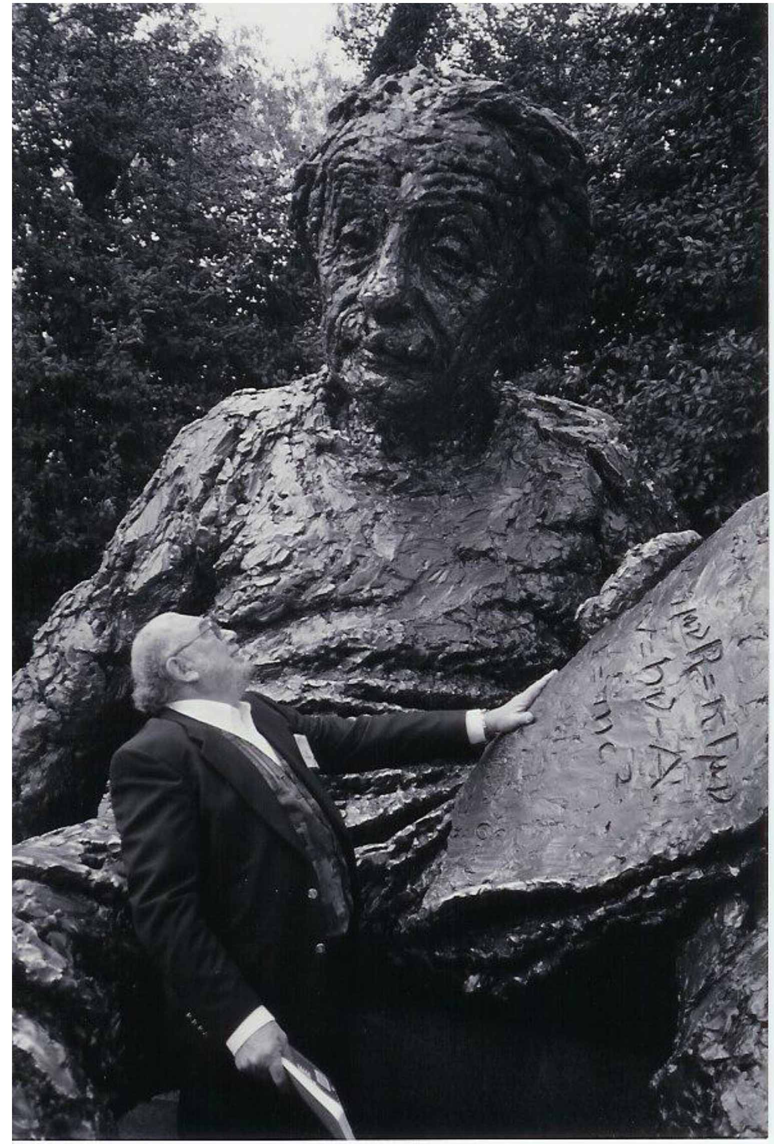
Random Forests

Adele Cutler
Utah State University

Random Forests

Leo Breiman

January 27, 1928 - July 5, 2005



Outline

- What are random forests?

- Background

- New features since Breiman (2001)
  - Proximities
    - Imputing missing values
    - Clustering
  - Unequal class sizes
  - Local variable importance
  - Visualization

Outline

- What are random forests?
- Background
- New features since Breiman (2001)
  - Proximities
    - Imputing missing values
    - Clustering
  - Unequal class sizes
  - Local variable importance
  - Visualization

Drawbacks of a classification tree:

- **Accuracy**: state-of-the-art methods have much lower error rates than a single classification tree.

- **Instability**: if you change the data a little, the tree picture can change a lot, so ***the interpretation is built on shifting sands.***

Today, we can do better!

Random Forests

What are Random Forests?

Grow a *forest* of trees:

- each tree is grown on an independent bootstrap sample from the training data.

- independently, for each node of each tree, find the best split on m randomly selected variables.

- grow deep trees.

Get the prediction for a new case by voting (averaging) the predictions from all the trees.

Properties of Random Forests

1. Accurate.
   – In independent tests on collections of data sets it's neck-and-neck with the best known machine learning methods (eg SVMs).

2. Fast.
   – With 100 variables, 100 trees in a forest can be grown in the same time as growing 3 single CART trees.

3. Do not overfit as we add more trees.

4. Handles
   - thousands of variables
   - many-valued categoricals
   - extensive missing values
   - badly unbalanced data sets.

5. Gives an internal estimate of test set error as trees are added to the ensemble.

6. Gives variable importance measures and proximities for visualization/clustering.

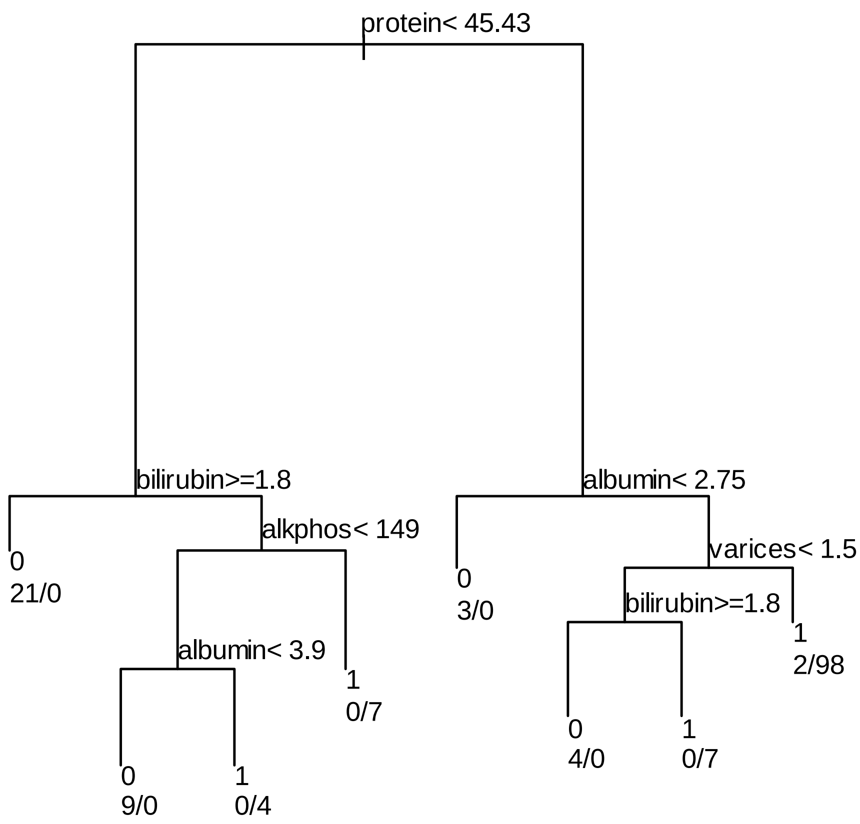
Leo: gives a wealth of scientifically important insights!

Outline

- What are random forests?
- Background
- New features since Breiman (2001)
  - Proximities
    - Imputing missing values
    - Clustering
  - Unequal class sizes
  - Local variable importance
  - Visualization

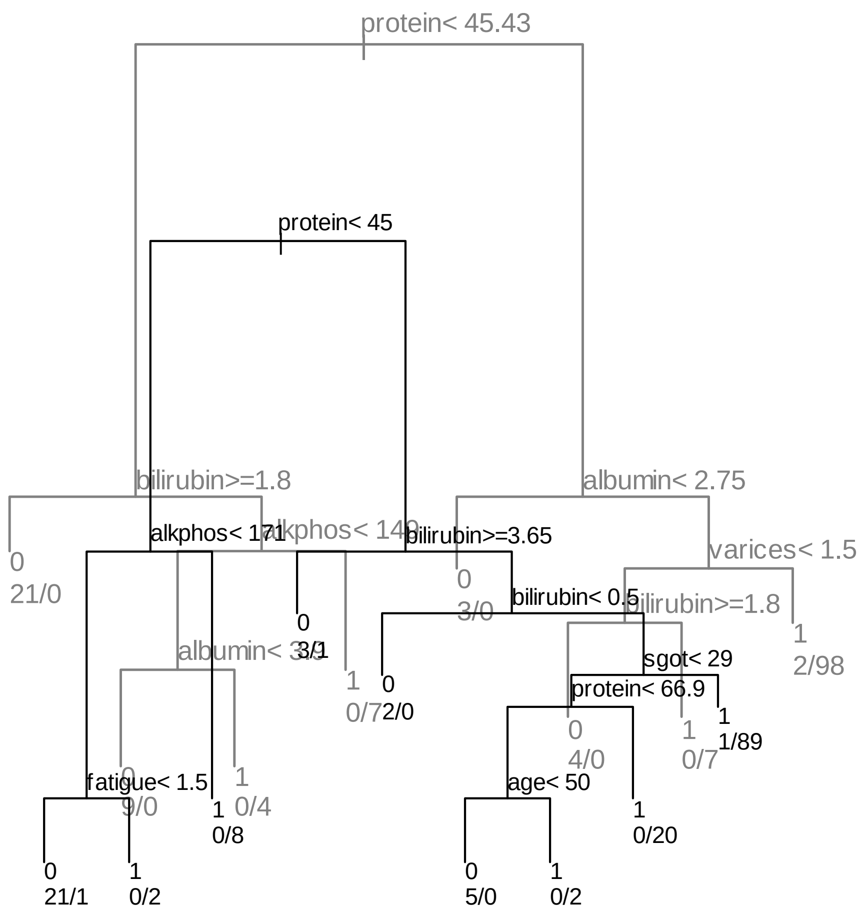
Random Forests

How do they work?



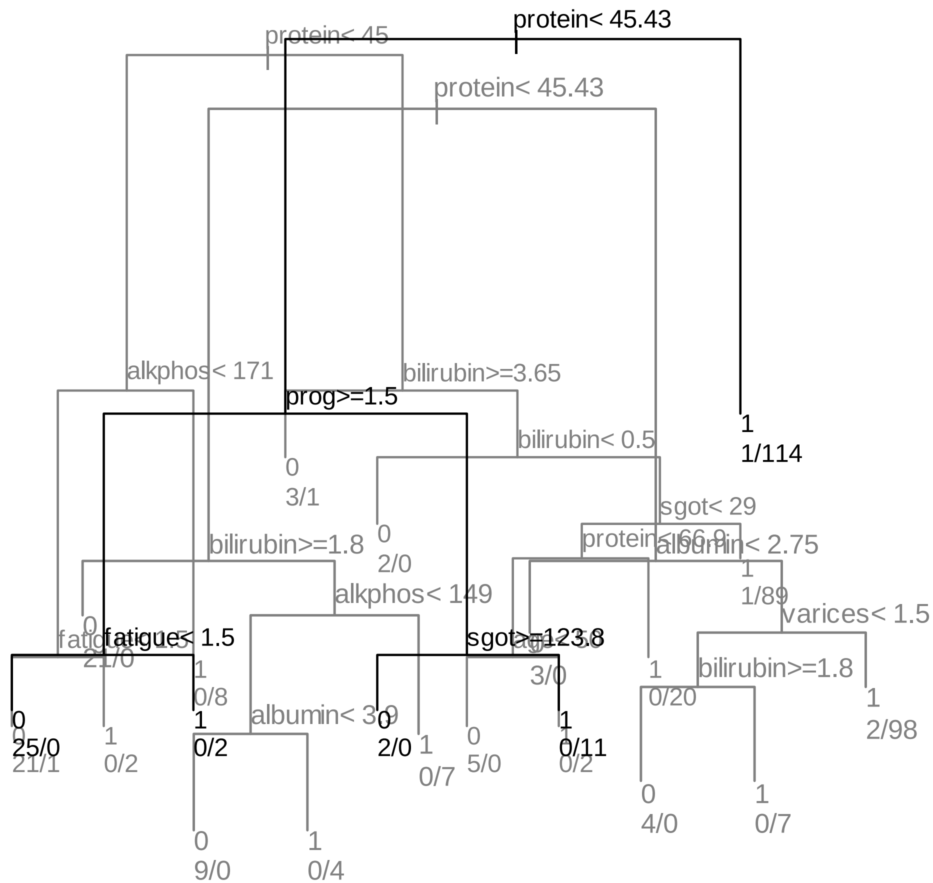
Random Forests

How do they work?



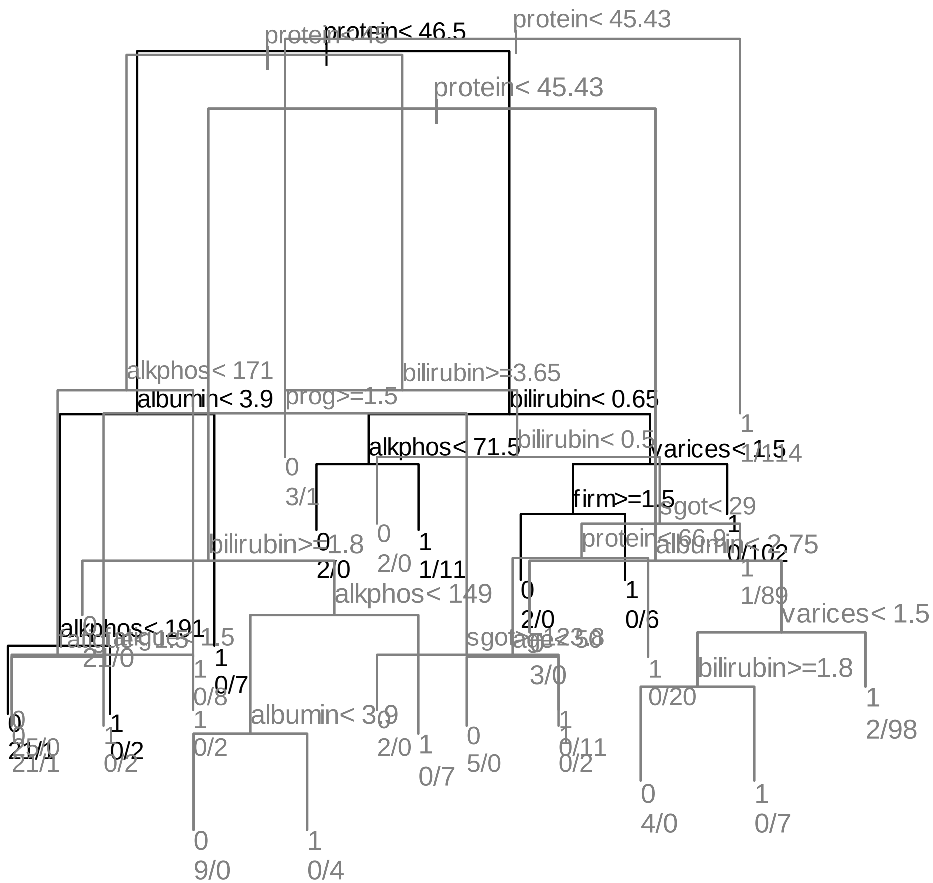
Random Forests

How do they work?



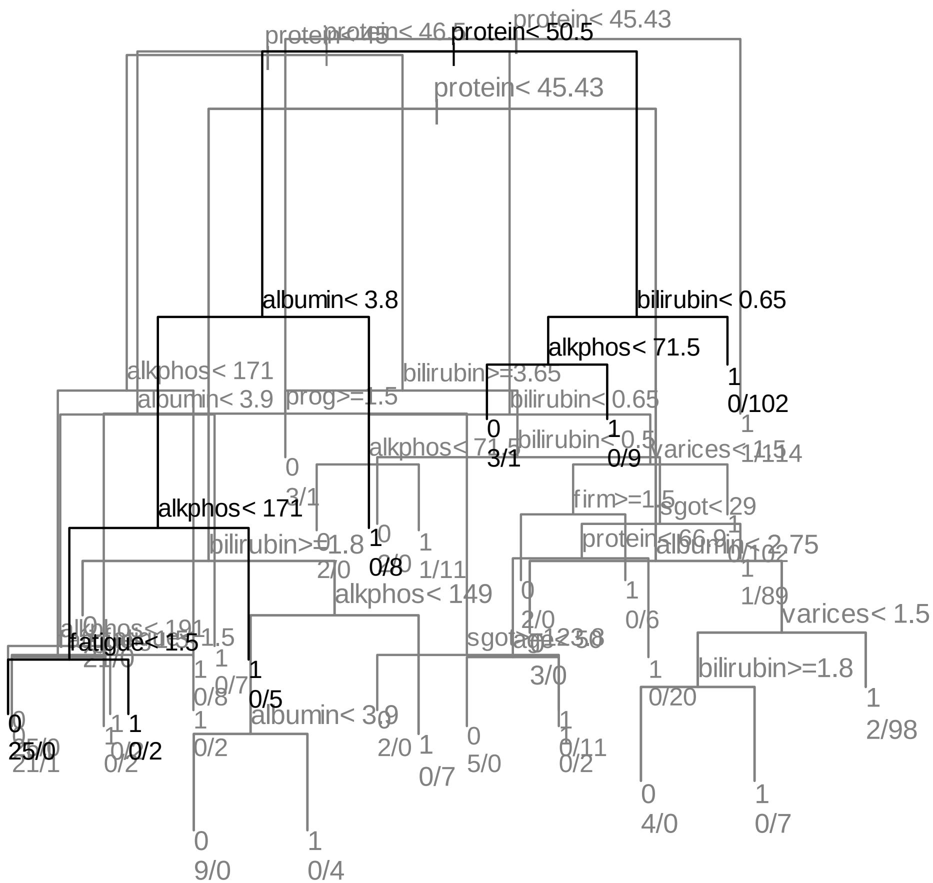
Random Forests

How do they work?



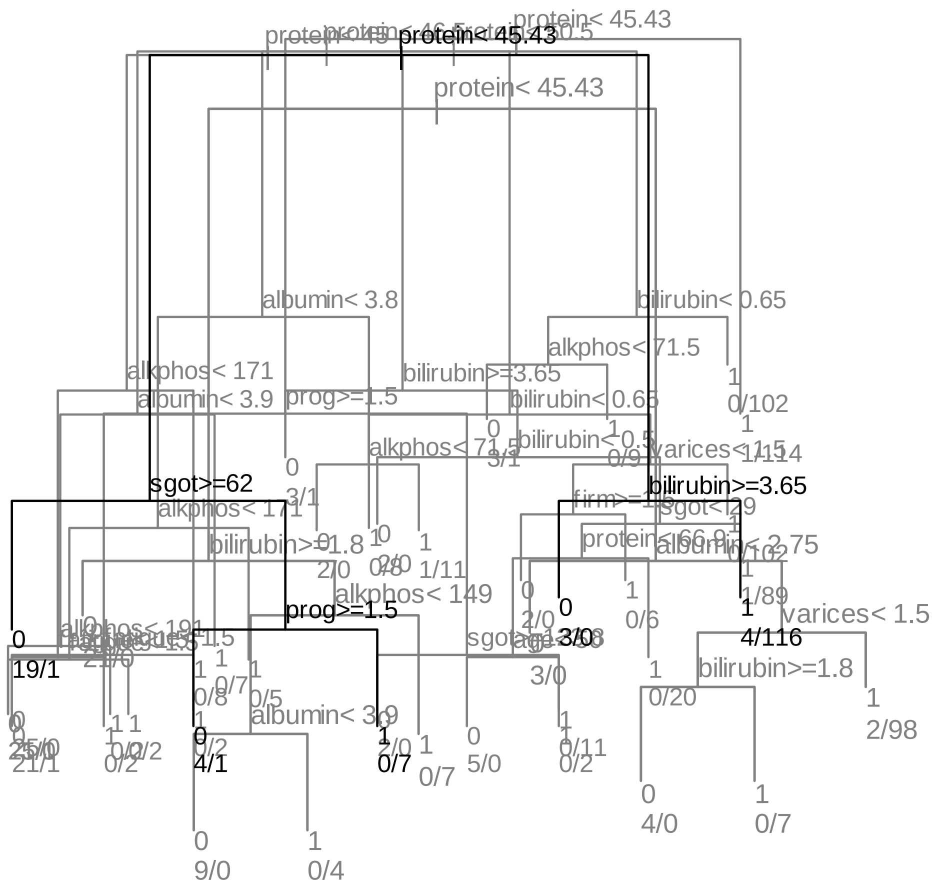
Random Forests

How do they work?



Random Forests

How do they work?



Leo: Looking at the trees is not going to tell us very much.

Illustration - Hepatitis

protein and alkaline phosphate

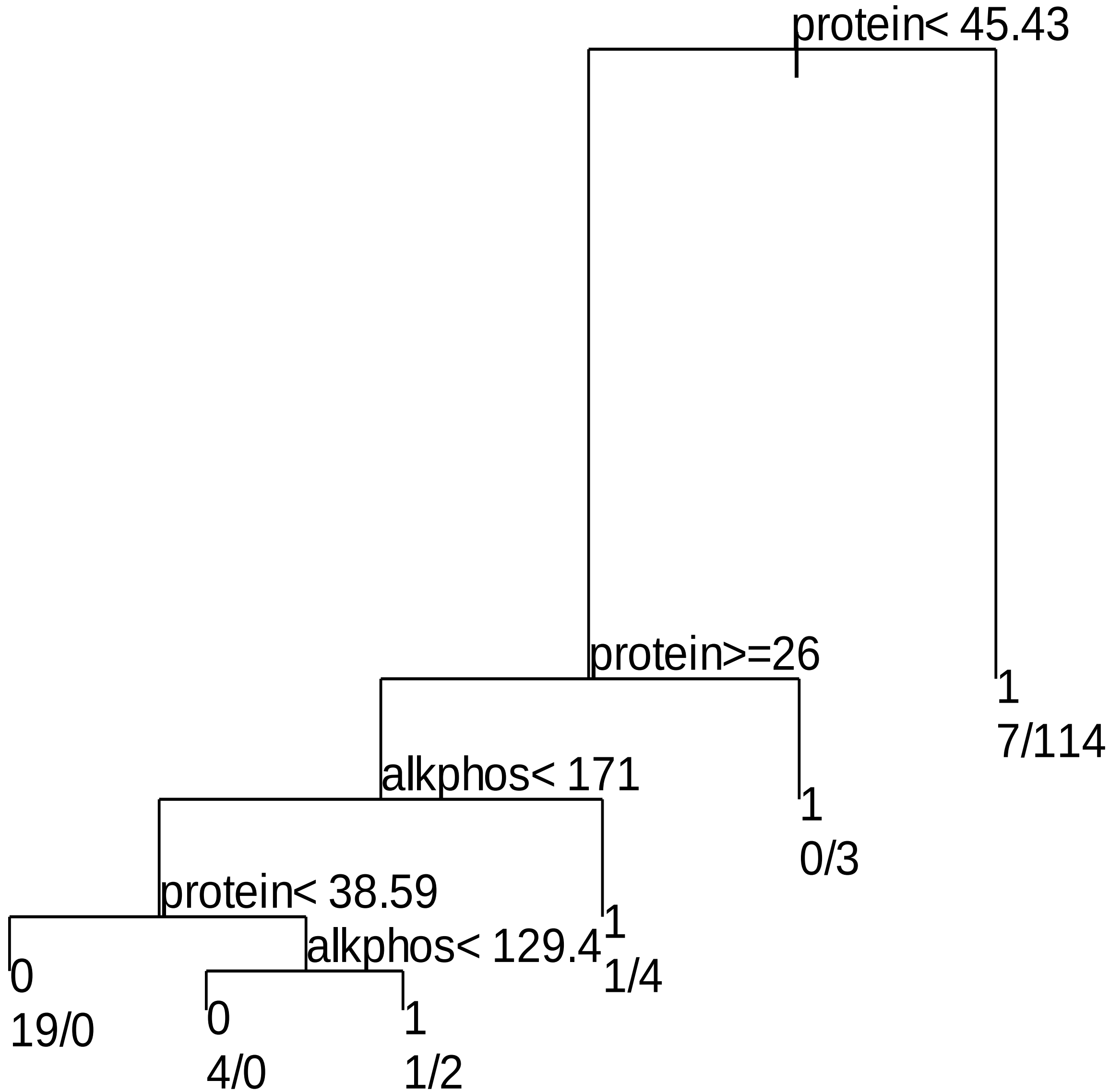
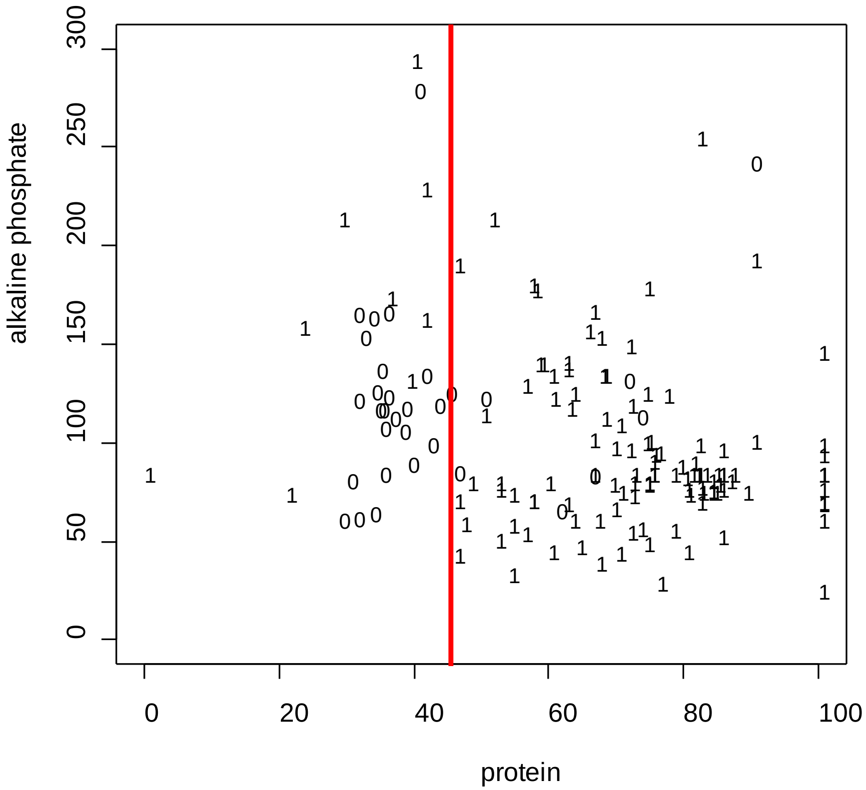


Illustration - Hepatitis

protein and alkaline phosphate



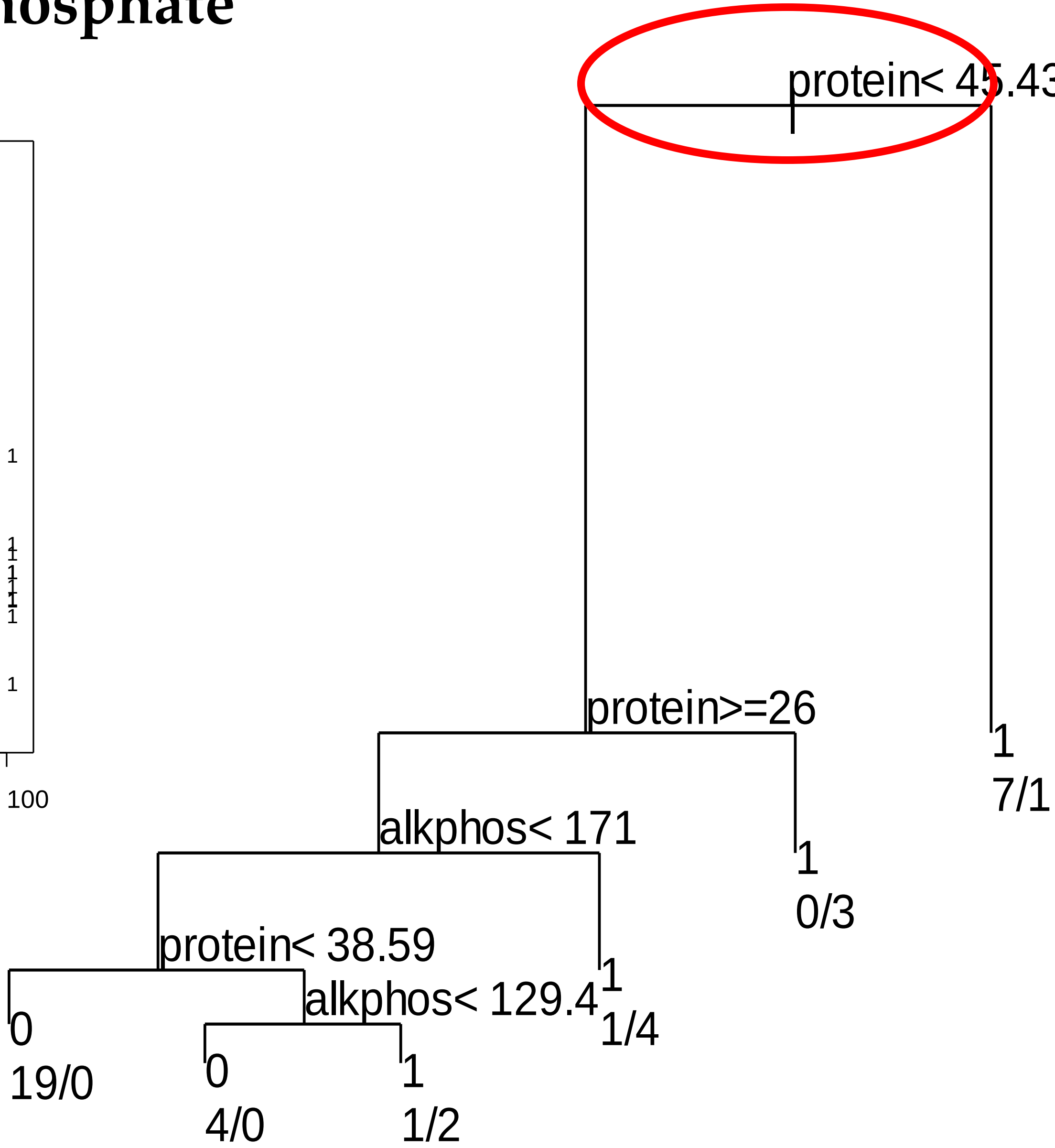
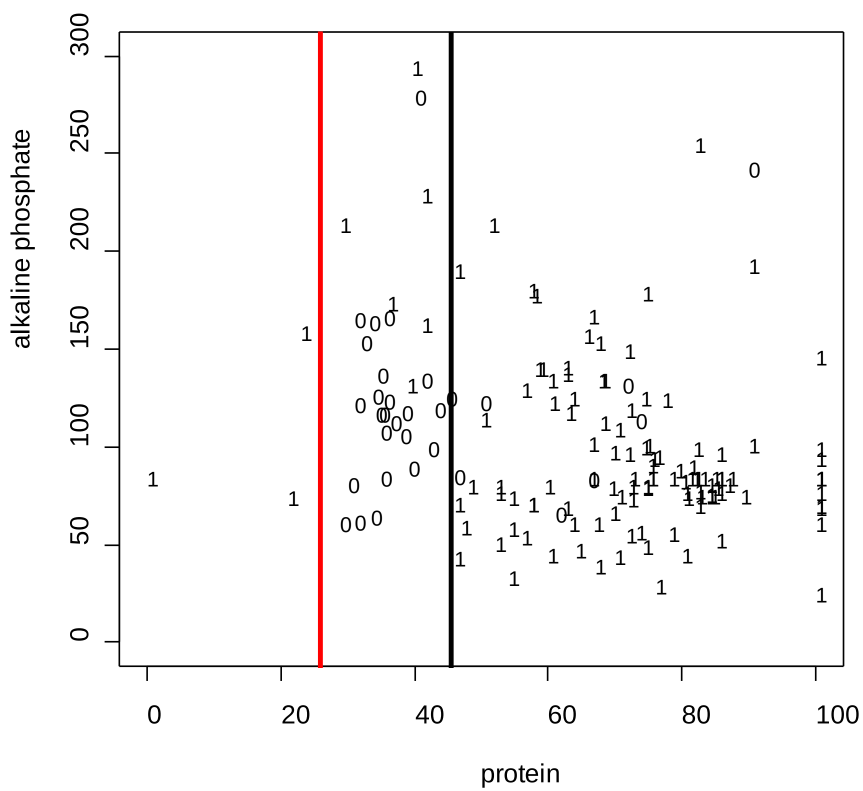


Illustration - Hepatitis

protein and alkaline phosphate



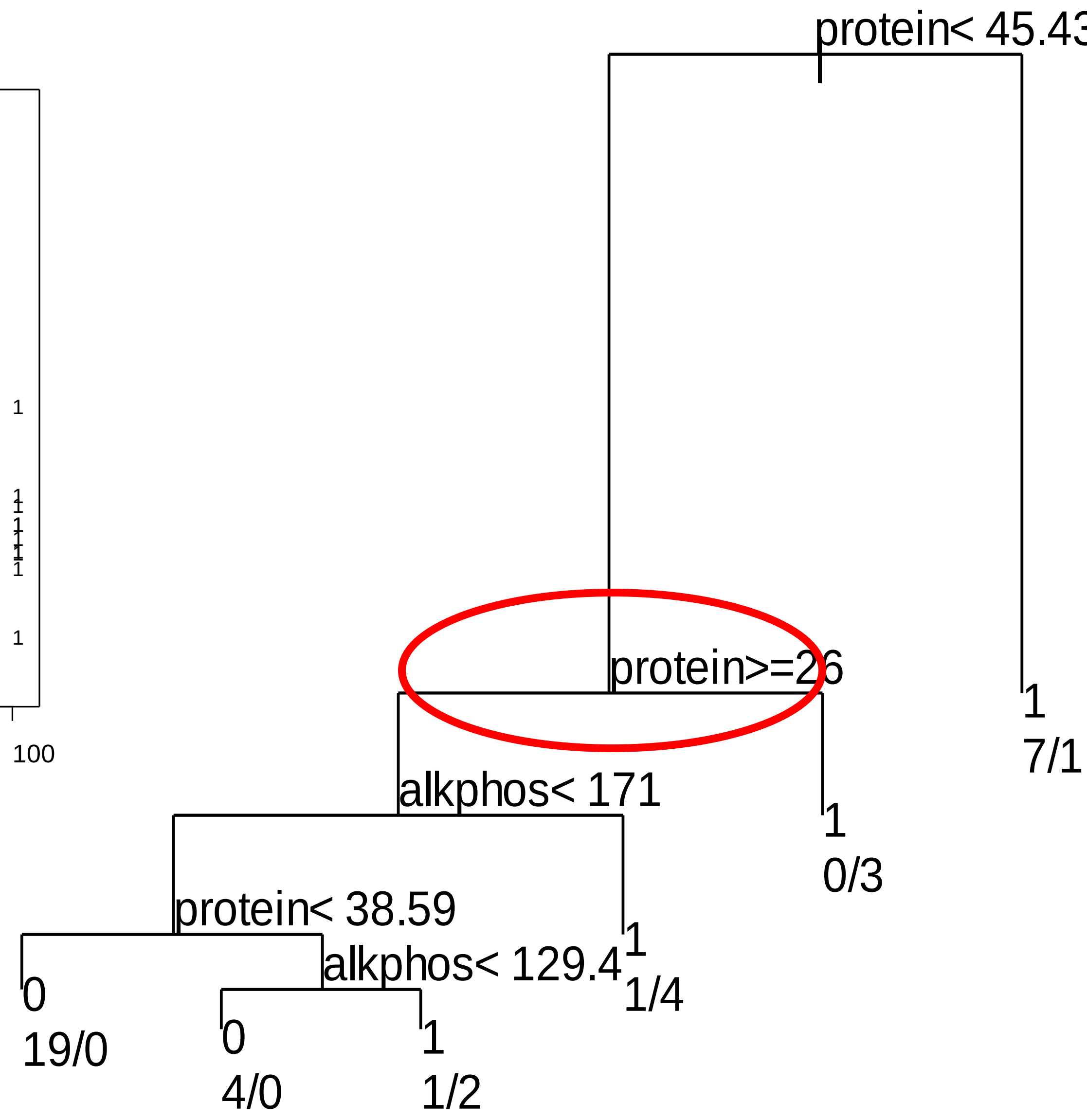
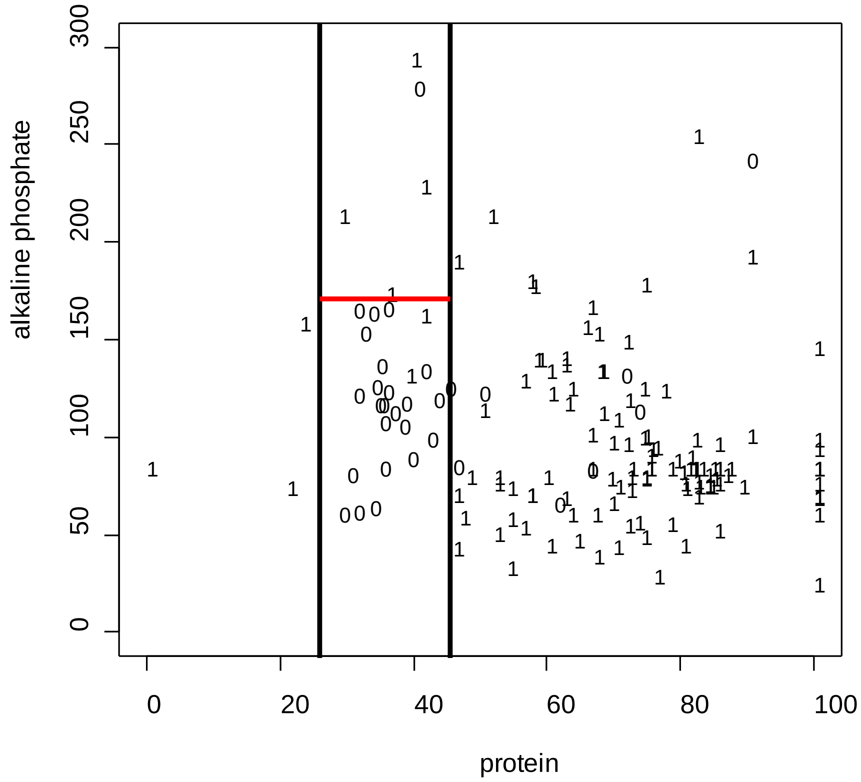


Illustration - Hepatitis

protein and alkaline phosphate



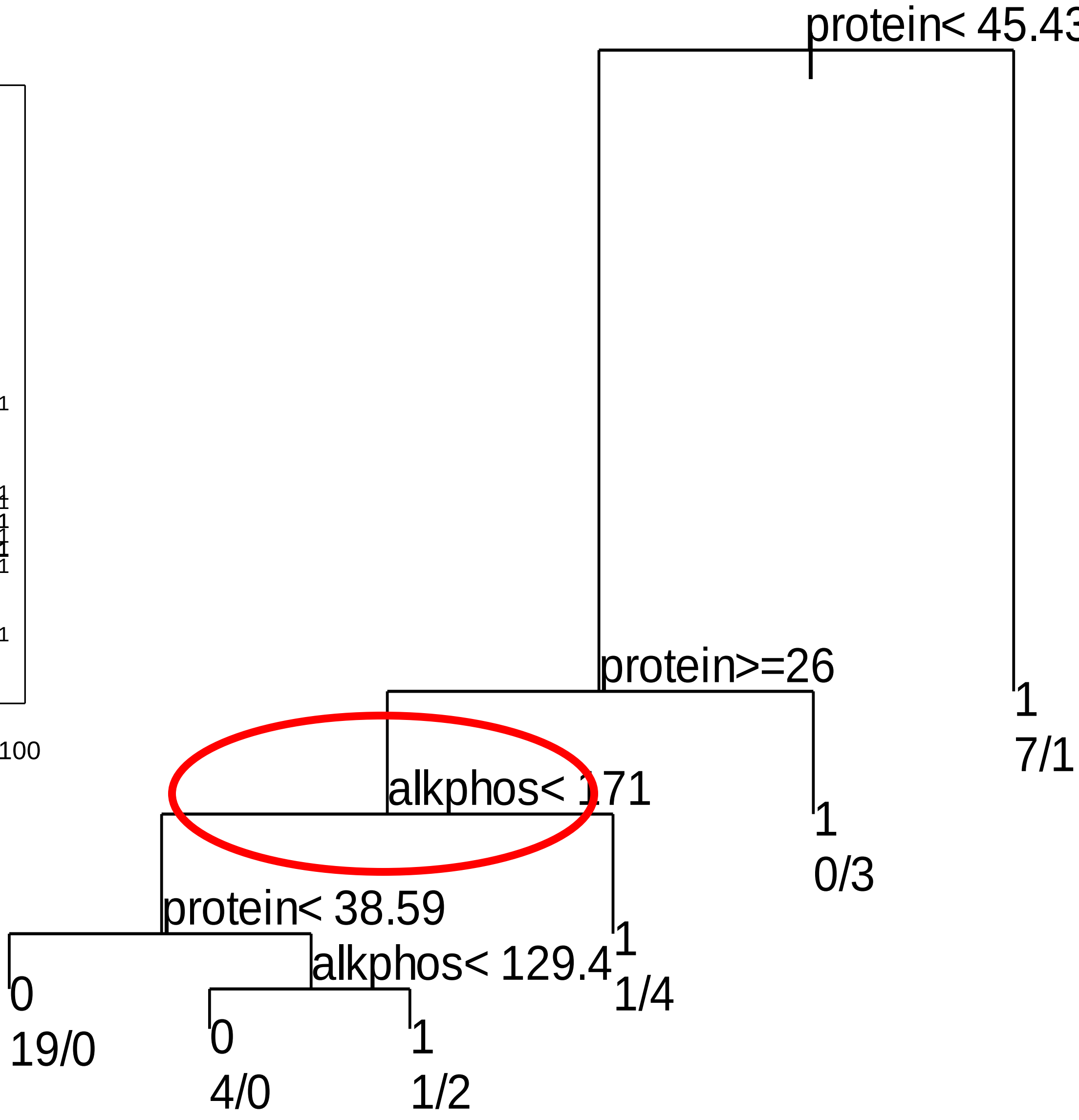
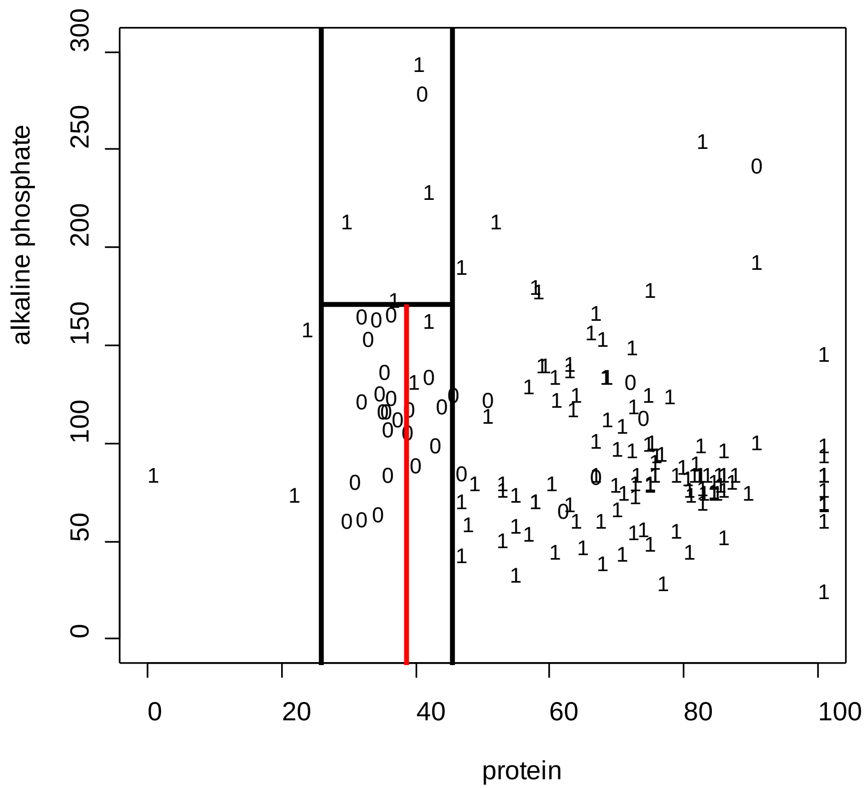


Illustration - Hepatitis

protein and alkaline phosphate



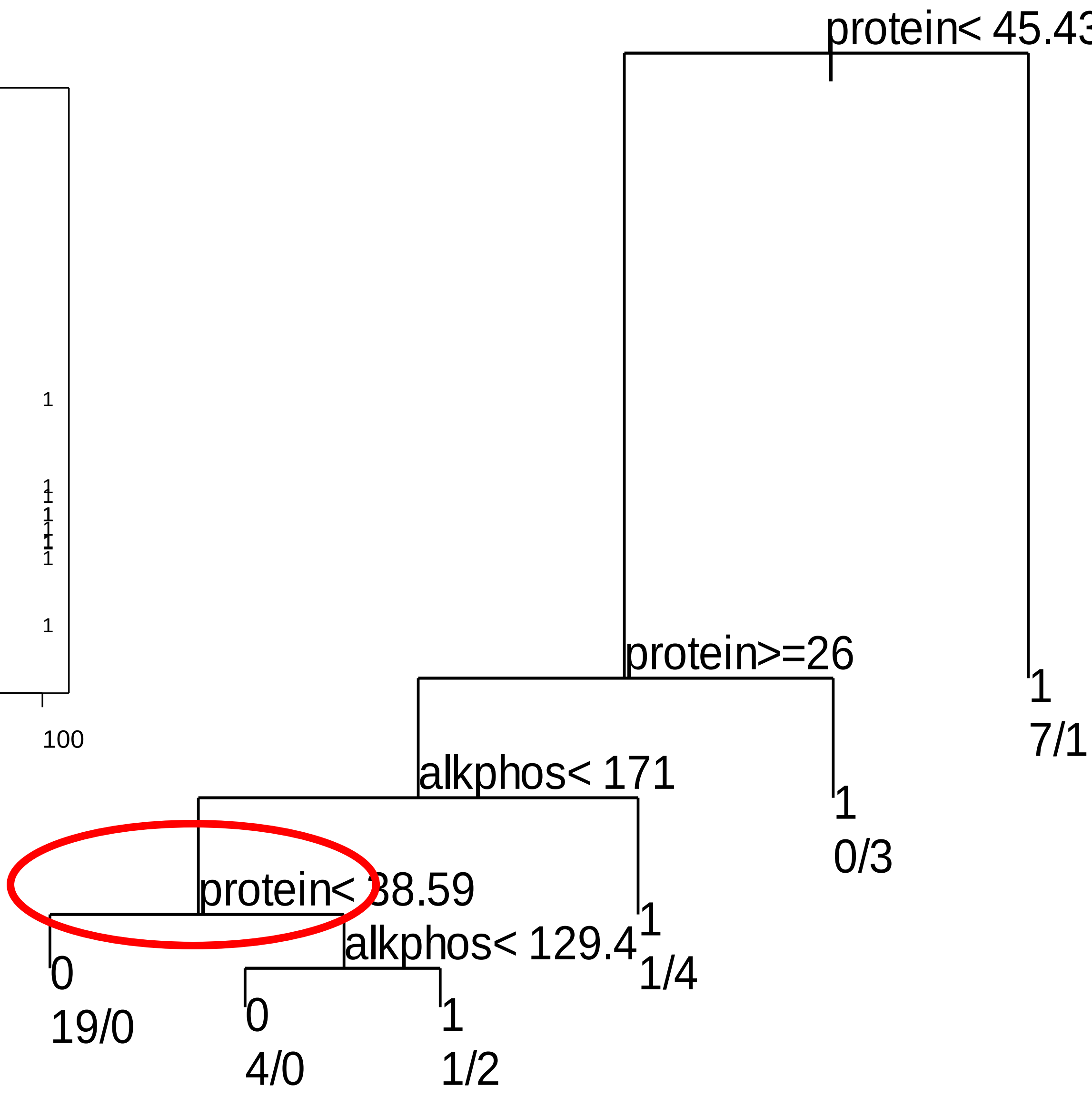
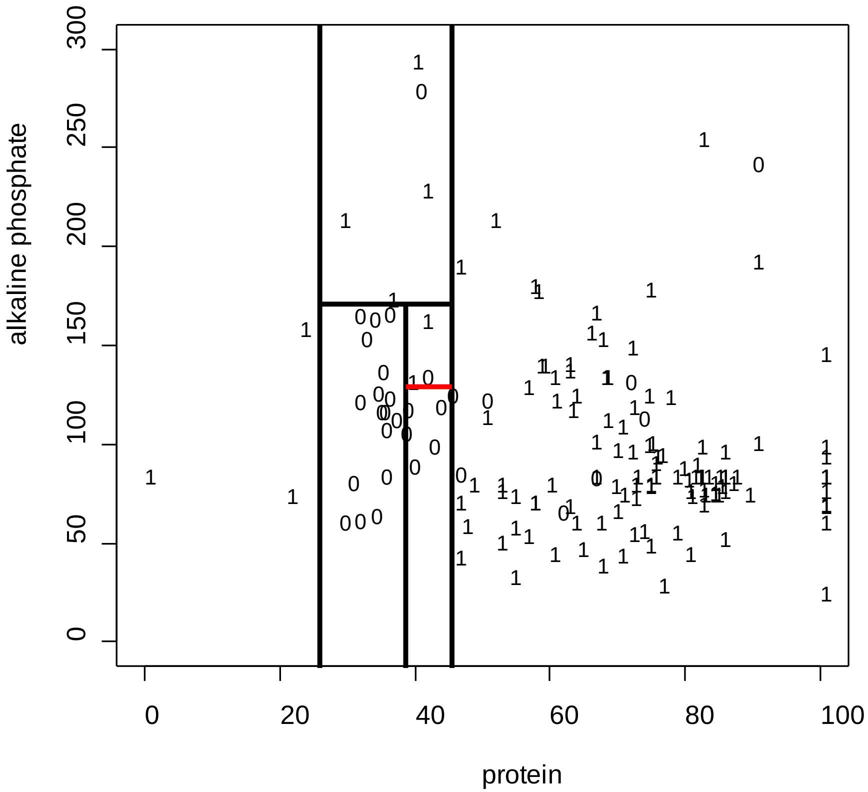
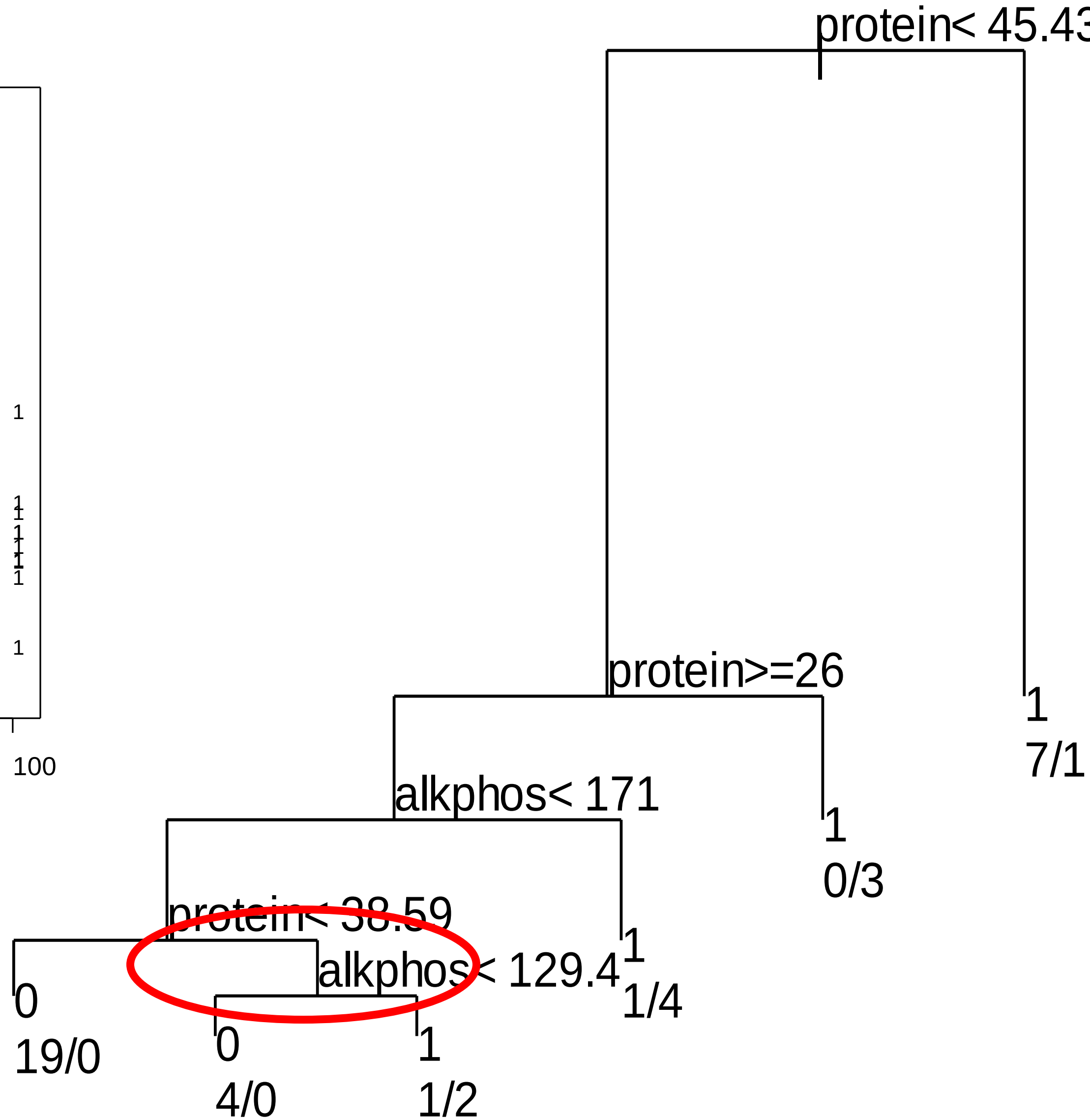


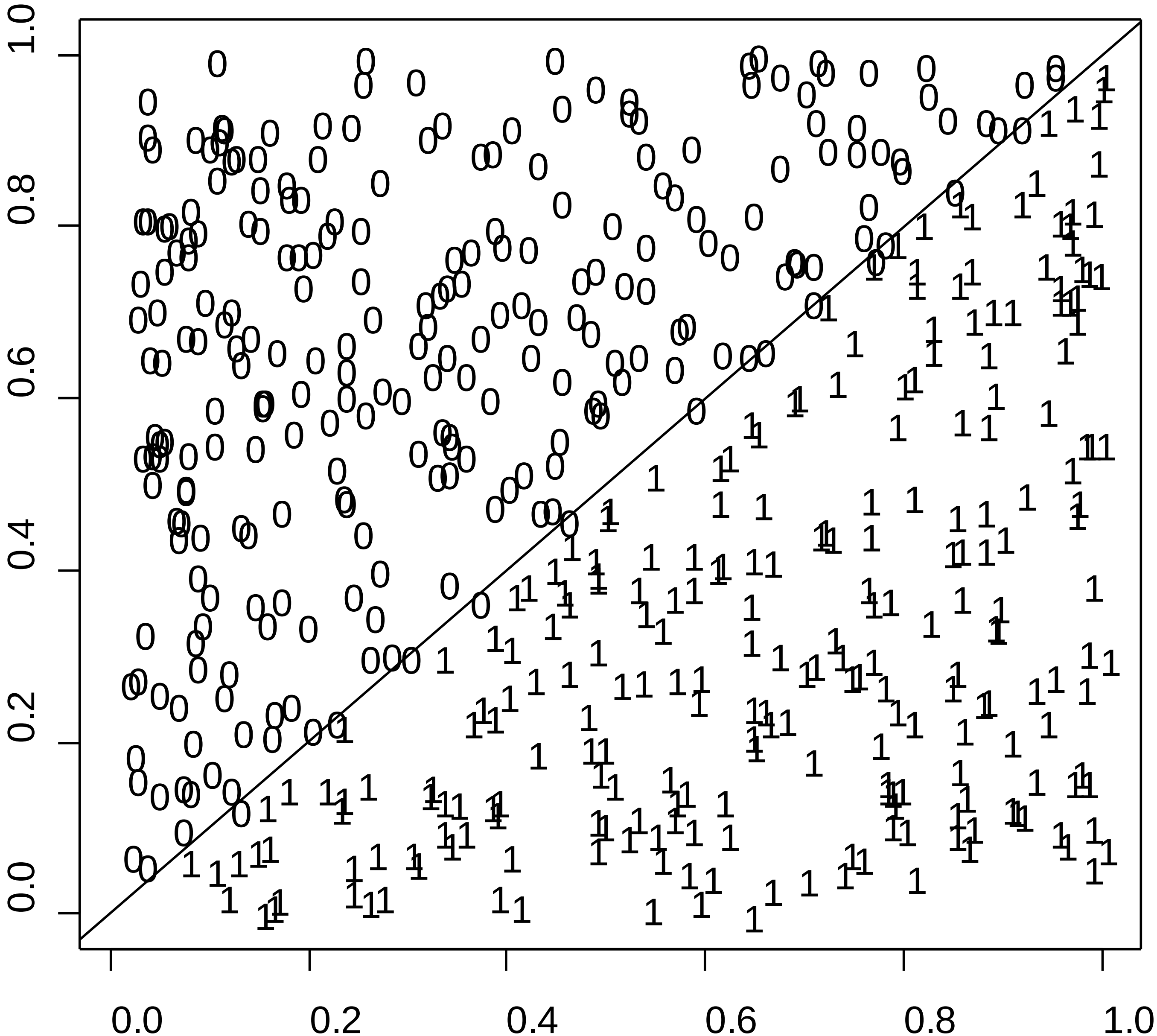
Illustration - Hepatitis

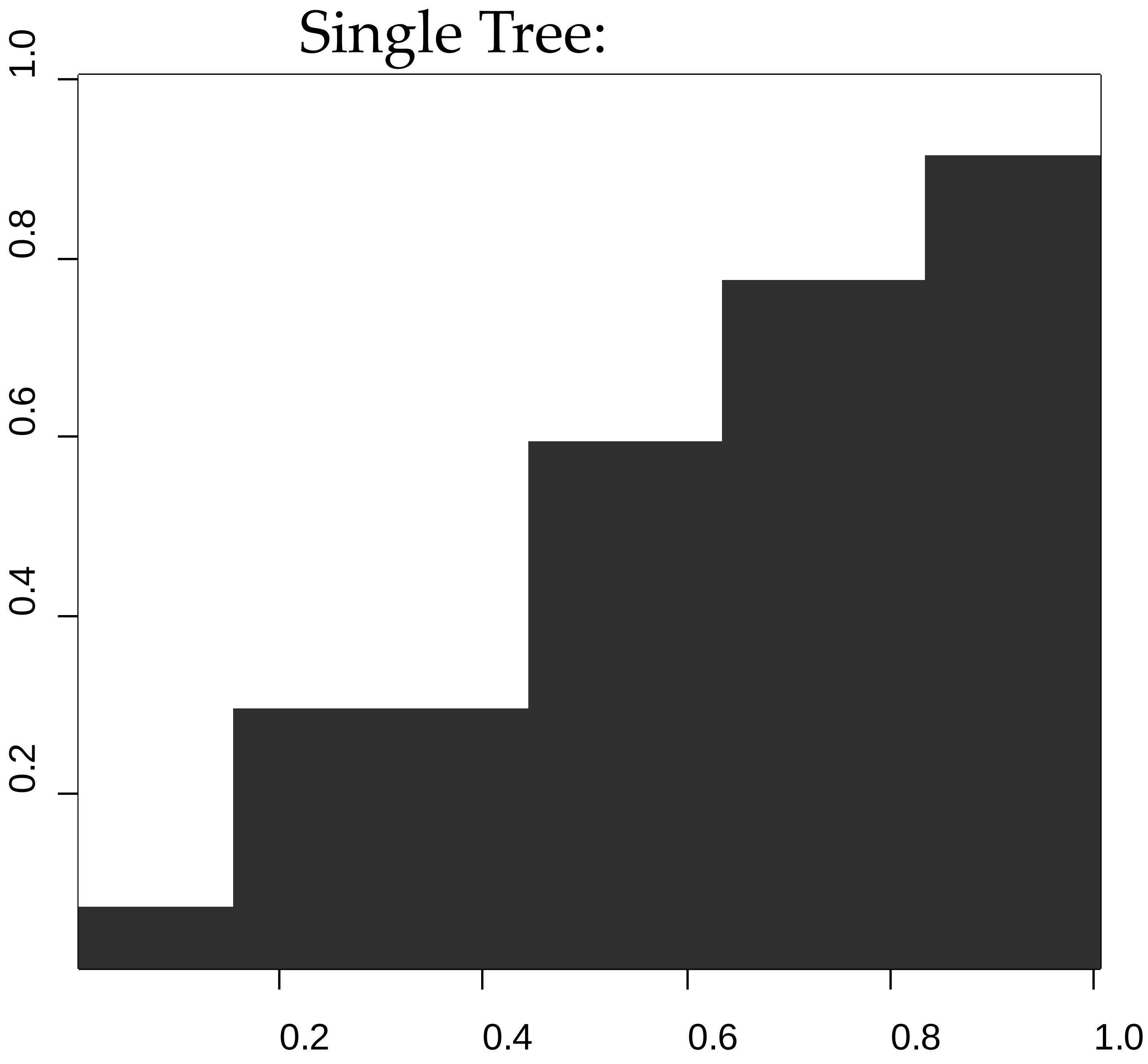
protein and alkaline phosphate



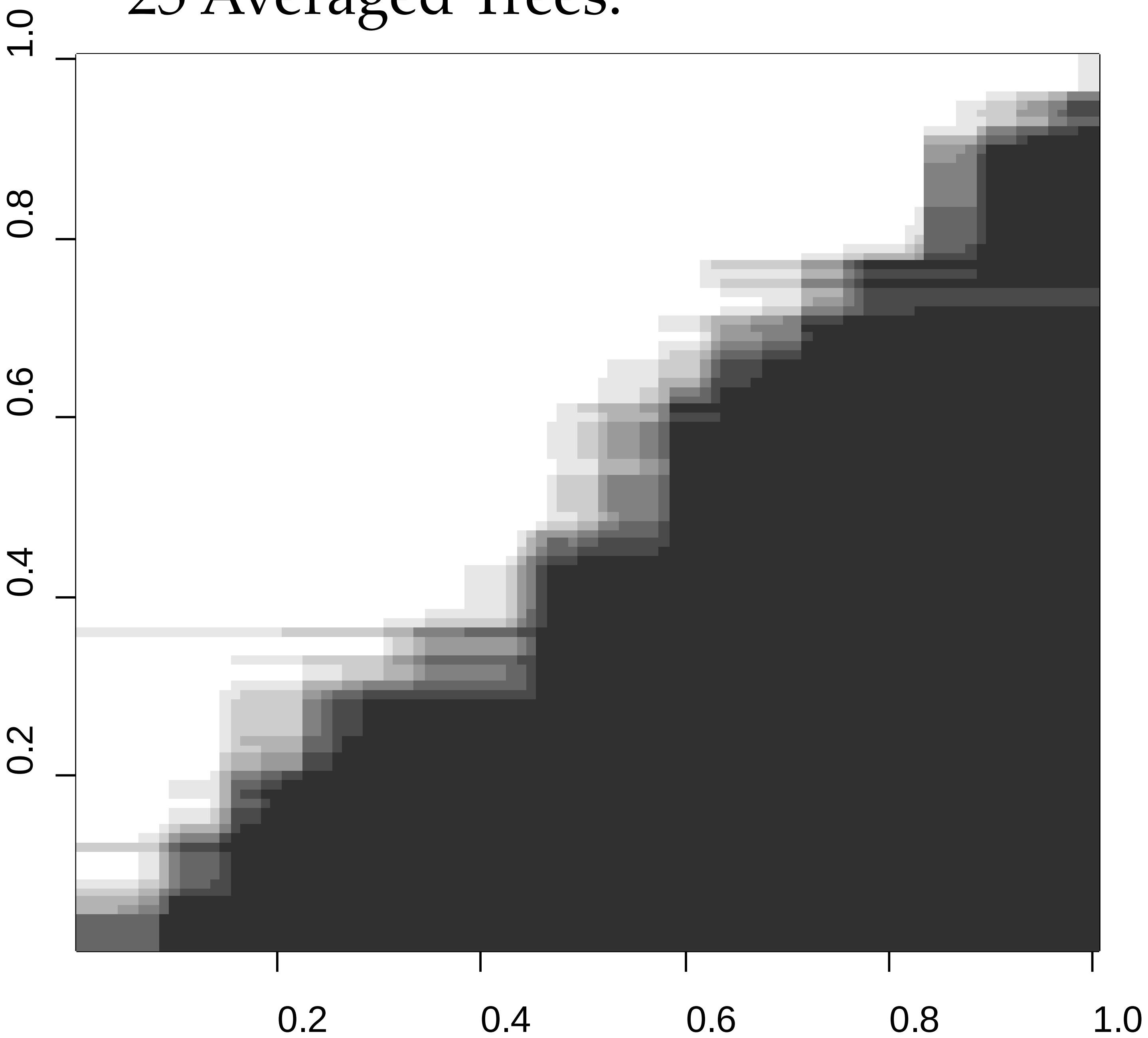


Hard for a single tree:

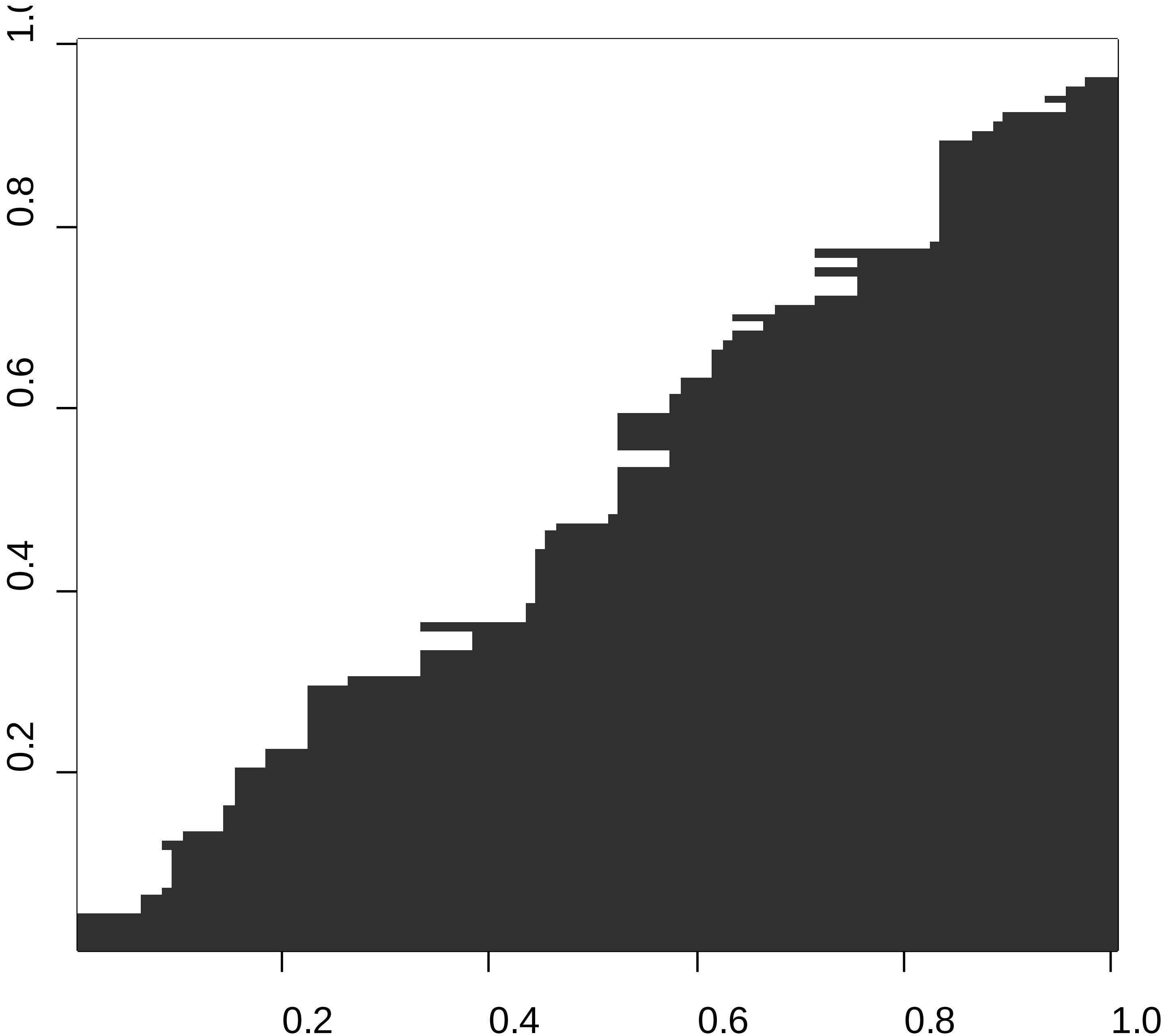



Single Tree:
0.2
0.4
0.6
0.8
1.0
0.2
0.4
0.6
0.8
1.0

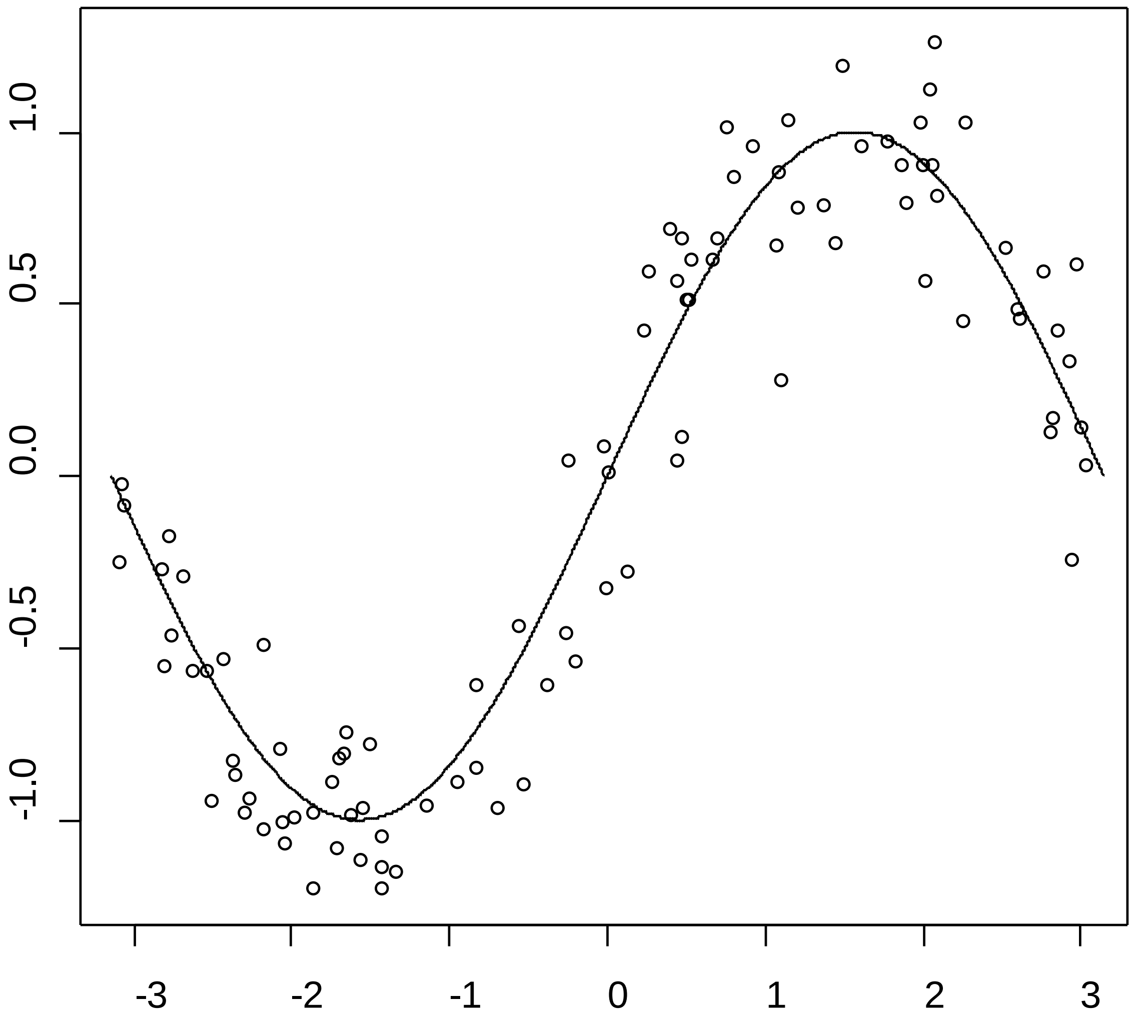
25 Averaged Trees:



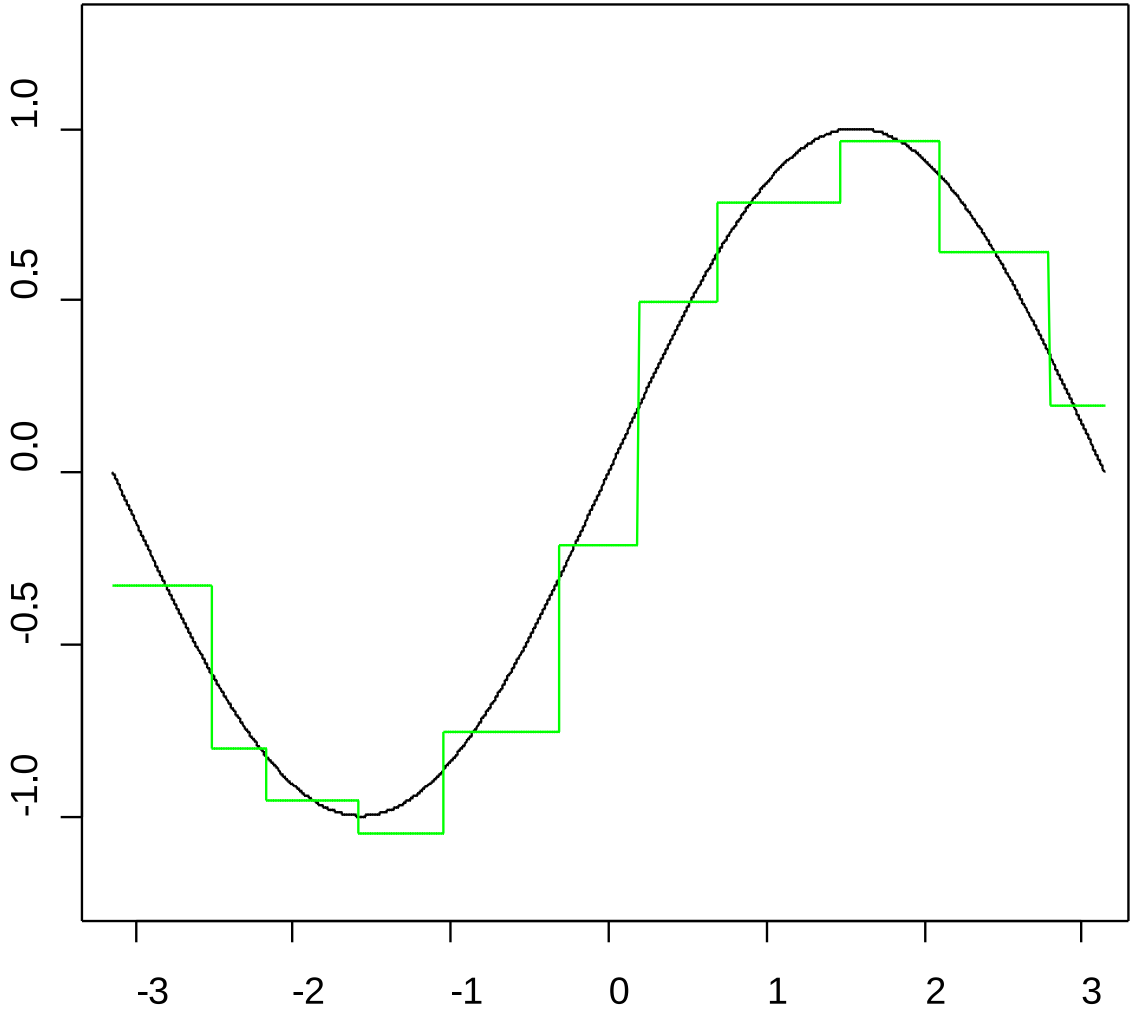
25 Voted Trees:



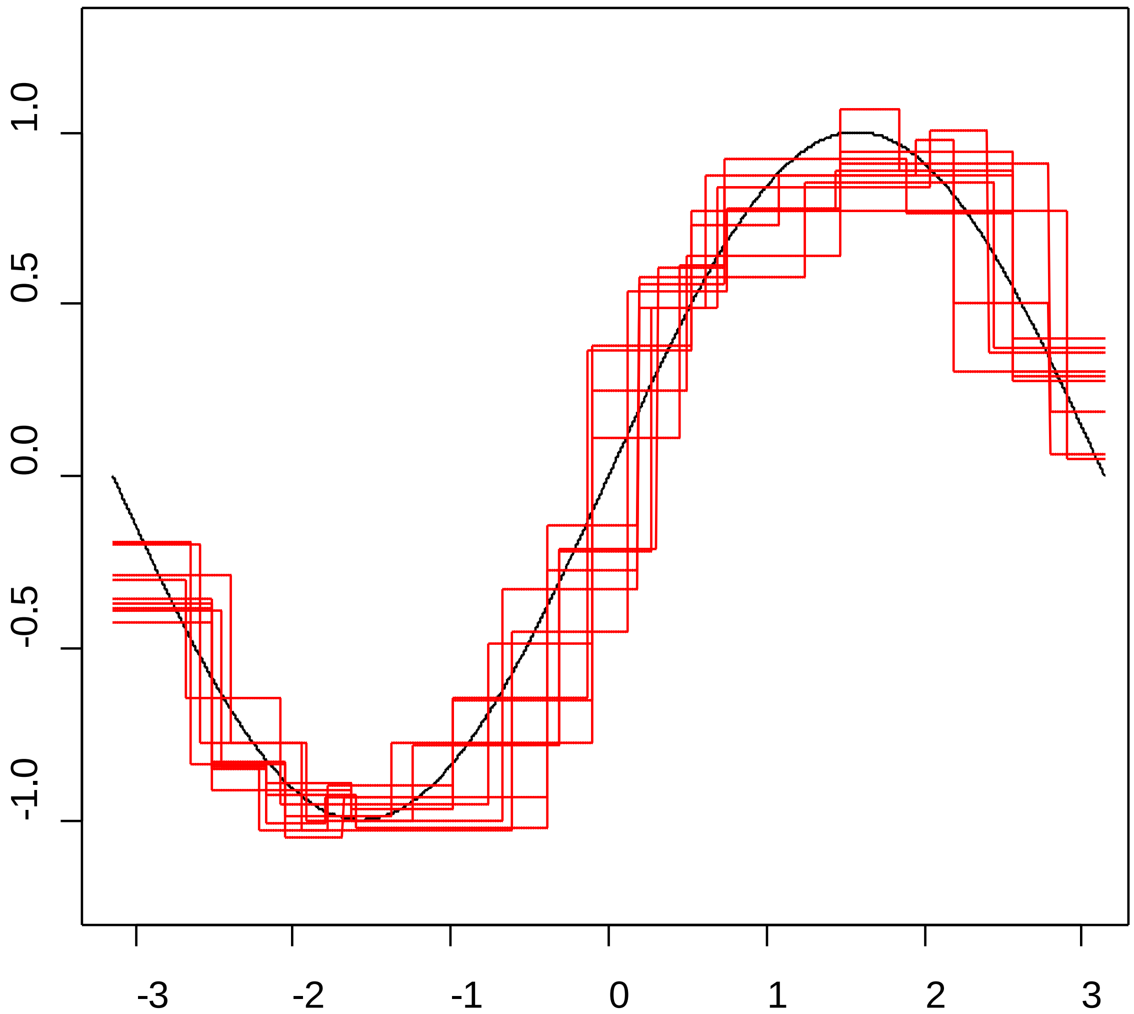
Data and Underlying Function



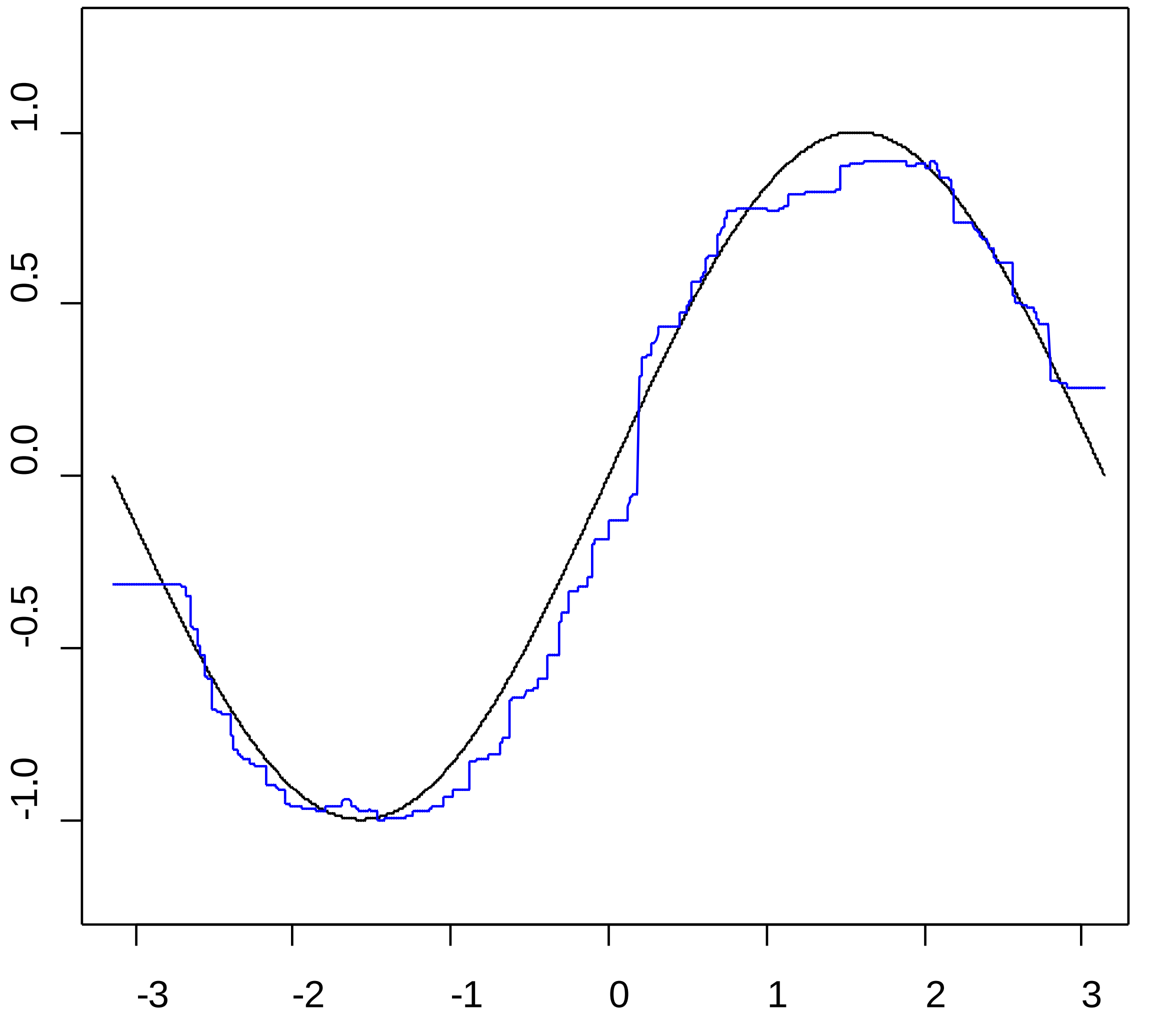
Single Regression Tree (all data)



10 Regression Trees (fit to boostrap samples)



Average of 100 Regression Trees (fit to bootstrap samples)



Useful by-products of Random Forests

Bootstrapping → out-of-bag data →

- Estimated error rate
- Variable importance

Leo: We use every bit of the pig except its squeal

Trees → proximities →

- Missing value fill-in
- Outlier detection
- Illuminating pictures of the data
  - Clusters
  - Structure
  - Outliers

Out-of-bag Data

Think about a single tree from a Forest:

- The tree is grown on a bootstrap sample ("the bag").
- The remaining data are said to be "out-of-bag" (about one-third of the cases).
- The out-of-bag data serve as a test set for this tree.

Out-of-bag data give

- Estimated error rate
- Variable importance

The out-of-bag Error Rate

Think of a ***single case*** in the training set:

- It will be out-of-bag in about 1/3 of the trees.
- Predict its class for each of these trees.
- Its **RF prediction** is the most common predicted class.

If we fit 1000 trees, and a case is out-of-bag in 339 of them, of which

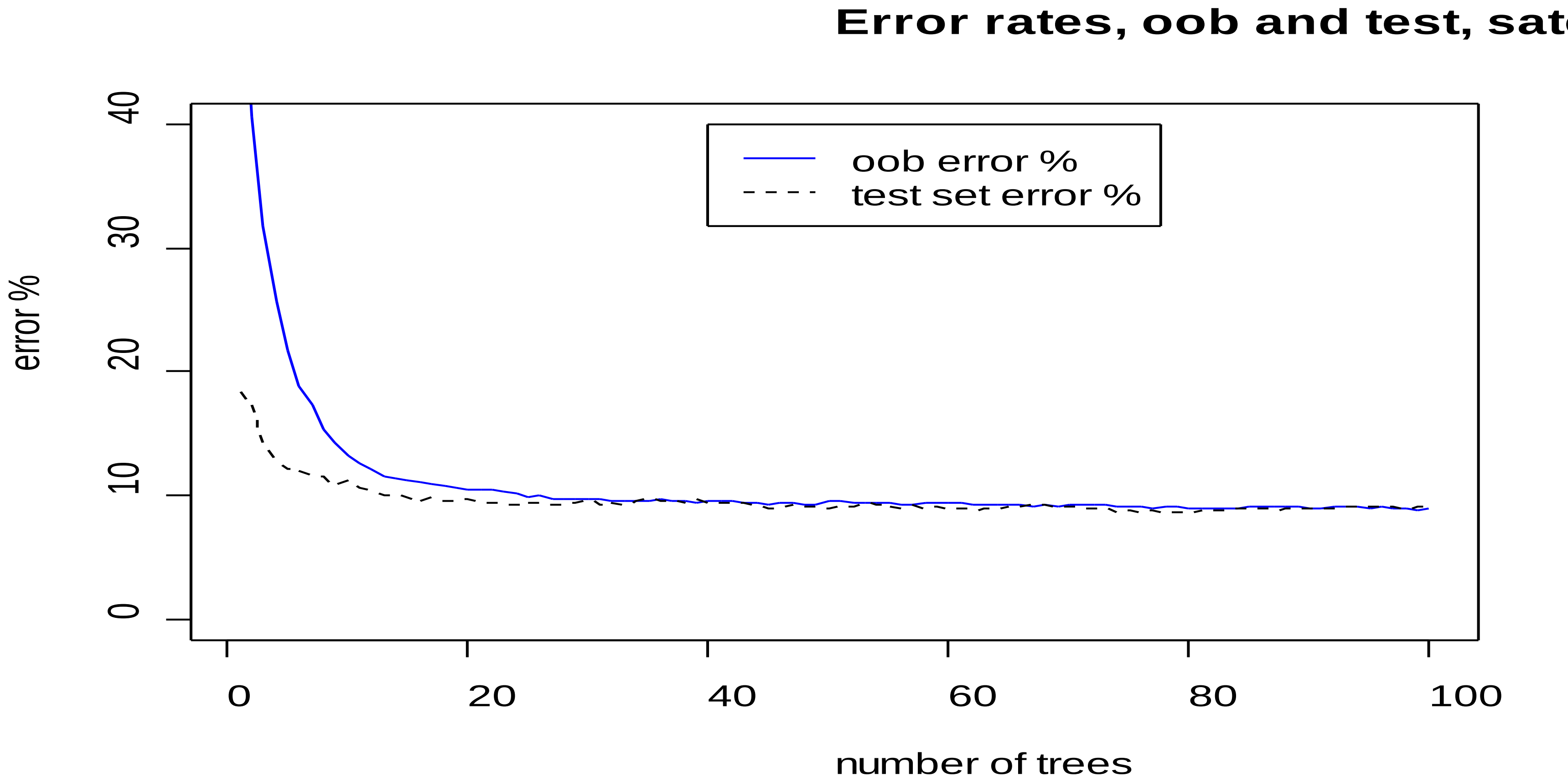
303 say "class 1"
36 say "class 2"

The **RF prediction** is "1".

The out-of-bag error rate is the **error rate of the RF predictor** (can be done for each class).

Illustration – Satellite Data

- 4435 cases, 36 variables.
- Test set: 2000 cases.



Variable Importance

For ***variable j***, look at the out-of-bag data for each tree:

- randomly permute the values of ***variable j***, holding the other variables fixed.
- pass these permuted data down the tree, save the classes.

Importance for ***variable j*** is

$$\left(\begin{array}{l}\text{error rate when}\\ \textbf{\textit{variable j}}\text{ is permuted}\end{array}\right) - \left(\begin{array}{l}\text{out-of-bag}\\ \text{error rate}\end{array}\right)$$

where the error rates are averaged over the out-of-bag data, then over the trees.

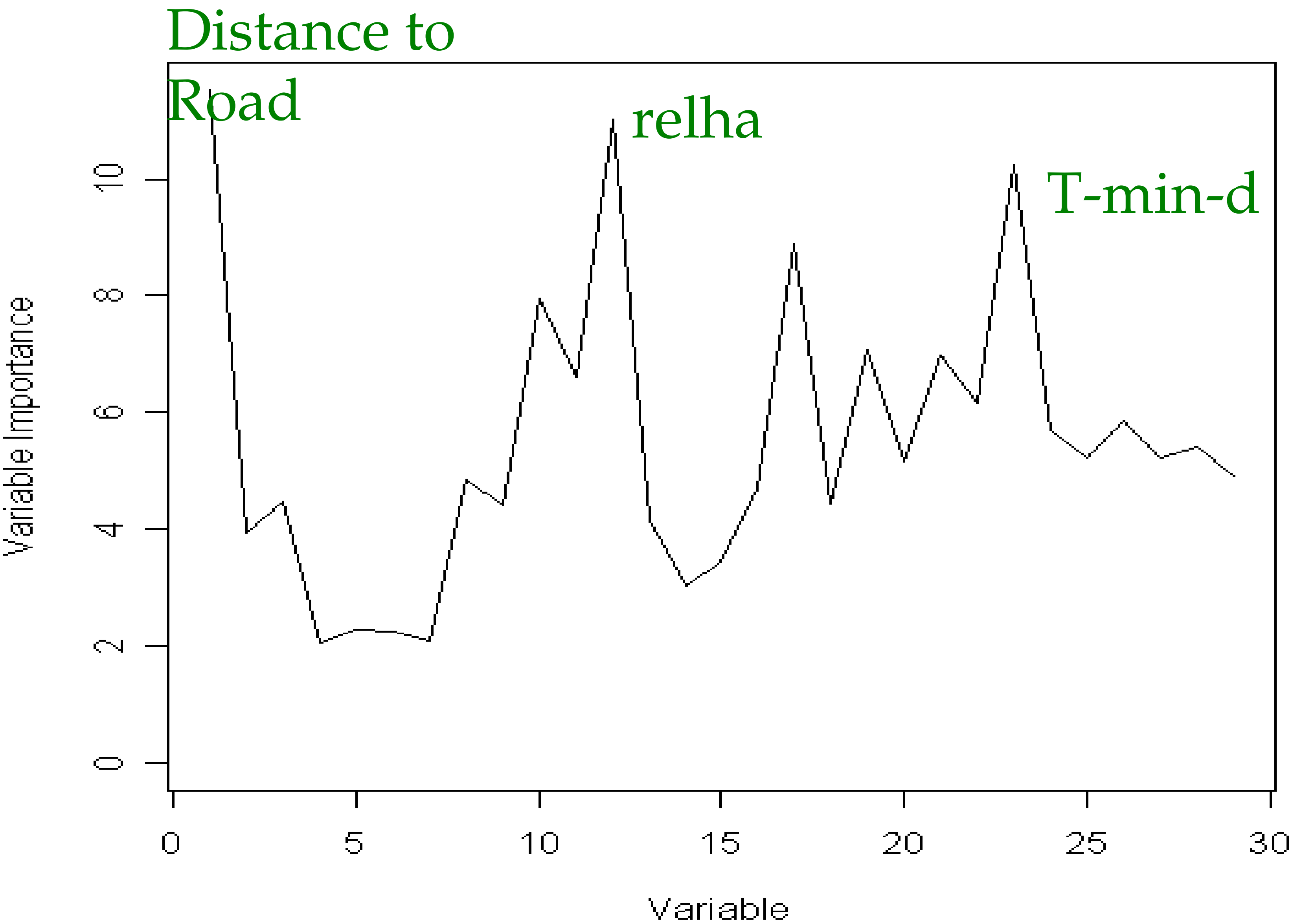
Case Study – Invasive Plants

Data courtesy of Richard Cutler, Tom Edwards

8251 cases, 30 variables, 2 classes:

- Absent (2204 cases)
- Present (6047 cases)

Illustration: Invasive Plants



Outline

- What are random forests?

- Background

- New features since Breiman (2001)
  - Proximities
    - Imputing missing values
    - Clustering
  - Unequal class sizes
  - Local variable importance
  - Visualization

Proximities

Proximity of two observations is the proportion of the time that they end up in the same node.

The proximities *don't* just measure similarity of the variables. They take into account the importance of the variables.

- Two observations that have quite ***different*** values on the variables might have ***large*** proximity if they differ only on variables that are ***not important***.

- Two observations that have quite ***similar*** values of the variables might have ***small*** proximity if they differ on inputs that are ***important.***

Illustration: Proximities

Synthetic data, 600 cases
2 meaningful variables and 48 “noise” variables
3 classes

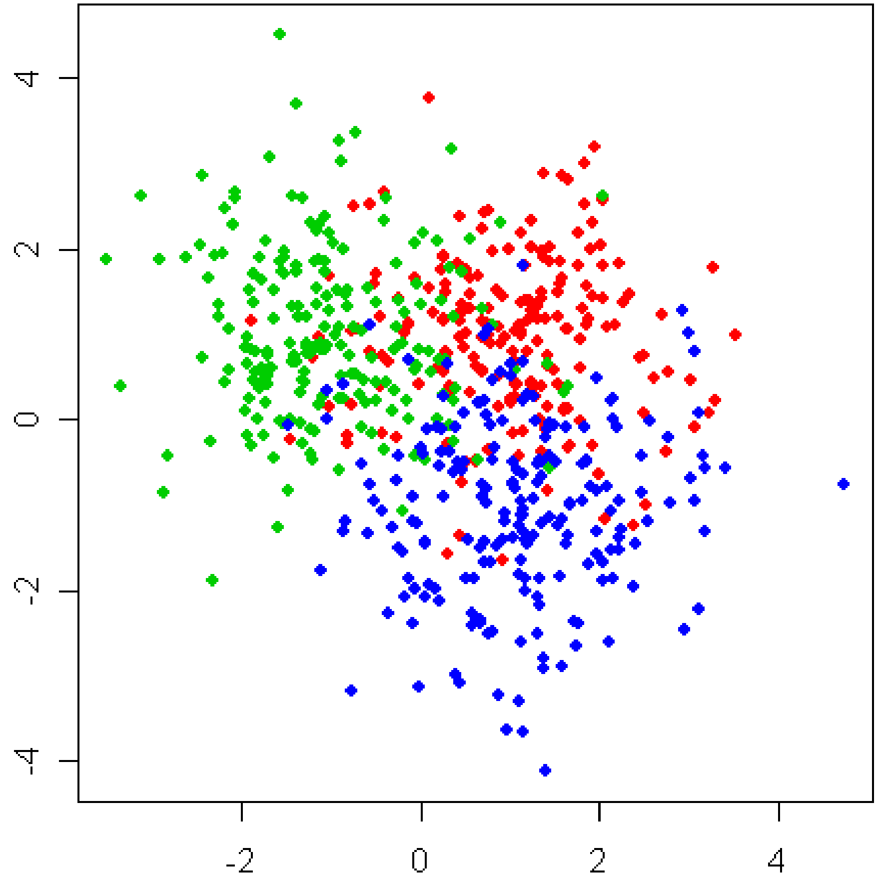
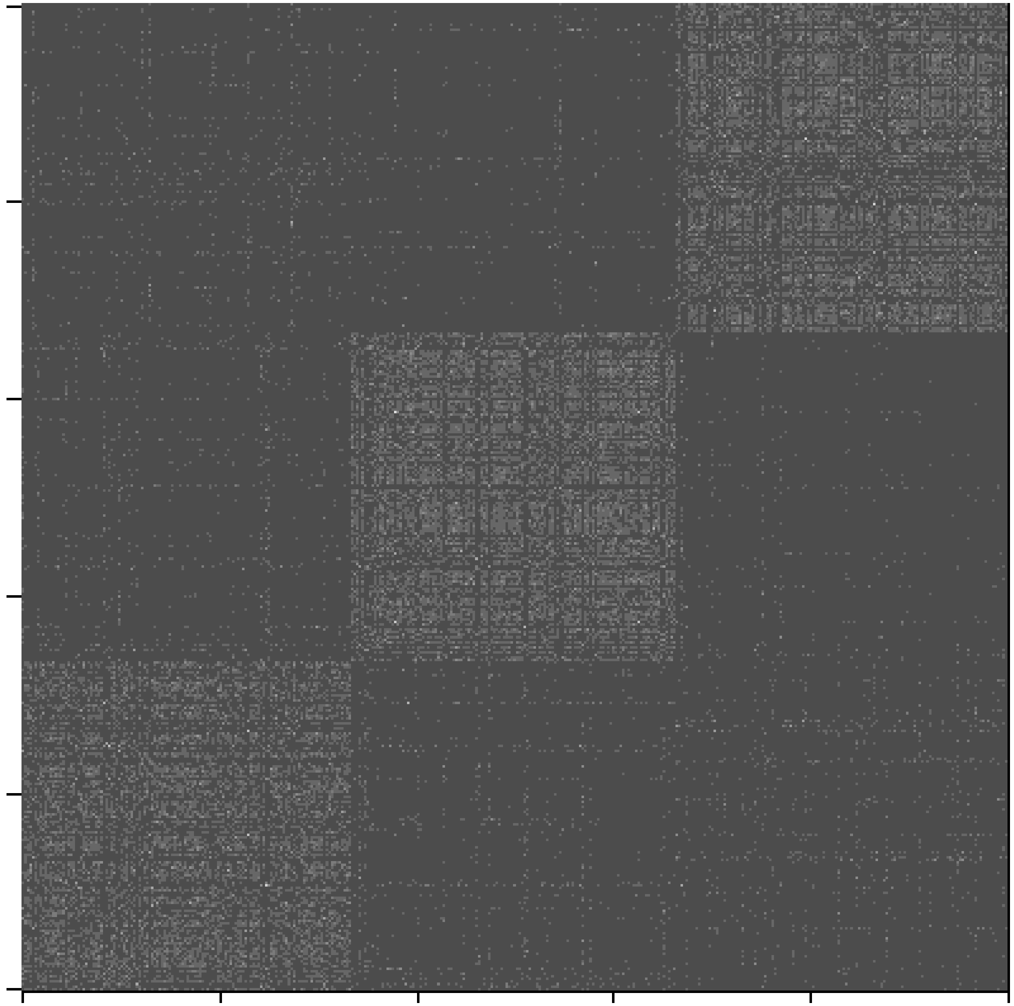


Illustration: Proximities



Proximities

Proximity of two observations is the proportion of the time that they end up in the same node.

Originally, we used all the data (in bag and out-of-bag). But we found that the proximities overfit the data…

Illustration: Proximities

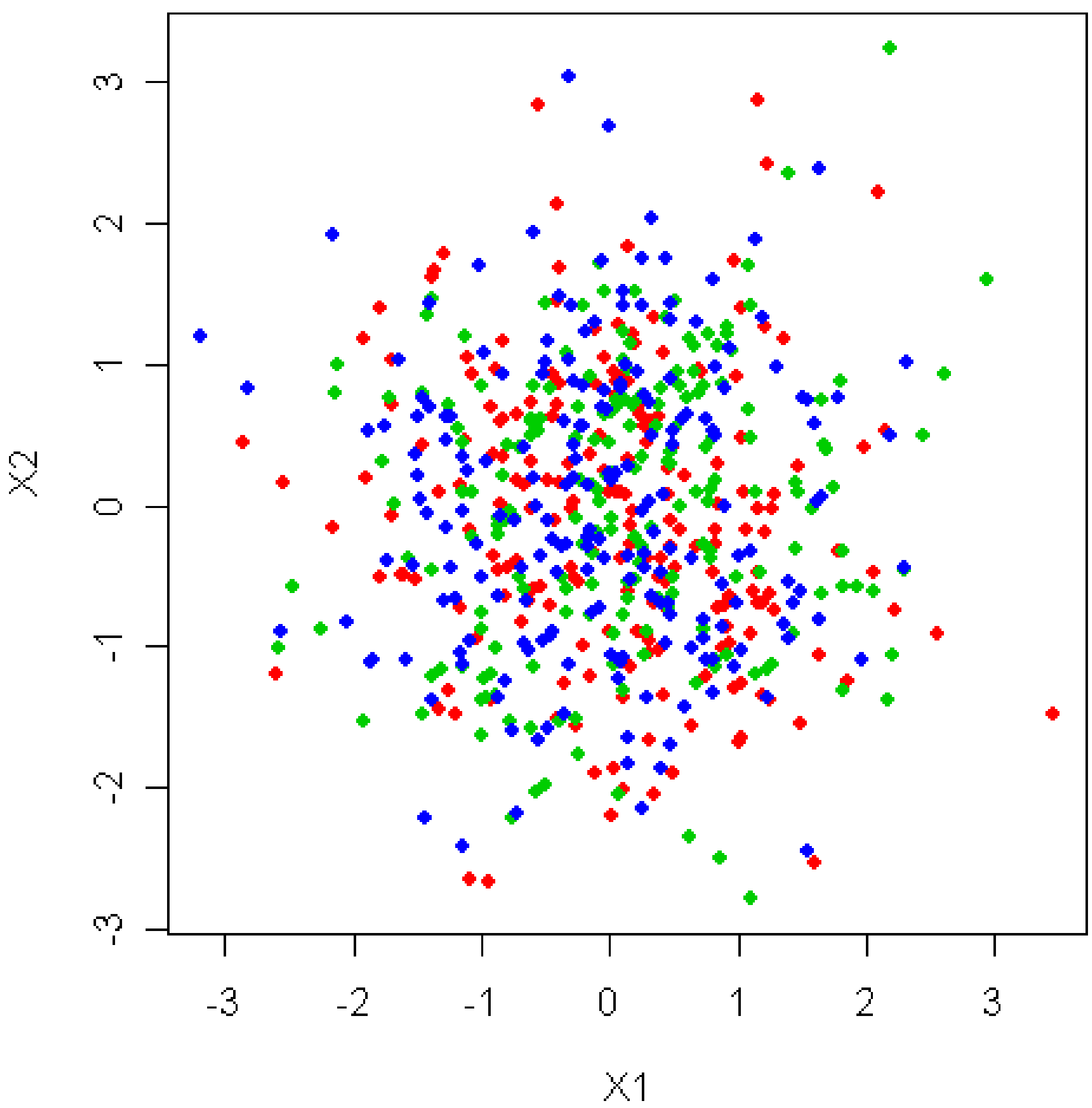
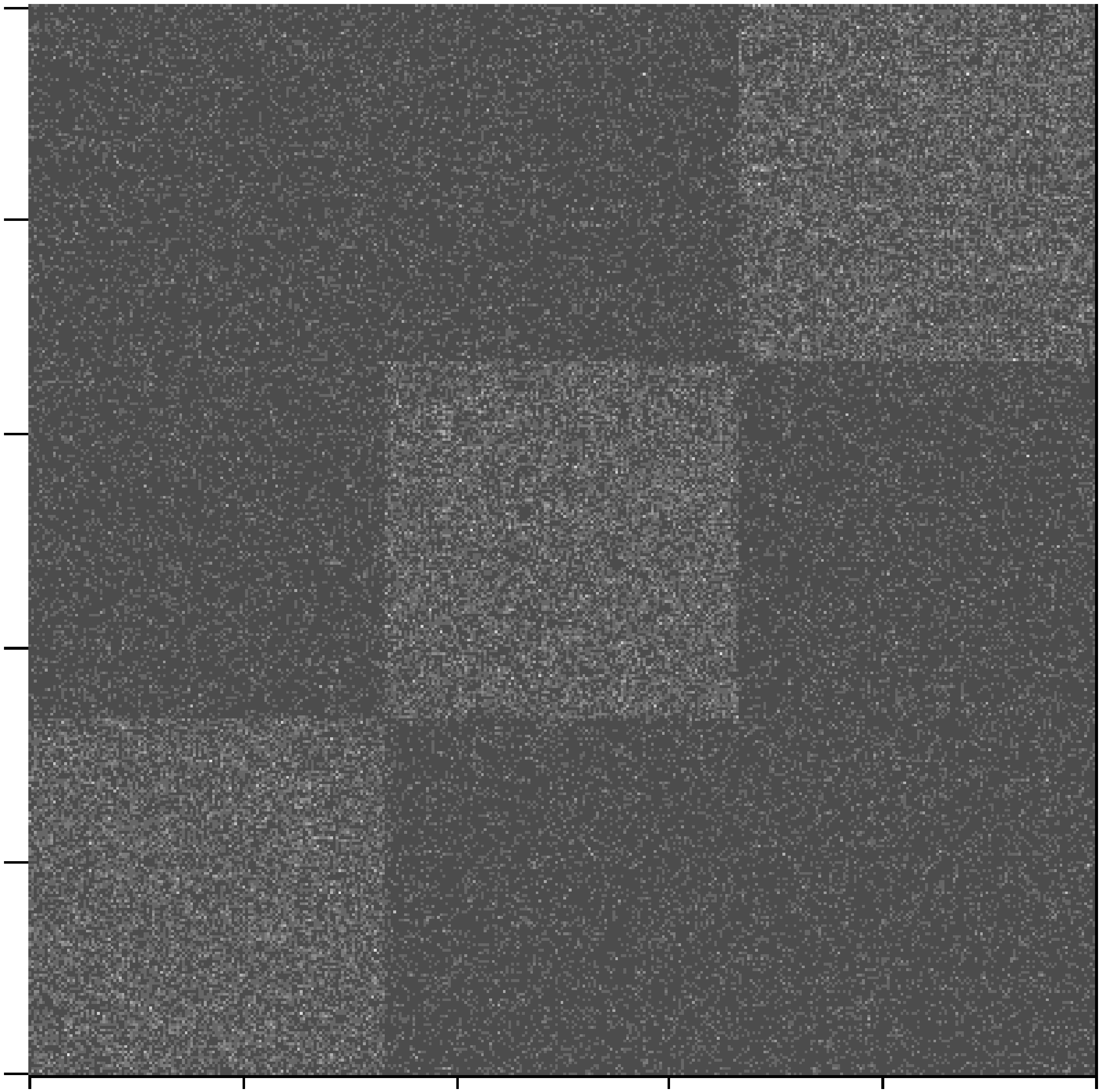


Illustration: Proximities



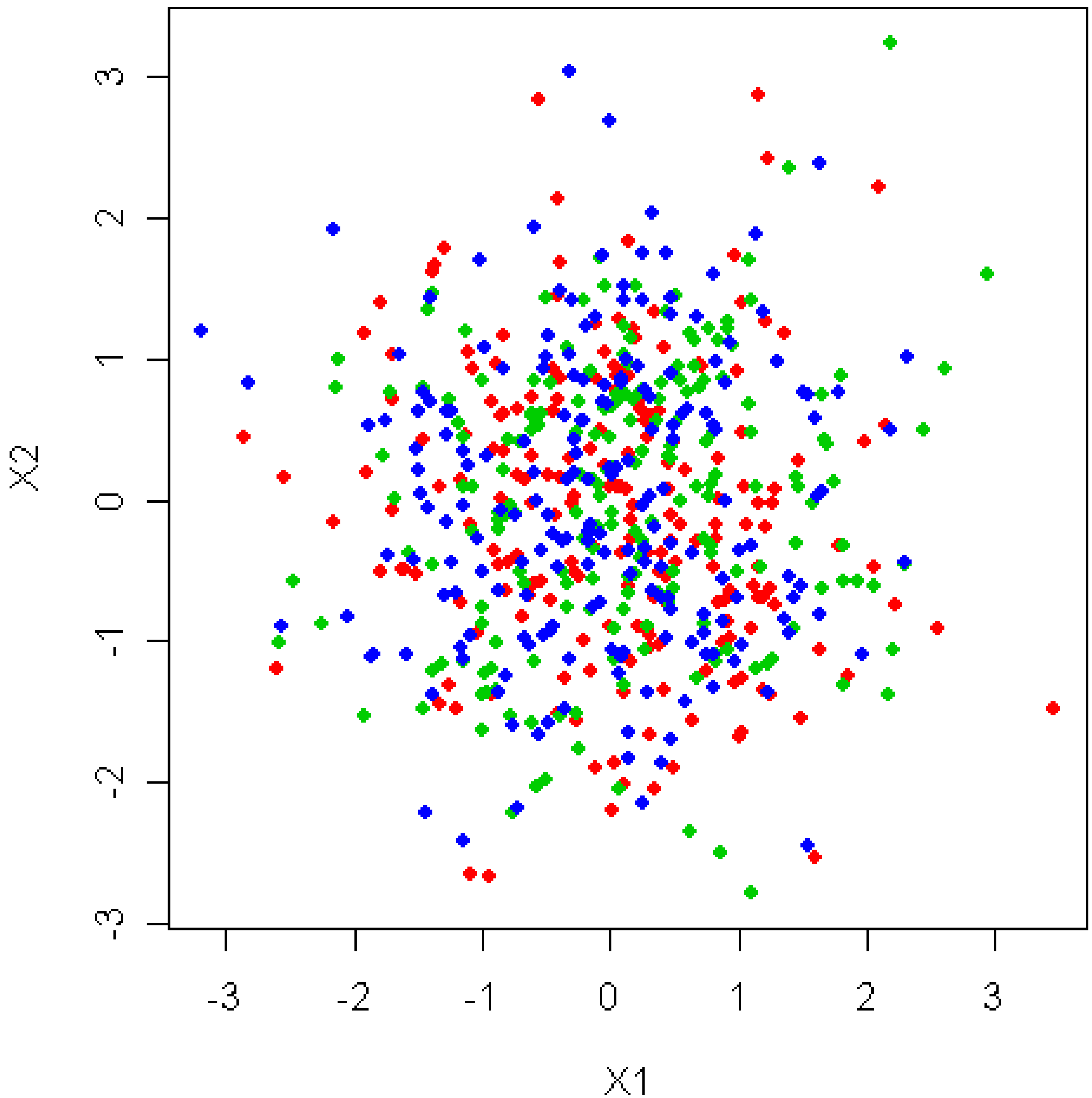
Proximities

Two modifications :

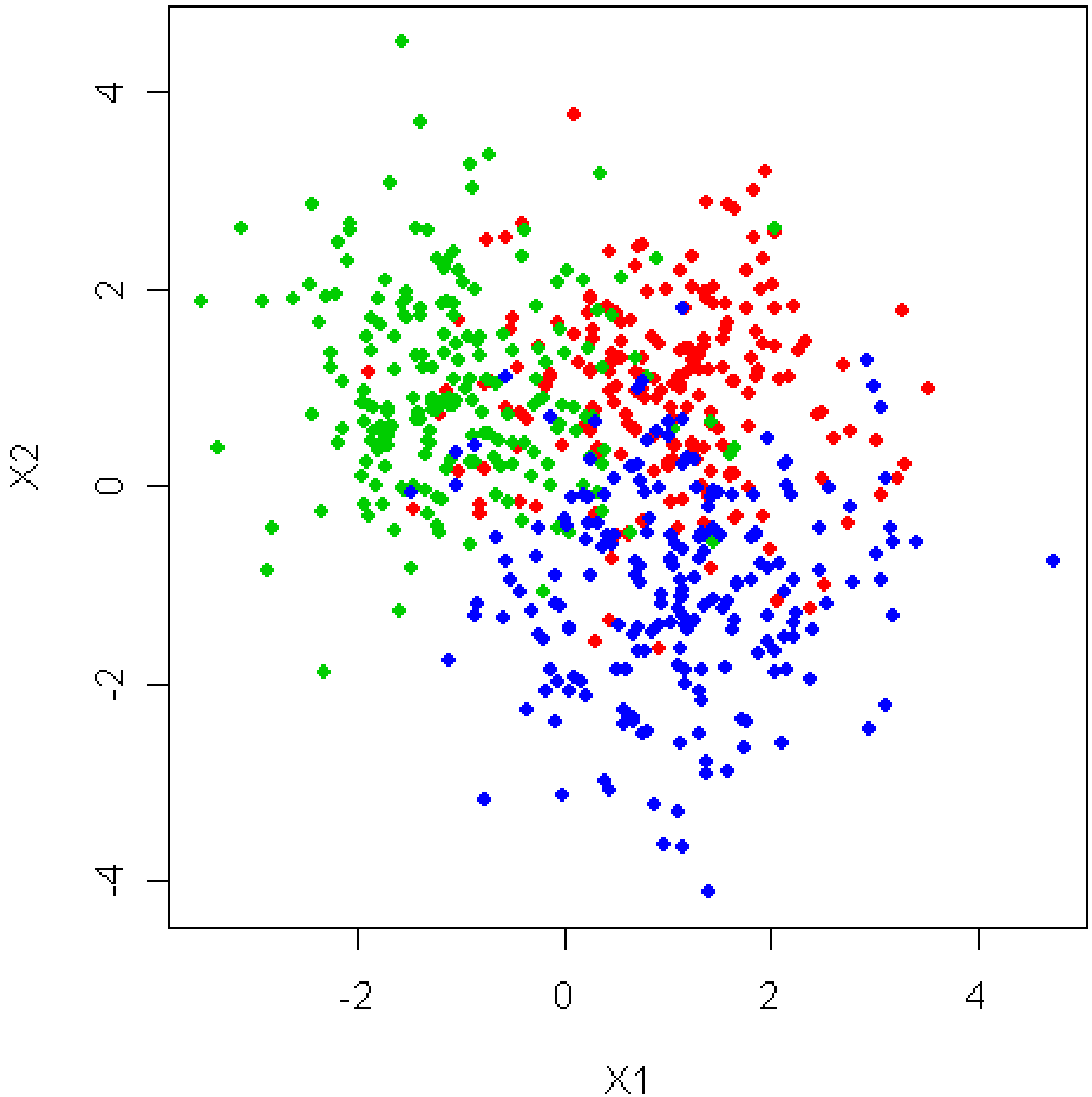
1. Out-of-bag. Proximity of two observations is the proportion of the time that they end up in the same node when they are both out-of-bag.

2. In and out. When observation *i* is out-of-bag, pass it down the tree and increment its proximity to all in-bag observations that end up in the same terminal node

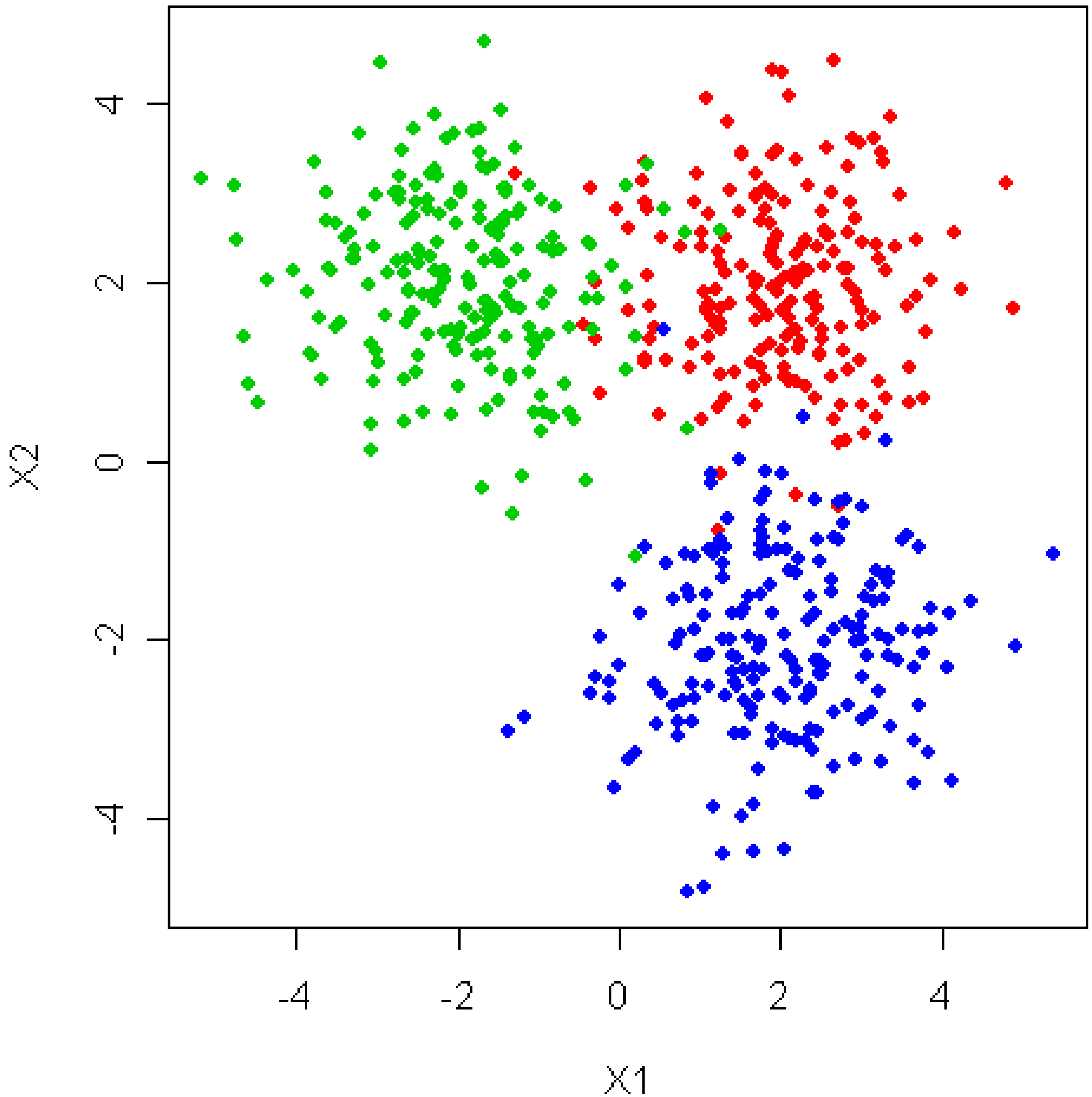
Data 1



Data 2



Data 3



Nearest-neighbor classifiers from proximities

% error	Data 1	Data 2	Data 3
Random Forests	64	23	4.7
Original	0	7	2.0
Out-of-bag	67	23	4.5
In and out	66	20	3.7

Nearest-neighbor classifiers from proximities

% Disagreement Compared to RF	Data 1	Data 2	Data 3
Original	64	16	3.0
Out-of-bag	48	5	0.5
In and out	15	3	1.0

Imputing Missing Values

Fast way: replace missing values for a given variable using the median of the non-missing values (or the most frequent, if categorical)

Better way (using proximities):

1. Start with the fast way.
2. Get proximities.
3. Replace missing values in case **n** by a weighted average of non-missing values, with weights proportional to the proximity between case **n** and the cases with the non-missing values.

Repeat steps 2 and 3 a few times (5 or 6).

Outline

- What are random forests?
- Background
- New features since Breiman (2001)
  - Proximities
    - Imputing missing values
    - Clustering
  - Unequal class sizes
  - Local variable importance
  - Visualization

Learning from Unbalanced Data

Increasingly often, data sets are occurring where the class of interest has a population that is a small fraction of the total population.

For such unbalanced data, a classifier can achieve great accuracy by classifying almost all cases into the majority class!

RF weights the classes to get similar error rates for each class.

Case Study – Invasive Plants

Data courtesy of Richard Cutler, Tom Edwards

8251 cases, 30 variables, 2 classes:

- Absent (2204 cases)
- Present (6047 cases)

The 3 most important variables are

Variable 1: distance to road

Variable 12: relha

Variable 23: t-min-d

Initial run, m=5, equal weights

Error rate = 6%

Out-of-bag confusion matrix

	Absent	Present
Called absent	1921	213
Called present	283	5834
Total	2204	6047
Error rate	**12.8%**	**3.5%**

Second run, m=5, weight 3 to 1

Error rate = 8.7%

Out-of-bag confusion matrix

	Absent	Present
Called absent	2099	614
Called present	105	5433
Total	2204	6047
Error rate	**4.8%**	**10.2%**

Third run, m=5, weight 2 to 1

Error rate = 7.0%

Out-of-bag confusion matrix

	Absent	**Present**
Called absent	2051	421
Called present	153	5626
Total	2204	6047
Error rate	**7.0%**	**7.0%**

Important Variables

30 variables in all

Weighted: Top 3 variables are 1, 12, 23

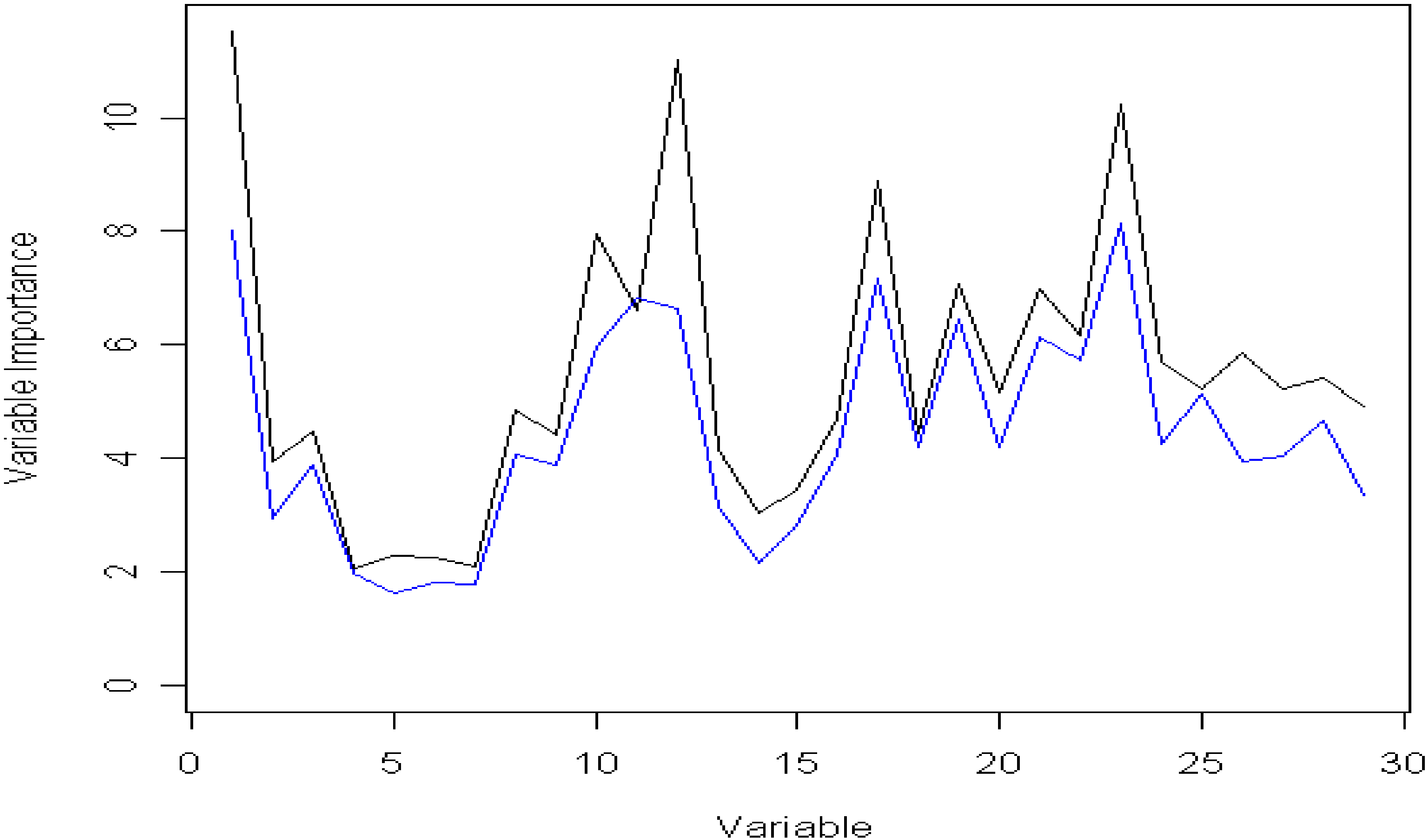
- Variable 1: distance to road
- Variable 12: relha
- Variable 23: t-min-d

Unweighted: Top 3 variables are 23, 1, 17

- Variable 17: t-ave-d

Variable Importance

Unweighted (blue) and weighted (black)



Outline

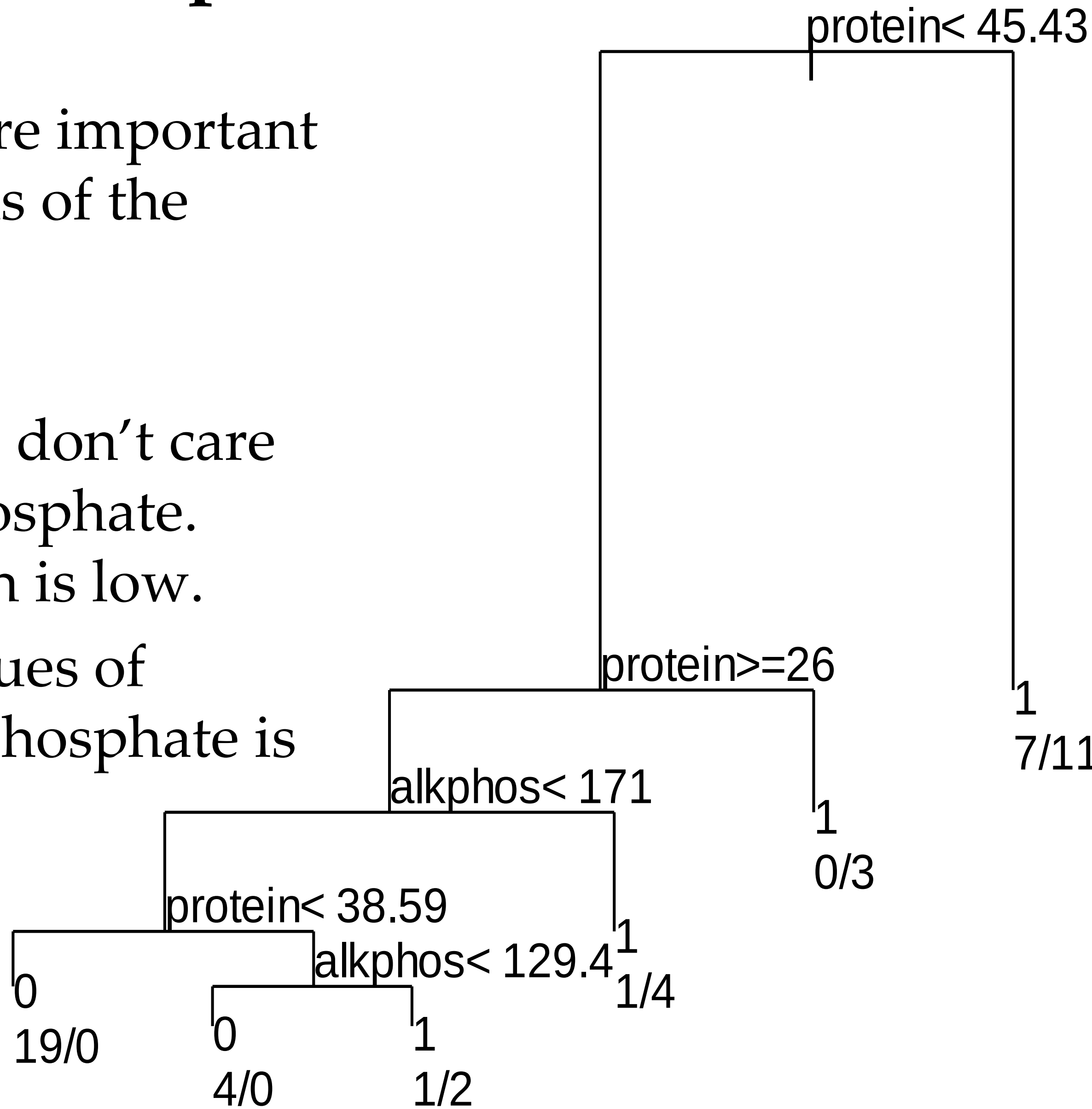
- What are random forests?
- Background
- New features since Breiman (2001)
  - Proximities
    - Imputing missing values
    - Clustering
  - Unequal class sizes
  - Local variable importance
  - Visualization

LOCAL Variable Importance

Different variables are important in different regions of the data.

If protein is high, we don't care about alkaline phosphate. Similarly if protein is low.

For intermediate values of protein, alkaline phosphate is important.



Estimating **Local** Variable Importance

For each tree, look at the out-of-bag data:

- randomly permute the values of variable *j*, holding the other variables fixed.
- pass these permuted data down the tree, save the classes.

Importance for **case *i*** and variable *j* is

$$\left(\begin{array}{l}\text{error rate } \textbf{for case } \boldsymbol{i} \\ \text{when variable } j \text{ is} \\ \text{permuted}\end{array}\right) - \left(\begin{array}{l}\text{out-of-bag} \\ \text{error rate}\end{array}\right)$$

where both error rates are taken over all trees for which case *i* is out-of-bag.

Variable importance for a single class 2 case

TREE	No permutation	Permute variable 1	…	Permute variable m
1	2	2	…	1
3	2	2	…	2
4	1	1	…	1
9	2	2	…	1
…	…	…	…	…
992	2	2	…	2
% Error	10%	11%	…	35%

Outline

- What are random forests?
- Background
- New features since Breiman (2001)
  - Proximities
    - Imputing missing values
    - Clustering
  - Unequal class sizes
  - Local variable importance
  - Visualization

Getting Pictures with Scaling Variables

To "look" at the data we use classical multidimensional scaling (MDS) to get a picture in 2-D or 3-D:

Proximities $\xrightarrow{\text{MDS}}$ scaling variables

Might see:

- clusters
- outliers
- other unusual structure.

Visualizing using proximities

- at-a-glance information about which classes are overlapping, which classes differ
- find clusters within classes
- find easy/hard/unusual cases

With a good tool we can also

- identify characteristics of unusual points
- see which variables are locally important
- see how clusters or unusual points differ

Case Study - Autism

Data courtesy of J.D.Odell and R. Torres, USU

154 subjects (308 chromosomes)

7 variables, all categorical (up to 30 categories)

2 classes:

- Normal, blue (69 subjects)
- Autistic, red (85 subjects)

Case Study – Invasive Plants

Data courtesy of Richard Cutler, Tom Edwards

8251 cases, 30 variables, 2 classes:

- Absent, blue (2204 cases)
- Present, red (6047 cases)

Current and Future Work

- Proximities and nonlinear MDS
- Detecting interactions
- Regression and Survival Analysis
- Visualization – regression