Decision Trees

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Course overview: http://openml.github.io/course

```
In [33]: options(warn=-1)
         library(mlr) # ML library
         library(OpenML) # Data import and sharing results
         library(ggplot2) # Plotting
         library(cowplot) # Plot styling
         library(rattle) # Plotting trees
```

1 Decision trees

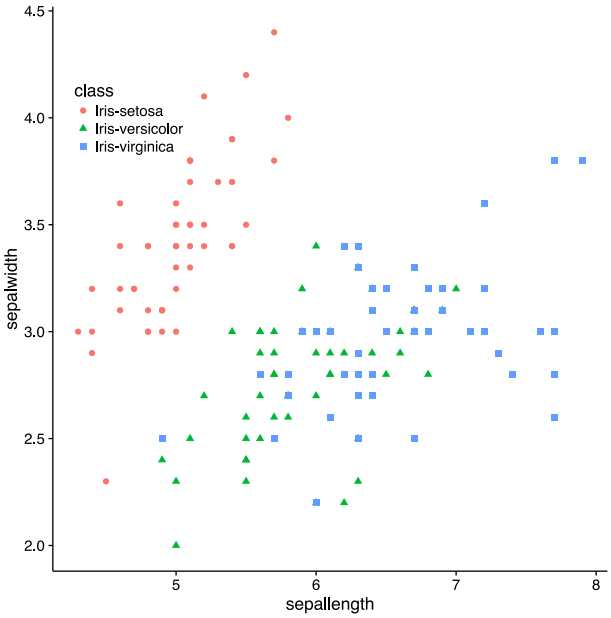
- Most widely-used machine learning algorithm
  - Fairly easy to understand and implement
  - Output (model) also easy to understand
  - Easy to use: you don't have to tweak many hyperparameters before it returns something useful
  - Pretty scalable (in number of features and instances)
  - Not top performance, but good place to start
- Depending on the type of the target feature
  - Classification tree (predicts class)
  - Regression tree (predicts numeric value)
- Predictive features can be discrete (categorical) or continuous (numeric), or mixed

1.1 Classification example

```
In [34]: iris = getOMLDataSet(did = 61, verbosity=0)$data
         iristask = makeClassifTask(data = iris, target = "class")
         head(iris)
```

	sepallength	sepalwidth	petallength	petalwidth	class
0	5.1	3.5	1.4	0.2	Iris-setosa
1	4.9	3	1.4	0.2	Iris-setosa
2	4.7	3.2	1.3	0.2	Iris-setosa
3	4.6	3.1	1.5	0.2	Iris-setosa
4	5	3.6	1.4	0.2	Iris-setosa
5	5.4	3.9	1.7	0.4	Iris-setosa

```
In [35]: ggplot(data=iris, aes(x=sepallength, y=sepalwidth, color=class, shape=class)) + geom_point(siz
```



1.2 Learning algorithms (recap)

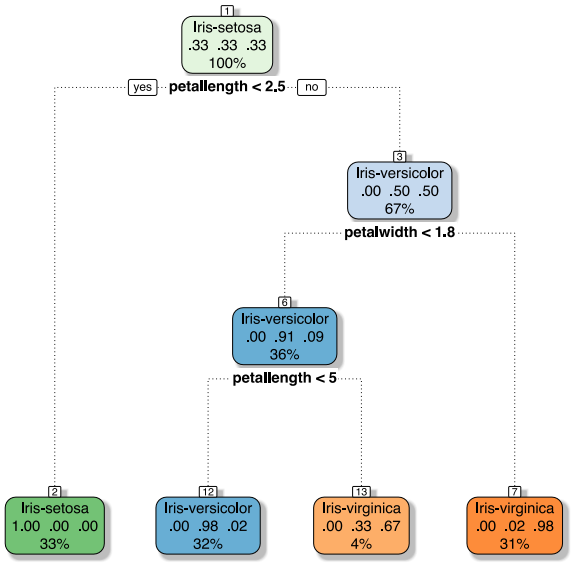
All learners consist of three main components:

- **Representation**: A model must be represented in a formal language that the computer can handle.
  - Defines the concepts it can learn: the hypothesis space
- **Evaluation function**: How to choose one hypothesis over the other?
  - Used internally, can differ from external measure
- **Optimization**: How do we search the hypothesis space?
  - Key to the efficiency of the learner

2 Decision trees: Representation

- **Internal nodes**: test value of one particular feature, divide all instances into branches according to the outcome
- **Leaf nodes**: make predictions based on remaining subset

```
In [36]: rpart = makeLearner("classif.rpart")
         rpart = setHyperPars(rpart, cp = 0, minbucket=4)
         model = train(rpart, iristask)
         fancyRpartPlot(model$learner.model, sub="")
```



Trees divide the feature space into (hyper)rectangular regions (leaves) and fit a simple model (or a constant) in each leaf:

$$f(x) = \sum_{m=1}^{M} c_m \; I(x \in R_m)$$

where: M rectangulars R_m are used, and c_m can be: - the most frequent class - the fitted class distribution (probabilistic classifier) - a simple classification model (linear model, naïve Bayes,...) - a fitted (e.g. average) value (regression) - a fitted regression model (linear,...)

Variants exist that create non-rectangular regions (e.g. oblique trees)

In [37]: *# Helper function for visualizing the hyperrectangles*

```
library("grid")
library("coin")
Colors <- colorspace::rainbow_hcl(3)
Colors_trans <- apply(rbind(col2rgb(colorspace::rainbow_hcl(3)), alpha = 100, maxColorValue = 1
                      function(x) do.call("rgb", as.list(x)))
plot_rectangles <- function(obj, x, y, class, depth) {
  xname <- paste(deparse(substitute(x), 500), collapse = "\n")
  yname <- paste(deparse(substitute(y), 500), collapse = "\n")
  grid.newpage()
  pushViewport(plotViewport(c(5, 4, 2, 2)))
  pushViewport(dataViewport(x,
                            y,
                            name="plotRegion"))
  grid.points(x, y, pch = 19,
              gp=gpar(cex=0.5, col = Colors[class]))
  grid.rect()
  grid.xaxis()
  grid.yaxis()
  grid.text(xname, y=unit(-3, "lines"))
```

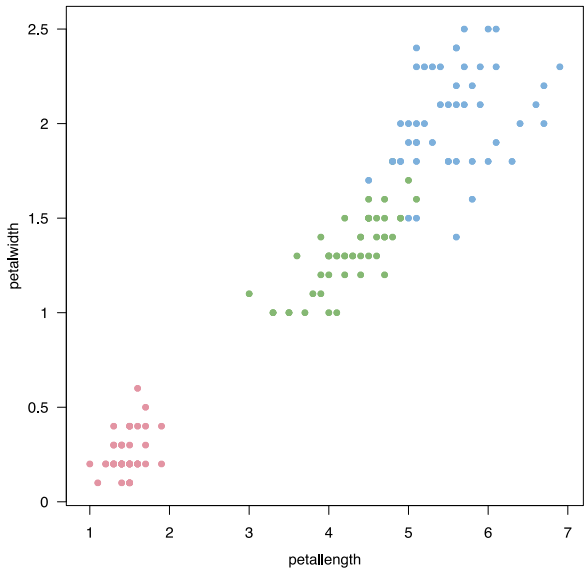
```
  grid.text(yname, x=unit(-3, "lines"), rot=90)
  seekViewport("plotRegion")
  plot_rect(obj@tree, xname = xname, depth)
  grid.points(x, y, pch = 19,
              gp=gpar(cex=0.5, col = Colors[class]))
}

plot_rect <- function(obj, xname, depth) {
  if (!missing(depth)) {
    if (obj$nodeID >= depth) return()
  }
  if (obj$psplit$variableName == xname) {
    x <- unit(rep(obj$psplit$splitpoint, 2), "native")
    y <- unit(c(0, 1), "npc")
  } else {
    x <- unit(c(0, 1), "npc")
    y <- unit(rep(obj$psplit$splitpoint, 2), "native")
  }
  grid.lines(x, y)
  if (obj$psplit$variableName == xname) {
    pushViewport(viewport(x = unit(current.viewport()$xscale[1], "native"),
                          width = x[1] - unit(current.viewport()$xscale[1], "native"),
                          xscale = c(unit(current.viewport()$xscale[1], "native"), x[1]),
                          yscale = current.viewport()$yscale,
                          just = c("left", "center")))
  } else {
    pushViewport(viewport(y = unit(current.viewport()$yscale[1], "native"),
                          height = y[1] - unit(current.viewport()$yscale[1], "native"),
                          xscale = current.viewport()$xscale,
                          yscale = c(unit(current.viewport()$yscale[1], "native"), y[1]),
                          just = c("center", "bottom")))
  }
  pred <- ifelse(length(obj$left$prediction) == 1, as.integer(obj$left$prediction > 0.5) + 1, v
  grid.rect(gp = gpar(fill = "white"))
  grid.rect(gp = gpar(fill = Colors_trans[pred]))
  if (!is(obj$left, "TerminalNode")) {
    plot_rect(obj$left, xname, depth)
  }
  popViewport()
  if (obj$psplit$variableName == xname) {
    pushViewport(viewport(x = unit(x[1], "native"),
                          width = unit(current.viewport()$xscale[2], "native")-x[1],
                          xscale = c(x[1], unit(current.viewport()$xscale[2], "native")),
                          yscale = current.viewport()$yscale,
                          just = c("left", "center")))
  } else {
    pushViewport(viewport(y = unit(y[1], "native"),
                          height = unit(current.viewport()$yscale[2], "native")-y[1],
                          xscale = current.viewport()$xscale,
                          yscale = c(y[1], unit(current.viewport()$yscale[2], "native")),
                            just = c("center", "bottom")))
  }
  pred <- ifelse(length(obj$right$prediction) == 1, as.integer(obj$right$prediction > 0.5) + 1
  grid.rect(gp = gpar(fill = "white"))
```

```
  grid.rect(gp = gpar(fill = Colors_trans[pred]))
  if (!is(obj$right, "TerminalNode")) {
    plot_rect(obj$right, xname, depth)
  }
  popViewport()
}
```

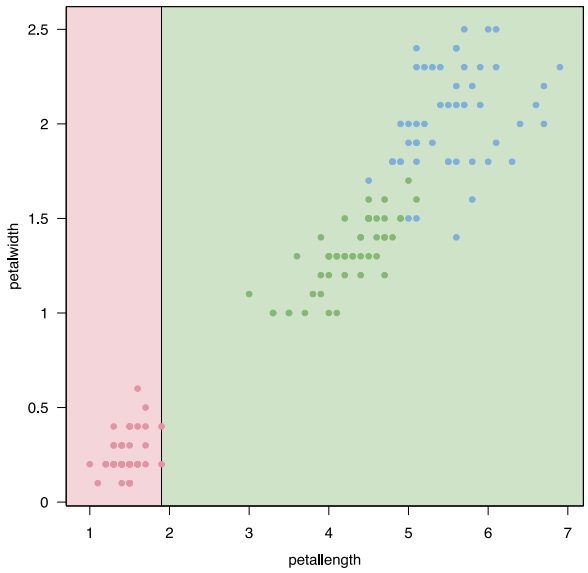
2.1 Can you predict the decision boundaries?

In [38]:
```
library(rpart)
library(party)
tree_iris <- ctree(class ~ ., data = iris)
```

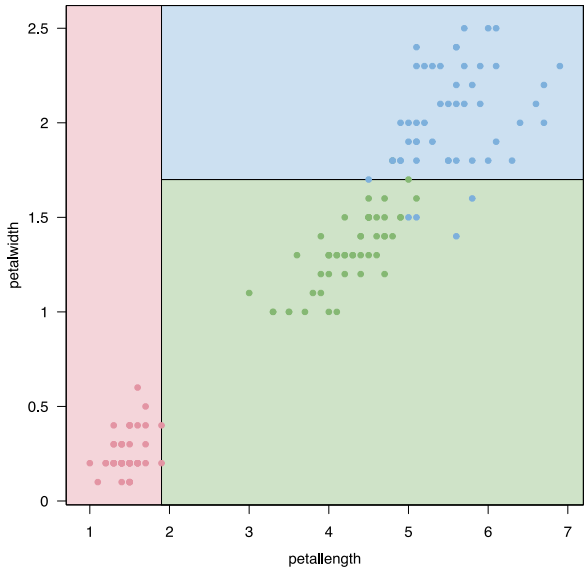
In [39]:
```
with(iris, plot_rectangles(tree_iris, petallength, petalwidth, class, 0))
```



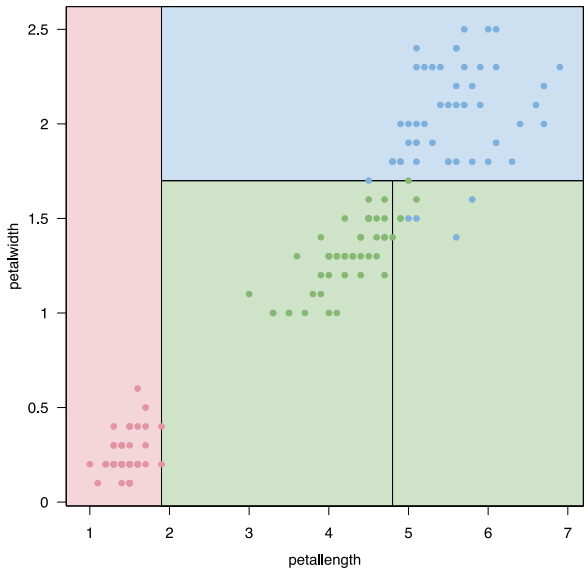
In [40]:
```
with(iris, plot_rectangles(tree_iris, petallength, petalwidth, class, 2))
```




```
In [41]: with(iris, plot_rectangles(tree_iris, petallength, petalwidth, class, 4))
```




```
In [42]: with(iris, plot_rectangles(tree_iris, petallength, petalwidth, class))
```

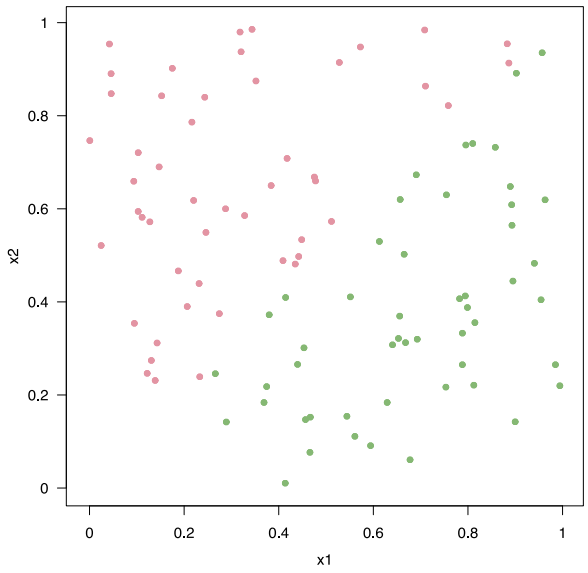


2.2 Representation: limitations

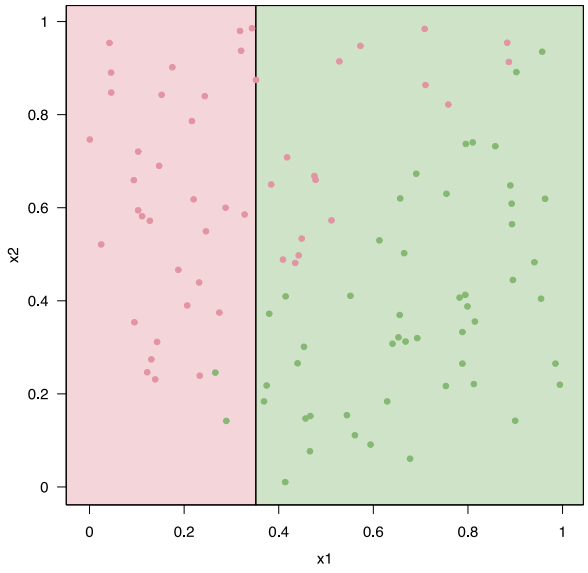
- High instability (variance) of the trees: small changes in data can lead to completely different splits
- Prediction function is not smooth (step function is fitted)
- Cannot learn (only approximate) linear dependencies
  - Still works well in many cases (in high dimensions a good splitting can be found)
- Linear dependencies must be modeled over several splits
  - Simple linear correlations translate into complex trees
- Worst case: parity problem (exponential number of leaves)

```
In [43]: set.seed(123)
         n <- 100
         linear <- data.frame(x1 = runif(n),
                              x2 = runif(n))
         linear$y <- with(linear, as.integer(x1 > x2))
         tree_example <- ctree(y ~ x1 + x2, data = linear)
```

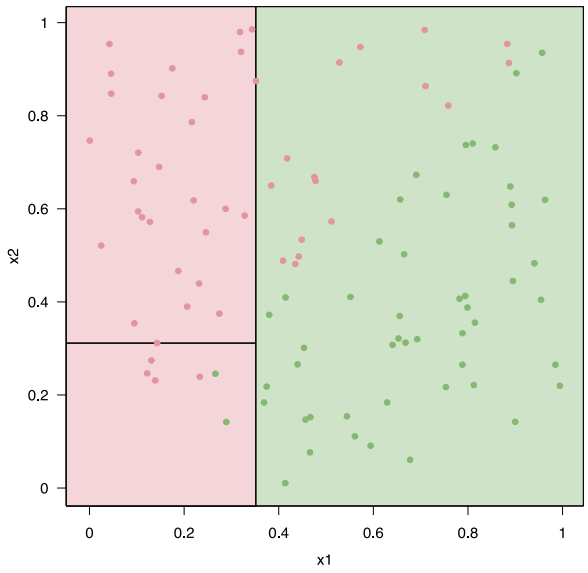
```
In [44]: with(linear, plot_rectangles(tree_example, x1, x2, y + 1, 0))
```



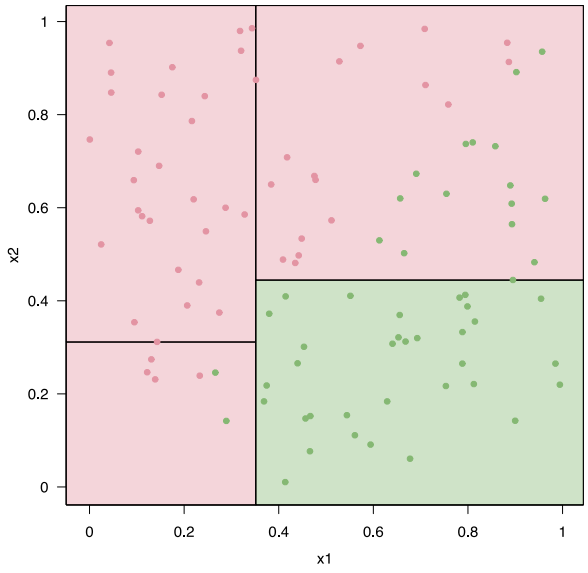

```
In [45]: with(linear, plot_rectangles(tree_example, x1, x2, y + 1, 2))
```



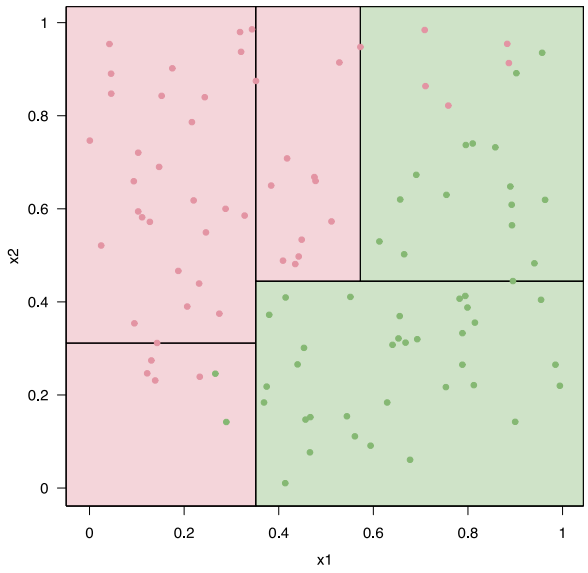

```
In [46]: with(linear, plot_rectangles(tree_example, x1, x2, y + 1, 3))
```



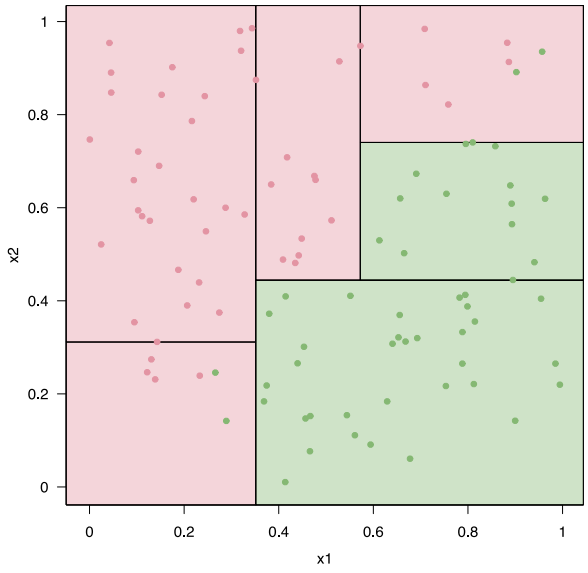

```
In [47]: with(linear, plot_rectangles(tree_example, x1, x2, y + 1, 6))
```




```
In [48]: with(linear, plot_rectangles(tree_example, x1, x2, y + 1, 8))
```




```
In [49]: with(linear, plot_rectangles(tree_example, x1, x2, y + 1, 10))
```



3 Evaluation: which split to choose?

3.1 Classification

For classification ($X_i \rightarrow class_k$): Impurity measures:

- Misclassification Error (leads to larger trees):

$$1 - \underset{k}{\operatorname{argmax}} \hat{p}_k$$

- Gini-Index (probabilistic predictions):

$$\sum_{k \neq k'} \hat{p}_k \hat{p}_{k'} = \sum_{k=1}^{K} \hat{p}_k (1 - \hat{p}_k)$$

with $\hat{p}_k$ = the relative frequency of class k in the leaf node

- Entropy (of the class attribute) measures unpredictability of the data:
  - How likely will random example have class k?

$$E(X) = -\sum_{k=1}^{K} \hat{p}_k \log_2 \hat{p}_k$$

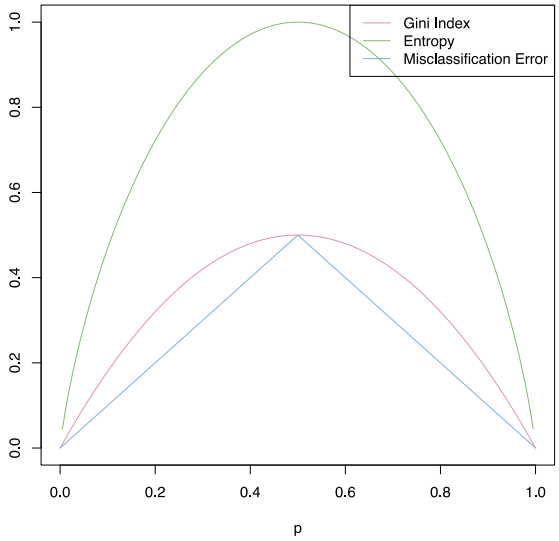
- Information Gain (a.k.a. Kullback–Leibler divergence) for choosing attribute X_i to split the data:

$$G(X, X_i) = E(X) - \sum_{v=1}^{V} \frac{|X_{i=v}|}{|X_i|} E(X_{i=v})$$

with $\hat{p}_k$ = the relative frequency of class k in the leaf node, X = the training set, containing i features (variables) X_i, v a specific value for X_i, $X_{i=v}$ is the set of examples having value v for feature X_i: $\{x \in X | X_i = v\}$

For binary target (K=2):

```
In [50]: p <- seq(0, 1, length.out = 200)
         entropy <- function(p) -((p * log2(p) + (1-p) * log2(1-p)))
         gini <- function(p) 2 * p * (1-p)
         misclassification <- function(p) (1 - max(p, 1-p))
         plot(p, entropy(p), type = "l", col = Colors[2], ylab = "", ylim = c(0, 1))
         lines(p, gini(p), col = Colors[1])
         lines(p, sapply(p, misclassification), col = Colors[3])
         legend("topright", c("Gini Index", "Entropy", "Misclassification Error"),
                col = Colors[1:3], lty = 1)
```



3.1.1 Example

Ex.	1	2	3	4	5	6
a1	T	T	T	F	F	F
a2	T	T	F	F	T	T
class	+	+	-	+	-	-

$E(X)$?
$G(X, X_{a2})$?
$G(X, X_{a1})$?
$E(X) = -(\frac{1}{2} * log_2(\frac{1}{2}) + \frac{1}{2} * log_2(\frac{1}{2})) = 1$ (classes have equal probabilities)
$G(X, X_{a2}) = 0$ (after split, classes still have equal probabilities, entropy stays 1)

Ex.	1	2	3	4	5	6
a1	T	T	T	F	F	F
a2	T	T	F	F	T	T
class	+	+	-	+	-	-

$$E(X) = -\sum_{k=1}^{K} \hat{p}_k \log \hat{p}_k \quad , \quad G(X, X_i) = E(X) - \sum_{v=1}^{V} \frac{|X_{i=v}|}{|X_i|} E(X_{i=v})$$

$$E(X_{a1=T}) = -\frac{2}{3}\log_2(\frac{2}{3}) - \frac{1}{3}\log_2(\frac{1}{3}) = 0.9183 \quad (= E(X_{a1=F}))$$

$$G(X, X_{a1}) = 1 - \frac{1}{2}0.9183 - \frac{1}{2}0.9183 = 0.0817$$

hence we split on a1

3.2 Regression

For regression ($x_i \rightarrow y_i \in \mathbb{R}$): Minimal quadratic distance

Dividing the data on split variable X_j at splitpoint s leads to the following half-spaces:

$$R_1(j, s) = X : X_j \leq s \quad and \quad R_2(j, s) = X : X_j > s$$

The best split variable and the corresponding splitpoint, with predicted value c_i and actual value Y_i:

$$\min_{j,s} \left(\min_{c_1} \sum_{x_i \in R_1(j,s)} (y_i - c_1)^2 + \min_{c_2} \sum_{x_i \in R_2(j,s)} (y_i - c_2)^2 \right)$$

Assuming that the tree predicts y_i as the average of all x_i in the leaf:

$$\hat{c}_1 = \text{avg}(y_i | x_i \in R_1(j, s)) \quad and \quad \hat{c}_2 = \text{avg}(y_i | x_i \in R_2(j, s))$$

with x_i being the i-th example in the data, with target value y_i

4 Optimization: how to grow the tree?

- Constructive search algorithm (like LEGO's): Start with one piece, add more pieces to build complex structure
- Greedy algorithm: Pick best features and splitpoint, from all features and all possible splitpoints

Options (depends on implementation): - Binary splits of multi-way splits - Criteria for the selection of a variable and its splitpoint(s) - Handling missing value - Stopping Criteria - Pruning (trimming leaves)

4.1 Binary or Multi-way splits

- Binary splits (e.g. CART algorithm)
  - No need to mind the penalization of multi-way splits when choosing the split criteria
  - Interpretability of the tree might suffer: multiple splits of the same variable in different levels

4.2 Selection of variable and splitpoints

- Choice of evaluation function (Information gain, Gini-index,...)
- Which splits to consider (for numeric features)?
  - Only split between data points of different classes
  - Split at the point, or halfway between points of different classes

4.3 Handling missing values

Strategies:

- Treat 'missing' as its own (new) catergory
- Missing value imputation (e.g. matrix decomposition)
- When considering feature for a split, ignore data points with missing value
  - To pass examples down the tree (while learning or predicting), find surrogate feature producing similar splits

4.4 Handling many-valued features

What happens when a feature has (almost) as many values as examples? - Information Gain will select it
One approach: use Gain Ratio instead:

$$GainRatio(X, X_i) = \frac{Gain(X, X_i)}{SplitInfo(X, X_i)}$$

$$SplitInfo(X, X_i) = -\sum_{v=1}^{V} \frac{|X_{i=v}|}{|X|} log_2 \frac{|X_{i=v}|}{|X|}$$

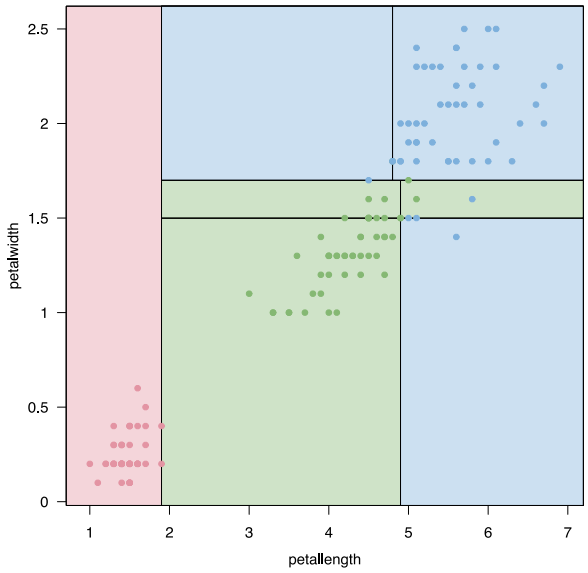
where $X_{i=v}$ is the subset of examples for which feature X_i has value v.
SplitInfo will be big if X_i fragments the data into many small subsets, resulting in a smaller Gain Ratio.

4.5 Avoiding overfitting

Complexity (and chance of overfitting) increase with size of the tree

- Controlled by regularization hyperparameters
  - Stopping criteria
  - Pruning

```
In [51]: tree_iris <- ctree(class ~ ., data = iris, controls = ctree_control(mincriterion = 0, minsplit
         with(iris, plot_rectangles(tree_iris, petallength, petalwidth, class))
```



4.6 Stopping criteria

Choose:

- A minimal number of examples for node before splitting
- A minimal number of examples that must be in each leaf
- A minimal increase in goodness of fit that must be reached before splitting (confidence)
- A maximum depth (number of levels) in the tree

4.7 Pruning

- Pruning optimizes trade-off between goodness of fit and complexity by cutting leaves
- Different strategies. Can you think of one?

4.7.1 Reduced error pruning

- Post-pruning, simple and fast
- Split (training) data into training and validation set
- Starting at leaves, prune: replace each node with most popular class
- Greedily remove the one that most improves performance on validation set

4.7.2 Cost Complexity Pruning

Cost function R_α = training error + complexity term

$$R_\alpha = R(T) + \alpha \cdot \#\text{leaves}$$

where $R(T)$ represents the error of tree T on the training set

- Generates series of trees

- For every α there is a distinctly defined smallest sub-tree of the original tree, which minimizes the cost function
- $\hat{\alpha}$ can be assessed with cross-validation
- Final tree is fitted on the whole data, where $\hat{\alpha}$ is used to find the optimal size of the tree

4.8 Questions?

4.9 Acknowledgements

Thanks to Bernd Bischl for help with many of the code examples.