Tree Methods

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Introduction

Classification and Regression Trees

The Generic Tree Algorithm

- Grow a binary tree.
- At each node, "split" the data into two "daughter" nodes.
- Splits are chosen using a splitting criterion.
- Bottom nodes are "terminal" nodes.

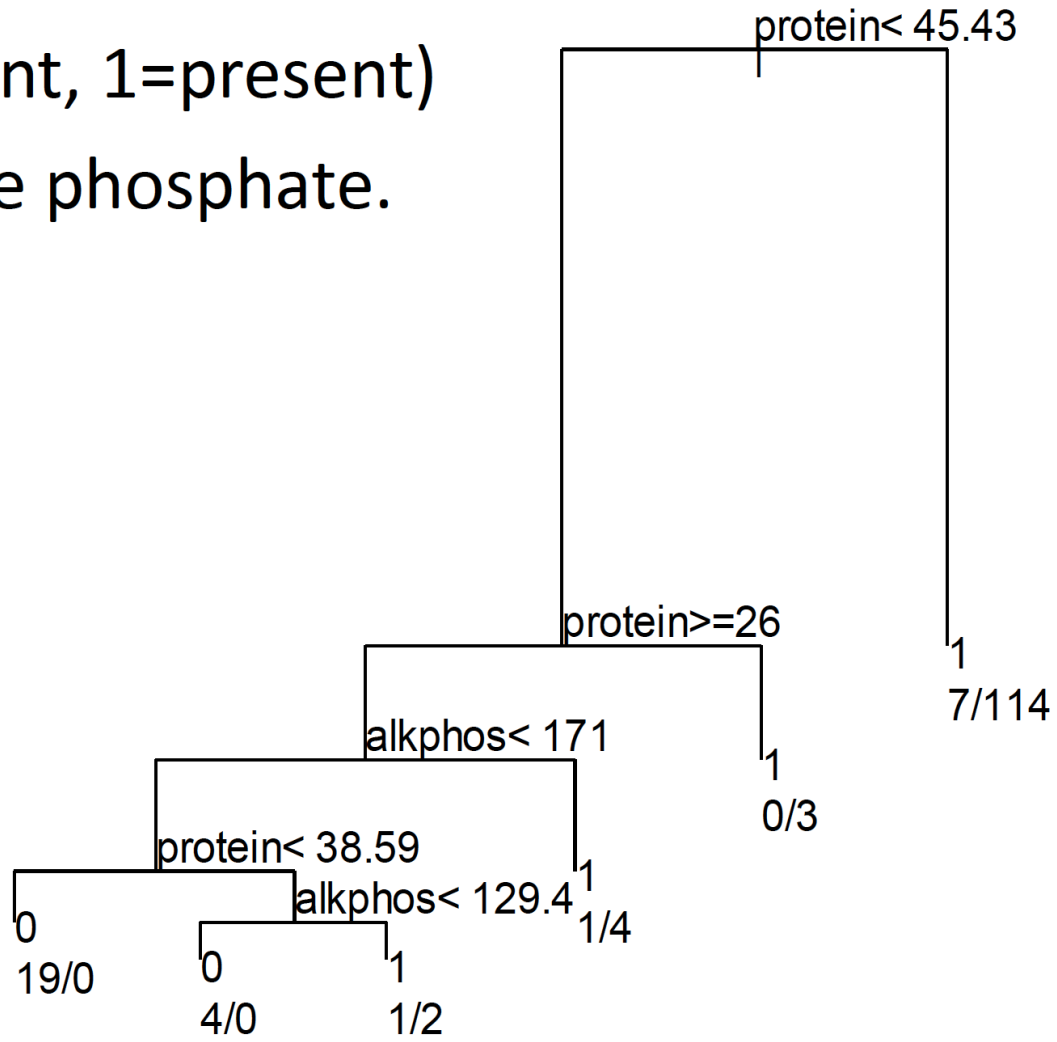
Remarks:

- For regression the predicted value at a node is the average response variable for all observations in the node.
- For classification the predicted class is the most common class in the node (majority vote).
- For classification trees, can also get estimated probability of membership in each of the classes

A Classification Tree

Predict hepatitis (0=absent, 1=present) using protein and alkaline phosphate.

"Yes" goes left.



Splitting criteria

- **Regression**: residual sum of squares

$$\text{RSS} = \sum_{\text{left}} (y_i - y_L^*)^2 + \sum_{\text{right}} (y_i - y_R^*)^2$$

where:

  - y_L^* = mean y-value for left node
  - y_R^* = mean y-value for right node

- **Classification**: Gini criterion

$$\text{Gini} = N_L \sum_{k=1}^{K} p_{kL}(1 - p_{kL}) + N_R \sum_{k=1}^{K} p_{kR}(1 - p_{kR})$$

where:

  - p_{kL} = proportion of class k in left node
  - p_{kR} = proportion of class k in right node

Tree Methods

Regression: Prostate Cancer

Example: Prostate Cancer Prognosis

After tumor detection, there are many treatment options.

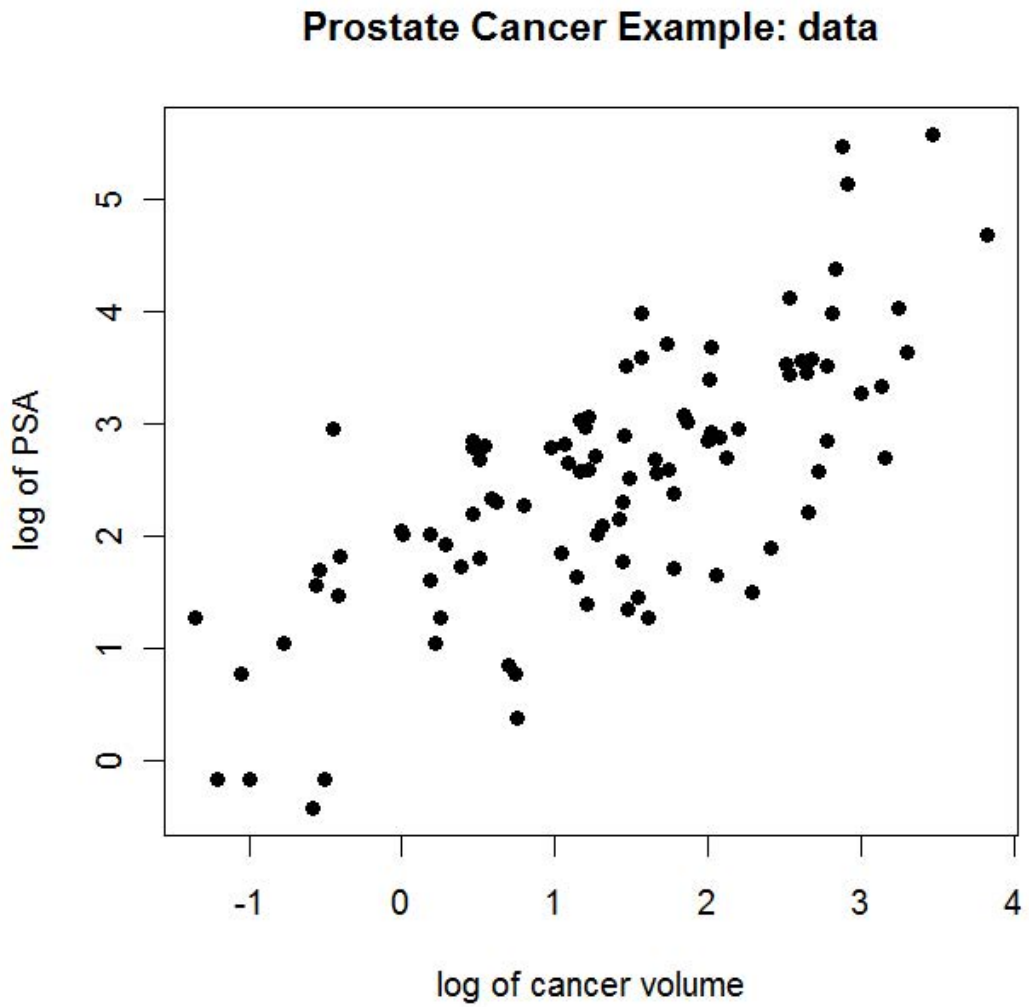
- Various chemo + radiation, surgical removal.

Biopsy information is useful to help in deciding treatment

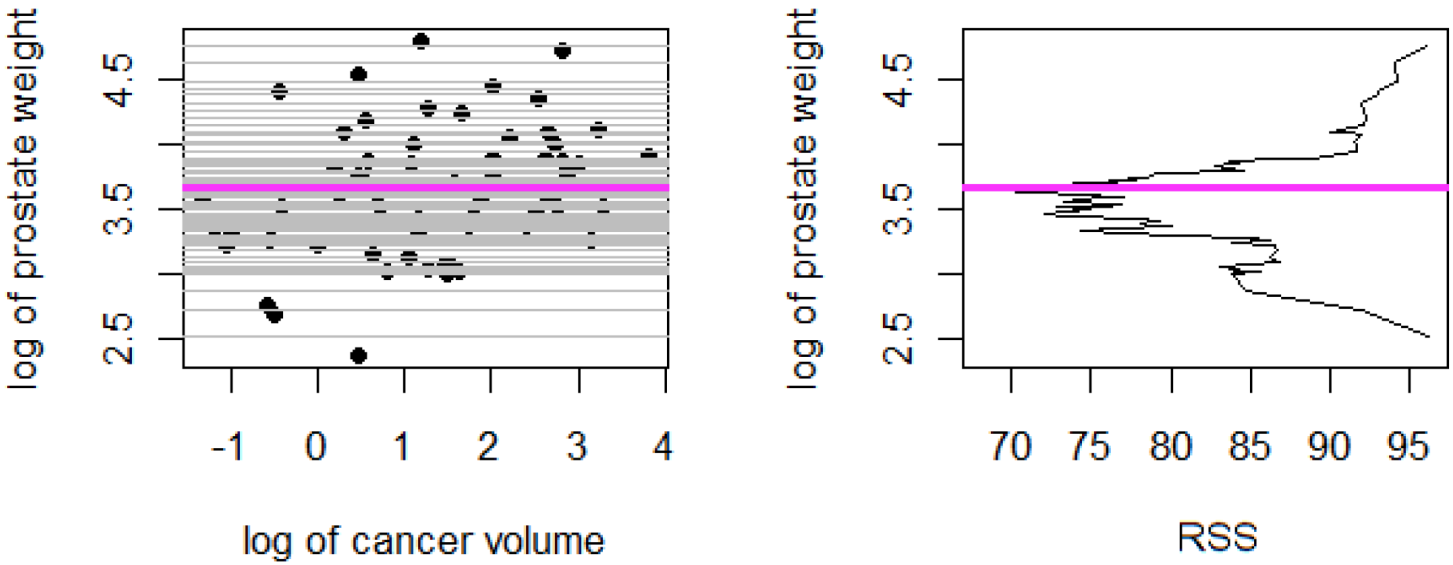
- *Prostate Specific Antigen, in Log (lpsa)*: protein production. (target)
- *Log of Prostate Volume (lcavol)*: predictor
- *Log of Prostate Weight (lweight)*: predictor

Data: `http://www.biostat.jhsph.edu/~ririzarr/Teaching/649/prostate.html`

Regression: Prostate Cancer

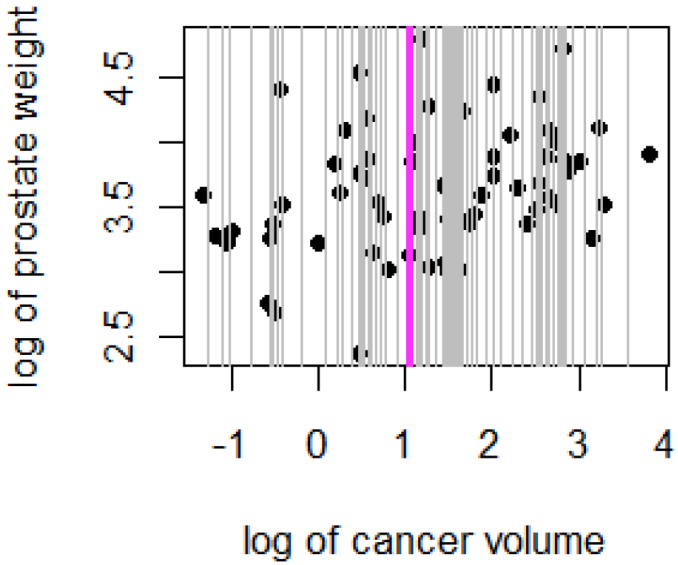


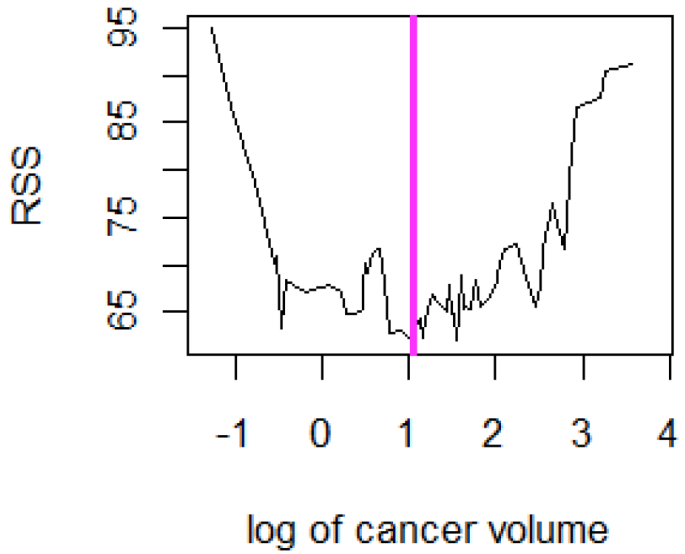
Choosing the best horizontal split



Best horizontal split is at 3.67 with RSS = 68.09.

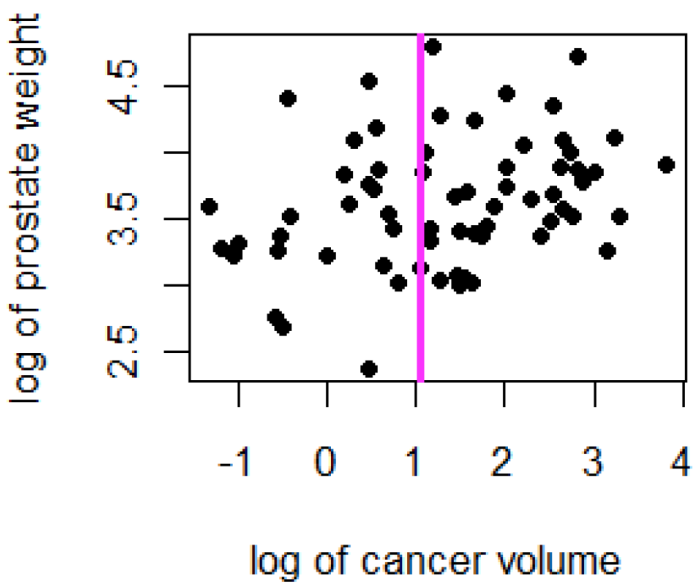
Choosing the best vertical split

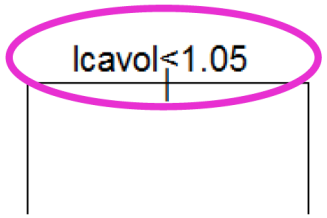




Best vertical split is at 1.05 with RSS = 61.76.

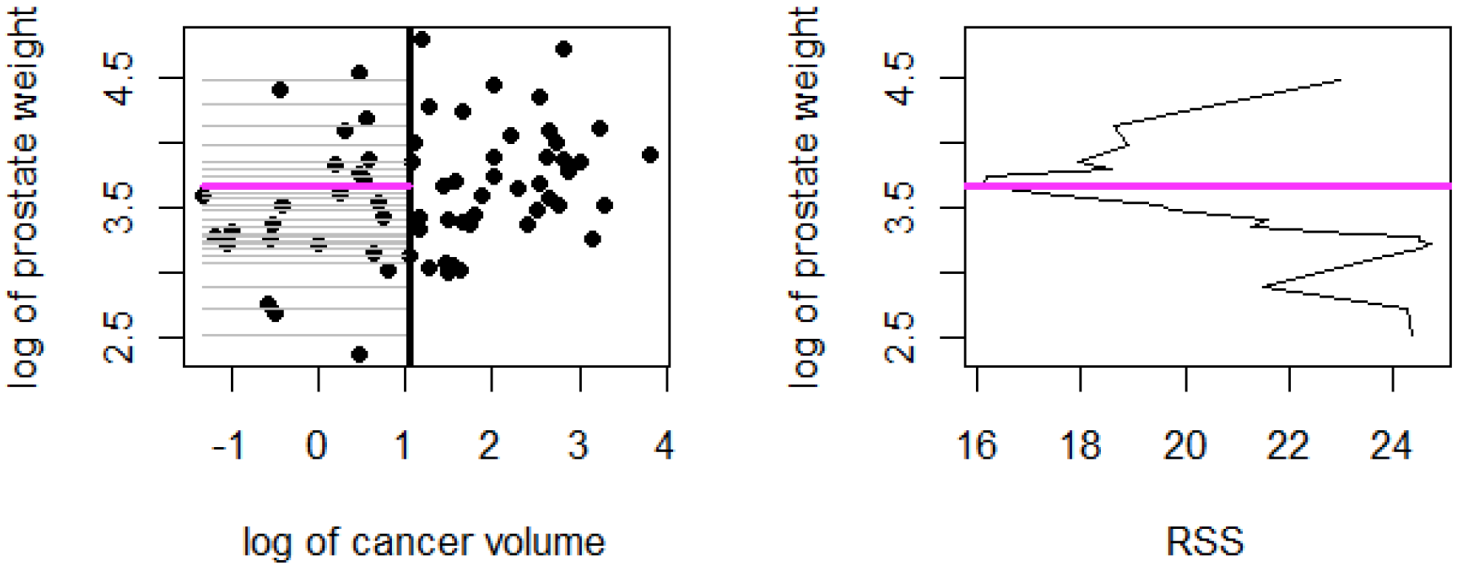
Regression tree (prostate cancer)





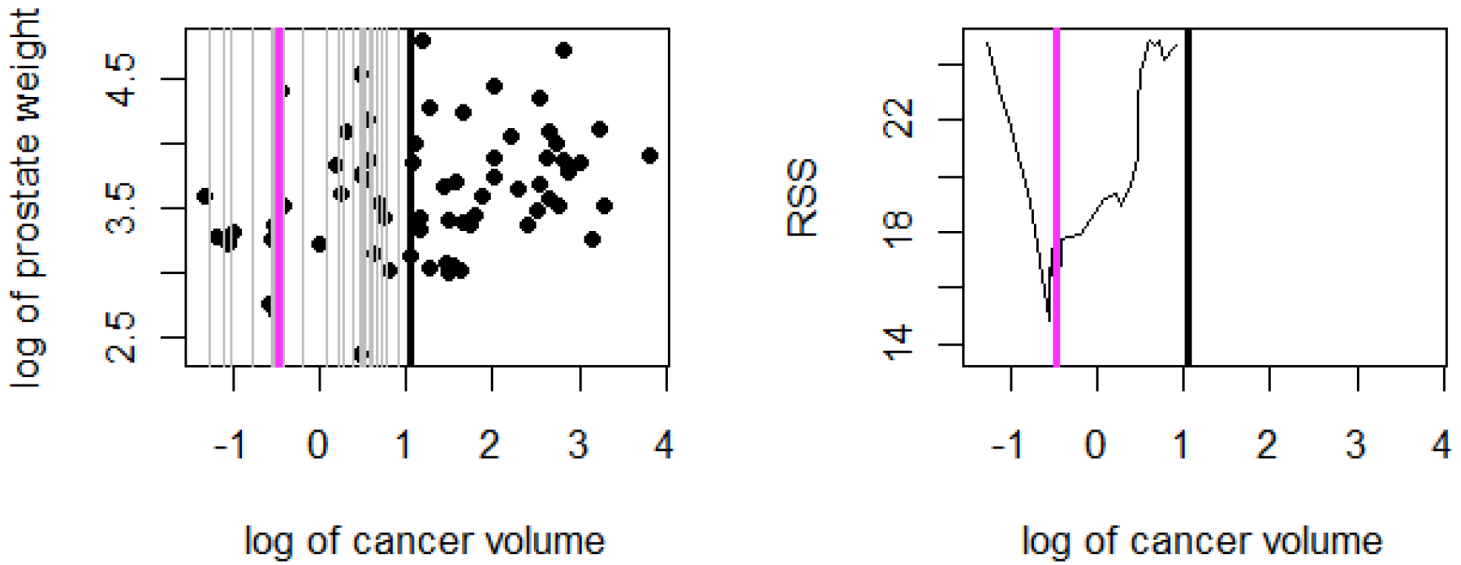
Use vertical as the first feature.

Choosing the best split in the left node



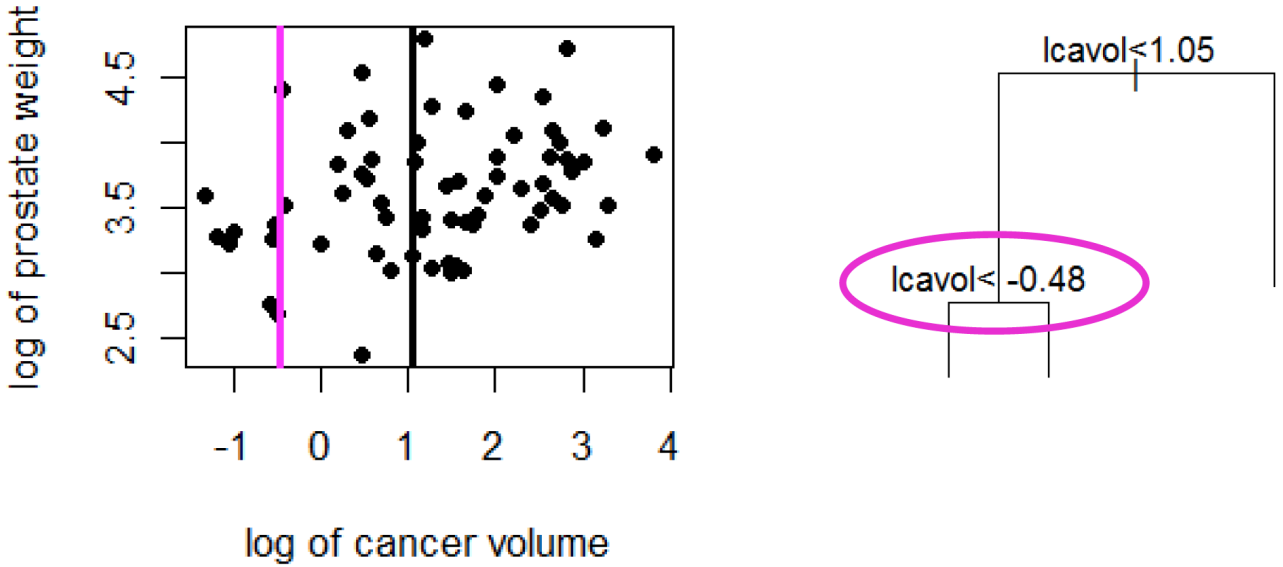
Best horizontal split is at 3.66 with RSS = 16.11.

Choosing the best split in the left node



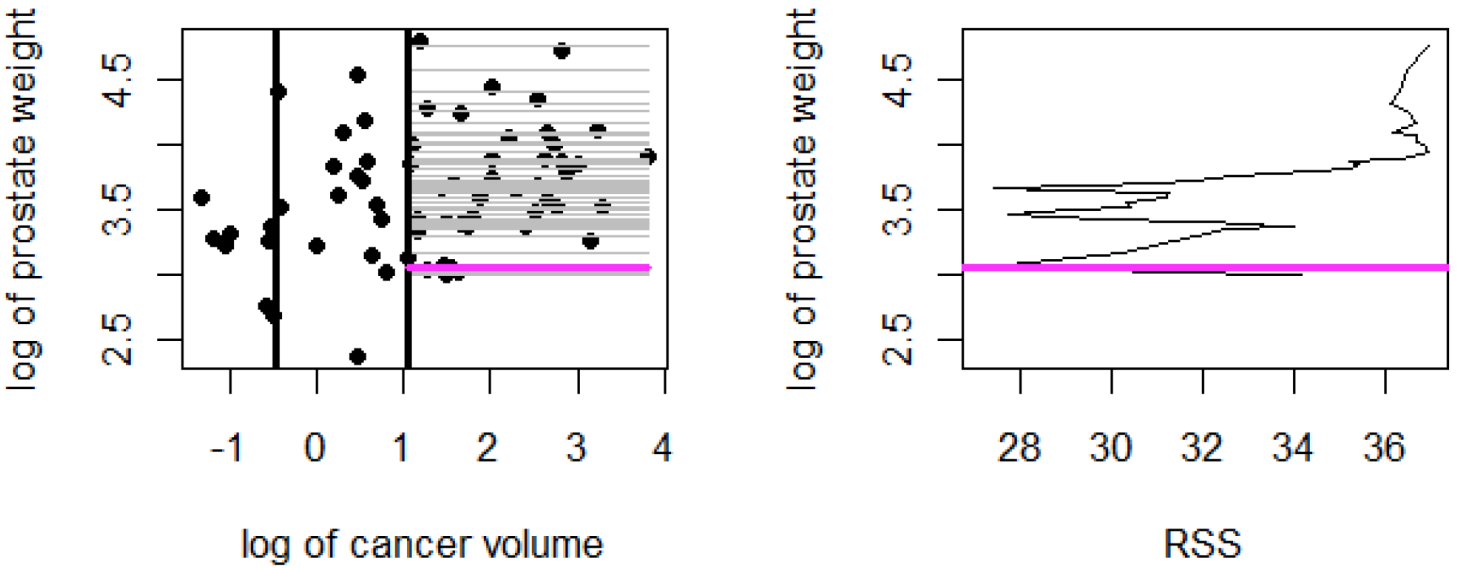
Best vertical split is at -.48 with RSS = 13.61.

Regression tree (prostate cancer)



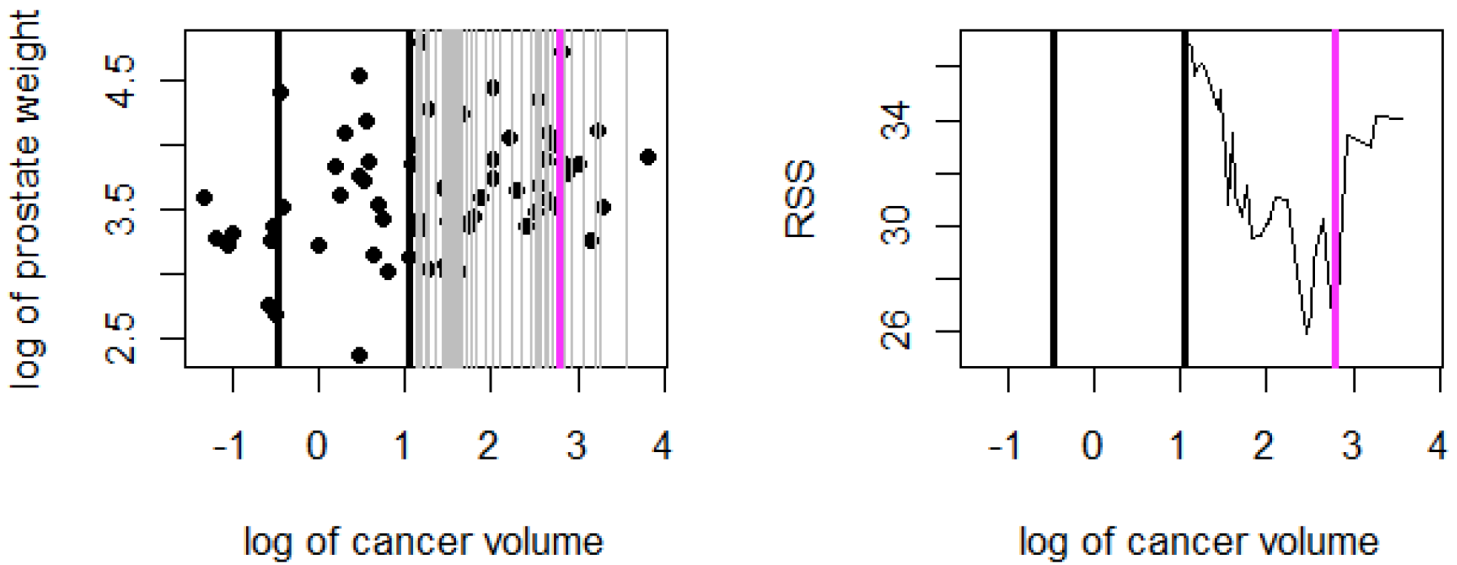
Use vertical as the feature for the left node.

Choosing the best split in the right node



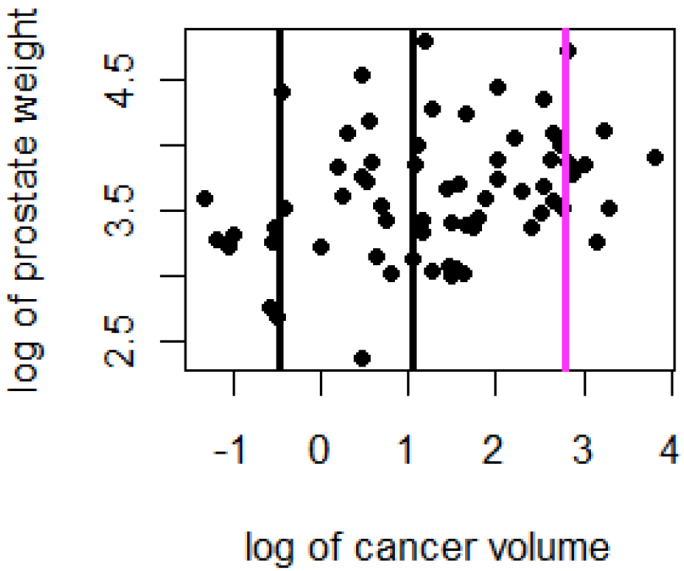
Best horizontal split is at 3.07 with RSS = 27.15.

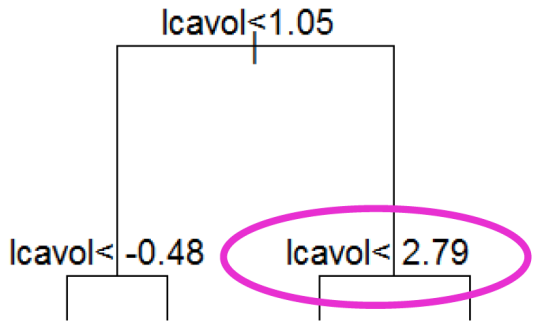
Choosing the best split in the right node



Best vertical split is at 2.79 with RSS = 25.11.

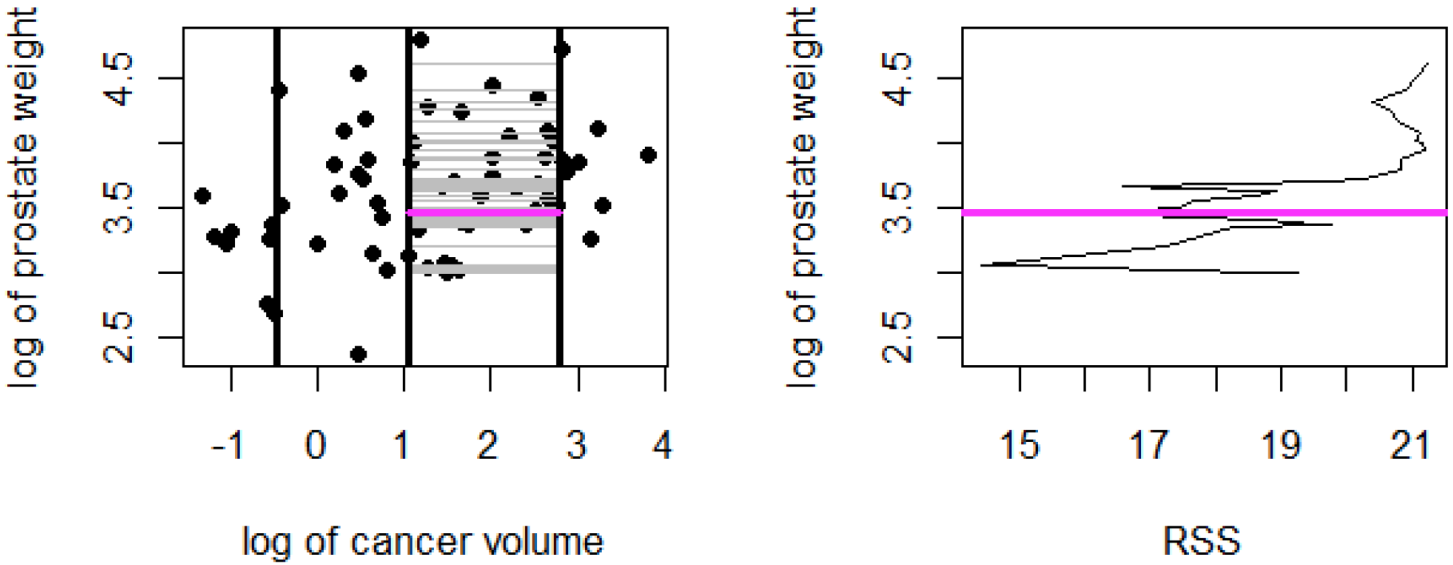
Regression tree (prostate cancer)





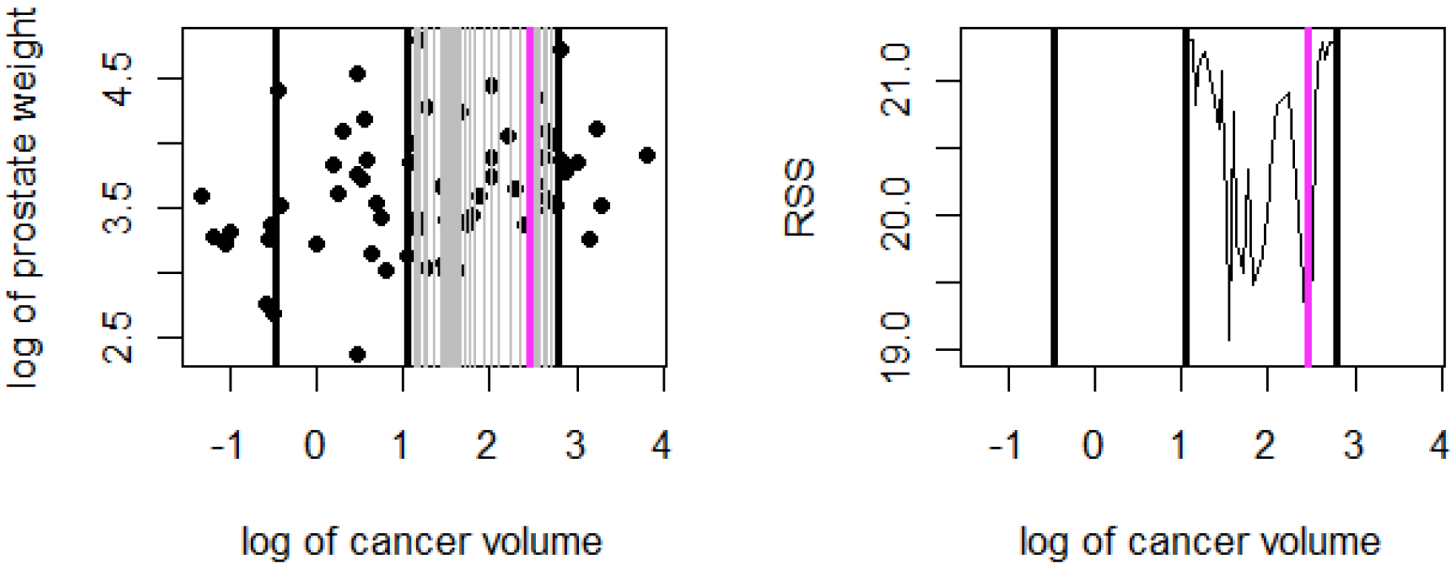
Use vertical as the feature for the right node.

Choosing the best split in the third node



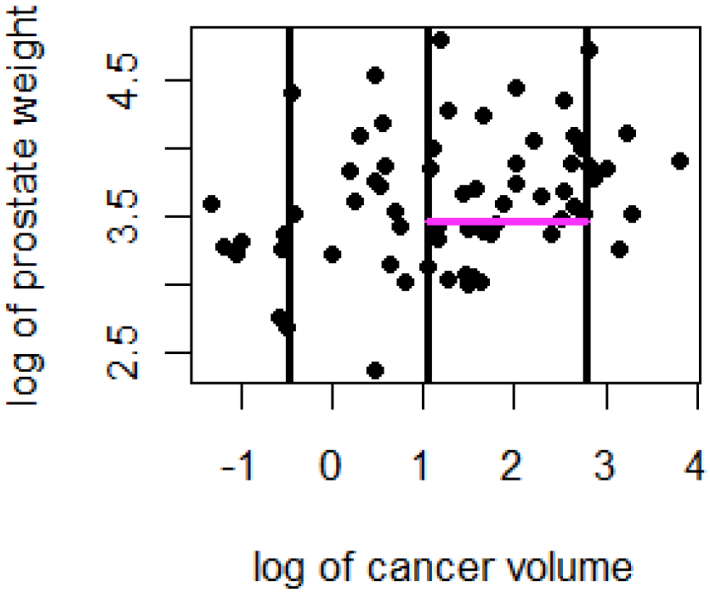
Best horizontal split is at 3.07 with RSS = 14.42, but this is too close to the edge. Use 3.46 with RSS = 16.14.

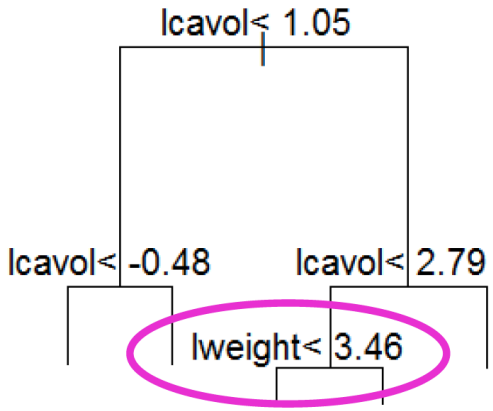
Choosing the best split in the third node



Best vertical split is at 2.46 with RSS = 18.97.

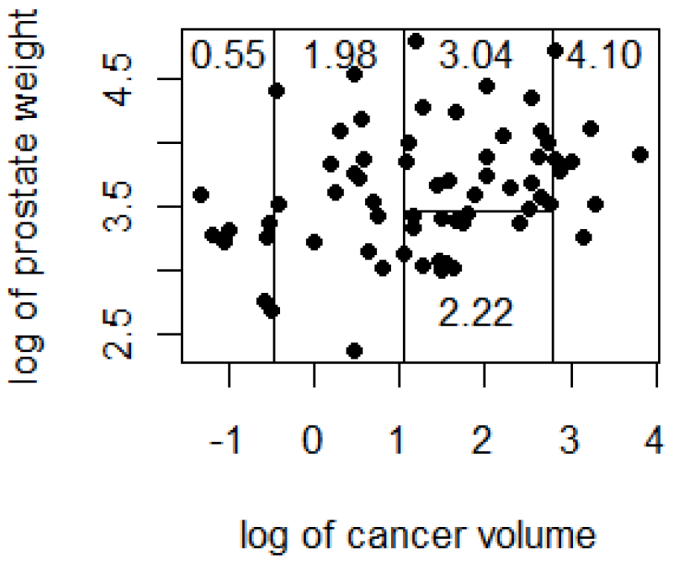
Regression tree (prostate cancer)

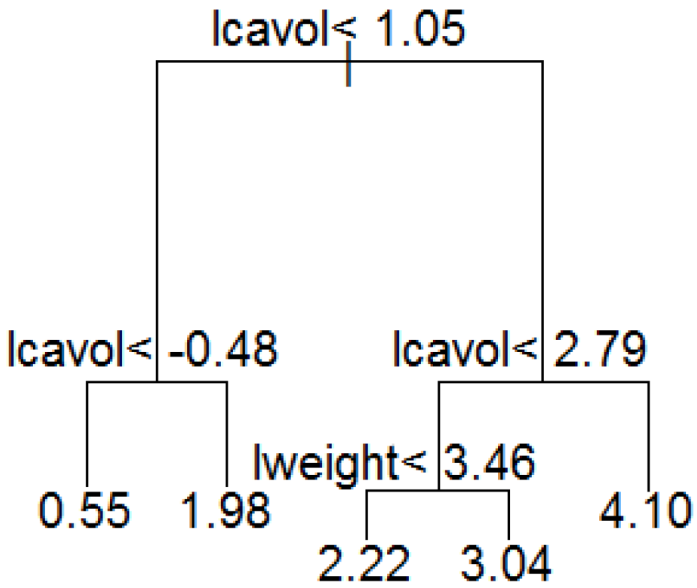




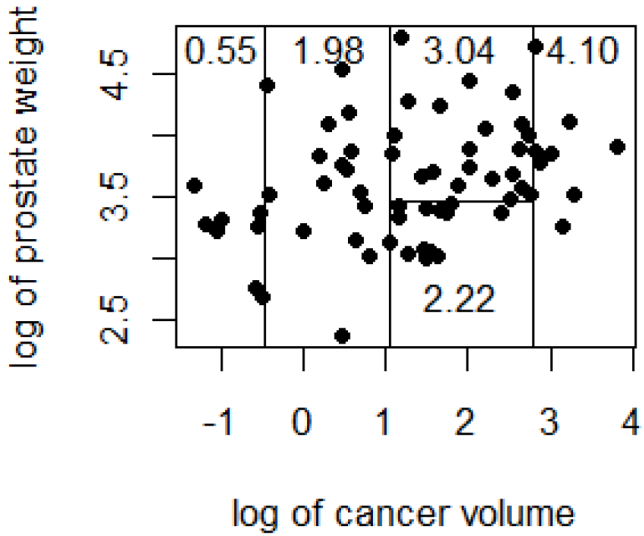
Use horizontal as the feature for the third node.

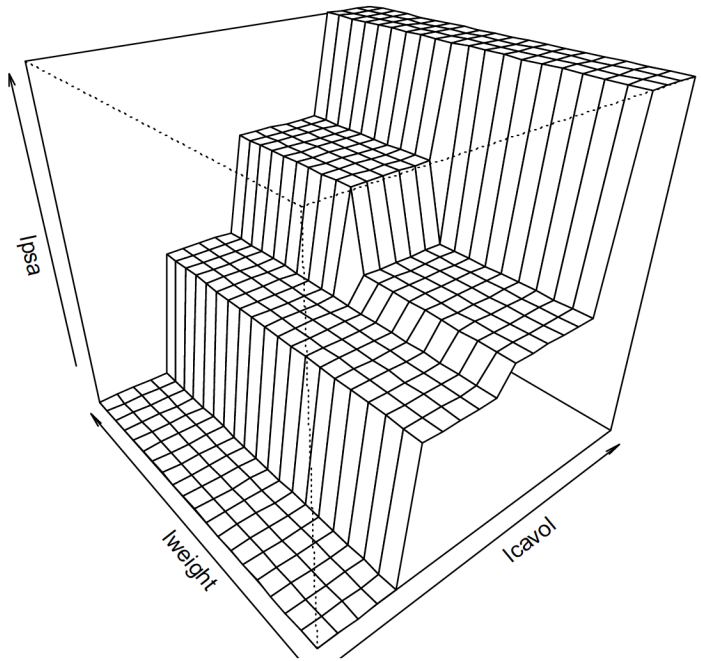
Regression tree (prostate cancer)



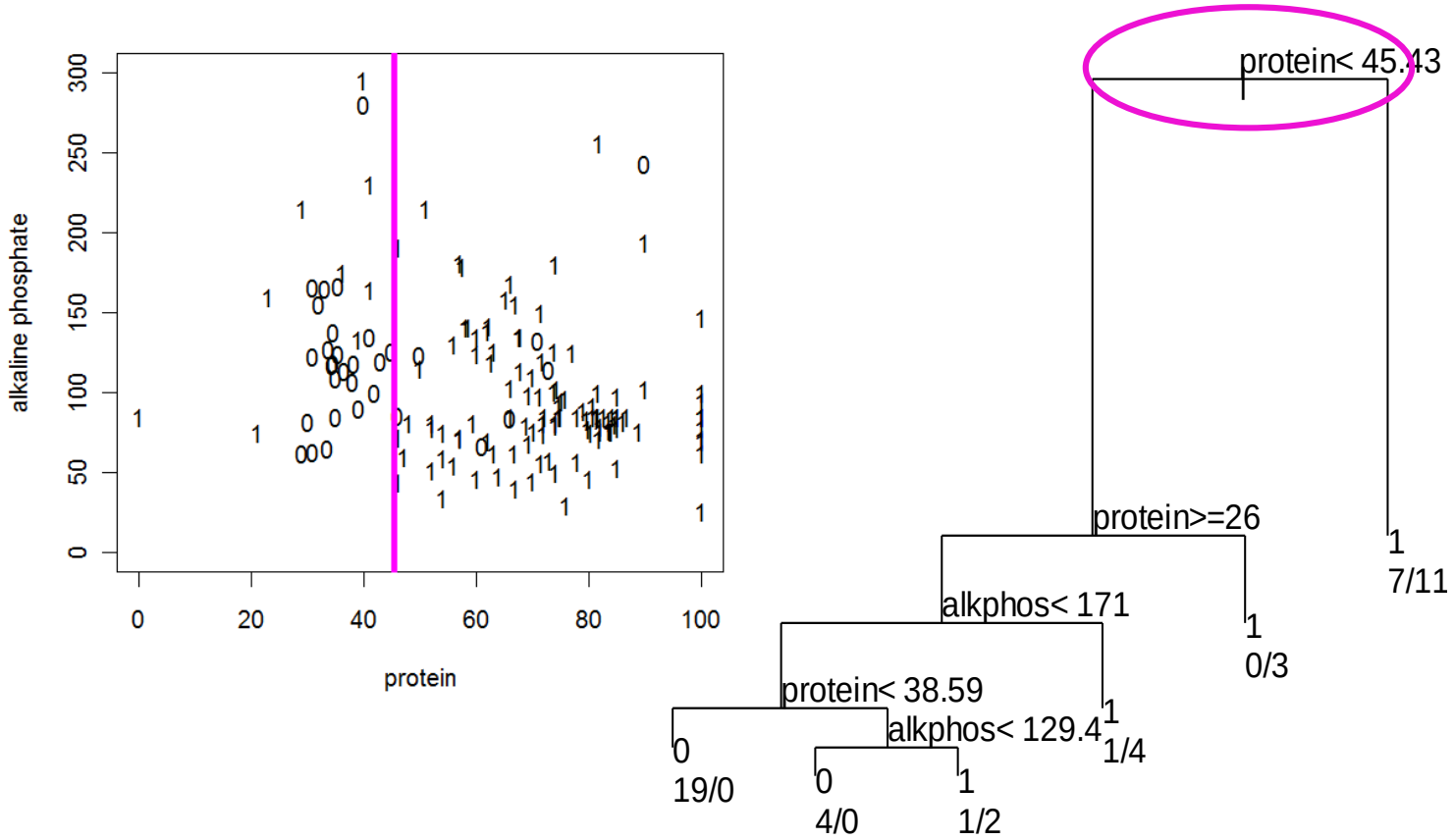


Regression tree (prostate cancer)





Classification tree (hepatitis)



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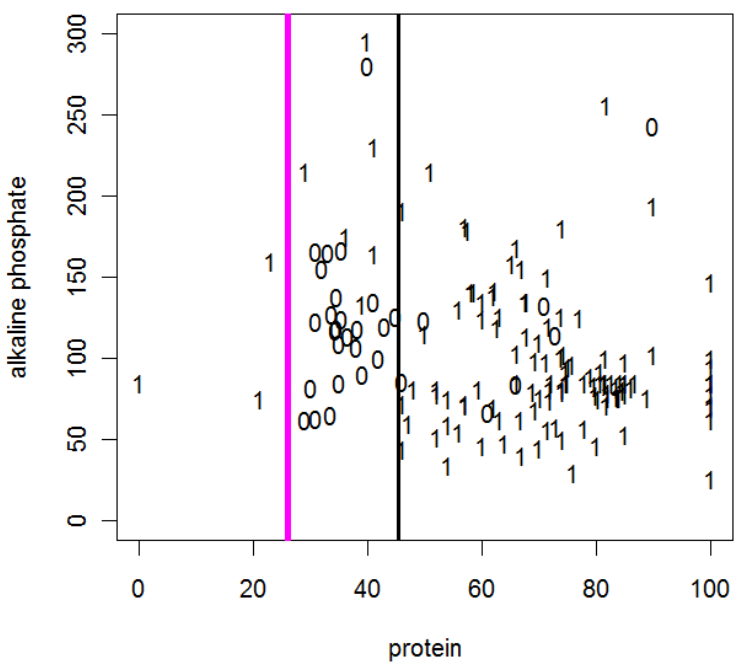

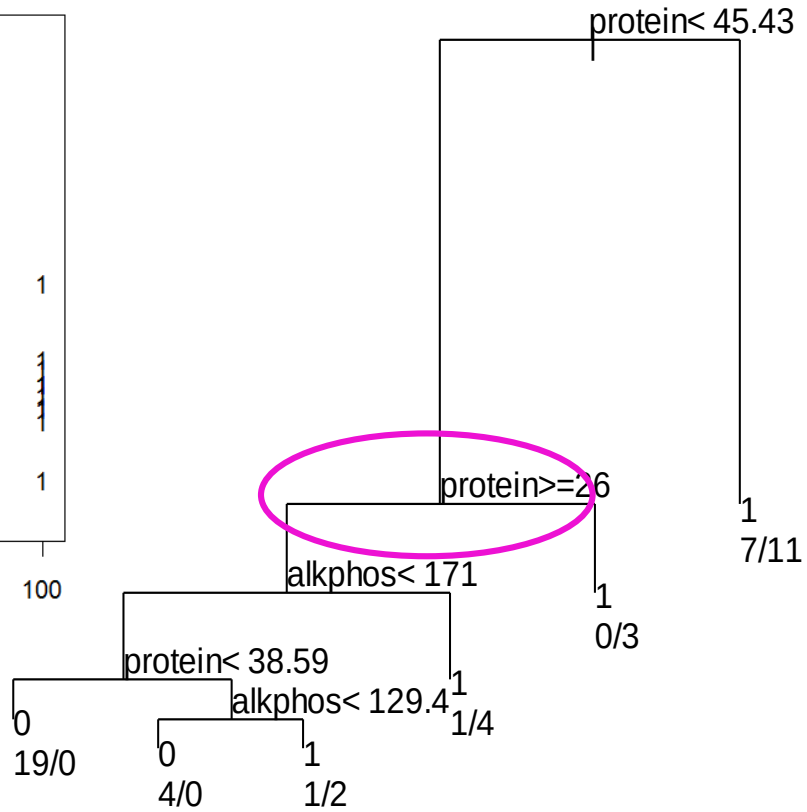

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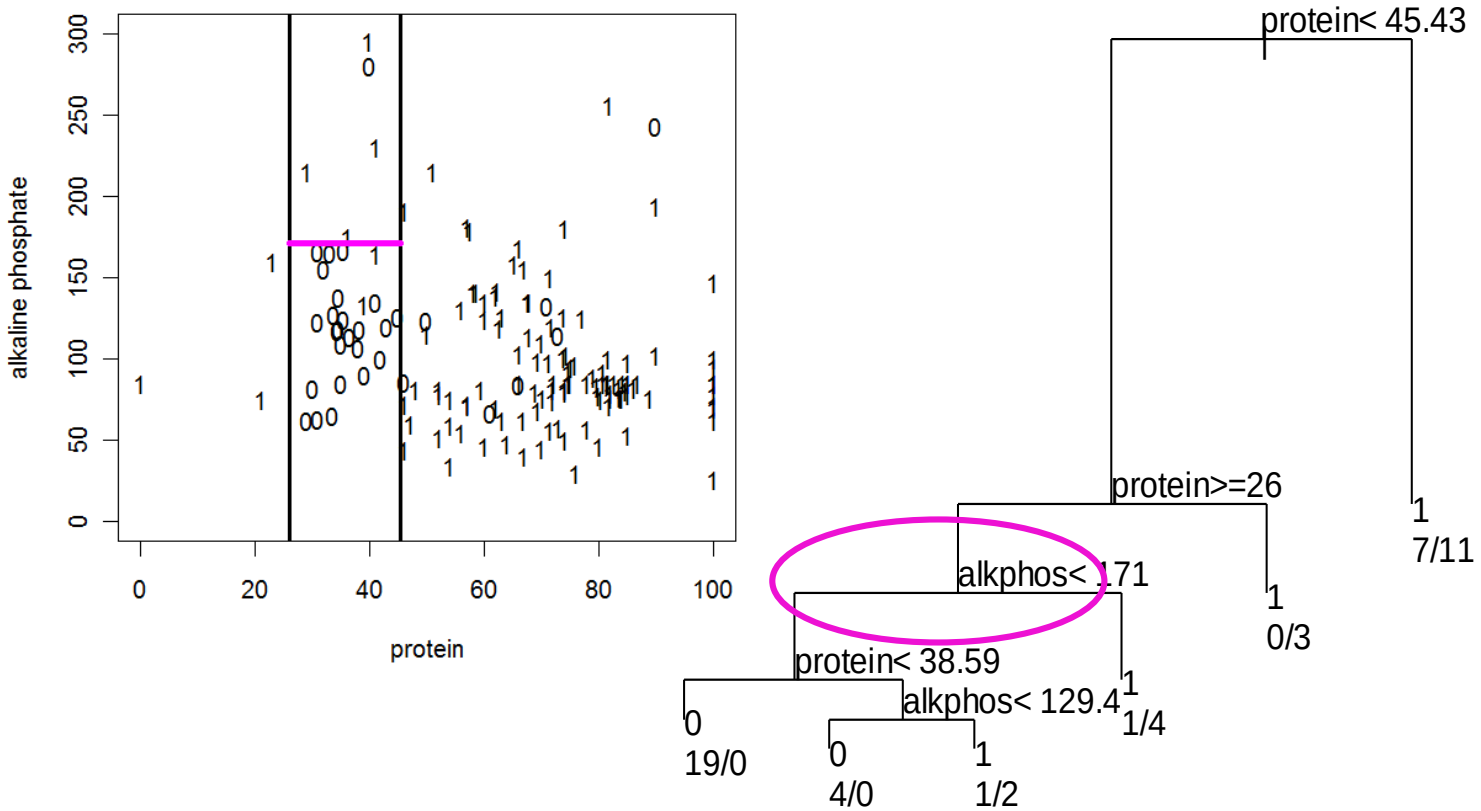

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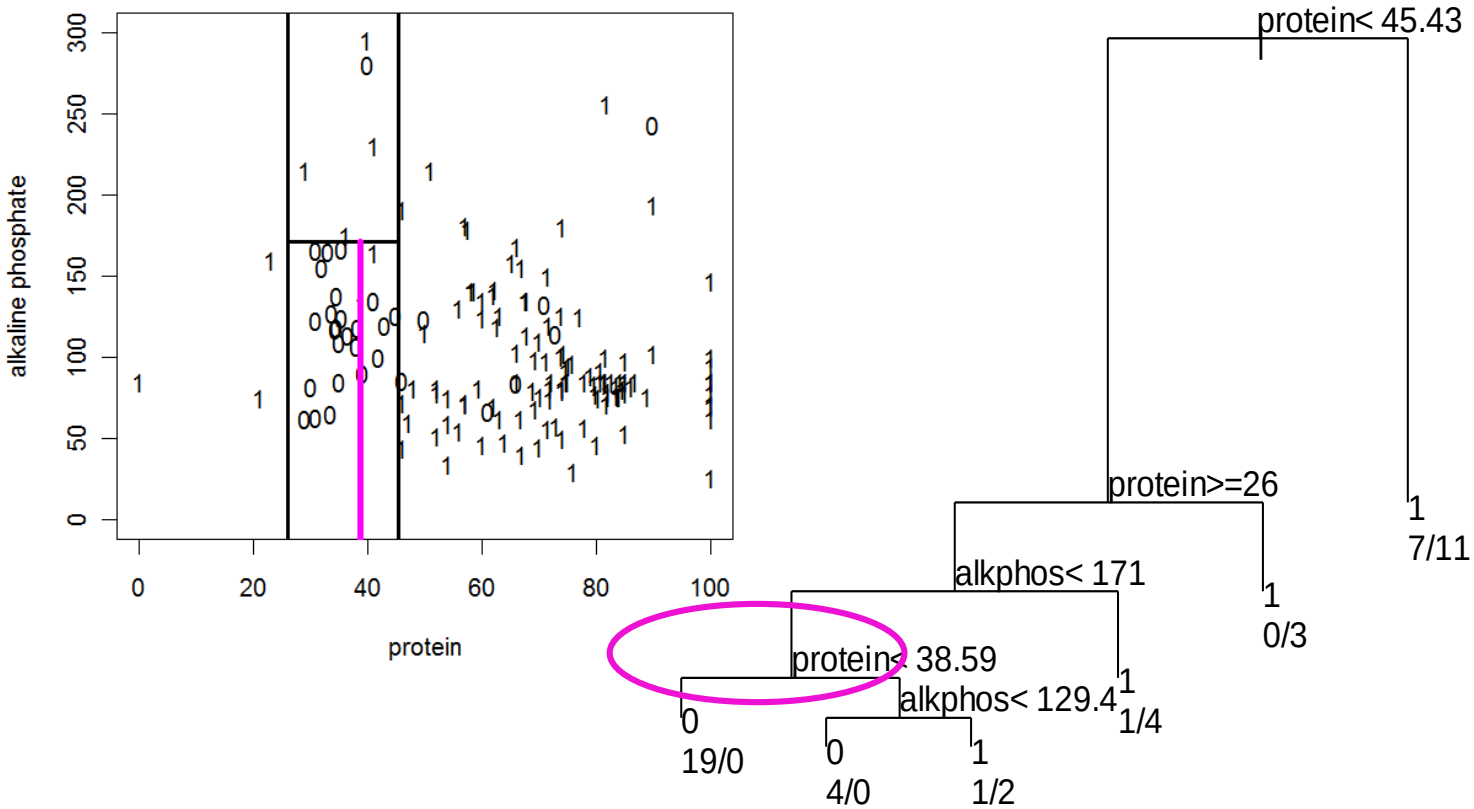

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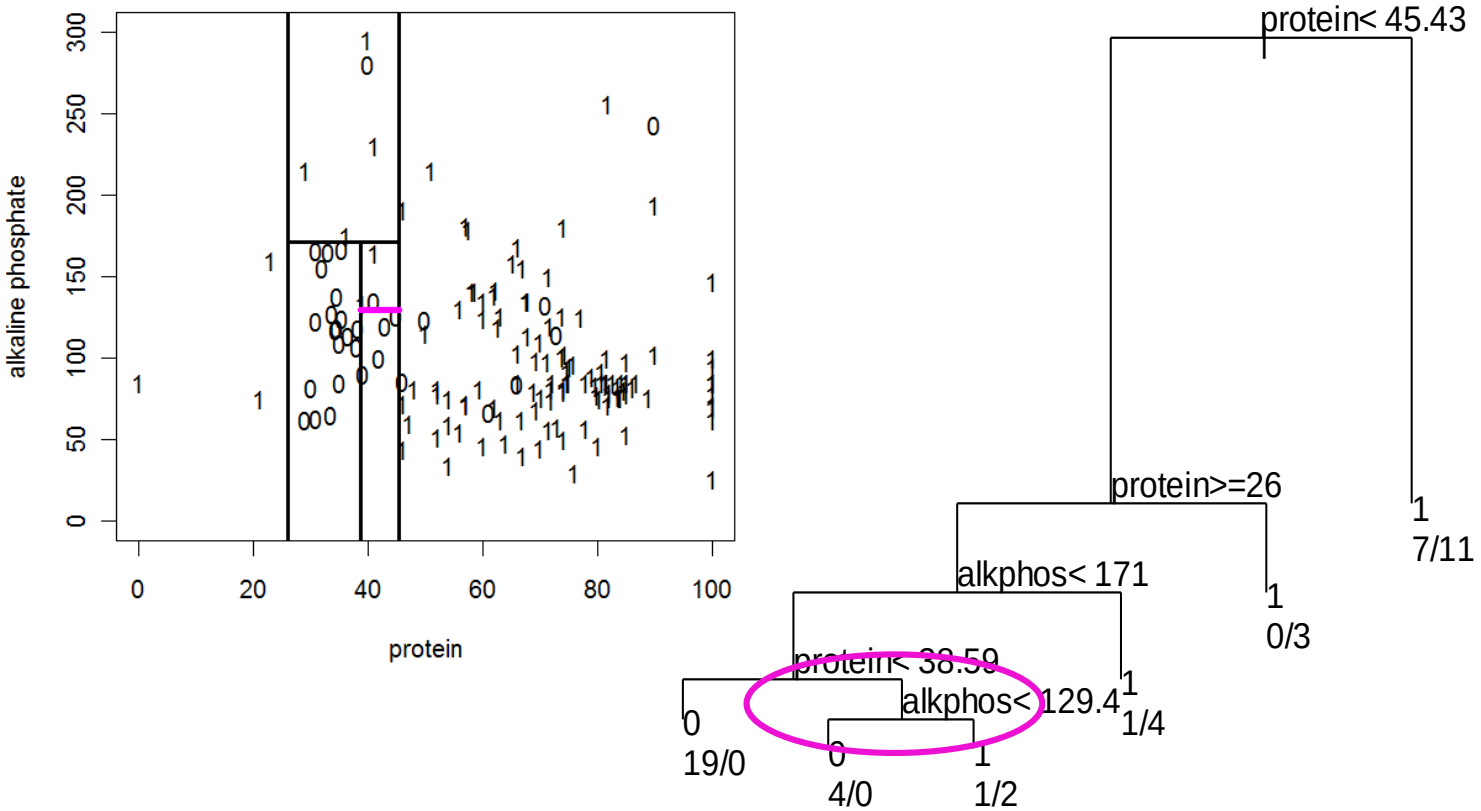


Pruning

- If the tree is too big, the lower "branches" are modeling noise in the data (overfitting).
- The usual paradigm is to grow the trees large and **prune** back unnecessary splits.
- Methods for **pruning** trees have been developed. Most use some form of cross-validation. Tuning may be necessary.

Classification and Regression Trees

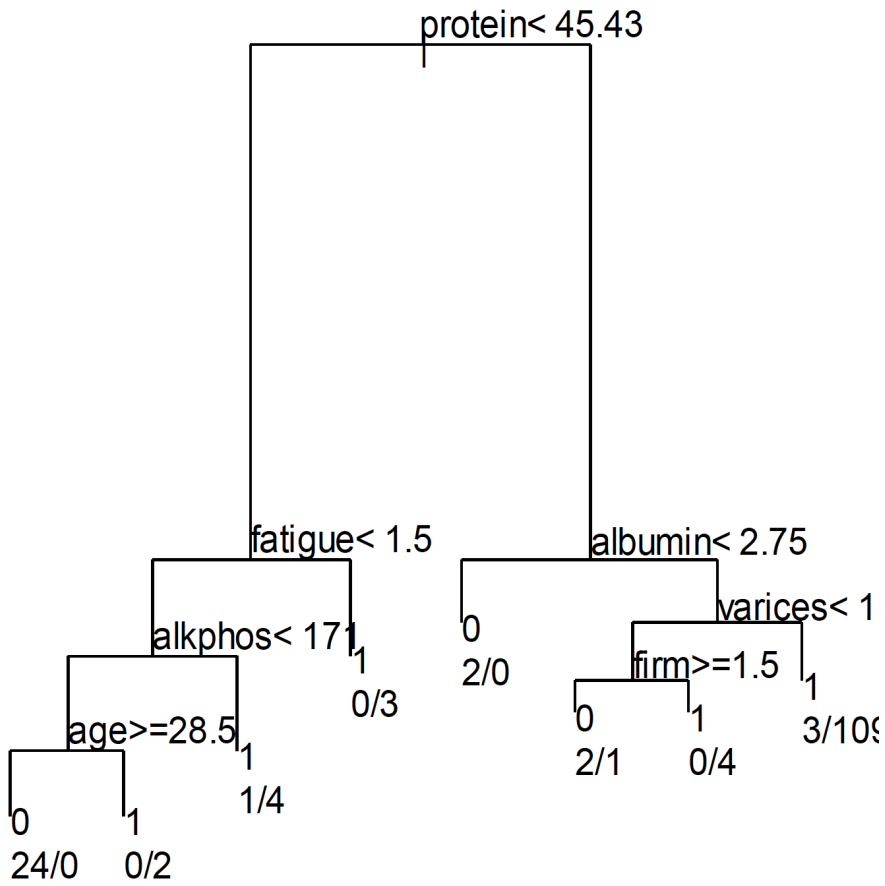
Advantages

- Applicable to both regression and classification problems.
- Handle categorical predictors naturally.
- Computationally simple and quick to fit, even for large problems.
- No formal distributional assumptions (non-parametric).
- Can handle highly non-linear interactions and classification boundaries.
- Automatic variable selection.
- Handle missing values through surrogate variables.
- Very easy to interpret if the tree is small.

Classification and Regression Trees

Advantages (cont.)

- The picture of the tree can give valuable insights into which variables are important and where.
- The terminal nodes suggest a natural clustering of data into homogeneous groups.



Classification and Regression Trees

Disadvantages

- **Accuracy** - current methods, such as support vector machines and ensemble classifiers often have 30% lower error rates than CART.
- **Instability** - if we change the data a little, the tree picture can change a lot. So the interpretation is not as straightforward as it appears.

Classification and Regression Trees

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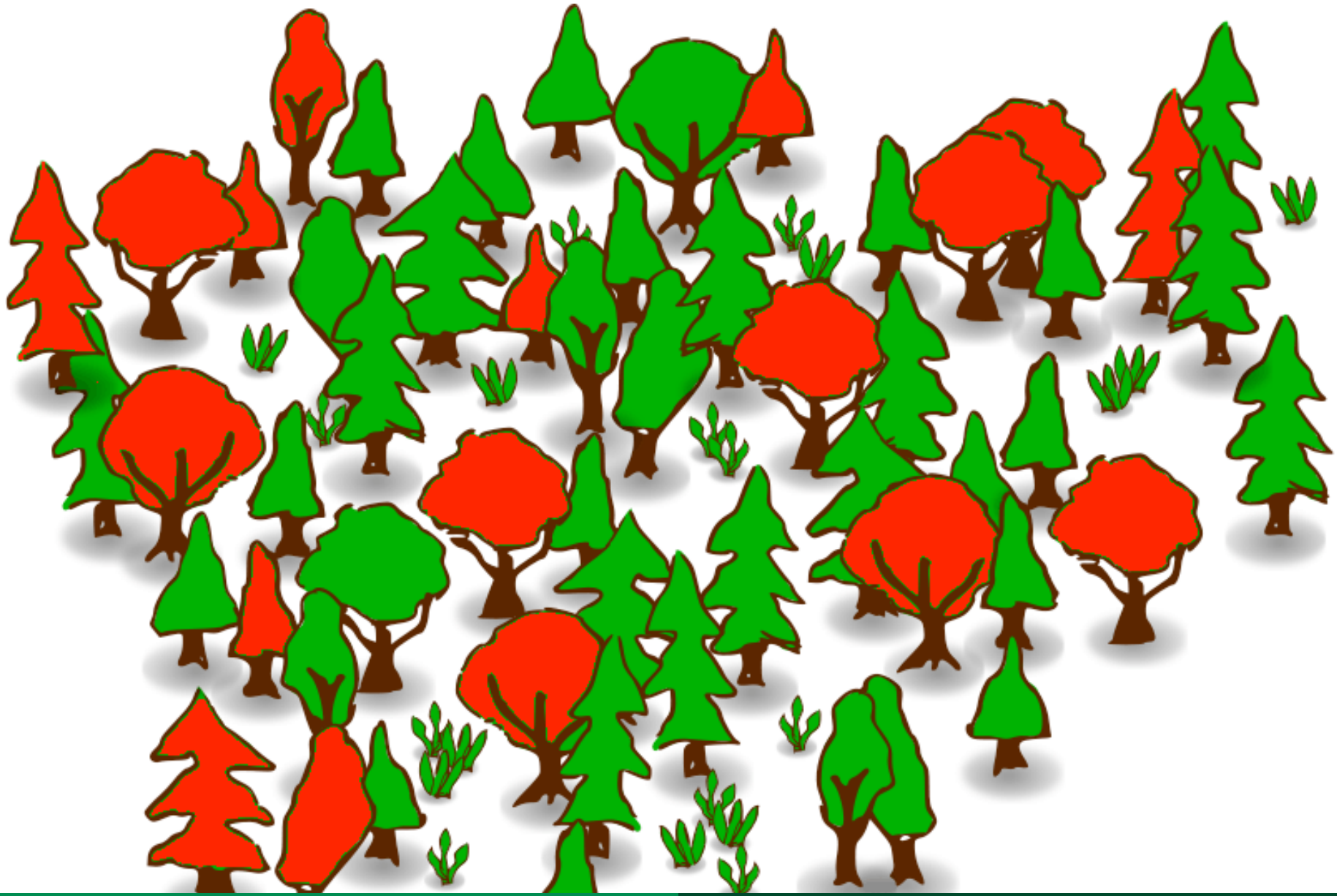
- **Accuracy** - current methods, such as support vector machines and ensemble classifiers often have 30% lower error rates than CART.
- **Instability** - if we change the data a little, the tree picture can change a lot. So the interpretation is not as straightforward as it appears.

Today, we can do better!

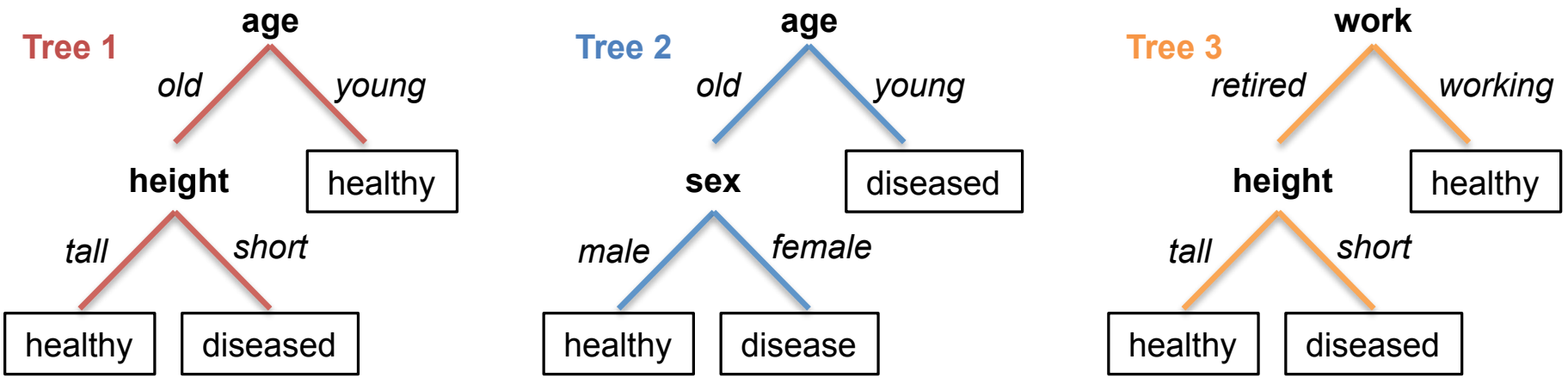
Random Forests

Random Forest

Random Forest

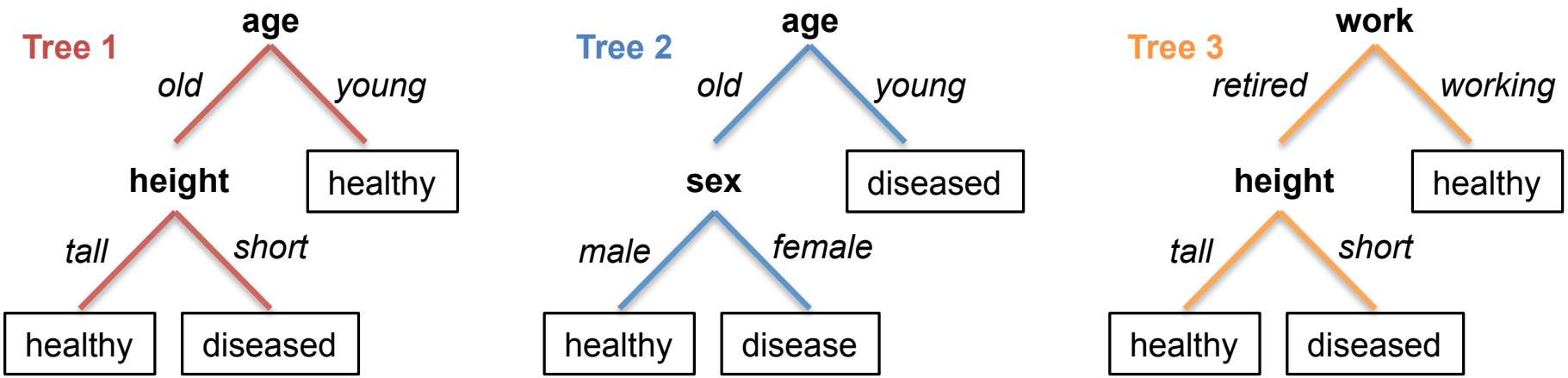


Example of Random Forest



- New sample: {old, retired, male, short}. Prediction?

Example of Random Forest



- New sample: {old, retired, male, short}. Prediction?
- Tree predictions: diseased, healthy, diseased
- Majority Rule: Diseased

The Random Forest Algorithm

1. For $b = 1$ to B
   1. Draw a bootstrap sample $\mathbf{Z}$ of size N from the training data
   2. Grow a random-forest tree T_b to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size $n_{\min}$ is reached.
      1. Select m variables at random from the p variables.
      2. Pick the best variable/split-point among the m
      3. Split the node into two daughter nodes
2. Output the ensemble of trees $\{T_b\}_1^B$

To make a prediction at a new point x:

- *Regression:* $\hat{f}_{\text{rf}}^B = \frac{1}{B}\sum_{b=1}^B T_b(x)$
- *Classification:* Let $\hat{C}_b(x)$ be the class prediction of the b-th random-forest tree. Then $\hat{C}_{\text{rf}}^B(x) = \text{majority vote}\{\hat{C}_b(x)\}_1^B$.

Differences to standard tree

- Train each tree on bootstrap resample of data
  Bootstrap resample of data set with N samples: Make new data set by drawing with replacement N samples; i.e., some samples will probably occur multiple times in new data set
- For each split, consider only m randomly selected variables
  Feature bagging
- Dont prune (why?)
- Fit a forest of B trees in such a way and use average or majority voting to aggregate results

Why Random Forest Works

- Mean Squared Error = Variance + Bias^2 + Noise
- If trees are sufficiently deep, they have very small bias (this is why we don't prune the trees)
- How could we improve the variance over that of a single tree?

Why Random Forest Works (cont.)

$$\text{Var}\left(\frac{1}{B}\sum_{i=1}^{B}T_i(c)\right) = \frac{1}{B^2}\sum_{i=1}^{B}\sum_{j=1}^{B}Cov(T_i(x),T_j(x))$$

$$= \frac{1}{B^2}\sum_{i=1}^{B}\left(\sum_{j\neq i}Cov(T_i(x),T_j(x)) + Var(T_i(x))\right)$$

Given that

$$Var(X+Y) = Var(X) + Var(Y) + 2Cov(X,Y), Var(X) = Cov(X,X)$$

$$Var(cX) = c^2 Var(X)$$

$$\rho(X,Y) = \frac{Cov(X,Y)}{\sqrt{Var(X), Var(Y)}}$$

A simplified setting: $\rho(T_i,T_j) = \rho, Var(T_i) = \sigma^2$

Why Random Forest Works (cont.)

$$\text{Var}\left(\frac{1}{B}\sum_{i=1}^{B}T_i(x)\right) = \frac{1}{B^2}\sum_{i=1}^{B}\sum_{j=1}^{B}Cov(T_i(x),T_j(x))$$

$$= \frac{1}{B^2}\sum_{i=1}^{B}\left(\sum_{j\neq i}^{B}Cov(T_i(x),T_j(x)) + Var(T_i(x))\right)$$

$$= \frac{1}{B^2}\sum_{i=1}^{B}\left((B-1)\sigma^2\rho + \sigma^2\right) = \frac{B(B-1)\rho\sigma^2 + B\sigma^2}{B^2}$$

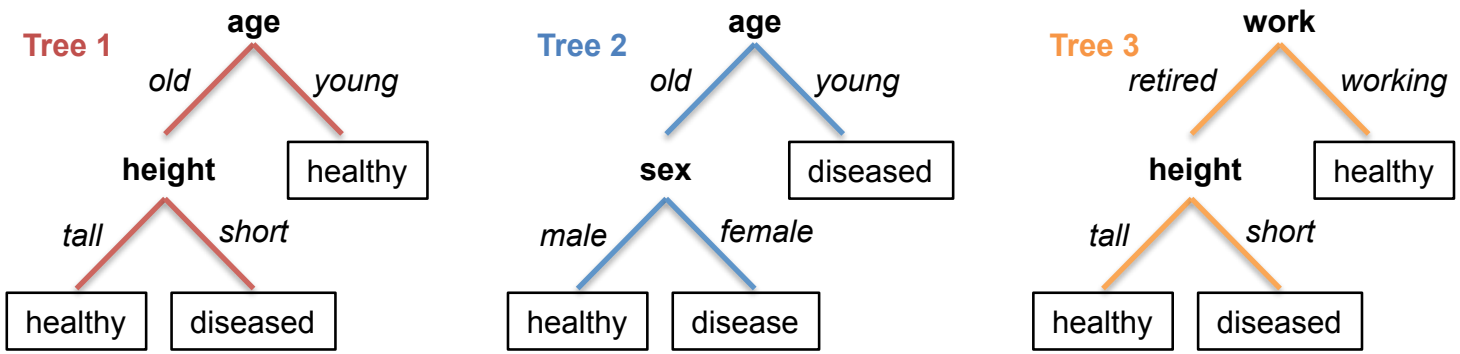
$$= \frac{(B-1)\rho\sigma^2}{B} + \frac{\sigma^2}{B} = \rho\sigma^2 - \frac{\rho\sigma^2}{B} + \frac{\sigma^2}{B}$$

$$= \rho\sigma^2 + \sigma^2(1-\rho)/B$$

Variance decreases if 1) correlation ρ decreases (i.e., if m decreases); 2) number of trees B increases (irrespective of ρ)

Variable Importance

- Advantage of tree methods is the intepretability.
- But we lose this property in random forest: what are the important variables in the forest?



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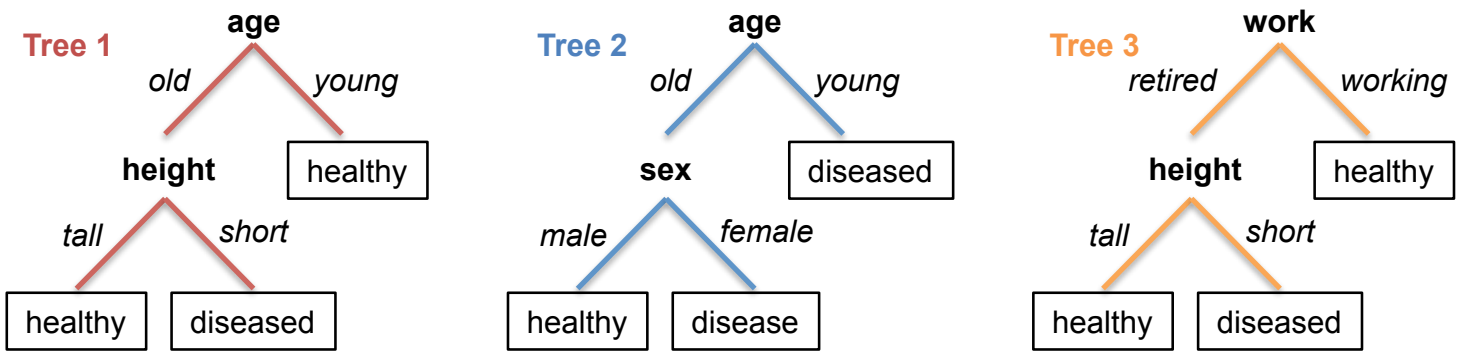
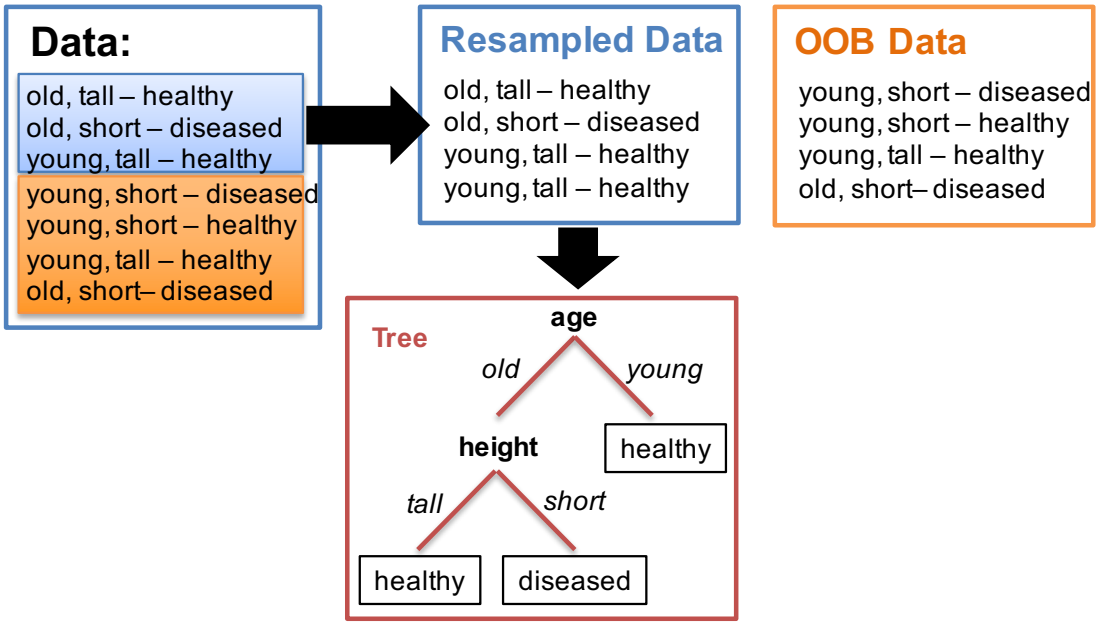


Good news. We can still identify important variables in the model.

Estimating Generalization Error

Out-of-Bag (OOB) Error

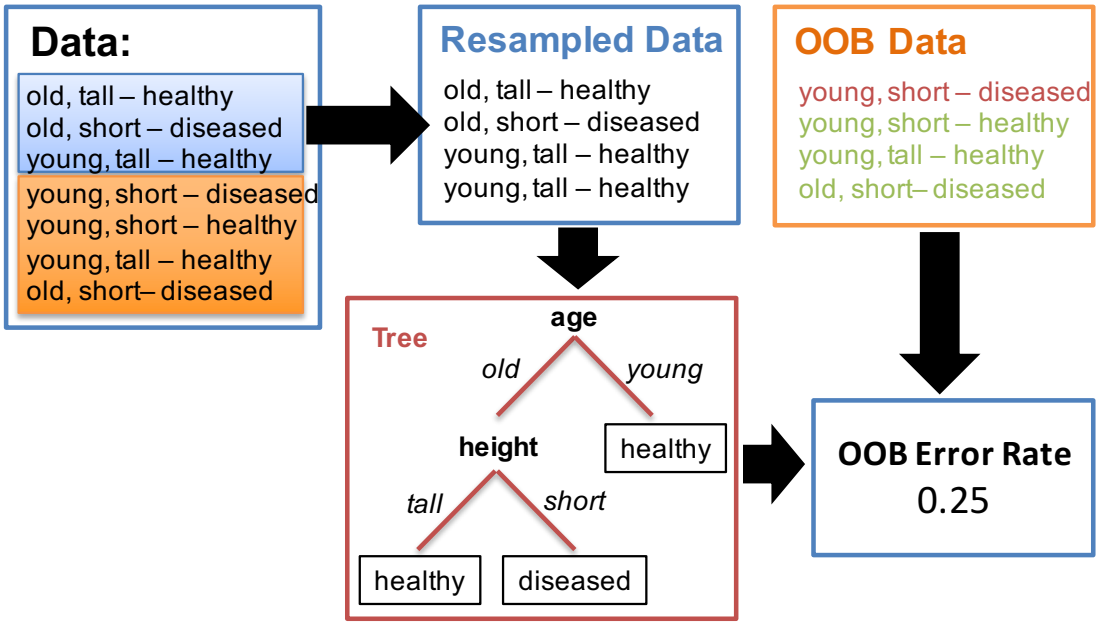
- Similar to leave-one-out cross-validation, but almost without any additional computational burden
- OOB error is a random number, since based on random resamples of the data



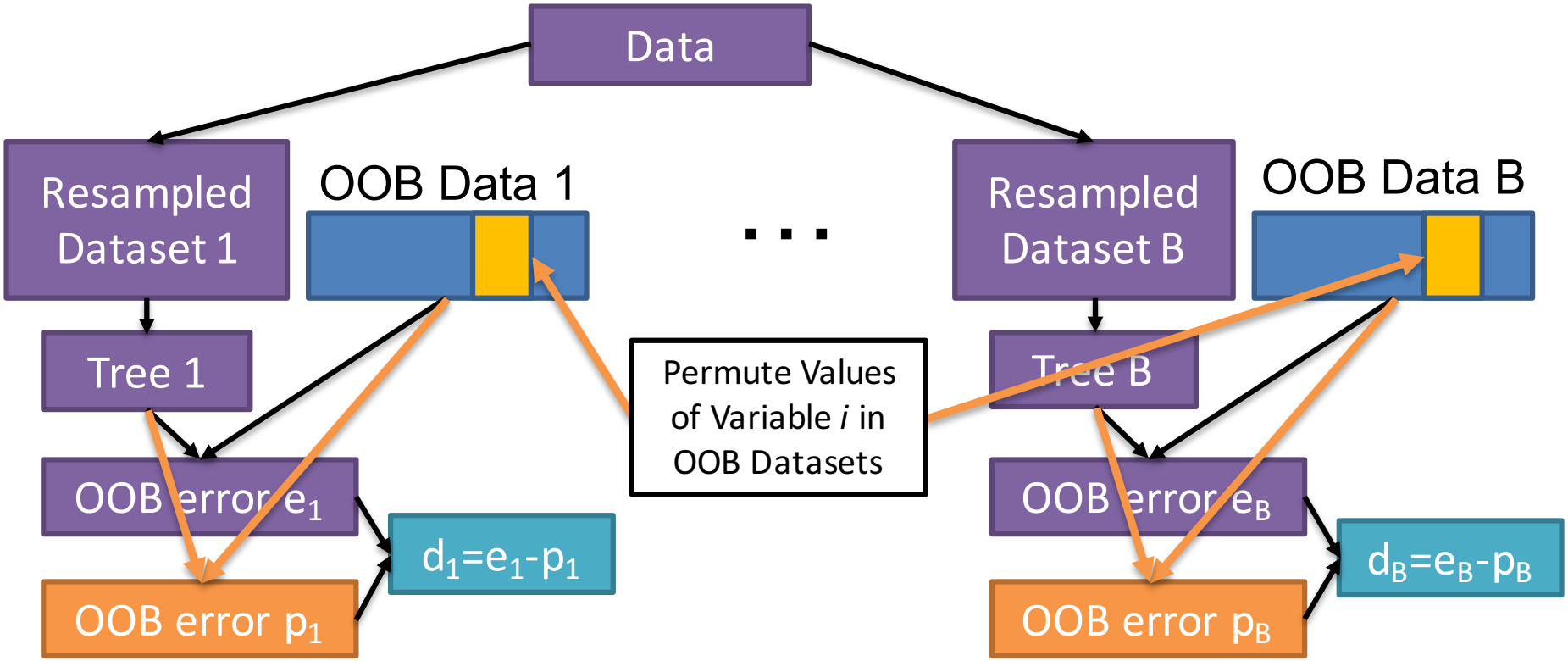
Estimating Generalization Error

Out-of-Bag (OOB) Error

- Similar to cross-validation, but almost without any additional computational burden
- OOB error is a random number, since based on random resamples of the data



Variable Importance for variable i using Permutations



- Average of d: $\bar{d} = \frac{1}{B}\sum_{j=1}^{B} d_j$
- Variance of d: $s_d^2 = \frac{1}{B-1}\sum_{j=1}^{B}(d_j - \bar{d})^2$
- Importance of feature i: $v_i = \bar{d}/s_d$

Tree and Random Forest

Trees

- \+ Trees yield insight into decision rules
- \+ Rather fast
- \+ Easy to tune parameters
- – Prediction of trees tend to have a high variance

Random Forest

- \+ RF has smaller prediction variance and therefore usually a better general performance
- \+ Easy to tune parameters
- – Rather slow
- – "Black Box": Rather hard to get insights into decision rules

Random Forest and LDA

Random Forest

- \+ Can model nonlinear class boundaries
- \+ OOB error "for free" (no CV needed)
- \+ Works on continuous and categorical responses (regression / classification)
- \+ Gives variable importance
- \+ Very good performance
- – Black box
- – Slow

LDA

- \+ Very fast
- \+ Discriminants for visualizing group separation
- \+ Can read off decision rule
- – Can model only linear class boundaries
- – Mediocre performance
- – No variable selection
- – Only on categorical response
- – Needs CV for estimating prediction error