S&DS 265 / 565

Introductory Machine Learning

Trees

Tuesday, October 5

Yale

Plan for this and next week

- Assn 2 due tonight
- Keep in mind reminders from last week (select pages in Gradescope, rerun notebook, length of output, line wrap)
- Assn 3 out today — decision trees
- Next week: Quiz 2 (Tuesday); SGD, bias-variance, CV, trees
- Midterm exam: Tuesday October 19 (in class); practice exam released next week
- Questions?

You are here

3	Sept 14, 16	Linear regression and classification	Covid trends (revisited) Classification examples	Tue: Assn1 out	Sept 14: Regression concepts Notes on regression Sept 16: Classification Notes on classification
4	Sept 21, 23	Stochastic gradient descent	SGD examples	Tue: Quiz 1 Thu: Assn 1 in Assn2 out	Sept 21: Classification (continued) Sept 23: Stochastic gradient descent
5	Sept 28, 30	Bias and variance, cross-validation	Bias-variance tradeoff Covid trends (revisited) California housing		Sept 28: Bias and variance Sept 30: Cross-validation
6	Oct 5, 7	Tree-based methods	Trees and forests	Tue: Assn 2 in; Assn 3 out	
7	Oct 12, 14	PCA and dimension reduction	PCA examples	Tue: Quiz 2 Thu: Assn 3 in; Assn 4 out	
8	Oct 19	Midterm exam (in class)			

Classification and Regression Trees (CART)

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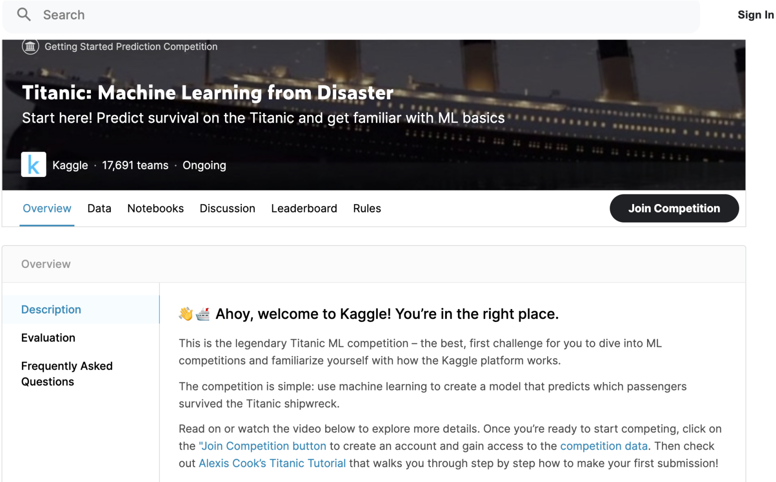
- Response variables can be categorical or quantitative.
- Yields a set of interpretable decision rules.
- Predictive ability is mediocre, *but* can be improved by combining multiple trees (resampling, ensemble methods)

Titanic data



Trees

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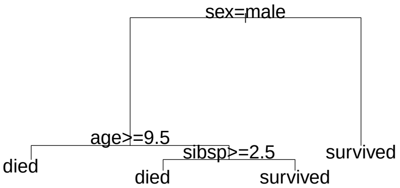
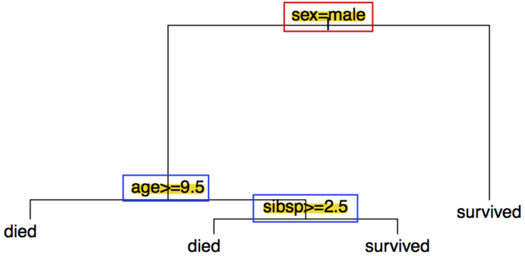
Modeling Titanic survival:



Tree terminology

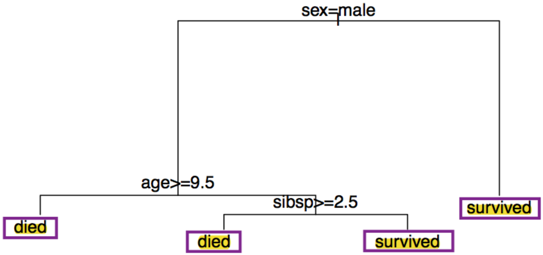
Internal nodes are points where the predictor space is split.



The internal node at the top is the **root** of the tree.

Tree terminology

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



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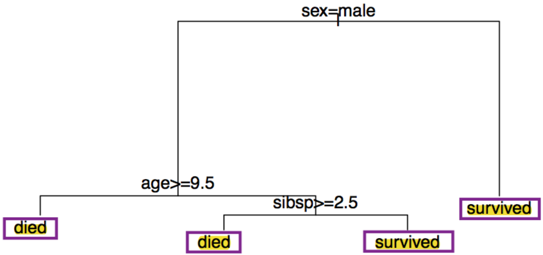
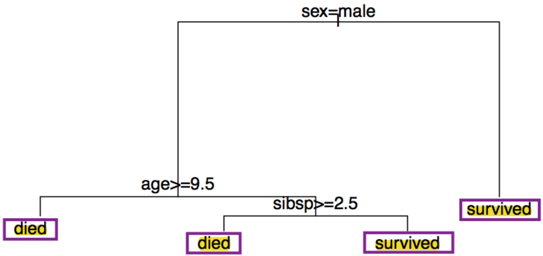


Denote these J regions as $R_1, \ldots, R_J$.

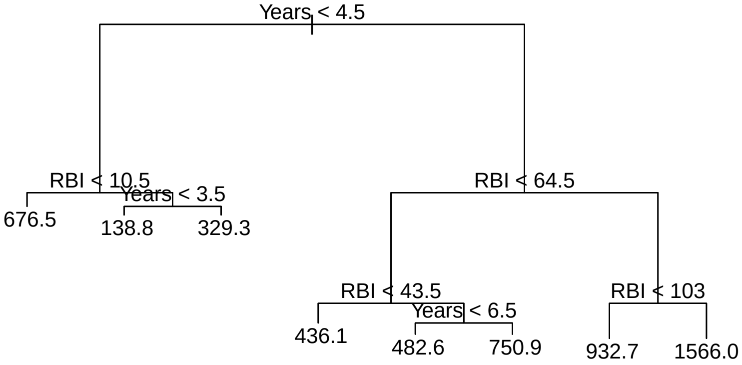
Tree terminology



- $R_1 = \{i : \text{sex}_i = \text{male} \cap \text{age}_i \geq 9.5\}$
- $R_2 = \{i : \text{sex}_i = \text{male} \cap \text{age}_i < 9.5 \cap \text{sibsp}_i \geq 2.5\}$
- $R_3 = \{i : \text{sex}_i = \text{male} \cap \text{age}_i < 9.5 \cap \text{sibsp}_i < 2.5\}$
- $R_4 = \{i : \text{sex}_i \neq \text{male}\}$

Regression tree example

Baseball hitter salaries (in $10,000s):



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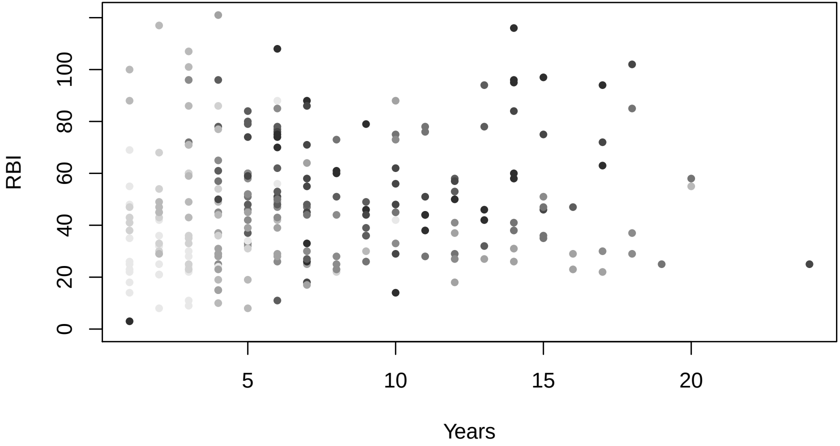

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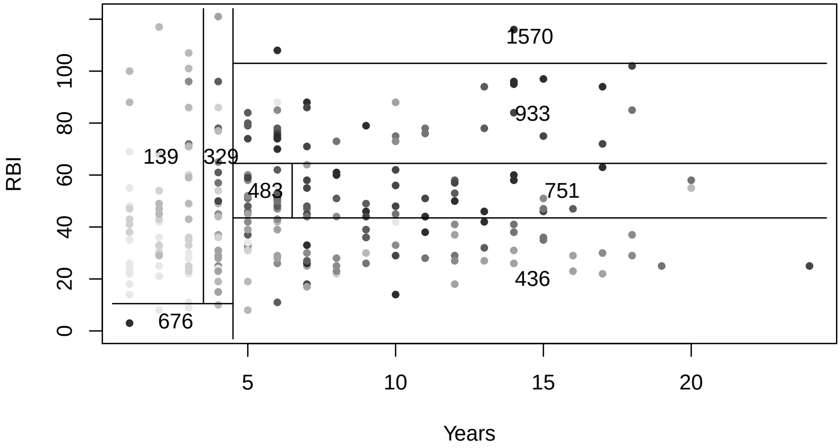

Prediction using trees

Trace each test observation into a leaf R_j based on the sequence of conditions. Predict $\widehat{y}_{R_j}$ for all observations in R_j.

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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.

Tree building

We want to choose $R_1, \ldots, R_J$ to minimize error:

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

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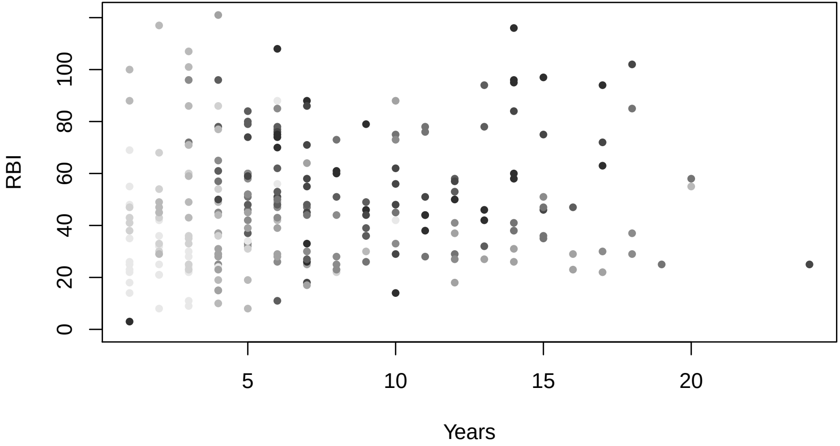
Tree building takes a *greedy* approach.

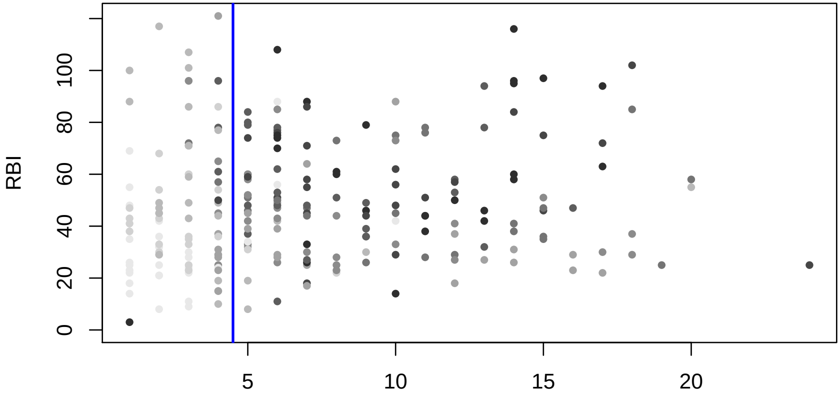
- Grow the tree by recursive binary splitting
- Prune back the tree

Tree growth



Tree growth

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



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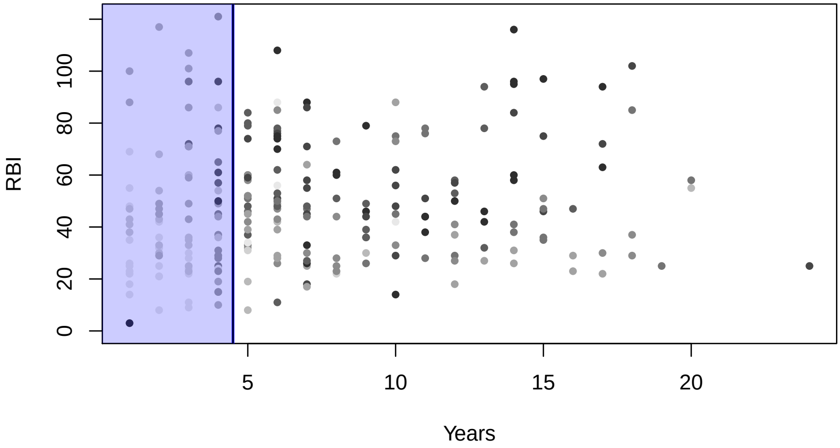

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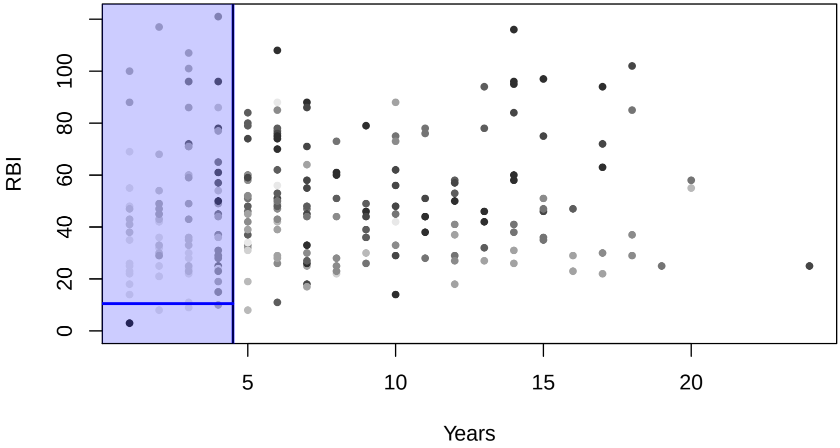

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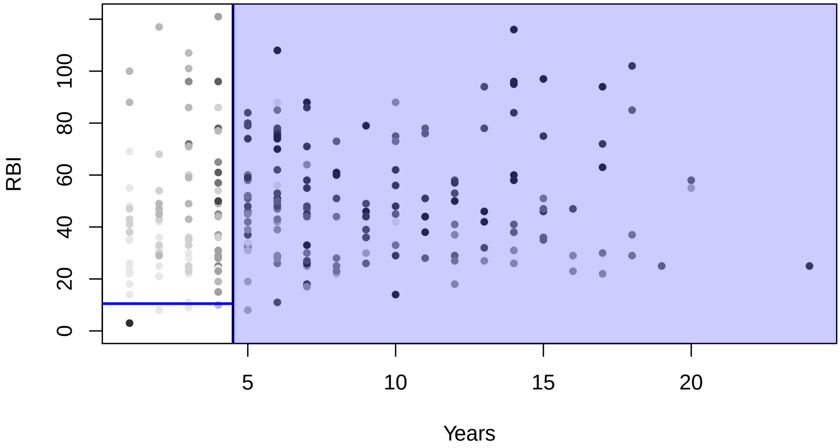

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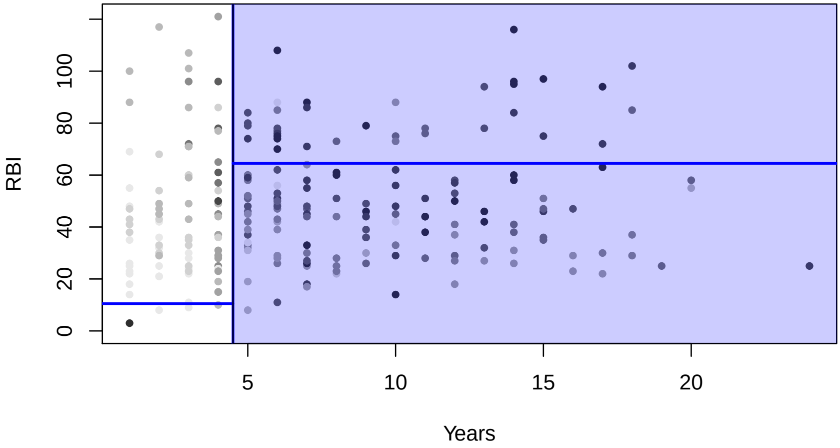

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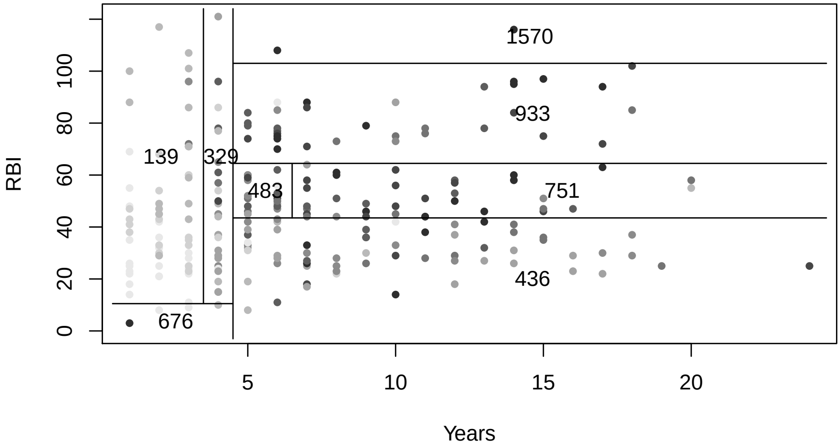

RBI
Years
0
20
40
60
80
100
5
10
15
20
1570
933
139
329
483
751
436
676

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   - Evaluate (for regression trees):

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

Example: Evaluating Q_{RBI}

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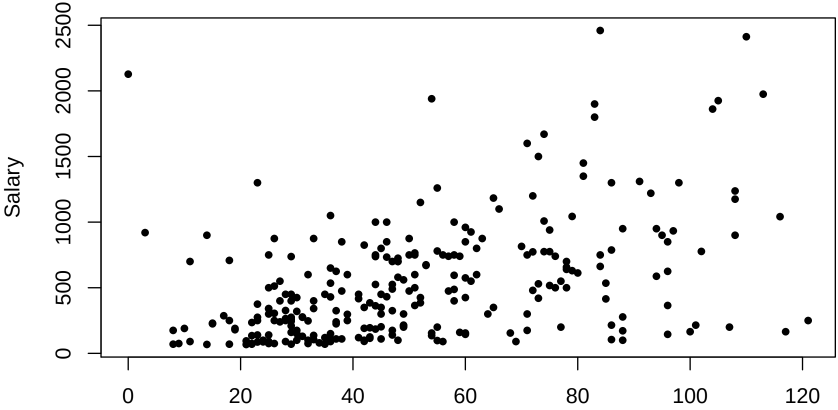

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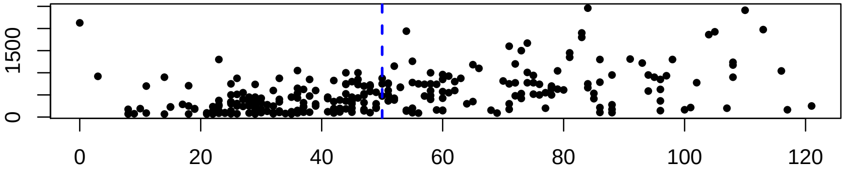

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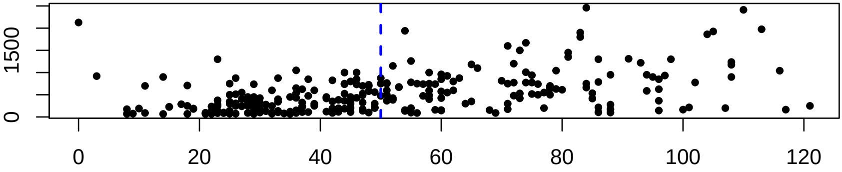

- $R_1(RBI, 50)$: $\bar{y}_{R_1} = 359$
- $R_2(RBI, 50)$: $\bar{y}_{R_2} = 753$
- $$\begin{aligned} Q_{RBI}(50) &= \sum_{i:i \in R_1} (y_i - 359)^2 + \sum_{i:i \in R_2} (y_i - 753)^2 \\ &= 13015000 + 30186039 \\ &= 43201039 \end{aligned}$$

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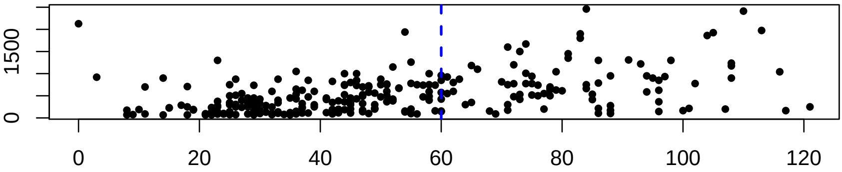

- $R_1(RBI, 60)$: $\bar{y}_{R_1} = 405$
- $R_2(RBI, 60)$: $\bar{y}_{R_2} = 802$
- $$\begin{aligned} Q_{RBI}(60) &= \sum_{i:i \in R_1} (y_i - 405)^2 + \sum_{i:i \in R_2} (y_i - 805)^2 \\ &= 19186489 + 24943383 \\ &= 44129872 \end{aligned}$$

Compute $Q_{RBI}(s)$ for all distinct values of RBI s.

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Every possible partition of the set of unique values into 2 subsets is considered, and again we identify the split producing the lowest resulting RSS.

Tree growth

1. Cycle through predictors X_k for $k = 1, \ldots, p$. For each X_k:
   - (Quantitative X_k) Consider cutpoints s (unique values of X_k) that divide up the region into two parts:

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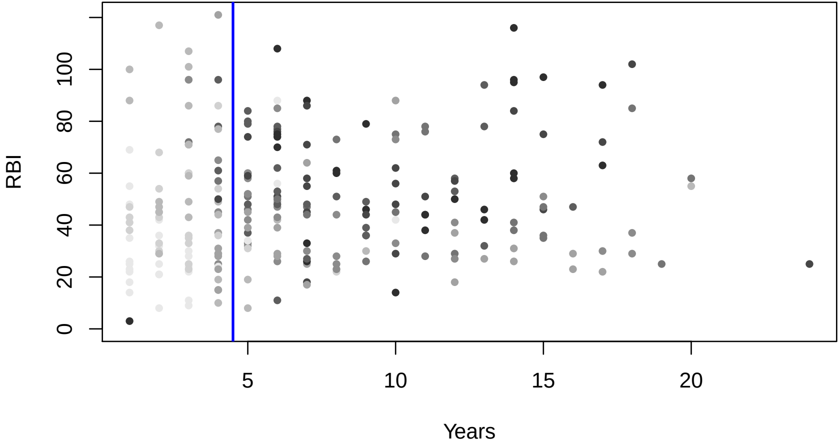
2. Find the predictor X_k with the minimum $Q_1(s_1), Q_2(s_2), \ldots, Q_p(s_p)$. Make the first binary partition along predictor X_k at cut point s_k.

Tree growth



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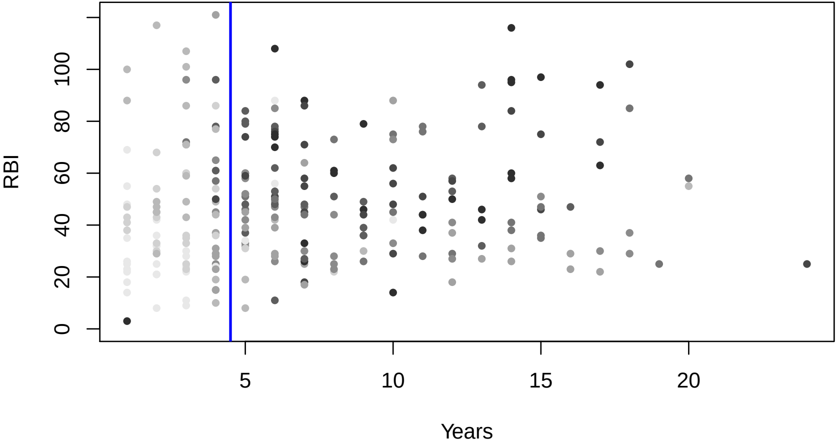

Essentially repeat the previous 2 steps on each of the resulting regions separately, iteratively. (Hence **recursive** binary partitioning.)

Bias-variance

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- As tree is grown deeper, bias decreases
- But the variance increases
- How to choose the right size of tree?

Stopping criterion

Once we stop, we relabel the terminal nodes to be $R_1, \ldots, R_J$ and compute $\bar{y}_{R_j}$ (means within each region) to serve as $\widehat{y}$ values.

But when do we stop?

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Many options – resulting in tuning parameters that are hard to deal with.

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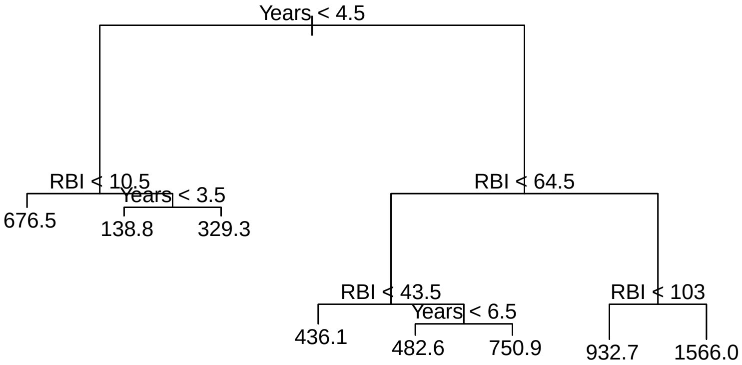

Tree pruning

How do we prune?

Tree pruning

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- cross validation

Tree pruning

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- cross validation
- cost-complexity pruning

Cost-complexity pruning

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

α is a tuning parameter that controls for the complexity of the model.

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It is possible to efficiently identify a sequence of nested subtrees that are optimal for a sequence of increasing α.

Tree pruning

1. Grow a big tree on a *training set*.
2. Obtain a nested set of subtrees $T_I \subset \cdots \subset T_2 \subset T_1 \subset T_0$ corresponding to a sequence of α values.
3. Use K-fold cross-validation to identify the subtree/α that does best.

Issues with trees

- Instability. Trees can have high variance. As data change, tree topology can change dramatically, making interpretation difficult
- Lack of smoothness. The splits lead to a “jagged” decision boundary. More of a problem for regression than classification
- Difficulty capturing additive structure, where the regression function is a sum of terms

Demos

Some nice demonstrations of decision trees:

`http://www.r2d3.us/visual-intro-to-machine-learning-part-1/`

`http://www.r2d3.us/visual-intro-to-machine-learning-part-2`

Summary from today

- Trees give interpretable, nonlinear prediction rules
- Deep trees have low bias, high variance
- Shallow trees have high bias, low variance
- Trees are grown greedily to be full, then pruned back