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08. Classification

Data Analysis for Networks - NDA'20
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Sorbonne-LIP6

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Bibliography

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B.1 Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani. “An introduction to statistical learning: with applications in R”. Springer Texts in Statistics. ISBN 978-1-4614-7137-0
Chapter 2, Chapter 4
DOI 10.1007/978-1-4614-7138-7

B.2 Nesrine Ammar, Ludovic Noirie, Sébastien Tixeuil. “Amélioration de l’identification du type des objets connectés par classification supervisée”, CORES 2019, Online: https://hal.archives-ouvertes.fr/hal-02126555

B.3 Giorgos Dimopoulos, Ilias Leontiadis, Pere Barlet-Ros, Konstantina Papagiannaki. “Measuring Video QoE from Encrypted Traffic”, IMC ’16 Proceedings of the 2016 Internet Measurement Conference Pages 513-526 .

Classification Setting

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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", "COVID") or more generally:

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

Application A: IoT Classifier

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☞ Example application: Internet-of-Things (IoT) for home networks. "Device identification assistant." from [B.2]

- Home devices can be controlled from distance. (Camera, Light, Sensor, Mobile, Switch, Alarm, Tablet, Speaker, TV.)
- For better quality-of-service these devices need to be identified **by type** from the network.
- Massive number of devices with heterogeneous functionality!

Use supervised learning to train an object classifier.

Input data:
(a) the data-flow information per device, i.e. traffic characteristics.
(b) a selected list of attributes (features).

A. IoT Features

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☞ Once a device is connected, a MAC address is attributed.

Feature set to use for classification:

- Flow-based statistics:
  - Packet size (mean, max, min)
  - Mean inter-arrival packet time in a flow.
  - Flow-size measured in number of packets.
  - Protocol type: HTTP, HTTPS, SSDP, mDNS, TFTP, etc.
- Textual attributes (Bag-of-words): 0 or 1 per word per object?
  - Fabrication mark from MAC address.
  - Model and Type from HTTP.

A. IoT Implementation

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- WiFi access connected to an Ethernet switch.
- A measurement computer is connected at the switch to trace traffic.
- The computer collects data from the new IoT device during 1 min.
- The computer contains the trained classifier, which decides the most relavant class the IoT device belongs to. The decision is probabilistic.

Types of classifier: K-Nearest Neighbours, Naive Bayes, Random Forest, Tree-based classifier, etc.

Application B: Classifying Video QoE

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☞ How to detect video streaming QoE issues from encrypted traffic? (see [B.3])

- Use predictive models to detect different levels of QoE degradation, due to: stalling, average video quality, quality variations.

Labels:

- Stalling: (None, Mild, Severe)
- Video Quality: (Low, Medium, High)
- Quality Switch: use frequency and amplitude of switches.

Features:
(a) Chunk size percentiles, and average.
(b) Packet retransmissions, (c) Bandwidth-Delay Product (BDP),
(d) Bytes-In-Flight (BIF).

Training Accuracy

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Suppose we have training observations:
$D_n = \{(x_1, y_1),\ (x_2, y_2), \ldots, (x_n, y_n)\}$, with $y_1,\ \ldots,\ y_n$ qualitative.

Consider a fitting model with an estimate $\hat{y}_i = \hat{f}(x_i)$.
We use the training error rate:

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

This is the fraction of incorrect classifications:

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

Test Accuracy

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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:

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

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

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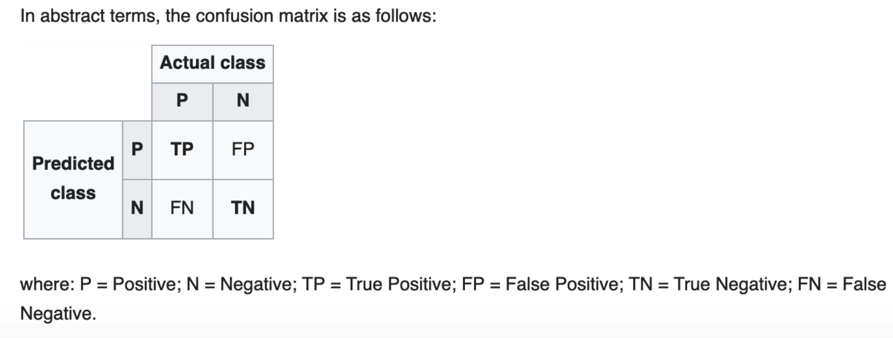
Confusion Matrix



In abstract terms, the confusion matrix is as follows:

		Actual class	
		P	**N**
Predicted class	**P**	**TP**	FP
	N	FN	**TN**

where: P = Positive; N = Negative; TP = True Positive; FP = False Positive; TN = True Negative; FN = False Negative.

Figure: (source: wikipedia "Confusion matrix")

☞ Two types of errors (False Negative, and False Positive)

- FP: Incorrectly assign an individual of Class N to Class P.
- FN: Incorrectly assign an individual of Class P to Class N.

Definitions of performance

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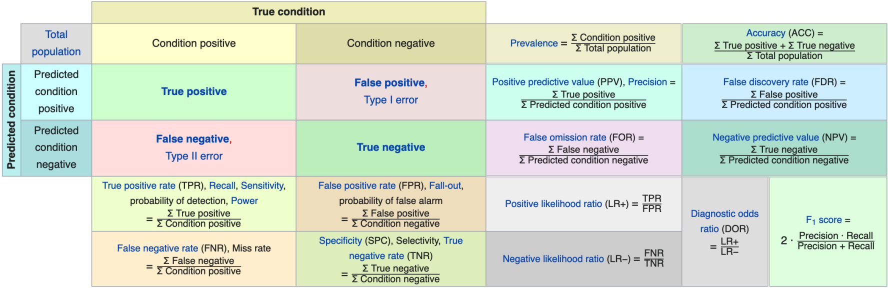

		True condition				
	Total population	Condition positive	Condition negative	Prevalence = $\frac{\Sigma\ \text{Condition positive}}{\Sigma\ \text{Total population}}$	Accuracy (ACC) = $\frac{\Sigma\ \text{True positive} + \Sigma\ \text{True negative}}{\Sigma\ \text{Total population}}$	
Predicted condition	Predicted condition positive	**True positive**	**False positive**, Type I error	Positive predictive value (PPV), Precision = $\frac{\Sigma\ \text{True positive}}{\Sigma\ \text{Predicted condition positive}}$	False discovery rate (FDR) = $\frac{\Sigma\ \text{False positive}}{\Sigma\ \text{Predicted condition positive}}$	
	Predicted condition negative	**False negative**, Type II error	**True negative**	False omission rate (FOR) = $\frac{\Sigma\ \text{False negative}}{\Sigma\ \text{Predicted condition negative}}$	Negative predictive value (NPV) = $\frac{\Sigma\ \text{True negative}}{\Sigma\ \text{Predicted condition negative}}$	
		True positive rate (TPR), Recall, Sensitivity, probability of detection, Power $= \frac{\Sigma\ \text{True positive}}{\Sigma\ \text{Condition positive}}$	False positive rate (FPR), Fall-out, probability of false alarm $= \frac{\Sigma\ \text{False positive}}{\Sigma\ \text{Condition negative}}$	Positive likelihood ratio (LR+) = $\frac{\text{TPR}}{\text{FPR}}$	Diagnostic odds ratio (DOR) $= \frac{\text{LR+}}{\text{LR–}}$	F_1 score = $2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$
		False negative rate (FNR), Miss rate $= \frac{\Sigma\ \text{False negative}}{\Sigma\ \text{Condition positive}}$	Specificity (SPC), Selectivity, True negative rate (TNR) $= \frac{\Sigma\ \text{True negative}}{\Sigma\ \text{Condition negative}}$	Negative likelihood ratio (LR–) = $\frac{\text{FNR}}{\text{TNR}}$		

Figure: (source: wikipedia "Confusion matrix")

Precision and Recall

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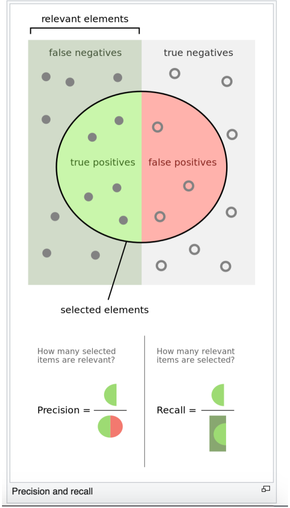

Precision and recall

Figure: (source: wikipedia "Precision and recall")

Metrics

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Accuracy (ACC)	$\frac{TP+TN}{TP+FP+TN+FN}$	
Precision Positive predictive value (PPV)	$\frac{TP}{TP+FP}$	
Recall (Sensitivity) True positive rate (TPR)	$\frac{TP}{TP+FN}$	**False negative rate** $FNR = 1 - TPR$
Specificity True negative rate (TNR)	$\frac{TN}{TN+FP}$	**False positive rate** $FPR = 1 - TNR$

ROC Curve

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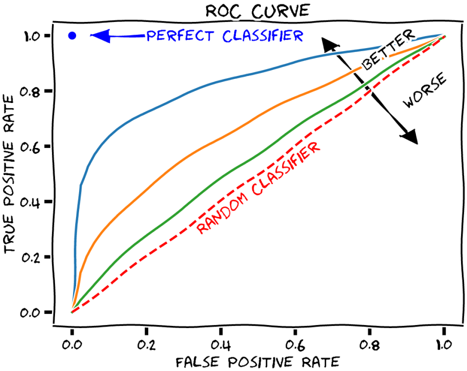

Figure: (source: wikipedia "Receiver operating characteristic")

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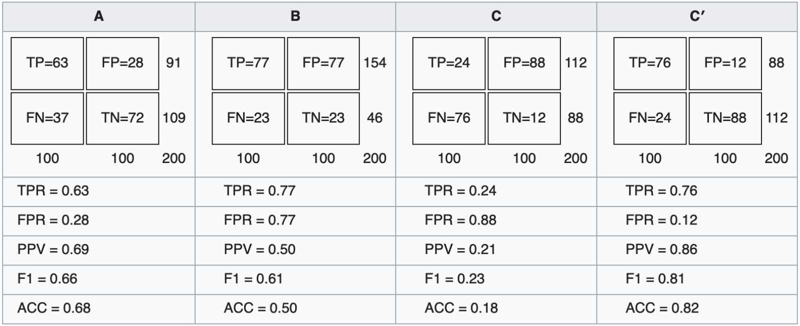
Examples



A			B			C			C′		
TP=63	FP=28	91	TP=77	FP=77	154	TP=24	FP=88	112	TP=76	FP=12	88
FN=37	TN=72	109	FN=23	TN=23	46	FN=76	TN=12	88	FN=24	TN=88	112
100	100	200	100	100	200	100	100	200	100	100	200
TPR = 0.63			TPR = 0.77			TPR = 0.24			TPR = 0.76		
FPR = 0.28			FPR = 0.77			FPR = 0.88			FPR = 0.12		
PPV = 0.69			PPV = 0.50			PPV = 0.21			PPV = 0.86		
F1 = 0.66			F1 = 0.61			F1 = 0.23			F1 = 0.81		
ACC = 0.68			ACC = 0.50			ACC = 0.18			ACC = 0.82		

Figure: Four confusion matrices (source: wikipedia "Receiver operating characteristic")

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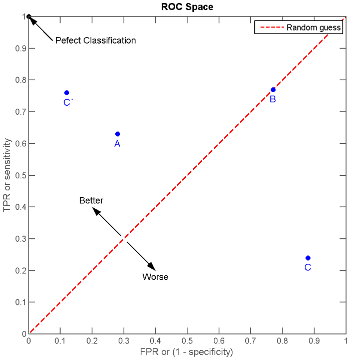

Figure: (source: wikipedia "Receiver operating characteristic")

Classifiers

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We will further consider in this lecture the following classifiers:

- ✯ (Wise) Bayes classifier
- ✯ K-Nearest-Neighbours classifier (KNN)
- ✯ Naive Bayes classifier
- ✯ Logistic Regression (LR)

Also: Linear Discriminant Analysis (LDA), Quadratic Discriminant Analysis (QDA)

Bayes Classifier

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Optimal Classifier: (If all misclassifications are equally important) Assign each observation to the most likely class, given its predictor values:

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

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

☞ In a two-class problem

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

$$\begin{array}{ll} \text{Class 1,} & \text{if } Pr\left(Y = 1 \mid X = x_o\right) > 0.5 \\ \text{Class 2,} & \text{if } Pr\left(Y = 2 \mid X = x_o\right) > 0.5 \end{array}$$

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

Bayes example

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

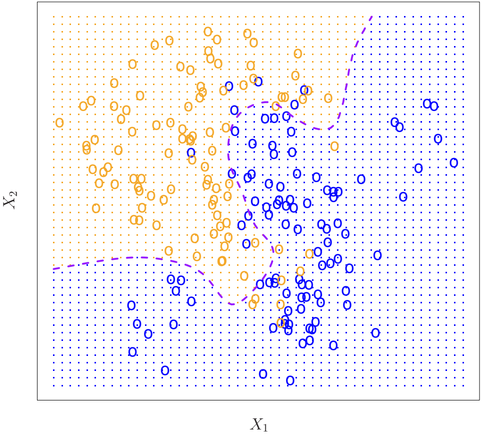

Figure: Bayes classifier : D_{100} data-set and 2 classes (blue, orange). [1]

[1] Source [B.1]

Bayes classifier cont'd

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

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

$$Test\ Error(x_o) = 1 - \max_j Pr\left(Y = j \mid X = x_o\right)$$

Drawback...

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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.

KNN classifier

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How does the KNN classifier work?

- Choose a positive integer $K > 0$.
- Given a test observation $x_o \notin D_n$, the KNN classifier identifies the K points in the training data-set closest to x_o, it is the set $\mathcal{N}_K(x_o)$.
- The conditional probability for class j at x_o is estimated as:

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

- Calculate the estimates for all classes $j = 1, \ldots, M$ and
- Finally, apply Bayes classification: classify x_o to the class with the largest estimated probability.

KNN example

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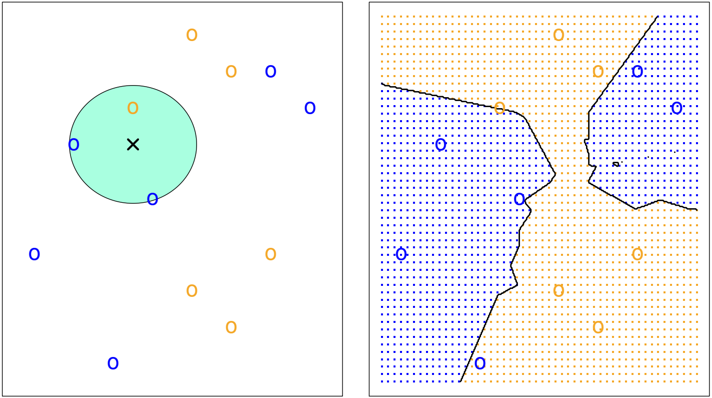

Figure: KNN classifier $(K = 3)$: D_{12} data-set and 2 classes. [2]

[2] Source [B.1]

Optimal Choice of K

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

- If $K = 1$, very flexible decision boundary → 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 ($\bigcup$ shape)
- If $K = 100$ decision boundary close to linear.

Variance vs Bias Tradeoff
or
Flexibility vs Interpretability

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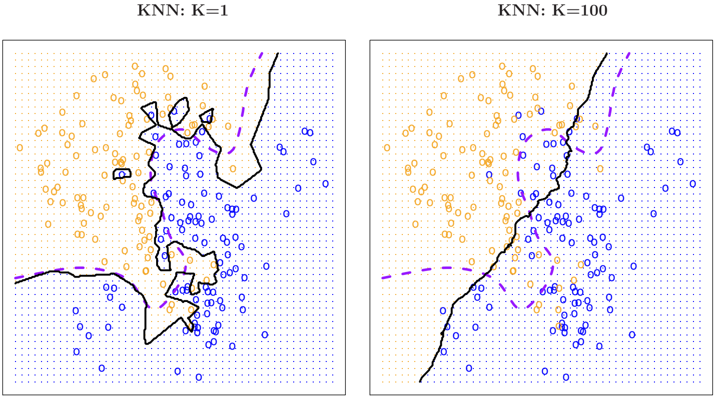

Figure: KNN with $K = 1$ (left) and $K = 100$ (right). [3]

[3] Source [B.1]

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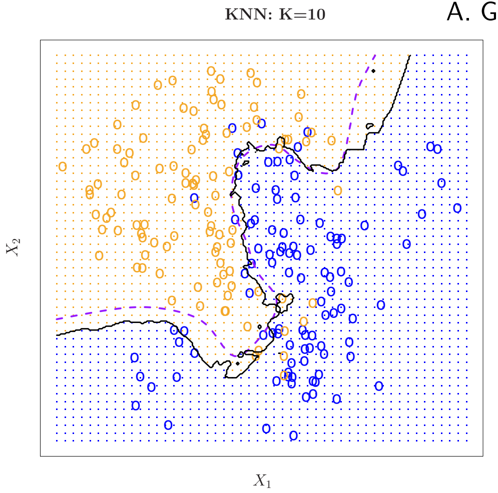

Figure: KNN with $K = 10$ close to Bayes optimal. [4]

[4] Source [B.1]

Variance vs Bias Tradeoff

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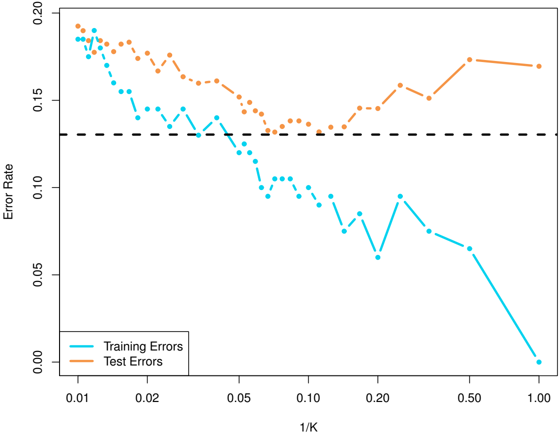

Figure: Training/Test Error Rate. [5]

[5] Source [B.1]

Naive Bayes

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☞ The Naive Bayes classifier:

- Assumes that the K features are independent.
- Uses a simple MAP or ML estimator

$$\begin{aligned} P(Y \mid \mathcal{D}_n) &\propto P(\mathcal{D}_n \mid Y)P(Y) \quad \textbf{[MAP]} \\ P(Y \mid \mathcal{D}_n) &\propto P(\mathcal{D}_n \mid Y) \qquad\quad \textbf{[ML]} \end{aligned}$$

where Y is the class label.
We choose MAP or ML, depending on the prior information over the class distribution Y.

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Naive Bayes with discrete features

✐ Let us classify texts (e.g. books, sentences) in one of two classes:

1. History
2. Science

To do so, we will use some features from the available data (texts). These are a certain bag-of-words: {'king', 'food', 'equals', 'proof'}

	Bag-Of-Words				Label	
	1:'king'	2:'food'	3:'equals'	4:'proof'	History	Science
Text 1	No	Yes	Yes	Yes	No	Yes
Text 2	No	No	Yes	No	No	Yes
Text 3	Yes	Yes	No	Yes	Yes	No
...	...	...	...	...	...	...
Text n	Yes	No	Yes	Yes	No	Yes

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Naive Bayes with discrete features (II)

✐ If X contains K binary state features, with $X_{t,k} \in \{0, 1\}$, then

$$X_t \quad = \quad (X_{t,1}, \dots, X_{t,K}), \quad t = 1, \dots, n.$$

$X_{t,k}$ says whether feature k appears or not in the t-th data sample of $\mathcal{D}_n$.

Also, Y is the label of each text. Then, let

$$Y_t = \begin{cases} 0 & \text{if 'History'} \\ 1 & \text{if 'Science'} \end{cases}$$

ML estimators

$$p_{Sc} = P(Y = 1) = \frac{1}{n} \sum_{t=1}^{n} Y_t, \qquad p_{Hi,k} = P(Y = 0) = \frac{1}{n} \sum_{t=1}^{n} (1 - Y_t)$$

$$p_{Sc,k} = P(Y = 1,\ X_k = 1) \quad = \quad \frac{\sum_{t=1}^{n} Y_t \cdot X_{t,k}}{\sum_{t=1}^{n} Y_t}$$

Naive Bayes with discrete features (III)

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☞ How does Naive Bayes work? Let's see for the 2 classes ('History'-'Science')

- Prior distribution over classes, i.e. $P(Y=0)$ and $P(Y=1)$.
- Suppose the distribution for each feature k per class j is $\mathrm{Bernoulli}(p_{j,k})$ and independent of other features.

$$P(\mathcal{D}_n \mid Y=j) \quad = \quad \prod_{t\in\mathcal{D}_n}\left(\prod_{k=1}^{K} p_{j,k}^{X_{t,k}}(1-p_{j,k})^{1-X_{t,k}}\right), \quad j=0,1$$

MAP posteriors:

$$P(Y=j \mid \mathcal{D}_n) \quad = \quad P(\mathcal{D}_n \mid Y=j)\cdot P(Y=j)$$

Naive Bayes with continuous features

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✐ Suppose that X contains K continuous state features.

- Prior distribution over classes, is assumed uniform, i.e. $P(Y = 0) = P(Y = 1) = 0.5$.
- Suppose the distribution for each feature k per class j is Gaussian $\mathcal{N}(\mu_{j,k}, \sigma^2_{j,k})$.

ML estimates for mean and variance

$$\overline{X}_{1,k} = \frac{1}{n} \sum_{t \in \mathcal{D}_n} Y_t \cdot X_{t,k}, \qquad \overline{X}_{0,k} = \frac{1}{n} \sum_{t \in \mathcal{D}_n} (1 - Y_t) \cdot X_{t,k}$$

$$\overline{S}^2_{1,k} = \frac{1}{n} \sum_{t \in \mathcal{D}_n} (Y_t \cdot X_{t,k} - \overline{X}_{1,k})^2, \qquad \overline{S}^2_{0,k} = \frac{1}{n} \sum_{t \in \mathcal{D}_n} ((1 - Y_t) \cdot X_{t,k} - \overline{X}_{0,k})^2$$

Naive Bayes with continuous features (II)

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Given a Test sample (x_o, y_o), the estimated class is the one which maximizes the ML (or MAP) estimator, i.e. the maximum between

$$P(Y = 0 \mid \mathcal{D}_n) = \prod_{k=1}^{K} \frac{1}{(2\pi \overline{S}_{0,k}^2)^{1/2}} \exp\left(-\frac{(x_o - \overline{X}_{0,k})^2}{2\overline{S}_0^2}\right) \quad \textit{for} \quad \textit{Class}\ 0$$

$$P(Y = 1 \mid \mathcal{D}_n) = \prod_{k=1}^{K} \frac{1}{(2\pi \overline{S}_{1,k}^2)^{1/2}} \exp\left(-\frac{(x_o - \overline{X}_{1,k})^2}{2\overline{S}_1^2}\right) \quad \textit{for} \quad \textit{Class}\ 1$$

What if... Linear Regression?

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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,

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

  and we look for the regression line

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

☞ 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

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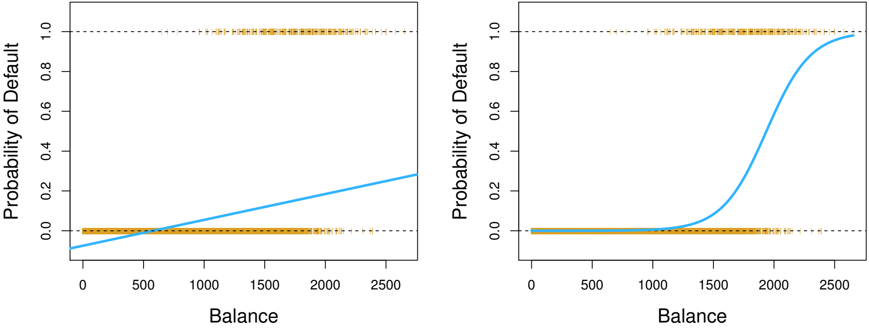

Figure: $Pr\left(Y=1|X\right)$. Linear vs Sigmoidal fit. [6]

[6] Source [B.1]

Logistic Regression

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

$$p(X) := Pr\,(Y=1|X) = \frac{e^{\beta_o+\beta_1 X}}{1+e^{\beta_o+\beta_1 X}}$$

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

☞ We need to fit $\beta_o,\ \beta_1$ in the non-linear logistic function.

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Logistic fit

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

- We don't want to use *MSE* fit → 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

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The log-likelihood function, is then equal to

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

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

Newton's algorithm

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We follow standard process:

- $\nabla \ell(\beta_0, \beta_1; D_n) = \left[\begin{array}{c} \frac{\partial \ell}{\partial \beta_o} \\ \frac{\partial \ell}{\partial \beta_1} \end{array} \right]$
- $\nabla^2 \ell(\beta_0, \beta_1; D_n) = \left[\begin{array}{cc} \frac{\partial^2 \ell}{\partial {\beta_0}^2} & \frac{\partial^2 \ell}{\partial \beta_o \partial \beta_1} \\ \frac{\partial^2 \ell}{\partial \beta_1 \partial \beta_0} & \frac{\partial^2 \ell}{\partial {\beta_1}^2} \end{array} \right] < 0$ negative-definite
- Hence the log-likelihood logistic function is strictly concave.

$$\left[\begin{array}{c} \beta_0^{(k+1)} \\ \beta_1^{(k+1)} \end{array} \right] = \left[\begin{array}{c} \beta_0^{(k)} \\ \beta_1^{(k)} \end{array} \right] - \left(\nabla^2 \ell(\beta_0, \beta_1; D_n)\right)^{-1} \cdot \nabla \ell(\beta_0, \beta_1; D_n)$$

"What are the odds?"

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

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

☞ 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)

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

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

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

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

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

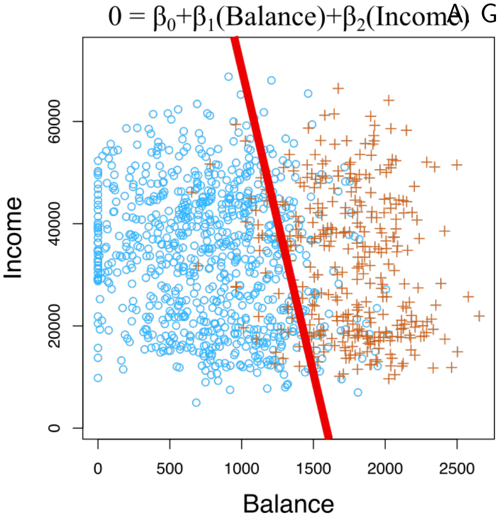

Figure: The boundary separates "blue" from "orange". [7]

[7] Source [B.1]

Test Data (Logistic)

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If we have test input data $x_o \notin D_n$, how do we choose its Class?
Say $x_o = (x_{o,1}, x_{o,2}, \ldots, x_{o,K})$.

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

- Either calculate $p(x_o) = \frac{e^{\beta_0+\beta_1 x_{o,1}+\ldots+\beta_K x_{o,K}}}{1+e^{\beta_0+\beta_1 x_{o,1}+\ldots+\beta_K x_{o,K}}}$ and check if $>, =, < 0.5$,
- or check the position of x_o related to the boundary: $\beta_0 + \beta_1 x_{o,1} + \beta_2 x_{o,2} + \ldots + \beta_K x_{o,K} >, =, < 0$.

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

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

Multiple Logistic Regression

A. Giovanidis 2020

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

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

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

Equivalently,

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

☞ $\beta_0, \ldots, \beta_K$ are estimated by the maximum likelihood method.

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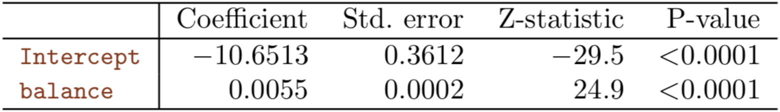
Example

Using the data set $\mathrm{Default}$ we want to decide, whether an individual is likely to default on its bank account, or not.

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

- First consider only $\mathrm{balance}$, $K = 1$.



	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 $\mathrm{balance}$ is associated to $\beta_1 = 0.0055$ units increase in log-odds of $\mathrm{default}$.

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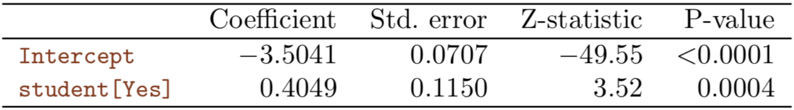
Example (predictions)

default[Yes] probability for an individual with $\text{balance} = 1000$ EUR

$$\hat{p}(\text{balance} = 1000) \quad = \quad \frac{e^{-10.6513+0.0055x1000}}{1 + e^{-10.6513+0.0055x1000}} = 0.00576$$

- 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

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

Conclusion 1: Students are more likely to default.

Example (multiple)

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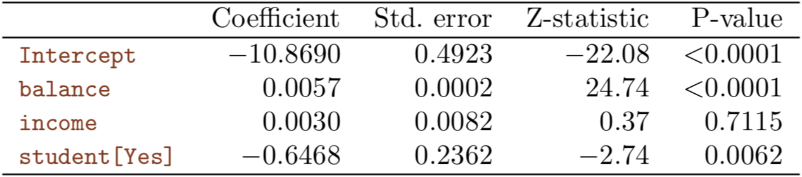
- Now consider the entire X vector, $K = 3$.



	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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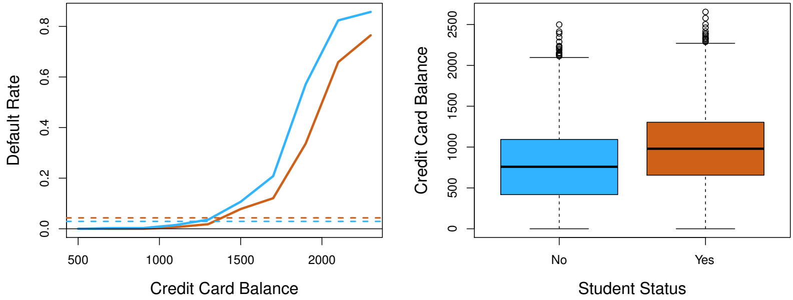

Figure: Students tend to have higher debts in the US/GB/D. [8]

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

[8] Source [B.1]

Logistic Regression for $>$ 2 Classes

A. Giovanidis 2020

We can easily generalise to M classes:

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

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

☞ For multiple classes, discriminant analysis is more popular...

Linear Discriminant Analysis (LDA)

A. Giovanidis 2020

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

A. Giovanidis 2020

We want to calculate the conditional probability for each class

$$\begin{aligned} Pr\left(Y=k|X=x\right) &\overset{Bayes'}{=} \frac{Pr\left(X=x|Y=k\right)Pr\left(Y=k\right)}{Pr\left(X=x\right)} \\ &\overset{Total}{=} \frac{Pr\left(X=x|Y=k\right)Pr\left(Y=k\right)}{\sum_{m=1}^{M} Pr\left(X=x|Y=m\right)Pr\left(Y=m\right)} \\ &= \frac{f_k(x)\cdot\pi_k}{\sum_{m=1}^{M} f_m(x)\cdot\pi_m} \end{aligned} \tag{1}$$

☞ 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 $\max_{1\leq j\leq M} Pr\left(Y=j|X=x_o\right)$ (Bayes classifier).

LDA for 1 predictor $K = 1$

A. Giovanidis 2020

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 $\sigma_1^2 = \sigma_2^2 = \ldots = \sigma_M^2 = \sigma^2$, 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 $(K = 1)$

A. Giovanidis 2020

Plugging in (1), we get:

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

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

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

Estimating the decision function

A. Giovanidis 2020

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

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

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

$$\begin{aligned}
\hat{\mu}_m &= \frac{1}{n_m} \sum_{i:y_i=m} x_i, \\
\hat{\sigma}^2 &= \frac{1}{n-M} \sum_{m=1}^{M} \sum_{i:y_i=m} \left(x_i - \hat{\mu}_m\right)^2, \\
\hat{\pi}_m &= \frac{n_m}{n}.
\end{aligned}$$

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2-class example

In the case of $M = 2$ classes, suppose $\pi_1 = \pi_2$ additionally.
Then the discriminant functions become:

$$\begin{aligned}\delta_1(x) &= x \cdot \frac{\mu_1}{\sigma^2} - \frac{\mu_1^2}{2\sigma^2} + \log(\pi_1) \\ \delta_2(x) &= x \cdot \frac{\mu_2}{\sigma^2} - \frac{\mu_2^2}{2\sigma^2} + \log(\pi_2)\end{aligned}$$

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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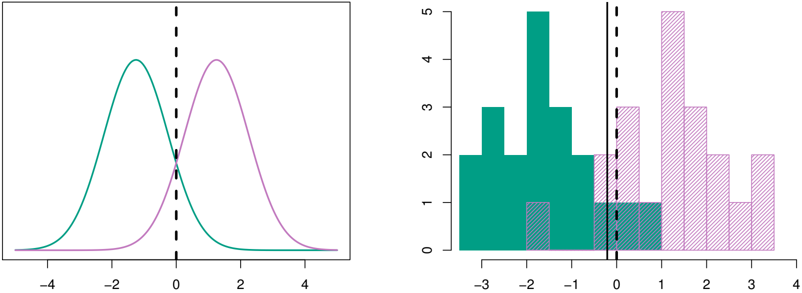

Figure: Two normal density functions and decision boundary. [9]

[9] Source [B.1]

LDA for $K > 1$ dimensions

A. Giovanidis 2020

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 $X \sim \mathcal{N}(\mu, \mathbf{\Sigma})$.

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

• mean $\mu = (\mu_1, \dots, \mu_K)$, • common covariance matrix $\mathbf{\Sigma}$.

Linear Discriminant Function:

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

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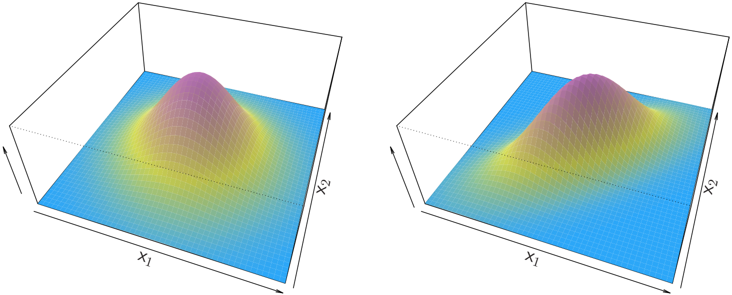

Figure: Examples of binormal distributions. [10]

[10] Source [B.1]

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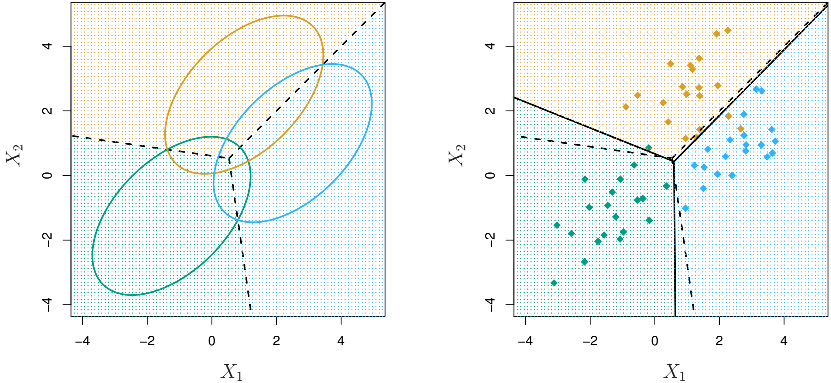

Figure: Classification for $M = 3$ classes and $K = 2$ dimensions. [11]

[11] Source [B.1]

Quadratic Discriminant Analysis (QDA)

A. Giovanidis 2020

LDA assumed for each class a different mean μ_k and same covariance matrix $\mathbf{\Sigma}$.

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

Quadratic Discriminant Function:

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

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

QDA examples

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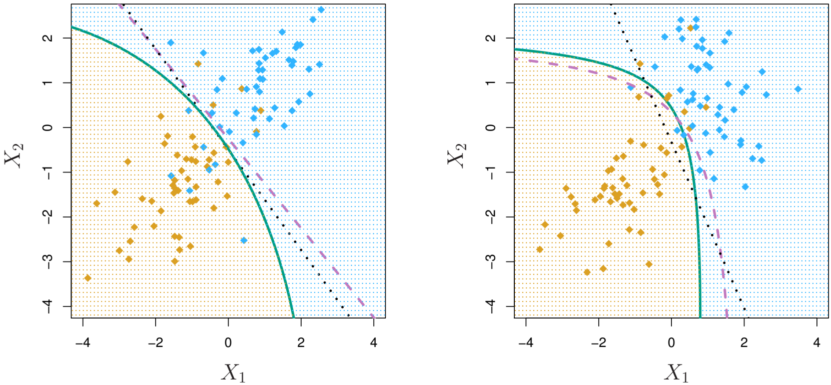

Figure: (left:) Truth common $\mathbf{\Sigma}$, (right:) Truth different $\mathbf{\Sigma}_1$, $\mathbf{\Sigma}_2$. [12]

[12] Source [B.1]

Method comparison: linear

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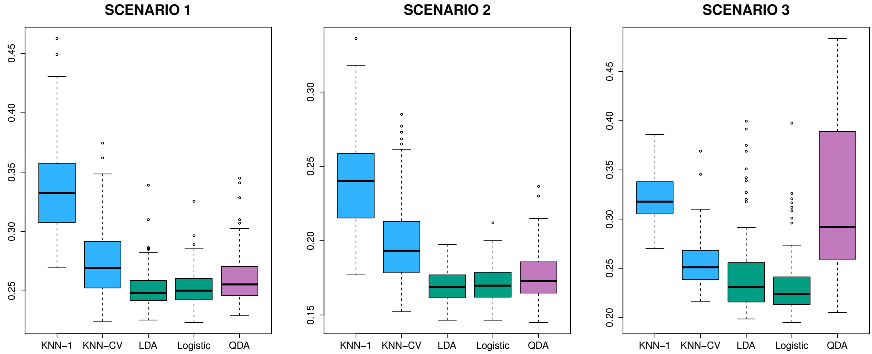

Figure: (1) uncorr., $\mathcal{N}$, $\mu_1 \neq \mu_2$, (2) corr., $\mathcal{N}$, (3) uncorr., t-distr.[13]

[13] Source [B.1]

Method comparison: non-linear

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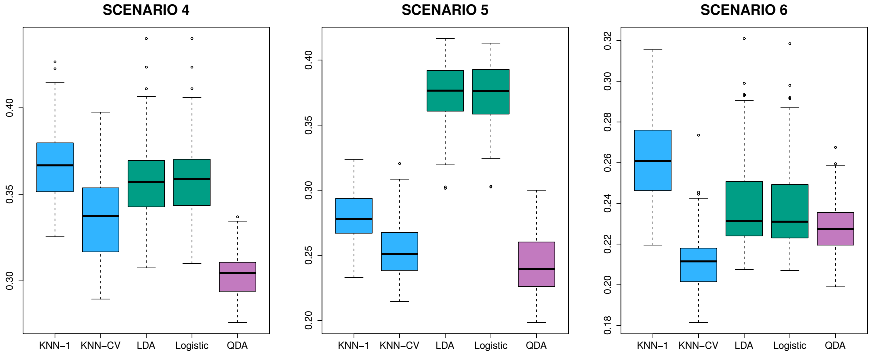

Figure: (4) corr. $\mathcal{N}$, $\mathbf{\Sigma}_1 \neq \mathbf{\Sigma}_2$, (5) logistic X_1^2, X_2^2, X_1X_2 (6) more-NL. [14]

[14] Source [B.1]

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END