STAT406- Methods of Statistical Learning Lecture 14

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Classification as prediction

- Most classifiers can be thought of as different ways to estimate or model

$$P\left(G = \mathbf{c}_j \,\middle|\, \mathbf{X} = \mathbf{x}\right)$$

- One way to model these probabilities is via Bayes' Thrm:

$$P\left(G = \mathbf{c}_j \,\middle|\, \mathbf{X} = \mathbf{x}\right) = \mathbf{f}\left(\mathbf{x} \,\middle|\, \mathbf{c}_j\right) P\left(G = \mathbf{c}_j\right) \big/ \mathbf{f}\left(\mathbf{x}\right)$$

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LDA vs QDA

LDA classifies an observation into the class c_j for which the estimated (under a normality assumption)

$$P\left(G = c_j \middle| \mathbf{X} = \mathbf{x}\right)$$

is highest.

If $\mathbf{X} | G = c_j \sim \mathcal{N}\left(\mu_j, \mathbf{\Sigma}\right)$ it means the class for which

$$\delta_j\left(\mathbf{x}\right) = \mathbf{x}' \, \mathbf{a}_j + b_j$$

is highest, where

$$\mathbf{a}_j = \mathbf{\Sigma}^{-1} \mu_j \quad \text{and} \quad b_j = -\frac{1}{2} \mu_j' \mathbf{\Sigma}^{-1} \mu_j + \log(p_j)$$

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QDA

If $\mathbf{X} | G = c_j \sim \mathcal{N}(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$ then, the estimated posterior probabilities look different.

QDA classifies an observation into the class c_j that maximizes

$$\delta_j(\mathbf{x}) = \mathbf{x}' \mathbf{A}_j \mathbf{x} + \mathbf{x}' \mathbf{d}_j + b_j$$

(see the book for details)

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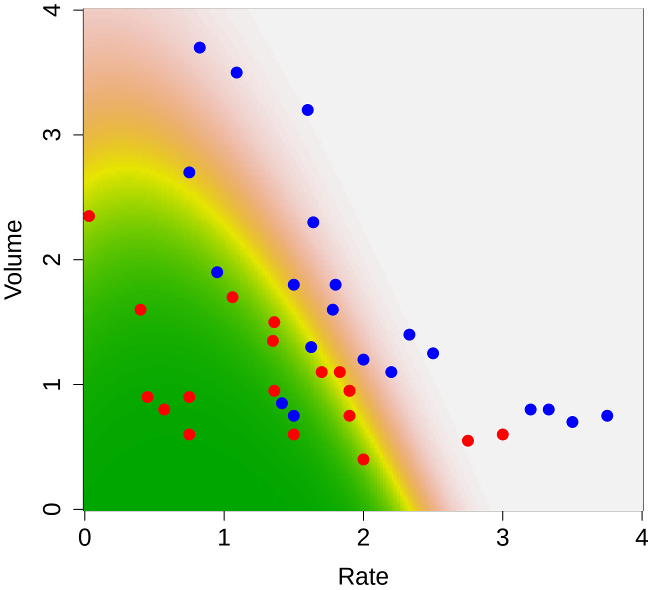
QDA-based probabilities



LDA - QDA - Logistic classifiers

- Multiclass: LDA, QDA and Logistic classifiers extend to the case of more than 2 classes
- Examples in R (Zip-code hand-written digits)

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LDA - QDA - Logistic classifiers

- LDA vs QDA: presents the usual "flexibility vs. variability" trade-off

- LDA & QDA vs Logistic classifiers: **Gaussian MLE estimates** (non-robust, sensitive to the Gaussian assumption) vs. **Binomial MLE estimates** (no distributional assumption of $\mathbf{X} | G = c_j$ required).

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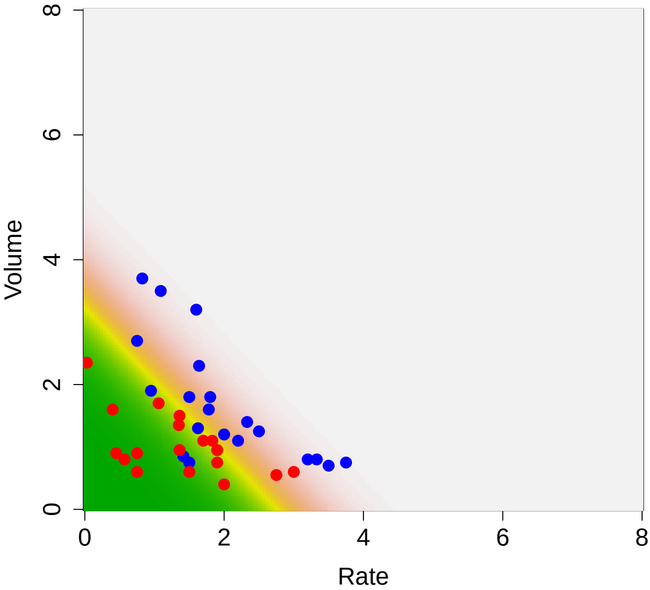
LDA



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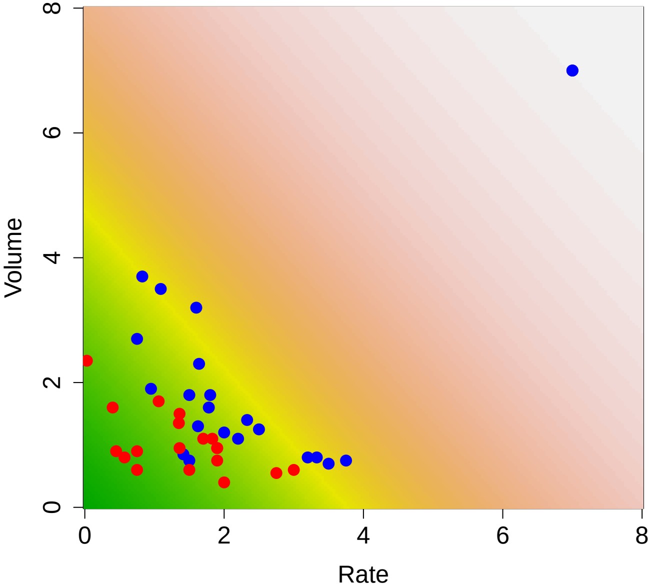
LDA + 2 “good outliers”



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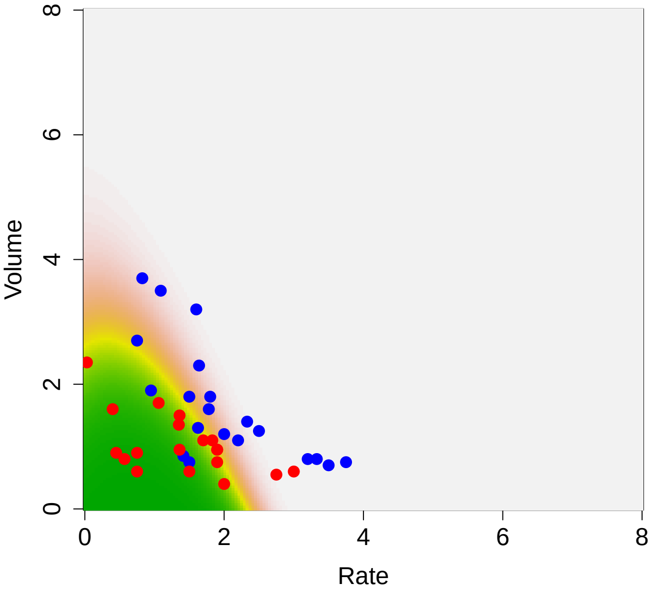
QDA



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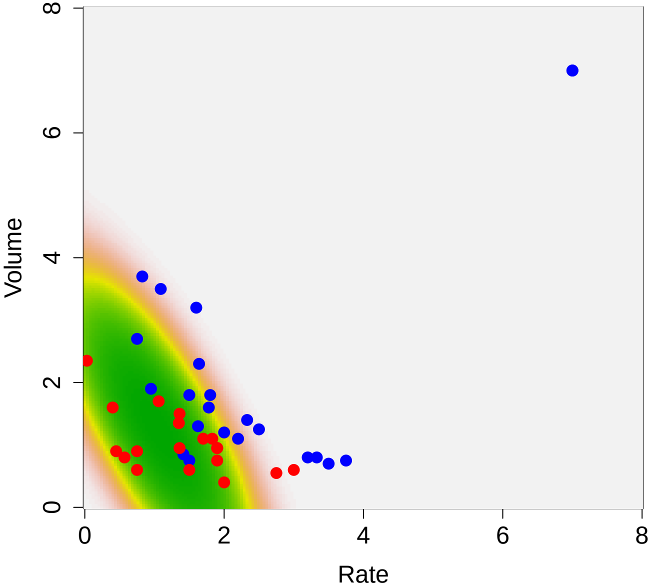
QDA + 2 “good outliers”



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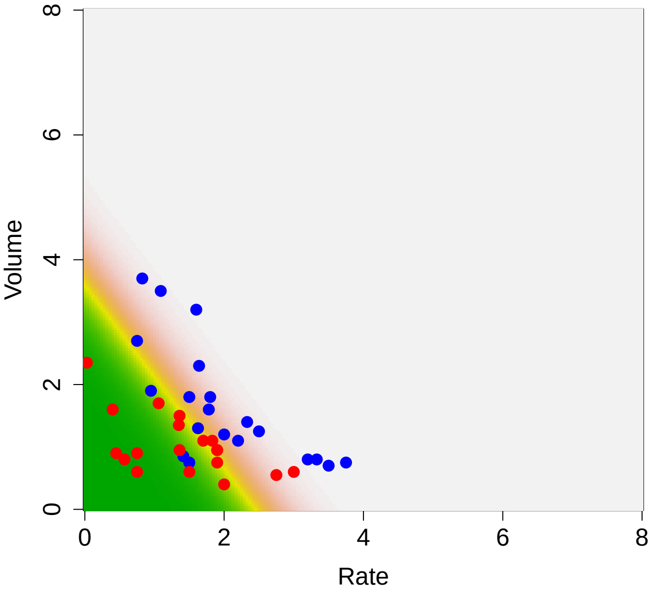
Logistic



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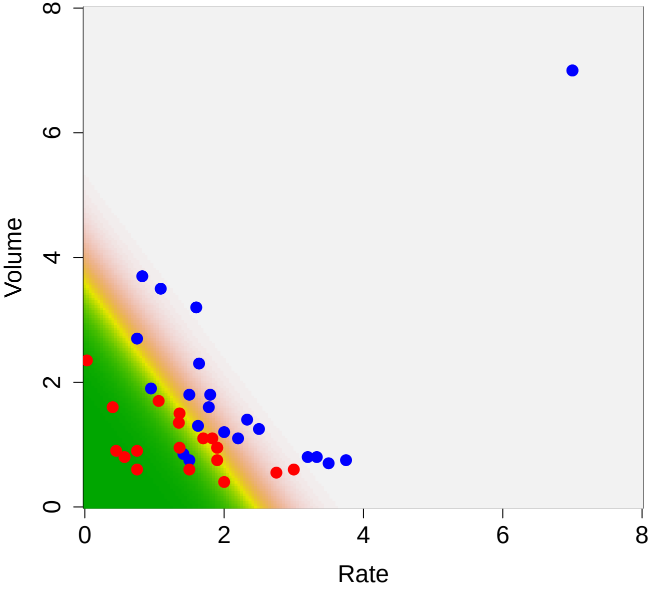
Logistic + 2 “good outliers”



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LDA - QDA - Logistic classifiers

Examples with R

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Nearest-neighbours

- We need to estimate

$$P\left(G = \mathbf{g} \middle| \mathbf{X} = \mathbf{x}\right)$$

- An intuitive and “model-free” estimator is the nearest-neighbours estimator

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Nearest-neighbours

- Same spirit as the local-constant (kernel) regression estimator
- The K-NN estimator is

$$\hat{P}\left(G = \mathbf{g} \middle| \mathbf{X} = \mathbf{x}\right) = \frac{1}{|N_{\mathbf{x}}^{K}|} \sum_{j \in N_{\mathbf{x}}^{K}} \mathbf{I}\left\{Y_j = \mathbf{g}\right\}$$

where

$$N_{\mathbf{x}}^{K} = \left\{i : d(\mathbf{X}_i, \mathbf{x}) \leq d_{(K)}\right\}$$

and $d_{(K)}$ is the distance from $\mathbf{x}$ to the K-th closest point in the sample $(\mathbf{X}_i)$

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Nearest-neighbours

- The K-NN estimator is the proportion of observations from class **g** among the closest K neighbours

- The K-NN classifier assigns a point to the class most represented among its K neighbours (“peer pressure”)

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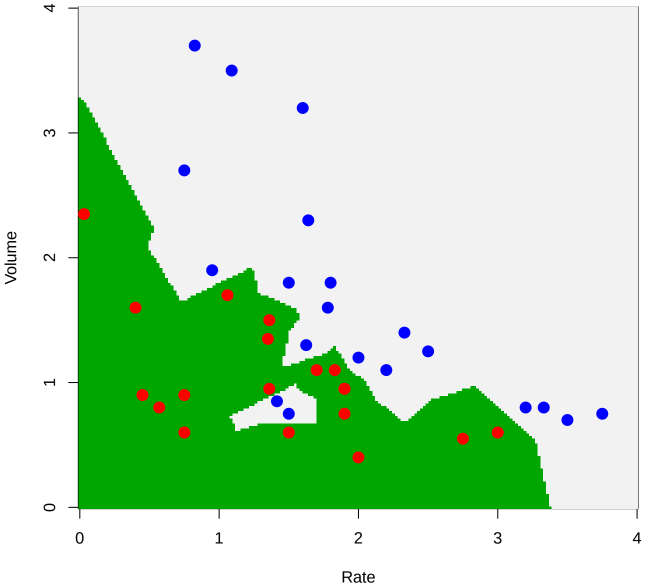
Vaso – 1-NN



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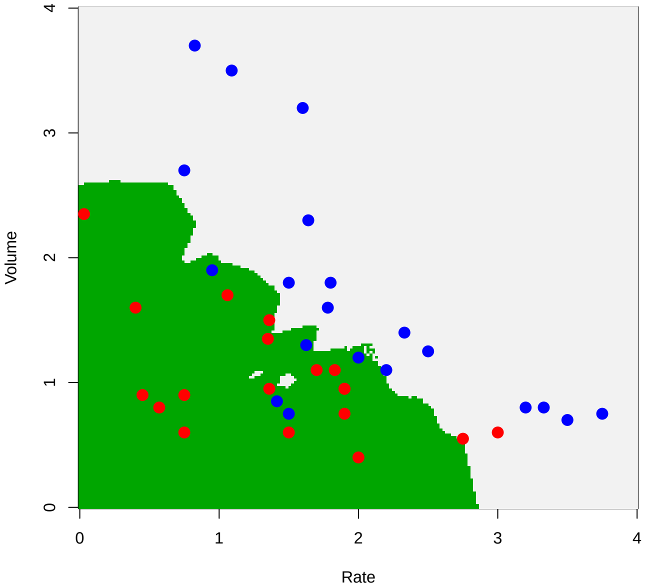
Vaso – 5-NN



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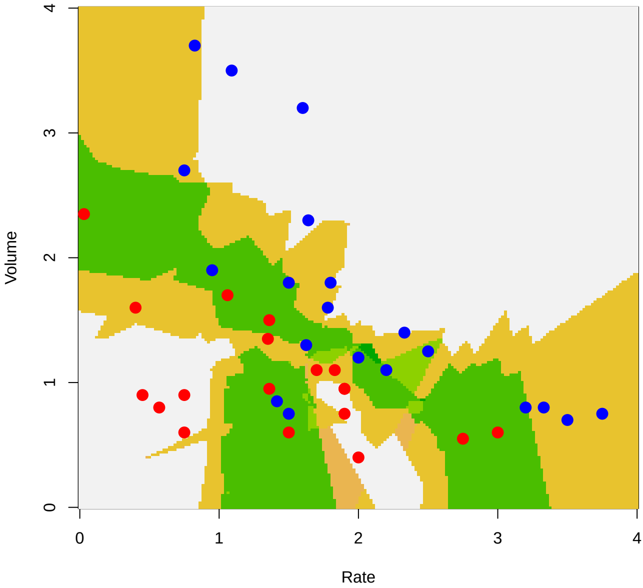
Vaso – 5-NN - votes



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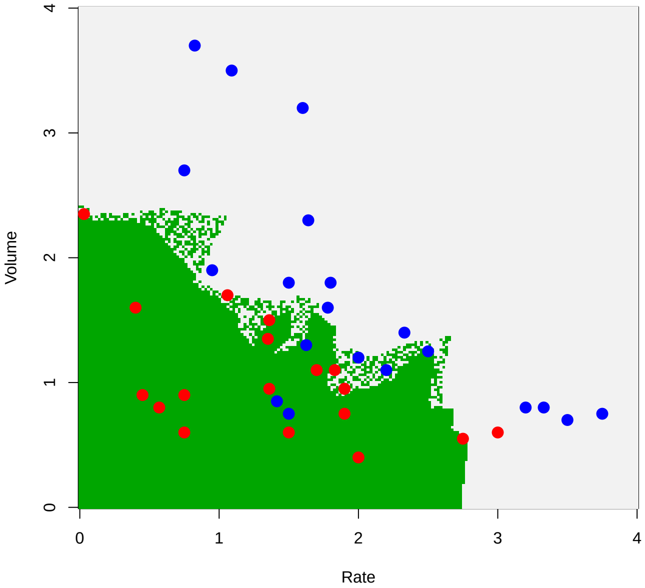
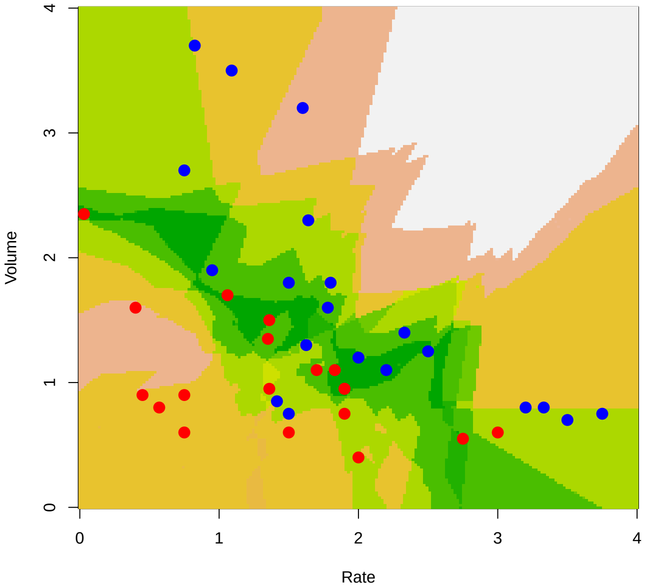
Vaso – 10-NN



Vaso – 10-NN - votes



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Nearest-neighbours

- How can we select the number K of neighbours?
- Zip-code example

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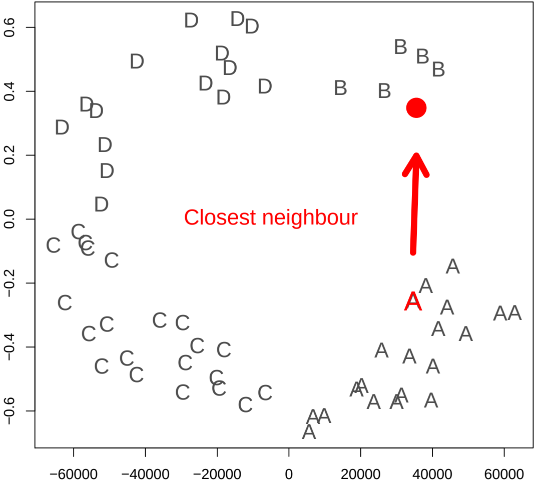
Nearest-neighbours - Challenge

- What's wrong with this picture?



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Classification Trees

- To estimate the probabilities of each class **g** for a particular value of the feature vector **x**, **nearest neighbours** constructs estimates

$$\widehat{P}\left(\mathbf{g} = \mathbf{g} \middle| \mathbf{X} = \mathbf{x}\right)$$
$$= \text{ prop. of objects of class } \mathbf{g} \text{ among } \mathbf{x}\text{'s neighbours}$$

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Classification Trees

- Drawback: may not be "local" for moderate number of features (hence, may not represent the distribution of $\mathbf{g}$ for $\mathbf{X} = \mathbf{x}$

- Yet another incarnation of the "curse of dimensionality"

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Classification Trees

- If we assume a model for the distribution of the features $\mathbf{X}$ for each class

$$f\left(\mathbf{x} \mid \mathbf{g} = \mathbf{g}\right) = f_{\mathbf{g}}\left(\mathbf{x}\right)$$

then we have a formula for

$$P\left(\mathbf{g} = \mathbf{g} \mid \mathbf{X} = \mathbf{x}\right) = \frac{f_{\mathbf{g}}\left(\mathbf{x}\right) P\left(\mathbf{g} = \mathbf{g}\right)}{\sum_{\mathbf{g}} f_{\mathbf{g}}\left(\mathbf{x}\right) P\left(\mathbf{g} = \mathbf{g}\right)}$$

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Classification Trees

- We typically have estimates for these probabilities
- Only the numerator is needed
- Drawback: the model may not be correct.
- Model-based inferences are typically more stable than model-free ones
- But they may be biased if the model is a poor approximation to the truth

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Classification Trees

- Classification trees provide another family of estimates for $P(\mathbf{g} = \mathbf{g} | \mathbf{X} = \mathbf{x})$
- They do not need a model
- Instead of estimating the local proportion (probability) of each class around a point $\mathbf{x}$, CART's attempt to find regions of the feature space that are "dominated" by one class.

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Classification Trees

- Classification trees try to identify regions of the domain where one class clearly dominates the others (i.e. where the class proportions are far from being “uniform”)
- They search for these regions in a very specific way.

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Classification Trees

- These regions are searched using a sequential algorithm that at each step partitions the current level ("leaf") into two "leaves" / "children" according to the value of one of the feature variables, for example:

$$X_j \leq \mathbf{a} \quad \text{versus} \quad X_j > \mathbf{a}$$

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Classification Trees

- At every step, the algorithm searches for the variable X_j and level **a** that produce the largest increase in "homogeneity" (alternatively: the largest decrease in "heteroscedasticity")
- We need a measure of "homogeneity" (or lack of it)

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Classification Trees

Some practical considerations in building (spanning) the tree:

- Do not partition nodes / leaves with fewer elements than a fixed threshold (say, 5)

- Do not partition a node if the “gain” in less homogeneity is less than a certain percentage of the current value

- Or both...

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Classification Trees

Let **N** denote a "node", that is: a subset of the data.

Let $\hat{p}_j$, $j = 1, \ldots, K$ be the proportion of observations of each class in this node

$$\hat{p}_j = \frac{\#\text{ of observations of class } j \text{ in node } \mathbf{N}}{\text{total } \#\text{ of observations in node } \mathbf{N}}$$

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Classification Trees

Maximum homogeneity when

$$\hat{p}_1 \approx \hat{p}_2 \approx \cdots \approx \hat{p}_K$$

Minimum homogeneity when $\hat{p}_r \approx 1$ for some $1 \leq r \leq K$

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Classification Trees

Measures of homogeneity

- Gini index:

$$Q_G\left(\hat{p}_1, \ldots, \hat{p}_K\right) = \sum_{j \neq i}^{K} \hat{p}_j \, \hat{p}_i = \sum_{j=1}^{K} \hat{p}_j \, \left(1 - \hat{p}_j\right)$$

- Entropy or deviance:

$$Q_D\left(\hat{p}_1, \ldots, \hat{p}_K\right) = -2 \sum_{j=1}^{K} \hat{p}_j \, \log\left(\hat{p}_j\right)$$

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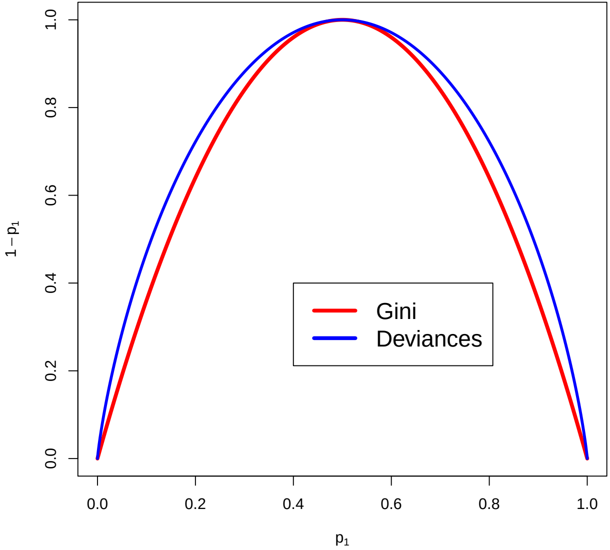
Gini & Deviances - 2 groups



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Classification Trees

Define the “homogeneity” of a node **N** as

$$Q(\mathbf{N}) = Q(\hat{p}_1, \ldots, \hat{p}_K)$$

where

$$\hat{p}_j = \frac{\#\text{ of observations of class } j \text{ in node } \mathbf{N}}{\text{total } \#\text{ of observations in node } \mathbf{N}}$$

Q could be Q_G or Q_D, for example.

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Classification Trees

(a) Start with a node $\mathbf{N}$ containing all data points

(b) Find the variable X_j and value $\mathbf{a}$ that minimize

$$\mathbf{n}_L\, Q\left(\mathbf{X} \in \mathbf{N} : X_j \le \mathbf{a}\right) + \mathbf{n}_R\, Q\left(\mathbf{X} \in \mathbf{N} : X_j > \mathbf{a}\right)$$

where $\mathbf{n}_L = \#\{\mathbf{X} \in \mathbf{N} : X_j \le \mathbf{a}\}$

(c) Define the corresponding two "children" of node $\mathbf{N}$

(d) Apply the same to each "child" / "leaf"

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Classification Trees

- In practice, we need to weight the homogeneity by the number of observations in each leaf.
- This reflects a probabilistic model for the tree, and represents the probability that a point is observed in this leaf
- In other words: minimize homogeneity more in “larger” (in average) leaves.

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Classification Trees

- Let n_c be the size of the node $\mathbf{N}_c$, its homogeneity is

$$n_c \, Q\left(\mathbf{N}_c\right) \propto \frac{n_c}{n} Q\left(\mathbf{N}_c\right)$$

- If we split $\mathbf{N}_c$ into $\mathbf{N}_1$ and $\mathbf{N}_2$ the homogeneity is

$$n_1 \, Q\left(\mathbf{N}_1\right) + n_2 \, Q\left(\mathbf{N}_2\right) \propto \frac{n_1}{n} Q\left(\mathbf{N}_1\right) + \frac{n_2}{n} Q\left(\mathbf{N}_2\right)$$

The homogeneity of any split is less than that of the parent node (Breiman, Friedman, Olshen, Stone; 1984).

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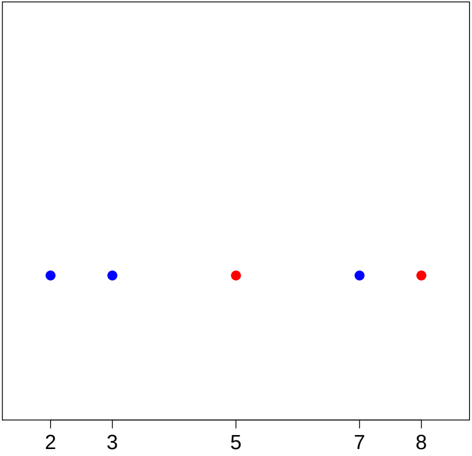
Classification Trees



$$(\hat{p}_R = 2/5 \quad \hat{p}_B = 3/5) \quad Q_G = \mathbf{2.4}$$

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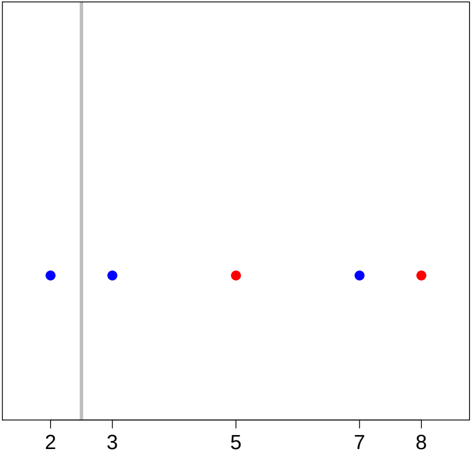
Classification Trees



$(\hat{p}_R = 0 \quad \hat{p}_B = 1)$ $\qquad (\hat{p}_R = 1/2 \quad \hat{p}_B = 1/2)$ $\quad Q_G = \mathbf{2}$

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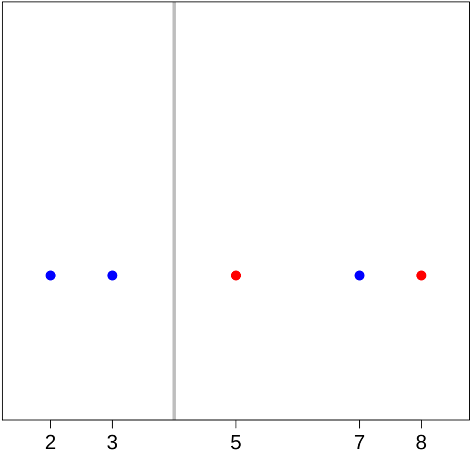
Classification Trees



$(\hat{p}_R = 0 \quad \hat{p}_B = 1)$ $(\hat{p}_R = 2/3 \quad \hat{p}_B = 1/3)$ $Q_G = \mathbf{1.33}$

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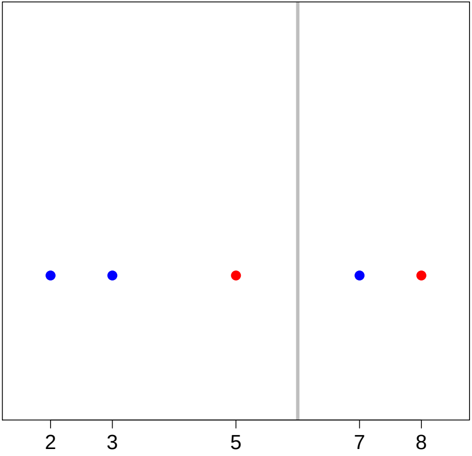
Classification Trees



$$(\hat{p}_R = 1/3 \quad \hat{p}_B = 2/3) \; (\hat{p}_R = 1/2 \quad \hat{p}_B = 1/2) \quad Q_G = \mathbf{2.33}$$

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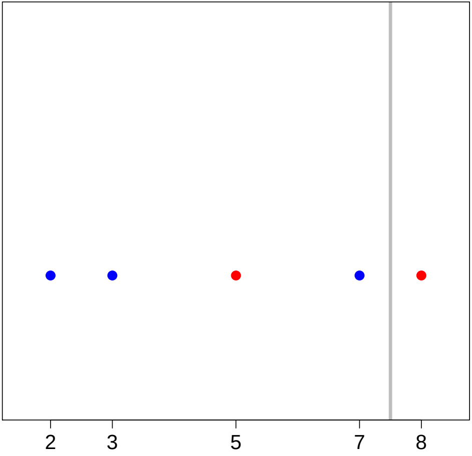
Classification Trees



$(\hat{p}_R = 1/4 \quad \hat{p}_B = 3/4) \qquad (\hat{p}_R = 1 \quad \hat{p}_B = 0) \quad Q_G = \mathbf{1.5}$

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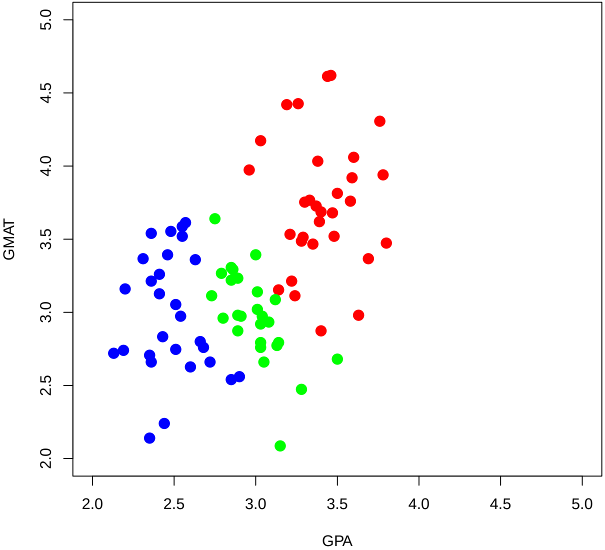
Grad admissions



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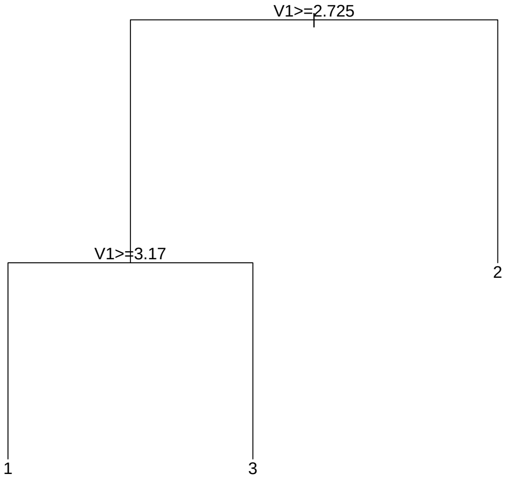
Grad admissions - Gini tree



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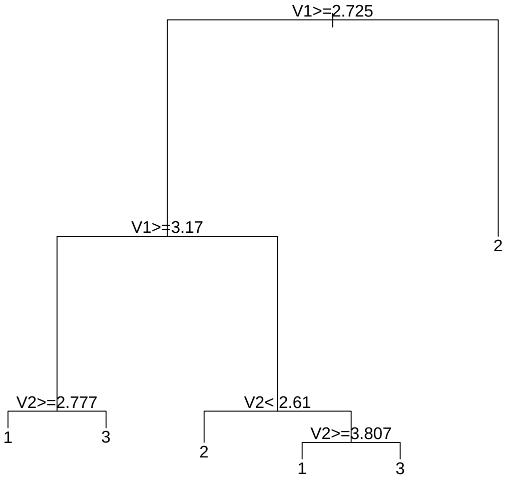
Grad admissions - Deviance tree



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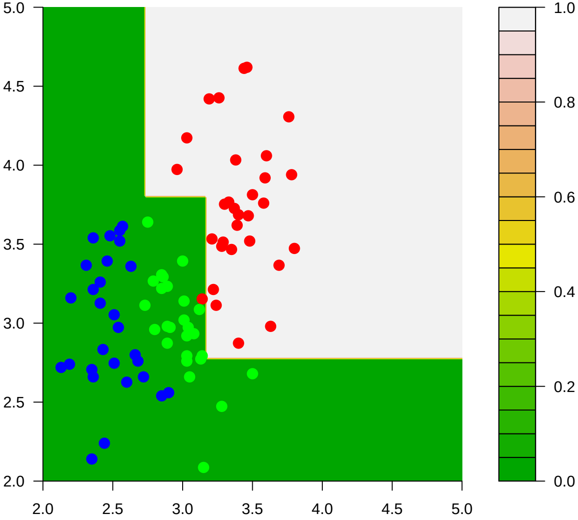
Grad admissions



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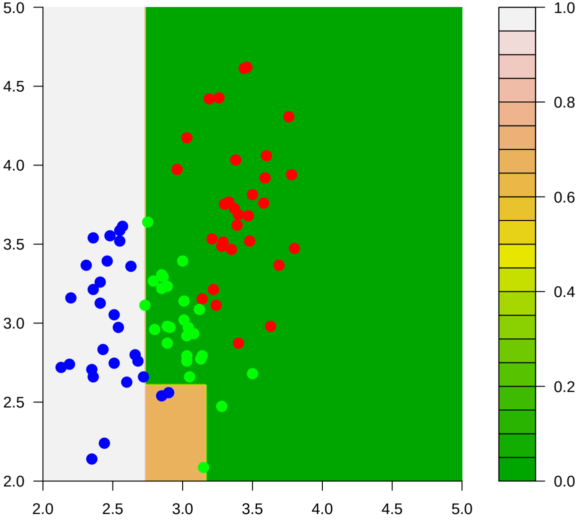
Grad admissions



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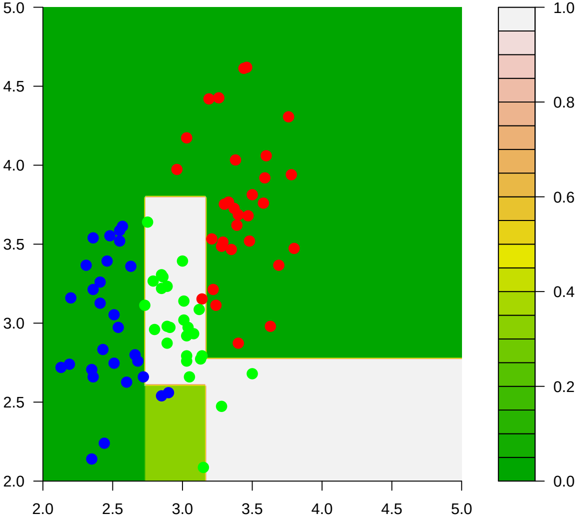
Grad admissions



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Classification example

- ISOLET data
  http://archive.ics.uci.edu/ml/datasets/ISOLET
- 150 subjects spoke the name of each letter twice
- 52 samples from each subject, 300 samples for each letter

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Classification example

- 617 features (explanatory variables). They include: spectral coefficients; contour features, sonorant features, pre-sonorant features, and post-sonorant features.
- Data are split into training ($n = 6238$) and test ($n = 1559$)
- Mission: build a classifier to identify future spoken letters

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Classification example

- I separated the letters C and Z

```
> x <- read.table('isolet-train.data', sep=',')
> # 3 and 26 --- "C" and "Z"
>
> xa <- x[ x$V618 == 3, ]
> xb <- x[ x$V618 == 26, ]
>
> xx <- rbind(xa, xb)
> xx$V618 <- as.factor(xx$V618)
```

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Classification example

- Fit a classification tree

```
> myc <- rpart.control(minsplit=7, cp=1e-7,
           xval=10)
>
>
> set.seed(123)
> a.t <- rpart(V618~., data=xx,
      parms = list(split = 'information'),
      control=myc)
> b <- a.t$cptable[
      which.min(a.t$cptable[,"xerror"]),"CP"]
> d.r <- prune(a.t, cp=b)
```

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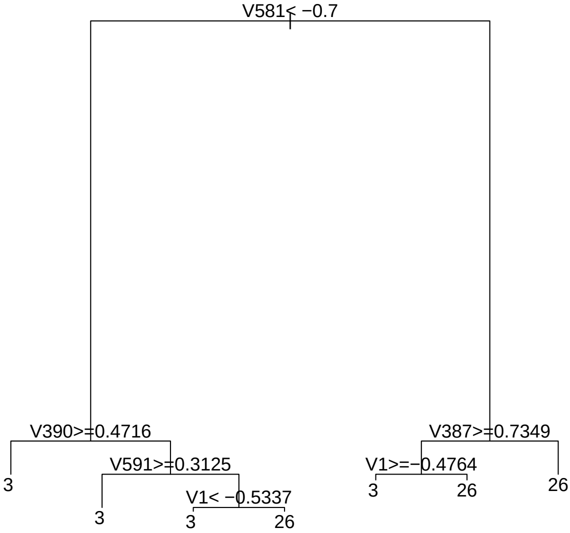
Classification example



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Classification example

- Predict on the test data

```
> d.pr <- predict(d.r, newdata=dd,
           type='class')
> table(truth, d.pr)
     d.pr
truth  3 26
   3  59  1
   26  0 60
```

- And we only used 5 explanatory variables!

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Classification example

- The problem is not trivial
- Let's try a 1-NN nearest neighbour classifier

```
> u1 <- knn(train=xx[,-618], test=dd[,-618],
     cl=xx[,618], k = 1)
>
> table(truth, u1)
     u1
truth  3 26
   3  57  3
   26  9 51
```

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Classification example

- With 5-NN is not much better

```
> u5 <- knn(train=xx[,-618],
     test=dd[,-618], cl=xx[,618],
     k = 5)
>
> table(truth, u5)
     u5
truth  3 26
   3  58  2
   26  5 55
```

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Classification example

- With a logistic classifier

```
> xx$V619 <- as.numeric(xx$V618==3)
> d.glm <- glm(V619 ~ . - V618, data=xx,
       family=binomial)
Warning message:
glm.fit: algorithm did not converge

[...]

> table(truth, pr.glm)
     pr.glm
truth  0  1
   3  25 35
   26 33 27
```

- Can we explain the problem?

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Classification example

- How about the approach based on the Gaussian distribution of the features (within each class)?

```
> library(MASS)
>
> d.lda <- lda(V618 ~ ., data=xx)
Warning message:
In lda.default(x, grouping, ...) :
    variables are collinear
```

- Can we explain the problem?

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