S&DS 355 / 555

Introductory Machine Learning

(Decision) Trees

Tuesday, September 24th

Prof. Elisa Celis

Yale

Updates and Announcements

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- Assignment 2 is due on Thursday, Sept 26.
- Quiz 1 will be given during the first 10 minutes of class on Oct 1 (includes this week's material!).

Classification and Regression Trees (CART)

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- Can be used for either classification or regression.
- Feature variables can be categorical or quantitative.
- Yields a set of interpretable decision rules (popular in medicine).
- Predictive ability is often mediocre, *but* can be improved with ideas of resampling (will be covered on Thursday).

Trees

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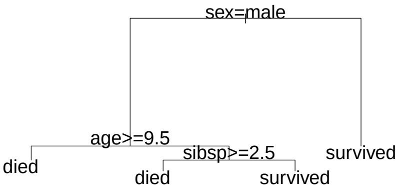
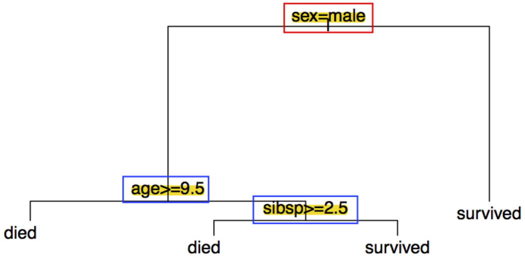
Modeling Titanic survival (classification tree):



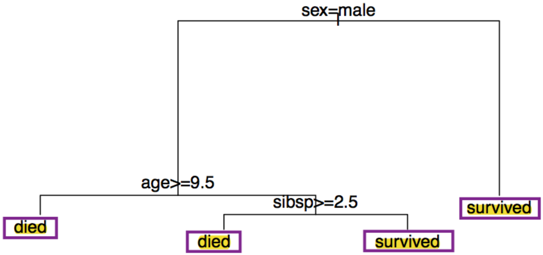
Tree terminology

Internal nodes are points where the predictor space is split.



Tree terminology

Terminal nodes (or **leaves**) are the ends of the tree where no further splitting occurs.



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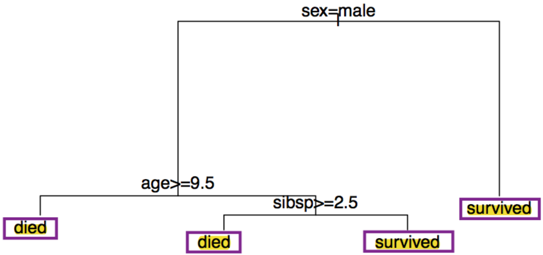
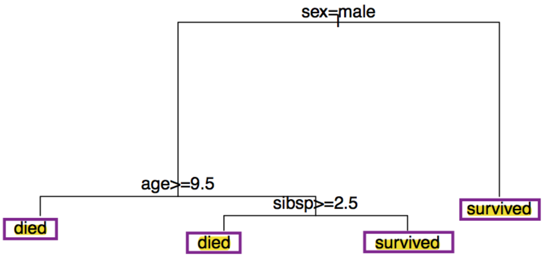


Denote these J regions as $R_1, \ldots, R_J$.

Tree terminology



- $R_1 = \{i : \text{sex}_i = \text{male} \cap \text{age}_i \geq 9.5\}$
- $R_2 = \{i : \text{sex}_i = \text{male} \cap \text{age}_i < 9.5 \cap \text{sibsp}_i \geq 2.5\}$
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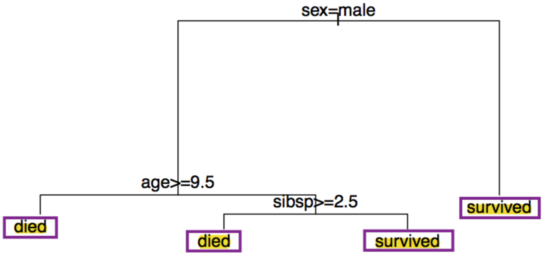

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Regions are disjoint and cover the whole space.

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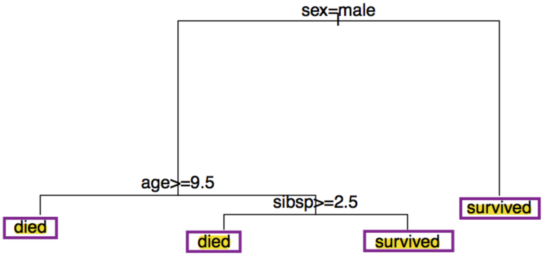

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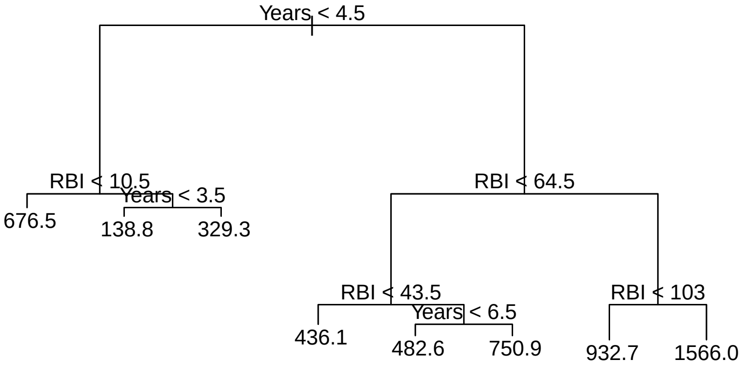
This is a classification tree – each region corresponds to a decision.

Regression tree example

Baseball hitter salaries (1987) (in $1,000s):



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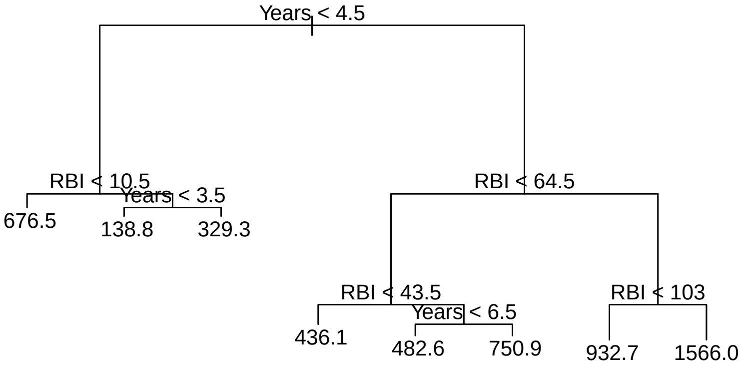

This is a regression tree – each region corresponds to an output value.

Prediction using trees

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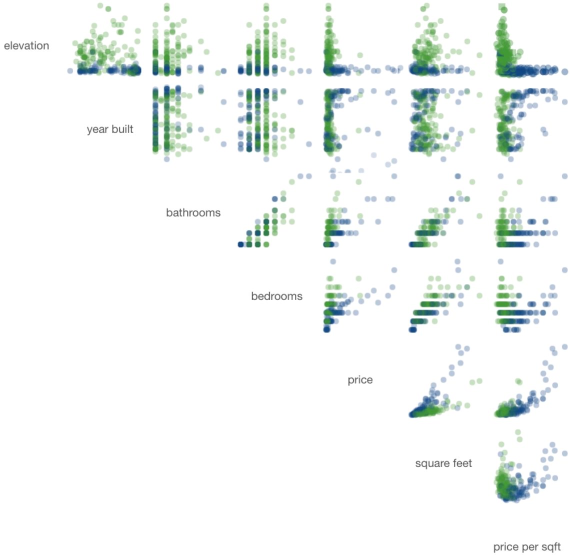
Fitting a tree boils down to identifying the appropriate set of regions $R_1, \ldots, R_J$ that "best" describes the relationship between X and y.

How to build a (classification) tree?

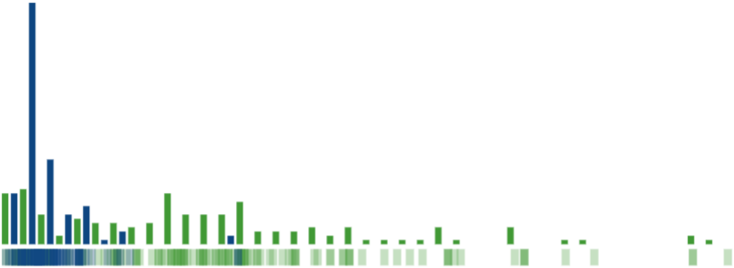
Example: New York vs San Francisco housing data.



How to build a (classification) tree?

Let's start with one feature: elevation.
Where should we create a split?

Rule of thumb: try to split the data into two homogeneous parts.



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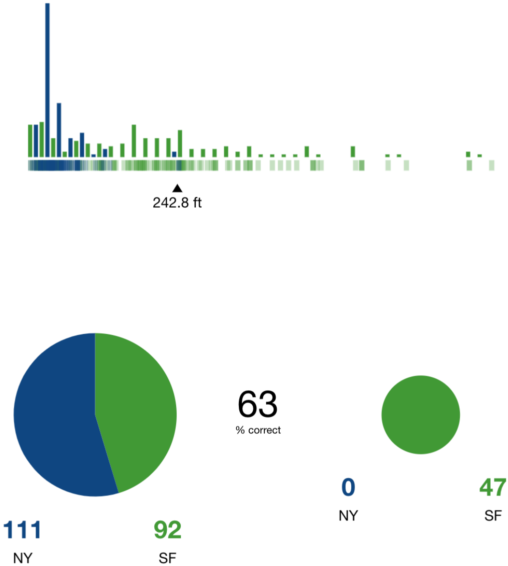

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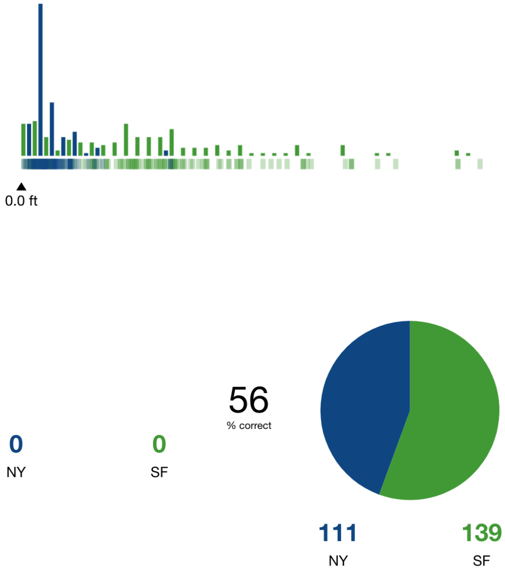

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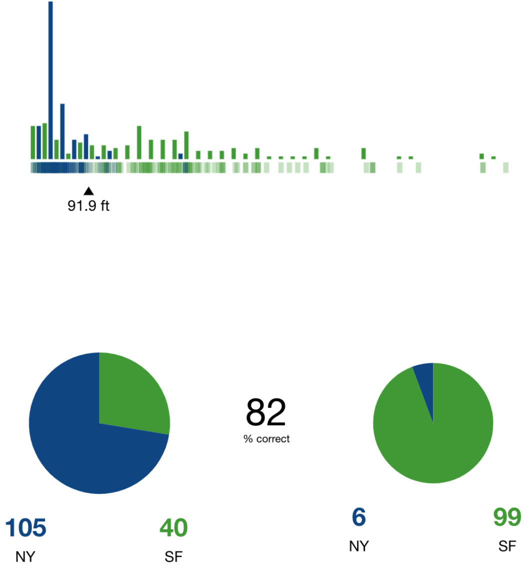

How to build a (classification) tree?

More formally...

Let $\widehat{p}_{jk}$ be the proportion of training observations of class k in R_j.

Recall: $\widehat{y}_j$ is *most commonly occurring class* of training observations in R_j: i.e., $\widehat{y}_j = \arg\max_k \widehat{p}_{jk}$

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- Classification error rate (as in the example above)

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- Other potential metrics...

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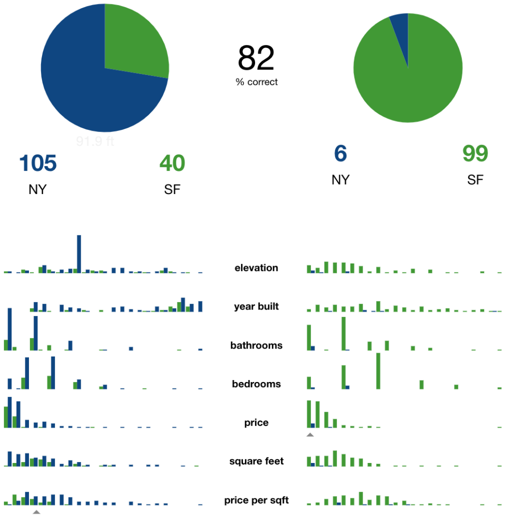

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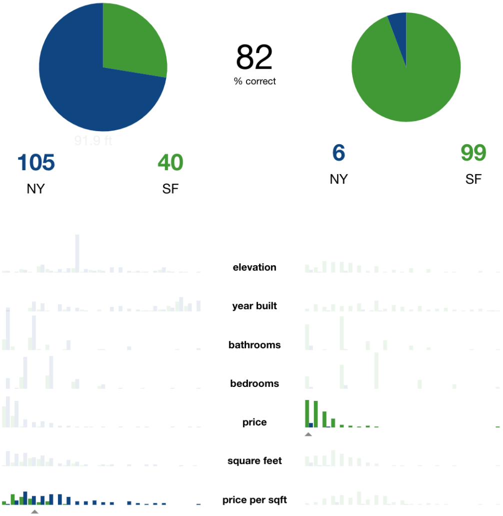

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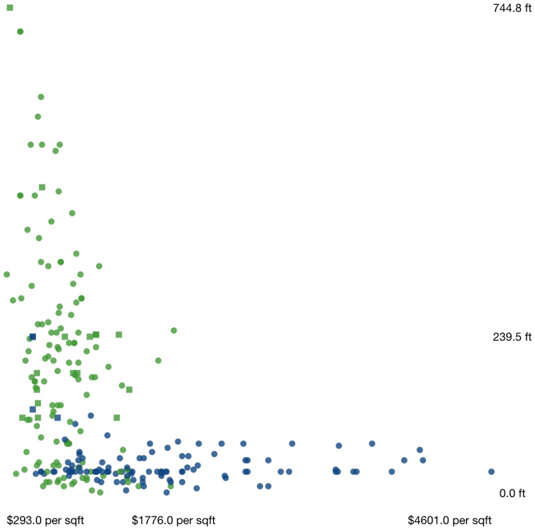
Alternate visualization for 2D:



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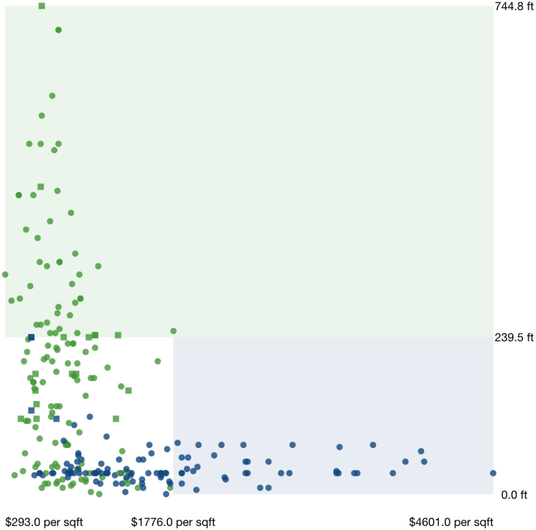
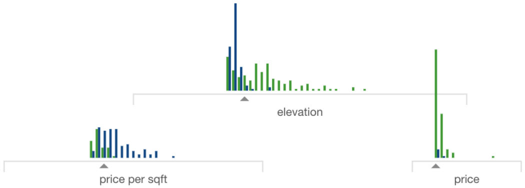


How to build a (classification) tree?

Recurse: For each branch, select another feature to split on until all leaves are pure.



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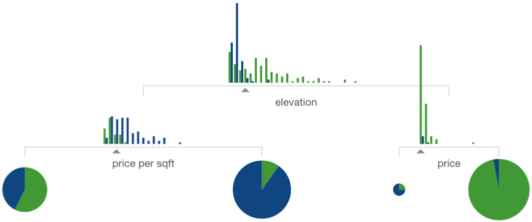

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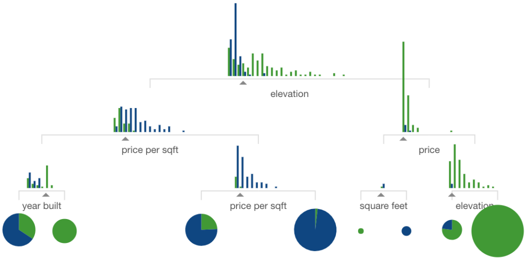

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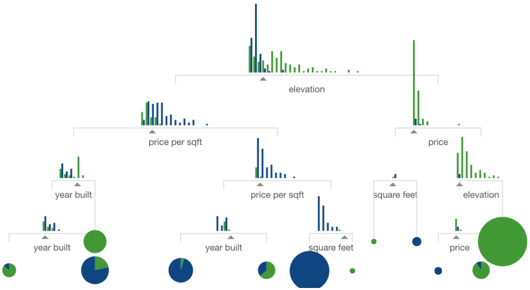

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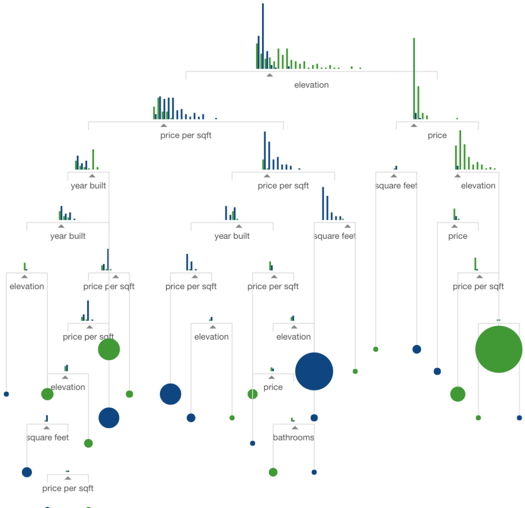

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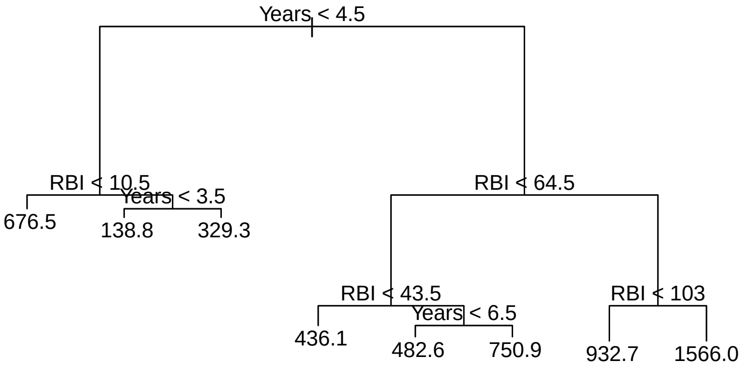

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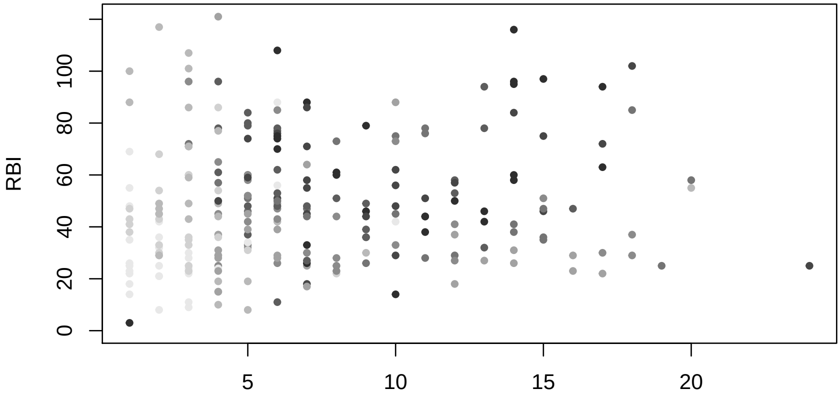
Let's look at the 2D version:

Where can we draw a horizontal or vertical line that best splits the data into two homogeneous parts?



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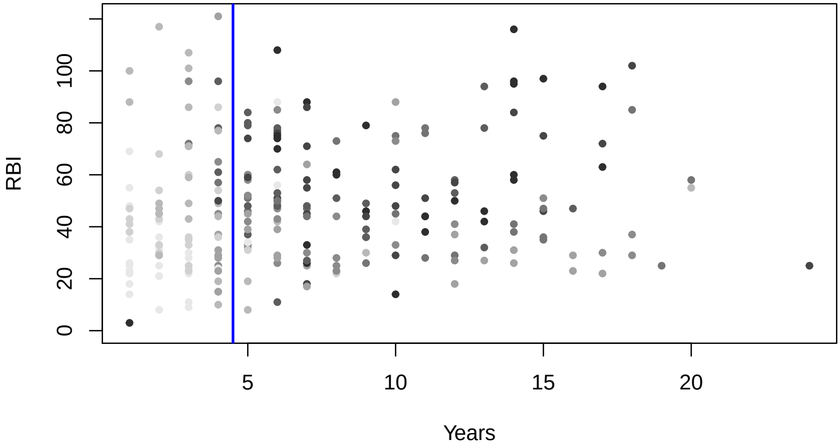

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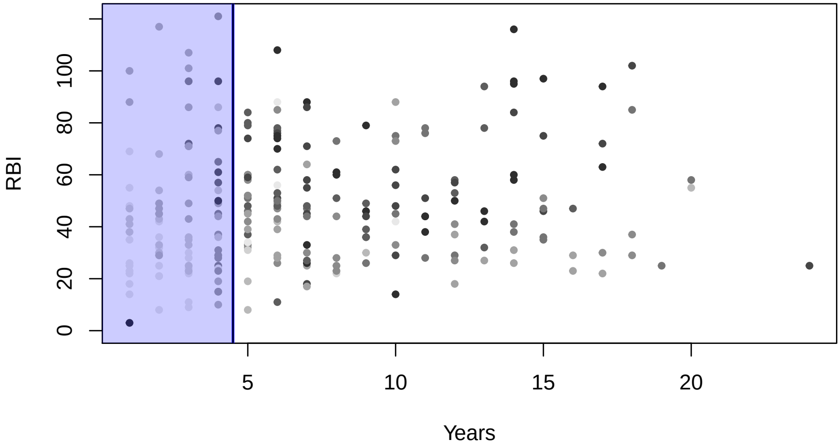

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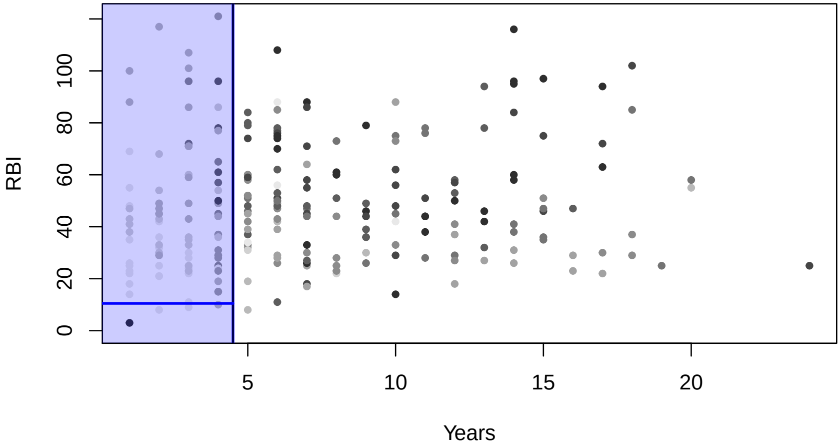

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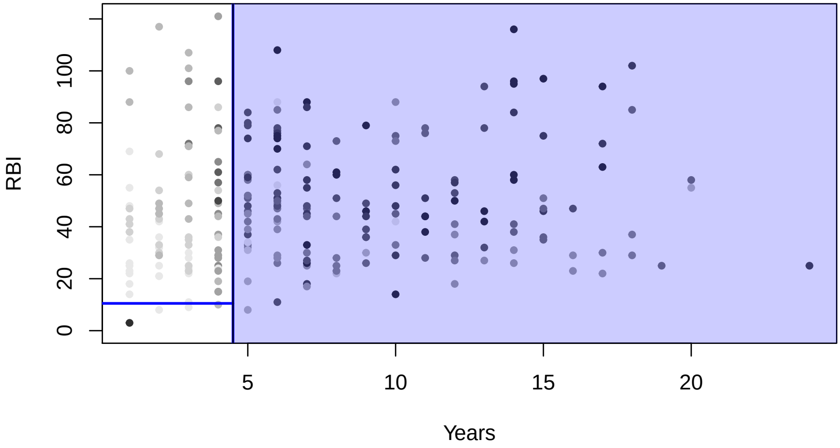

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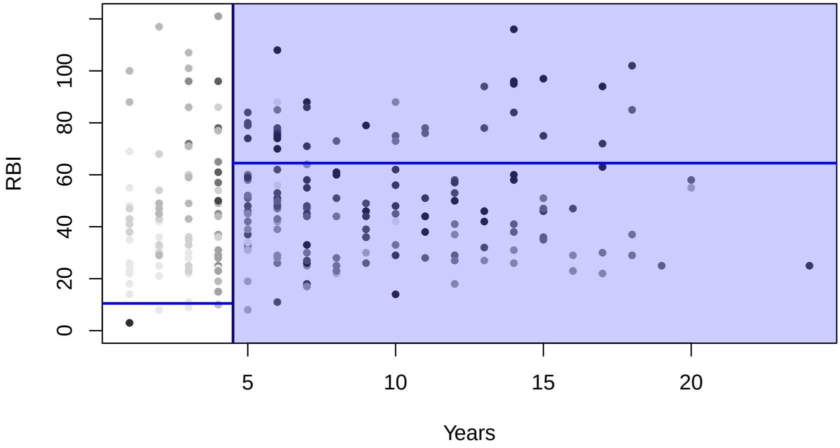

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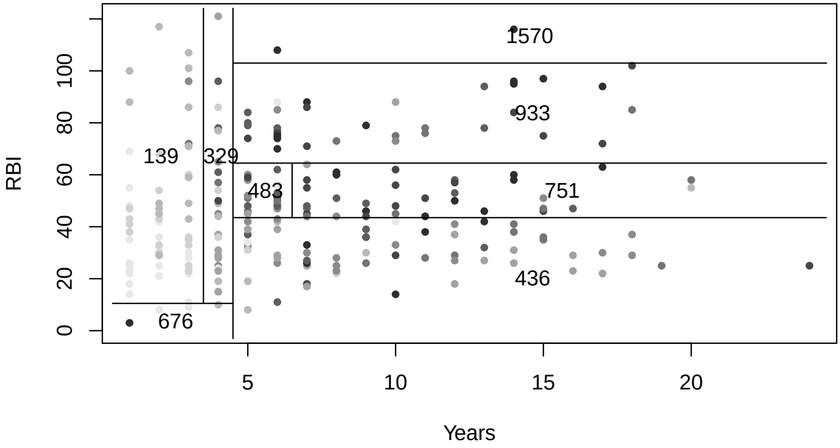

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More formally...

We again want to choose $R_1, \ldots, R_J$ to minimize error. In this case, the residual sum of squares:

$$RSS = \sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \bar{y}_{R_j})^2$$

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This is called a **stopping criterion** – we will consider others later.

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   - Consider cutpoints s (i.e., unique values of X_k) that divide the training points in region R_v into two parts. E.g.:

$$R_{v1}(k, s) = \{i \mid X_{ik} < s\} \quad \text{and} \quad R_{v2}(k, s) = \{i \mid X_{ik} \geq s\}$$

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   - Evaluate metric $Q_k(s)$ for each. E.g., for regression trees:

$$Q_k(s) = \sum_{i:i \in R_1(k,s)} (y_i - \bar{y}_{R_1})^2 + \sum_{i:i \in R_2(k,s)} (y_i - \bar{y}_{R_2})^2$$

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Repeat until all leaves have met stopping criterion.

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Then, the possible splits include:

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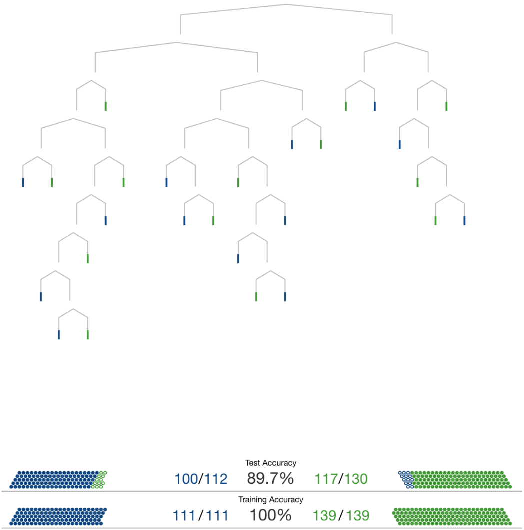
Every possible partition of the set into 2 subsets are considered, and we proceed as before.

Perfect Trees?

Using the above we built perfect trees... **for the training data.**
In reality:



Errors: Variance

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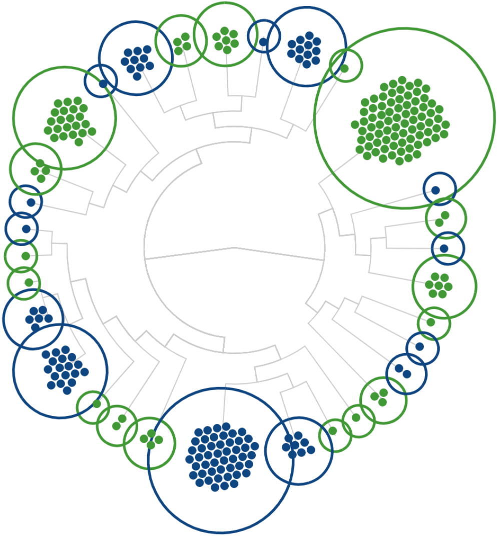

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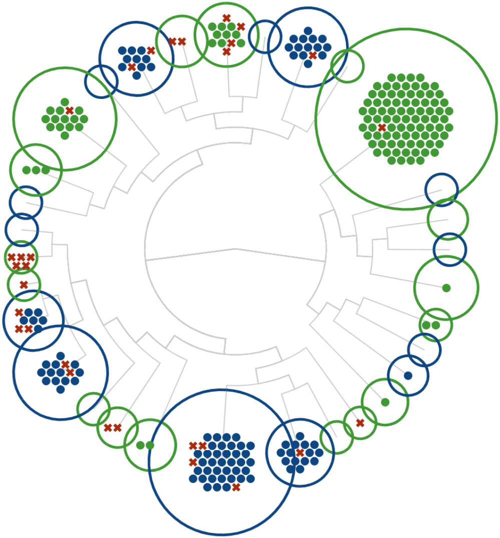

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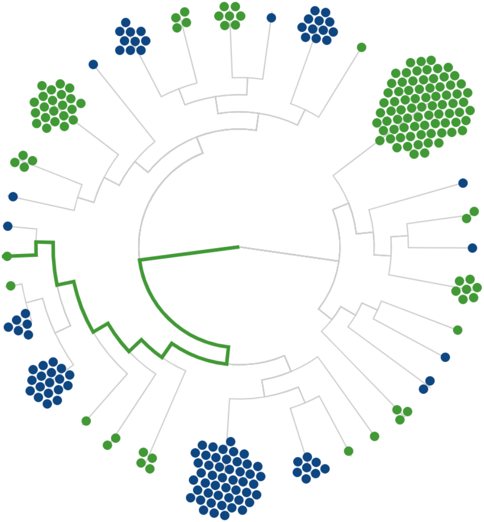

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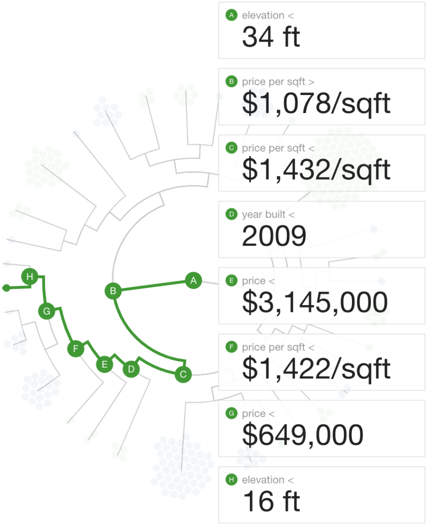

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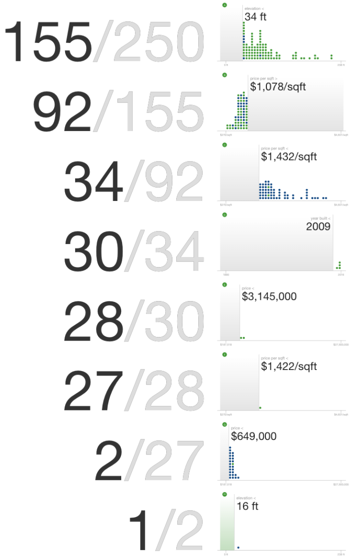

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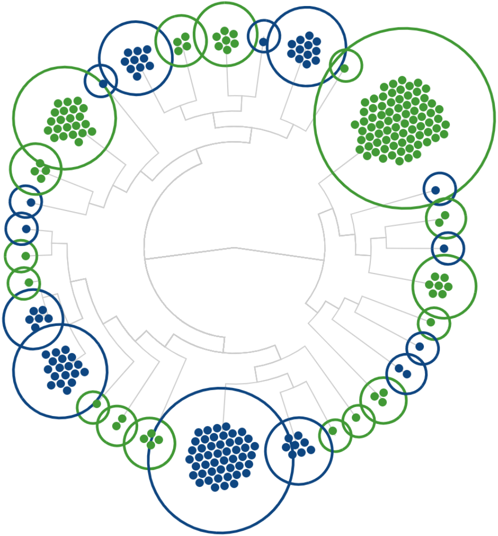

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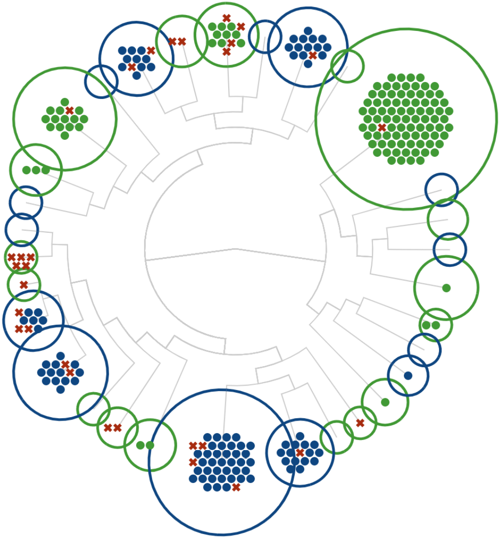

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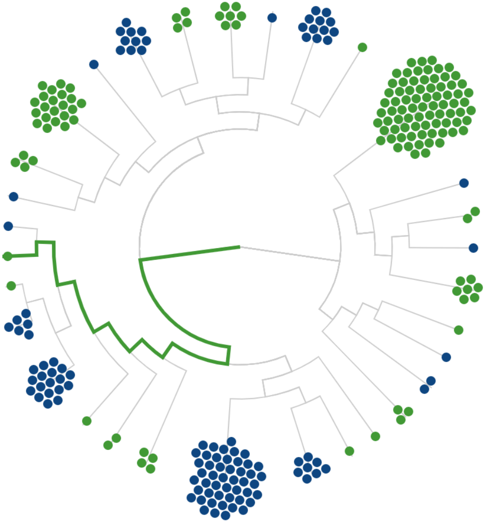

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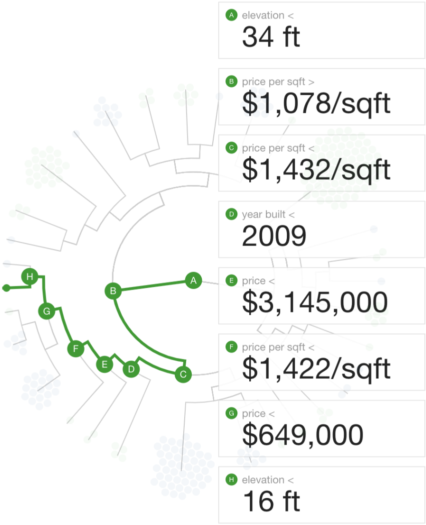

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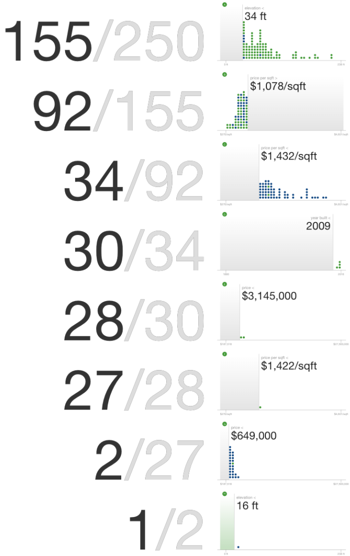

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What if we had a shorter tree?

Errors: Bias

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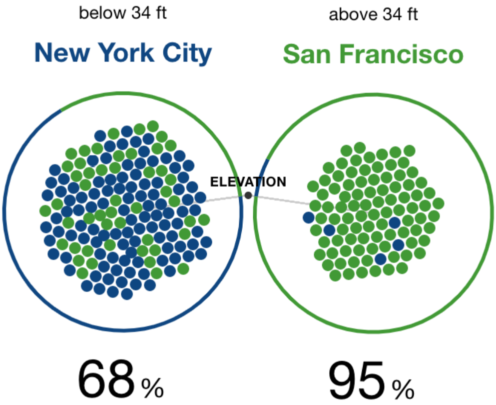

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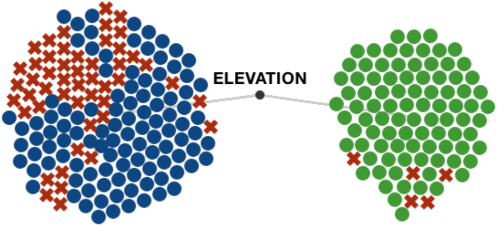
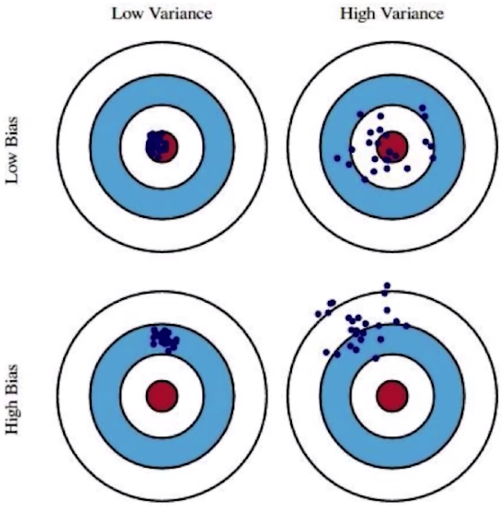


Bias vs Variance



Bias vs Variance

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Option 1: Change the stopping criterion.

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Some possibilities:

- number of observations in a node has reached a minimum

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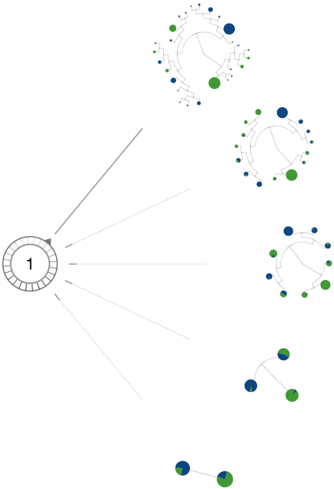
Many options – often resulting in tuning parameters that may be hard to deal with.

Stopping criterion

Example: Number of observations in a node has reached a minimum.



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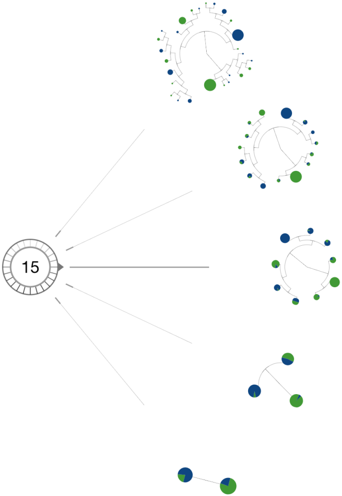
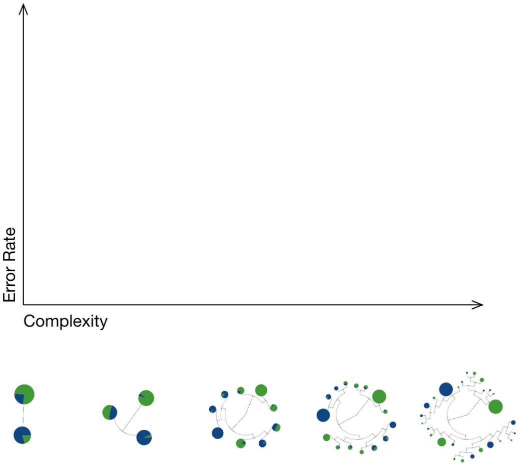


Bias vs Variance

Have to tune this parameter:



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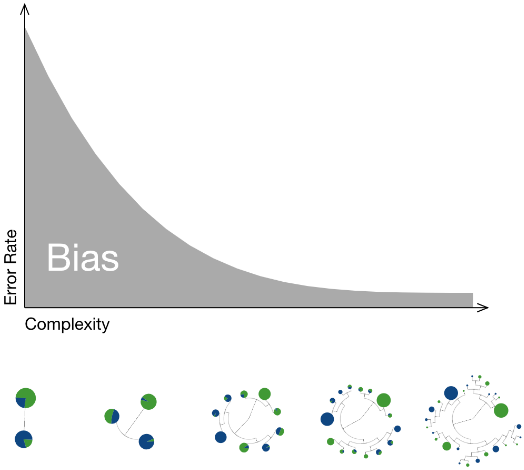

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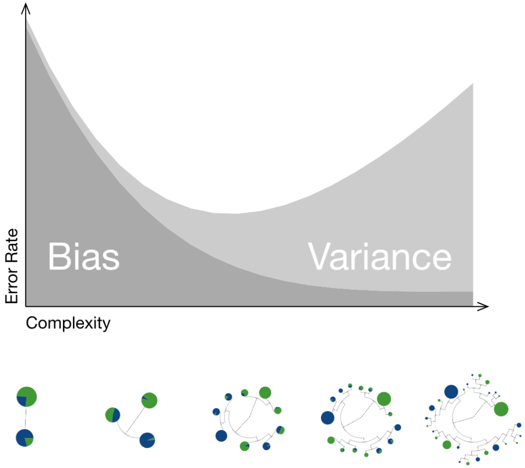

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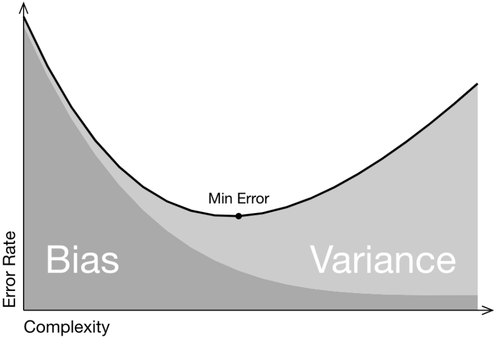

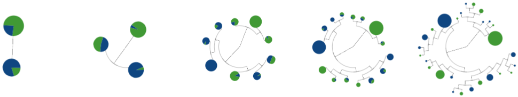

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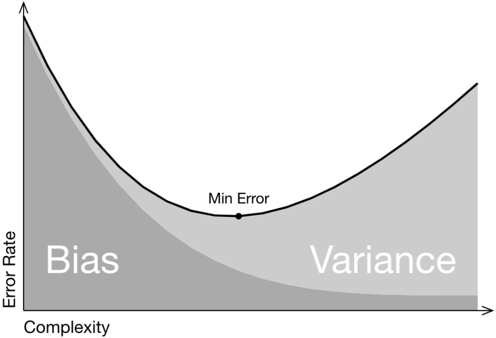

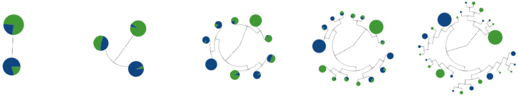

In general, these are coarse rules and not always ideal even when tuned.

Tree pruning

Option 2: Grow a large tree and then **prune** it back.

I.e., look at subtrees of the fully-grown tree, and comparing how well they perform.

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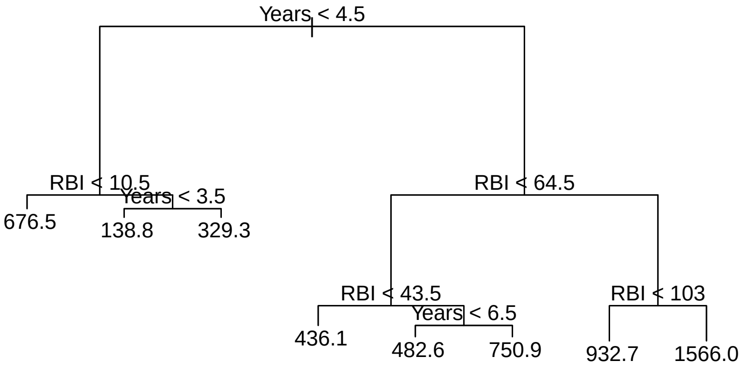

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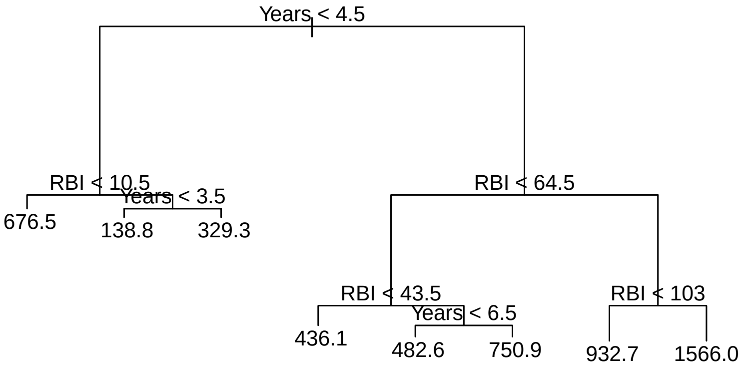

Cost-complexity pruning

$$C(T) = \sum_{m=1}^{|T|} \sum_{i \in R_m} (y_i - \widehat{y}_{R_m})^2 + \alpha |T|$$

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The set of trees corresponding to the various α form a sequence of nested subtrees!

Tree pruning

1. Grow a big tree on a *training set*.
2. Obtain the optimal set of nested subtrees $T_l \subset \cdots \subset T_2 \subset T_1 \subset T_0$ corresponding to the cost complexity minimization problem.
3. Identify the subtree/α that does best.

Nice properties of trees

- Interpretable.
- Inbuilt feature selection – irrelevant covariates won't be used as often as splits.
- Simple, fast implementation – (mostly) performs well with large datasets.

Problems with trees

- Instability – tree topology can change dramatically with slight changes to data. Interpretability kind of an illusion.
- Greedy – cannot guarantee to find the globally optimal decision tree.
- Lack of smoothness – the splits lead to a “jagged” decision boundary.
- Difficulty capturing additive structure – if the actual model is additive, this may not be captured by the tree with limited data.

What did we learn today?

- Trees are a nonparametric method
- Gives interpretable decision rules
- Shallow trees have high bias and low variance, deep trees have low bias, high variance
- Trees are grown greedily to the full, then pruned back