

A. Giovanidis 2019

Classification

Data Analysis for Networks - DataNets'19
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Sorbonne-LIP6



February 8, 2019

Bibliography

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[Chapter 2](#), [Chapter 4](#)
DOI 10.1007/978-1-4614-7138-7

Classification Setting

We have seen how to fit models to data when the response y_i to the input x_i is **quantitative** (e.g. "0.57", "24", "-24.3", etc.)

Question: How do we choose models and define their accuracy, when y_i 's are **qualitative**?

Examples: ("Yes", "No"), ("Red", "Blue", "Green"), ("Malaria", "Yellow Fever", "Flu") or more generally:

☞ ("Class 1", "Class 2", ..., "Class M")

Training Accuracy

Suppose we have training observations:

$D_n = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$, with y_1, \dots, y_n qualitative.

Consider a fitting model with an estimate $\hat{y}_i = \hat{f}(x_i)$.

We use the **training error rate**:

$$\frac{1}{n} \sum_{i=1}^n \mathbf{1}(y_i \neq \hat{y}_i).$$

This is the **fraction of incorrect classifications**:

- ▶ \hat{y}_i is the predicted class label for the i -th observation using \hat{f} .
- ▶ $\mathbf{1}(y_i \neq \hat{y}_i) = 0$ for correct classification, else 1.
- ▶ Similar to MSE_{train} in regression!

Test Accuracy

Most interested in the error rates of the classifier to test observations $(x_o, y_o) \notin D_n$, not used in training.

Again for an estimate $\hat{y}_o = \hat{f}(x_o)$ we use the **test error rate**:

$$\text{Ave}(\mathbf{1}(y_o \neq \hat{y}_o)).$$

☞ A **good classifier** is the one for which the **test error is smallest** !

Bayes Classifier

Optimal Classifier: Assign each observation to **the most likely class**, given its predictor values:

$$\max_{1 \leq j \leq M} Pr(Y = j \mid X = x_o)$$

- We consider *conditional probabilities* given the observed x_o .

☞ In a two-class problem

$$Pr(Y = 1 \mid X = x_o) + Pr(Y = 2 \mid X = x_o) = 1:$$

Class 1, if $Pr(Y = 1 \mid X = x_o) > 0.5$

Class 2, if $Pr(Y = 2 \mid X = x_o) > 0.5$

- ☞ Decision boundary $Pr(Y = 1 \mid X = x_o) = Pr(Y = 2 \mid X = x_o)$

Bayes example

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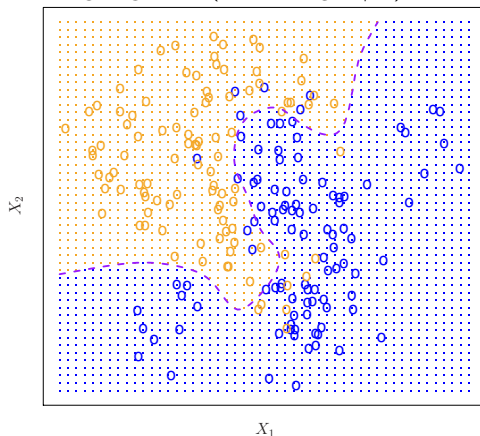
orange region: $Pr(Y = \text{"orange"} \mid X) > 0.5$ 

Figure: Bayes classifier : D_{100} data-set and 2 classes (blue, orange). ¹

¹Source [B.1]

Bayes classifier cont'd

- ▶ Orange shaded region: $Pr(Y = \text{"orange"} \mid X) > 0.5$.
- ▶ Blue shaded region: $Pr(Y = \text{"blue"} \mid X) > 0.5$.
- ▶ The dashed line: Bayes decision boundary.
- ▶ Circles that fall in regions with different colour: **misclassifications**

☞ Bayes classifier produces lowest test error rate (**irreducible**) !

$$\text{Test Error}(x_o) = 1 - \max_j Pr(Y = j \mid X = x_o)$$

Drawback...

There is one problem however: For real data we do not know the conditional distribution $P(Y|X)$,

(unless we have generated data ourselves, in which case we know the joint distribution $P(X, Y)$).

Bayes classifier serves as an unreachable gold standard!

If we do not know exactly $P(Y|X)$ we can try to **estimate it**.

Classifiers

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We will consider in this lecture the following classifiers:

- ▶ K-Nearest-Neighbours classifier ([KNN](#))
- ▶ Logistic Regression ([LR](#))
- ▶ Linear Discriminant Analysis ([LDA](#))
- ▶ Quadratic Discriminant Analysis ([QDA](#))

KNN classifier

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So, how does the KNN classifier works?

- ▶ Choose a positive integer K .
- ▶ Given a test observation $x_o \notin D_n$, the KNN classifier identifies the **K points in the training data closest to x_o** , the set $\mathcal{N}_K(x_o)$.
- ▶ The conditional probability for class j at x_o is **estimated as**:

$$Pr(Y = j \mid X = x_o) = \frac{1}{K} \sum_{i \in \mathcal{N}_K(x_o)} \mathbf{1}(y_i = j). \quad (1)$$

- ▶ Calculate the estimates for all classes $j = 1, \dots, M$ and
- ▶ Finally, **Apply Bayes**: classify x_o to the class with the largest estimated probability.

KNN example

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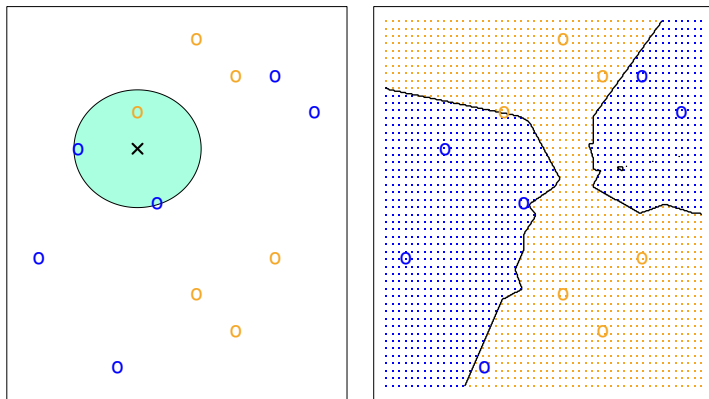


Figure: KNN classifier ($K = 3$) : D_{12} data-set and 2 classes. ²

²Source [B.1]

Optimal Choice of K

Despite its simplicity KNN can give classifiers surprising close to Bayes.
Choice of K is important:

- ▶ If $K = 1$, **very flexible** decision boundary \rightarrow
Low Training Error ($= 0$) but! High Test Error.
- ▶ As K increases (less flexibility)
Training Error increases but the Test Error may not !
- ▶ Find optimal K^* with minimum Test Error (**U** shape)
- ▶ If $K = 100$ decision boundary close to linear.

Variance vs Bias Tradeoff
or
Flexibility vs Interpretability

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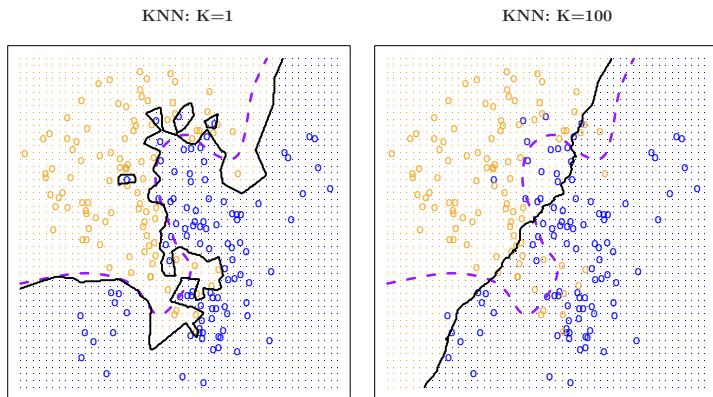


Figure: KNN with $K = 1$ (left) and $K = 100$ (right). ³

³Source [B.1]

KNN: $K=10$

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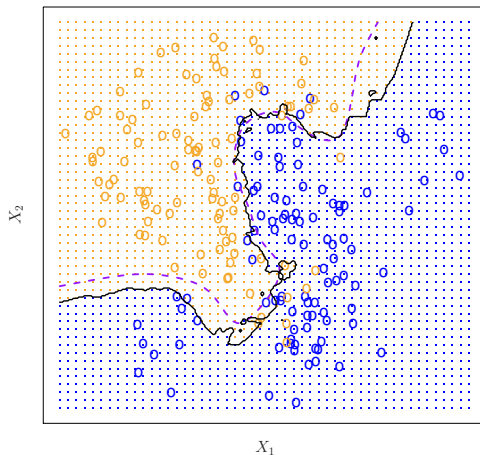


Figure: KNN with $K = 10$ close to Bayes optimal. ⁴

⁴Source [B.1]

Variance vs Bias Tradeoff

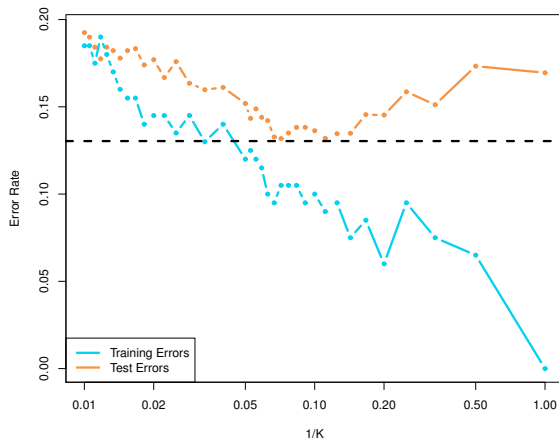


Figure: Training/Test Error Rate. ⁵

⁵Source [B.1]

What if... Linear Regression?

Suppose we have again two classes: 'Class 1', 'Class 2'.

- ▶ What if we used Linear Regression for the $P(Y|X)$?
- ▶ Let 'Class 1': $Y = 0$ and 'Class 2': $Y = 1$.
- ▶ We assume that the linear model describes the 0/1 data,

$$y_i = \beta_0 + \beta_1 x_i + \epsilon$$

and we look for the regression line

$$\mathbb{E}[y_i|x_i] = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

☞ Since $y_i \in \{0, 1\}$ then $\mathbb{E}[y_i|x_i] = \Pr(y_i = 1|x_i) = \hat{\beta}_0 + \hat{\beta}_1 x_i$.

Wrong Shape ! less than 0, more than 1

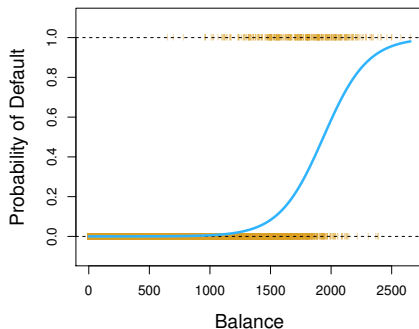
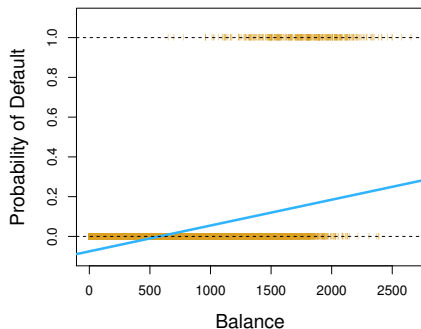


Figure: $Pr(Y = 1|X)$. Linear vs Sigmoidal fit. ⁶

⁶Source [B.1]

Logistic Regression

Suppose for the two-class problem $Pr(Y = 1|X)$ follows the **logistic function**.

$$p(X) := Pr(Y = 1|X) = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}} \quad (2)$$

- ▶ For $X \rightarrow -\infty$: $p(X) \rightarrow 0$
- ▶ For $X \rightarrow +\infty$: $p(X) \rightarrow 1$
- ▶ It is an **S-shaped curve**.

☞ We need to fit β_0 , β_1 in the non-linear logistic function.

Logistic fit

We consider a Training data-set D_n with $Y_n = (0, 0, 1, \dots, 0, 1)$.

- ▶ We don't want to use *MSE* fit \rightarrow complicated expressions.
- ▶ Better use: **log-likelihood** function.

What is the **likelihood** $g(D_n)$ of the data-sample?

$$g(D_n) = \prod_{i: y_i=1} p(x_i) \prod_{i': y_{i'}=0} (1 - p(x_{i'}))$$

because we assumed that for any X

$$Y = \begin{cases} 1, & p(X) \\ 0, & 1 - p(X) \end{cases}$$

and for all $x_i \in D_n$ we know what is the y_i answer.

Log-likelihood maximization

The log-likelihood function, is then equal to

$$\begin{aligned}\ell(\beta_0, \beta_1; D_n) &= \log(g(D_n)) & (3) \\ &= \sum_{i: y_i=1} \log p(x_i) + \sum_{i': y_{i'}=0} \log(1 - p(x_{i'})) \\ &= \sum_{i=1}^n \{y_i \log p(x_i) + (1 - y_i) \log(1 - p(x_i))\} \\ &= \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}} \sum_{i=1}^n \{y_i (\beta_0 + \beta_1 x_i) - \log(1 + e^{\beta_0 + \beta_1 x_i})\}\end{aligned}$$

☞ We want to $\max_{\beta_0, \beta_1} \ell(\beta_0, \beta_1; D_n)$.

Newton's algorithm

We follow standard process:

- ▶ $\nabla \ell(\beta_0, \beta_1; D_n) = \begin{bmatrix} \frac{\partial \ell}{\partial \beta_0} \\ \frac{\partial \ell}{\partial \beta_1} \end{bmatrix}$
- ▶ $\nabla^2 \ell(\beta_0, \beta_1; D_n) = \begin{bmatrix} \frac{\partial^2 \ell}{\partial \beta_0^2} & \frac{\partial^2 \ell}{\partial \beta_0 \partial \beta_1} \\ \frac{\partial^2 \ell}{\partial \beta_1 \partial \beta_0} & \frac{\partial^2 \ell}{\partial \beta_1^2} \end{bmatrix} < 0$ **negative-definite**
- ▶ Hence the log-likelihood logistic function is **strictly concave**.

$$\begin{bmatrix} \beta_0^{(k+1)} \\ \beta_1^{(k+1)} \end{bmatrix} = \begin{bmatrix} \beta_0^{(k)} \\ \beta_1^{(k)} \end{bmatrix} - (\nabla^2 \ell(\beta_0, \beta_1; D_n))^{-1} \cdot \nabla \ell(\beta_0, \beta_1; D_n)$$

"What are the odds?"

One can see the logistic expression of the predictions from a different point-of-view:

$$q(x_i) := \frac{p(x_i)}{1 - p(x_i)} = e^{(\beta_0 + \beta_1 x_i)}.$$

👉 **odds function**: often used in... Horse-racing!

"What are the odds ?"

- ▶ If $q(x_i) = 1/4$, then $p(x_i = 1) = 0.2$
- ▶ If $q(x_i) = 9/1$, then $p(x_i = 1) = 0.9$.

The logits (or log-odds)

One can see the logistic expression from a different point-of-view:

$$Q(x_i) := \log \left(\frac{p(x_i)}{1 - p(x_i)} \right) = \beta_0 + \beta_1 x_i.$$

Here we come back to the expression for the Linear Regression!

Separating hyperplane: For $p = 0.5$, we get the "linear" boundary

$$0 = \beta_0 + \beta_1 x_{i,1} \quad (+\beta_2 x_{i,2} + \dots + \beta_K x_{i,K}), \quad \text{for } K \geq 1.$$

e.g. for $K = 1$, it is a point $x_{\text{bound}} = -\beta_0/\beta_1$. (**left**: 1, **right**: 0)

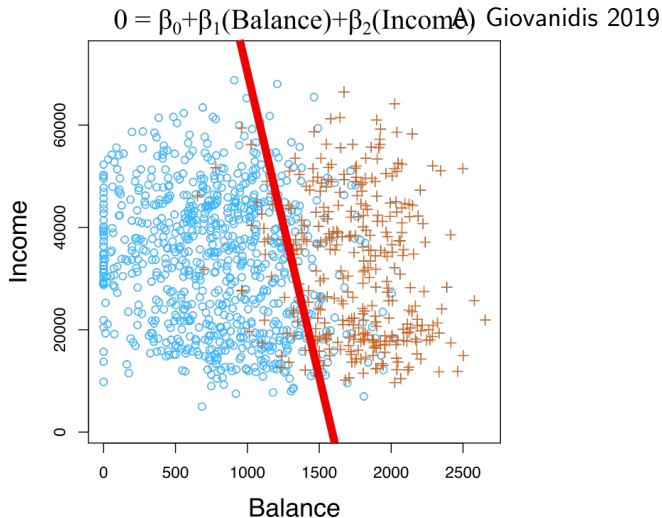


Figure: The boundary separates "blue" from "orange". ⁷

⁷ Source [B.1]

Test Data (Logistic)

If we have test input data $x_o \notin D_n$, how do we choose its Class?

Say $x_o = (x_{o,1}, x_{o,2}, \dots, x_{o,K})$.

Use the fitted values of $\beta_0, \beta_1, \dots, \beta_K$

► Either calculate $p(x_o) = \frac{e^{\beta_0 + \beta_1 x_o}}{1 + e^{\beta_0 + \beta_1 x_o}}$ and check if $>, =, < 0.5$,

► or check the position of x_o related to the boundary:

$$\beta_0 + \beta_1 x_{o,1} + \beta_2 x_{o,2} + \dots + \beta_K x_{o,K} >, =, < 0.$$

e.g. $\beta_0 + \beta_1 x_{o,1} + \beta_2 x_{o,2} + \dots + \beta_K x_{o,K} > 0 \Rightarrow p(x_o) > 0.5$

👉 We need not always use the value of 0.5 for the boundary...

Multiple Logistic Regression

We have implied that the Logistic Regression is generalised to higher than 1 dimension:

$$\log \left(\frac{p(X)}{1 - p(X)} \right) = \beta_0 + \beta_1 X_1 + \dots + \beta_K X_K,$$

where $X = (X_1, \dots, X_K)$ are K predictors.

Equivalently,

$$p(X) = \frac{e^{\beta_0 + \beta_1 X_1 + \beta_K X_K}}{1 + e^{\beta_0 + \beta_1 X_1 + \beta_K X_K}}.$$

☞ β_0, \dots, β_K are estimated by the **maximum likelihood method**.

Example

Using the data set Default we want to decide, whether an individual is likely to default on its bank account.

$X = (\text{balance}, \text{income}, \text{student}[\text{Yes}])$, so $K = 3$.

$Y = \text{default}[\text{Yes}]$.

- First consider only balance, $K = 1$.

	Coefficient	Std. error	Z-statistic	P-value
Intercept	-10.6513	0.3612	-29.5	<0.0001
balance	0.0055	0.0002	24.9	<0.0001

☞ 1-unit increase in balance is associated to $\beta_1 = 0.0055$ units increase in log-odds of default.

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Example (predictions)

default[Yes] probability for an individual with balance = 1000 EUR

$$\hat{p}(\text{balance} = 1000) = \frac{e^{-10.6513+0.0055 \times 1000}}{1 + e^{-10.6513+0.0055 \times 1000}} = 0.00576$$

- Now consider binary student[Yes], $K = 1$.

	Coefficient	Std. error	Z-statistic	P-value
Intercept	-3.5041	0.0707	-49.55	<0.0001
student[Yes]	0.4049	0.1150	3.52	0.0004

$$\hat{p}(\text{student[Yes]} = 1) = 0.0431 > \hat{p}(\text{student[Yes]} = 0) = 0.0292$$

Conclusion 1: Students are more likely to default.

Example (multiple)

- Now consider the entire X vector, $K = 3$.

	Coefficient	Std. error	Z-statistic	P-value
Intercept	-10.8690	0.4923	-22.08	<0.0001
balance	0.0057	0.0002	24.74	<0.0001
income	0.0030	0.0082	0.37	0.7115
student[Yes]	-0.6468	0.2362	-2.74	0.0062

Paradox: Conclusion 2: Students are **less** likely to default !!!!

$$(\beta_{\text{student[Yes]}} < 0)$$

Why? The student[Yes] and balance predictors are correlated.

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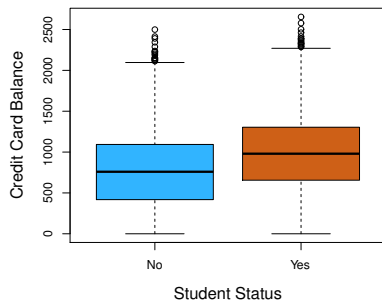
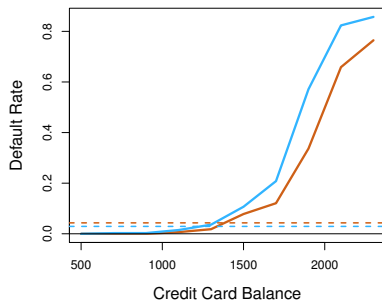


Figure: Students tend to have higher debts in the US/GB/D.⁸

Conclusion 1: For the same credit-card balance a student is less likely to default.

⁸Source [B.1]

Logistic Regression for > 2 Classes

We can easily generalise to M classes:

$$\begin{aligned} \log \frac{Pr(Class = 1|X = x)}{Pr(Class = M|X = x)} &= \beta_{1,0} + \beta_1^T x \\ &\dots \\ \log \frac{Pr(Class = M-1|X = x)}{Pr(Class = M|X = x)} &= \beta_{M-1,0} + \beta_{M-1}^T x \\ Pr(Class = M|X = x) &= \frac{1}{1 + \sum_{m=1}^{M-1} \exp(\beta_{m,0} + \beta_m^T x)} \end{aligned}$$

- We need $M - 1$ log-odds.
- The probabilities sum-up to 1.
- The choice of denominator class is arbitrary.
- Max likelihood.

☞ For multiple classe, **discriminant analysis** is more popular...

Linear Discriminant Analysis (LDA)

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For classification of two or multiple classes, we often use the LDA classifier:

- ▶ Again, the class boundaries are **linear**.
- ▶ Instead of modelling $Pr(Y = k|X = x)$ directly as in LR, it does this indirectly by modelling $Pr(X = x|Y = k)$.
- ▶ It makes use of the **Bayes' Theorem** and the **Bayes classifier**.
- ▶ It assumes that the distribution of X 's is approximately **Normal**, (or **Gaussian**).

Bayes' Theorem in Classification

We want to calculate the conditional probability for each class

$$\begin{aligned}
 Pr(Y = k|X = x) &\stackrel{\text{Bayes'}}{=} \frac{Pr(X = x|Y = k) Pr(Y = k)}{Pr(X = x)} \\
 &\stackrel{\text{Total}}{=} \frac{Pr(X = x|Y = k) Pr(Y = k)}{\sum_{m=1}^M Pr(X = x|Y = m) Pr(Y = m)} \\
 &= \frac{f_k(x) \cdot \pi_k}{\sum_{m=1}^M f_m(x) \cdot \pi_m} \quad (4)
 \end{aligned}$$

☞ We need the **conditional probability of X** given the class, and the **frequency** of each class.

☞ Given these, we can choose for $X = x_o$, the class with $\max_{1 \leq j \leq M} Pr(Y = j|X = x_o)$ (**Bayes classifier**).

LDA for 1 predictor $K = 1$

We can **assume** that $f_k(x)$ is **normal** or **Gaussian**.

- For $K = 1$:

$$f_k(x) = \frac{1}{\sigma_k \sqrt{2\pi}} \exp \left(-\frac{1}{2\sigma_k^2} (x - \mu_k)^2 \right),$$

μ_k and σ_k^2 are the **mean** and **variance** for the k -th class.

- Let us further assume that $\sigma_1^2 = \sigma_2^2 = \dots = \sigma_M^2 = \sigma^2$, hence there is a shared variance among all classes.
- The π_m 's are also called **prior probabilities**.

Q: Is the gaussian assumption reasonable?

LDA ($K = 1$)

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Plugging in (4), we get:

$$Pr(Y = k|X = x) = \frac{\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2}(x - \mu_k)^2\right) \cdot \pi_k}{\sum_{m=1}^M \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2}(x - \mu_m)^2\right) \cdot \pi_m}$$

Unknowns: π_m , μ_m , $\forall m$, and σ .

LDA ($K = 1$) classification

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We take the log in the above expression. We then assign for $X = x$, the class m^* such that

$$\begin{aligned} m^* &= \arg \max_{1 \leq m \leq M} \Pr(Y = m | X = x) \\ &= \arg \max_{1 \leq m \leq M} \log \Pr(Y = m | X = x) \\ &= \arg \max_{1 \leq m \leq M} \left\{ x \cdot \frac{\mu_m}{\sigma^2} - \frac{\mu_m^2}{2\sigma^2} + \log(\pi_m) \right\} \quad (5) \\ &= \arg \max_{1 \leq m \leq M} \{x \cdot c_1 + c_0\} \quad (\text{linear!}) \end{aligned}$$

Estimating the decision function

For each m we have the **linear discriminant function** function of x :

$$\delta_m(x) = x \cdot \frac{\mu_m}{\sigma^2} - \frac{\mu_m^2}{2\sigma^2} + \log(\pi_m),$$

and to calculate it from the dataset D_n we use the estimates:

$$\hat{\mu}_m = \frac{1}{n_m} \sum_{i:y_i=m} x_i,$$

$$\hat{\sigma}^2 = \frac{1}{n - M} \sum_{m=1}^M \sum_{i:y_i=m} (x_i - \hat{\mu}_m)^2,$$

$$\hat{\pi}_m = \frac{n_m}{n}.$$

2-class example

In the case of $M = 2$ classes, suppose $\pi_1 = \pi_2$ additionally.

Then the discriminant functions become:

$$\delta_1(x) = x \cdot \frac{\mu_1}{\sigma^2} - \frac{\mu_1^2}{2\sigma^2} + \log(\pi_1)$$

$$\delta_2(x) = x \cdot \frac{\mu_2}{\sigma^2} - \frac{\mu_2^2}{2\sigma^2} + \log(\pi_2)$$

so that x is assigned class 1, if $\delta_1(x) > \delta_2(x)$ or,

$$2x(\mu_1 - \mu_2) > \mu_1^2 - \mu_2^2$$

The decision boundary are the points x , s.t.

$$x = \frac{\mu_1 + \mu_2}{2}.$$

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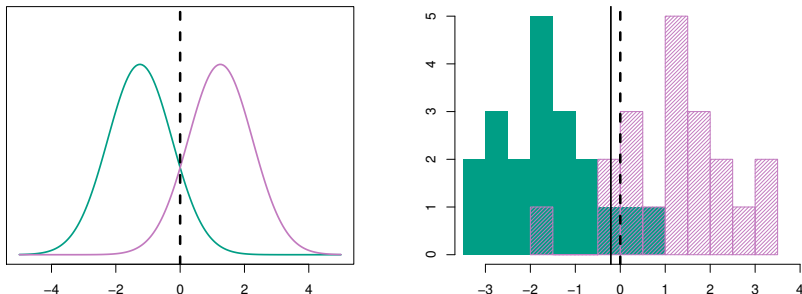


Figure: Two normal density functions and decision boundary. ⁹

⁹Source [B.1]

LDA for $K > 1$ dimensions

How does the LDA perform, when the predictors X have more than 1 dimension? say $X = (X_1, \dots, X_K)$.

☞ Assume a **multivariate Gaussian distribution** instead of a 1-dimensional $X \sim \mathcal{N}(\mu, \Sigma)$.

$$f(x) = \frac{1}{(2\pi)^{K/2} |\Sigma|^{1/2}} \exp \left(-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right).$$

- **mean** $\mu = (\mu_1, \dots, \mu_K)$,
- common **covariance matrix** Σ .

Linear Discriminant Function:

$$\delta_k(x) = x^T \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k^T \Sigma^{-1} \mu_k + \log(\pi_k)$$

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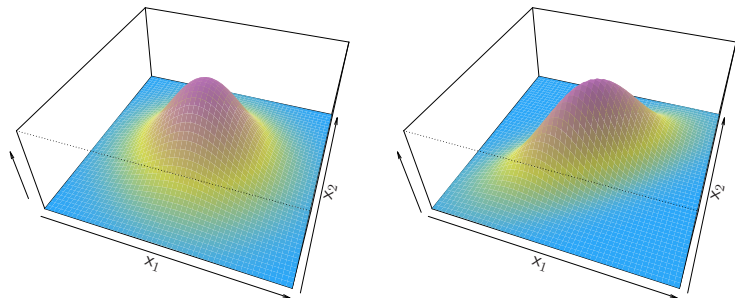


Figure: Examples of binormal distributions. ¹⁰

¹⁰Source [B.1]

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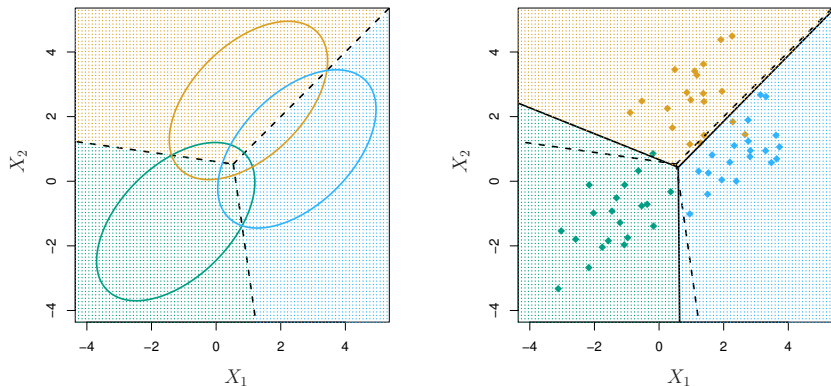


Figure: Classification for $M = 3$ classes and $K = 2$ dimensions. ¹¹

¹¹Source [B.1]

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		<i>True default status</i>		
		No	Yes	Total
<i>Predicted default status</i>	No	9,644	252	9,896
	Yes	23	81	104
	Total	9,667	333	10,000

Figure: Confusion Matrix: Predicted vs True default status. ¹²

$$\text{Error} \left[\widehat{\text{Default}} = \text{"Yes"} \mid \text{Default} = \text{"No"} \right] = 23/9667 \approx 0.2\%$$

$$\text{Error} \left[\widehat{\text{Default}} = \text{"No"} \mid \text{Default} = \text{"Yes"} \right] = 252/333 \approx 75.7\%$$

¹²Source [B.1]

Quadratic Discriminant Analysis (QDA)

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LDA assumed for each class a different mean μ_k and same covariance matrix Σ .

☞ QDA assumes **different covariance matrix per class**. That is, an observation from the k -th class is of the form $X \sim \mathcal{N}(\mu_k, \Sigma_k)$.

Quadratic Discriminant Function:

$$\begin{aligned}\delta_k(x) = & -\frac{1}{2}x^T \Sigma_k^{-1}x + x^T \Sigma_k^{-1}\mu_k - \frac{1}{2}\mu_k^T \Sigma_k^{-1}\mu_k - \\ & -\frac{1}{2}\log |\Sigma_k| + \log(\pi_k)\end{aligned}$$

QDA is more flexible than LDA: Bias vs Variance tradeoff !

QDA examples

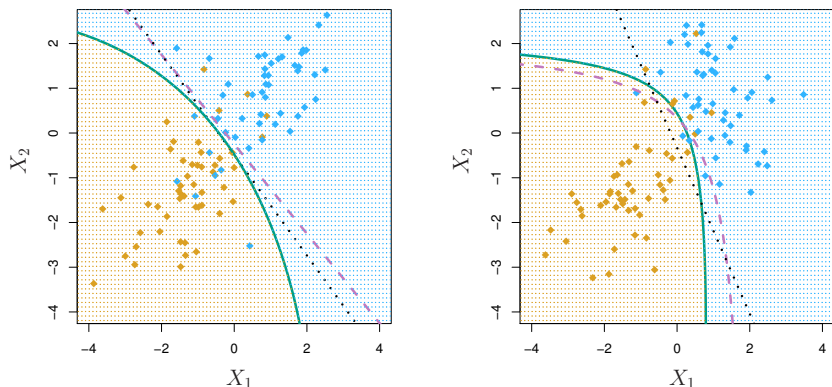


Figure: (left:) Truth common Σ , (right:) Truth different Σ_1, Σ_2 .¹³

¹³Source [B.1]

Method comparison: linear

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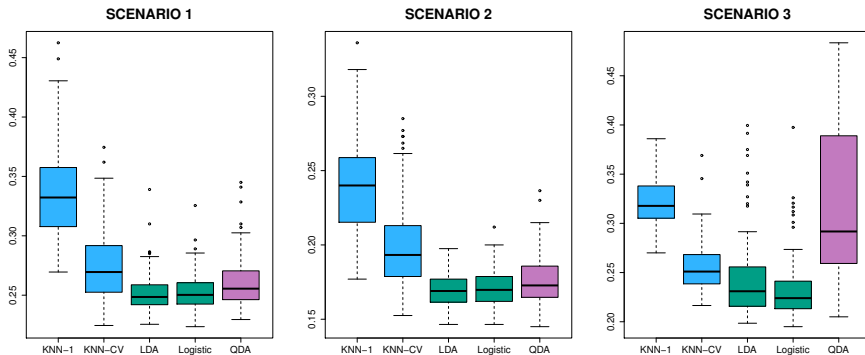


Figure: (1) uncorr., \mathcal{N} , $\mu_1 \neq \mu_2$, (2) corr., \mathcal{N} , (3) uncorr., t-distr.¹⁴

¹⁴Source [B.1]

Method comparison: non-linear

A. Giovanidis 2019

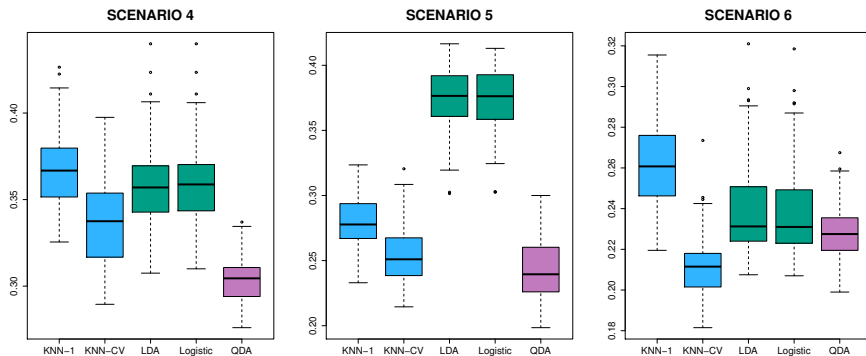


Figure: (4) corr. \mathcal{N} , $\Sigma_1 \neq \Sigma_2$, (5) logistic $X_1^2, X_2^2, X_1 X_2$ (6) more-NL. ¹⁵

¹⁵Source [B.1]

A. Giovanidis 2019

END