# ELEN 4720: Machine Learning for Signals, Information and Data

## Lecture 12

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# Decision Trees

# Decision Trees

A *decision tree* maps input $x \in \mathbb{R}^d$ to output $y$ using binary decision rules:

- Each node in the tree has a *splitting rule*.
- Each leaf node is associated with an output value (outputs can repeat).

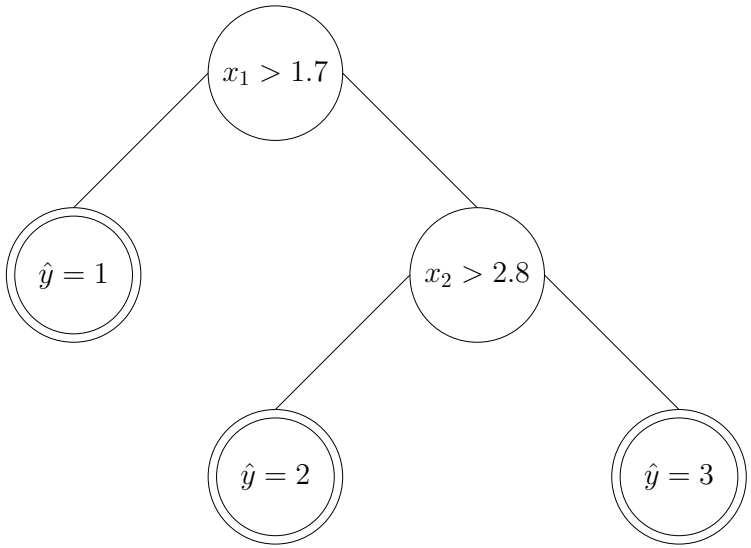
Each splitting rule is of the form

$$h(x) = \mathbb{1}\{x_j > t\}$$

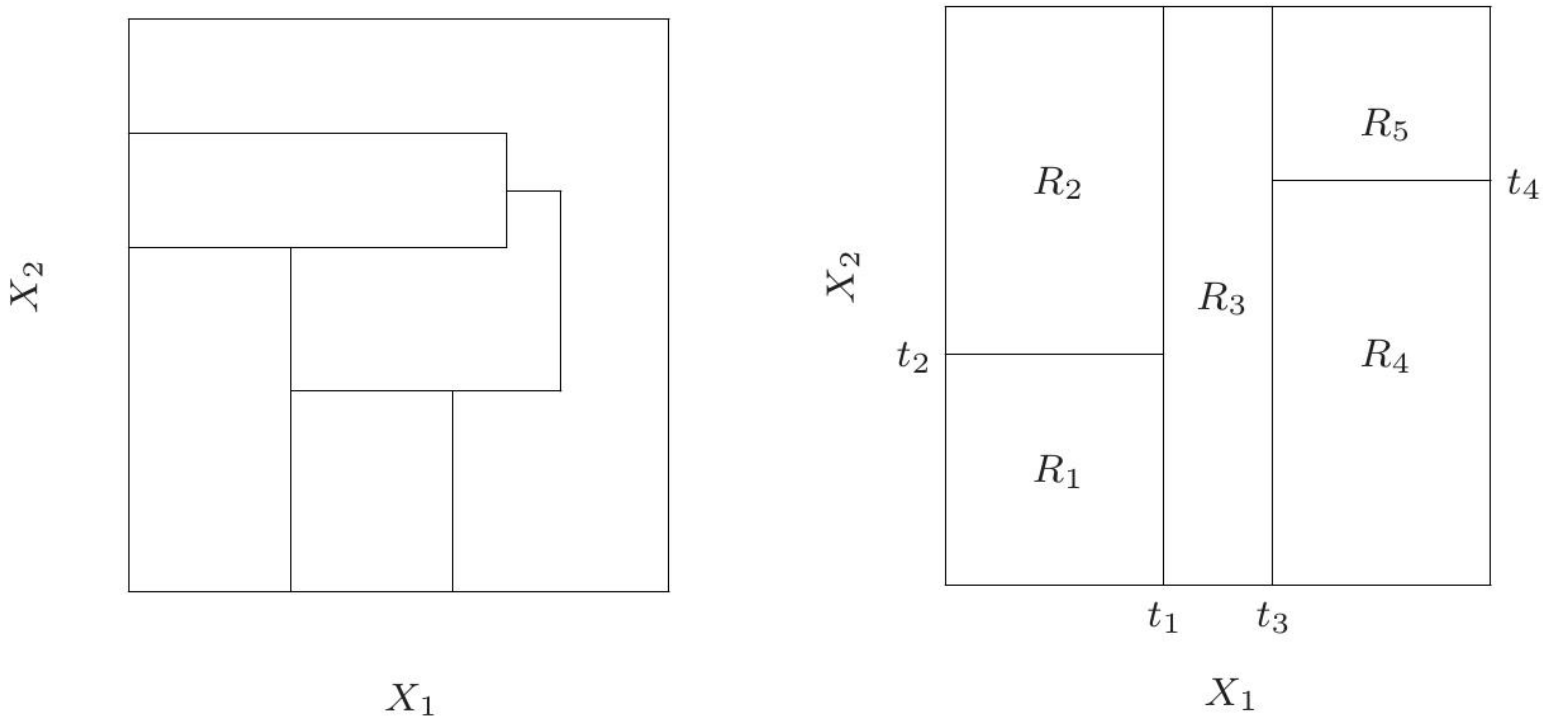
for some dimension $j$ of $x$ and $t \in \mathbb{R}$.

Using these transition rules, a path to a *leaf node* gives the prediction.

(One-level tree = *decision stump*)



# Regression Trees

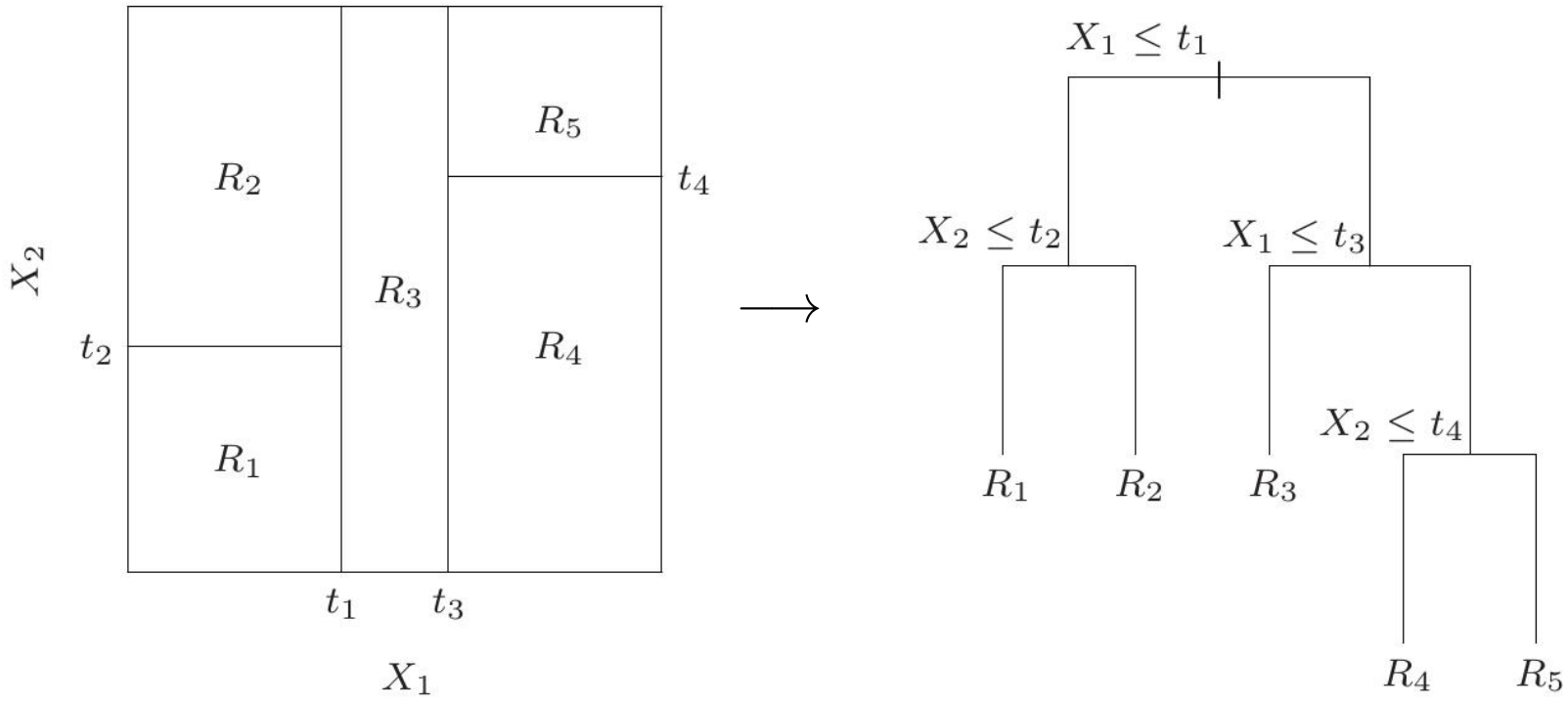



**Motivation**: Partition the space so that data in a region have same prediction

Left: Difficult to define a "rule".

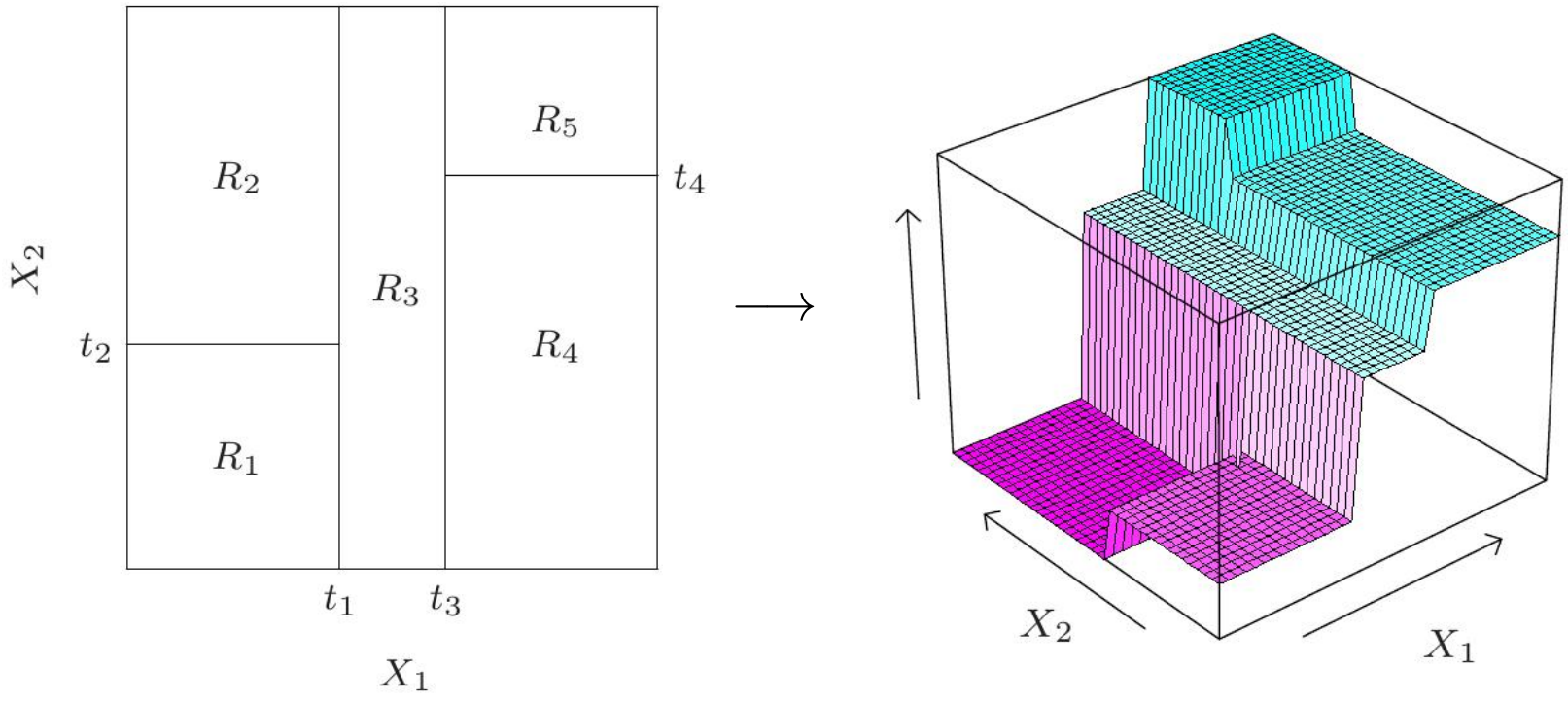
Right: Easy to define a recursive splitting rule.

# Regression Trees



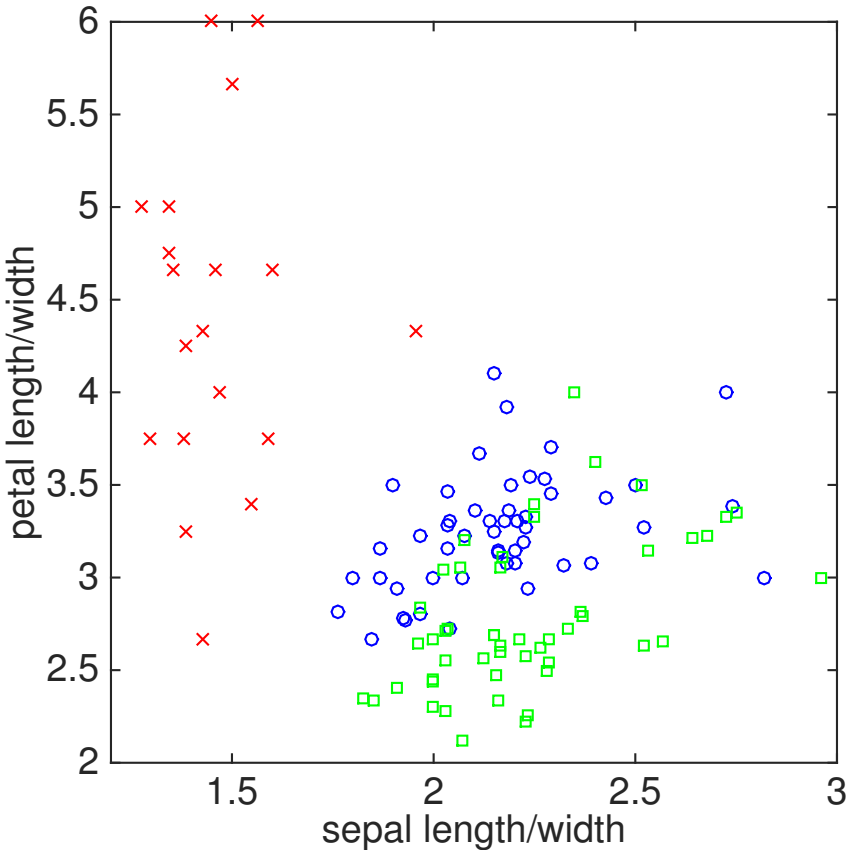

If we think in terms of trees, we can define a simple rule for partitioning the space. The left and right figures represent the same regression function.

# Regression Trees




Adding an output dimension to the figure (right), we can see how regression trees can learn a step function approximation to the data.

# Classification Trees (Example)




Classifying irises using sepal and petal measurements:

- $x \in \mathbb{R}^2, y \in \{1, 2, 3\}$
- $x_1 =$ ratio of sepal length to width
- $x_2 =$ ratio of petal length to width

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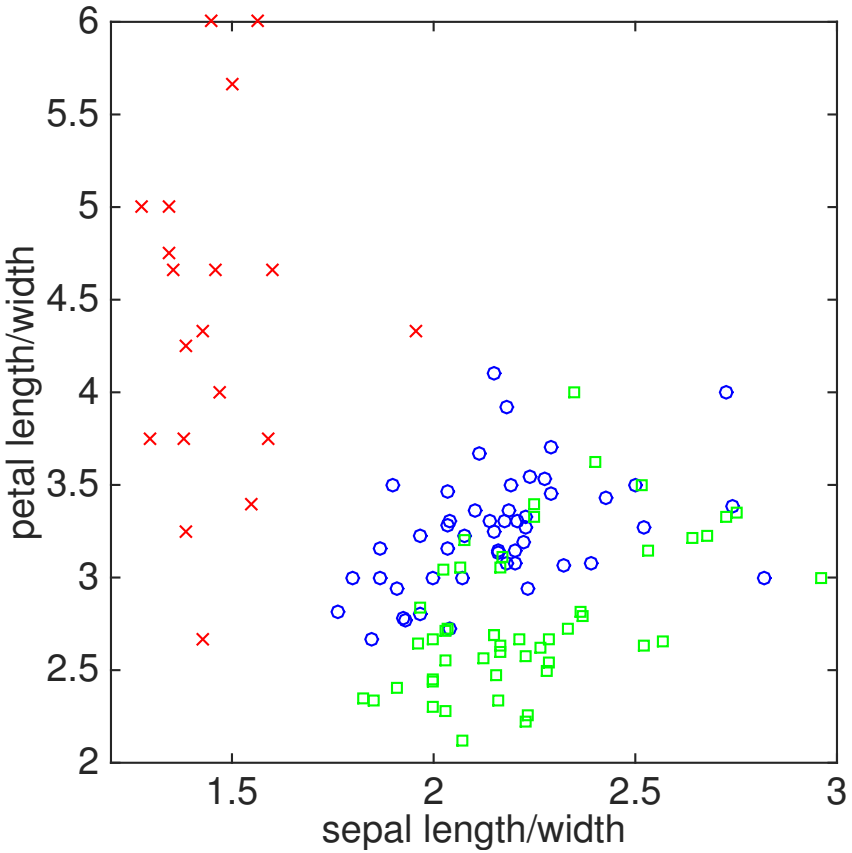


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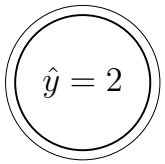

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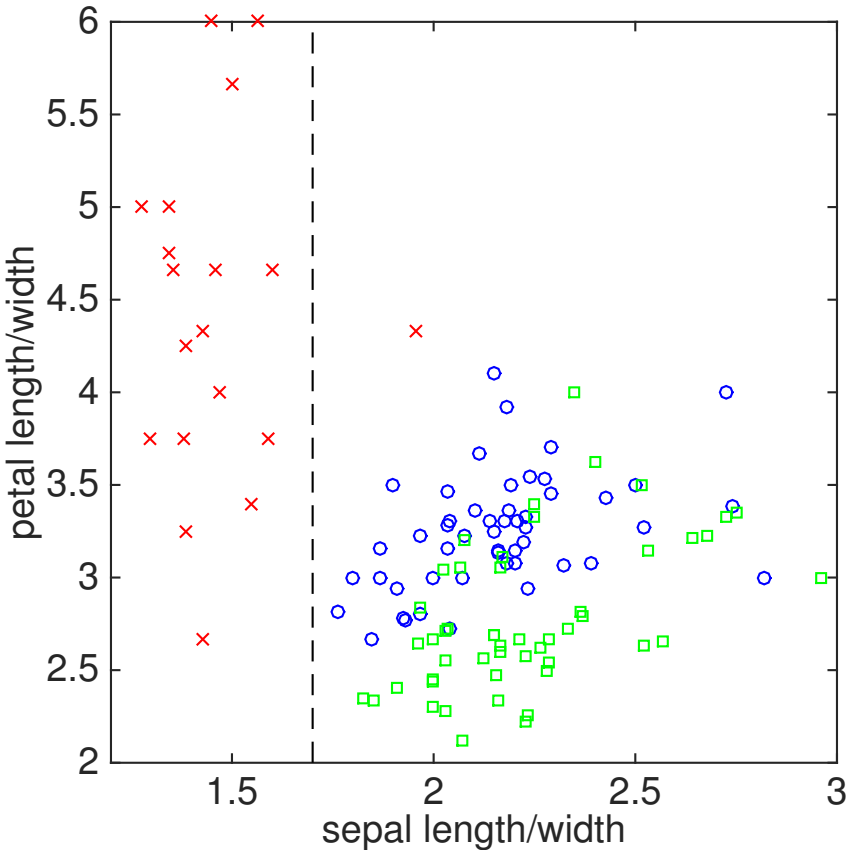


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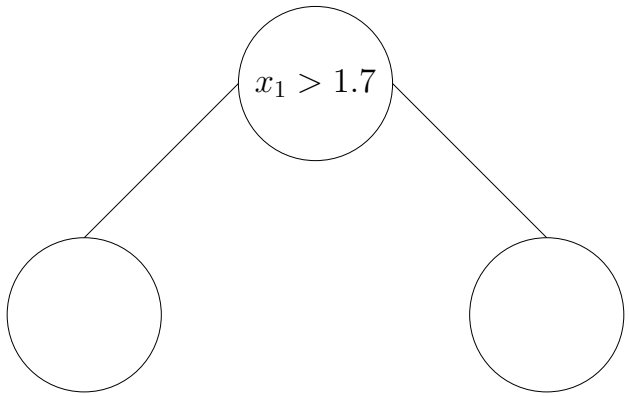

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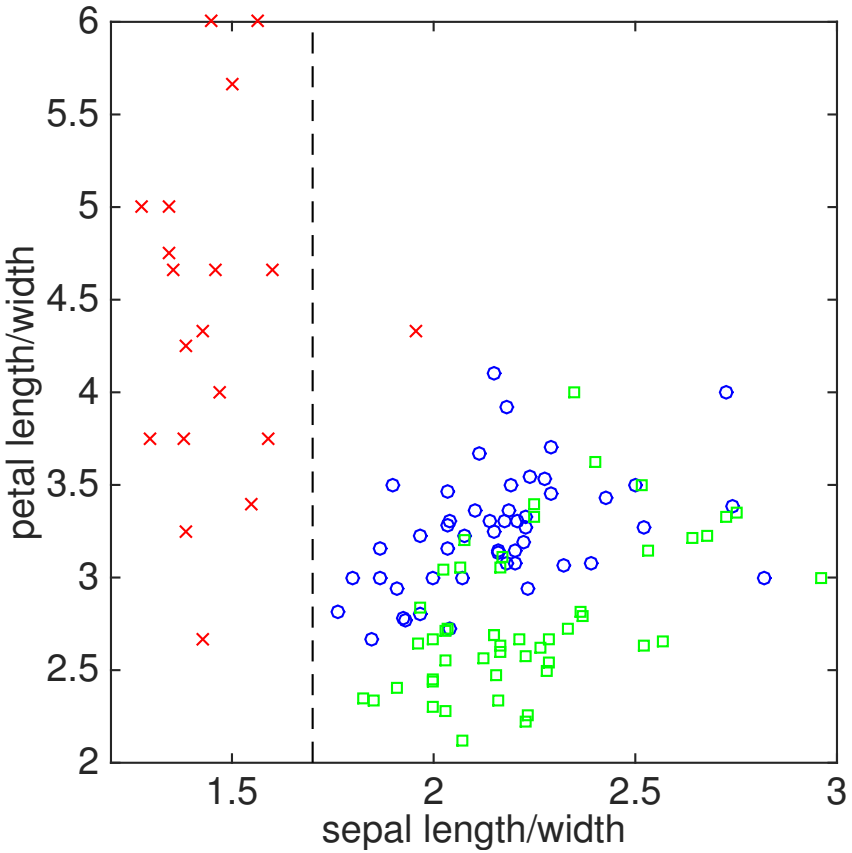


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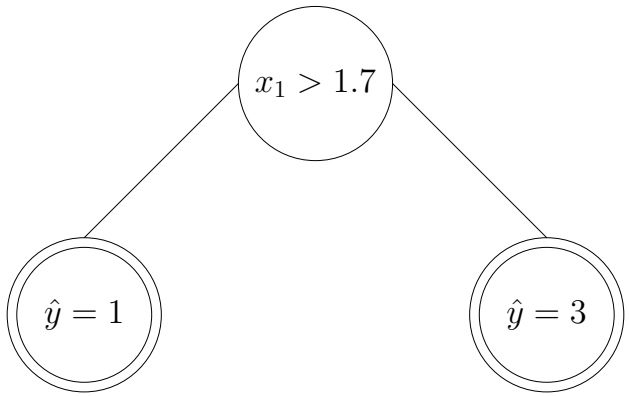

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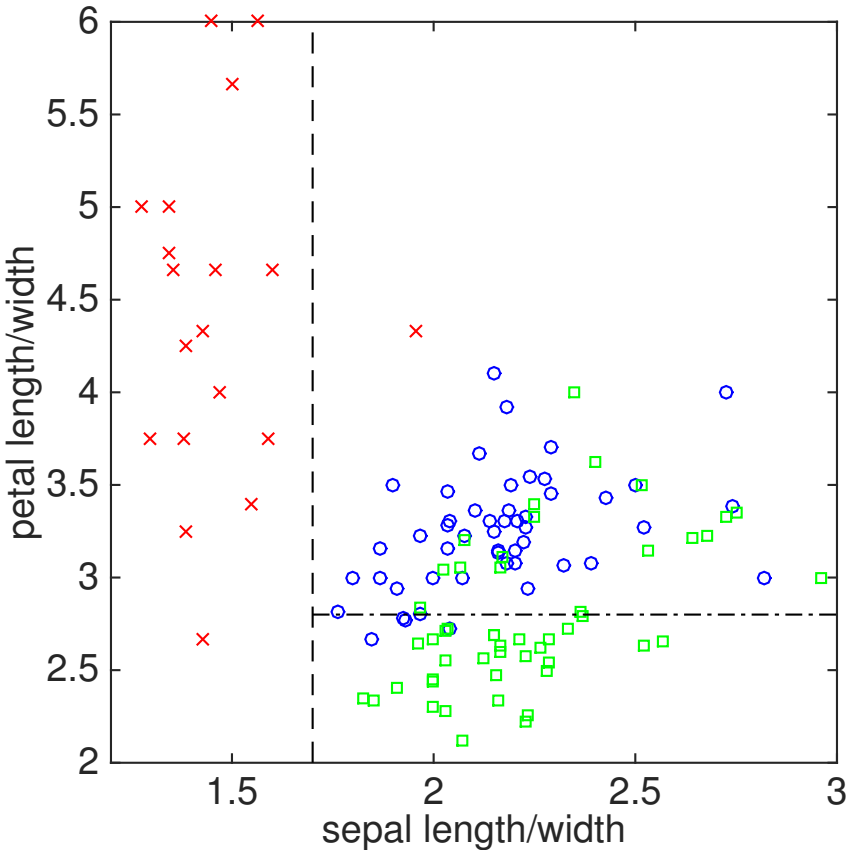


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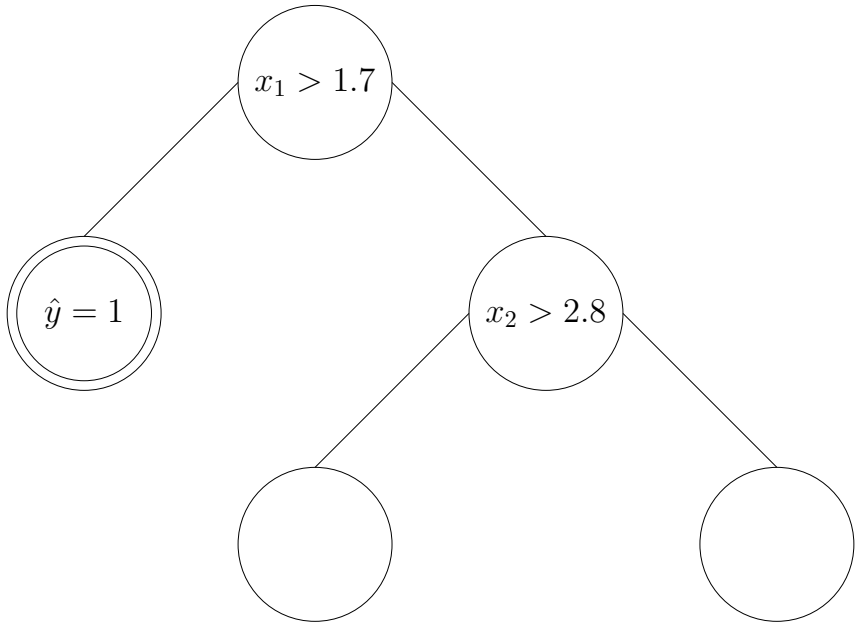

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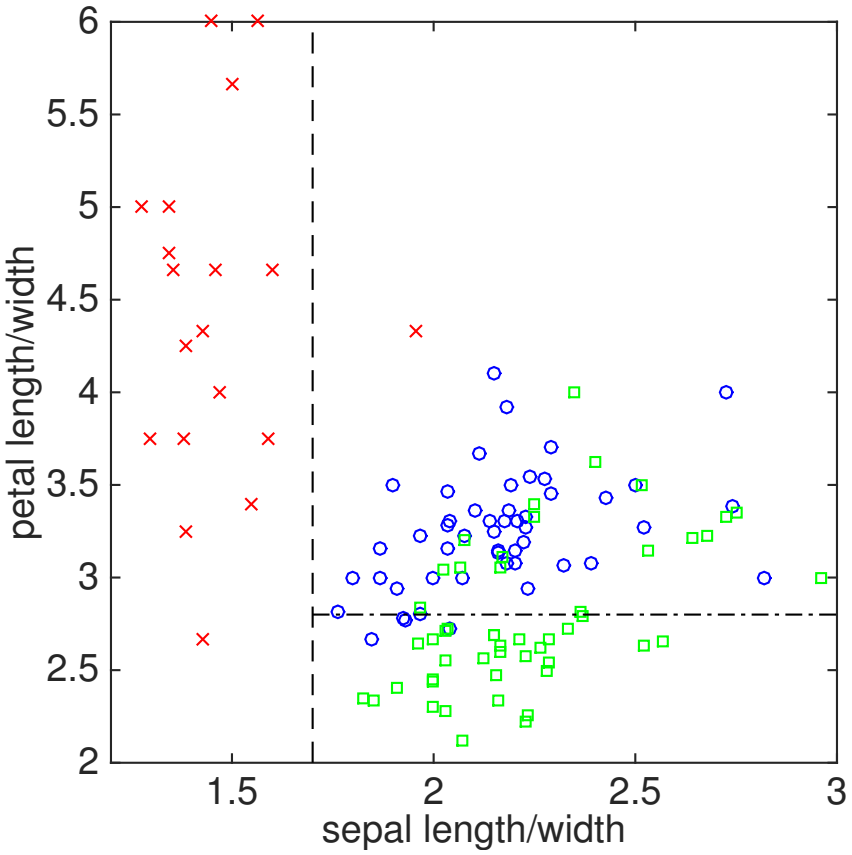


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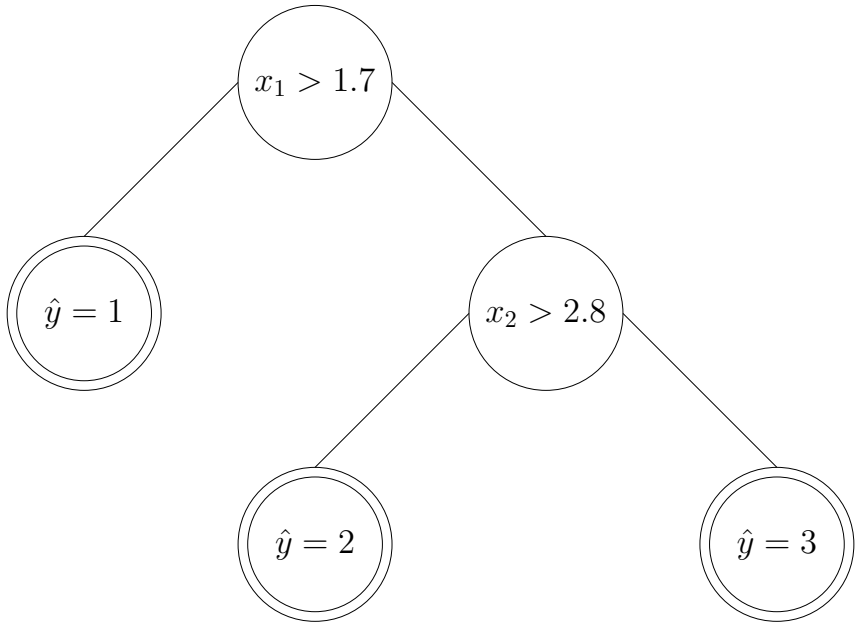
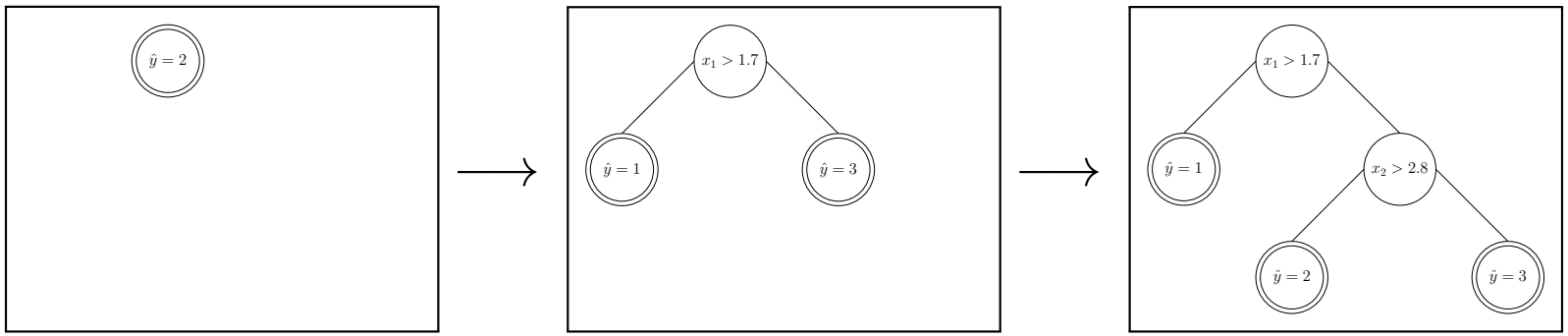


# BASIC DECISION TREE LEARNING ALGORITHM




The basic method for learning trees is with a top-down greedy algorithm.

- Start with a single leaf node containing all data
- Loop through the following steps:
  - Pick the leaf to split that reduces uncertainty the most.
  - Figure out the $\lessgtr$ decision rule on one of the dimensions.
- Stopping rule discussed later.

Label/response of the leaf is majority-vote/average of data assigned to it.

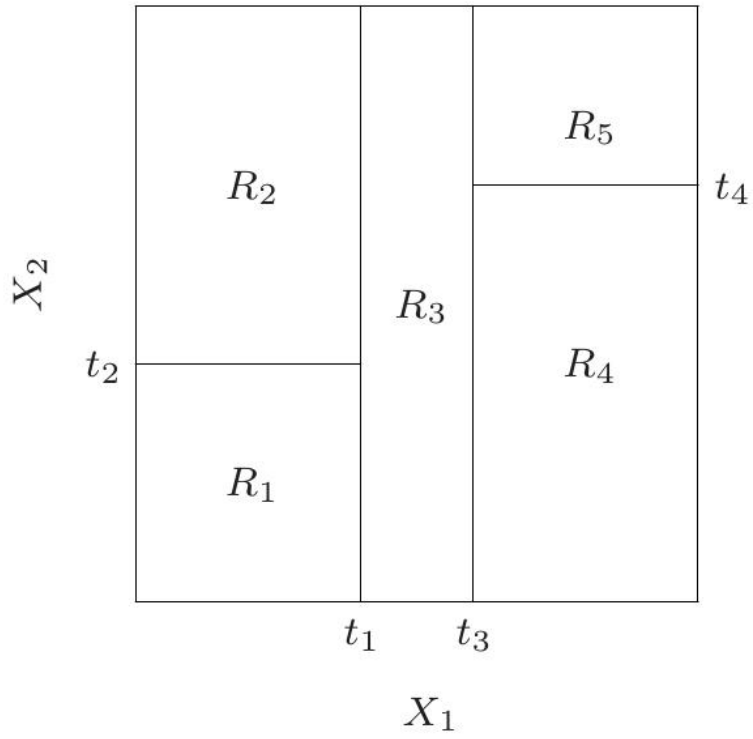
# GROWING A REGRESSION TREE

How do we grow a regression tree?

- For $M$ regions of the space, $R_1, \ldots, R_M$, the prediction function is

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

So for a fixed $M$, we need $R_m$ and $c_m$.




Goal: Try to minimize $\sum_i (y_i - f(x_i))^2$.

1. Find $c_m$ given $R_m$: Simply the average of all $y_i$ for which $x_i \in R_m$.
2. How do we find regions? Consider splitting region $R$ at value $s$ of dim $j$:
   - Define $R^-(j,s) = \{x_i \in R | x_i(j) \leq s\}$ and $R^+(j,s) = \{x_i \in R | x_i(j) > s\}$
   - For each dimension $j$, calculate the best splitting point $s$ for that dimension.
   - Do this for each region (leaf node). Pick the one that reduces the objective most.

# GROWING A CLASSIFICATION TREE

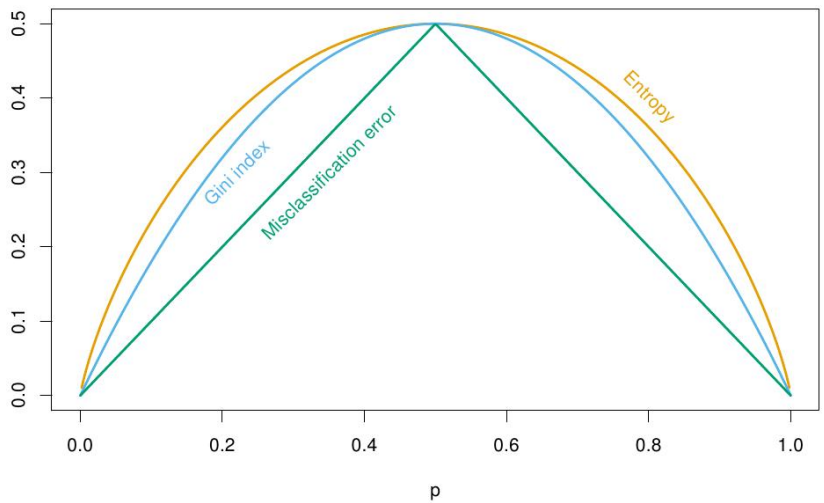
**For regression**: Squared error is a natural way to define the splitting rule.

**For classification**: Need some measure of how badly a region classifies data and how much it can improve if it's split.

**K-class problem**: For all $x \in R_m$, let $p_k$ be empirical fraction labeled $k$.

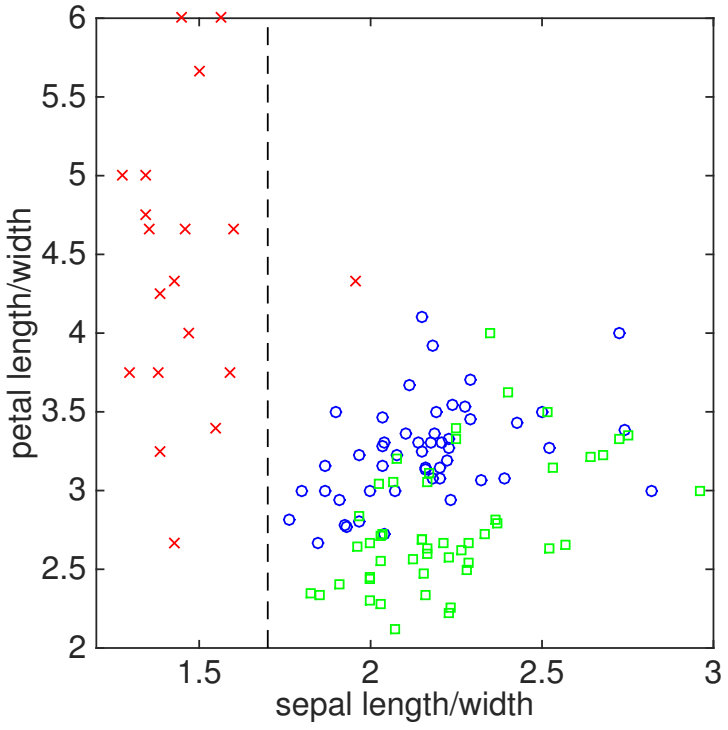
Measures of quality of $R_m$ include

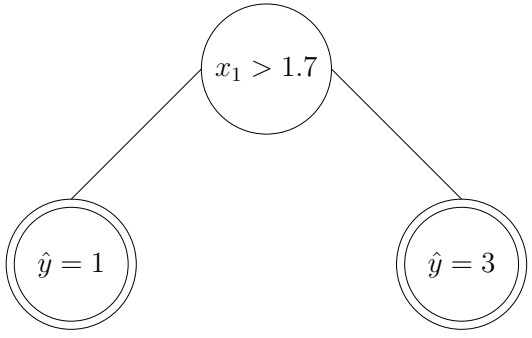
1. Classification error: $1 - \max_k p_k$
2. Gini index: $1 - \sum_k p_k^2$
3. Entropy: $-\sum_k p_k \ln p_k$




- These are all *maximized* when $p_k$ is uniform on the $K$ classes in $R_m$.
- These are *minimized* when $p_k = 1$ for some $k$ ($R_m$ only contains one class)

# GROWING A CLASSIFICATION TREE




Search $R_1$ and $R_2$ for splitting options.

1. $R_1$: $y = 1$ leaf classifies perfectly
2. $R_2$: $y = 3$ leaf has Gini index

$$u(R_2) = 1 - \left(\frac{1}{101}\right)^2 - \left(\frac{50}{101}\right)^2 - \left(\frac{50}{101}\right)^2$$
$$= 0.5098$$

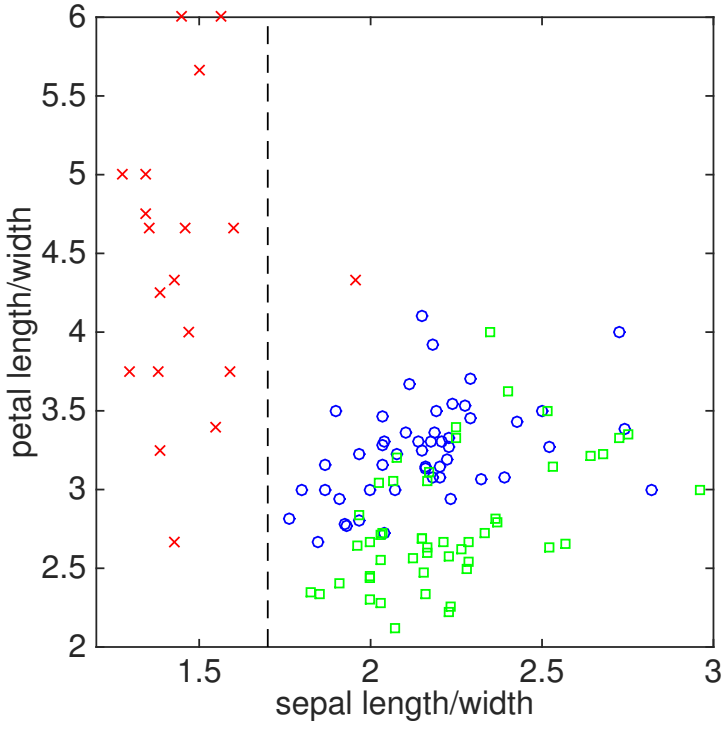
Gini improvement from split $R_2$ to $R_2^-$ & $R_2^+$ at point $t$ in dimension $j$ (not written):

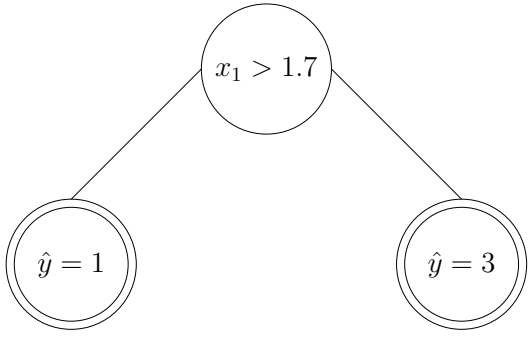
$$u(R_2) - \left(p_{R_2^-} \cdot u(R_2^-) + p_{R_2^+} \cdot u(R_2^+)\right)$$

$p_{R_m^+}$ : Fraction of data in $R_2$ split into $R_2^+$.

$u(R_2^+)$ : New quality measure in region $R_2^+$.

# GROWING A CLASSIFICATION TREE

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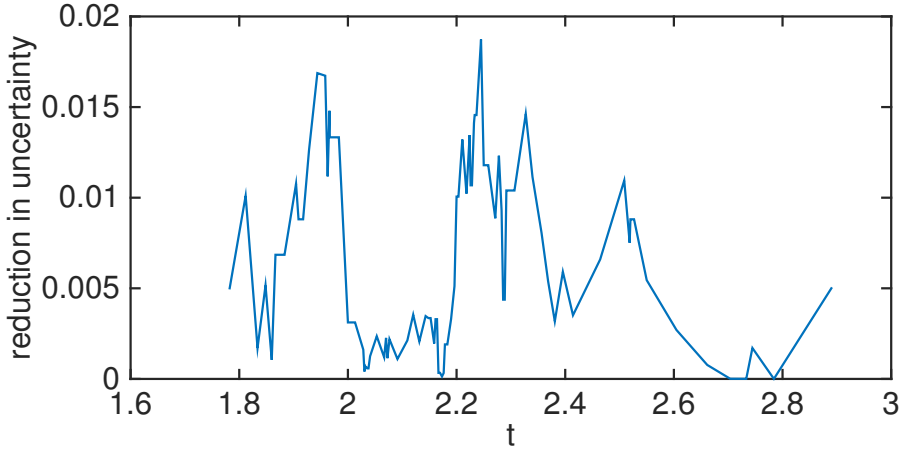
Check split $R_2$ with $\mathbb{1}\{x_1 > t\}$



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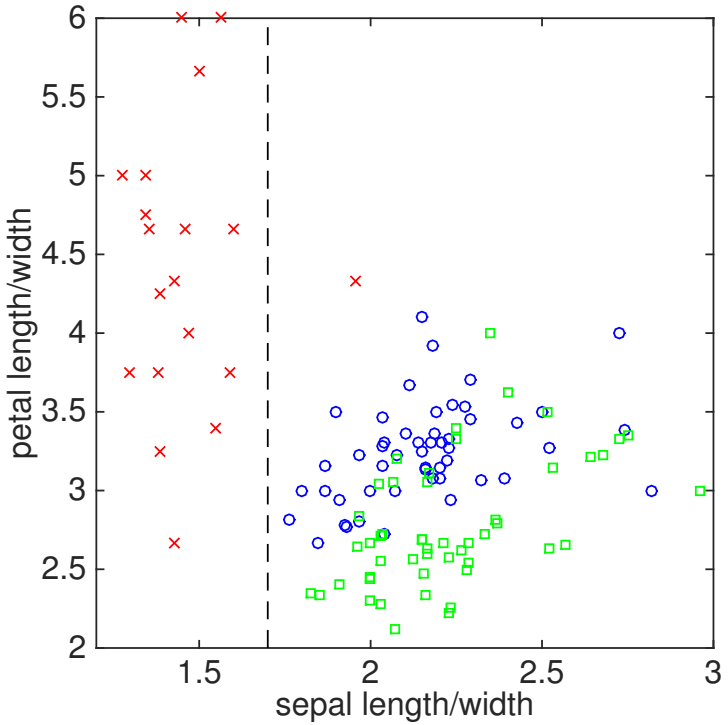


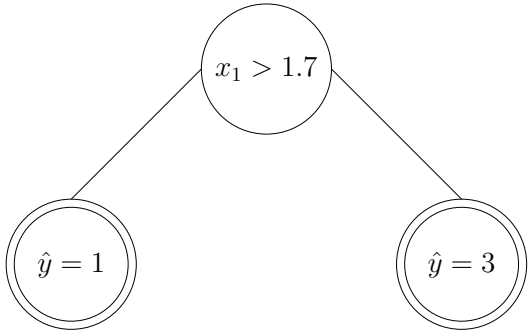


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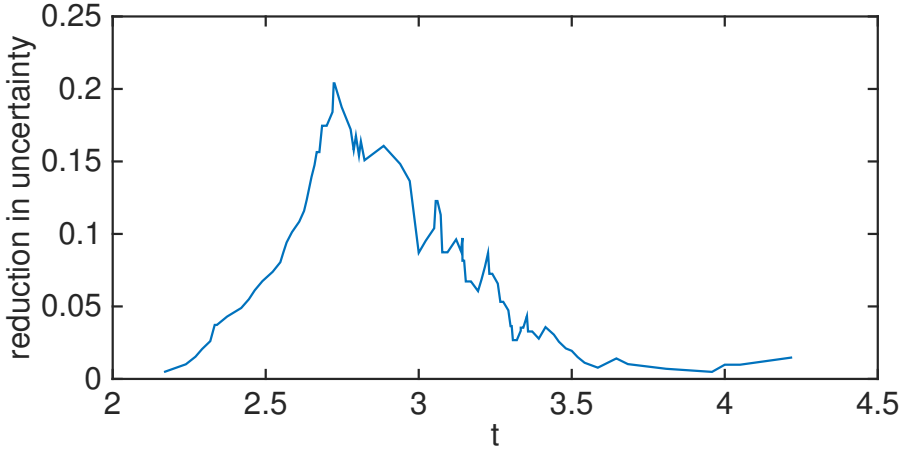

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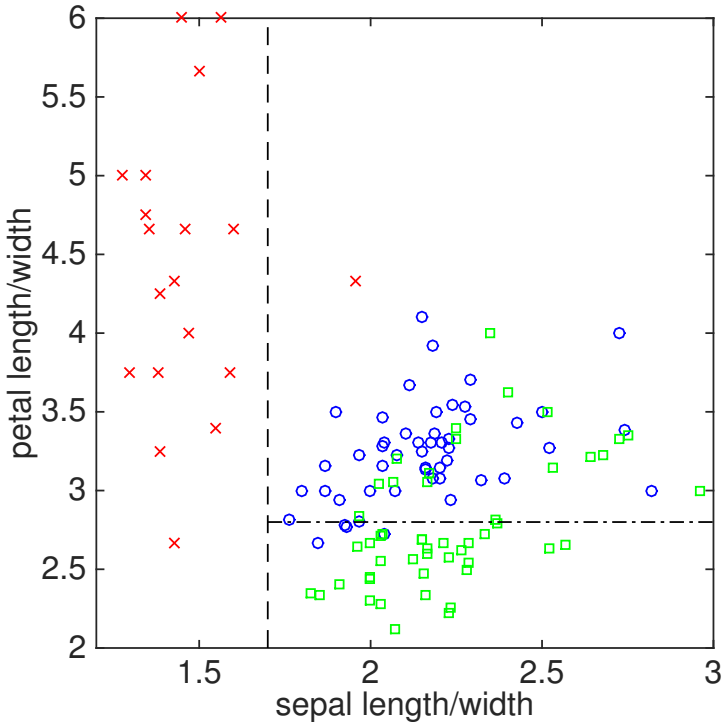


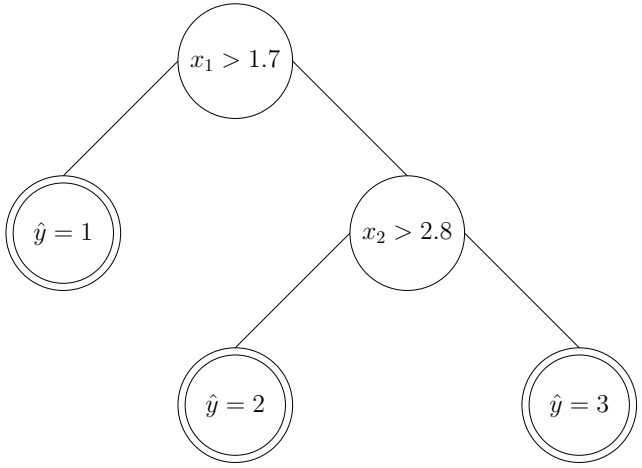


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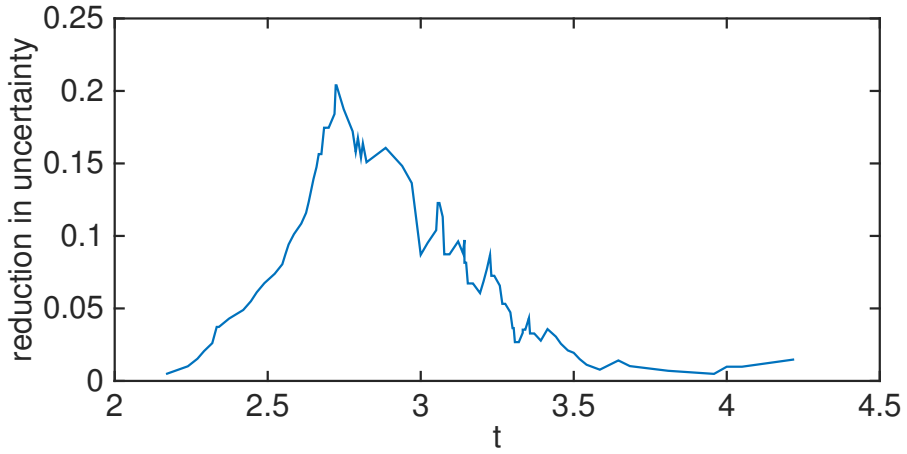


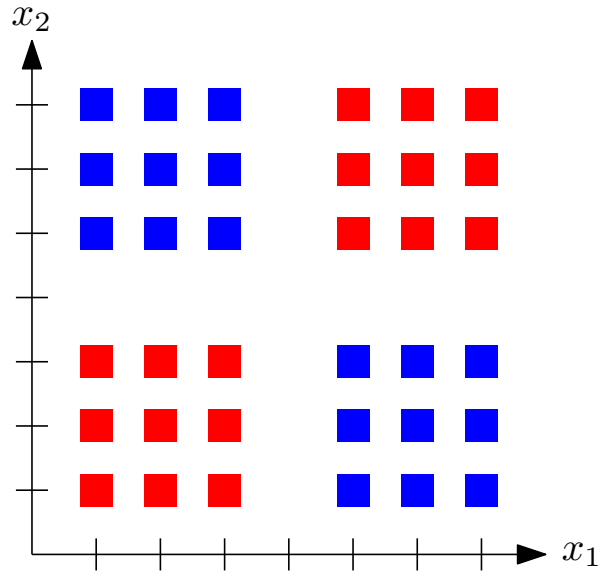
# PRUNING A TREE

**Q**: When should we stop growing a tree?

**A**: Uncertainty reduction is not best way.

**Example**: Any split of $x_1$ or $x_2$ at right will show *zero* reduction in uncertainty.

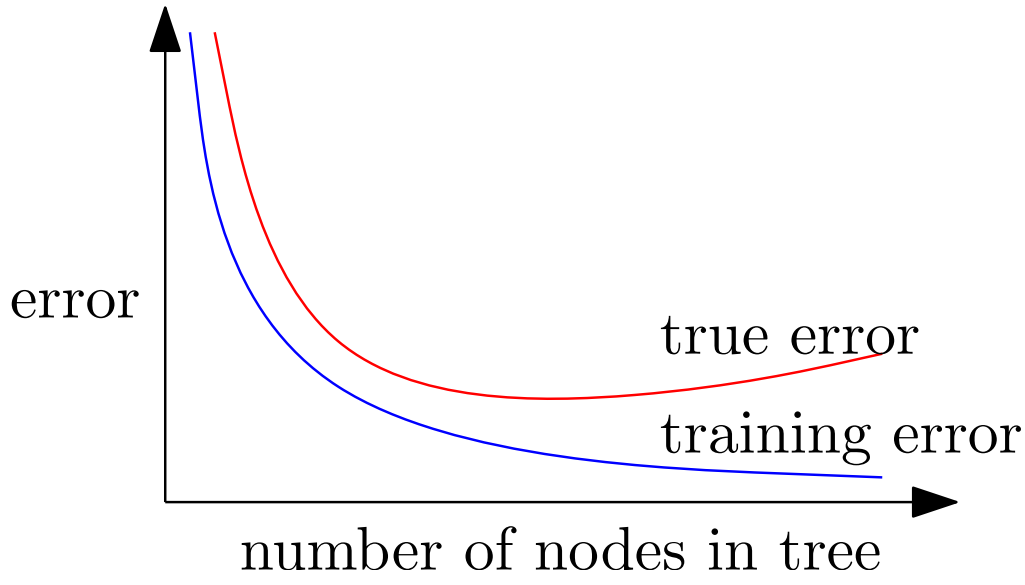
However, we can learn a perfect tree on this data by partitioning in quadrants.




*Pruning* is the method most often used. Grow the tree to a very large size. Then use an algorithm to trim it back.

(We won't cover the algorithm, but mention that it's non-trivial.)

# OVERFITTING




- *Training error* goes to zero as size of tree increases.
- *Testing error* decreases, but then increases because of *overfitting*.

# THE BOOTSTRAP

# The Bootstrap: A Resampling Technique

We briefly present a technique called the *bootstrap*. This statistical technique is used as the basis for learning *ensemble classifiers*.

## Bootstrap

*Bootstrap* (i.e., resampling) is a technique for improving estimators.

> Resampling = Sampling from the empirical distribution of the data

## Application to ensemble methods

- We will use resampling to generate many "mediocre" classifiers.
- We then discuss how "bagging" these classifiers improves performance.
- First, we cover the bootstrap in a simpler context.

# Bootstrap: Basic algorithm

## Input

- A sample of data $x_1, \ldots, x_n$.
- An estimation rule $\hat{S}$ of a statistic $S$. For example, $\hat{S} = \text{med}(x_{1:n})$ estimates the true median $S$ of the unknown distribution on $x$.

## Bootstrap algorithm

1. Generate *bootstrap samples* $\mathcal{B}_1, \ldots, \mathcal{B}_T$.
   - Create $\mathcal{B}_t$ by picking points from $\{x_1, \ldots, x_n\}$ randomly $n$ times.
   - A particular $x_i$ can appear in $\mathcal{B}_t$ many times (it's simply duplicated).
2. Evaluate the estimator on each $\mathcal{B}_t$ by pretending it's the data set:

$$\hat{S}_t := \hat{S}(\mathcal{B}_t)$$

3. Estimate the mean and variance of $\hat{S}$:

$$\mu_B = \frac{1}{T}\sum_{t=1}^{T} \hat{S}_t, \quad \sigma_B^2 = \frac{1}{T}\sum_{t=1}^{T} (\hat{S}_t - \mu_B)^2$$

# EXAMPLE: VARIANCE ESTIMATION OF THE MEDIAN

- The median of $x_1, \ldots, x_n$ (for $x \in \mathbb{R}$) is found by simply sorting them and taking the middle one, or the average of the two middle ones.

- How confident can we be in the estimate median$(x_1, \ldots, x_n)$?
  - Find it's variance.
  - But how? Answer: By bootstrapping the data.

1. Generate bootstrap data sets $\mathcal{B}_1, \ldots, \mathcal{B}_T$.

2. Calculate: (notice that $\hat{S}_{mean}$ is the mean of the sampled medians)

$$\hat{S}_{mean} = \frac{1}{T}\sum_{t=1}^{T} \text{median}(\mathcal{B}_t), \quad \hat{S}_{var} = \frac{1}{T}\sum_{t=1}^{T} \left(\text{median}(\mathcal{B}_t) - \hat{S}_{mean}\right)^2$$

- The procedure is remarkably simple, but has a lot of theory behind it.

# Bagging and Random Forests

# Bagging

Bagging uses the bootstrap for regression or classification:

$$\textbf{Bagging} \;=\; \textbf{B}\text{ootstrap } \textbf{agg}\text{regation}$$

## Algorithm

For $t = 1, \ldots, T$:

1. Draw a bootstrap sample $\mathcal{B}_t$ of size $n$ from training data.
2. Train a classifier or regression model $f_t$ on $\mathcal{B}_t$.

- For a new point $x_0$, compute:

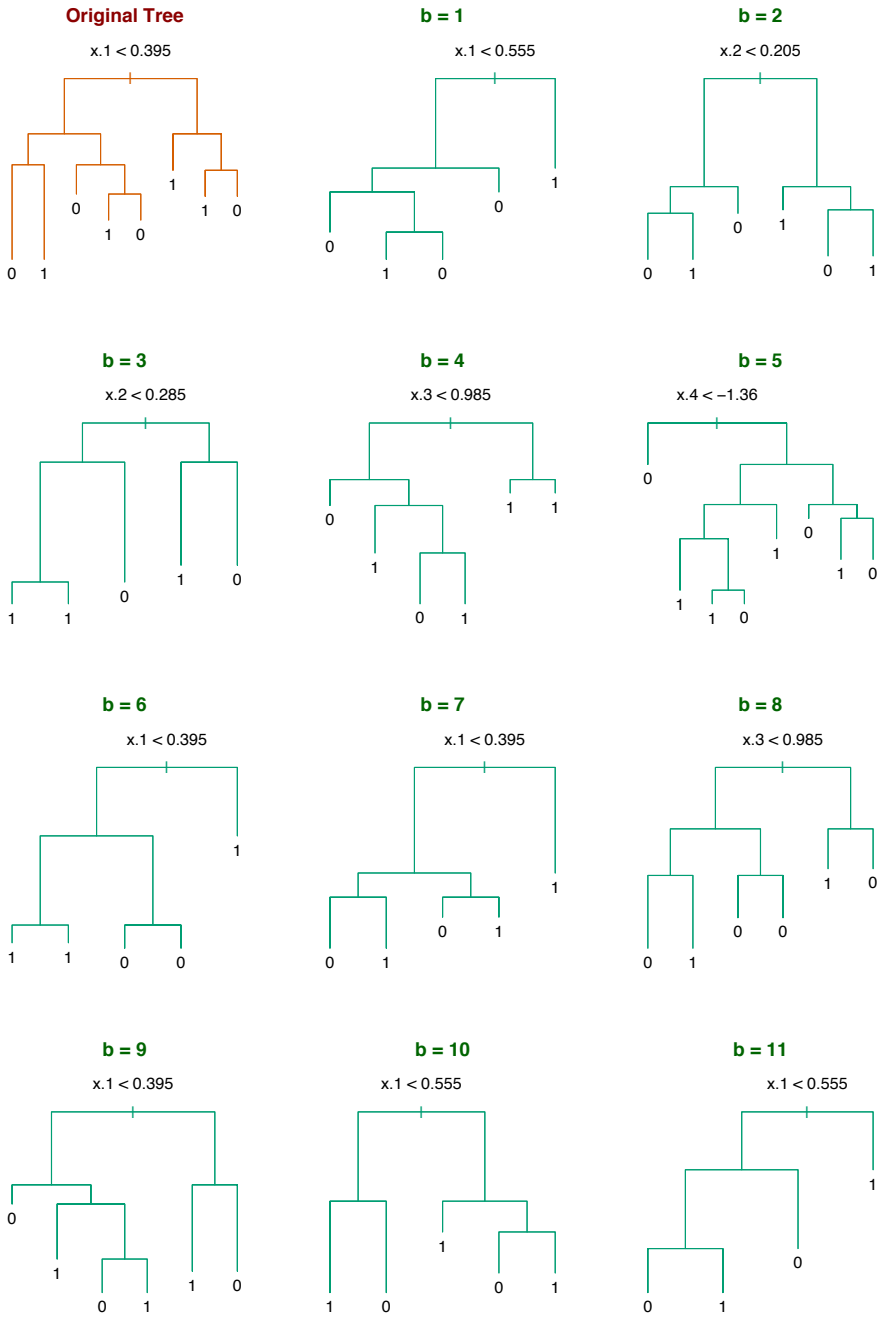
$$f_{\text{avg}}(x_0) = \frac{1}{T}\sum_{t=1}^{T} f_t(x_0)$$

  - For regression, $f_{\text{avg}}(x_0)$ is the prediction.
  - For classification, view $f_{\text{avg}}(x_0)$ as the distribution of $T$ votes. Pick the majority.

# Example: Bagging Trees

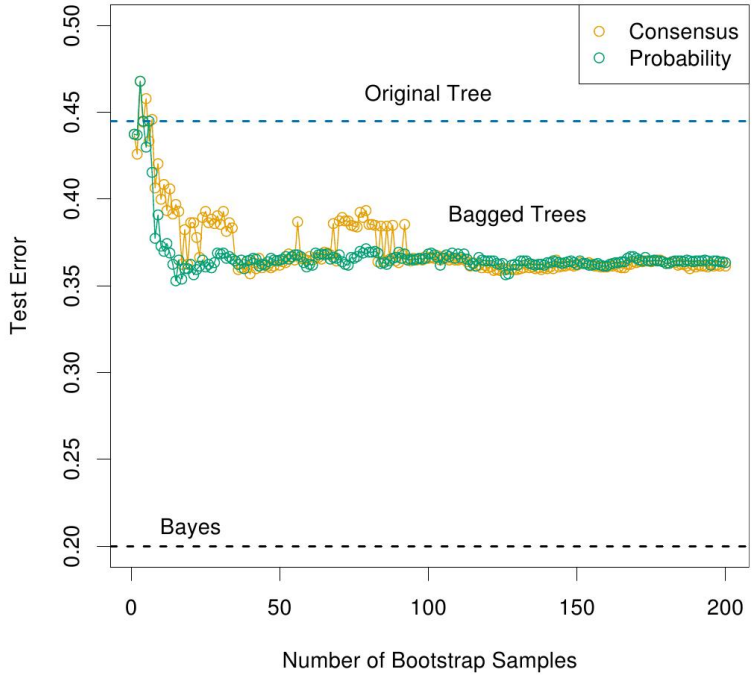
- Binary classification, $x \in \mathbb{R}^5$.
- Note the variation among bootstrapped trees.
- Take-home message:

  With bagging, each tree doesn't have to be great, just "ok".
- Bagging often improves results *when the function is non-linear*.



## Drawbacks of Bagging

- Bagging works on trees because of the bias-variance tradeoff ($\uparrow$ bias, $\downarrow$ variance).
- However, the bagged trees are correlated.
- In general, when bootstrap samples are correlated, the benefit of bagging decreases.




## Random Forests

Modification of bagging where trees are designed to reduce correlation.

- A very simple modification.
- Still learn a tree on each bootstrap set, $\mathcal{B}_t$.
- To split a region, only consider random subset of dimensions of $x \in \mathbb{R}^d$.

# Random Forests: Algorithm

## Training

Input parameter: $m$ — a positive integer with $m < d$, often $m \approx \sqrt{d}$

For $t = 1, \ldots, T$:

1. Draw a bootstrap sample $\mathcal{B}_t$ of size $n$ from the training data.
2. Train a tree classifier on $\mathcal{B}_t$, where each split is computed as follows:
   - Randomly select $m$ dimensions of $x \in \mathbb{R}^d$, newly chosen for each split.
   - Make the best split restricted to that subset of dimensions.

- Bagging for trees: Bag trees learned using the original algorithm.
- Random forests: Bag trees learned using algorithm on this slide.

# Random Forests

## Example problem

- Random forest classification.
- Forest size: A few hundred trees.
- Notice there is a tendency to align decision boundary with the axis.