ARISTOTLE UNIVERSITY OF THESSALONIKI

FACULTY OF ENGINEERING

Pattern Recognition & Machine Learning

Model Combination - Trees

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Until now…

- We have talked about many different models for classification.
- It is often the case that the overall performance could be improved by model combination!
- Example: You have multiple NN models trained on different datasets for the same regression problem. For a new, test sample, the average of the predictions made by each model would probably lead to a better result than the outcome of a single model.
- The group of models that are combined like this are called *committees*!
  - Why *committees* lead to better results?

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Test error of a classifier

- You can think about test error in terms of a decomposition into **two terms**.
- Let f be a learned classifier, selected from a set $\mathcal{F}$, i.e., all possible classifiers using a fixed representation, e.g., trees with certain depth, NNs with certain number of neurons in the hidden layer etc.
- Then the error of the classifier on a test set can be decomposed as:

$$error(f) = \mathbb{E}_{\mathcal{D}}\left[\left(f(\boldsymbol{x};\mathcal{D}) - h(\boldsymbol{x})\right)^2\right] =$$

$$= \left(\mathbb{E}_{\mathcal{D}}[f(\boldsymbol{x};\mathcal{D})] - h(\boldsymbol{x})\right)^2 + \mathbb{E}_{\mathcal{D}}[(f(\boldsymbol{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[f(\boldsymbol{x};\mathcal{D})])^2]$$

where $\mathcal{D}$ is a particular dataset and $h(\boldsymbol{x})$ is the function to be approximated.

Bias/Variance Trade-off

$$\mathbb{E}_{\mathcal{D}}\left[\left(f(\boldsymbol{x};\mathcal{D}) - h(\boldsymbol{x})\right)^2\right] = \underbrace{\left(\mathbb{E}_{\mathcal{D}}[f(\boldsymbol{x};\mathcal{D})] - h(\boldsymbol{x})\right)^2}_{\text{Bias}} + \underbrace{\mathbb{E}_{\mathcal{D}}[(f(\boldsymbol{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[f(\boldsymbol{x};\mathcal{D})])^2]}_{\text{Variance}}$$

- Bias: measures the quality of the model family (e.g., NNs with certain number of neurons in hidden layer).
  - Suppose someone gave you infinite data to train your model; How well would you do with this particular model family?

- Variance: measures how far the actual, learned classifier (train over limited data) is from the optimal classifier of the family, i.e., the one trained with infinite data.
  - In essence, this tells you how much you have to pay due to the fact that you do not have infinite amount of data!
  - Sensitivity of the model to the individual dataset it was trained on.

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- There is a fundamental trade-off between Bias and Variance in practical applications.

- As you make your model family more complex, e.g., complex NN architecture, you make $\mathcal{F}$ bigger. This, will cause a decrease in bias term as the approximation with infinite data will be much better.

- On the other hand this will also cause and increase in the variance term as more complex representation with limited data will most probably lead to overfitting!

Bias/Variance Trade-off - Example

- Assume we have L datasets of N points to approximate the function:

$$h(x) = \sin(2\pi x) + \varepsilon$$

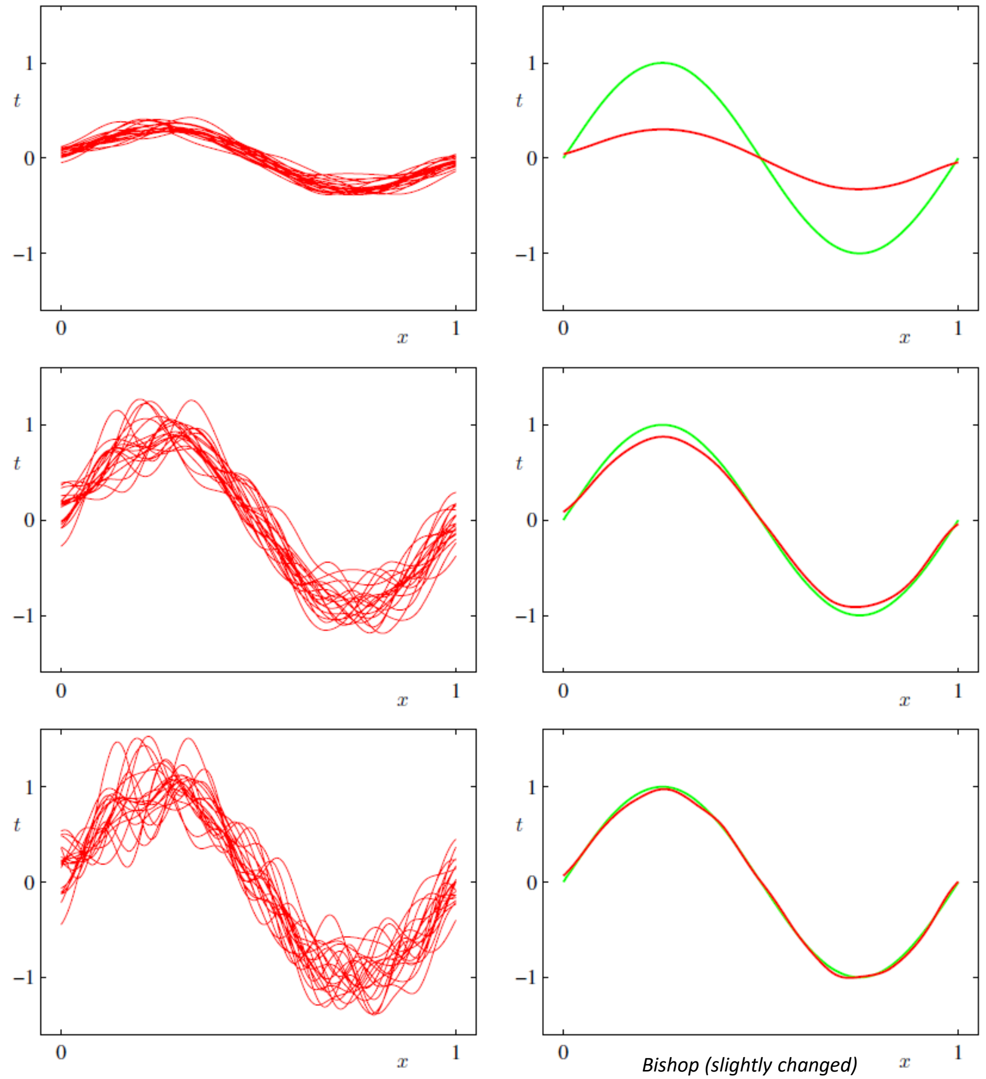
The final outcome of the committee will be:

$$\mathbb{E}_{\mathcal{D}}[f(\boldsymbol{x};\mathcal{D})] = \frac{1}{L}\sum_{l=1}^{L} f^{l}(x)$$

first row: high bias, low variance

second row: lower bias, high variance

third row: low bias, higher variance



Bishop (slightly changed)

Averaging predictions

- Averaging predictions of models trained on different datasets leads to reduction of the variance!
  - Low bias/high variance leads to low variance/low bias after averaging
- Thus, when we average a set of low-bias (high variance) models, i.e., complex models, we obtain accurate predictions. That's why committees work!
- Pitfall: we only have one single dataset!
- How could we artificially introduce variability between different models within a committee?

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- Pitfall: we only have one single dataset!
- How could we artificially introduce variability between different models within a committee?
  - Bootstrap datasets!

Bootstrapping Datasets

- Suppose we have the dataset $\boldsymbol{X} = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$
- we can create B new datasets by simply drawing N points at random from $\boldsymbol{X}$ with replacement!
  - Some samples may appear multiple times in a new dataset after bootstrapping.
  - Some samples of the initial dataset may not appear at all.
- Thus, I get B new datasets: $\{\boldsymbol{X}_1, \dots, \boldsymbol{X}_B\}$.

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- Thus, I get B new datasets: $\{\boldsymbol{X}_1, \dots, \boldsymbol{X}_B\}$.
- Now we can use these B training sets to train B different models (committee members).
- The final decision of the committee will be: $f_{com} = \frac{1}{B}\sum_{b=1}^{B} f_b(\boldsymbol{x})$
  - Bootstrap aggregation/bagging

Regression with bootstrapping

- Suppose the ground truth function that we need to predict is $h(\boldsymbol{x})$.
- Each model gives a prediction: $f_b(\boldsymbol{x}) = h(\boldsymbol{x}) + \epsilon_b(\boldsymbol{x})$
  - error of the model: $\epsilon_b(\boldsymbol{x})$
- The average sum-of-squares error of model b is :

$$\mathbb{E}_{\boldsymbol{x}}\left[\left(f_b(\boldsymbol{x}) - h(\boldsymbol{x})\right)^2\right] = \mathbb{E}_{\boldsymbol{x}}[\epsilon_b(\boldsymbol{x})\ ^2]$$

- The average error of b individual models is:

$$E_{ave} = \frac{1}{B}\sum_{b=1}^{B} \mathbb{E}_{\boldsymbol{x}}[\epsilon_b(\boldsymbol{x})\ ^2]$$

Regression with bootstrapping

- The expected error of the committee is:

$$E_{com} = \mathbb{E}_{\boldsymbol{x}}\left[\left(f_{com}(\boldsymbol{x}) - h(\boldsymbol{x})\right)^2\right] = \mathbb{E}_{\boldsymbol{x}}\left[\left(\frac{1}{B}\sum_{b=1}^{B} f_b(\boldsymbol{x}) - h(\boldsymbol{x})\right)^2\right]$$

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- Nevertheless, the way we defined the datasets after bootstrapping, it is not possible that the errors are not correlated.
- Even in the correlated case, it can be proved that: $E_{com} \le E_{ave}$
- Basic strategy: choose B models with low bias (complex models that can overfit). Then bootstrap aggregated error will be lower than the average error of the individual models.

Feature Bagging

- Feature Bagging: create new datasets by sampling **subsets of features** of length $M < D$ for each learner.
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- Example:
  - Assume dataset $\boldsymbol{X} = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$ with samples $\boldsymbol{x}_n = \{x_1, x_2, x_3, x_4, x_5, x_6\}$. I create new datasets $\boldsymbol{Y}^1 = \left\{\boldsymbol{y}_1^1, \dots, \boldsymbol{y}_N^1\right\}$ with $\boldsymbol{y}_n^1 = \{x_1, x_2, x_6\}$ and $\boldsymbol{Y}^2 = \left\{\boldsymbol{y}_1^2, \dots, \boldsymbol{y}_N^2\right\}$ with $\boldsymbol{y}_n^2 = \{x_3, x_4, x_6\}$.
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  - Train different models with different datasets after feature bagging

- It works well if features are uncorrelated.

- Advantage: pushes learners to **not** over focus on features that predict well on certain training set but do not generalize well to new data!

- Works well when I have too many features and too few samples.

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- Thus,
  - Bootstrap-bagging: Complex model with low bias. Decrease variance by averaging.
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  - Bootstrap-bagging: Complex model with low bias. Decrease variance by averaging.
  - Boosting: Simple models with high bias (underfit). Decrease bias (and variance) by focusing on error of previous models.
- Boosting, final decision: $Y_{com}(\boldsymbol{x}) = sign\left(\sum_{m=1}^{M} a_m y_m(\boldsymbol{x})\right)$, $y_m(\boldsymbol{x}) \in \{-1,1\}$

Boosting: Binary Classification

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- The most popular boosting algorithm is AdaBoost (Adaptive Boosting)
    - At each step a new classifier is trained on weighted dataset
    - Weights of misclassified data samples increase.
    - Committee decision is formed by weighted base classifiers.

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   b) Compute weighted error rates $\varepsilon_m = \frac{\sum_{n=1}^{N} w_n^m I[y_m(\boldsymbol{x}_n) \neq t_n]}{\sum_{n=1}^{N} w_n^m}$

      and model weight $a_m = ln\left(\frac{1-\varepsilon_m}{\varepsilon_m}\right)$

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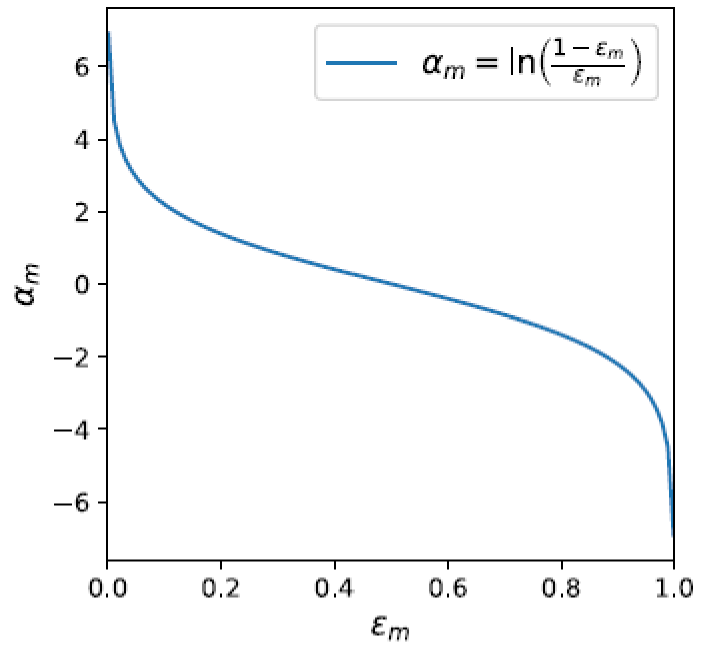
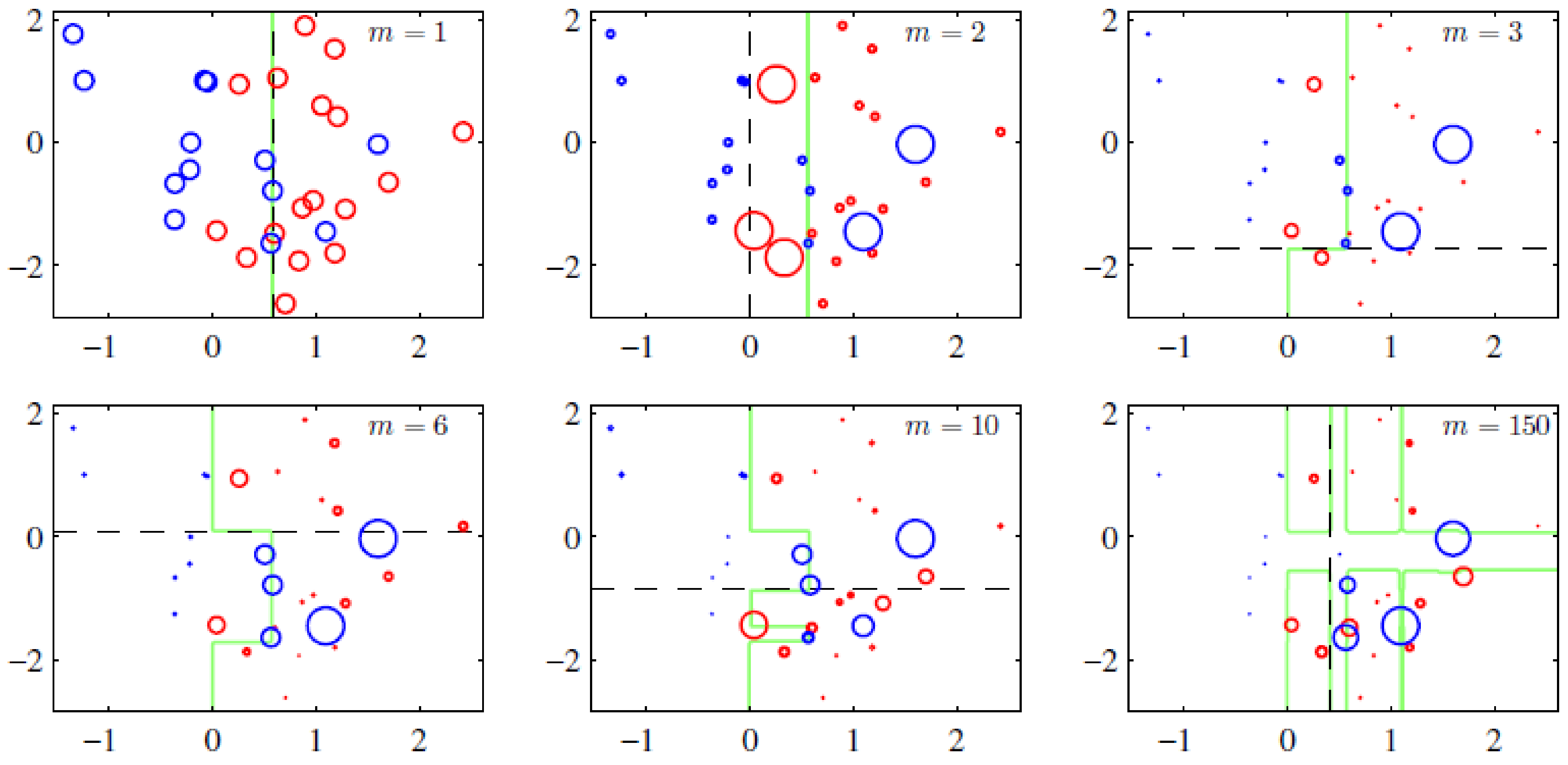


AdaBoost Algorithm - Example



Bishop

Dashed line: current base classifier boundary, green line: committee's decision boundary, cycles: training samples, radius of cycles: weight of the sample for current base classifier.

Interpretation of AdaBoost

- AdaBoost is actually minimizing an exponential error function:

$$E_m = \sum_{n=1}^{N} \exp[-t_n f_m(\boldsymbol{x}_n)]$$

where $t_n f_m(\boldsymbol{x}_n) > 0$ if the sample $\boldsymbol{x}_n$is correctly classified and $t_n f_m(\boldsymbol{x}_n) \leq 0$ otherwise.

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$$f_m(\boldsymbol{x}_n) = \frac{1}{2}\sum\nolimits_{i=1}^{m} a_i y_i(\boldsymbol{x}_n)$$

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- Goal: minimize E_m w.r.t. a_i and the parameters of $y_i(\boldsymbol{x}_n)$
  - *Sequential minimization:* fix $y_1(\boldsymbol{x}), \dots, y_{m-1}(\boldsymbol{x})$ and $a_1, \dots, a_{m-1}$ and minimize E_m w.r.t. a_m and the parameters of $y_m(\boldsymbol{x}_n)$

Derivation of AdaBoost - 1

$f_m(\boldsymbol{x}_n) = \frac{1}{2}\sum_{i=1}^{m} a_i y_i(\boldsymbol{x}_n)$

- Error function:

$$E_m = \sum_{n=1}^{N} \exp\left(-t_n f_{m-1}(\boldsymbol{x}_n) - \frac{1}{2} t_n a_m y_m(\boldsymbol{x}_n)\right)$$
$$= \sum_{n=1}^{N} w_n^m \exp\left(-\frac{1}{2} t_n a_m y_m(\boldsymbol{x}_n)\right)$$

where $w_n^m = exp\left(-t_n f_{m-1}(\boldsymbol{x}_n)\right)$ is known (fixed) based on the trainings so far!

- Assume:
  - C_m to be the set of samples that are correctly classified by $y_m(\boldsymbol{x})$, i.e., $t_n y_m(\boldsymbol{x}_n) = 1$
  - M_m to be the set of samples that are misclassified by $y_m(\boldsymbol{x})$, i.e., $t_n y_m(\boldsymbol{x}_n) = -1$

- Then we can rewrite error function as:

Derivation of AdaBoost - 2

$$E_m = \sum_{n=1}^{N} w_n^m \exp\left(-\frac{1}{2} t_n a_m y_m(\boldsymbol{x}_n)\right) = e^{-\frac{a_m}{2}} \sum_{n \in C_m} w_n^m + e^{\frac{a_m}{2}} \sum_{n \in M_m} w_n^m$$

$$= \left(e^{\frac{a_m}{2}} - e^{-\frac{a_m}{2}}\right) \sum_{n=1}^{N} w_n^m I[y_m(\boldsymbol{x}_n) \neq t_n] + e^{-\frac{a_m}{2}} \sum_{n=1}^{N} w_n^m$$

- Thus, minimization of E_m w.r.t. $y_m(\boldsymbol{x}_n)$ minimizes $J_m = \sum_{n=1}^{N} w_n^m I[y_m(\boldsymbol{x}_n) \neq t_n]$

- minimization of E_m w.r.t. a_m: $\frac{\partial E_m}{\partial a_m} = 0$:

$$a_m = ln\left(\frac{1-\varepsilon_m}{\varepsilon_m}\right) \text{ where } \varepsilon_m = \frac{\sum_{n=1}^{N} w_n^m I[y_m(\boldsymbol{x}_n) \neq t_n]}{\sum_{n=1}^{N} w_n^m}$$

Derivation of AdaBoost - 3

- As soon as we have found $y_m(\boldsymbol{x}_n)$ and a_m, we subsequently minimize E_{m+1} w.r.t. $y_{m+1}(\boldsymbol{x}_n)$ and a_{m+1}:

$$E_{m+1} = \sum_{n=1}^{N} \exp[-t_n f_{m+1}(\boldsymbol{x}_n)] =$$

$$= \sum_{n=1}^{N} w_n^m \exp\left(-\frac{1}{2} t_n a_m y_m(\boldsymbol{x}_n)\right) \exp\left(-\frac{1}{2} t_n a_{m+1} y_{m+1}(\boldsymbol{x}_n)\right) =$$

$$= \sum_{n=1}^{N} w_n^{m+1} \exp\left(-\frac{1}{2} t_n a_{m+1} y_{m+1}(\boldsymbol{x}_n)\right)$$

where

$$w_n^{m+1} = w_n^m exp\left(-\frac{1}{2} t_n a_m y_m(\boldsymbol{x}_n)\right)$$

Derivation of AdaBoost - 4

- Weight updates:

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- The term $\exp\left(-\frac{a_m}{2}\right)$ is independent of n and, thus, can be discarded.
- Finally, $sign(f_m(\boldsymbol{x}_n)) = sign\left(\frac{1}{2}\sum_{i=1}^m a_i y_i(\boldsymbol{x}_n)\right) = sign(\sum_{i=1}^m a_i y_i(\boldsymbol{x}_n))$

Pros and Cons of AdaBoost

- The selection of the exponential error function, makes AdaBoost a very simple algorithm with easy implementation.

- It is sensitive to large negative outliers of the term $t_n y_m(\boldsymbol{x}_n)$ (in case there is not suitable activation function to get +1 or -1).

- Exponential error function can not be interpreted as a well defined probabilistic model.

- AdaBoost does not generalize easily to $c > 2$
    - There are many alterations of the algorithm, though.

Decision Trees (revisited)

Combining models

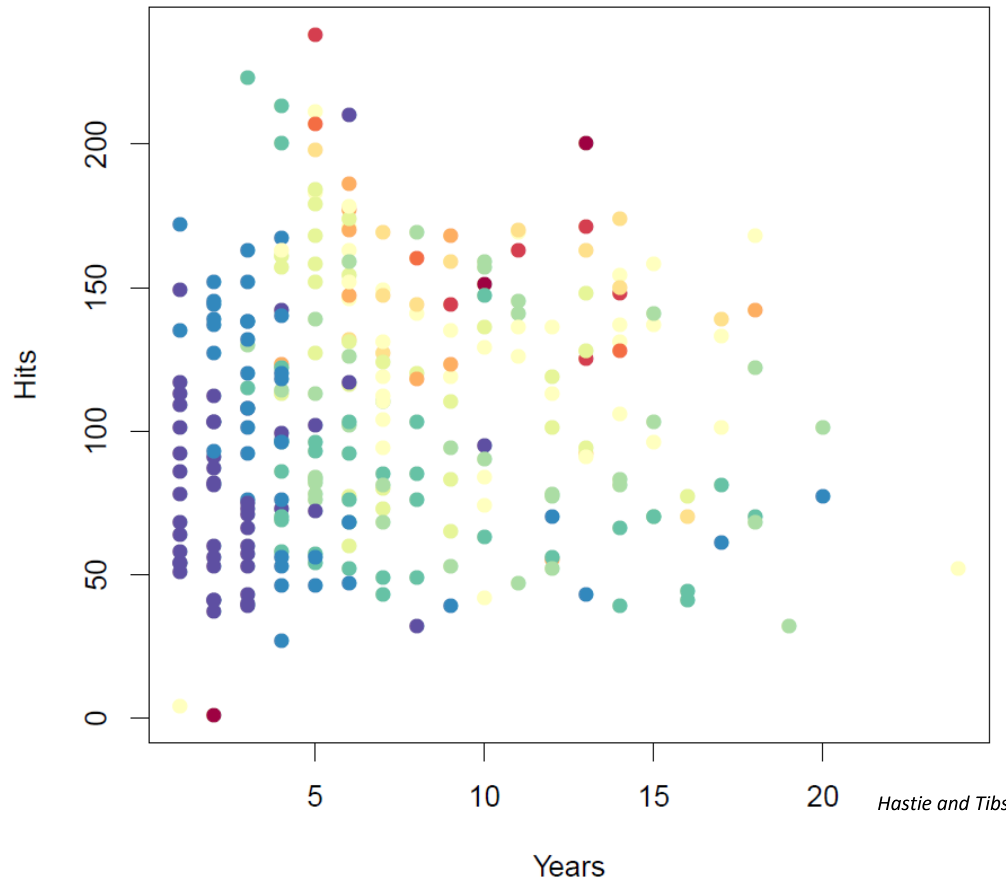
- Committees
  - Bootstrap Aggregation
  - Random Subspace methods (feature bagging)
  - Boosting
- We will now revisit the Decision Tree model and will extend the approach to Random Forests.
- In essence, decisions trees with bootstrapping and random subspaces methods lead to the random forests realization.

Decision Trees (DT)

- DT methods can be used both for regression and classification
- They result in stratification of segmentation of the feature space into a number of rectangular regions.
- The rules that segment the feature space into distinct regions can be summarized using tree, thus the term Decision Trees.
- DT are suitable for intuitive interpretation of the outcome!
- Nevertheless, they are in general weak classifiers (or regressors) and cannot compete with the supervised approaches that we have seen so far.
- Combining a large number of DT grown with bagging and/or boosting approaches can often result in great improvement in prediction accuracy at the expense of loss interpretation.

DT - Regression

- Baseball salary data
  - Salary is color-coded from low (blue, green) to high (yellow, red)



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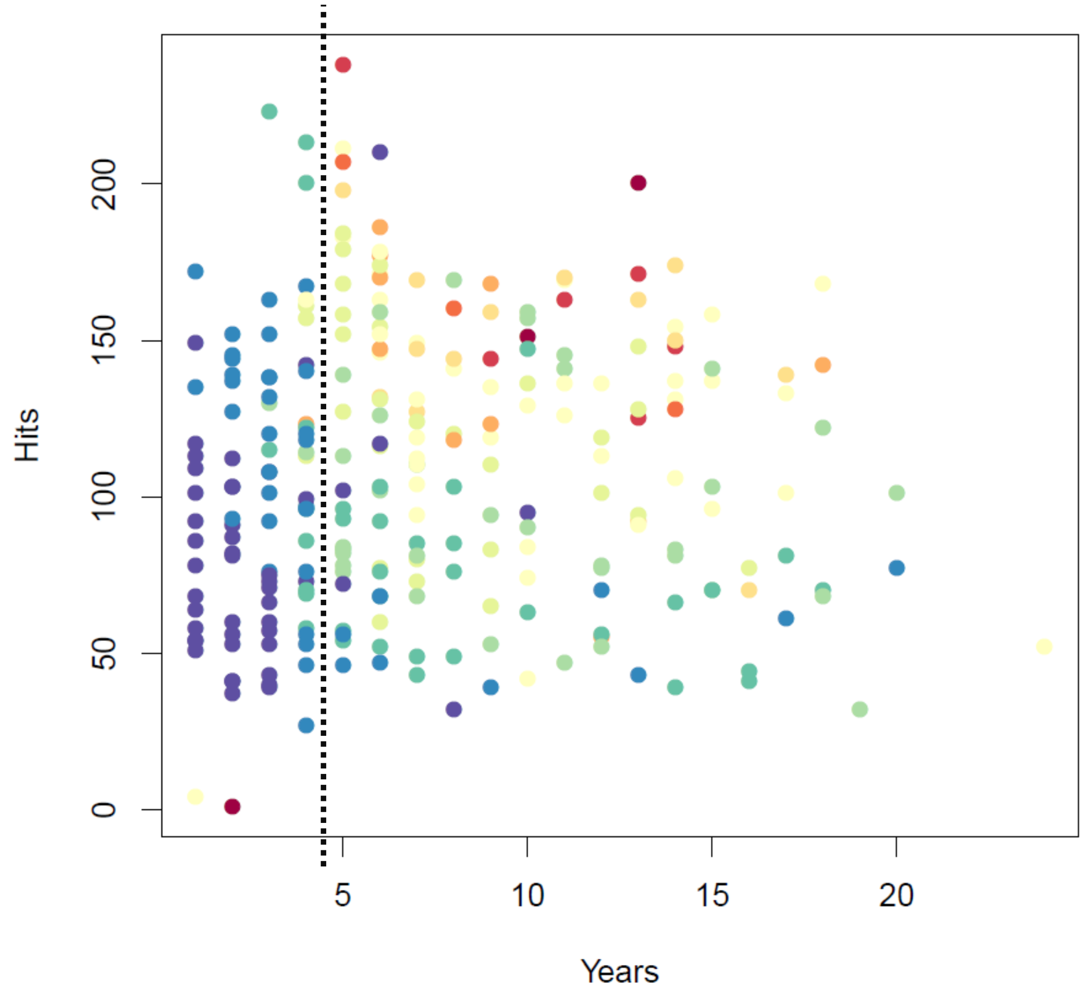
Baseball salary data



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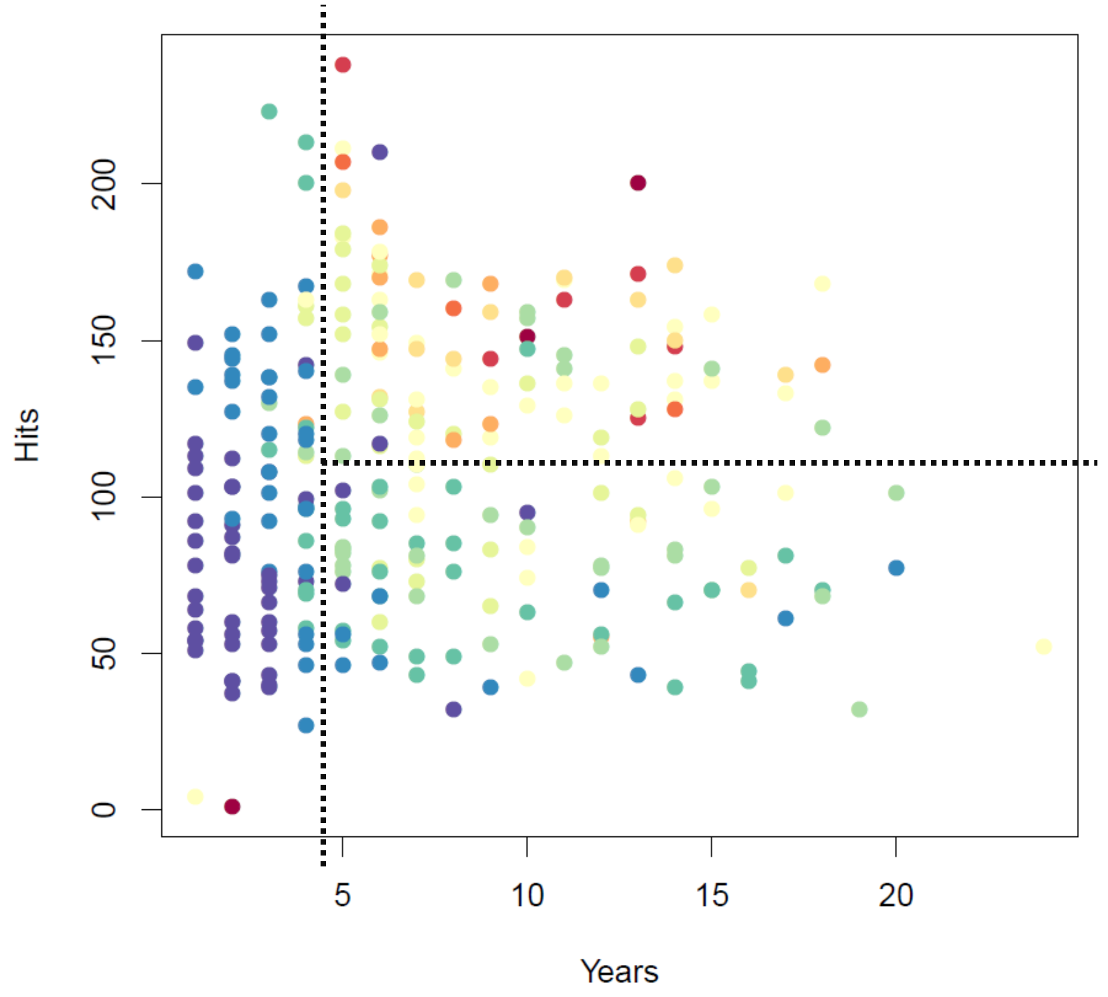

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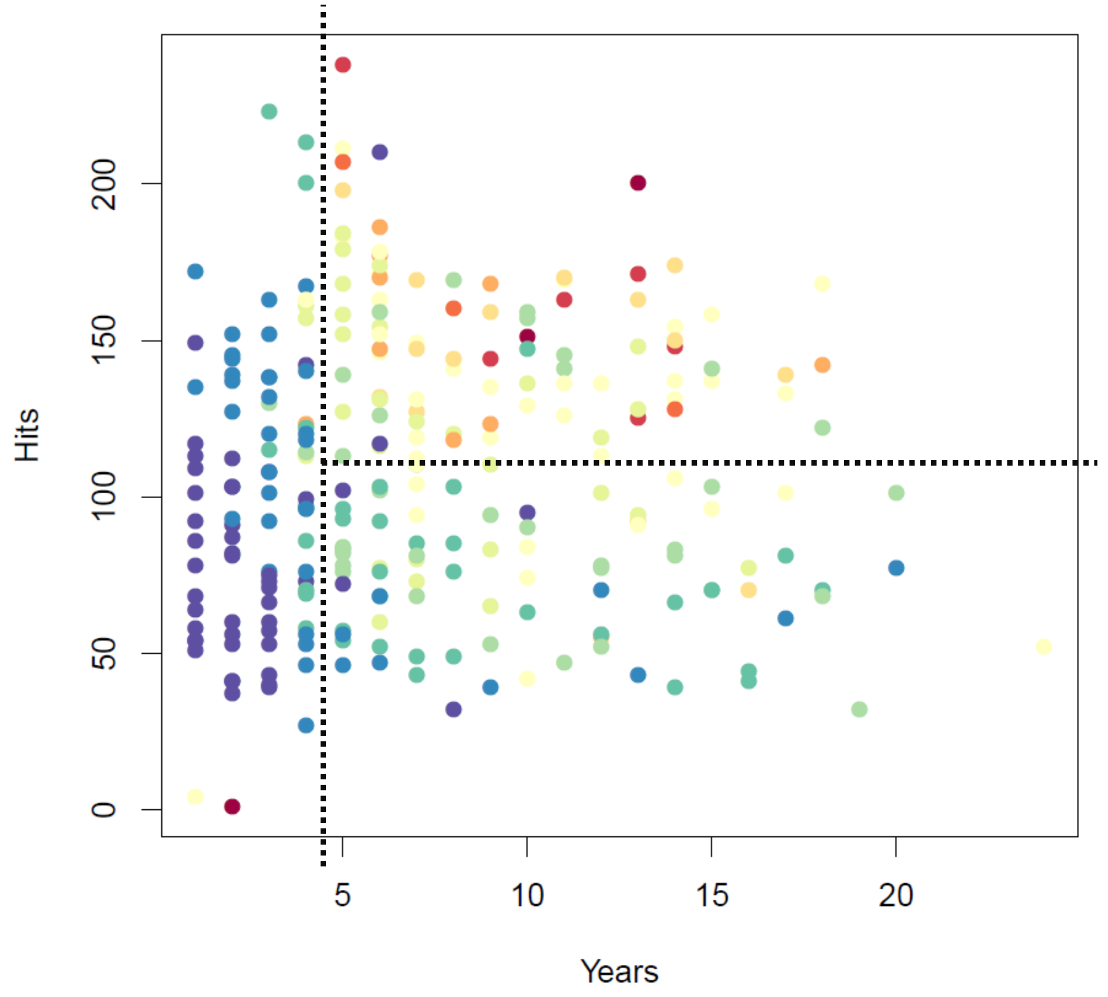

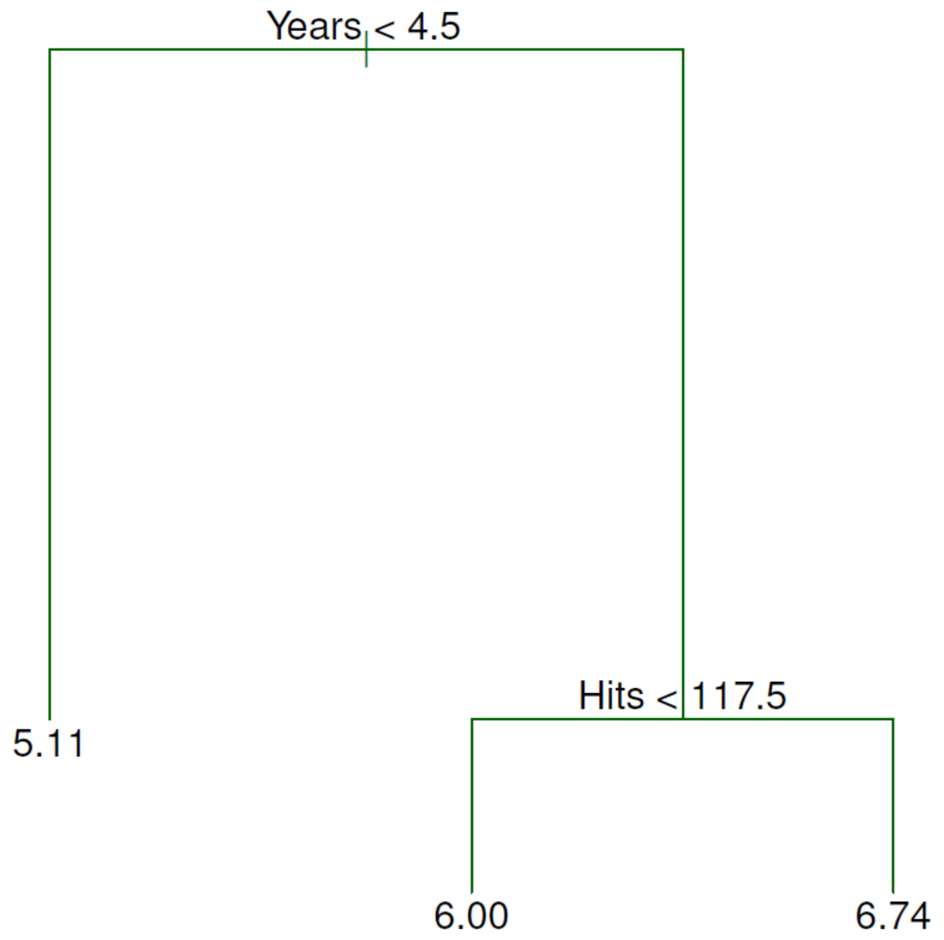

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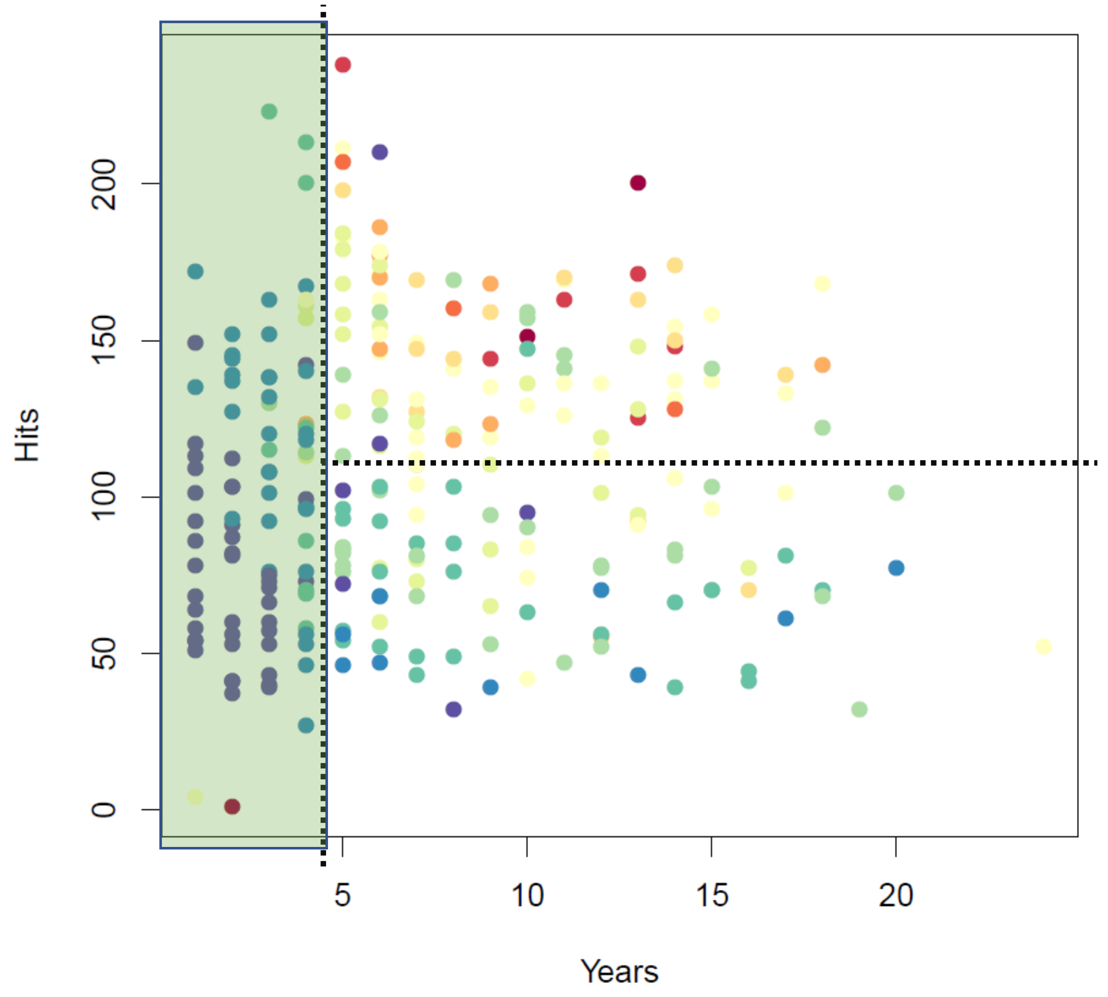

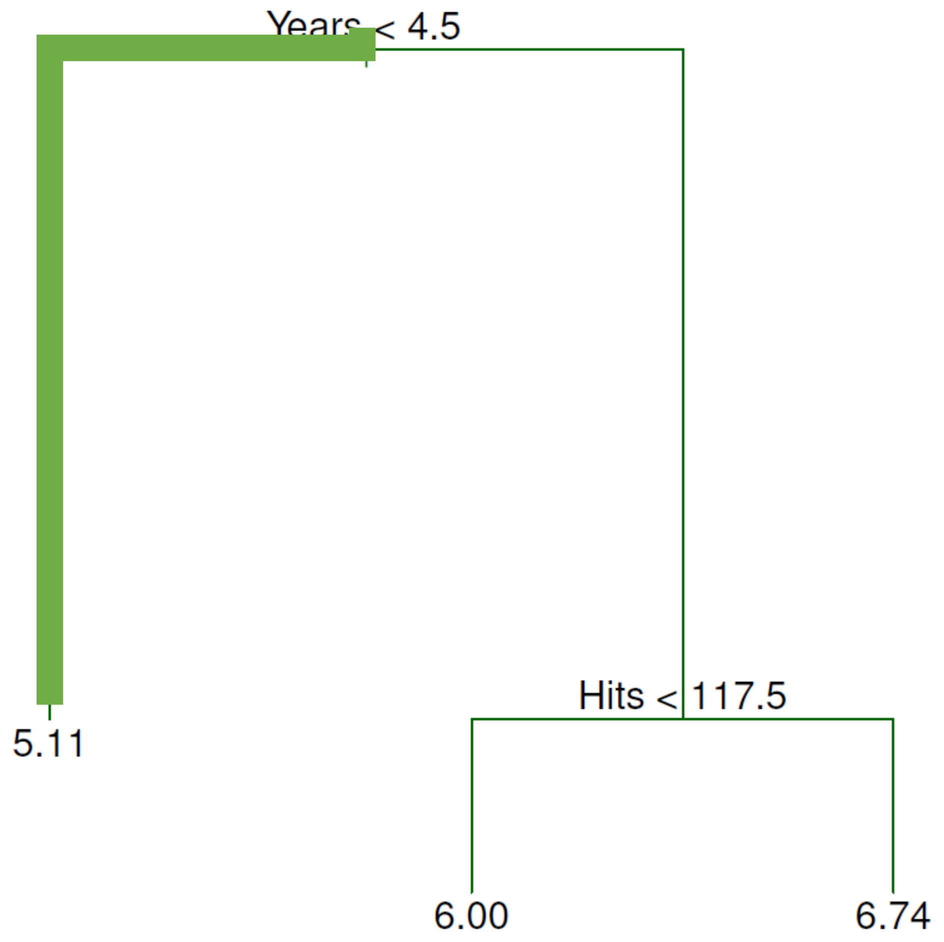

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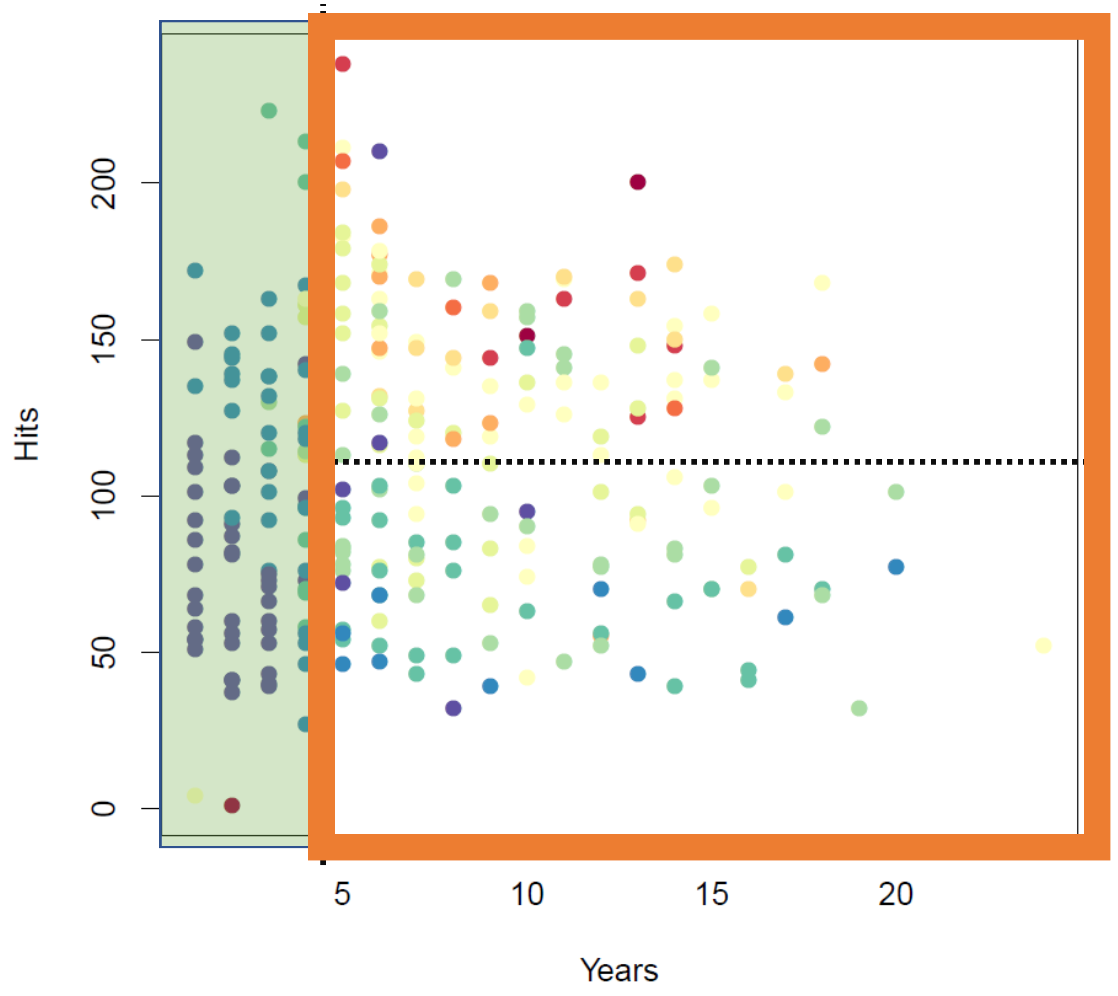

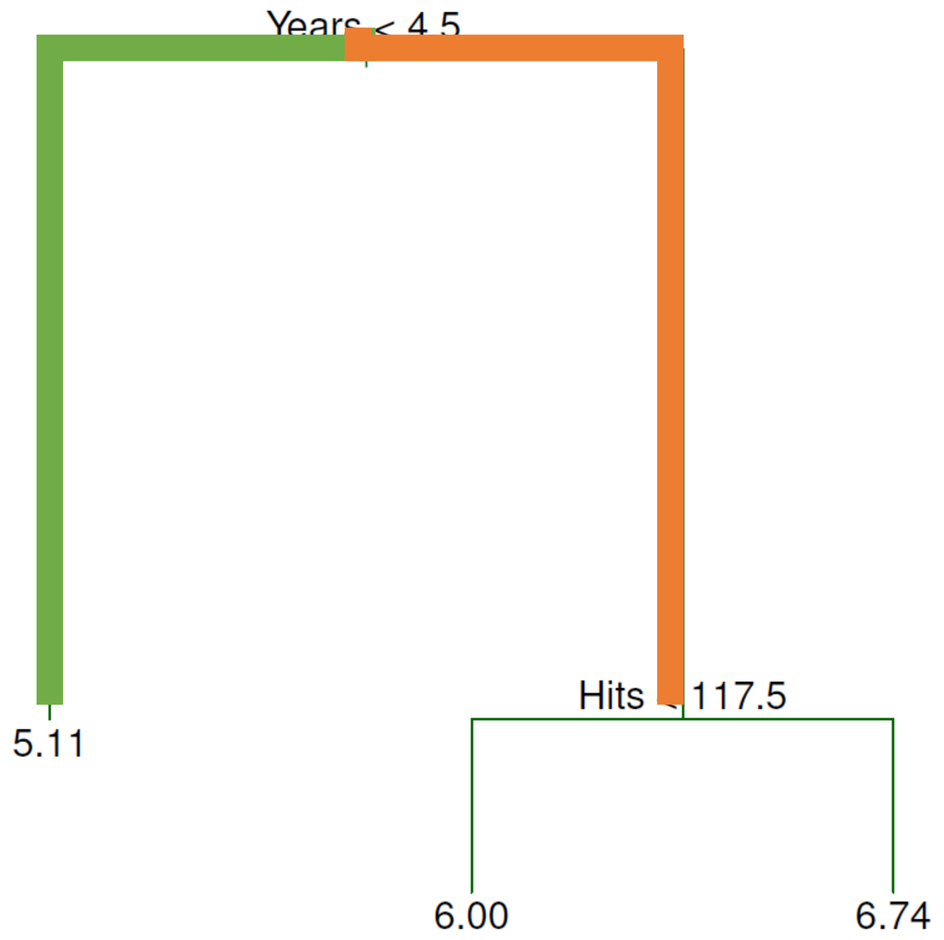

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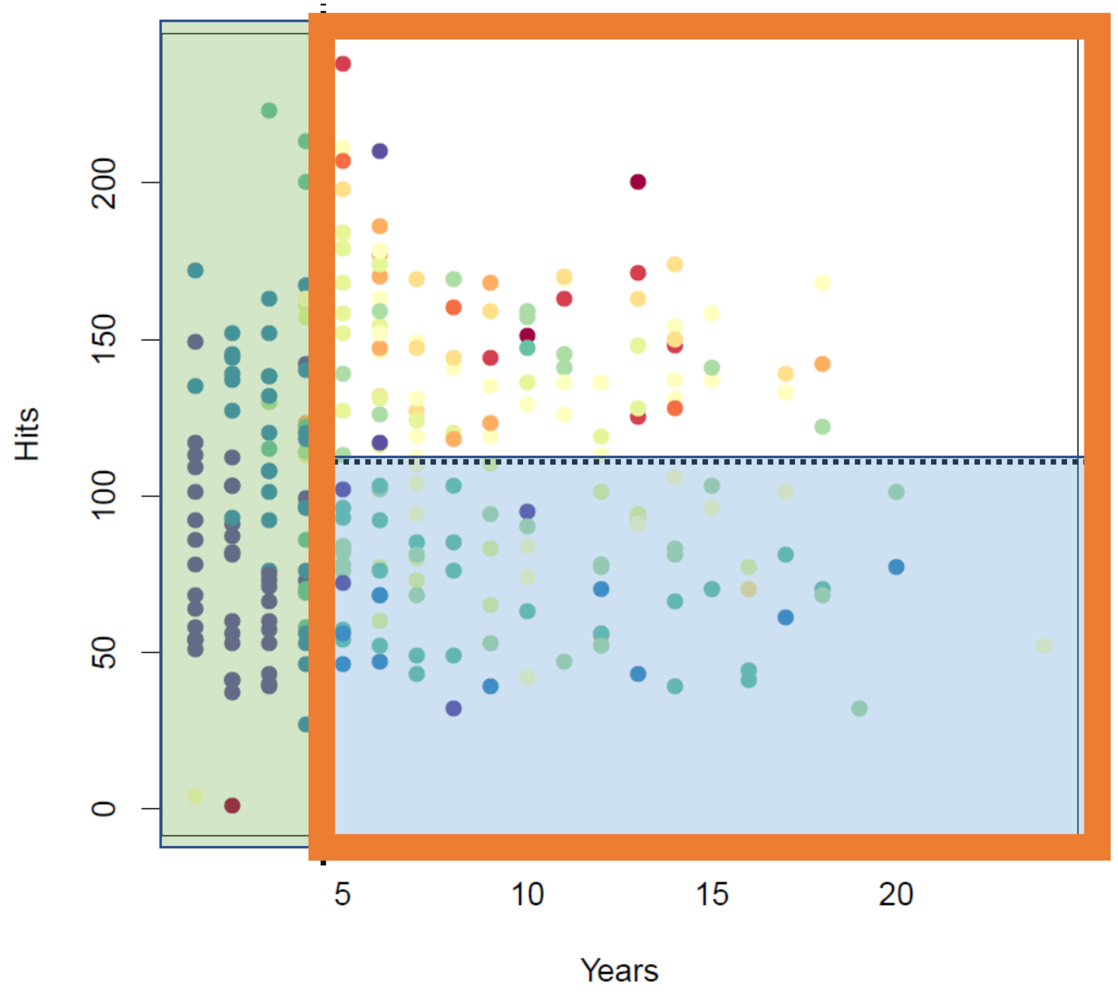

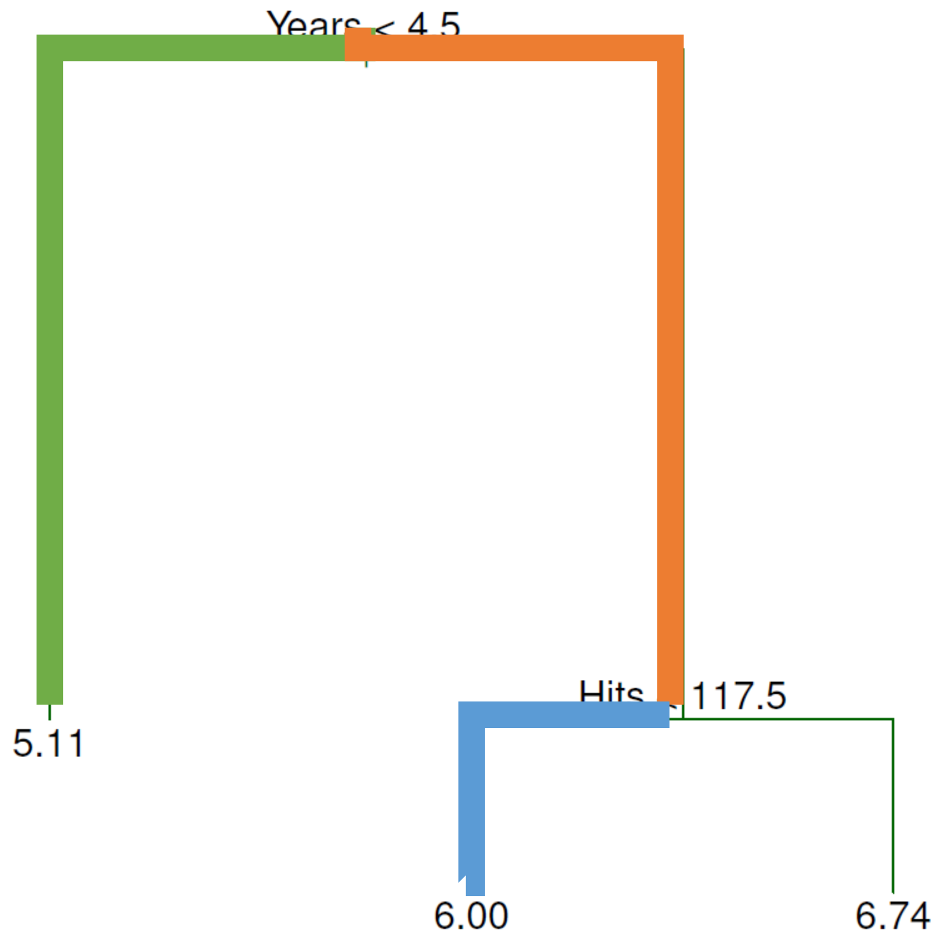

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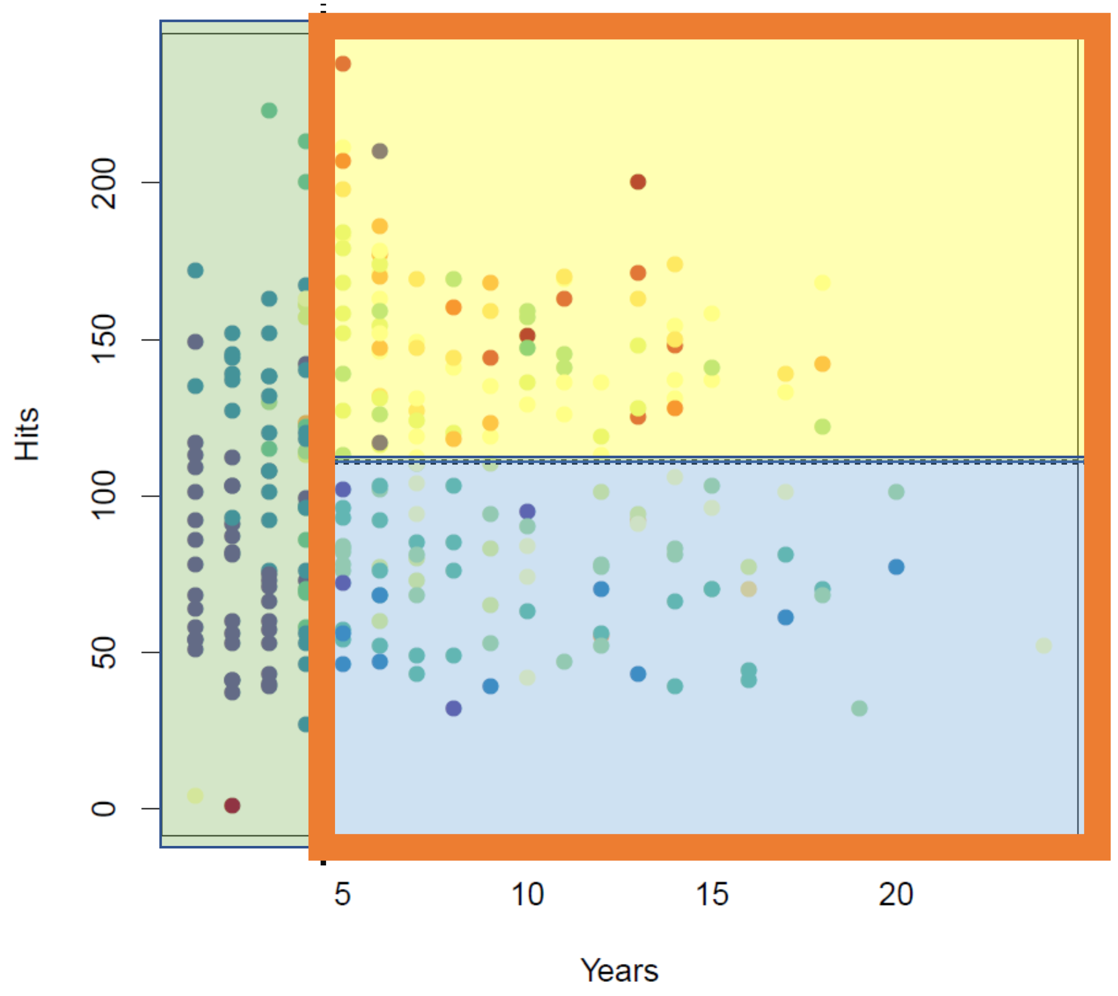

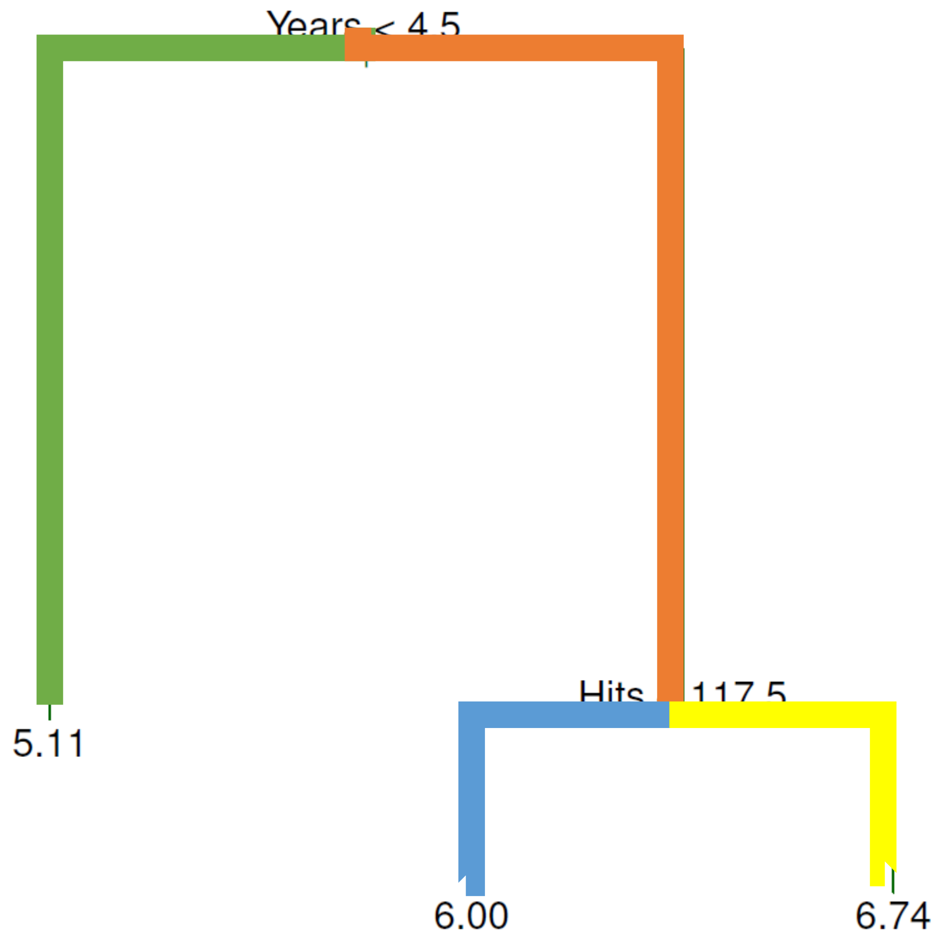

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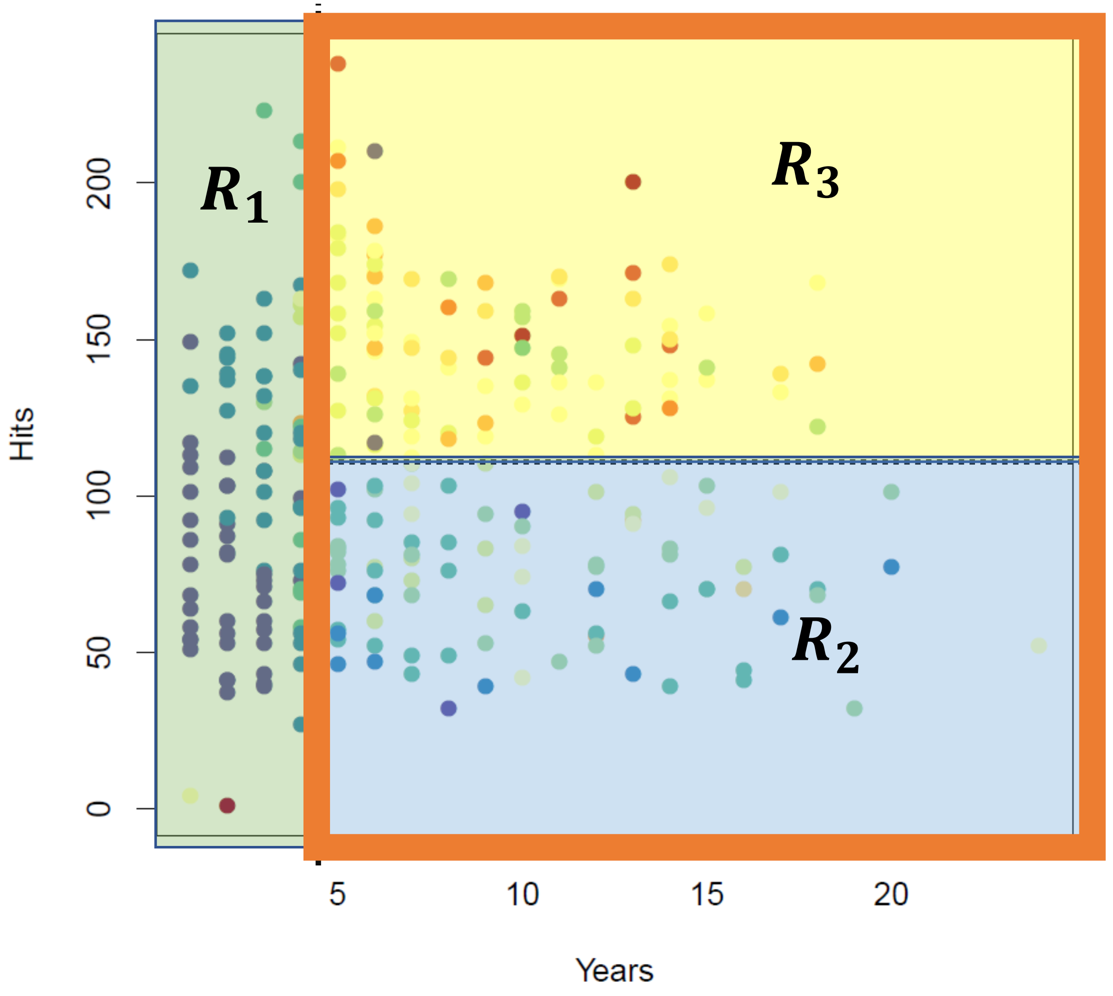

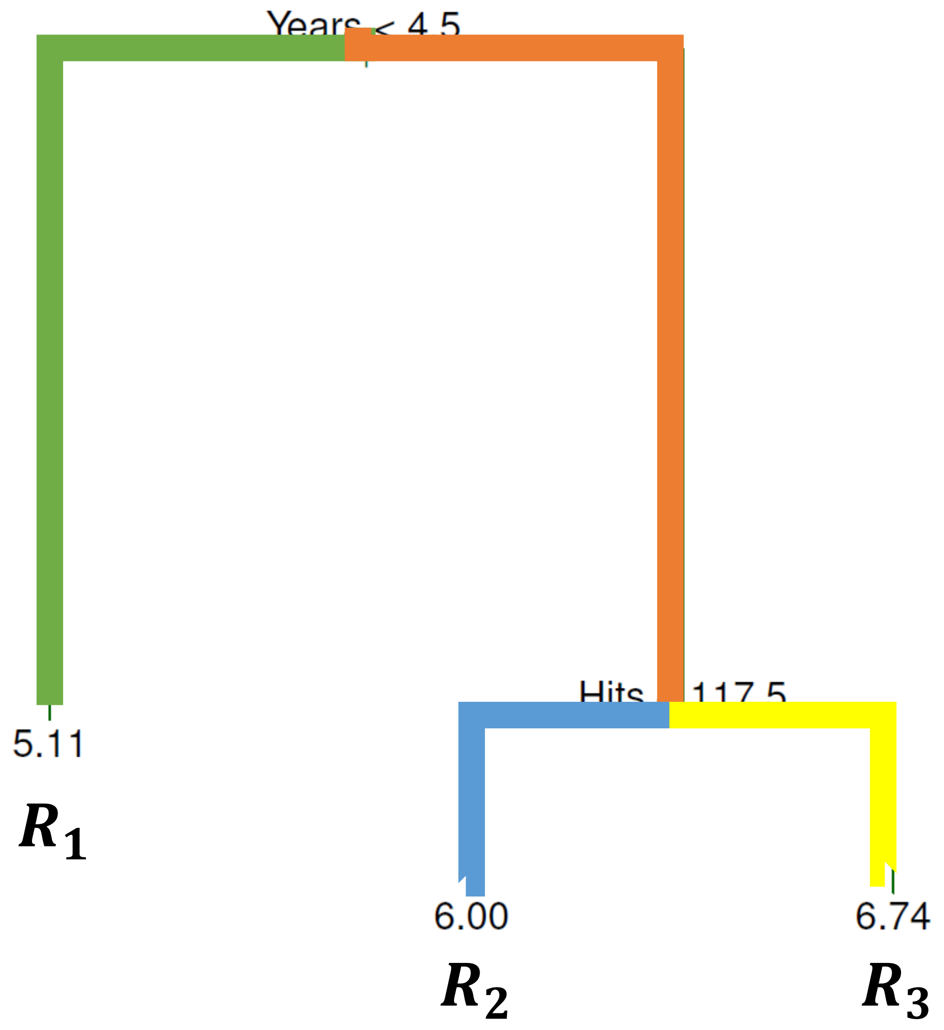

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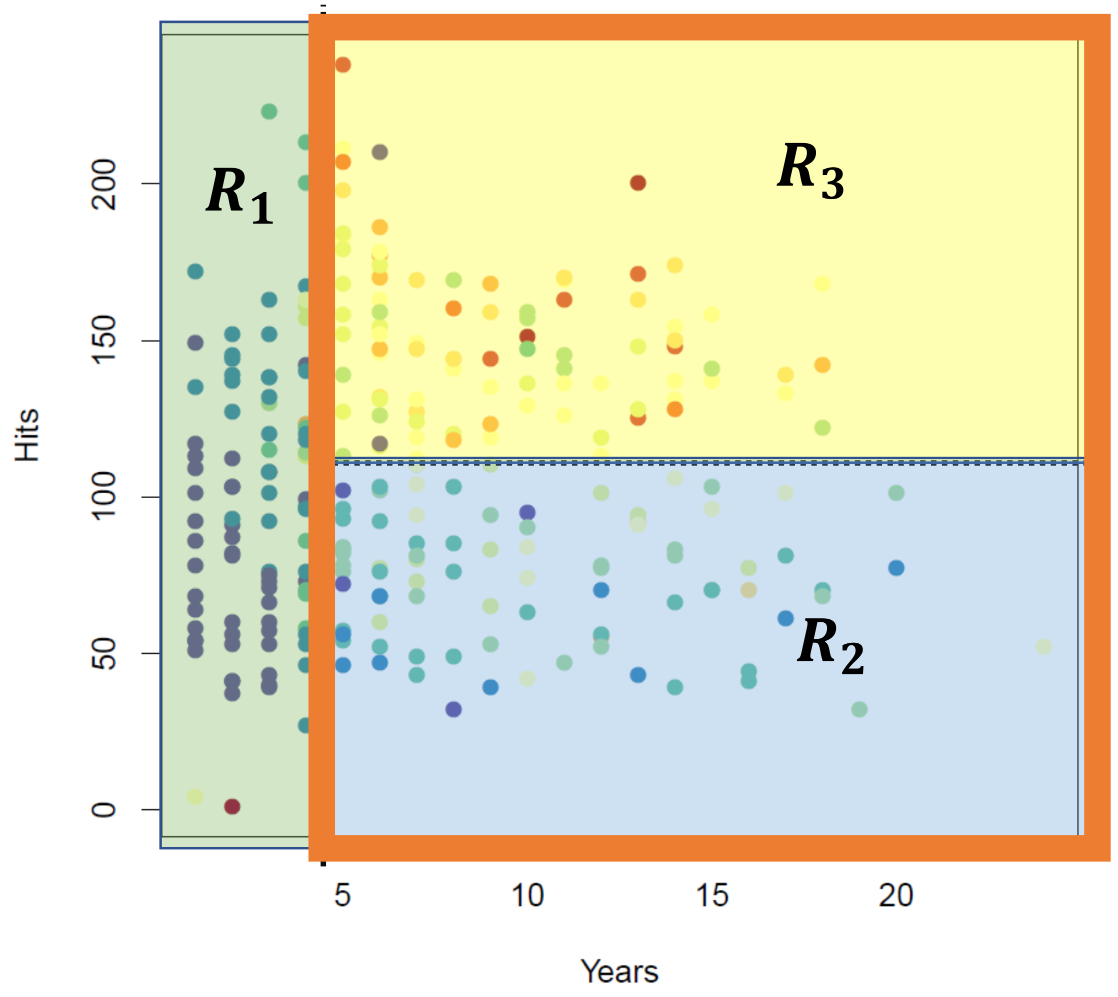

Overall the tree segments the feature space into three regions:

$$R_1 = \{\boldsymbol{x}; Years < 4.5\}$$

$$R_2 = \{\boldsymbol{x}; Years < 4.5, Hits < 117.5\}$$

$$R_3 = \{\boldsymbol{x}; Years < 4.5, Hits \geq 117.5\}$$

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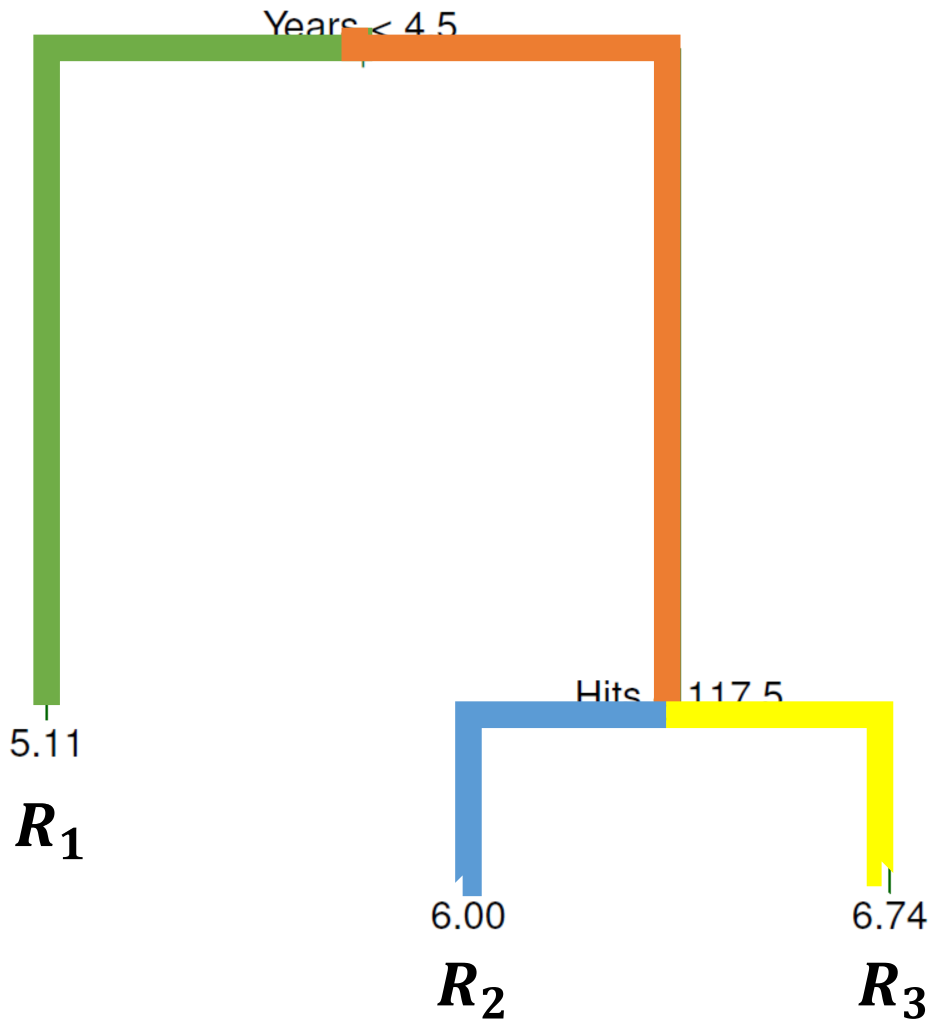

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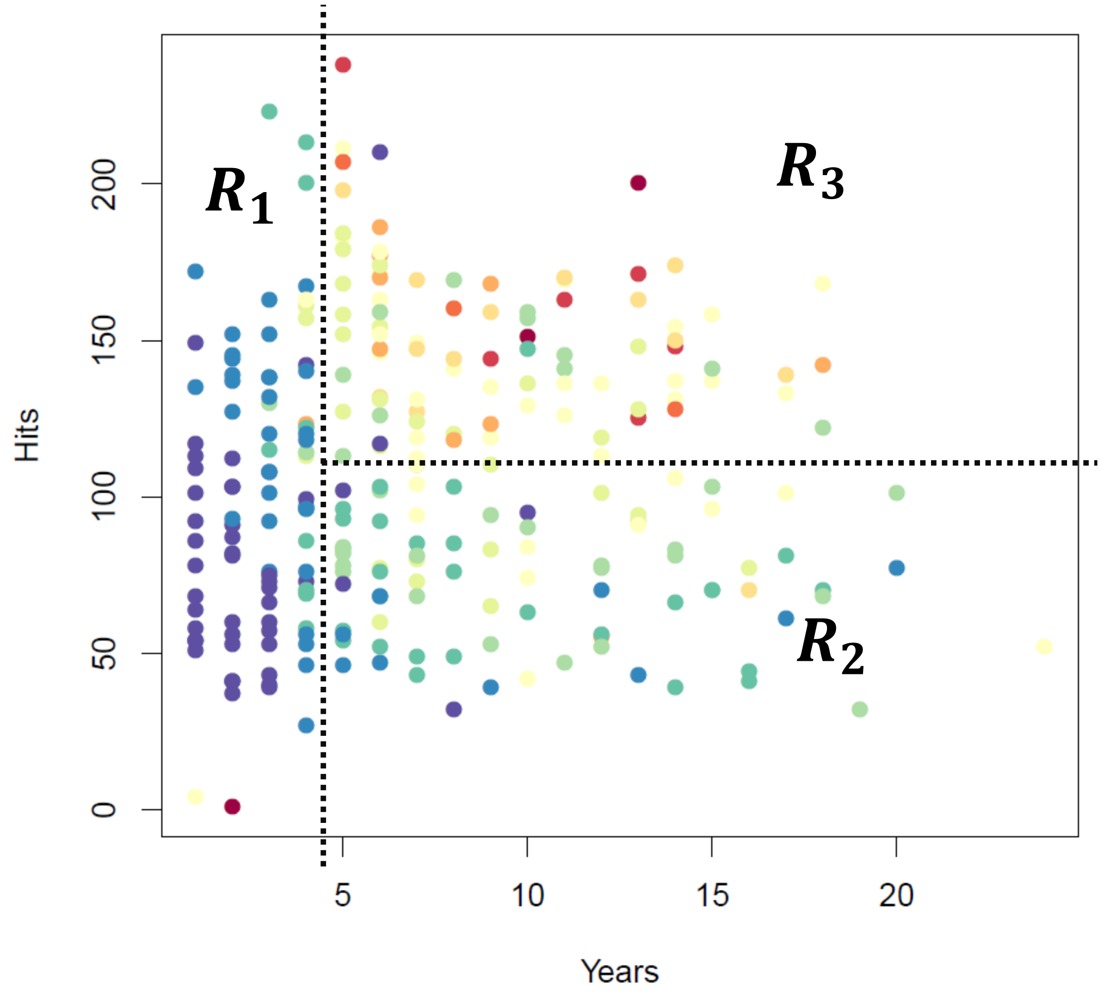
- In tree terminology, R_1, R_2, R_3 are known as terminal nodes whereas the nodes where the feature space is split are referred to as internal nodes.

Interpretation of Results



- *Years* is the most important factor in determining salary. Players with less experience earn lower salaries than more experienced players.

- Given that a player is less experienced, the number of *Hits* that he made in the previous year seems to play little role in his salary.

- Among players who have been in the major leagues for five or more years, the number of *Hits* does affect salary

Tree-building process - Regression

- Divide feature space into high-dimensional rectangles.
- The goal is to find rectangular regions $R_1, R_2, \ldots, R_J$ minimize error function:

$$E = \sum_{j=1}^{J} \sum_{i \in R_j} \left(x_i - \bar{x}_{R_j} \right)^2$$

where $\bar{x}_{R_j}$ is the mean of the training samples within region R_j .

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- Well… this is computationally infeasible! Thus we follow a greedy approach:
  - top-down approach: successively split feature space; each split is indicated via two new branches further down on the tree.
  - At each step, best split is made at that particular step, instead of looking ahead and picking a split that will lead to a better tree in some future step. (greedy approach)

Tree-building process - 2

- First select the feature x_i and the cutpoint s in order to split the feature space into two regions: $\{\boldsymbol{x}: x_i < s\}$ and $\{\boldsymbol{x}: x_i \geq s\}$ for which E is minimized.

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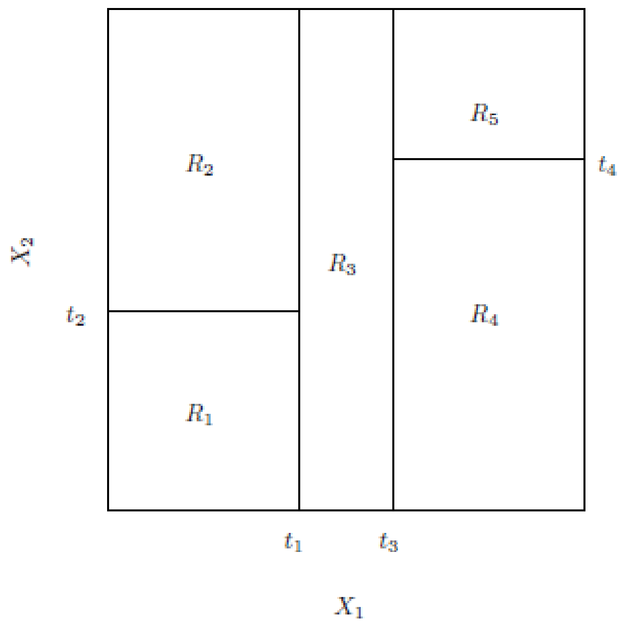
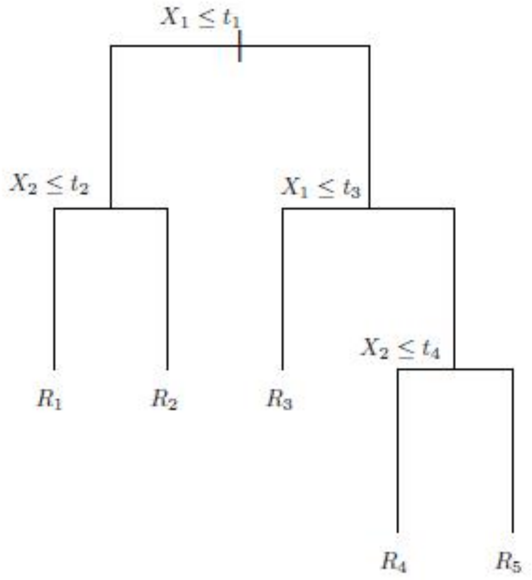
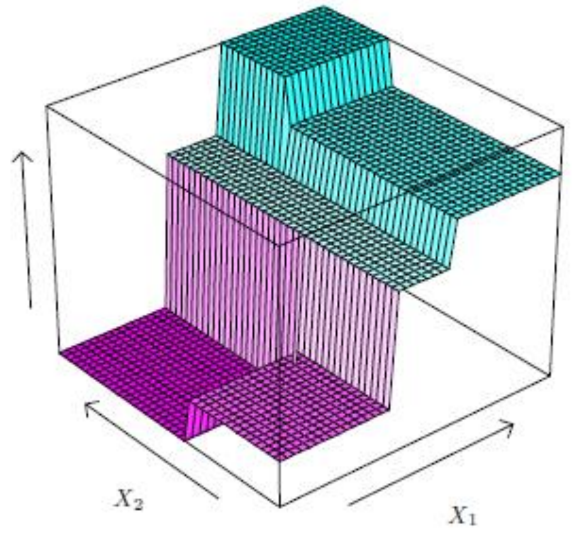
- Predict the response for a given test sample by assigning the mean (regression) of the training samples in the region where the test sample belongs.

Example







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- Left: The output of recursive binary splitting on a two-dimensional example.
- Center: A tree corresponding to the partition in the top right panel.
- Right: A perspective plot of the prediction surface corresponding to that tree.

Tree Pruning

- The abovementioned process may result in overfitting (really large trees). (remember with shallow trees I may get underfitted models).

- An alternate approach would be to grow a tree only so long as E decreases more than a certain threshold.

- This would result in medium sized trees but would cause the loss of larger decrease later on the training process.
    - seemingly worthless split early on in the tree might be followed by a very good split later on.

- A better strategy would be to grow a very large tree T_0 and then prune it in order to obtain a subtree that meet certain restrictions.
    - Grow T_0 and then prune it to T with a smaller number of terminal nodes $|T|$.

Decision Tree – Classification (K classes)

- Same as in the regression case but we now split the feature space by minimizing

$$E = \sum_{j=1}^{J} Q_j$$

where Q_j can be one of the following options:

- Misclassification rate: $Q_j = 1 - \max_k(p_{jk})$
- Negative cross entropy: $Q_j = -\sum_{k=1}^{K} p_{jk} ln p_{jk}$
- Gini index: $Q_j = \sum_{k=1}^{K} p_{jk}(1 - p_{jk})$

where p_{jk} represents the proportion of training observations in the jth region that are from the kth class.

Ensemble methods

- DT are easily interpretable and nice to visualize. It is said that DTs more closely mirror human decision-making than other ML approaches.

- Unfortunately, DT have not the same level of predictive accuracy as other classification approaches we have seen so far.

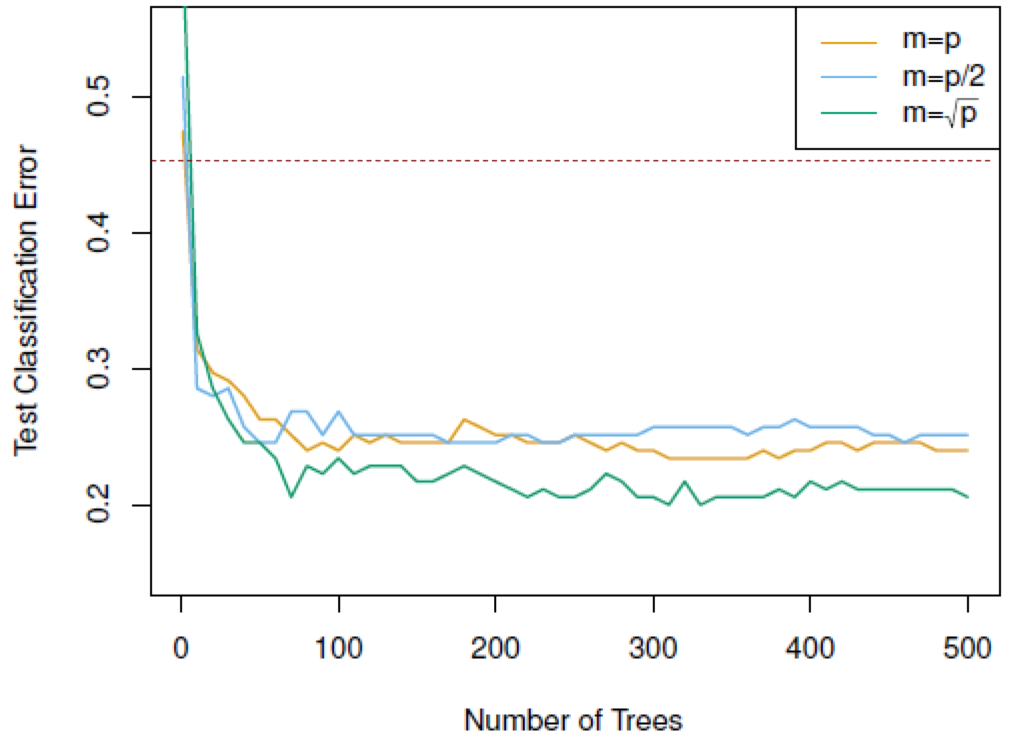
- Solution: Create ensembles of DTs!
  - Bagging/bootstrap aggregation with trees
  - Random Forests: bagging + random subspace methods
  - Boosting

Random Forests

- Bootstrapping can lead to highly correlated DT.
  - If there are a few very strong features in the dataset all bootstrapped trees will use these features to split space.
- Solution:
  - Build an ensemble of trees by bootstrapping the dataset.
  - Use a feature bagging/random subspace method: for each tree, every time a split is under consideration, a random selection of m out of p features is chosen as a split candidate.
  - At each split a new selection is made

Random Forests - Example

- Gene expression dataset
- Task: classify cancer type based on $p = 500$ gene expressions (features).
- Random Forests $(m < p)$
- Just bootstrapping $(m = p)$
- Random Forests exhibit small improvement over just bootstrapping.
- Single tree performance (red dashed line) is much worse (45.7%)



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Sum up

- We can combine multiple models using different methods
  - Bootstrapping/Bagging
  - Random subspace methods/Feature Bagging
  - Boosting

- Trees are weak classifiers but with nice interpretability.

- Bagging, random forests and boosting are good methods for improving the prediction accuracy of trees.

- Random Forests and boosting are among the state-of-the-art methods for supervised learning but their results can be difficult to interpret.
  - The more complexity we add the more difficult it becomes to interpret out results.

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Questions?

Pattern Recognition & Machine Learning

Model Combination - Trees

Fall Semester