S&DS 265 / 565

Introductory Machine Learning

Trees

October 4

Yale

Plan for this and next week

- Notes on assignments: select pages in Gradescope, rerun notebook, limit length of output, line wrap
- Assn 2 is out — decision tree problem
- Quiz 3 Thursday; classification, SGD, bias-variance, trees
- Midterm exam: Tuesday October 18 (in class); practice exams posted to Canvas
- Review sessions next week (TBA)
- Questions?

You are here

4	Sept 20, 22	Stochastic gradient descent	SGD examples	Sept 20: Classification (continued) Sept 22: Stochastic gradient descent	ISL Section 6.2.2 ISL Section 10.7.2	Thu: Quiz 2
5	Sept 27, 29	Bias and variance, cross-validation	Bias-variance tradeoff Covid trends (revisited) California housing	Sept 27: Bias and variance Sept 29: Cross-validation	ISL Section 2.2 ISL Section 5.1	Thu: Assn 1 in Assn2 out
6	Oct 4, 6	Tree-based methods	Trees and forests Visualizing trees	Oct 4: Trees Oct 6: Forests	ISL Sections 8.1, 8.2	Thu: Quiz 3
7	Oct 11, 13	PCA and dimension reduction	PCA examples PCA revisited Used for regression	Oct 11: PCA Oct 13: PCA and review	ISL Section 12.2	Thu: Assn 2 in Assn3 out
8	Oct 18	Midterm exam (in class)			On Canvas: Practice midterms / Sample solns Midterm / Sample	

Classification and Regression Trees (CART)

Trees provide ways of modeling nonlinear relationships by carving out *rectangular regions* in the feature space.

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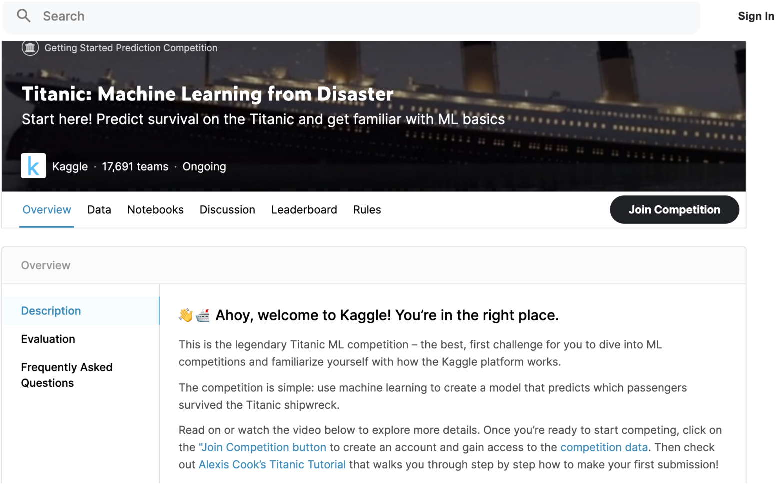
- Response variables can be categorical or quantitative
- Yields a set of interpretable decision rules
- Predictive ability is mediocre, *but* can be improved by combining multiple trees (resampling, ensemble methods)

Titanic data



Titanic data

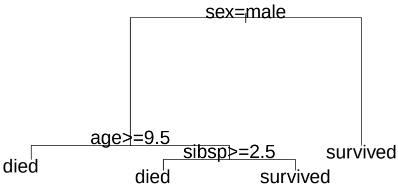
- **Survived**: Outcome of survival (0 = No; 1 = Yes)
- **Pclass**: Socio-economic class (1 = Upper class; 2 = Middle class; 3 = Lower class)
- **Name**: Name of passenger
- **Sex**: Sex of the passenger
- **Age**: Age of the passenger (Some entries contain `NaN`)
- **SibSp**: Number of siblings and spouses of the passenger aboard
- **Parch**: Number of parents and children of the passenger aboard
- **Ticket**: Ticket number of the passenger
- **Fare**: Fare paid by the passenger
- **Cabin** Cabin number of the passenger (Some entries contain `NaN`)
- **Embarked**: Port of embarkation of the passenger (C = Cherbourg; Q = Queenstown; S = Southampton)

Trees

Trees

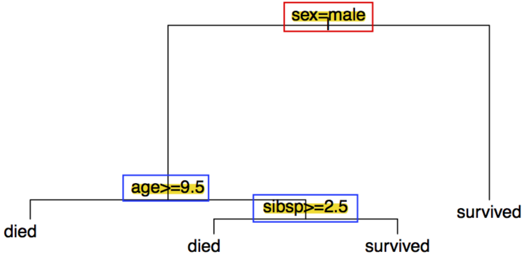
Trees

Modeling Titanic survival:



Tree terminology

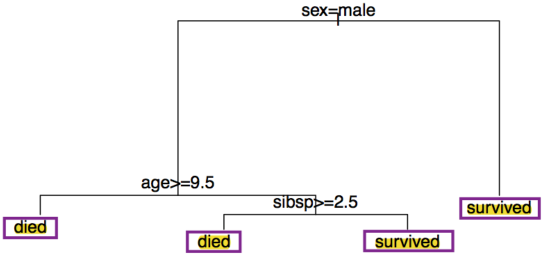
Internal nodes are points where the predictor space is split.



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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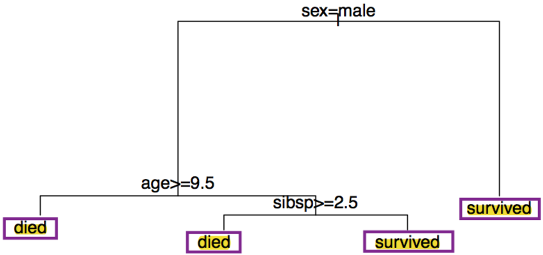
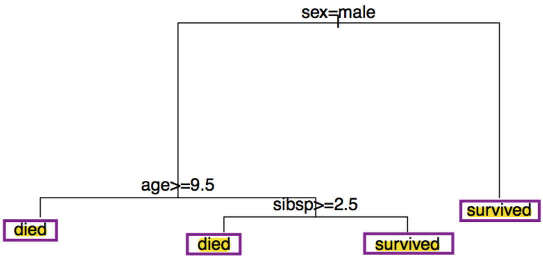


Denote these J regions as $R_1, \ldots, R_J$.

Tree terminology



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

Let's go to the Titanic demo

Runs batted in (RBI)

MAJOR LEAGUE BASEBALL

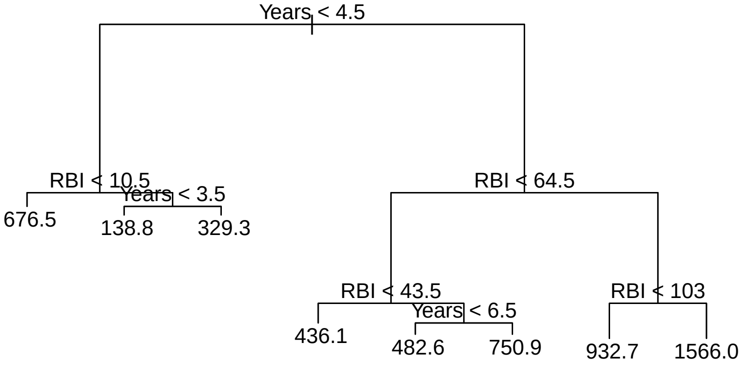
BATTING STATS

2022 REGULAR SEASON

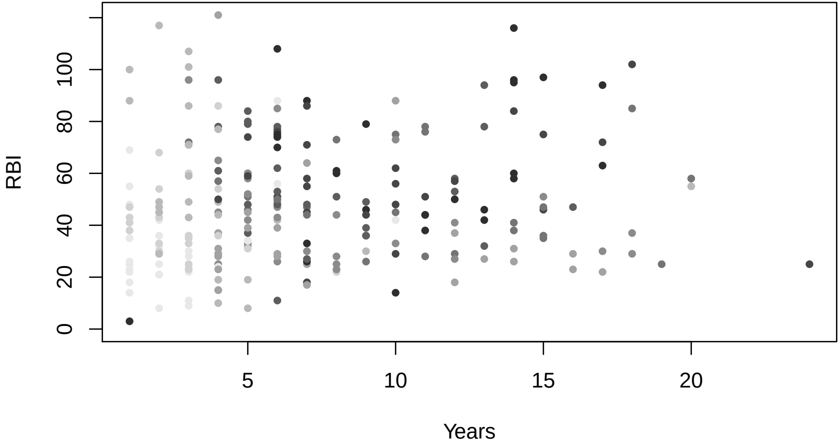
	PLAYERS	G	PA	AB	H	R	2B	3B	HR	RBI	SB	CS
1	P. Alonso NYM	158	678	592	159	94	27	0	40	**131**	5	1
2	A. Judge NYY	155	689	563	175	131	28	0	61	**130**	16	3
3	J. Ramírez CLE	155	676	592	163	88	42	5	29	**122**	20	7

Regression tree example

Baseball hitter salaries (in $1,000s — old data!):



Regression tree example



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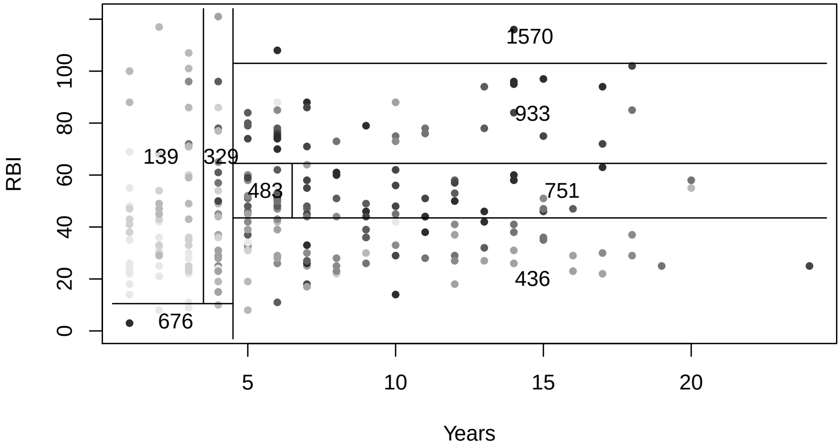

Prediction using trees

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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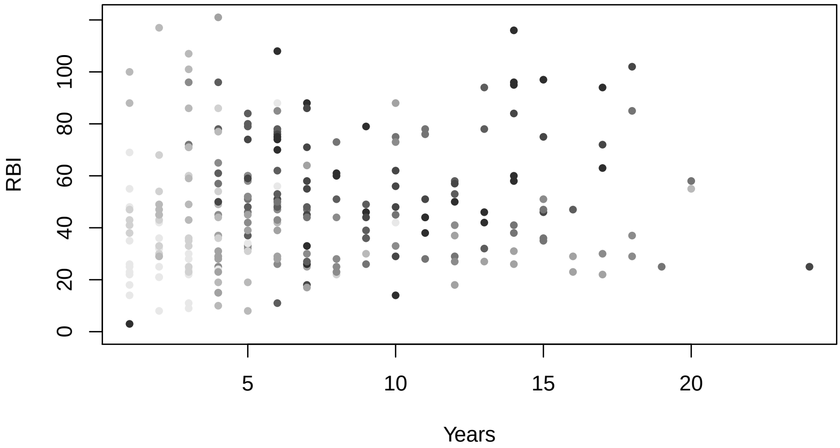
Tree building takes a *greedy* approach.

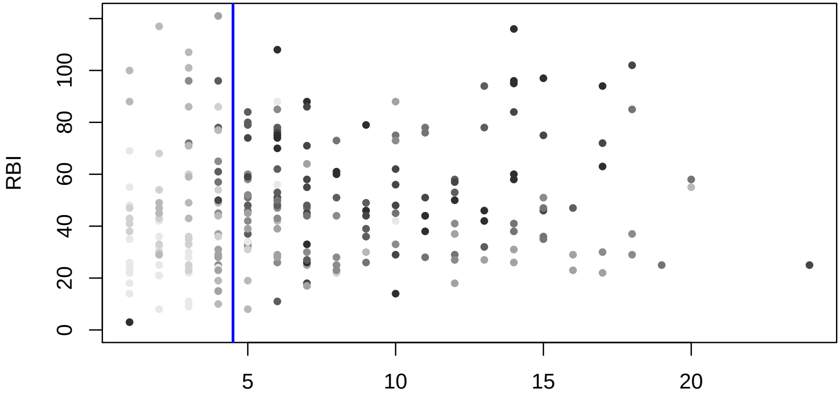
- Grow the tree by recursive binary splitting
- Prune back the tree

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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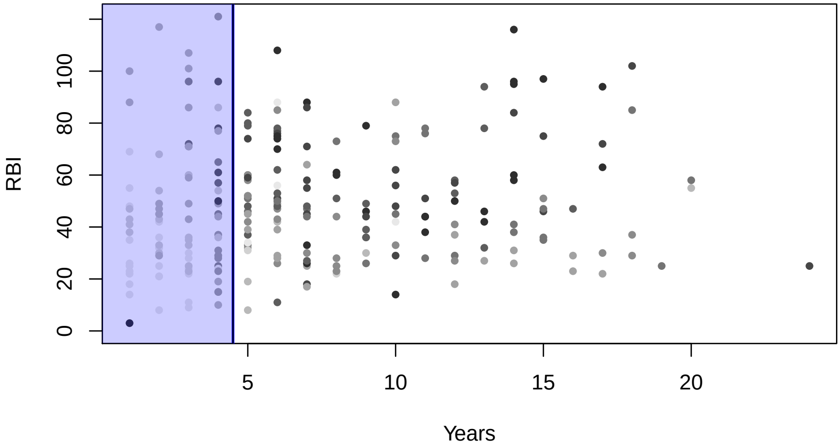

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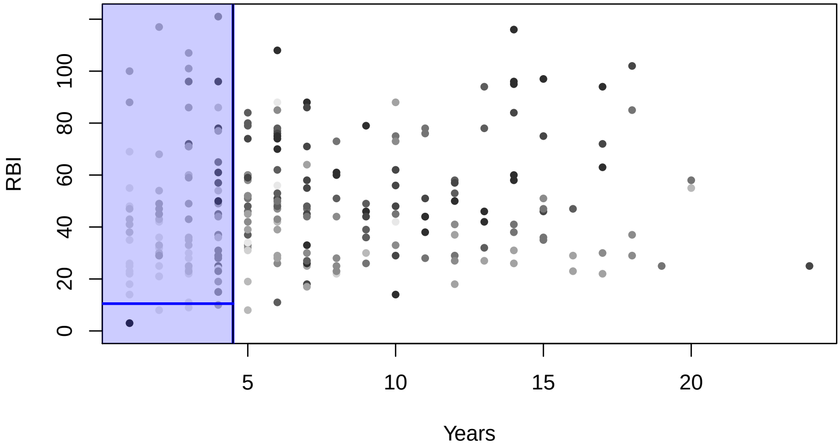

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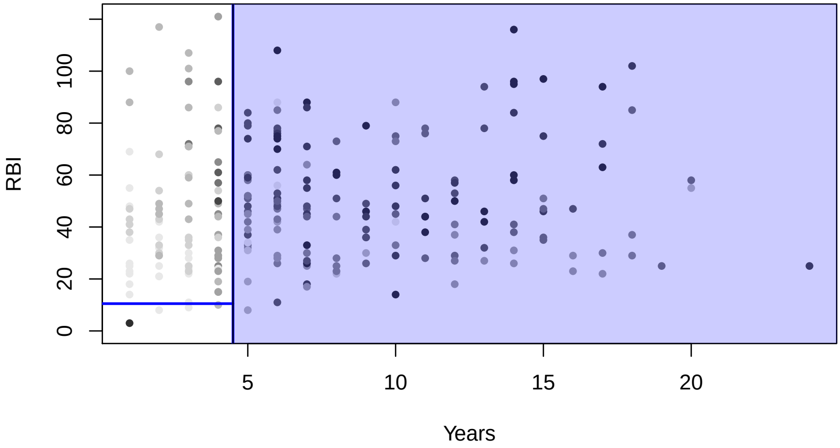

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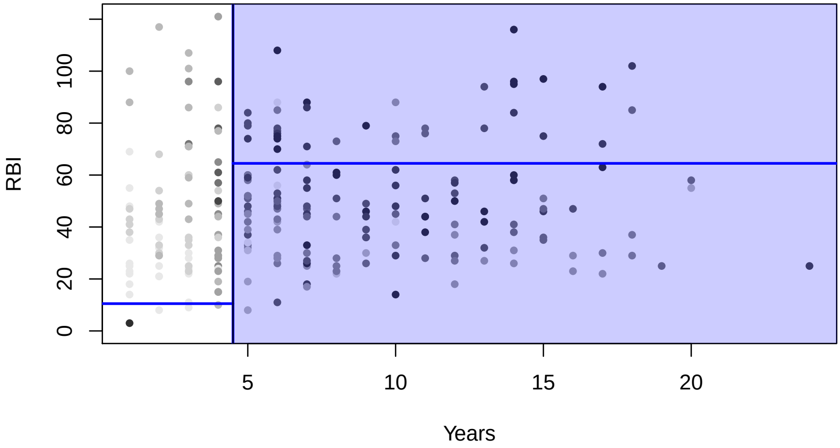

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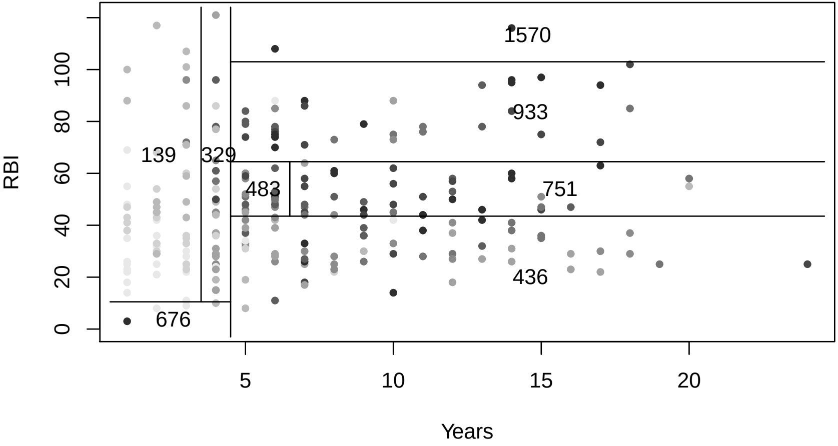

1570
933
139
329
483
751
436
676
RBI
Years
0
20
40
60
80
100
5
10
15
20

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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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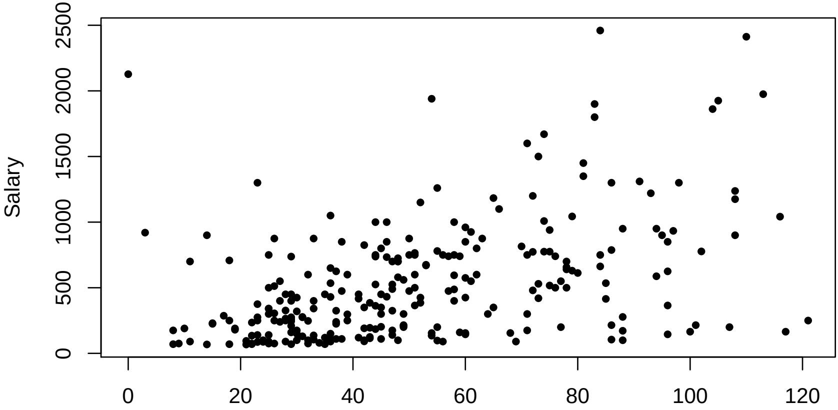

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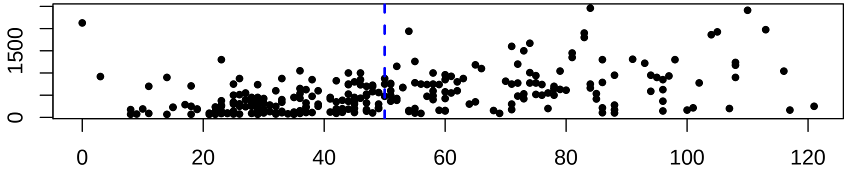

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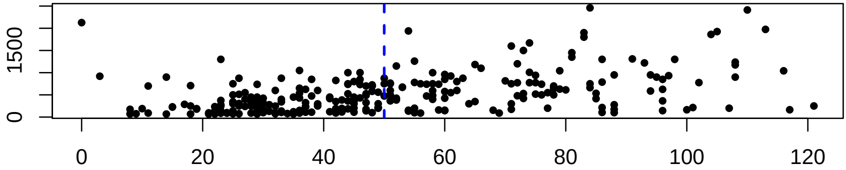
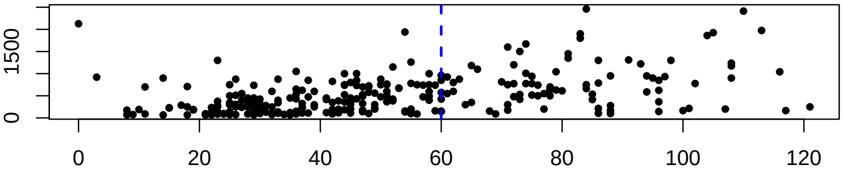


- $R_1(RBI, 50)$: $\bar{y}_{R_1} = 359$
- $R_2(RBI, 50)$: $\bar{y}_{R_2} = 753$
-

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

Example: Evaluating Q_{RBI}



- $R_1(RBI, 60)$: $\bar{y}_{R_1} = 405$
- $R_2(RBI, 60)$: $\bar{y}_{R_2} = 802$
-

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

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:

$$R_1(k, s) = \{i | X_{ik} < s\} \quad \text{and} \quad R_2(k, s) = \{i | X_{ik} \geq s\}$$

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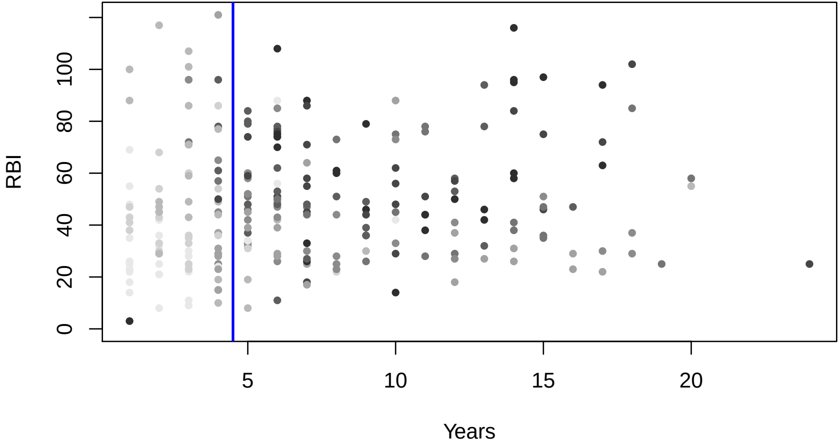
2. Find the predictor X_k with the minimum $Q_1(s_1), Q_2(s_2), \ldots, Q_p(s_p)$. Make the first binary partition along predictor X_k at cut point s_k.

Tree growth



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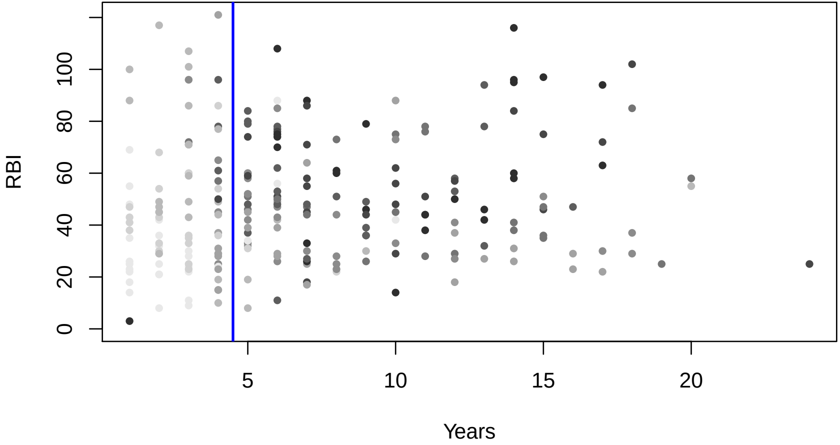

Repeat the previous 2 steps on each of the resulting regions separately, iteratively. (Hence **recursive** binary partitioning.)

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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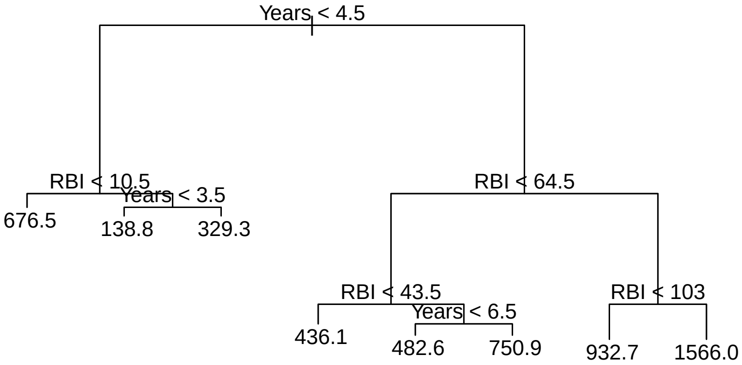

Tree pruning

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 $T_L \subset \cdots \subset T_2 \subset T_1 \subset T_0$ 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
- Predictive power is...meh

We’ll talk about ways of addressing some of these next time

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
- Deep trees are pruned back using cross-validation to find best bias/variance tradeoff.