# Outline

| Week | Topic | Chapter | Lecturer |
|---|---|---|---|
| 1 | Introduction to business analytics & R | 1 | Souhaib |
| 2 | Statistical learning | 2 | Souhaib |
| 3 | Regression for prediction | 3 | Souhaib |
| 4 | Resampling | 5 | Souhaib |
| 5 | Dimension reduction | 6,10 | Souhaib |
| 6 | Visualization | | Di |
| 7 | Visualization | | Di |
| 8 | Classification | 4,8 | Di |
| 9 | Classification | 4,9 | Di |
| | - | | |
| 10 | Classification | 8 | Souhaib |
| 11 | Advanced regression | 6 | Souhaib |
| 12 | Clustering | 10 | Souhaib |

# Optimal classifier

The Bayes classifier is the **optimal classifier** under the error rate:

$$E[I(Y \neq \hat{f}(X))] = P(Y \neq \hat{f}(X))$$

The Bayes classifier at $x$ is given by

$$C(x) = j \quad \text{if } p_j(x) = \max\{p_1(x), p_2(x), \dots, p_K(x)\}$$

where

$$p_k(x) = \Pr(Y = k \mid X = x), \qquad k = 1, 2, \dots, K.$$

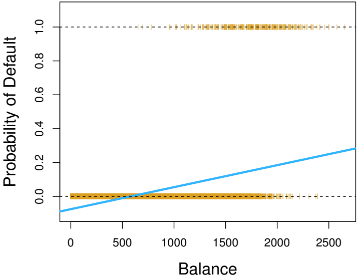
# Logistic regression

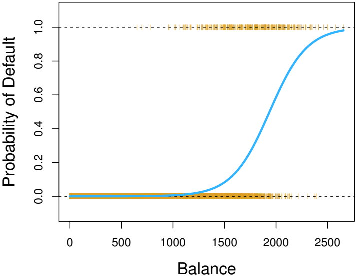
$$p(X) = P(Y = 1|X)$$

Linear reg. $p(X) = \beta_0 + \beta_1 X$

Logistic reg. $p(X) = \text{logistic}(\beta_0 + \beta_1 X) = \dfrac{e^{\beta_0+\beta_1 X}}{1 + e^{\beta_0+\beta_1 X}}$

$$\rightarrow log(\frac{p(X)}{1 - p(X)}) = \beta_0 + \beta_1 X$$



# Linear/Quadratic Discriminant Analysis

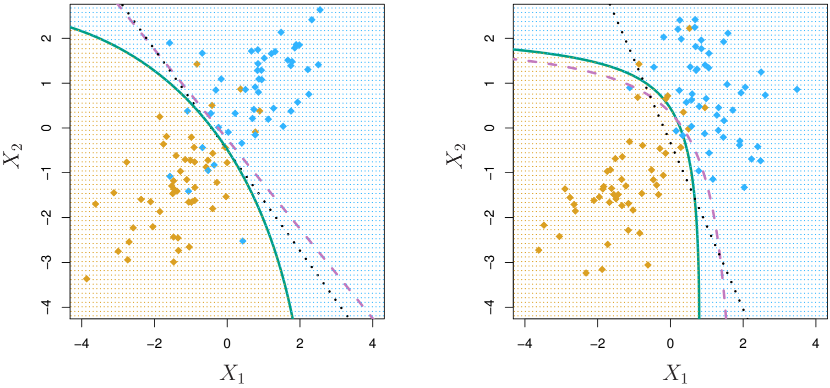
- Linear Discriminant Analysis (LDA)
  - Observations from the $k$th class: $X \sim N(\mu_k, \Sigma)$

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

- Quadratic Discriminant Analysis (QDA)
  - Observations from the $k$th class: $X \sim N(\mu_k, \Sigma_{\boldsymbol{k}})$

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

## LDA vs QDA: Bias and variance tradeoff




- Bayes (purple dashed)
- QDA (green solid)
- LDA (black dotted)

# Logistic regression and LDA

- Logistic regression
  - $log(\frac{p(x)}{1-p(x)}) = \beta_0 + \beta_1 x$
  - $\beta_0$ and $\beta_1$ estimated using maximum likelihood
- Linear Discriminant Analysis
  - $log(\frac{p_1(x)}{1-p_1(x)}) = c_0 + c_1 x$
  - $c_0$ and $c_1$ computed using the estimated mean and variance of a normal distribution

→ Both logistic regression and LDA produce linear decision boundaries.

→ However, they make different assumptions and use a different fitting procedure

# kNN Classifier

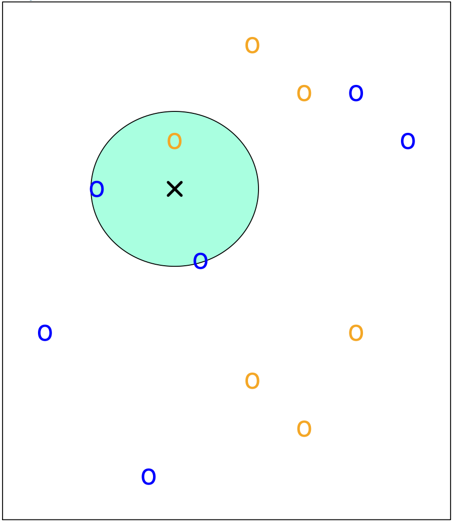
One of the simplest classifiers. Given a test observation $x_0$:

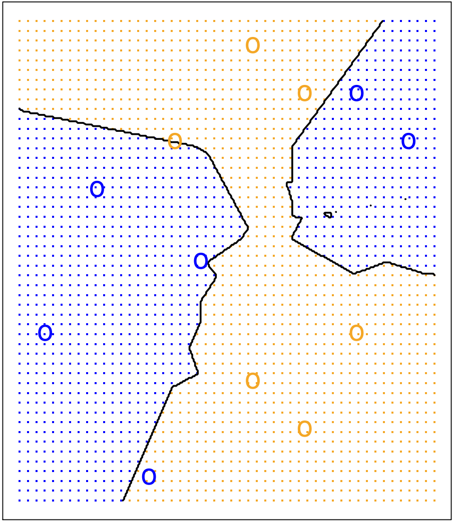
- Find the $K$ nearest points to $x_0$ in the training data: $\mathcal{N}_0$.
- Estimate conditional probabilities $\Pr(Y = j \mid X = x_0) = \frac{1}{K} \sum_{i \in \mathcal{N}_0} I(y_i = j)$.
- Classify $x_0$ to class with largest probability.

→ Nonparametric approach: no assumptions about the shape of the decision boundary

→ No table of coefficients as in logistic regression

# kNN Classifier

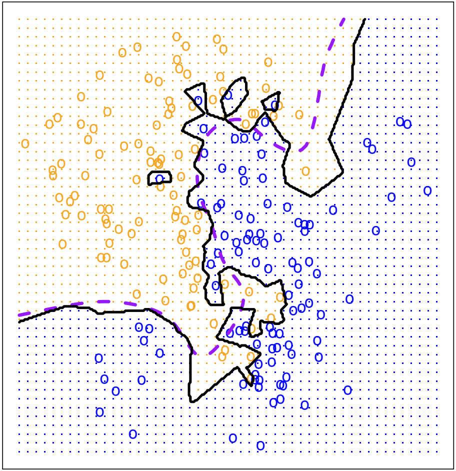




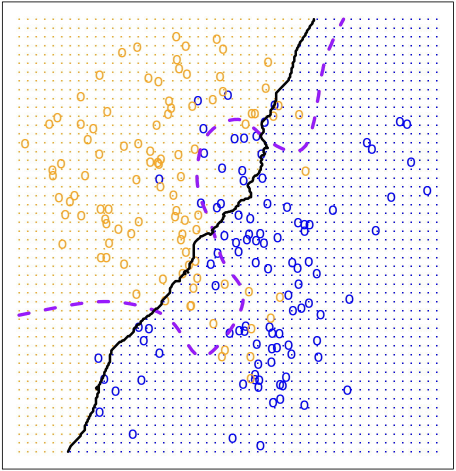
$K = 3$.

# kNN Classifier

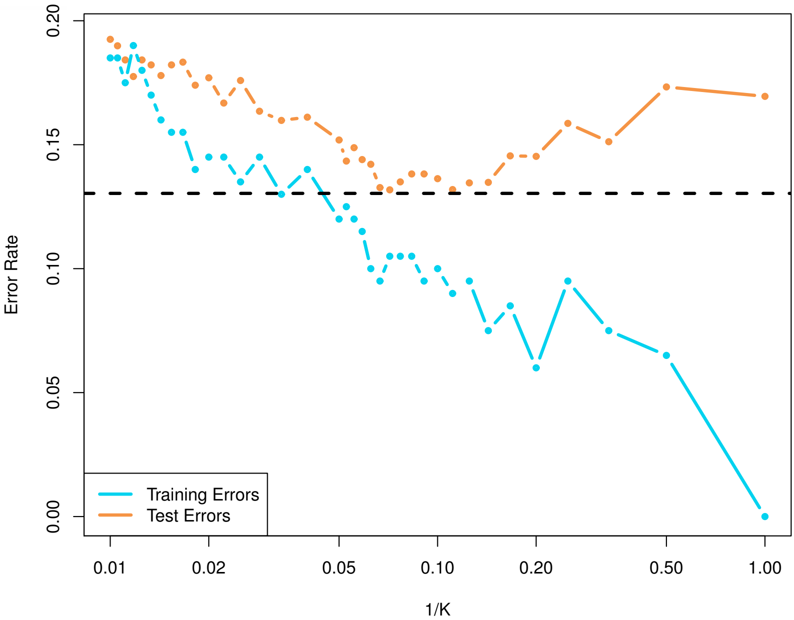
KNN: K=1



KNN: K=100

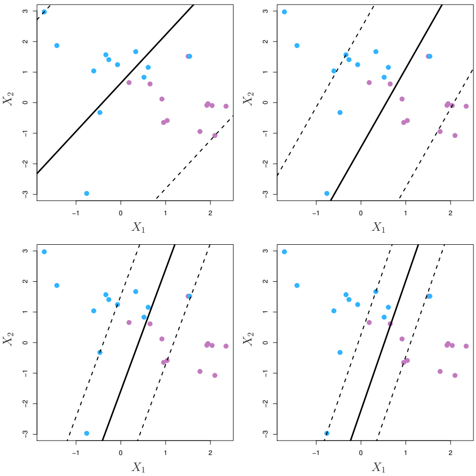


# kNN Classifier

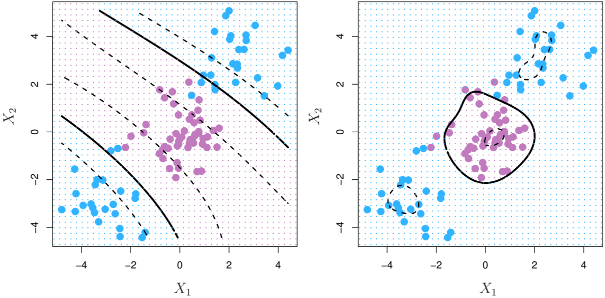


# Support Vector Classifier

Classification for decreasing values of the tuning parameter $C$.

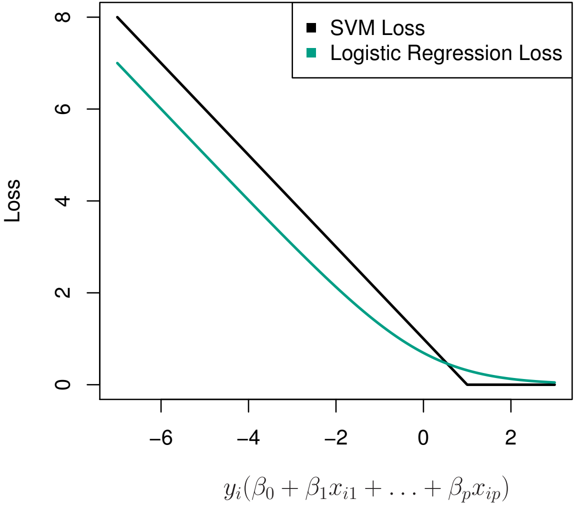


# Support Vector Machines




polynomial and radial kernel

# SVM and logistic regression



# Classification methods

- Logistic regression
- Linear Discriminant Analysis
- Quadratic Discriminant Analysis
- k-Nearest Neighbours
- Support Vector Machines
- Trees and Random Forests

# Which classification method?

- Is it binary or multi-class classification?
- How many training examples do we have?
- What is the dimensionality of the problem?
- How many categorical variables do we have?
- Are features independent?
- Do we expect the classes to be linearly separable?
- Any requirements in terms of computational time/performance/memory usage?
- Importance of interpretability?

# Empirical comparison of classifiers

- We compare the following classifiers: KNN-1, KNN-CV, LDA, Logistic and QDA
- We consider **six different scenarios** for the data generating process
- Scenarios 1-3 are **linear**, and scenarios 4-6 are **nonlinear**
- In each scenario, we generate 100 **random training data sets**. For each of these training sets, we fit each model to the data and compute the test error rate on a **large test set**

# Scenario 1

There were 20 training observations in each of two classes. The observations within each class were uncorrelated random normal variables with a different mean in each class.

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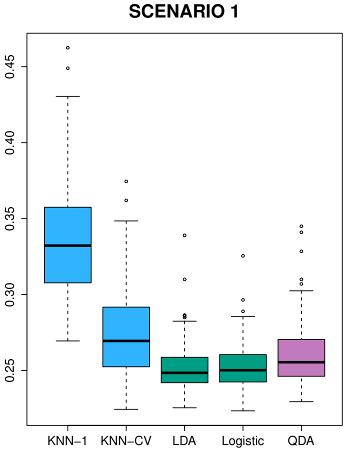

# Scenario 2

Details are as in Scenario 1, except that within each class, the two predictors had a correlation of -0.5.

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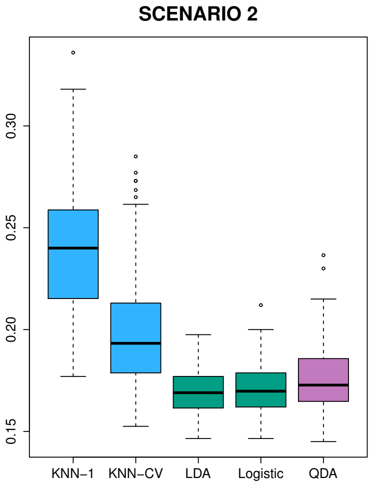

# Scenario 3

We generated $X_1$ and $X_2$ from the $t$-distribution, with 50 observations per class.

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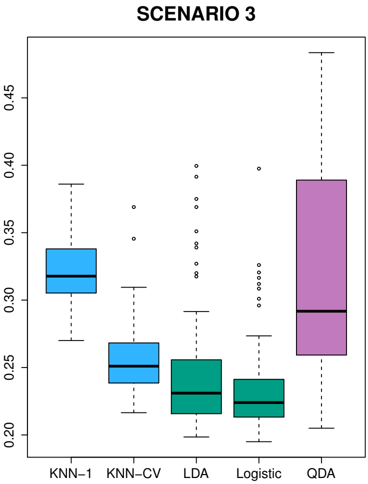

# Scenario 4

The data were generated from a normal distribution, with a correlation of 0.5 between the predictors in the first class, and correlation of -0.5 between the predictors in the second class.

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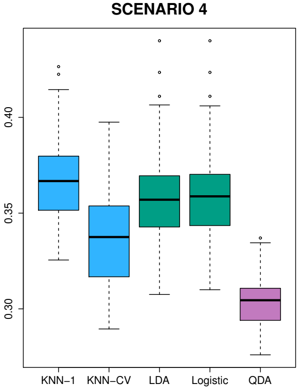

# Scenario 5

Within each class, the observations were generated from a normal distribution with uncorrelated predictors. However, the responses were sampled from the logistic function using $X_1^2$, $X_2^2$ and $X_1 \times X_2$ as predictors.

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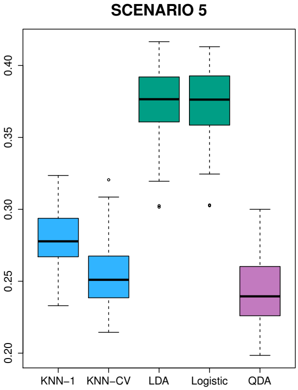

# Scenario 6

Details are as in the previous scenario, but the responses were sampled from a more complicated non-linear function.

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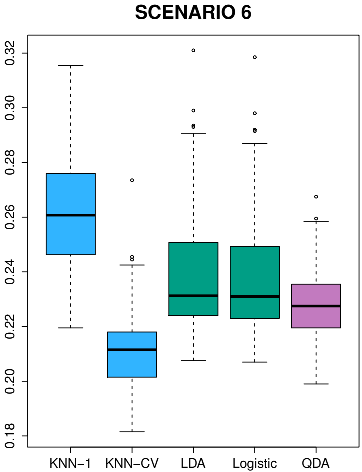

# Summary

- When the true decision boundaries are linear, LDA and logistic regression will perform well
- When the boundaries are moderately non-linear, QDA may give better results
- For more complicated boundaries, a non-parametric approach such as KNN can be superior
- Do not forget the importance of other criteria: number of samples and predictors, computational time, interpretability, etc.
- In many data analytics competitions, tree-based methods such as Boosting and Random Forests are often among the best methods