https://github.com/tedinburgh/ads2023

Decision trees

Tom Edinburgh
te269

Schedule

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1. Supervised learning
    - Regression, model fitting
    - Classification
    - k-nearest neighbours, SVM
    - Tree-based methods
2. Unsupervised learning
    - Dimensionality reduction
    - Clustering
3. Intro to neural networks
    - Neurons, perceptrons and back-propagation

Schedule

1. Supervised learning ← Irina
   - Regression, model fitting
   - Classification
   - k-nearest neighbours, SVM
   - Tree-based methods ← Tom
2. Unsupervised learning
   - Dimensionality reduction
   - Clustering
3. Intro to neural networks ← Miles
   - Neurons, perceptrons and back-propagation

Today: Decision trees

- Overview
- How to grow a tree (recursive binary partition)
- Decision trees for regression (example: baseball salary)
- Decision trees for classification (example: playing outdoors)
- Summary

Questions: halfway through, at the end, or by email (te269)

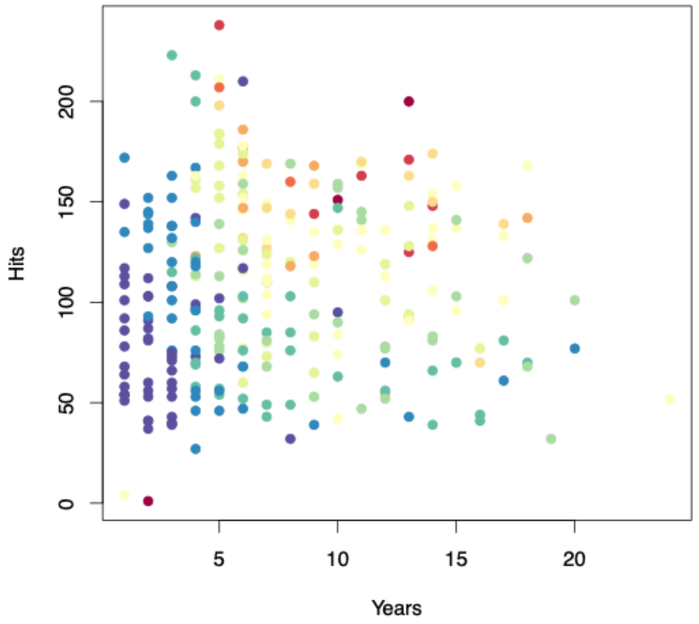
Resources

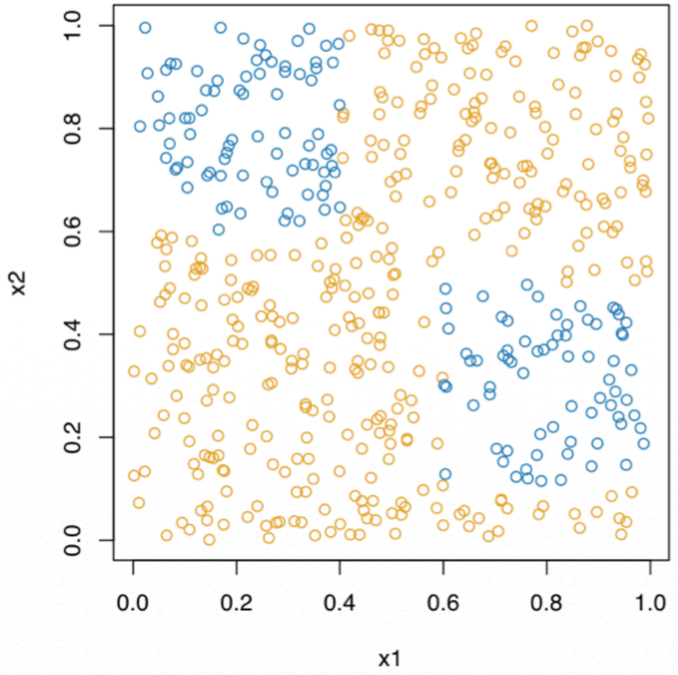
- An Introduction to Statistical Learning with Applications in R/Python (James, Witten, Hastie, Tibshirani, Taylor; 2013/2023)

- Slides adapted from:
  - Prof Alexandra Chouldechova, Carnegie Mellon
  - Prof Stephen Eglen, Cambridge

Overview

- Tree-based methods **segment** the feature space into simple regions (e.g. high-dimensional rectangles)
- **Predict** using the average (mean, mode), **classify** using the most common class
- Origins: CART (Breiman, 1984), identification trees (ID3) (Quinlan, 1986)





Overview

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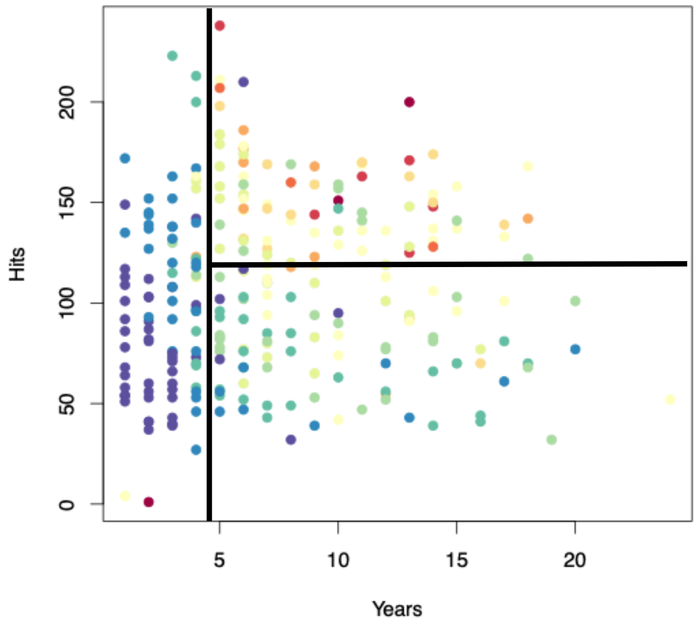
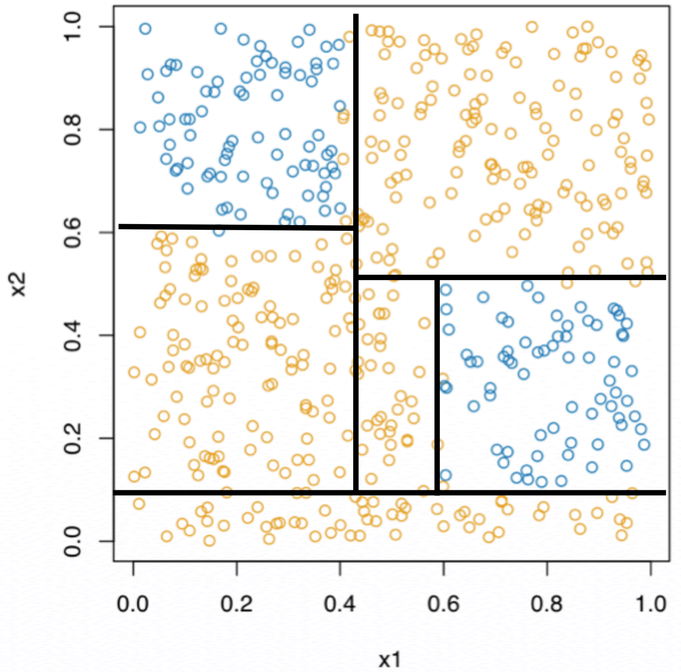
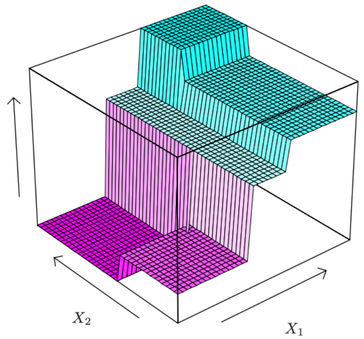
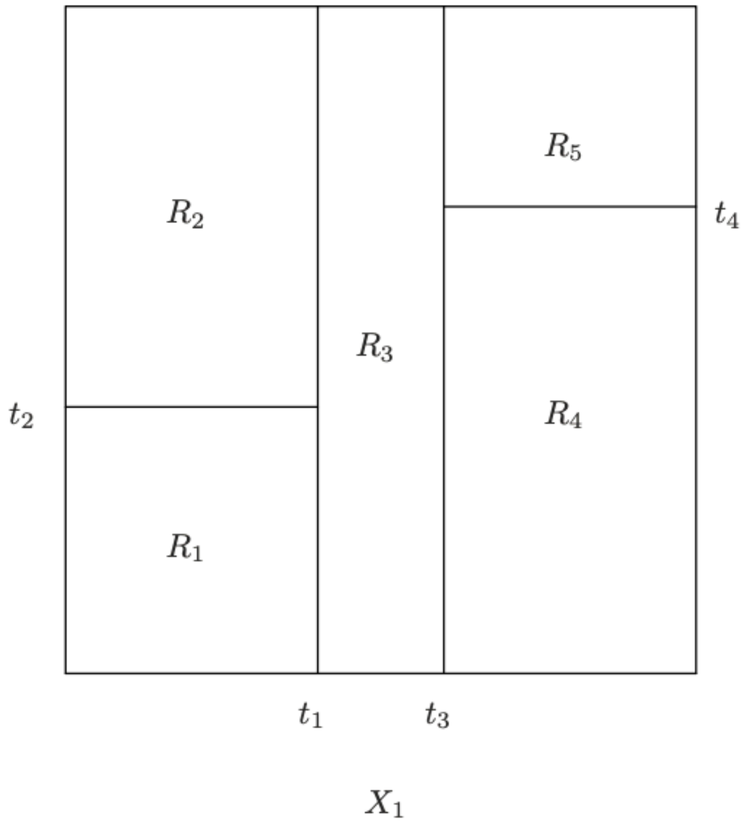
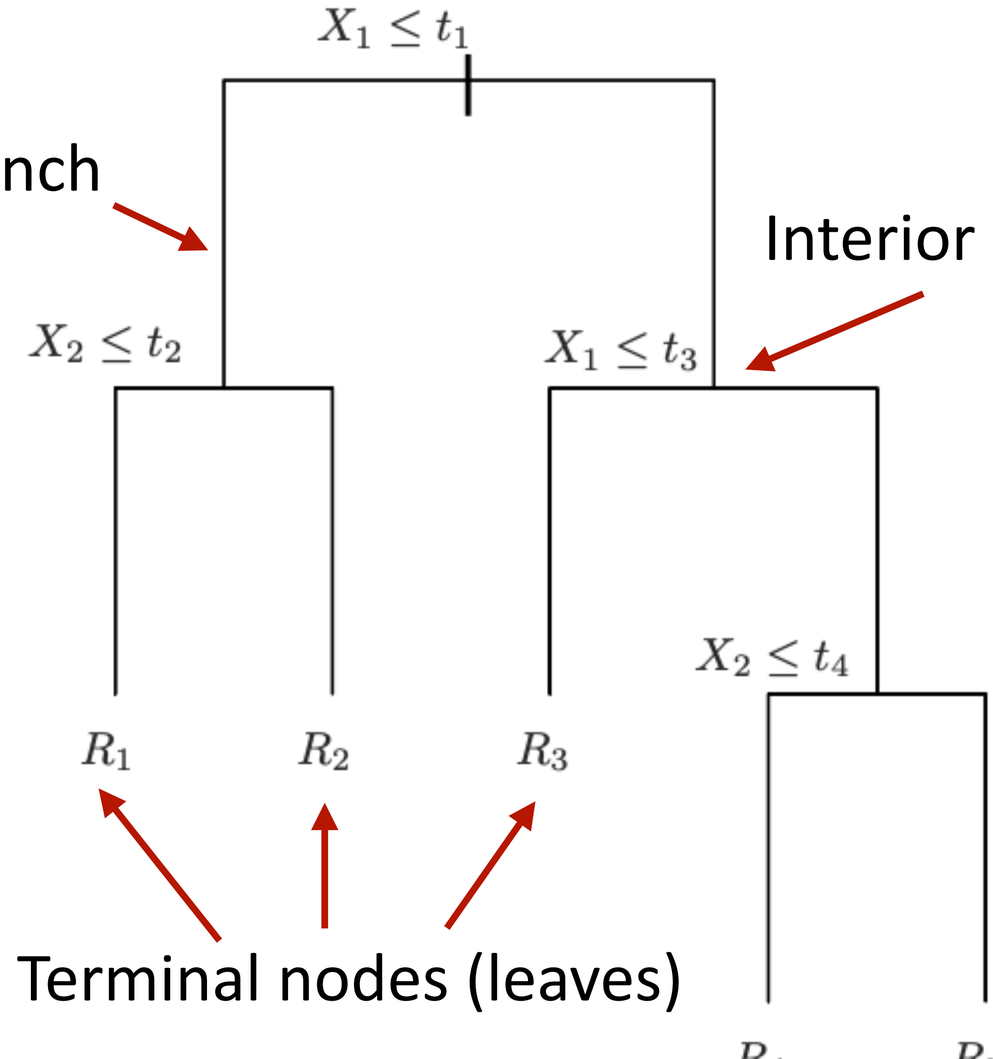


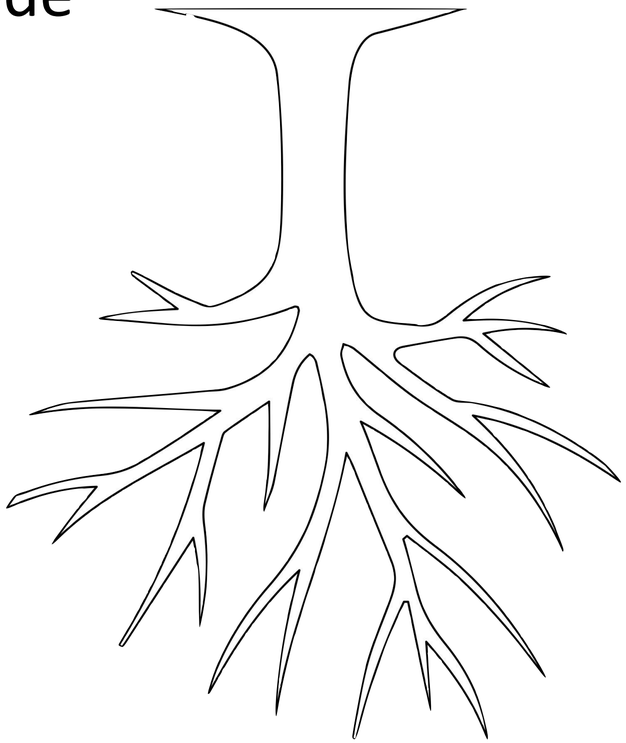


Why is this called a decision tree?









Format of the data

$$X = \begin{pmatrix} X_1 & X_2 & \cdots & X_p \end{pmatrix} = \begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix} \qquad y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

- Each of the features (predictors) X_j can be qualitative or quantitative, no need to re-scale
- The output (response) y can be qualitative (for classification) or quantitative (for regression)

How to grow the tree?

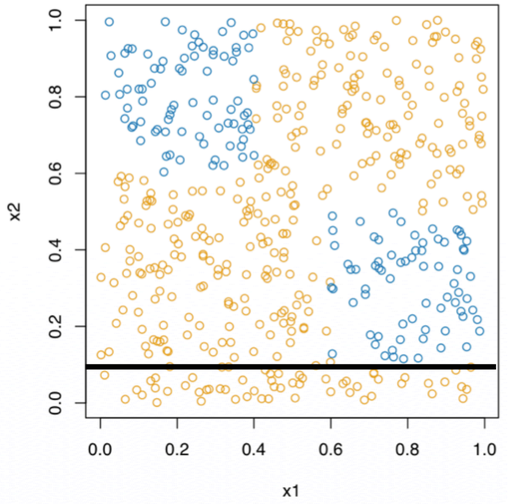
- General process:

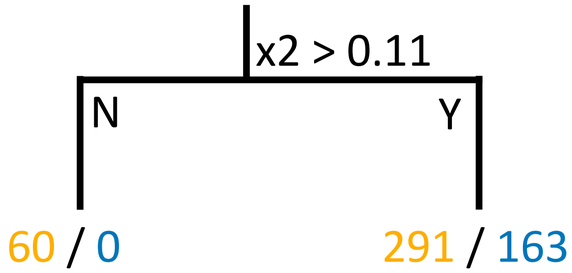
    1. Partition the predictor space (i.e. all possible values of $X_1, X_2, \ldots, X_p$) into J distinct, non-overlapping regions, labelled $R_1, \ldots, R_J$

    2. Each observation in a given region R_j is given the same predicted value (or class), which is the mean (or mode) of all response variables in that region

- How do we choose the partitions? e.g. high-dimensional rectangles

How to grow the tree?





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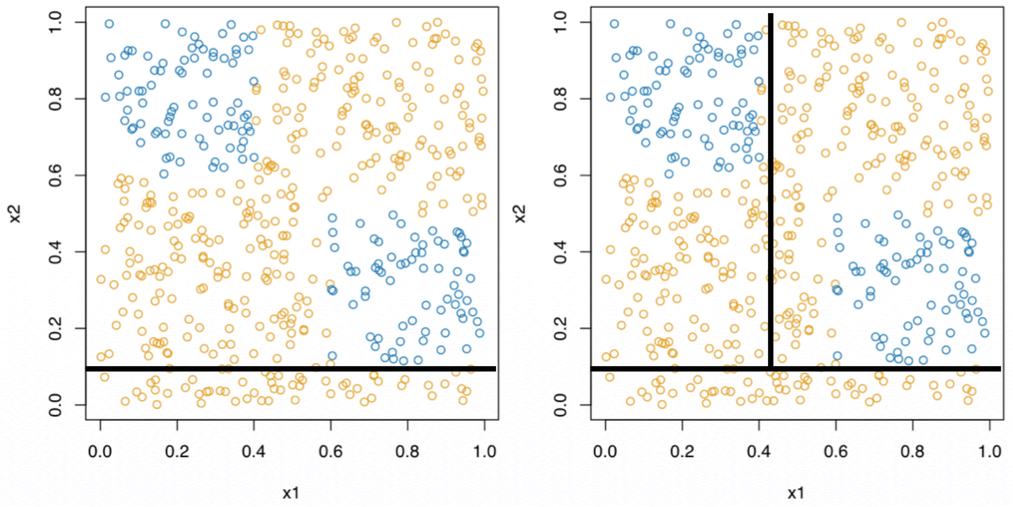

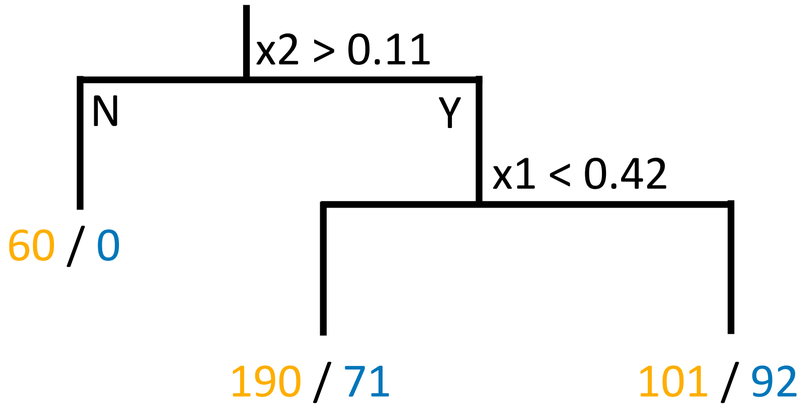

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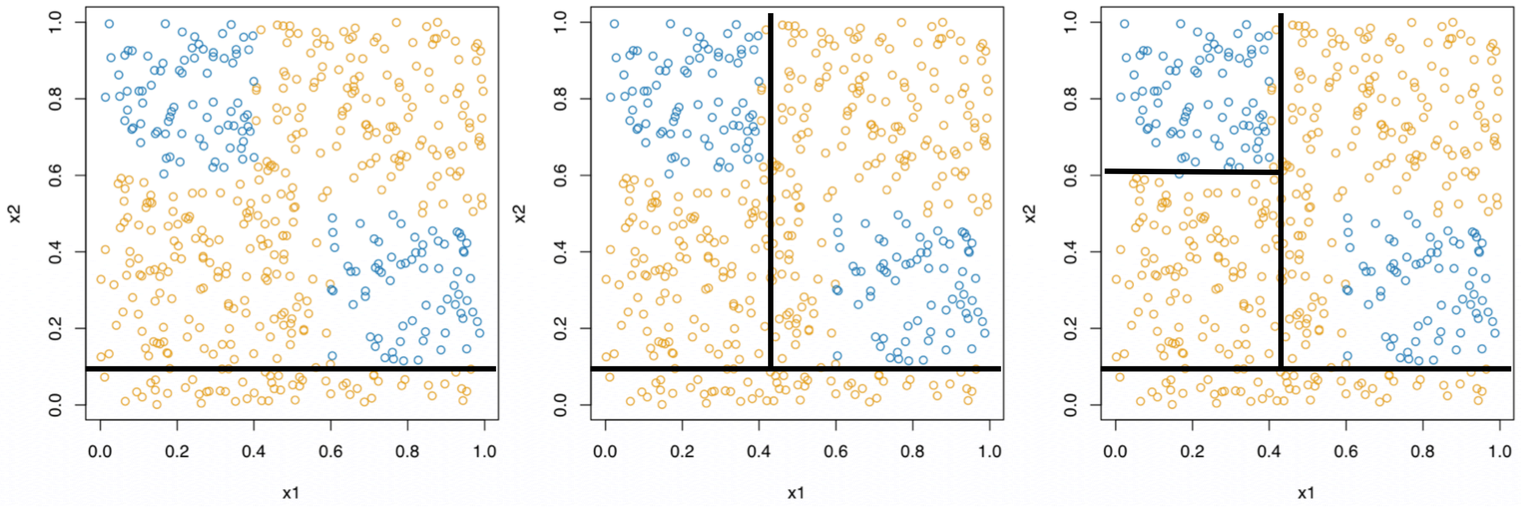

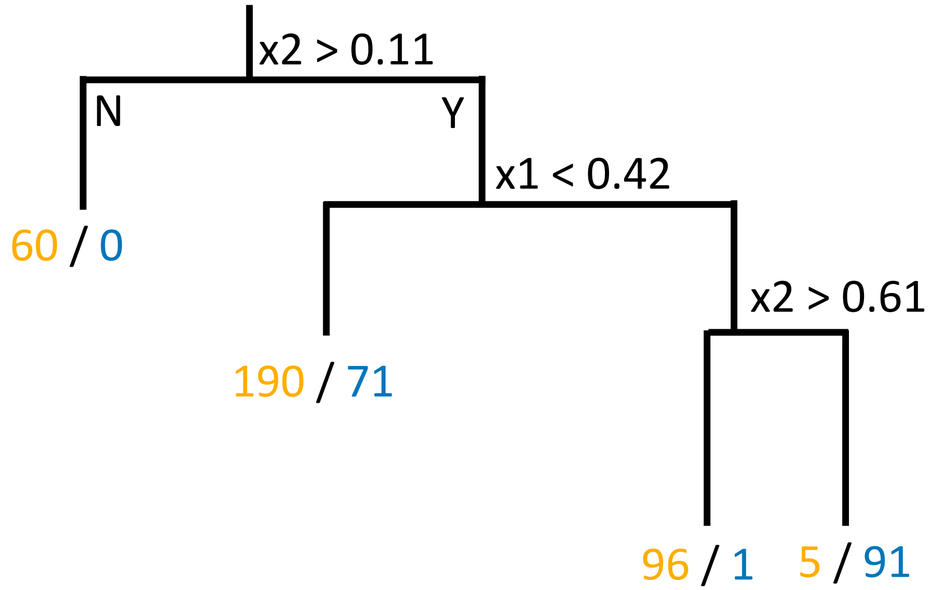

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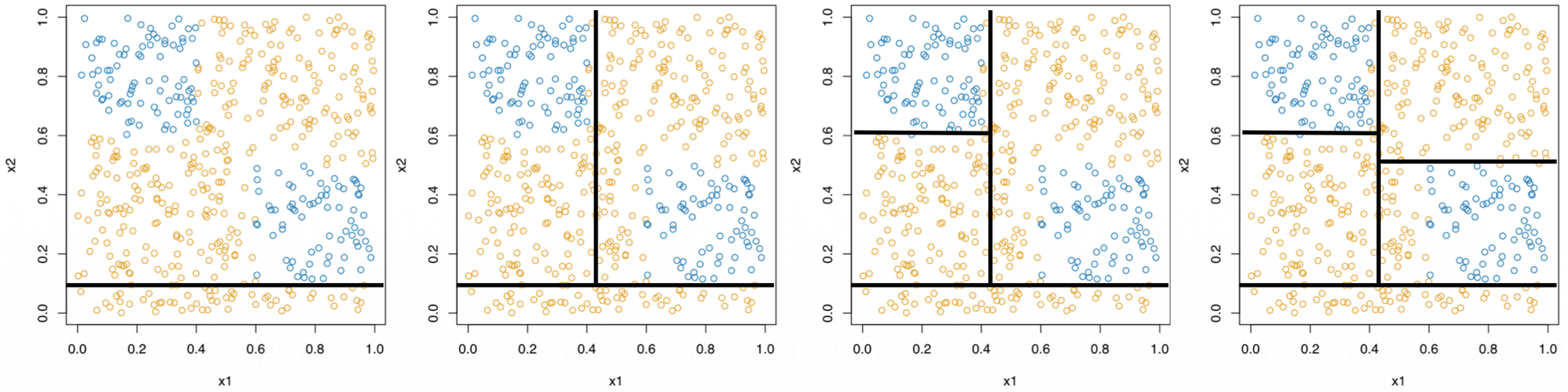

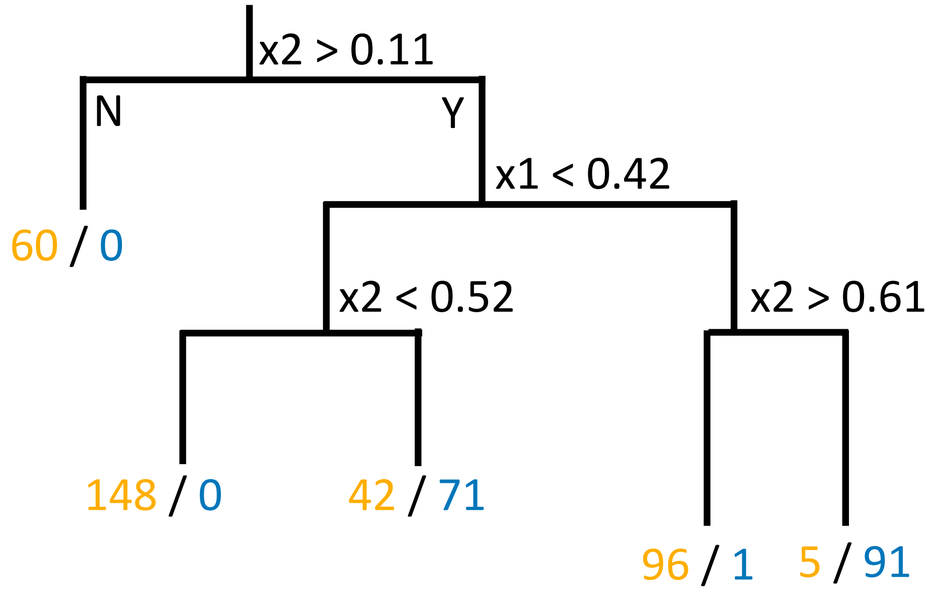

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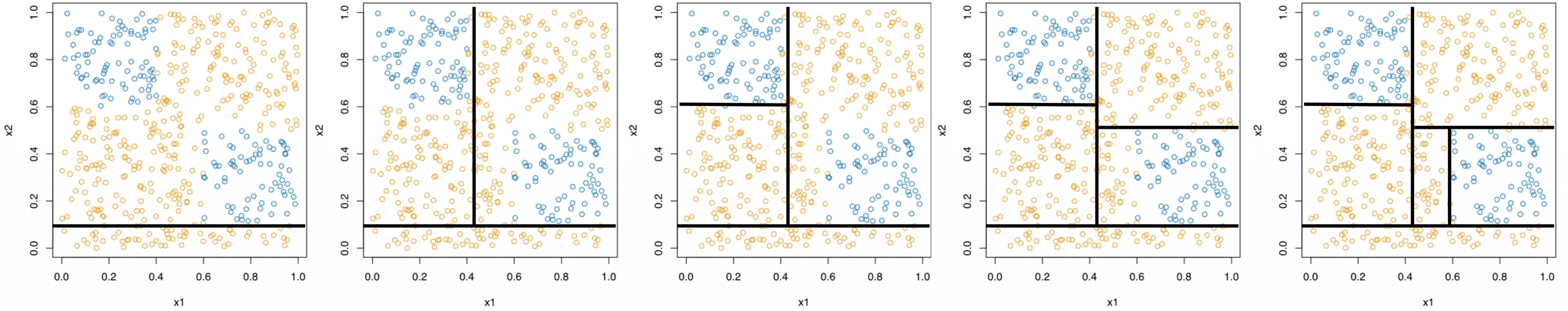

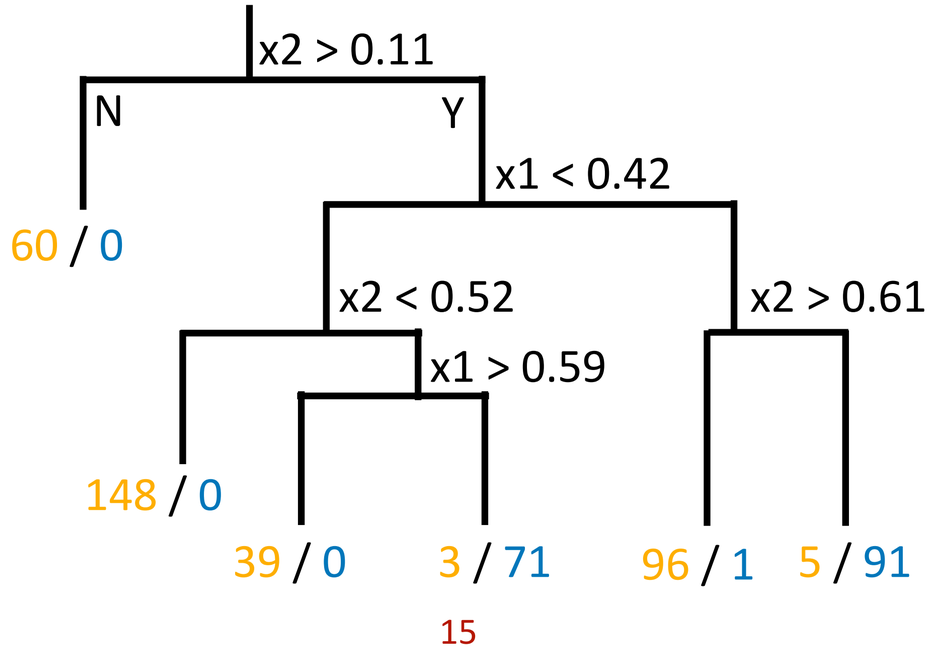

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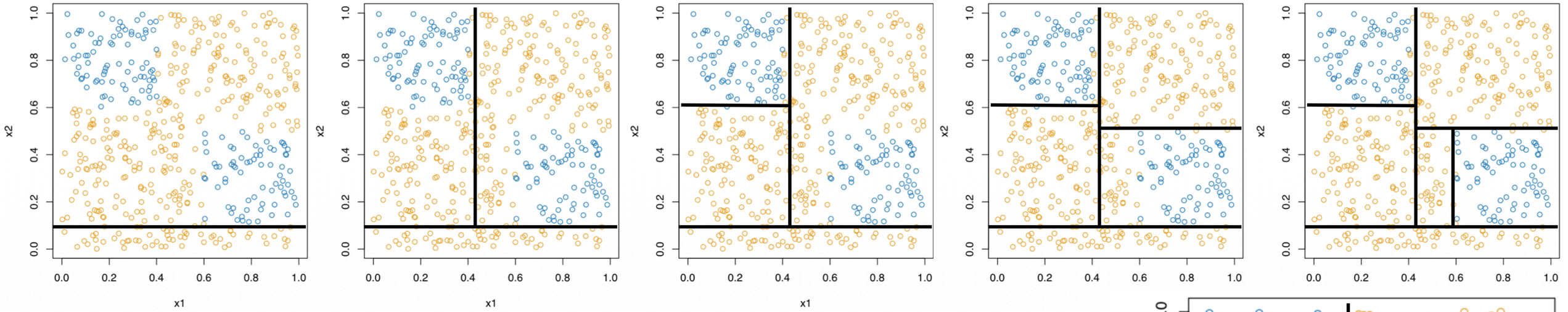
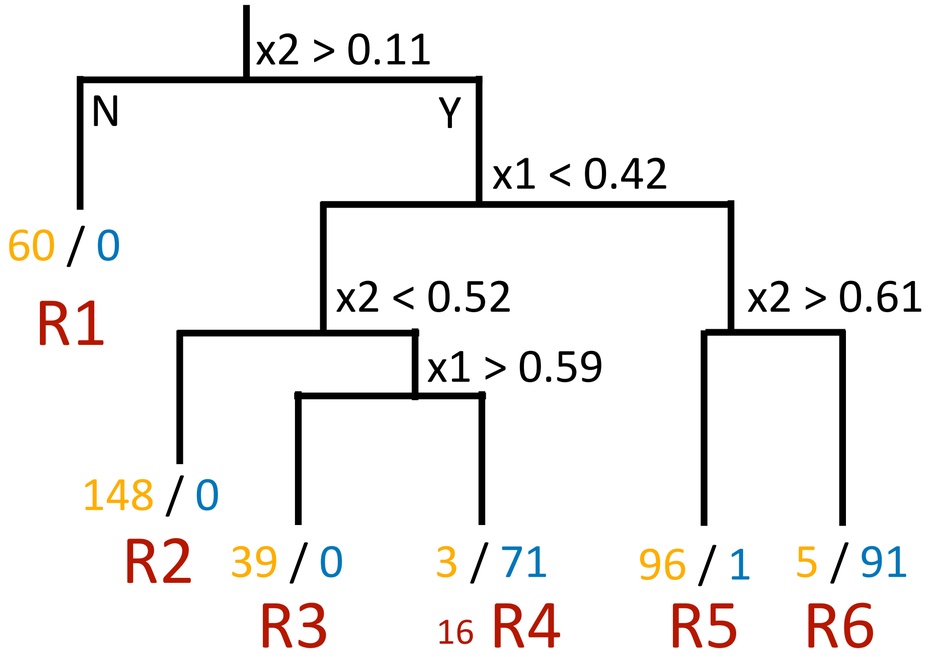
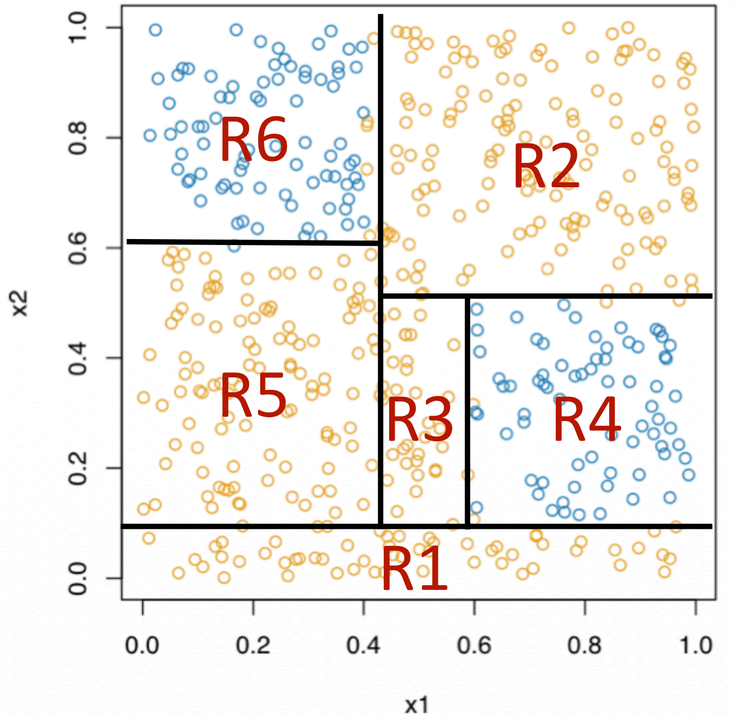


Confusion matrix

True \ Predicted	Yellow	Blue
Yellow	343	8
Blue	1	162





How to grow the tree?

- This is called recursive binary partitioning
- A **greedy** algorithm
- At each step, we only care about the best partition at that moment
    - All past partitions are fixed
    - It doesn’t worry about any future partitions
- When do we stop? e.g.
    - Same number of leaves as observations, or
    - Each leaf has fewer than a small fixed number of observations

Regression trees

- For one of the predictors X_j with a cutoff threshold c, we define two regions:
  $R_1(j, c) = \{X \mid X_j < c\}$ and $R_2(j, c) = \{X \mid X_j \geq c\}$
- An observation x_i is in region $R_1(j, c)$ if $x_{ij} < c$ and in region $R_2(j, c)$ if $x_{ij} \geq c$
- For the first iteration, $R_1(j, c)$ and $R_2(j, c)$ partitions the entire predictor space
- For later iterations, $R_1(j, c)$ and $R_2(j, c)$ partitions a previous 'parent' region (so inherits any previous conditions of that 'parent' region)

Regression trees

- Suppose there are n_1 observations in $R_1(j, c)$ and n_2 observations in $R_2(j, c)$
- The prediction in each region is the mean response for observations in that region, i.e. $\hat{y}_{R_1} = \frac{1}{n_1} \sum_{i:\ x_i \in R_1(j,c)} y_i$ and $\hat{y}_{R_2} = \frac{1}{n_2} \sum_{i:\ x_i \in R_2(j,c)} y_i$
- Select the current partition to minimise the residual sum of squares (RSS), i.e. choose j and c to minimise:

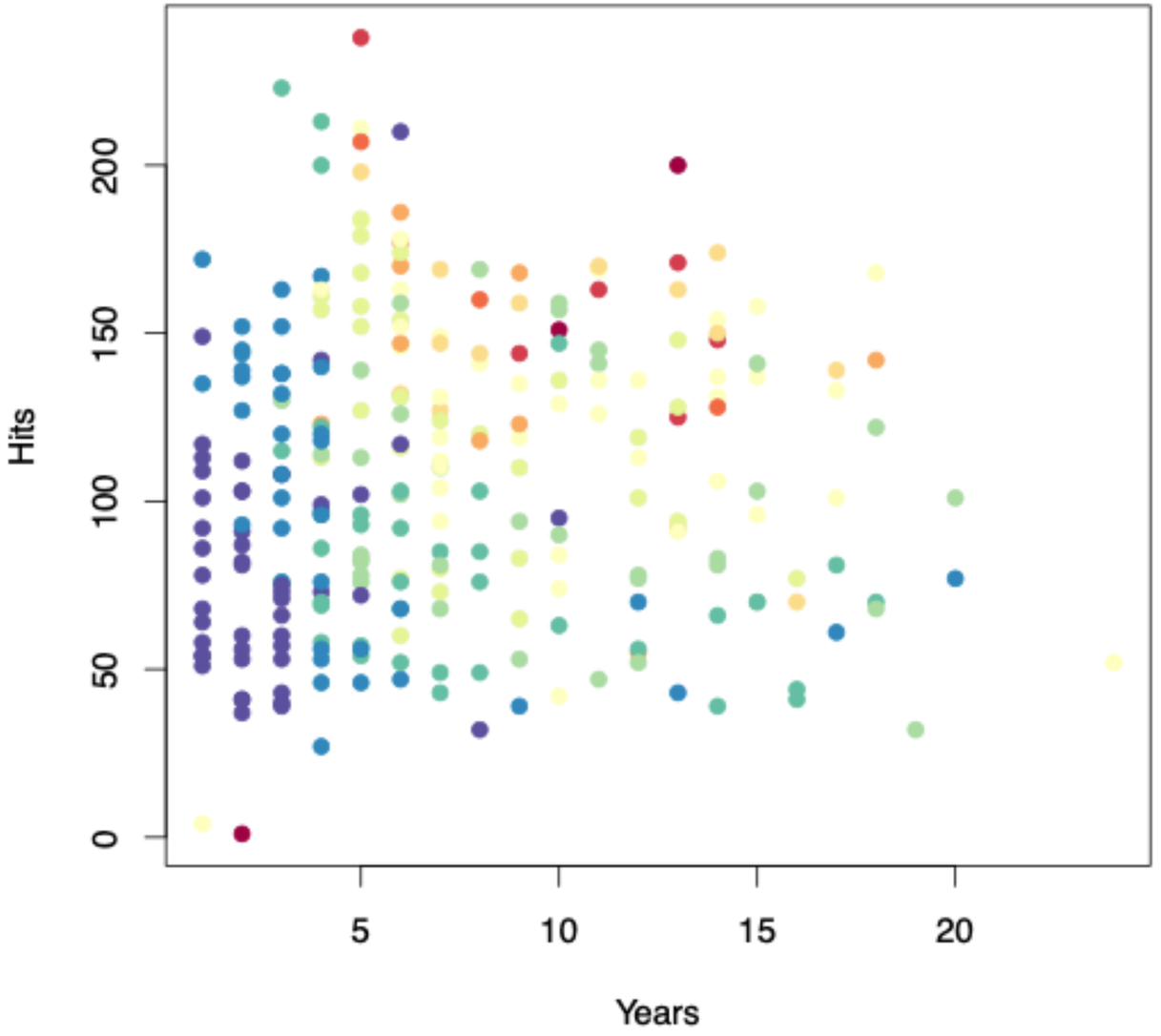
$$RSS(j, c) = \sum_{i:\ x_i \in R_1(j,c)} (y_i - \hat{y}_{R_1})^2 + \sum_{i:\ x_i \in R_2(j,c)} (y_i - \hat{y}_{R_2})^2$$

- How much does this reduce the RSS before the partition? $RSS = \sum_i (y_i - \hat{y})^2$

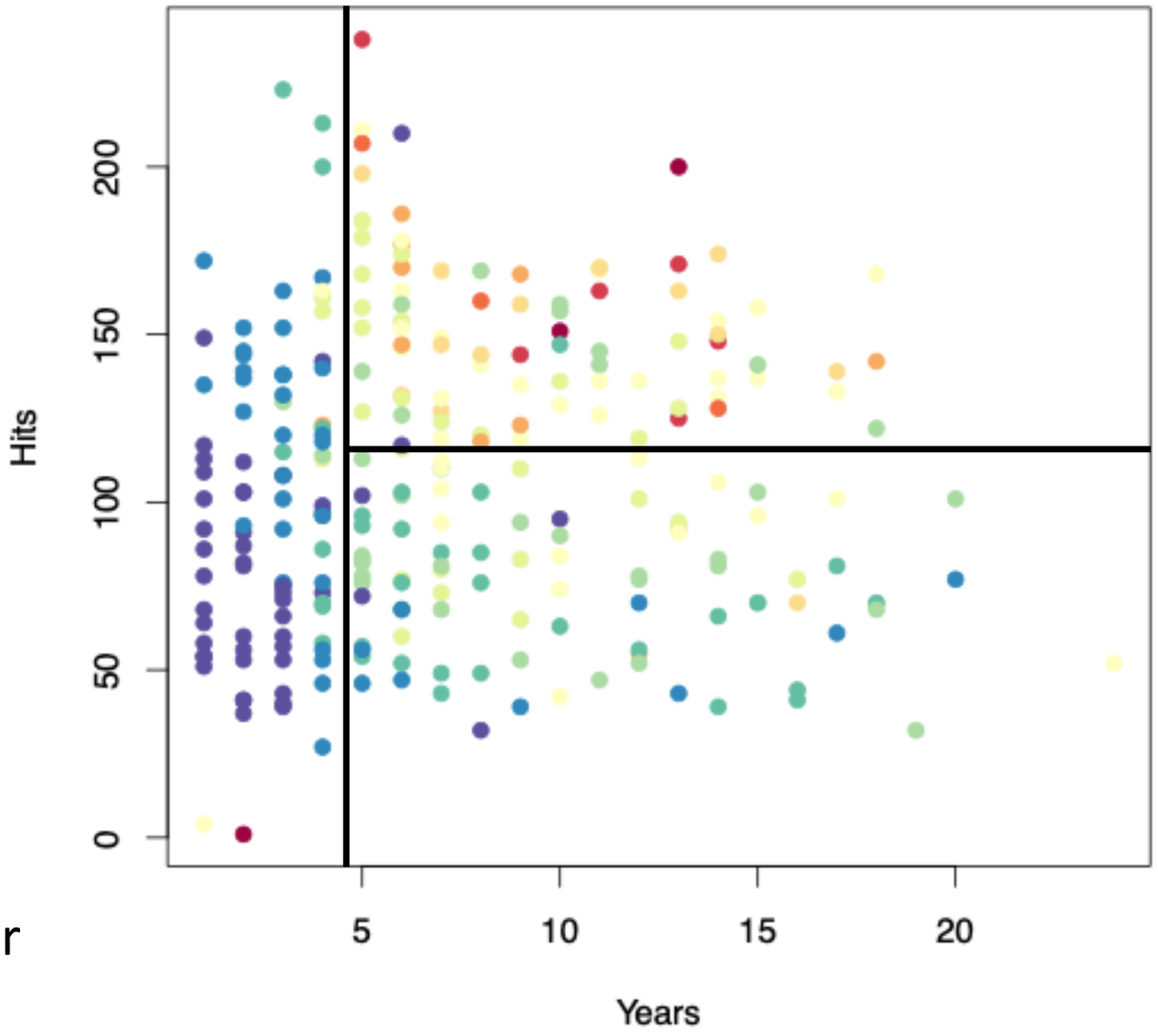
Example: baseball salaries

- X_1 is number of years experience
- X_2 is number of hits last year
- y is a log-transform of salary, measured in thousands of dollars i.e. the player's salary is $\$1000e^y$

- In the figure, y is represented by the colour of the dot (low - medium - high)

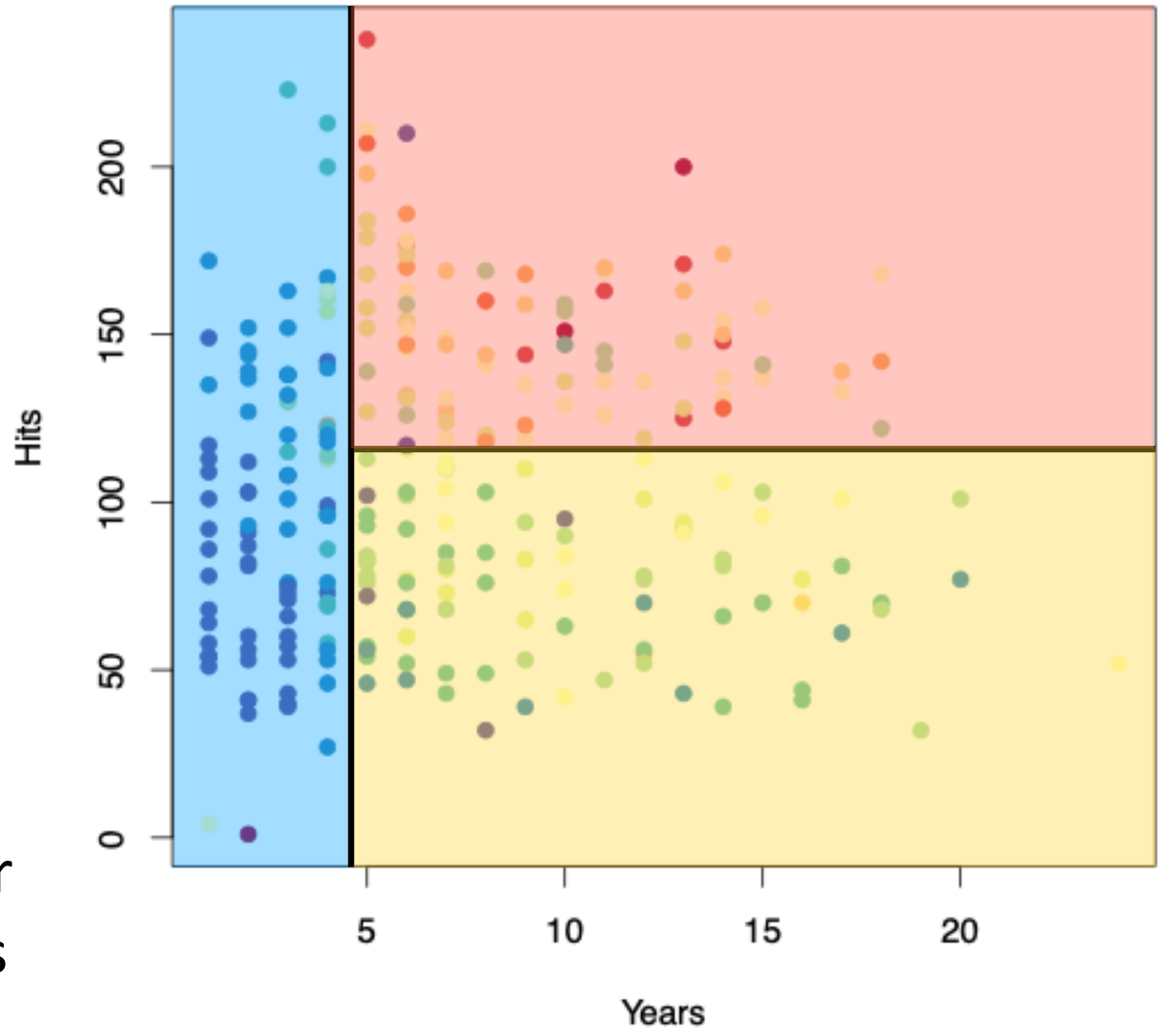


Baseball salary example



- How to interpret this?
  - Experience most important feature
  - If limited experience, hits isn't a big factor
  - If lots of experience, hits is a big factor

Baseball salary example



- How do we make predictions?
- How much do we expect a new player with 10 years experience and 200 hits to make? $\$1000e^{6.74} = \$845{,}346$

Questions?

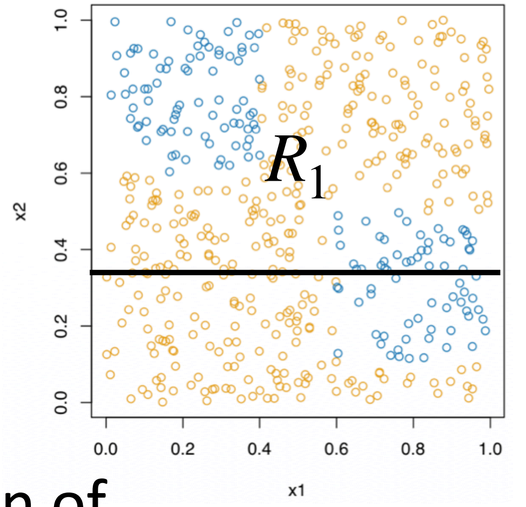
Classification trees

- The tree building process is very similar to before
- Now the output y is qualitative rather than quantitative, e.g. with K classes
- Instead of RSS, there are various criteria for making each partition, where $\hat{p}_{mk}$ is the proportion of observations within the region $R_m(j, c)$ belonging to the k^{th} class:
  - Classification error, $E_m(j, c) = 1 - \max_k(\hat{p}_{mk})$
  - Gini index, $G_m(j, c) = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk}) = 1 - \sum_{k=1}^{K} \hat{p}_{mk}^2$
  - Entropy, $H_m(j, c) = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$

Classification trees

- What is the total classification error or Gini index after the partition?
- A weighted average of the scores for each region (weighted by the number of observations in each region, n_1 and n_2)
  - Classification error, $E(j,c) = \frac{n_1}{n} E_1(j,c) + \frac{n_2}{n} E_2(j,c)$
  - Gini index, $G(j,c) = \frac{n_1}{n} G_1(j,c) + \frac{n_2}{n} G_2(j,c)$
- We'll come back to entropy shortly

Classification trees



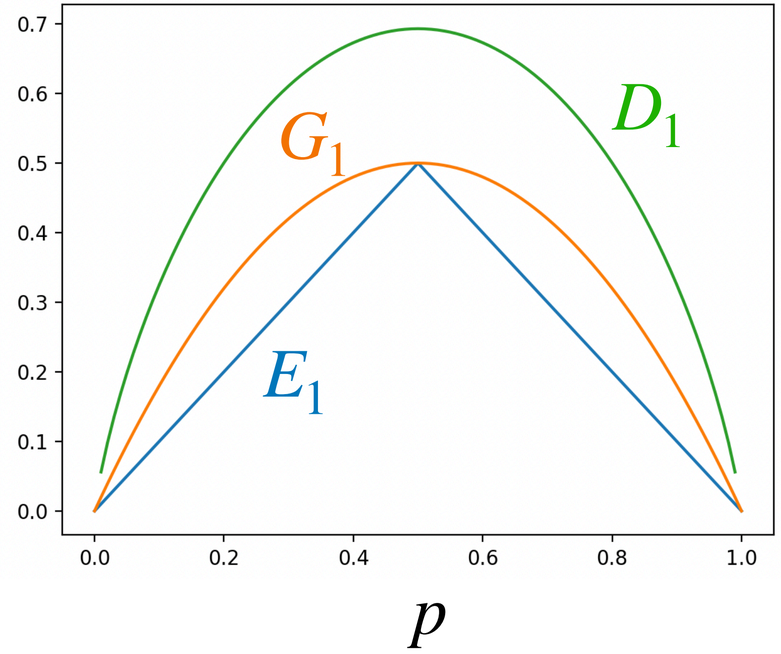
- What do this look like if there are $K = 2$ classes?

- Consider just region R_1 (with j and c fixed). If we write the proportion of observations in class $k = 1$ (e.g. yellow) as $\hat{p}_{11} = p$, then the proportion of observations in class $k = 2$ (e.g. blue) is $\hat{p}_{12} = (1 - p)$.

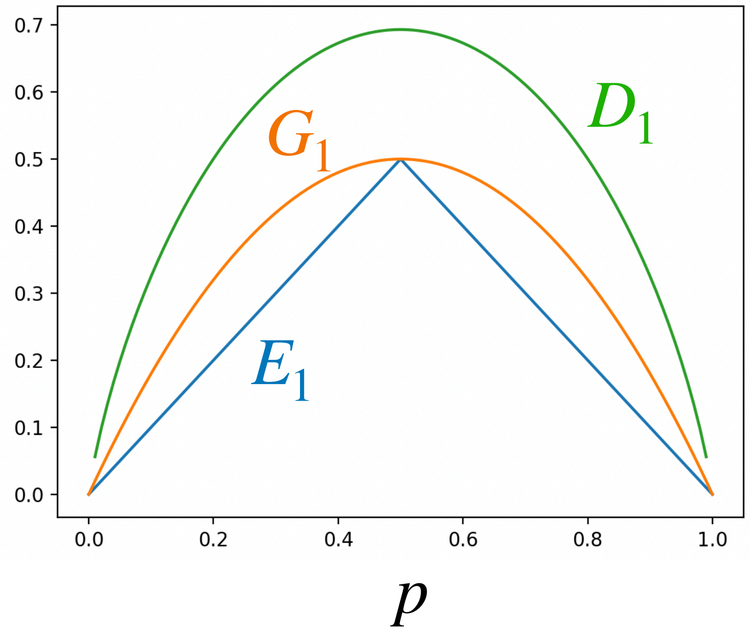
  - Classification error, $E_1 = \begin{cases} 1 - p & \text{if } p > 0.5 \\ p & \text{if } p < 0.5 \end{cases}$

  - Gini index, $G_1 = 1 - p^2 - (1 - p)^2 = 2p(1 - p)$

  - Entropy, $H_1 = -p \log p - (1 - p)\log(1 - p)$



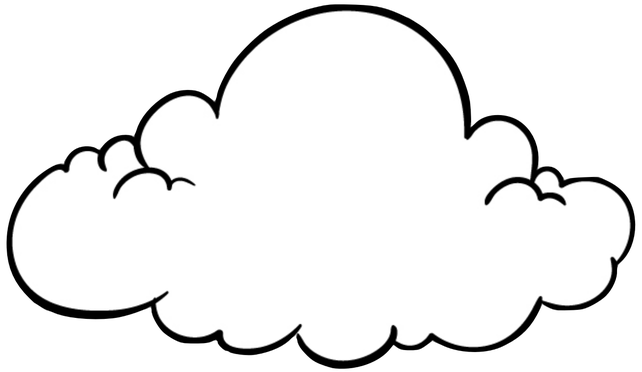
Classification trees



- We want **pure nodes** (almost all observations from one class), i.e. p close to 0 or close to 1
- The classification error is not particularly good at this!
- E.g. we would rather choose a partition that goes from $\hat{p}_{mk} = 0.8$ to $\hat{p}_{mk} = 0.9$ than a partition that goes from $\hat{p}_{mk} = 0.5$ to $\hat{p}_{mk} = 0.6$. The classification error improves by 0.1 in both cases.
- The Gini index improves by 0.14 when the partition goes from $\hat{p}_{mk} = 0.8$ to $\hat{p}_{mk} = 0.9$ and only by 0.02 when the partition goes from $\hat{p}_{mk} = 0.5$ to $\hat{p}_{mk} = 0.6$

Example: playing outdoors

Day	Weather	Temperature	Wind	Play?
1	Sun	Hot	Weak	No
2	Cloud	Hot	Weak	Yes
3	Sun	Mild	Strong	Yes
4	Cloud	Mild	Strong	Yes
5	Rain	Mild	Strong	No
6	Rain	Cool	Strong	No
7	Rain	Cool	Weak	Yes
8	Sun	Mild	Strong	No
9	Cloud	Hot	Weak	Yes
10	Rain	Mild	Strong	No



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7	Rain	Cool	Weak	Yes
8	Sun	Mild	Strong	No
9	Cloud	Hot	Weak	Yes
10	Rain	Mild	Strong	No

- Discrete predictors, binary outcome
- Class $k = 1$ is Play?=Yes, with proportion $\hat{p}_{11} = p = 0.5$
- Class $k = 2$ is Play?=No, with proportion $\hat{p}_{12} = 0.5$
- Initial classification (assume we classify all observations as Play?=Yes):
  - $E(\text{Init}) = 1 - 0.5 = 0.5$
  - $G(\text{Init}) = 1 - 0.5^2 - 0.5^2 = 0.5$

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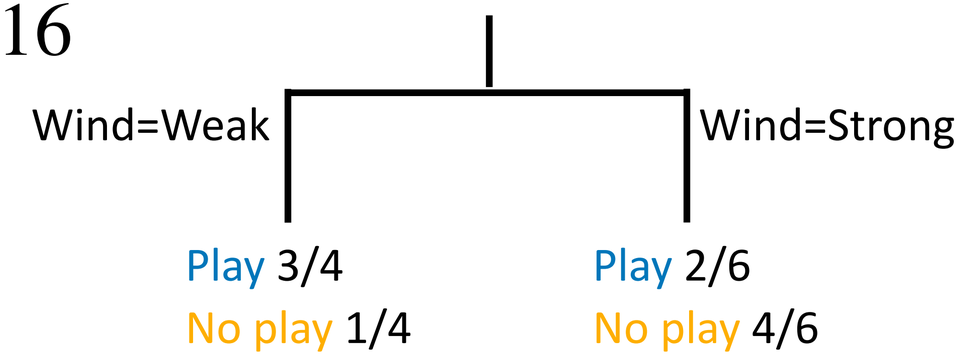
- Partition into R_1 (Wind=Weak) vs R_2 (Wind=Strong)
- $E_1 = 1 - 3/4 = 0.25$

  $E_2 = 1 - 2/3 \approx 0.33$

  $E(\text{Wind}) = 4/10 \times 0.25 + 6/10 \times 0.33 = 0.3$
- $G_1 = 1 - (3/4)^2 - (1/4)^2 = 0.375$

  $G_2 = 1 - (1/3)^2 - (2/3)^2 = 4/9 \approx 0.44$

  $G(\text{Wind}) = 4/10 \times 0.375 + 6/10 \times 0.44 \approx 0.416$



Example: playing outdoors

- Temperature has 3 categories, so partition into 3 branches
- E.g. partition into R_1 (Temp=Hot) vs R_2 (Temp=Mild/Cool), then partition R_2 into R_3 (Temp=Cool) vs R_4 (Temp=Mild)

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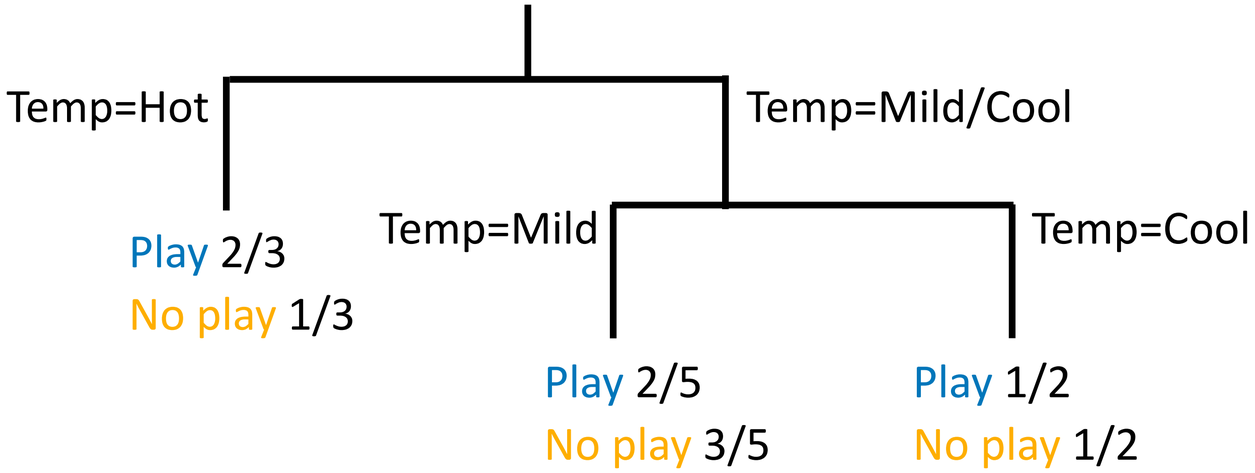

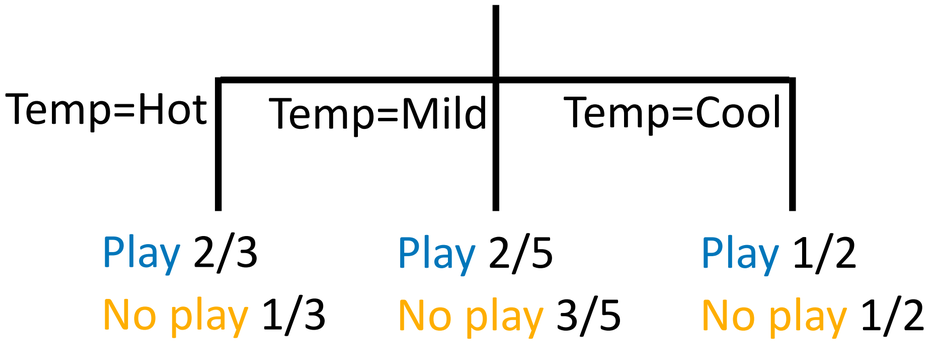

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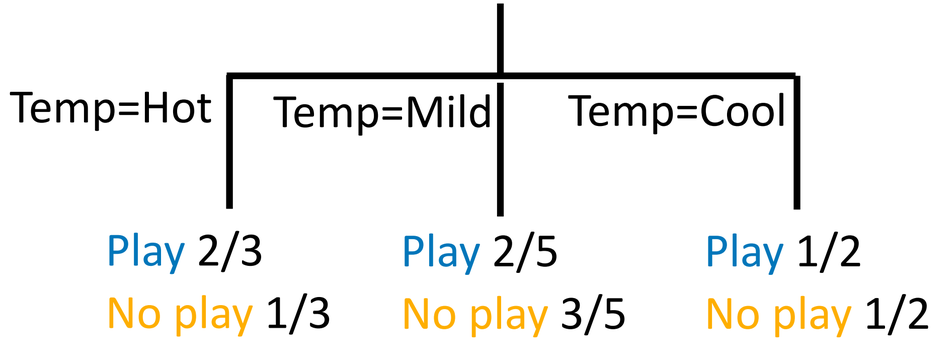
3	Sun	Mild	Strong	Yes
4	Cloud	Mild	Strong	Yes
5	Rain	Mild	Strong	No
6	Rain	Cool	Strong	No
7	Rain	Cool	Weak	Yes
8	Sun	Mild	Strong	No
9	Cloud	Hot	Weak	Yes
10	Rain	Mild	Strong	No

- Partition into R_1 (Temp=Hot) vs R_2 (Temp=Mild) vs R_3 (Temp=Cool) (renaming R_4 from previous slide to R_2)
- $E_1 = 1 - 2/3 \approx 0.33, \quad E_2 = 1 - 3/5 = 0.4$

  $E_3 = 1 - 1/2 = 0.5$

  $E(\text{Temp}) = 3/10 \times 0.33 + 5/10 \times 0.4 + 2/10 \times 0.5 = 0.4$



- $G_1 = 1 - (2/3)^2 - (1/3)^2 \approx 0.44$

  $G_2 = 1 - (2/5)^2 - (3/5)^2 = 0.48$

  $G_3 = 1 - (1/2)^2 - (1/2)^2 = 0.5$

  $G(\text{Temp}) = 3/10 \times 0.44 + 5/10 \times 0.48 + 2/10 \times 0.5 \approx 0.473$

Example: playing outdoors

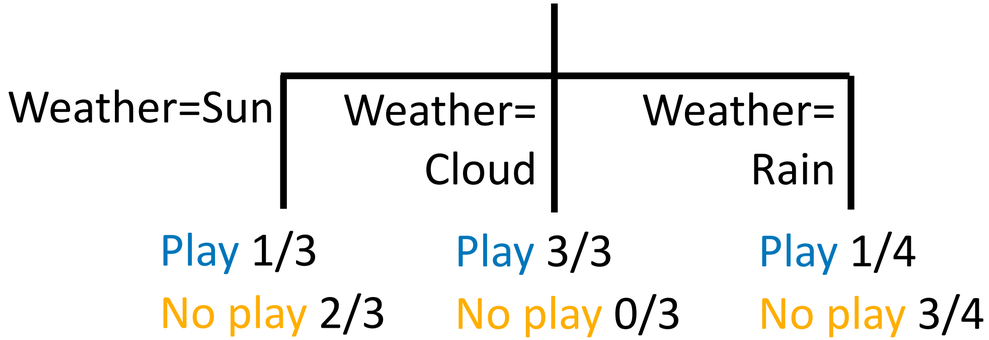
Day	Weather	Temperature	Wind	Play?
1	Sun	Hot	Weak	No
2	Cloud	Hot	Weak	Yes
3	Sun	Mild	Strong	Yes
4	Cloud	Mild	Strong	Yes
5	Rain	Mild	Strong	No
6	Rain	Cool	Strong	No
7	Rain	Cool	Weak	Yes
8	Sun	Mild	Strong	No
9	Cloud	Hot	Weak	Yes
10	Rain	Mild	Strong	No

- Partition into R_1 (Weather=Sun) vs R_2 (Weather=Cloud) vs R_3 (Weather=Rain)

- $E_1 = 1 - 2/3 \approx 0.33, \quad E_2 = 1 - 3/3 = 0$

  $E_3 = 1 - 3/4 = 0.25$

  $E(\text{Weather}) = 3/10 \times 0.33 + 3/10 \times 0 + 4/10 \times 0.25 = 0.2$



- $G_1 = 1 - (1/3)^2 - (2/3)^2 \approx 0.44$

  $G_2 = 1 - (3/3)^2 - (0/3)^2 = 0$

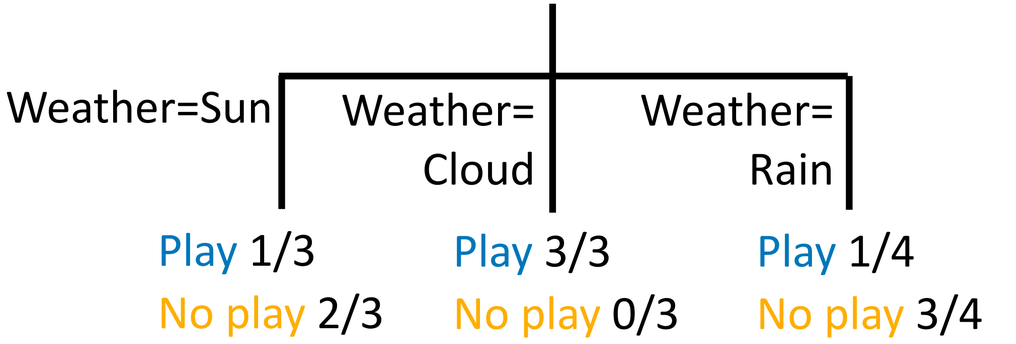
  $G_3 = 1 - (1/4)^2 - (3/4)^2 = 0.375$

  $G(\text{Weather}) = 3/10 \times 0.44 + 3/10 \times 0 + 4/10 \times 0.375 \approx 0.282$

Example: playing outdoors

Day	Weather	Temperature	Wind	Play?
1	Sun	Hot	Weak	No
2	Cloud	Hot	Weak	Yes
3	Sun	Mild	Strong	Yes
4	Cloud	Mild	Strong	Yes
5	Rain	Mild	Strong	No
6	Rain	Cool	Strong	No
7	Rain	Cool	Weak	Yes
8	Sun	Mild	Strong	No
9	Cloud	Hot	Weak	Yes
10	Rain	Mild	Strong	No

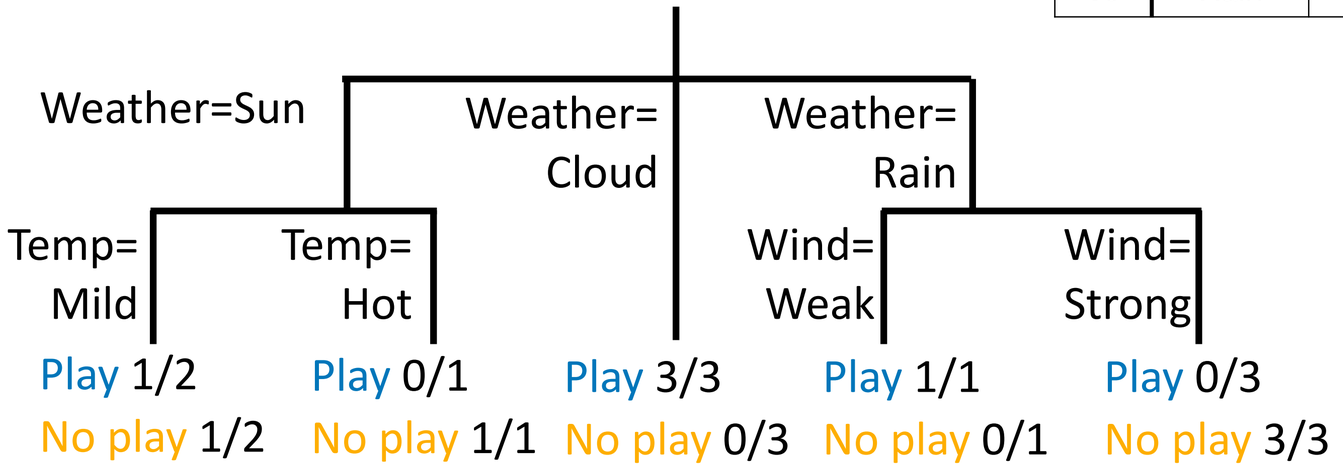
- $E(\text{Init}) = 0.5$
  $E(\text{Wind}) = 0.3,\ E(\text{Temp}) = 0.4,\ E(\text{Weather}) = 0.2$
- $G(\text{Init}) = 0.5$
  $G(\text{Wind}) \approx 0.416,\ G(\text{Temp}) \approx 0.473$
  $G(\text{Weather}) \approx 0.282$
- The best partition (biggest decrease) is by Weather, using either the classification error or the Gini index



Example: playing outdoors

- Next: consider partitioning R_1 (Weather=Sun) by Temp or Wind OR partitioning R_3 (Weather=Rain) by Temp or Wind
- A final decision tree:

Day	Weather	Temperature	Wind	Play?
1	Sun	Hot	Weak	No
2	Cloud	Hot	Weak	Yes
3	Sun	Mild	Strong	Yes
4	Cloud	Mild	Strong	Yes
5	Rain	Mild	Strong	No
6	Rain	Cool	Strong	No
7	Rain	Cool	Weak	Yes
8	Sun	Mild	Strong	No
9	Cloud	Hot	Weak	Yes
10	Rain	Mild	Strong	No

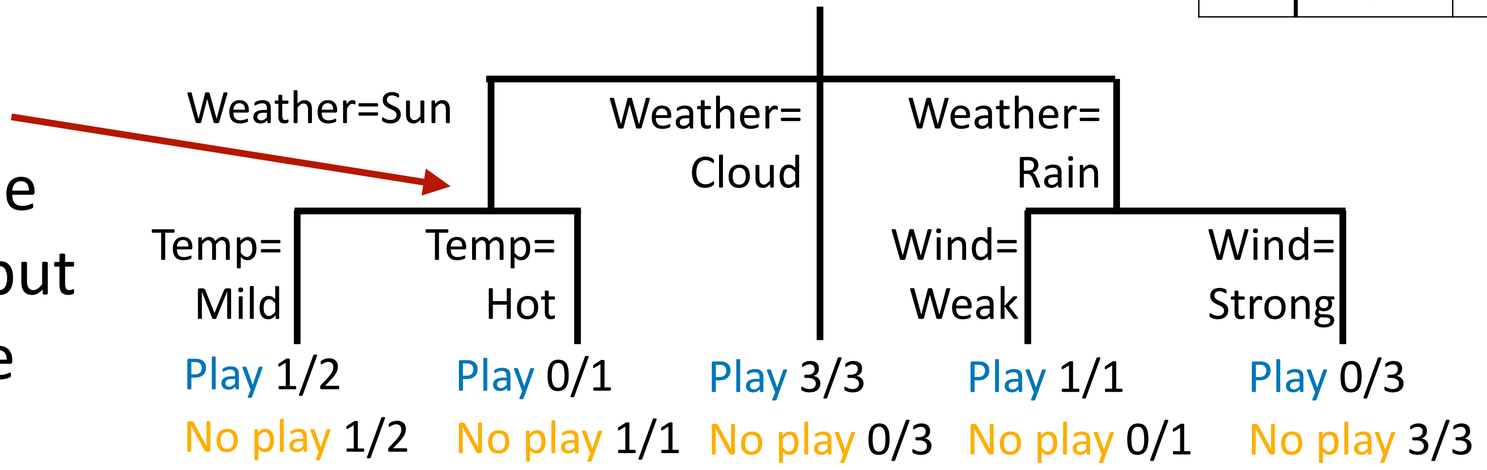


Example: playing outdoors

- Next: consider partitioning R_1 (Weather=Sun) by Temp or Wind OR partitioning R_3 (Weather=Rain) by Temp or Wind
- A final decision tree:

Day	Weather	Temperature	Wind	Play?
1	Sun	Hot	Weak	No
2	Cloud	Hot	Weak	Yes
3	Sun	Mild	Strong	Yes
4	Cloud	Mild	Strong	Yes
5	Rain	Mild	Strong	No
6	Rain	Cool	Strong	No
7	Rain	Cool	Weak	Yes
8	Sun	Mild	Strong	No
9	Cloud	Hot	Weak	Yes
10	Rain	Mild	Strong	No

Note: this partition doesn't decrease the classification error but it does decrease the Gini index!



Entropy and information gain

- Entropy, measured in nats:

$$H(Y) = -\sum_k P(Y=k)\log P(Y=k) = -\sum_k p_k \log p_k$$

- Entropy, measured in bits: $H(Y) = -\sum_k p_k \log_2 p_k$ (we'll use this for now)

- Suppose we know $X_j = x$, then

$$H(Y \mid X_j = x) = -\sum_k P(Y=k \mid X_j = x)\log_2 P(Y=k \mid X_j = x)$$

- The **information gain** is the amount that this reduces the entropy of Y, i.e.

$$IG(Y, X_j = x) = H(Y) - H(Y \mid X_j = x)$$

Entropy and information gain

- We can use the **average information gain** as another way to calculate the 'best' partition, i.e. $IG(Y, X_j) = H(Y) - \sum_x p(X_j = x) H(Y \mid X_j = x)$

Entropy and information gain

- We can use the **average information gain** as another way to calculate the 'best' partition, i.e. $IG(Y, X_j) = H(Y) - \sum_x p(X_j = x) H(Y \mid X_j = x)$

Day	Weather	Temperature	Wind	Play?
1	Sun	Hot	Weak	No
2	Cloud	Hot	Weak	Yes
3	Sun	Mild	Strong	Yes
4	Cloud	Mild	Strong	Yes
5	Rain	Mild	Strong	No
6	Rain	Cool	Strong	No
7	Rain	Cool	Weak	Yes
8	Sun	Mild	Strong	No
9	Cloud	Hot	Weak	Yes
10	Rain	Mild	Strong	No

- For the example, $H(\text{Play}) = -\sum_k P(\text{Play} = k) \log_2 P(\text{Play} = k)$

  $= -5/10 \log_2(5/10) - 5/10 \log_2(5/10) = 1$

- $H(\text{Play} \mid \text{Wind} = \text{Strong}) = -3/4 \log(3/4) - 1/4 \log(1/4) \approx 0.811$

  $H(\text{Play} \mid \text{Wind} = \text{Weak}) = -2/3 \log(2/3) - 1/3 \log(1/3) \approx 0.918$

Entropy and information gain

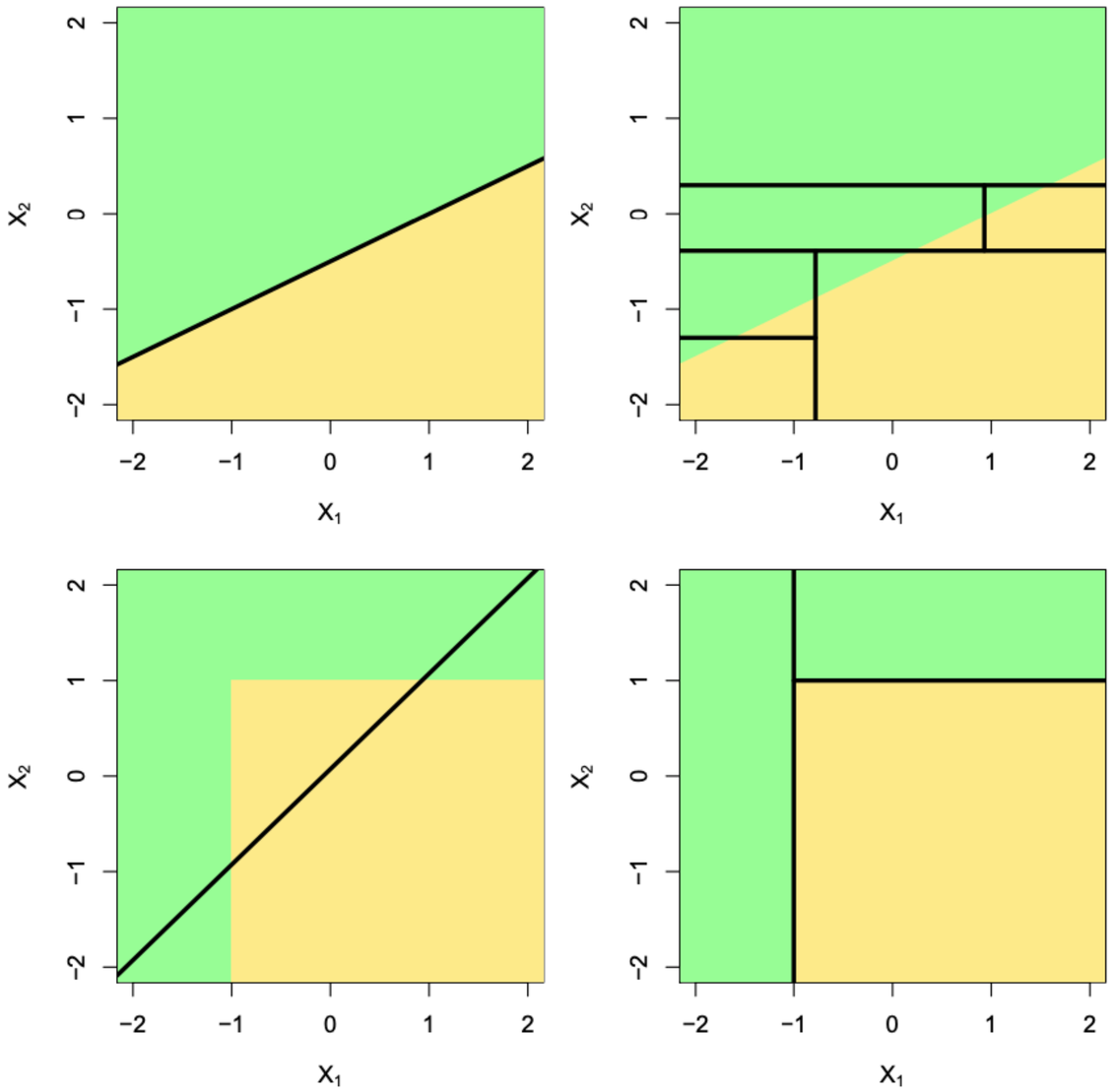
- We can use the **average information gain** as another way to calculate the 'best' partition, i.e. $IG(Y, X_j) = H(Y) - \sum_x p(X_j = x) H(Y \mid X_j = x)$

Day	Weather	Temperature	Wind	Play?
1	Sun	Hot	Weak	No
2	Cloud	Hot	Weak	Yes
3	Sun	Mild	Strong	Yes
4	Cloud	Mild	Strong	Yes
5	Rain	Mild	Strong	No
6	Rain	Cool	Strong	No
7	Rain	Cool	Weak	Yes
8	Sun	Mild	Strong	No
9	Cloud	Hot	Weak	Yes
10	Rain	Mild	Strong	No

- For the example, $H(\text{Play}) = -\sum_k P(\text{Play} = k) \log_2 P(\text{Play} = k)$
  $= -5/10 \log_2(5/10) - 5/10 \log_2(5/10) = 1$
- $H(\text{Play} \mid \text{Wind} = \text{Strong}) = -3/4 \log(3/4) - 1/4 \log(1/4) \approx 0.811$
  $H(\text{Play} \mid \text{Wind} = \text{Weak}) = -2/3 \log(2/3) - 1/3 \log(1/3) \approx 0.918$
- $IG(\text{Play}, \text{Wind}) = 1 - 4/10 \times 0.811 - 6/10 \times 0.918 \approx 0.1245$
- Similarly, $IG(\text{Play}, \text{Temp}) \approx 0.2116$, $IG(\text{Play}, \text{Weather}) = 0.4$

Largest information gain

Decision trees vs linear regression



$$y \approx f(X) = \beta_0 + \sum_j X_j \beta_j$$

$$y \approx f(X) = \sum_m c_m 1\{X \in R_m\}$$

Decision trees: pros and cons

- Trees are very interpretable! You can easily read off why the model gave a particular prediction (it's a white box model) ✓
- Trees are non-parametric, they don't require assumptions about the data or residuals ✓
- Trees handle mixed data types (both predictors and response variables) ✓
- Trees can handle missing data (e.g. using surrogate variables) ✓
- Trees are not very robust. Small changes to the input data can completely change the tree structure. ✘
- Most of the time, trees aren't particularly good at prediction. ✘
- Does this mirror human intuition better than other methods for prediction or classification?

When do we stop growing the tree?

- Which is better: small trees or big trees?

Questions?

- Feel free to email me at te269@cam.ac.uk

- These slides will go on GitHub later today,

  https://github.com/tedinburgh/ads2023

Next time

- Pruning
- Ensembles and aggregates
  - Bagging
  - Boosting
  - Random forests