannot capture this.
- **LDA** and **QDA** uses the assumption of gaussian distribution of X|Y and **Logistic regression** does not assume any distribution on X and is thus more robust to the outliers.
- **Least-squares** is sensitive to outliers as loss function used is the square of residuals. The heavy penalization makes it less robust to outlier. Logistic regression used is logistic loss which behaves linearly for highly negative values.
- This explains why compared to dataset B, after adding outliers, the slope of LDA and Least-Squares strongly shifted, and not so much for Logistic Regression.

Exercise 1: Learning in discrete graphical models

Let $(z_i, x_i)_{i=1,...,n}$ an i.i.d. sample of observations.

The negative log-likelihood of the distribution of z is given by:

$$-l(\pi) = -log(p(z_1, ..., z_n)) = -log(\prod_{i=1}^{n} p(z_i)) = -\sum_{i=1}^{n}\sum_{m=1}^{M} log(\pi_m^{1_{z_i=m}}) = -\sum_{m=1}^{M} n_m log(\pi_m) = -n\sum_{m=1}^{M}\frac{n_m}{n}log(\pi_m)$$

with $\boxed{n_m = \sum_{i=1}^{n} 1_{z_i=m}}$ We want to minimize the negative log-likelihood over π with constraints $\sum_{m=1}^{M}\pi_m = 1$ and $\pi > 0$, which can be seen as the cross-entropy between discrete distributions z and $\tilde{z}$. ($\tilde{z}$ the empirical discrete variable with $p(\tilde{z} = m) = \frac{n_m}{n}$ such that $-l(\pi) = nH(z, \tilde{z})$. Here $\tilde{z}$ is fixed, cross-entropy takes on its minimal value for $z = \tilde{z}$ i.e. $\boxed{\hat{\pi_m} = \frac{n_m}{n}}$ as the maximum likelihood estimator.

The negative log-likelihood of $x|z$ is given by:

$$-l(\theta) = -log(\prod_{i=1}^{n} p(x_i|z_i)) = -\sum_{i=1}^{n}\sum_{k,m} log(\theta_{k,m}^{1_{z_i=m,x_i=k}}) = -\sum_{k,m} n_{k,m}log(\theta_{k,m})$$

with $\boxed{n_{k,m} = \sum_{i=1}^{n} 1_{z_i=m,x_i=k}}$. As $\sum_{k,m} n_{k,m} = 1$. With the same cross-entropy argument, we can derive the maximum likelihood estimator $\boxed{\hat{\theta_{k,m}} = \frac{n_{k,m}}{n}}$

Exercise 2.1.(a): LDA formulas

Let $(x_i, y_i)_{i=1,...,n}$ an i.i.d. sample of observations, we want to find the maximum likelihood estimator of π, Σ, μ_1 and μ_0. Let $\boxed{n_j = \sum_{i=1}^{n} 1_{y_i=j}}$, $\boxed{\widetilde{\Sigma_j} = \frac{\sum_i^n 1_{y_i=j}(x_i - \mu_j)(x_i - \mu_j)^T}{n_j}}$ for $j \in \{0, 1\}$. For estimating π, we consider the distribution of $y \sim Bernoulli(p)$, hence $\boxed{\hat{\pi} = \frac{\sum_{i=1}^{n} y_i}{n}}$. For the rest, we consider the negative log-likelihood of $x|y$ distribution knowing that $p(X|Y = j) = Normal(\mu_j, \Sigma)$:

$$\begin{aligned}
-l(\mu_0, \mu_1, \Sigma) &= -log(\prod_i p(x = x_i|y = 0)^{1_{y_i=0}} p(x = x_i|y = 1)^{1_{y_i=1}}) \\
&= \sum_{i=1}^{n} -log(\frac{\exp(\frac{-(x_i-\mu_1)^T\Sigma^{-1}(x_i-\mu_1)}{2})^{y_i} \exp(\frac{-(x_i-\mu_0)^T\Sigma^{-1}(x_i-\mu_0)}{2})^{1-y_i}}{2\pi\sqrt{\det(\Sigma)}}) \\
&= n\log(2\pi) + \frac{n}{2}\log(\det(\Sigma)) + \frac{1}{2}\sum_{i,y_i=0}(x_i - \mu_0)^T\Sigma^{-1}(x_i - \mu_0) + \frac{1}{2}\sum_{i,y_i=1}(x_i - \mu_1)^T\Sigma^{-1}(x_i - \mu_1) \\
&= n\log(2\pi) - \frac{n}{2}\log(\det(\Sigma^{-1})) + \frac{n_1}{2}Tr(\Sigma^{-1}\widetilde{\Sigma_1}) + \frac{n_0}{2}Tr(\Sigma^{-1}\widetilde{\Sigma_0})
\end{aligned}$$

For $j \in \{0, 1\}$, $\nabla_{\mu_j}(-l) = \sum_{i,y_i=j}\Sigma^{-1}(\mu_j - x_i) = \Sigma^{-1}(\sum_{i,y_i=j}\mu_j - x_i) = 0$, if and only if $\boxed{\hat{\mu_j} = \frac{\sum_i^n x_i 1_{y_i=j}}{n_j}}$, it's minimum as $-l$ is strictly convex w.r.t to μ_j since $\nabla^2_{\mu_j}(-l) = \Sigma^{-1}n_j$ is symmetric positive-semidefinite. Since $\nabla_\Sigma(\frac{n_j}{2}Tr(\Sigma^{-1}\widetilde{\Sigma_j})) = \frac{n_j}{2}\widetilde{\Sigma_j}$ and $\nabla_\Sigma(-\frac{n}{2}\log(\det(\Sigma^{-1}))) = -\frac{n}{2}\Sigma$, $\nabla_\Sigma(-l) = \frac{n}{2}\Sigma - \frac{n_1\widetilde{\Sigma_1}+n_0\widetilde{\Sigma_0}}{2} = 0$ if and only if $\boxed{\hat{\Sigma} = \frac{n_1\widetilde{\Sigma_1} + n_0\widetilde{\Sigma_0}}{n}}$, it's the minimum as $-l$ is strictly convex w.r.t to Σ since $\nabla^2_\Sigma(-l) = \frac{n}{2}I_n$ is symmetric positive-semidefinite.

With Bayes formula, we have $p(y = 1|x) = \frac{\pi p(x|y=1)}{\pi p(x|y=1)+(1-\pi)p(x|y=0)} = \frac{1}{1+\frac{1-\pi}{\pi}\frac{p(x|y=0)}{p(x|y=1)}}$

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

with $\omega = \Sigma^{-1}(\mu_0 - \mu_1)$, C a constant wrt to x and σ the sigmoid function. Hence $\boxed{p(y=1|x) = \sigma(\omega^T x + C)}$: we recognize the logistic regression model. The assumption of equal covariance matrices cancel the quadratic part in the exponents. The decision boundary are then linear in x: classifications regions will be separated by hyperplanes.

Exercise 2.5.(a): QDA formulas

We will keep the same notations and we want to find the maximum likelihood estimator of π, Σ_1, Σ_0, μ_1 and μ_0. We still have $\boxed{\hat{\pi} = \frac{\sum_{i=1}^n y_i}{n}}$. For the rest, we consider the negative log-likelihood of $x|y$ distribution knowing that $p(X|Y=j) = Normal(\mu_j, \Sigma_j)$:

$$\begin{aligned}
-l(\mu_0, \mu_1, \Sigma_0, \Sigma_1) &= -log(\prod_i p(x = x_i|y=0)^{1_{y_i=0}} p(x = x_i|y=1)^{1_{y_i=1}}) \\
&= n\log(2\pi) - \frac{n_1}{2}\log(\det(\Sigma_1^{-1})) - \frac{n_0}{2}\log(\det(\Sigma_0^{-1})) + \frac{n_1}{2}Tr(\Sigma_1^{-1}\widetilde{\Sigma_1}) + \frac{n_0}{2}Tr(\Sigma_0^{-1}\widetilde{\Sigma_0})
\end{aligned}$$

For $j \in \{0, 1\}$, we also obtain $\boxed{\hat{\mu_j} = \frac{\sum_{i=1}^n x_i 1_{y_i=j}}{n_j}}$, it's the minimum as $-l$ is strictly convex w.r.t to μ_j since $\nabla^2_{\mu_j}(-l) = \Sigma_j^{-1} n_j$ is symmetric positive-semidefinite. $\nabla_{\Sigma_j}(\frac{n_j}{2}Tr(\Sigma_j^{-1}\widetilde{\Sigma_j})) = \frac{n_j}{2}\widetilde{\Sigma_j}$ and $\nabla_{\Sigma_j}(-\frac{n_j}{2}\log(\det(\Sigma_j^{-1}))) = -\frac{n_j}{2}\Sigma_j$, $\nabla_{\Sigma_j}(-l) = \frac{n_j}{2}\Sigma_j - \frac{n_j}{2}\widetilde{\Sigma_j} = 0$, if and only if $\boxed{\hat{\Sigma_j} = \widetilde{\Sigma_j}}$, it's the minimum as $-l$ is strictly convex w.r.t to Σ_j since $\nabla^2_{\Sigma_j}(-l) = \frac{n_j}{2} I_n$ is symmetric positive-semidefinite.