Computational Data Analysis

Classification And Regression Trees

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Todays Lecture

- Recap
- Regression Trees
- Classification Trees

Recap

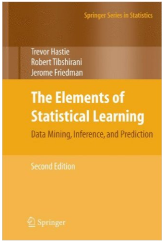
Unsupervised clustering

- Dissimilarity measures
- K-means clustering
- K-medoids clustering
- Hierarchical clustering
  - cluster-cluster distance
- Gaussian mixture
- Validation and model selection
  - CV?
  - Gap-statistics
  - BIC

Classification And Regression Trees

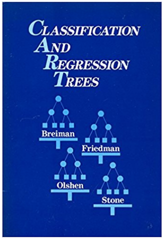
CART

Classification **A**nd **R**egression **T**rees



The Elements of Statistical Learning:

"Tree based methods partition the feature space into a set of rectangles, and then fit a simple model (like a constant) in each one."

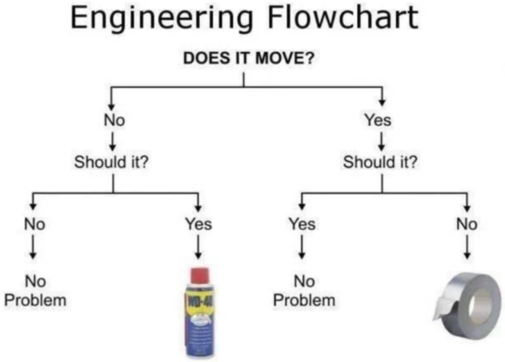


Classification And Regression Trees (1984) by Breiman, Friedman, Olshen and Stone introduced,

- CART
- The one-standard-error rule

Decision trees

Like a decision tree but built on data instead of expert knowledge

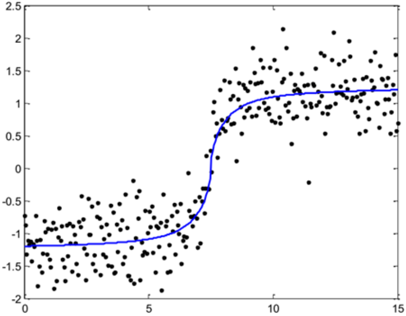


Regression trees

A simple example

Regression

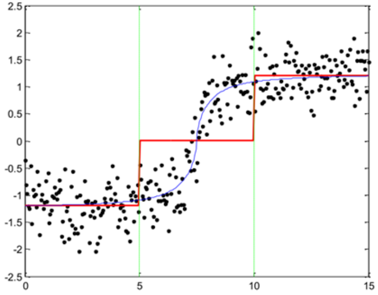
- True function: $y = f(x)$ (blue)
- Observation with noise: (x_i, y_i) (black)

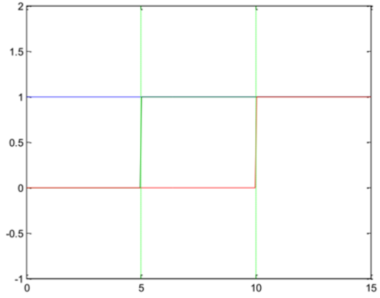


A simple example

Fit a piecewise polynomial

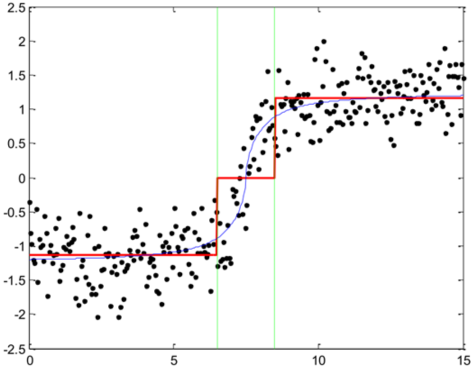
- `X = [ones(n,1) double(x>5) double(x>10)];`
- A constant in each interval
- Evenly spaced knots





A simple example

Can we place the knots in a better way?



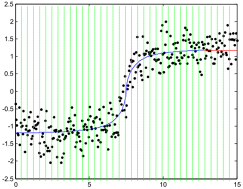
A simple example

Algorithm attempt:

- Choose a number of knots k.
- try all possible positions for each knot k
  - Infinite number of combinations

Try e.g. 100 positions on the x-axis for each knot

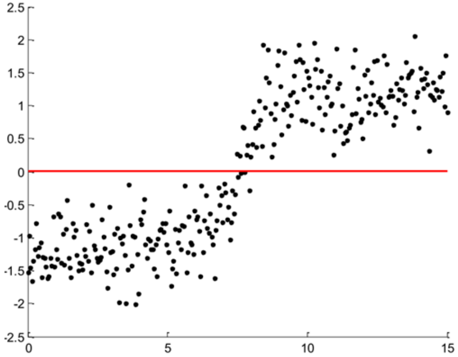
- 100^k positions to try
- E.g. $100^5 = 10\,000\,000\,000$ combinations
- With more than one input variable it gets even worse



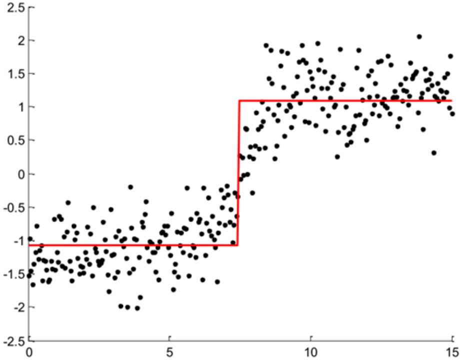
A simple example

New idea:

- Place the knots one after another
- Place each knot such that the fit is as good as possible



A simple example



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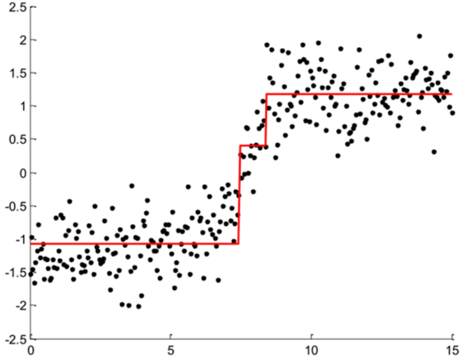

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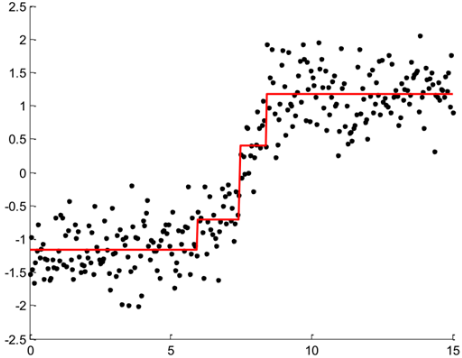

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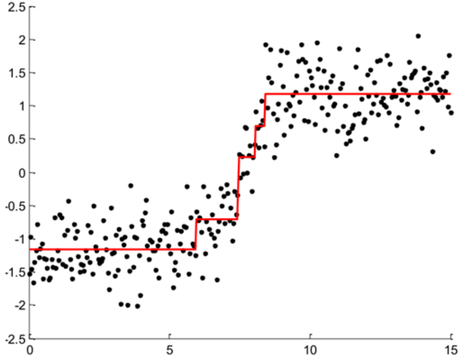
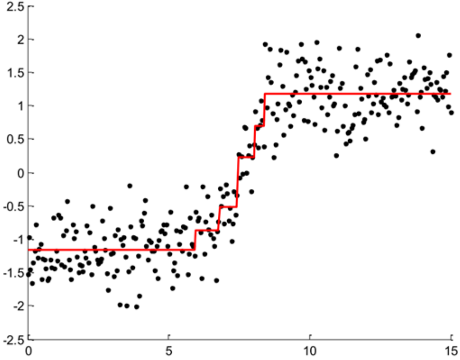


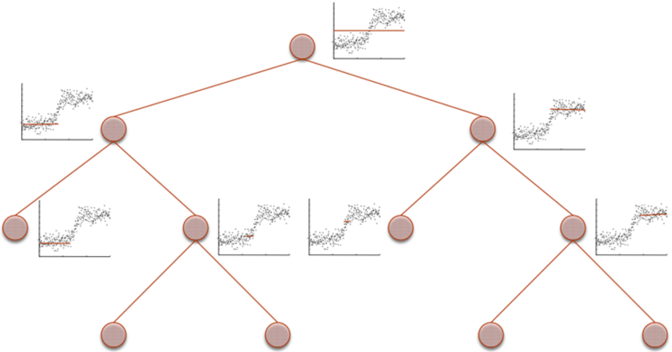
A simple example

At this point, the regression function is pretty good!



Tree representation

Each split can be represented by a parent node split into two child nodes



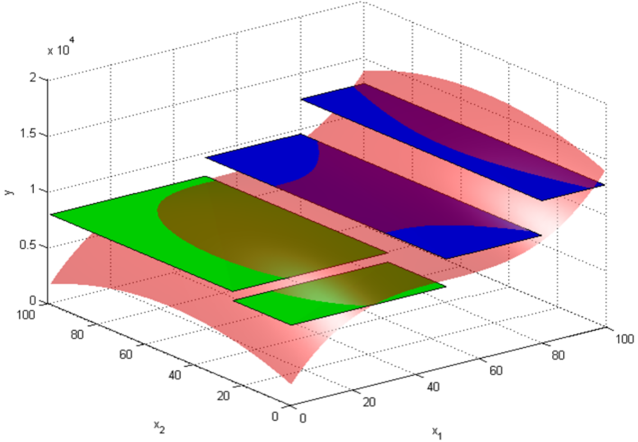
More than one input variable

Handled in the simplest way possible

```
For each input variable
    For each split
        Evaluate split point
    End
End
```

Choose the best variable and split

More than one input variable



Questions

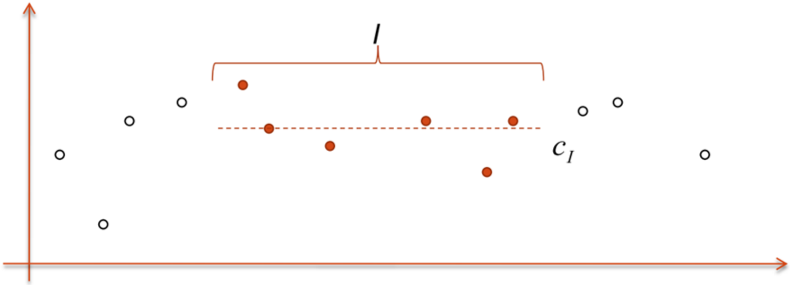
- What is a good split?
  - We need to know this to decide where to split
- How many splits should we try?
  - We used 100 before - is there a better choice?
- When do we stop splitting?

What is a good split?

- The terminal nodes each represent an interval of the input variable(s).
- We choose to represent the outcome in this interval by a **constant** function.
- As for most regression problems, we say that a constant function is good if it has low **residual sum of squares** when compared to training outcome data

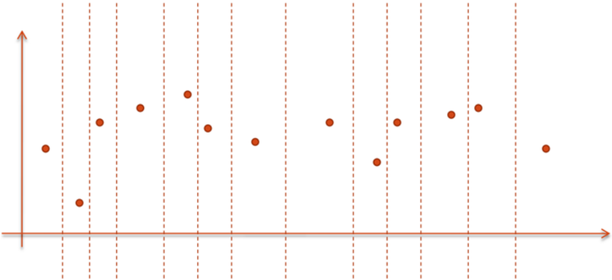
What is a good split?

- Prediction $\hat{y}$ is a constant in each interval.
- Residual sum of squares (RSS) in interval I: $RSS_I = \sum_{i \in I}(y_i - \hat{y}_i)^2$
- Minimal when $\hat{y} = \sum_{i \in I} y_i / n$



How many splits?

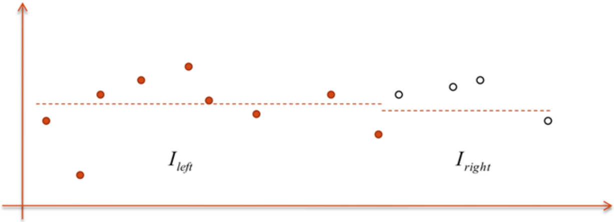
- Optimal constant function is the average of the outcome in the interval.
- Only important if observations are in the interval or not.
- Split somewhere in each gap between observations.



How many splits?

In an interval with n_I observations we have n_I possible splits

- Nothing fancy here, just try them all
- Chose the one with the lowest total RSS on the interval



$$RSS_I = RSS_{I_{left}} + RSS_{I_{right}}$$

Splitting categorical predictors

- Consider a two-category input (e.g. male-female)
  - Only one way to split, men versus women
  - Empty groups are not allowed
  - {male},{female} and {female},{male} is the same split
- Consider a three-category input {apple, orange, banana}
  - Three possible splits
    {apple} , {orange, banana}
    {apple, orange} , {banana}
    {apple, banana} , {orange}
- How many splits for a variable with k categories?
  - In today's exercises!

How large do we grow the tree?

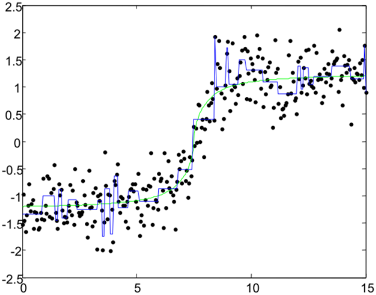
- Stop splitting when a node contains too few observations
- For instance, do not split nodes with 10 or less observations
- This variable is called `MinParent` in Matlab's `fitrtree` function

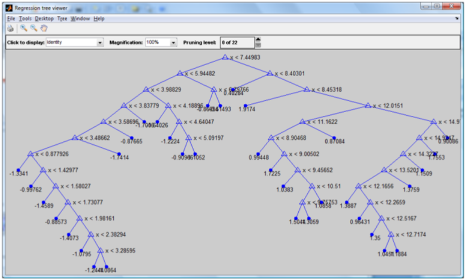
Tree-growing procedure

- First interval (node) is the entire range of X.
- For each variable
  - For each splitting position, calculate $RSS = RSS_{left} + RSS_{right}$
  - Remember position with the lowest RSS
- Split the variable with the lowest RSS at the corresponding position
- This produces a left and right sub-interval (child-nodes)
  - Split each of these into child nodes as above
  - Keep splitting nodes until a node contains too few observations
- Assign a constant function to terminal nodes, the average of the observations

Resulting tree

`MinParent = 10`

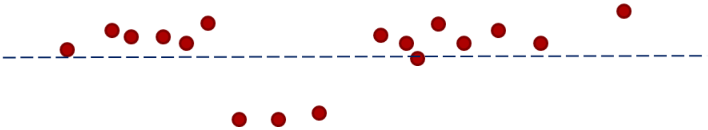




Finding the right sized tree

- The tree was split too far - overfitting
- How do we know when to stop splitting?

  Answer: we don't
  - A seemingly worthless split may lead to excellent splits below



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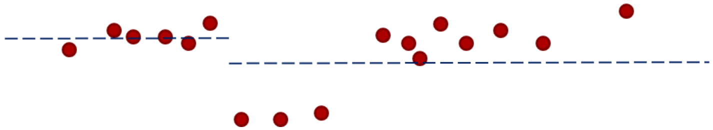

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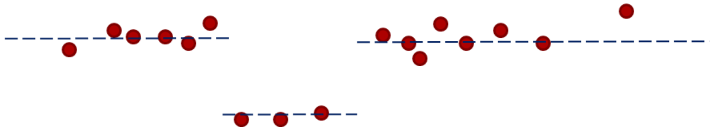


Finding the right sized tree

- We don't want to miss out on good splits
- Strategy: grow the tree really large (small `MinParent`)and then decide which splits were unnecessary and remove these.
- This is called **pruning** the tree
  - Pruning a node amounts to removing its sub-tree, thereby making a terminal node

Pruning rule

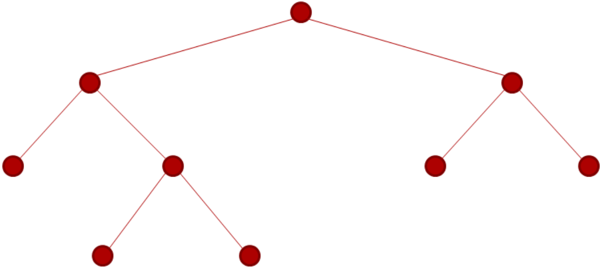
Prune the non-terminal node whose sub-tree gives the smallest **per node** reduction in RSS.

- Divide the reduction by the number of terminal nodes minus one

Pruning the tree

Weakest-link pruning: prune branches that contribute the least to lowering RSS

Example:



Pruning the tree

Weakest-link pruning: prune branches that contribute the least to lowering RSS

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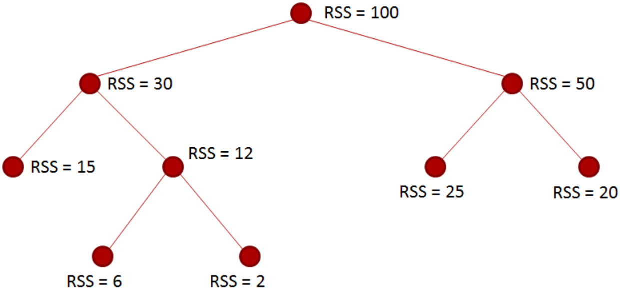

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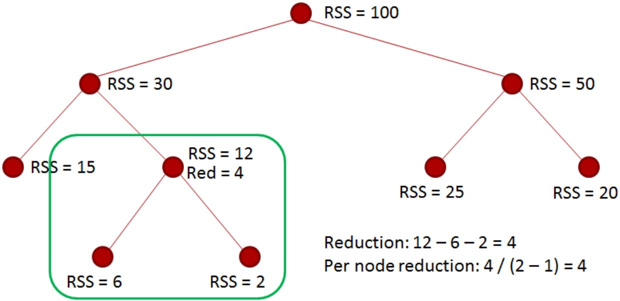

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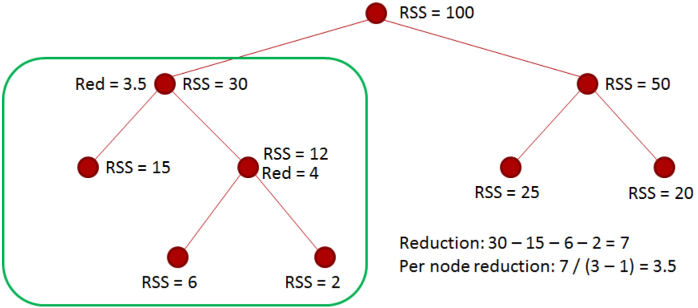

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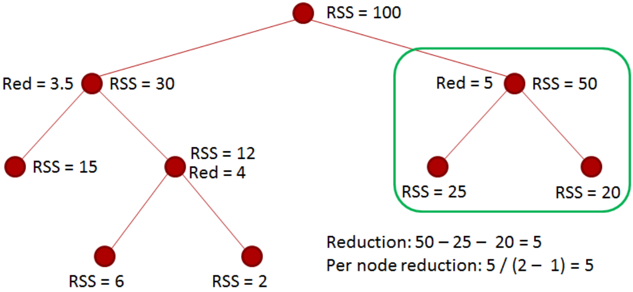

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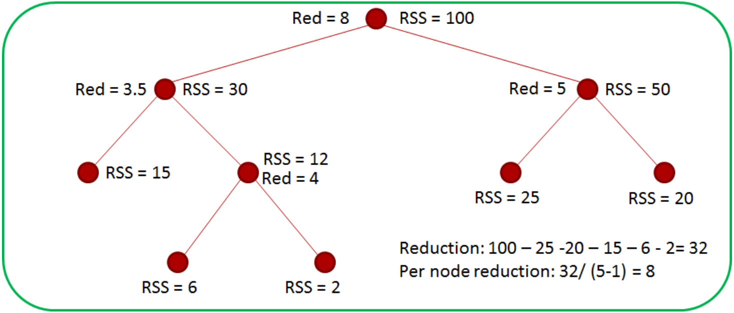

Pruning the tree

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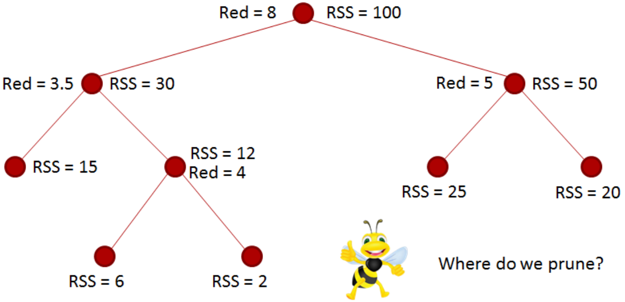
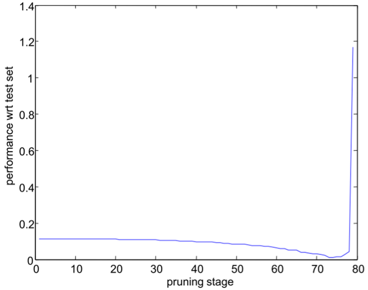


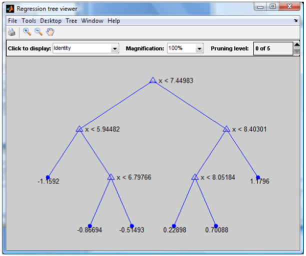
When to stop pruning?

- If we keep pruning, we will end up with just the root node
- Which of all these sub-trees do we choose?
- Two approaches
  - Independent test set
  - Cross-validation

Using a independent test set

- As we prune our way towards the root node, evaluate the performance of each sub-tree with respect to the test set.
- Continue all the way to the root node
  - Choose sub-tree with best performance





Using cross-validation

Three alternatives...

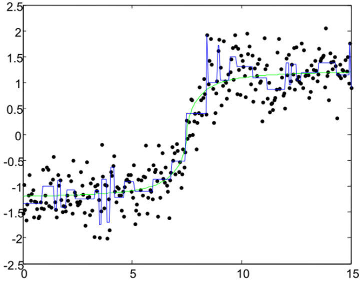
- Cross validate **all possible trees**, does not work in practice - too many trees.
- Use a **tuning parameter**. Choose the tree that minimizes,

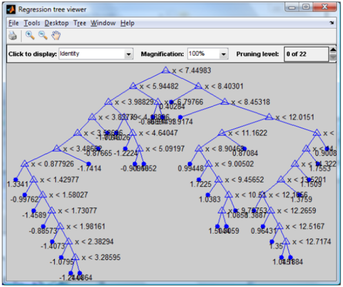
  $$RSS(T) + \alpha|T|$$
  $$|T| = \text{ \# end-nodes}$$

  Find the tuning parameter α using cross validation
- Use the cross validation to determine the optimal value of the minimum number of **observations in a terminal node**. Matlab parameter '`MinLeaf`'. Then use the full grown tree without pruning.

Regression example revisited

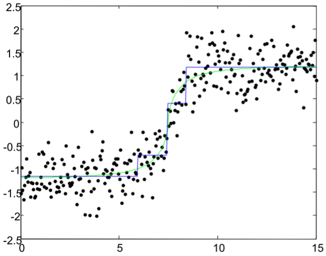
`MinParent = 20` full tree

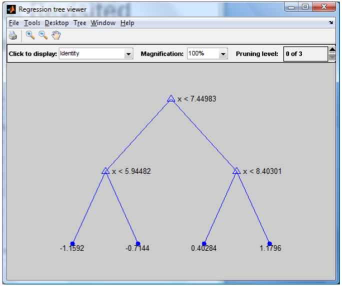




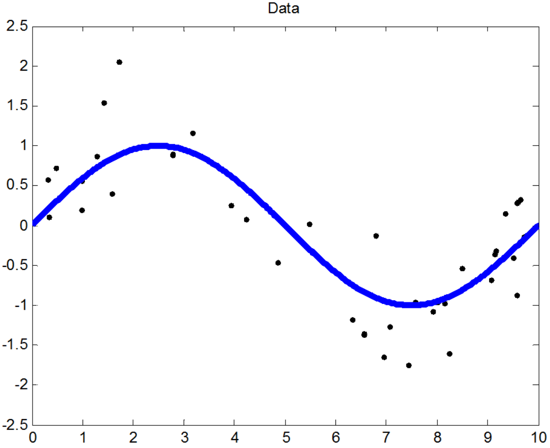
Regression example revisited

Best sub-tree chosen by 10-fold cross-validation.





Bias and variance trade-off



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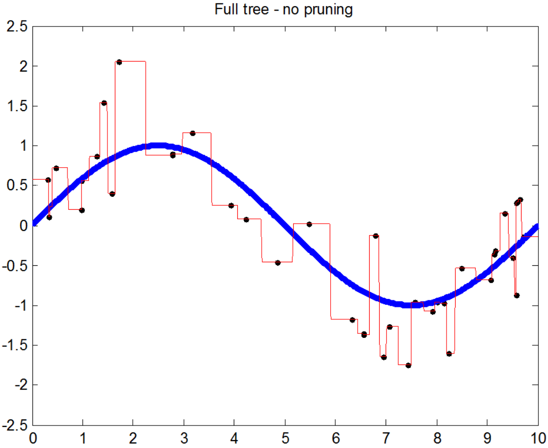

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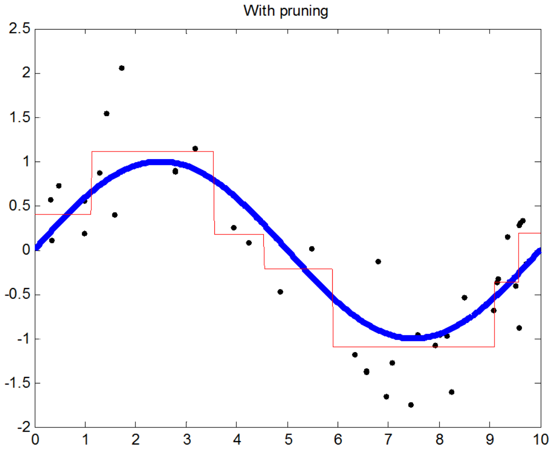

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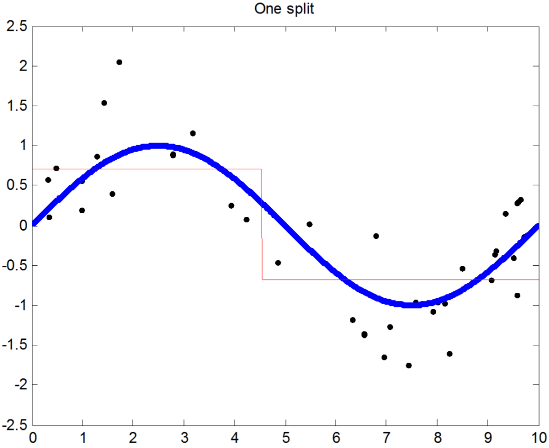

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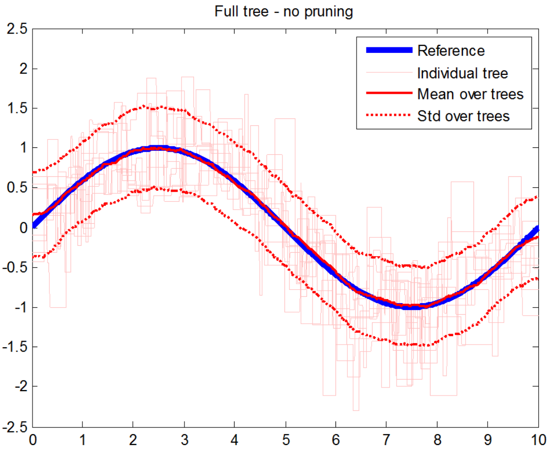

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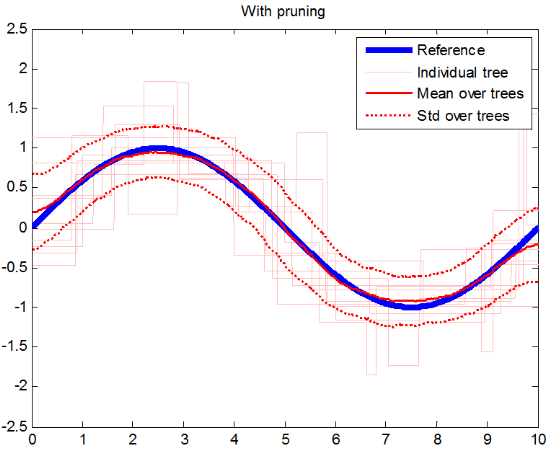

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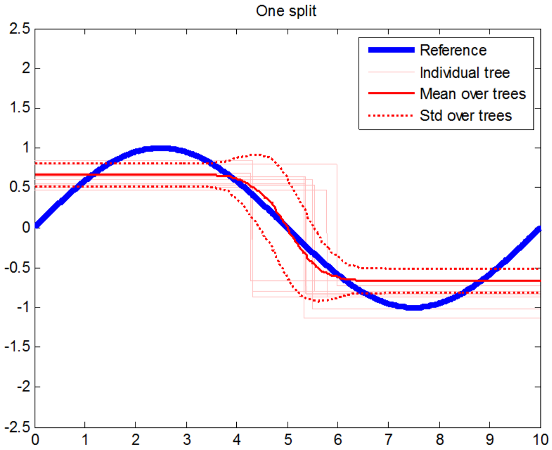


Bias and variance trade-off

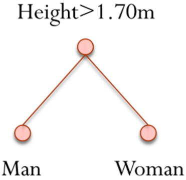
What do we conclude about regression trees in terms of

- Bias
- Variance

Classification trees

Classification trees

Terminal node assigns a class instead of a constant



Only difference: criteria for splitting nodes and pruning the tree

Node values

With **regression trees** we transform a new observation into a constant.

- The constant was derived from the training data.
- It was the **mean** of the output variable of the training observations in the node.

For **classification trees** we assign new observations to a certain class

- The class is derived from training data
- It is the **majority class** of the training observations in the node

Model error

Regression trees

- For regression trees we used RSS as a measure of node impurity

Classification trees

- For classification trees we have a few options
  - Missclassification rate
  - Gini index
  - Cross-entropy
- They all favor the split that increases purity the most.
  - Typically the predictive performance is not that different
  - The shape of the trees might, however, be very different

Node impurity for classification trees

In a specific node, representing a region R with N observations, let

$$\hat{p}_k = \frac{1}{N} \sum_{x_i \in R} \mathbb{1}(y_i = k)$$

Classify observations in the node to class,

$$K = \arg\max_k \hat{p}_k$$

Measures of impurity within a node,

Misclassification error:	$Q = \frac{1}{N} \sum_{i \in R} \mathbb{1}(y_i \neq K) = 1 - \hat{p}_K$
Gini index:	$Q = \sum_{k \neq k'} \hat{p}_k \hat{p}_{k'} = \sum_k \hat{p}_k (1 - \hat{p}_k)$
Cross-entropy (deviance):	$Q = -\sum_k \hat{p} \log \hat{p}_k$

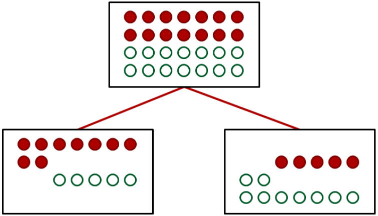
From node impurity to split criterion

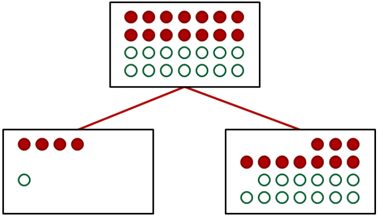
- The node impurity is weighted with the number of observations in each node.
- The split decision is based on the split that **minimizes**,

$$N_{left} Q_{left} + N_{right} Q_{right}$$

N, the number of observations in left and right node
Q, node impurity for left and right node

Comparing splits



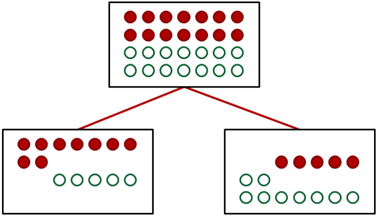


Missclassification error
Left node: 5/14
Right node: 5/14
Split criterion
14(5/14) + 14(5/14) = 10

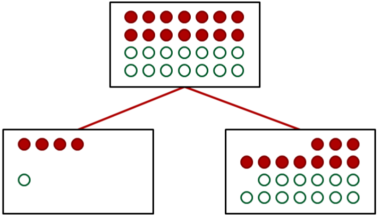
Missclassification error
Left node: 1/5
Right node: 10/23
Split criterion
5(1/5) + 23(10/23) = 11

Lower is better!

Comparing splits



Gini index
Left node: ...
Right node: ...
Split criterion
...

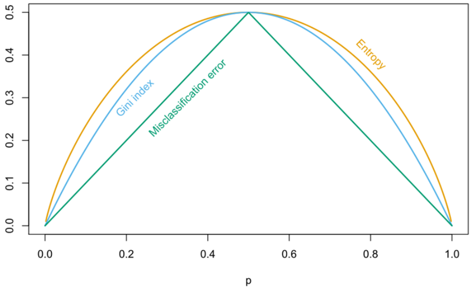


Gini index
Left node: ...
Right node: ...
Split criterion
...

Calculate split criterion based on the Gini index!

Node impurity for classification trees

- Node impurity measures for a two-class problem.
- X-axis: proportion of samples belonging to class 2.



- Entropy and Gini index are better measures for growing tree because they are more sensitive to node probabilities.

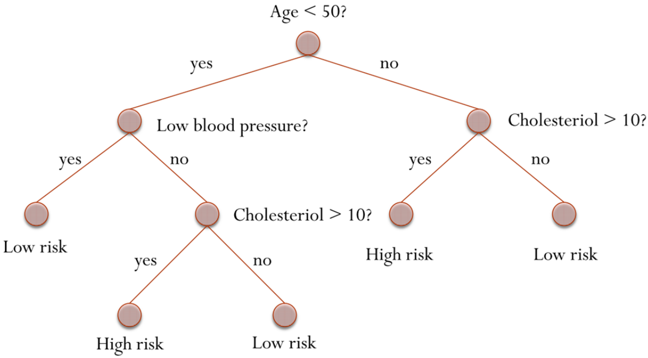
Standard practice

- Use **Gini index** as split criterion when **building** the tree.
- Use **missclassification rate** as criterion when deciding which node to **prune**.

Benefits of a tree structure

Interpretability!

Consider the following (classification) tree on heart diseases



Interpretability

- CART is popular in medical sciences because it may represent the way doctors reason.
- A single tree describes the entire partitioning on the input space.
- With $p > 3$ input variables, the partition (cf. knot positions) are difficult to visualize.
  - But a tree representation is always possible.
- A large tree might be difficult to interpret anyway...

Missing data

Incomplete data are common in many applications.

We can always

- Delete the observation
- Replace with mean or median

For trees we can

- Introduce and **extra category** “missing” - if it is a categorical variable.
- Use a **surrogate variable**. In each branch, have a list of alternative variables and split points - as a backup.
  - Matlab does this.

Questions?