STAT406- Methods of Statistical Learning Lecture 15

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Classification Trees

- To estimate the probabilities of each class **g** for a particular value of the feature vector **x**, **nearest neighbours** constructs estimates

$$\widehat{P}\left(\mathbf{g} = \mathbf{g} \middle| \mathbf{X} = \mathbf{x}\right)$$

$$= \text{ prop. of objects of class } \mathbf{g} \text{ among } \mathbf{x}\text{'s neighbours}$$

Classification Trees

- Drawback: may not be “local” for moderate number of features (hence, may not represent the distribution of $\mathbf{g}$ for $\mathbf{X} = \mathbf{x}$
- Yet another incarnation of the “curse of dimensionality”

Classification Trees

- If we assume a model for the distribution of the features $\mathbf{X}$ for each class

$$f(\mathbf{x}|\,\mathbf{g}=\mathbf{g}) = f_{\mathbf{g}}(\mathbf{x})$$

then we have a formula for

$$P(\mathbf{g}=\mathbf{g}|\,\mathbf{X}=\mathbf{x}) = \frac{f_{\mathbf{g}}(\mathbf{x})\,P(\mathbf{g}=\mathbf{g})}{\sum_{\mathbf{g}} f_{\mathbf{g}}(\mathbf{x})\,P(\mathbf{g}=\mathbf{g})}$$

Classification Trees

- We typically have estimates for these probabilities
- Only the numerator is needed
- Drawback: the model may not be correct.
- Model-based inferences are typically more stable than model-free ones
- But they may be biased if the model is a poor approximation to the truth

Classification Trees

- Classification trees provide another family of estimates for $P(\mathbf{g} = \mathbf{g}|\mathbf{X} = \mathbf{x})$
- They do not need a model
- Instead of estimating the local proportion (probability) of each class around a point **x**, CART's attempt to find regions of the feature space that are "dominated" by one class.

Classification Trees

- Classification trees try to identify regions of the domain where one class clearly dominates the others (i.e. where the class proportions are far from being “uniform”)
- They search for these regions in a very specific way.

Classification Trees

- These regions are searched using a sequential algorithm that at each step partitions the current level ("leaf") into two "leaves" / "children" according to the value of one of the feature variables, for example:

$$X_j \leq \mathbf{a} \quad \text{versus} \quad X_j > \mathbf{a}$$

Classification Trees

- At every step, the algorithm searches for the variable X_j and level **a** that produce the largest increase in "homogeneity" (alternatively: the largest decrease in "heteroscedasticity")
- We need a measure of "homogeneity" (or lack of it)

Classification Trees

Some practical considerations in building (spanning) the tree:

- Do not partition nodes / leaves with fewer elements than a fixed threshold (say, 5)
- Do not partition a node if the "gain" in less homogeneity is less than a certain percentage of the current value
- Or both...

Classification Trees

Let **N** denote a "node", that is: a subset of the data.

Let $\hat{p}_j$, $j = 1, \ldots, K$ be the proportion of observations of each class in this node

$$\hat{p}_j = \frac{\#\text{ of observations of class } j \text{ in node } \mathbf{N}}{\text{total } \#\text{ of observations in node } \mathbf{N}}$$

Classification Trees

Maximum homogeneity when

$$\hat{p}_1 \approx \hat{p}_2 \approx \cdots \approx \hat{p}_K$$

Minimum homogeneity when $\hat{p}_r \approx 1$ for some $1 \leq r \leq K$

Classification Trees

Measures of homogeneity

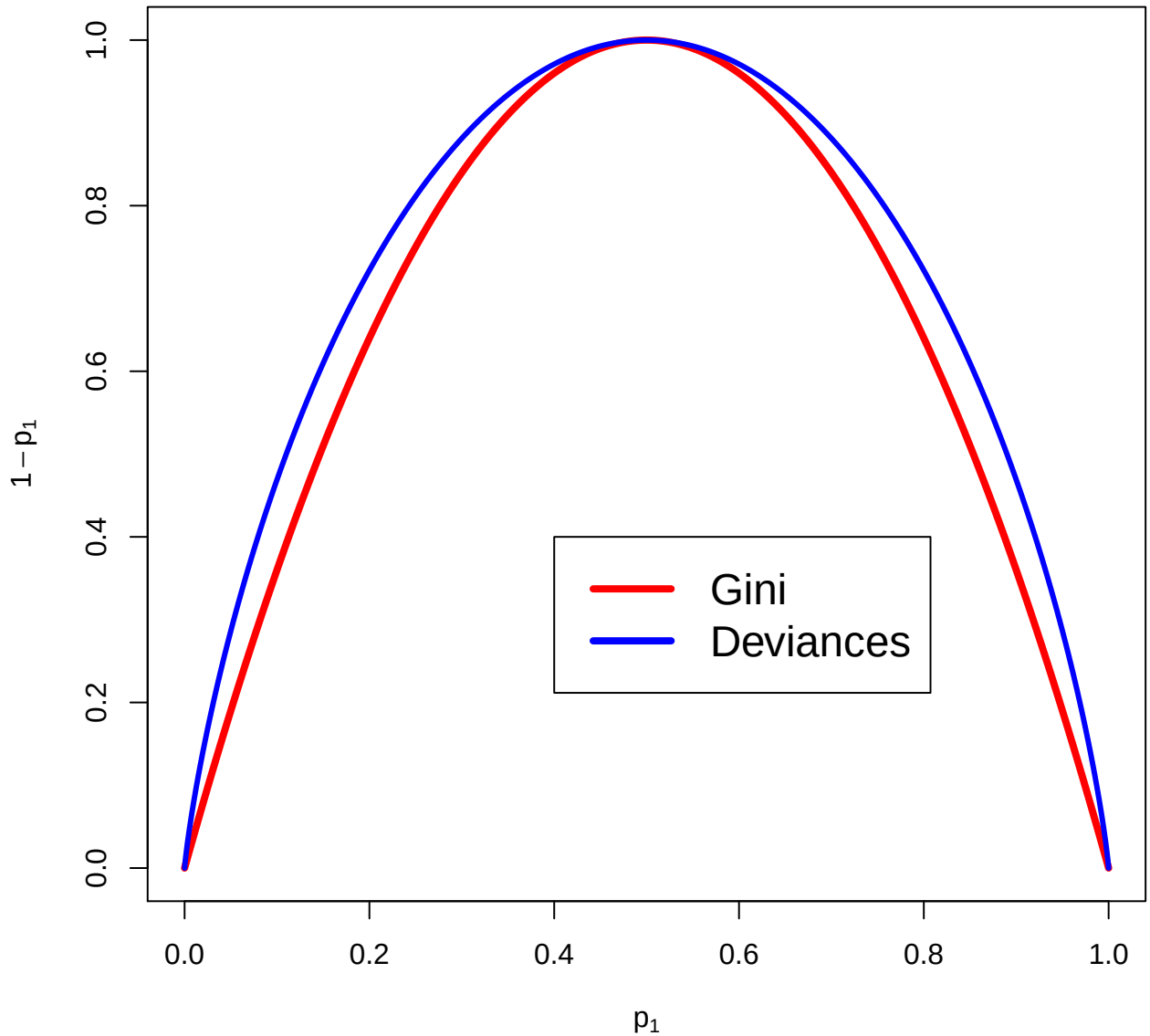
- Gini index:

$$Q_G(\hat{p}_1, \ldots, \hat{p}_K) = \sum_{j \neq i}^{K} \hat{p}_j \hat{p}_i = \sum_{j=1}^{K} \hat{p}_j \left(1 - \hat{p}_j\right)$$

- Entropy or deviance:

$$Q_D(\hat{p}_1, \ldots, \hat{p}_K) = -2 \sum_{j=1}^{K} \hat{p}_j \log\left(\hat{p}_j\right)$$

Gini & Deviances - 2 groups



Classification Trees

Define the "homogeneity" of a node **N** as

$$Q(\mathbf{N}) = Q(\hat{p}_1, \ldots, \hat{p}_K)$$

where

$$\hat{p}_j = \frac{\#\text{ of observations of class } j \text{ in node } \mathbf{N}}{\text{total }\#\text{ of observations in node } \mathbf{N}}$$

Q could be Q_G or Q_D, for example.

Classification Trees

(a) Start with a node **N** containing all data points

(b) Find the variable X_j and value **a** that minimize

$$\mathbf{n}_L \, Q\left(\mathbf{X} \in \mathbf{N} : X_j \leq \mathbf{a}\right) + \mathbf{n}_R \, Q\left(\mathbf{X} \in \mathbf{N} : X_j > \mathbf{a}\right)$$

where $\mathbf{n}_L = \#\{\mathbf{X} \in \mathbf{N} : X_j \leq \mathbf{a}\}$

(c) Define the corresponding two "children" of node **N**

(d) Apply the same to each "child" / "leaf"

Classification Trees

- In practice, we need to weight the homogeneity by the number of observations in each leaf.
- This reflects a probabilistic model for the tree, and represents the probability that a point is observed in this leaf
- In other words: minimize homogeneity more in “larger” (in average) leaves.

Classification Trees

- Let n_c be the size of the node $\mathbf{N}_c$, its homogeneity is

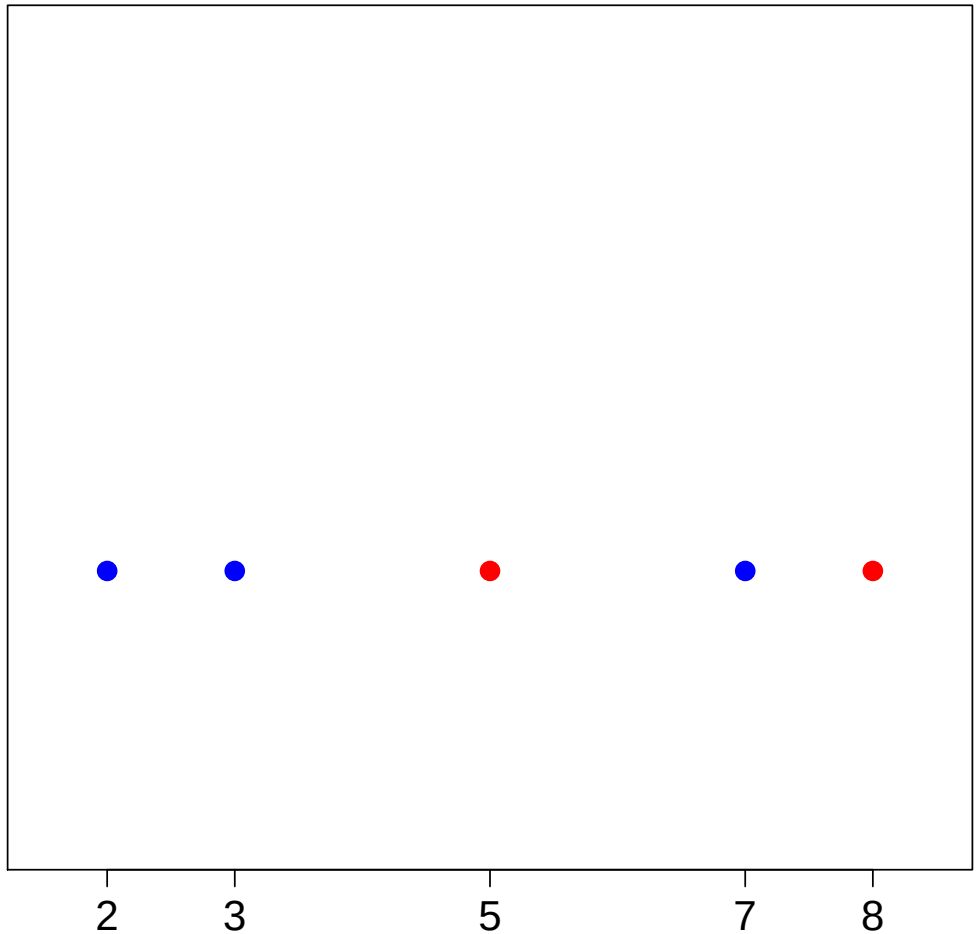
$$n_c Q(\mathbf{N}_c) \propto \frac{n_c}{n} Q(\mathbf{N}_c)$$

- If we split $\mathbf{N}_c$ into $\mathbf{N}_1$ and $\mathbf{N}_2$ the homogeneity is

$$n_1 Q(\mathbf{N}_1) + n_2 Q(\mathbf{N}_2) \propto \frac{n_1}{n} Q(\mathbf{N}_1) + \frac{n_2}{n} Q(\mathbf{N}_2)$$

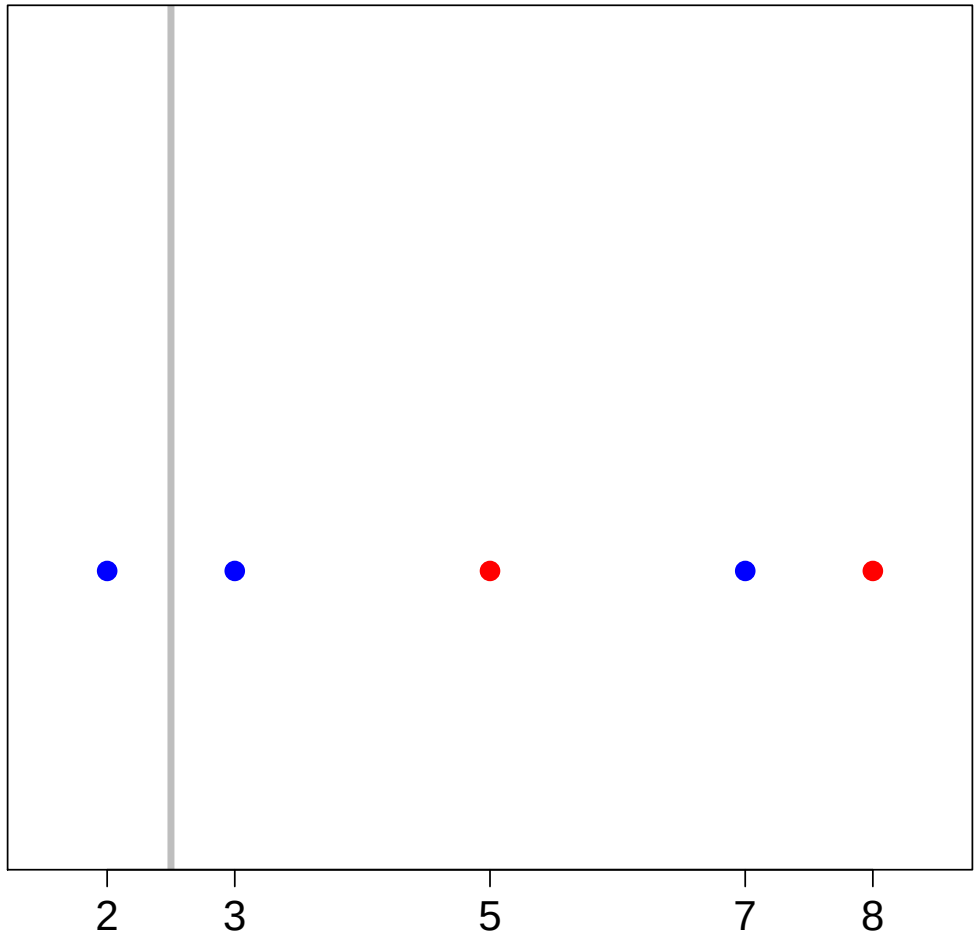
The homogeneity of any split is less than that of the parent node (Breiman, Friedman, Olshen, Stone; 1984).

Classification Trees



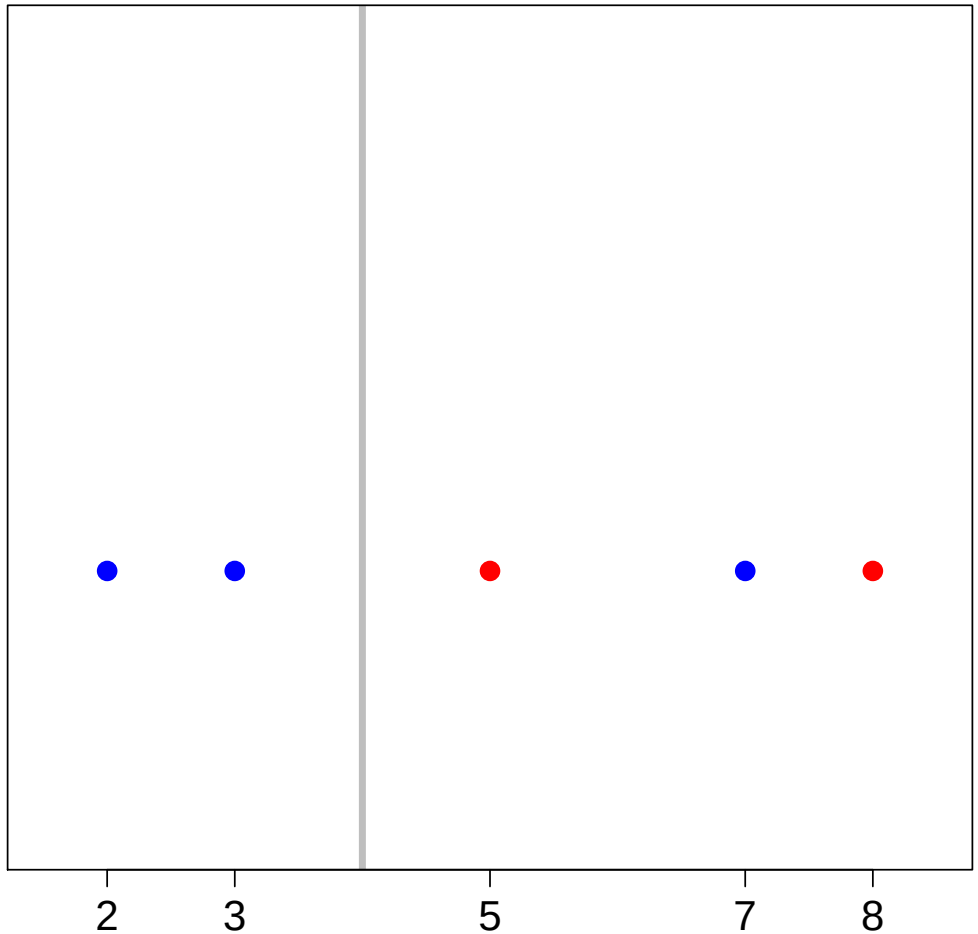
$$(\hat{p}_R = 2/5 \quad \hat{p}_B = 3/5) \quad Q_G = \mathbf{2.4}$$

Classification Trees



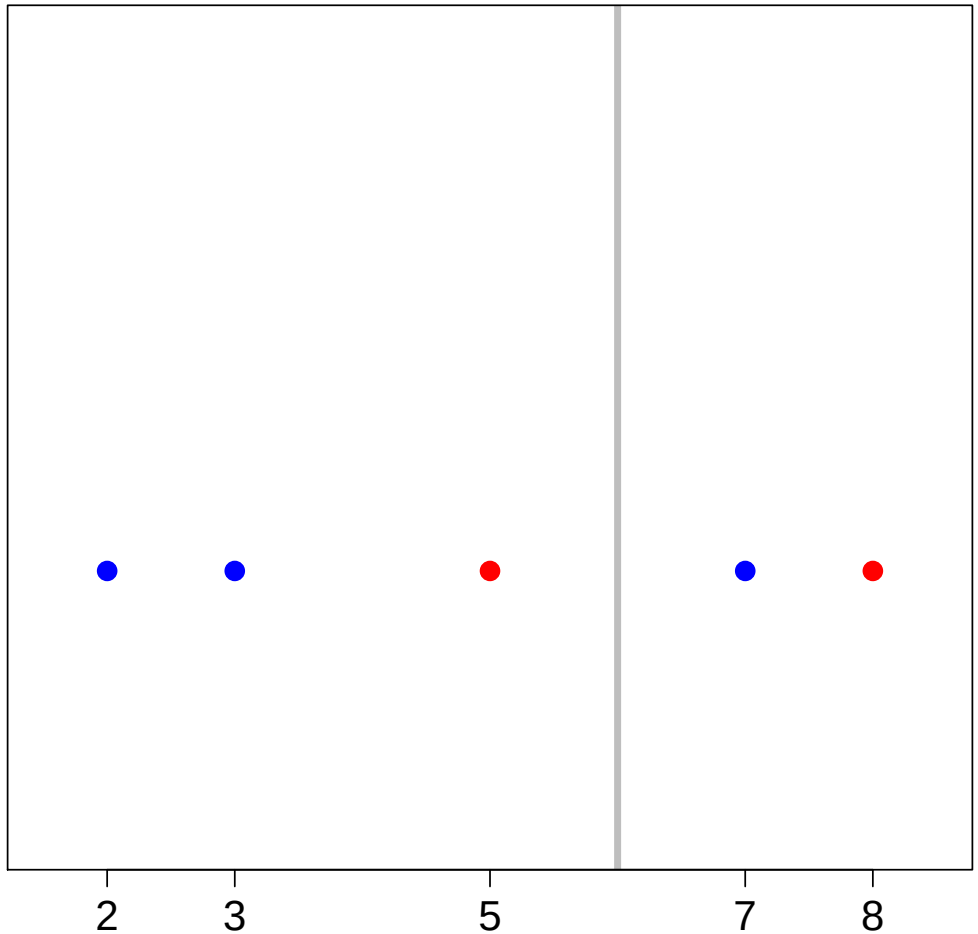
$(\hat{p}_R = 0 \quad \hat{p}_B = 1) \qquad (\hat{p}_R = 1/2 \quad \hat{p}_B = 1/2) \quad Q_G = \mathbf{2}$

Classification Trees



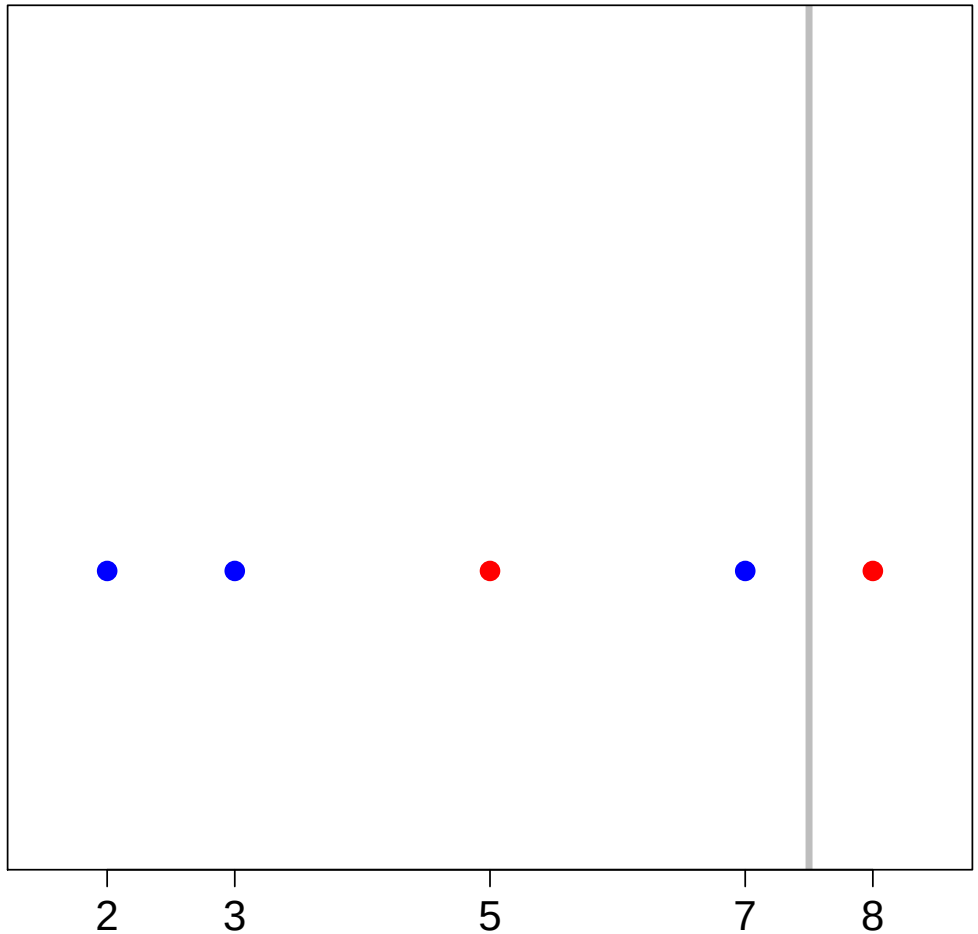
$(\hat{p}_R = 0 \quad \hat{p}_B = 1)$ $(\hat{p}_R = 2/3 \quad \hat{p}_B = 1/3)$ $Q_G = \mathbf{1.33}$

Classification Trees



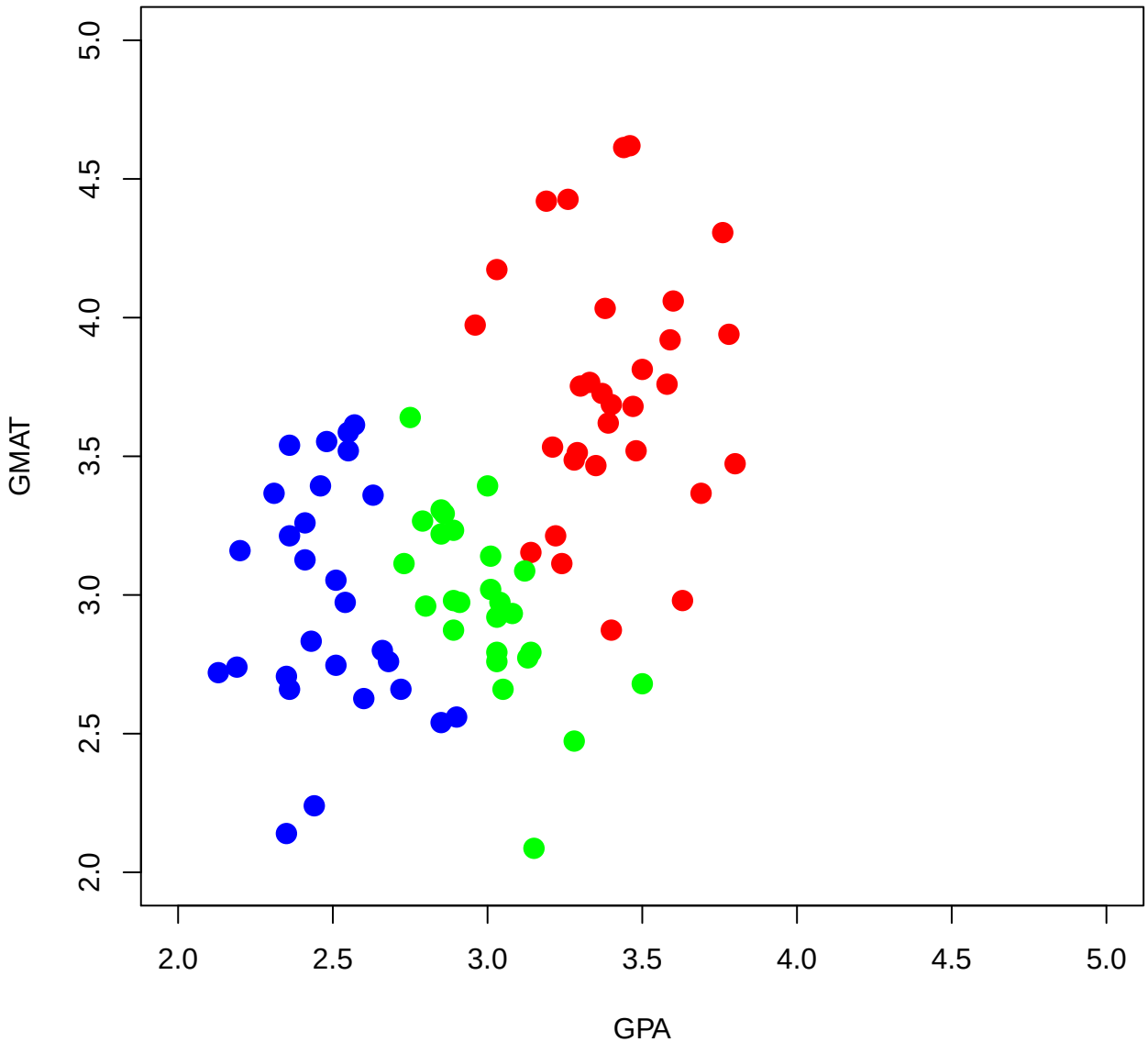
$(\hat{p}_R = 1/3 \quad \hat{p}_B = 2/3)$ $(\hat{p}_R = 1/2 \quad \hat{p}_B = 1/2)$ $Q_G = \mathbf{2.33}$

Classification Trees

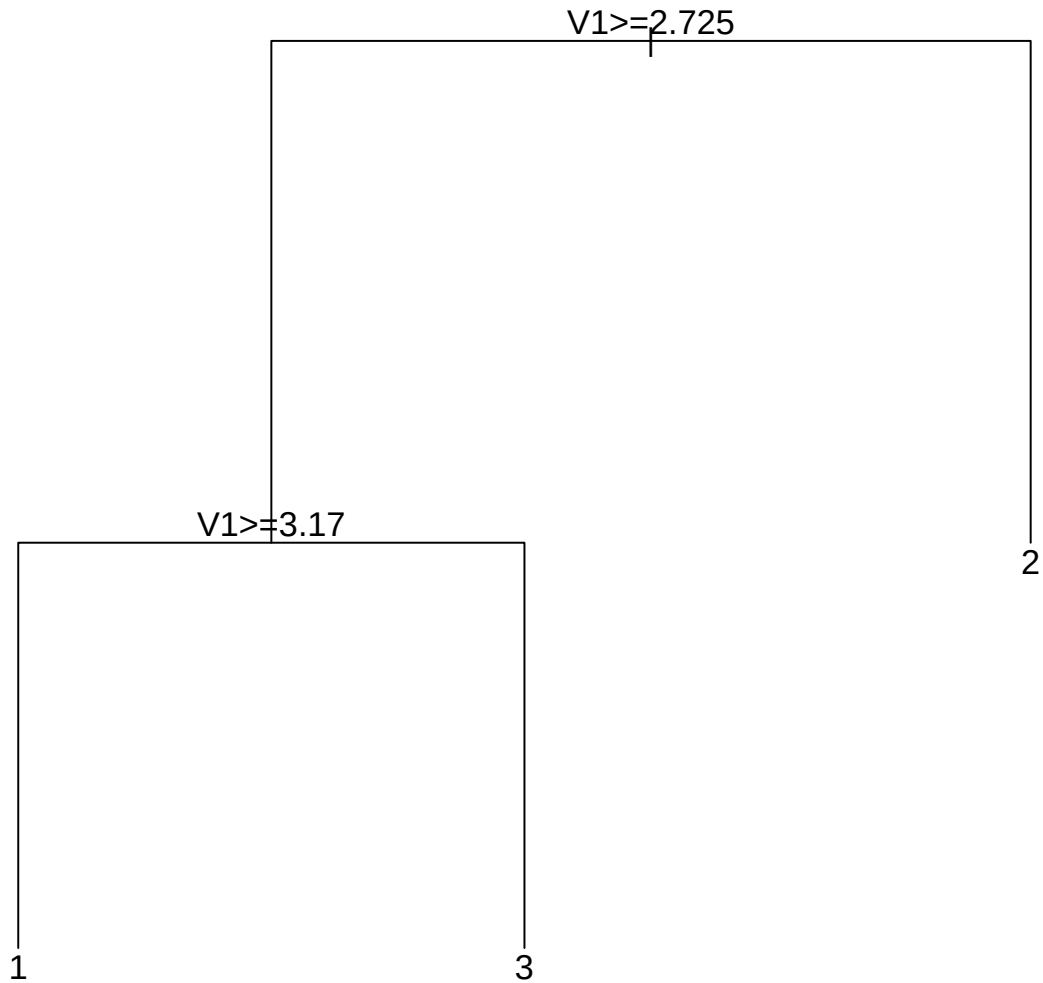


$(\hat{p}_R = 1/4 \quad \hat{p}_B = 3/4)$ $(\hat{p}_R = 1 \quad \hat{p}_B = 0)$ $Q_G = \mathbf{1.5}$

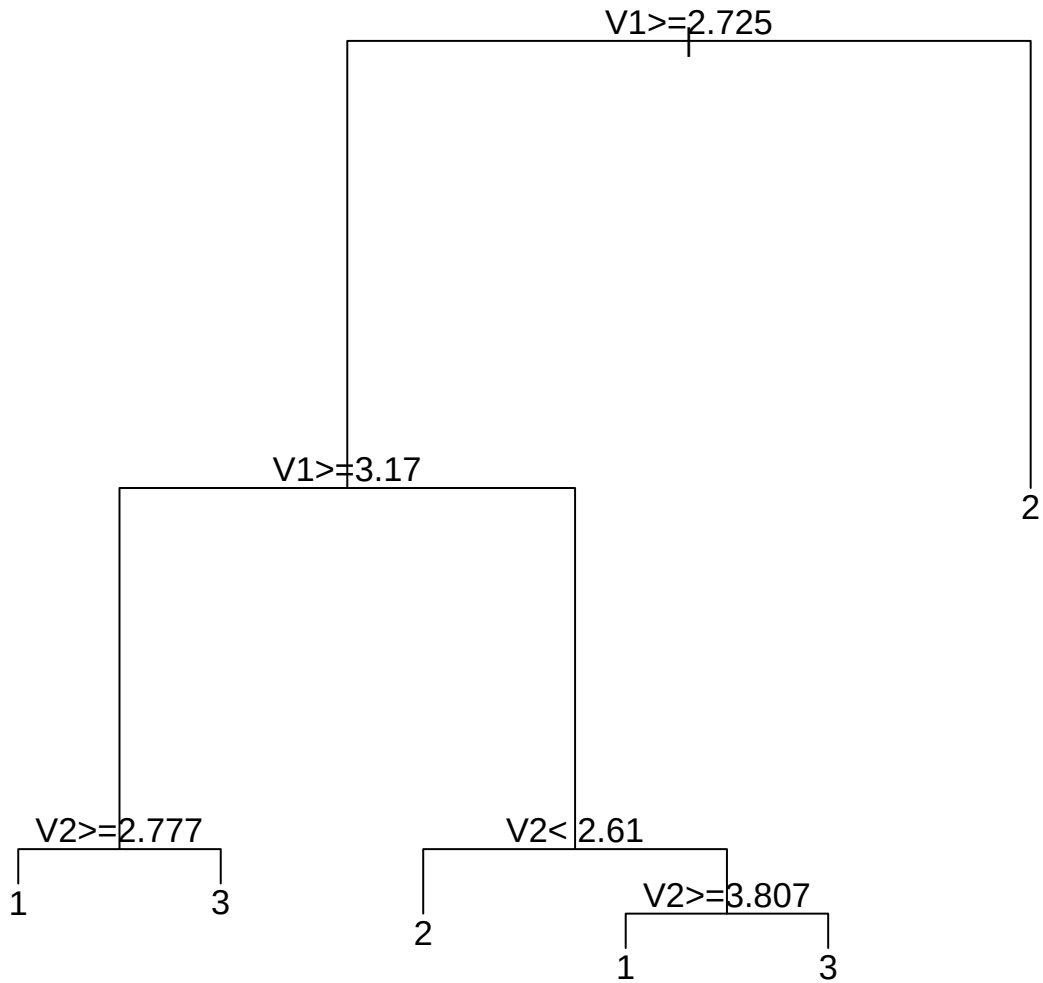
Grad admissions



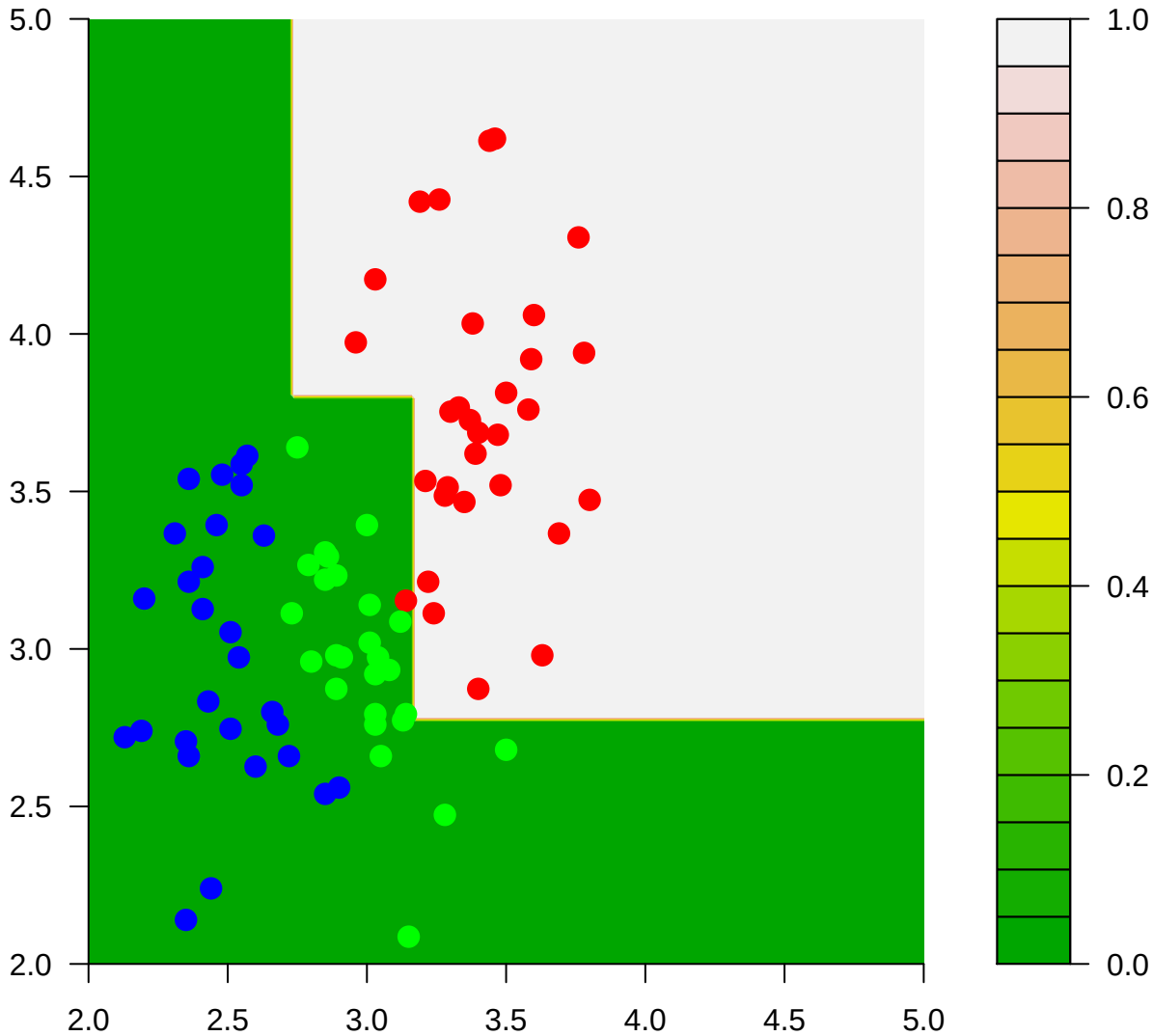
Grad admissions - Gini tree



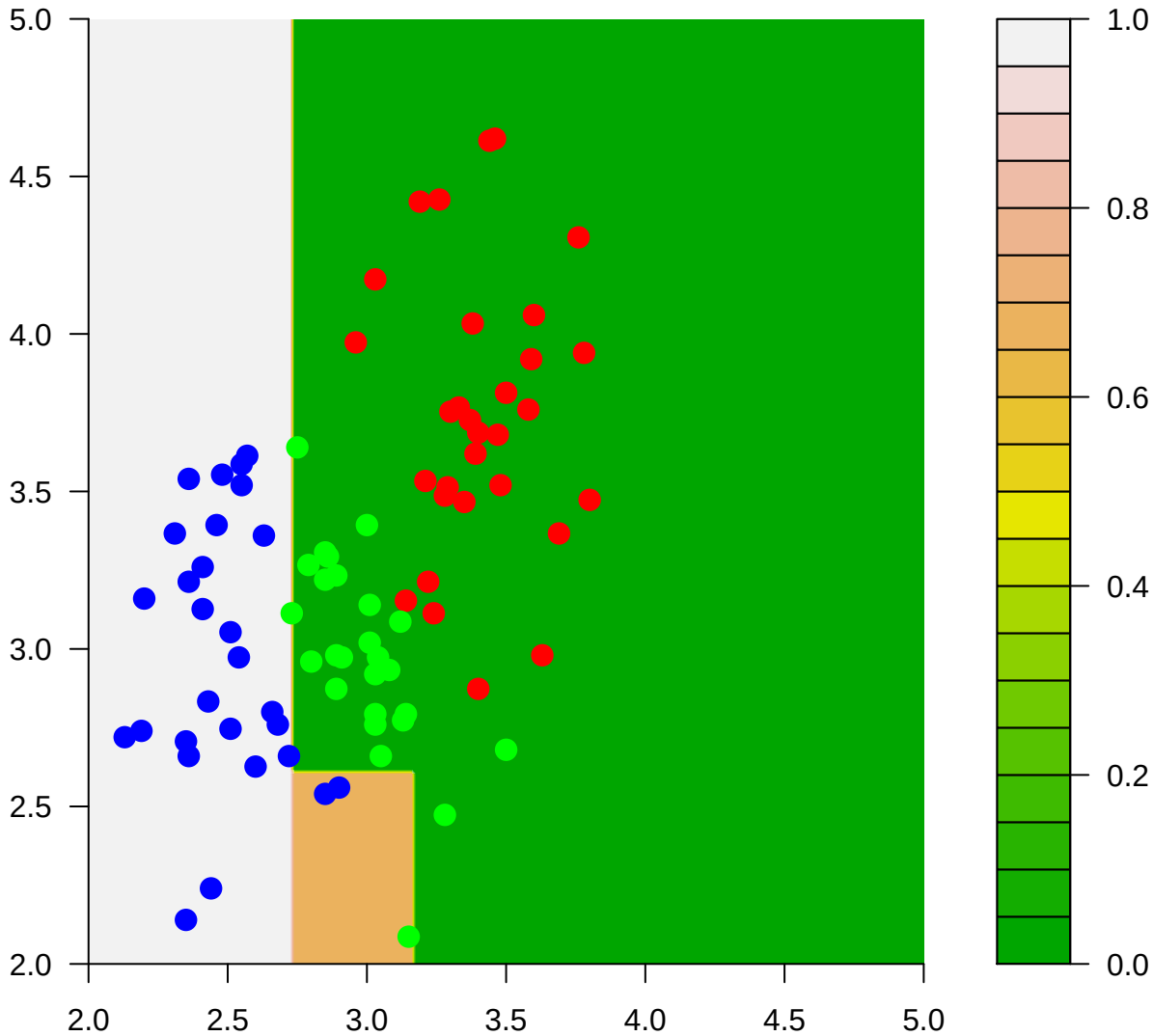
Grad admissions - Deviance tree



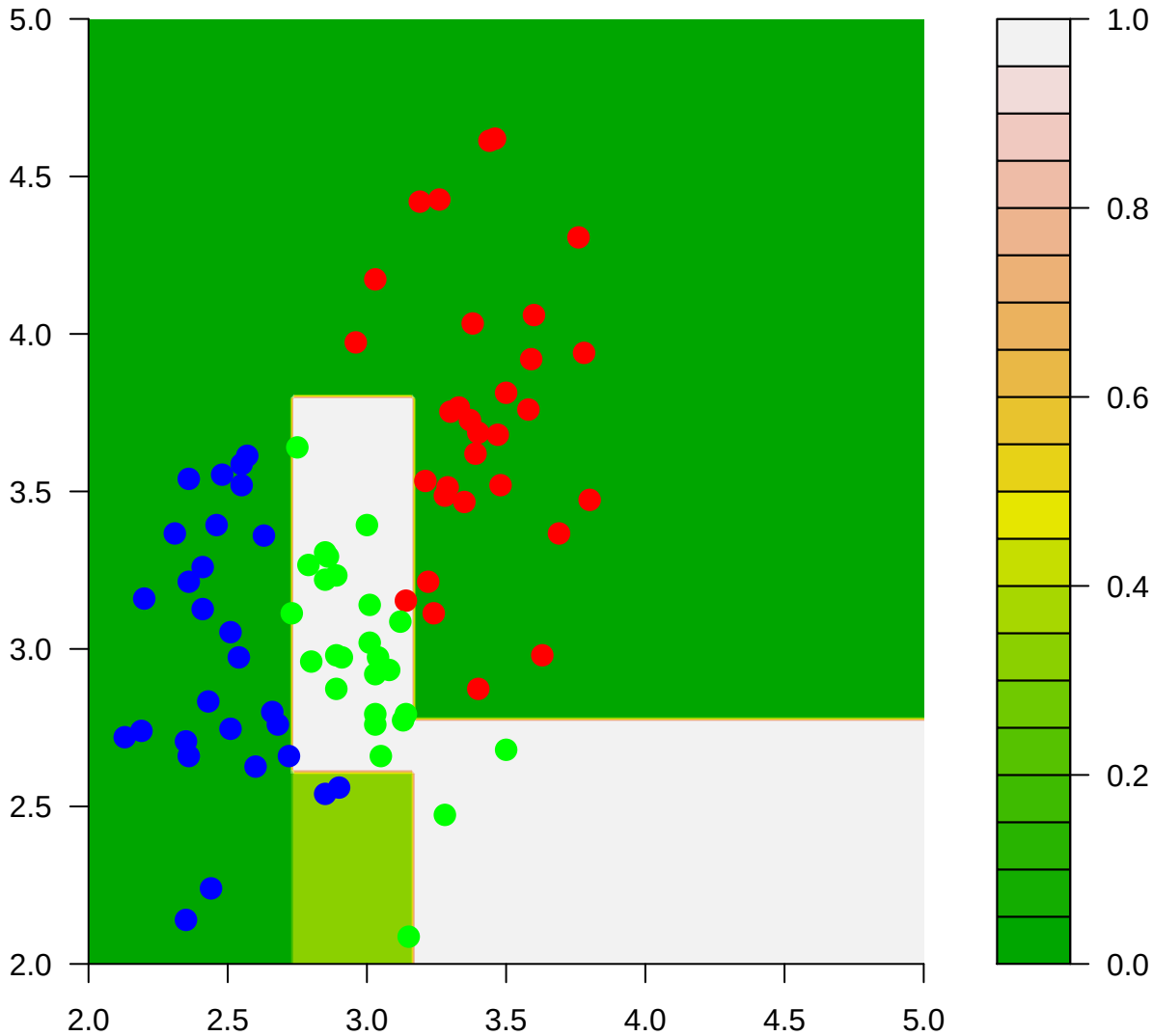
Grad admissions



Grad admissions



Grad admissions



Classification example

- ISOLET data
  http://archive.ics.uci.edu/ml/datasets/ISOLET
- 150 subjects spoke the name of each letter twice
- 52 samples from each subject, 300 samples for each letter

Classification example

- 617 features (explanatory variables). They include: spectral coefficients; contour features, sonorant features, pre-sonorant features, and post-sonorant features.
- Data are split into training ($n = 6238$) and test ($n = 1559$)
- Mission: build a classifier to identify future spoken letters

Classification example

- I separated the letters C and Z

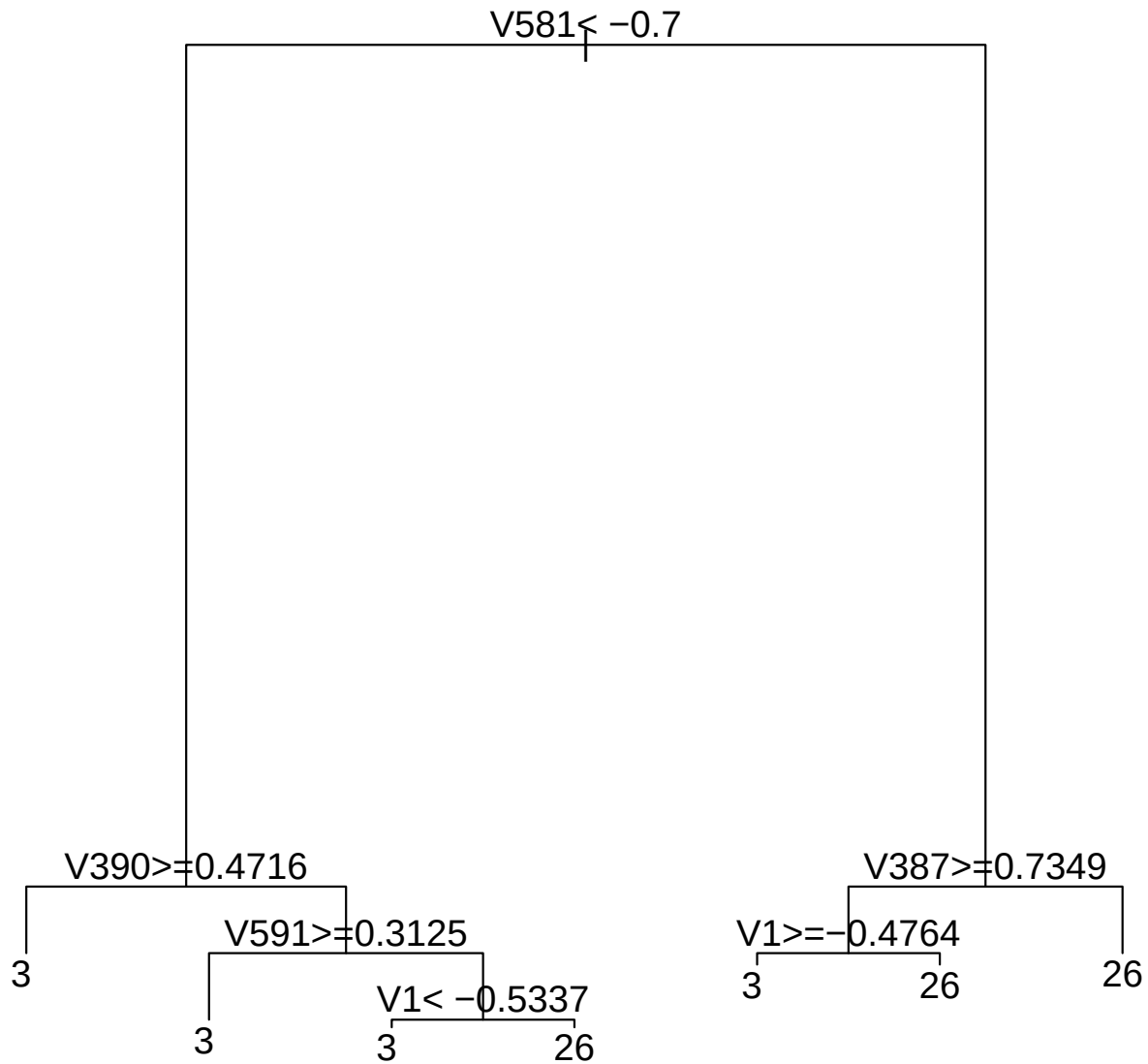
```
> x <- read.table('isolet-train.data', sep=',')
> # 3 and 26 --- "C" and "Z"
>
> xa <- x[ x$V618 == 3, ]
> xb <- x[ x$V618 == 26, ]
>
> xx <- rbind(xa, xb)
> xx$V618 <- as.factor(xx$V618)
```

Classification example

- Fit a classification tree

```
> myc <- rpart.control(minsplit=7, cp=1e-7,
            xval=10)
>
>
> set.seed(123)
> a.t <- rpart(V618~., data=xx,
      parms = list(split = 'information'),
      control=myc)
> b <- a.t$cptable[
      which.min(a.t$cptable[,"xerror"]),"CP"]
> d.r <- prune(a.t, cp=b)
```

Classification example



Classification example

- Predict on the test data

```
> d.pr <- predict(d.r, newdata=dd,
                  type='class')
> table(truth, d.pr)
      d.pr
truth  3 26
   3  59  1
   26  0 60
```

- And we only used 5 explanatory variables!

Classification example

- The problem is not trivial
- Let's try a 1-NN nearest neighbour classifier

```
> u1 <- knn(train=xx[,-618], test=dd[,-618],
     cl=xx[,618], k = 1)
>
> table(truth, u1)
     u1
truth  3 26
   3  57  3
   26  9 51
```

Classification example

- With 5-NN is not much better

```
> u5 <- knn(train=xx[,-618],
      test=dd[,-618], cl=xx[,618],
      k = 5)
>
> table(truth, u5)
      u5
truth  3 26
    3  58  2
    26  5 55
```

Classification example

- With a logistic classifier

```
> xx$V619 <- as.numeric(xx$V618==3)
> d.glm <- glm(V619 ~ . - V618, data=xx,
      family=binomial)
Warning message:
glm.fit: algorithm did not converge

[...]

> table(truth, pr.glm)
      pr.glm
truth  0  1
    3  25 35
    26 33 27
```

- Can we explain the problem?

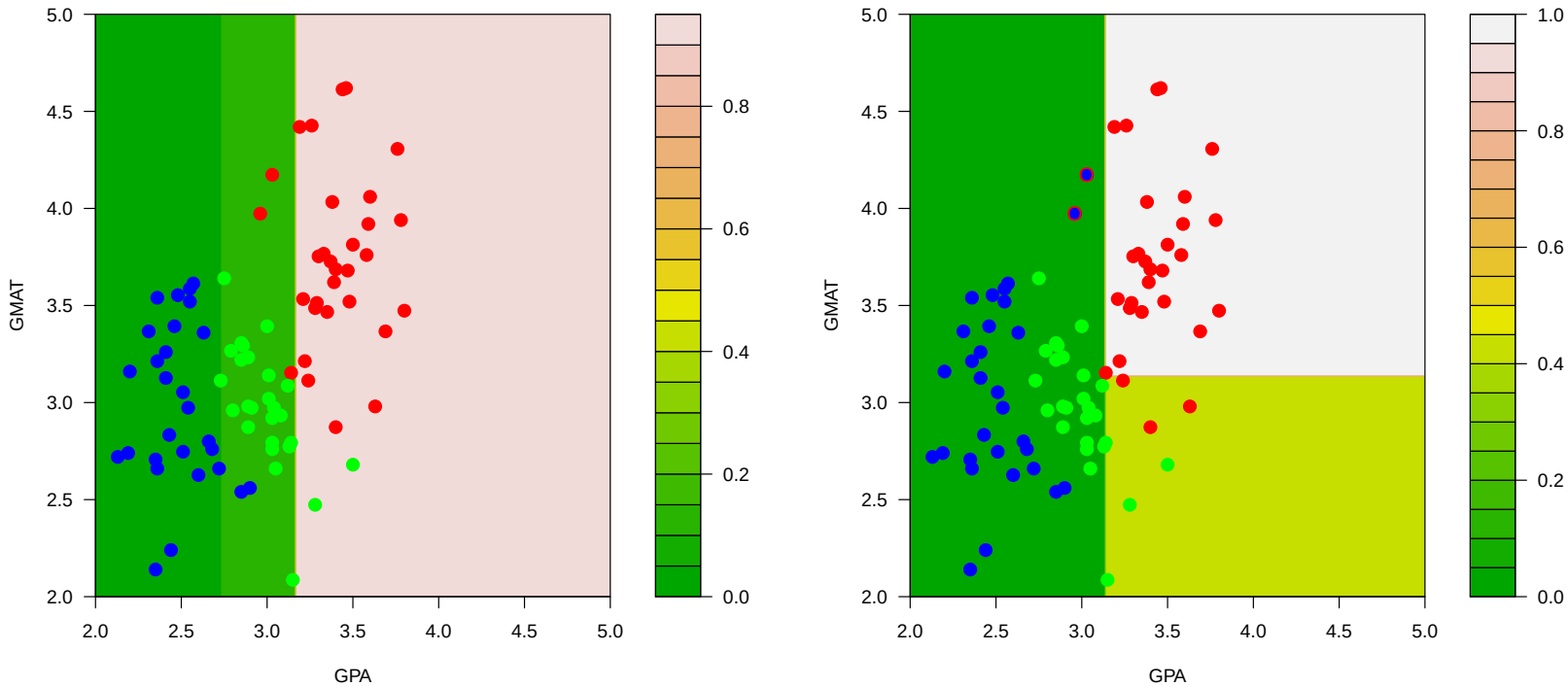
Classification example

- How about the approach based on the Gaussian distribution of the features (within each class)?

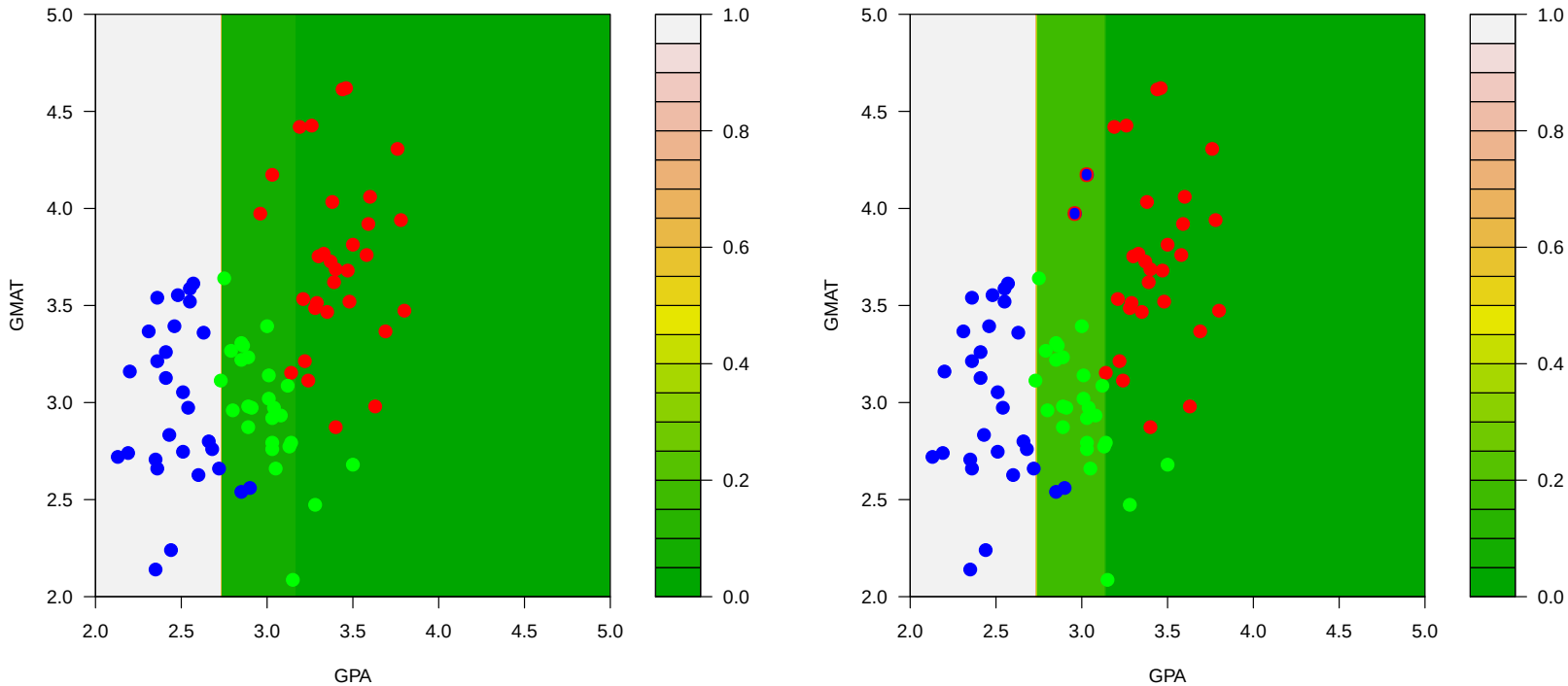
```
> library(MASS)
>
> d.lda <- lda(V618 ~ ., data=xx)
Warning message:
In lda.default(x, grouping, ...) :
    variables are collinear
```

- Can we explain the problem?

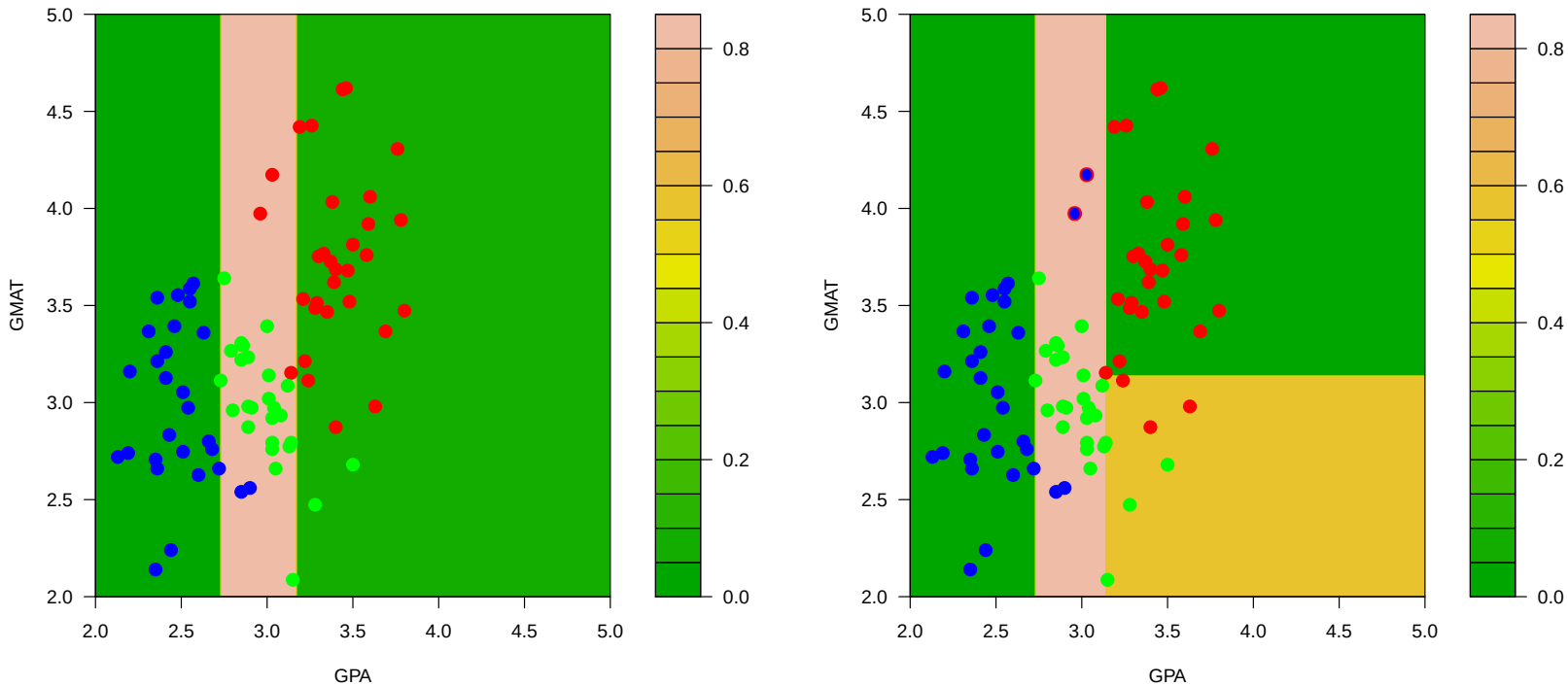
Trees are unstable...



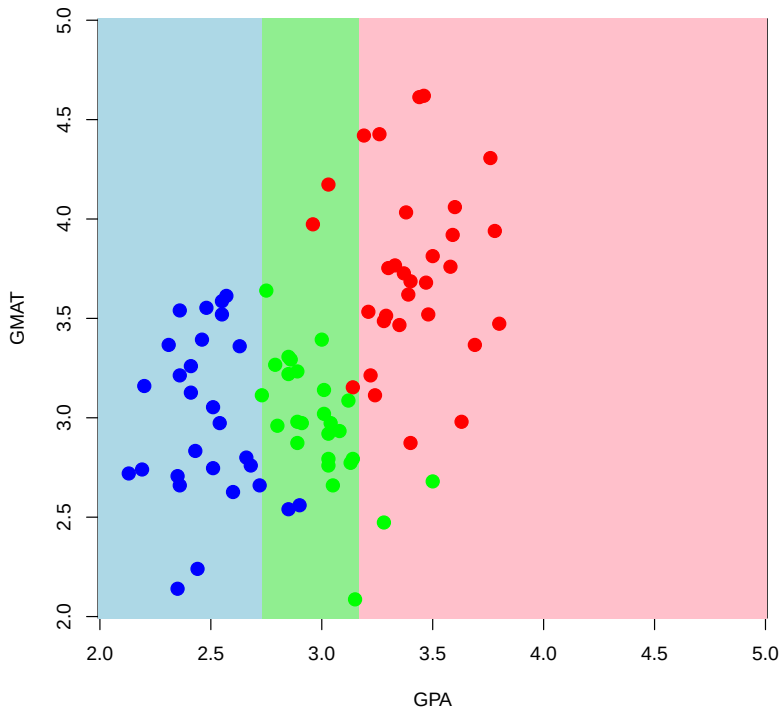
Trees are unstable...

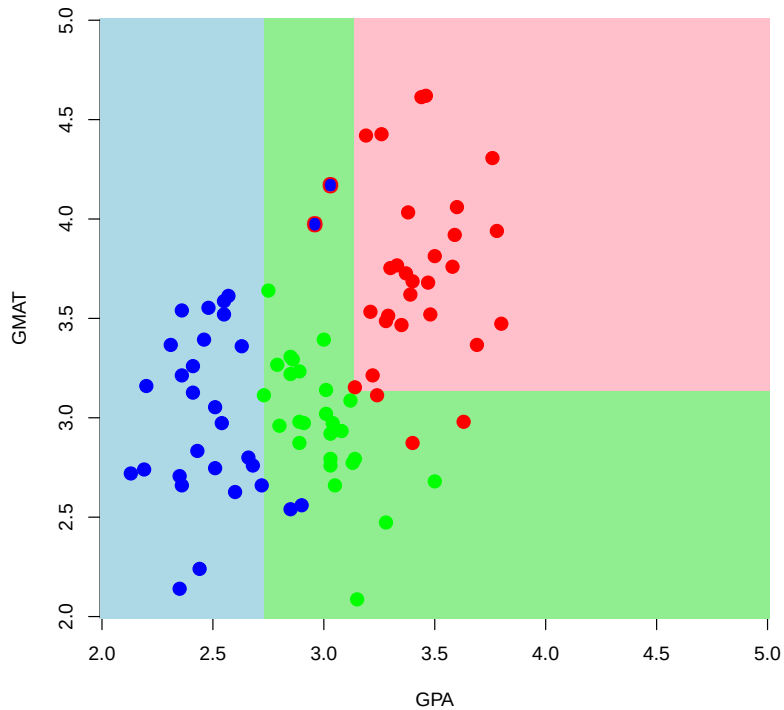


Trees are unstable...



Trees are unstable...





Classification Trees - Bagging

- This problem can be alleviated sometimes using “Bagging” (Bootstrap aggregation)
- It is a general principle, applies to any classifier / estimator
- But its not always equally effective (see the Midterm)

Classification Trees - Bagging

- Consider the predicted class $\hat{g}(\mathbf{X})$ or predicted probabilities $\hat{P}(g|\mathbf{X})$

$$\hat{f}(\mathbf{X}) = \left\{ \begin{array}{c} \left(\hat{P}(g_1|\mathbf{X}), \ldots, \hat{P}(g_K|\mathbf{X})\right) \\ \\ \arg\max_g \hat{P}(g|\mathbf{X}) \end{array} \right\}$$

Classification Trees - Bagging

- If we had several independent samples, we could obtain a more stable (less variable) $\hat{f}(\mathbf{X})$ by using the average over the samples.

- Using our sample distribution as an estimator of the population distribution, the bootstrap simulates independent samples by randomly drawing samples from our data

Classification Trees - Bagging

- We can obtain a “large” number of trees and have them “vote” on the classification of future observations, or average their conditional probabilities estimates $\hat{P}\left(g_j \middle| \mathbf{X}\right)$

Classification Trees - Bagging

- Our aggregated classifier is

$$\bar{f}(\mathbf{X}) = \left\{ \begin{array}{c} \left(\bar{P}(g_1|\mathbf{X}), \ldots, \bar{P}(g_K|\mathbf{X})\right) \\ \\ \arg\max\ (n_1, n_2, \ldots, n_K) \end{array} \right\}$$

where $\left(\bar{P}(g_1|\mathbf{X}), \ldots, \bar{P}(g_K|\mathbf{X})\right)$ are averaged conditional probabilities over the boostrap samples;

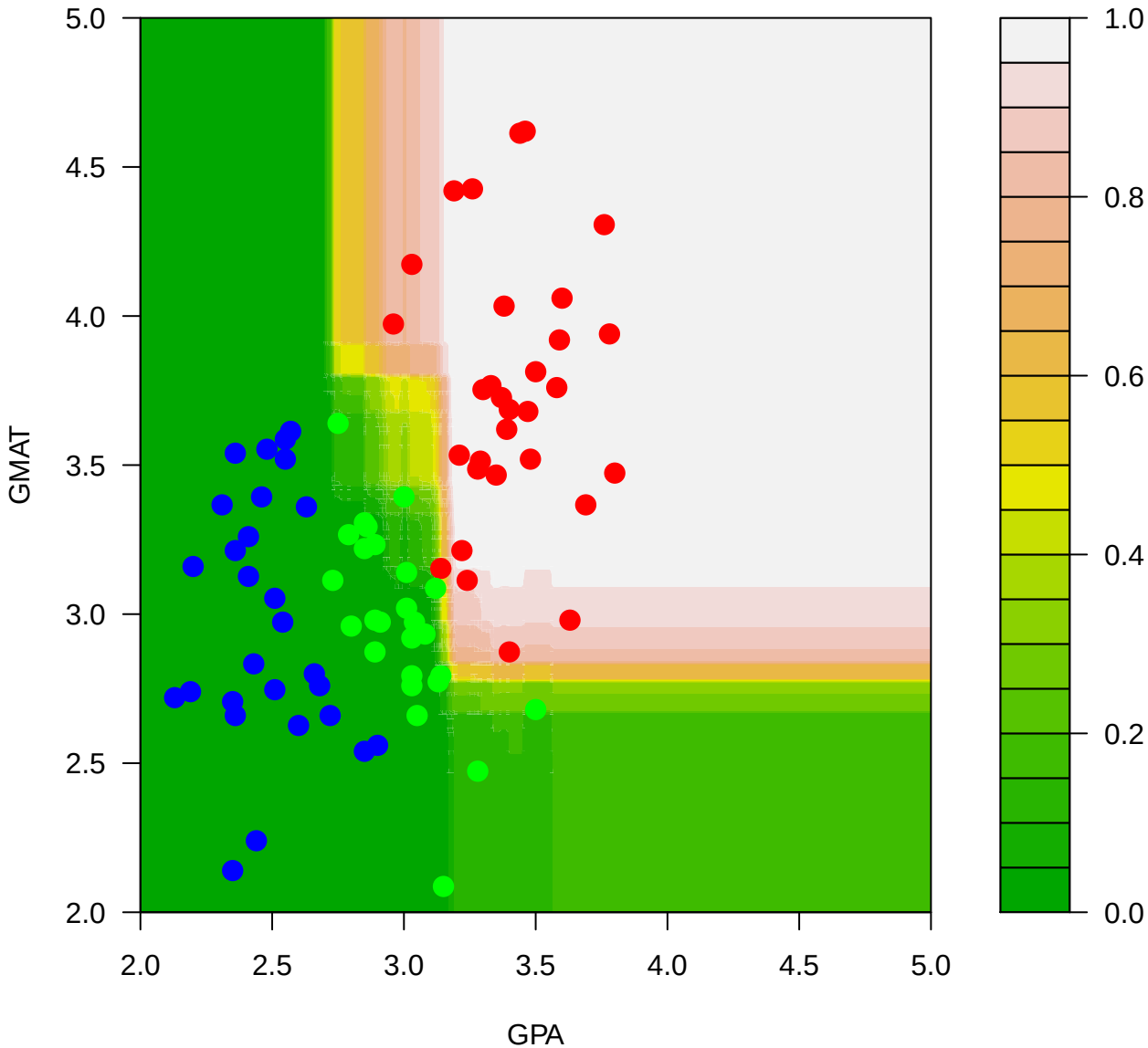
$(n_1, n_2, \ldots, n_K)$ are the number of times each class was selected and

$n_1 + n_2 + \cdots + n_K =$ number of bootstrap samples

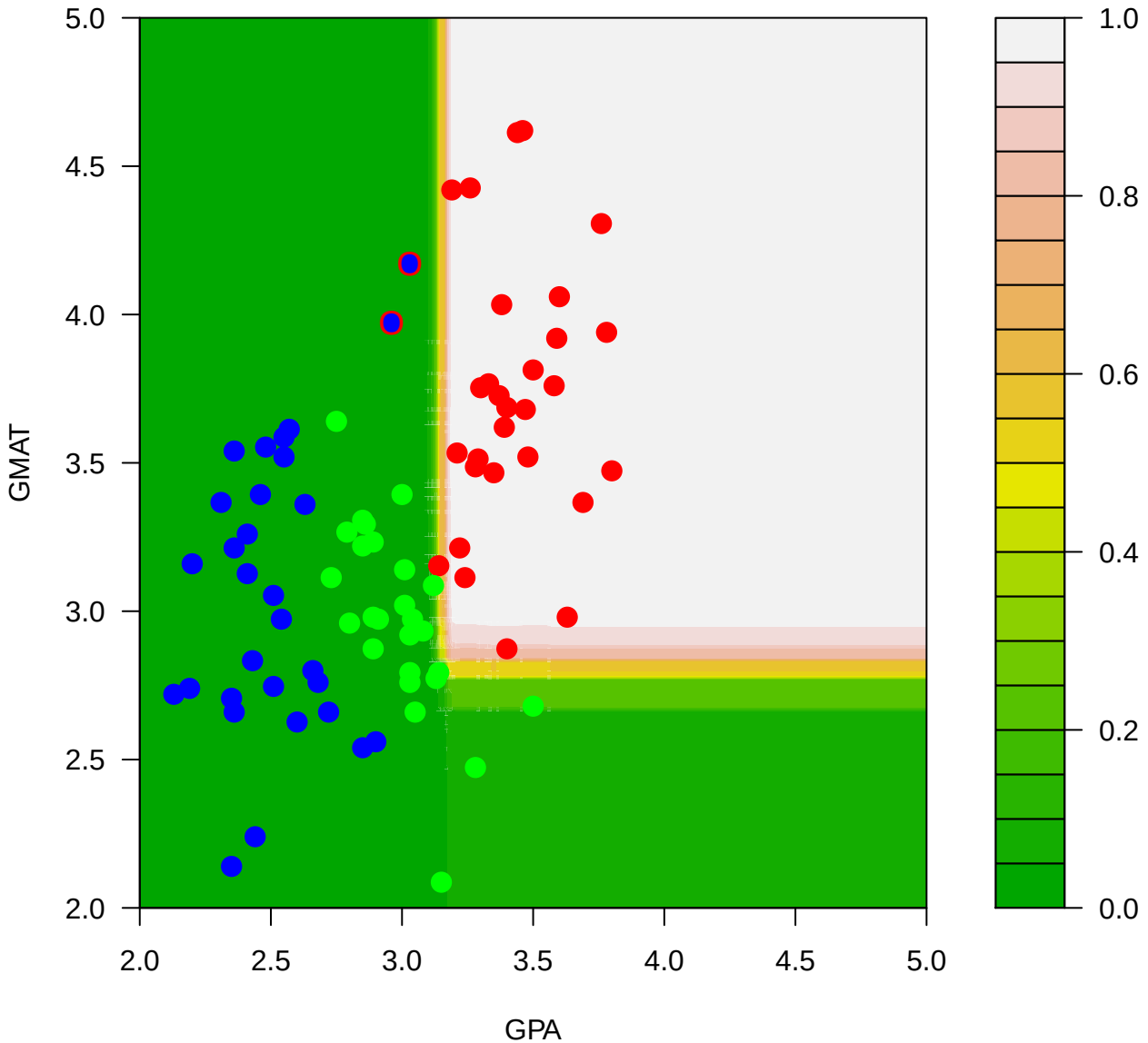
Example

Example

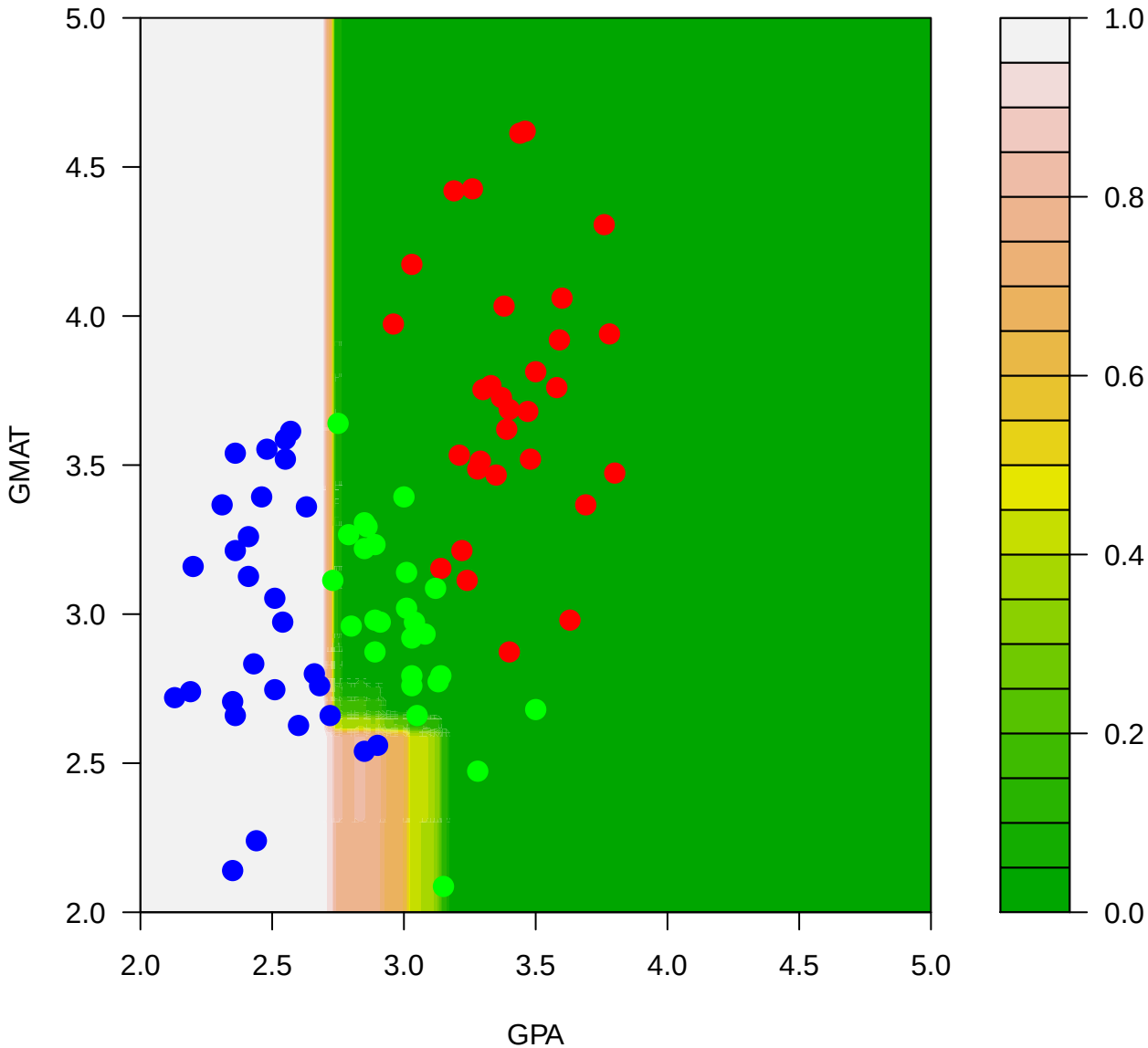
Bagged trees -original data



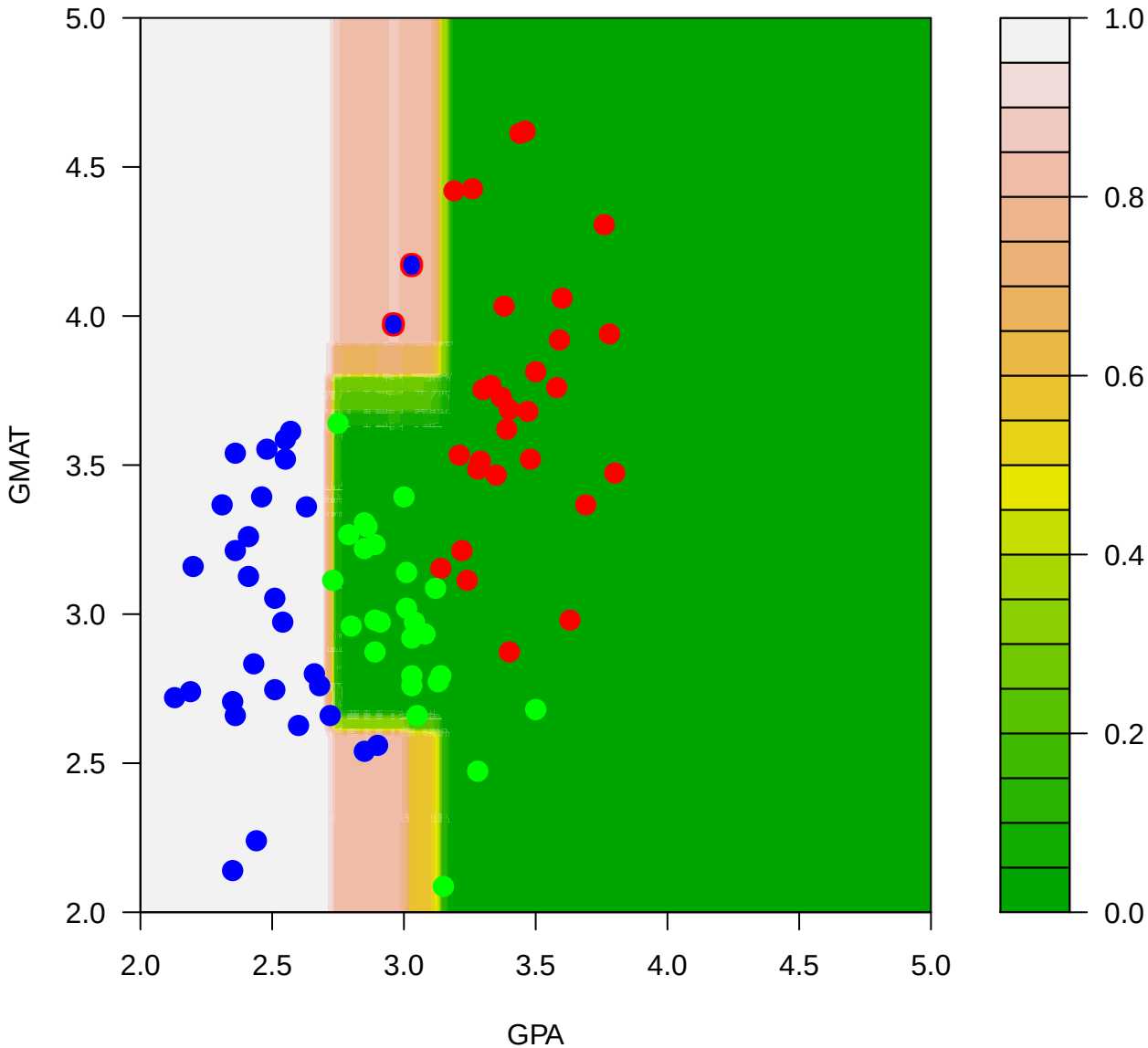
Bagged trees -modified data



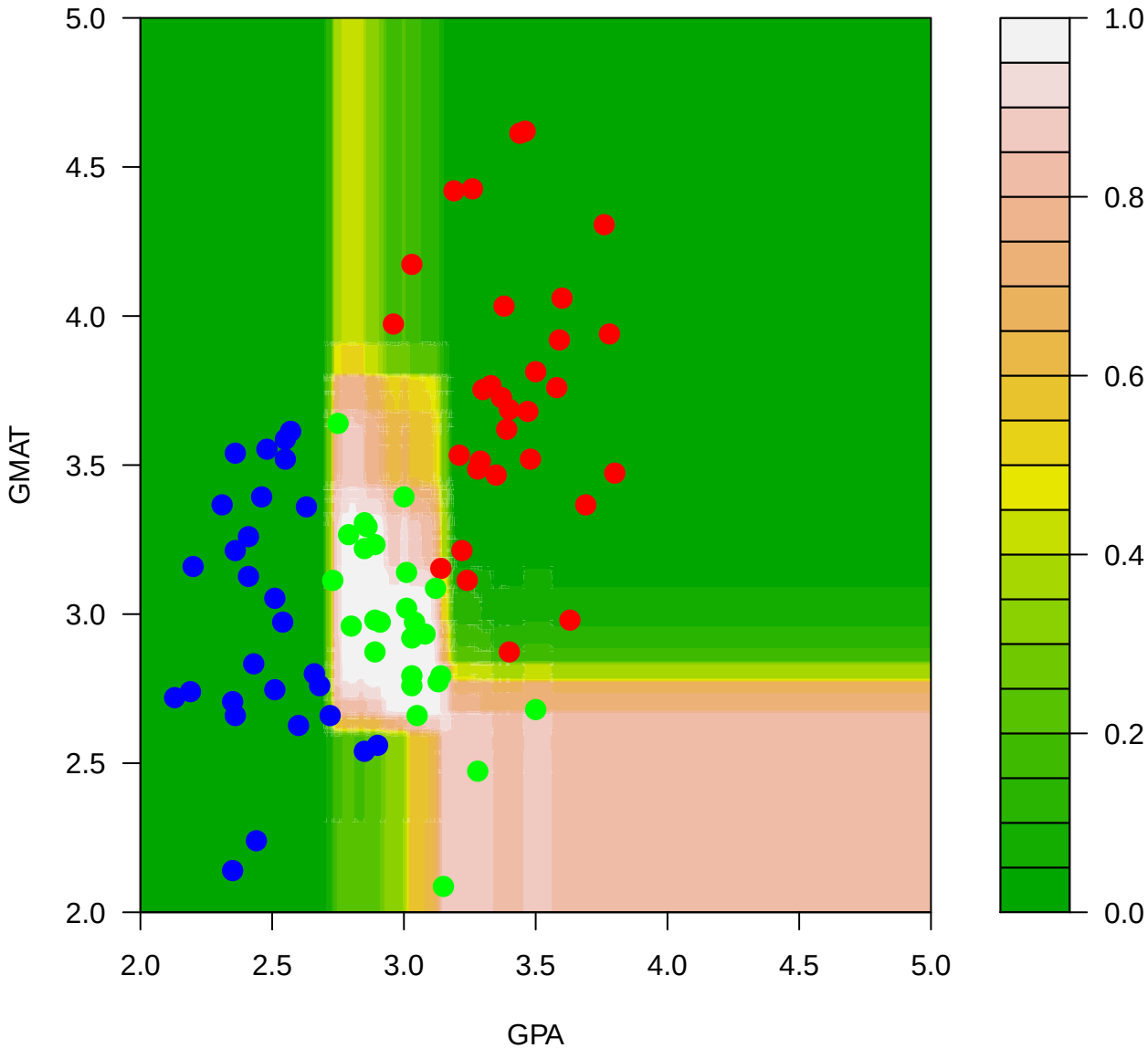
Bagged trees -original data



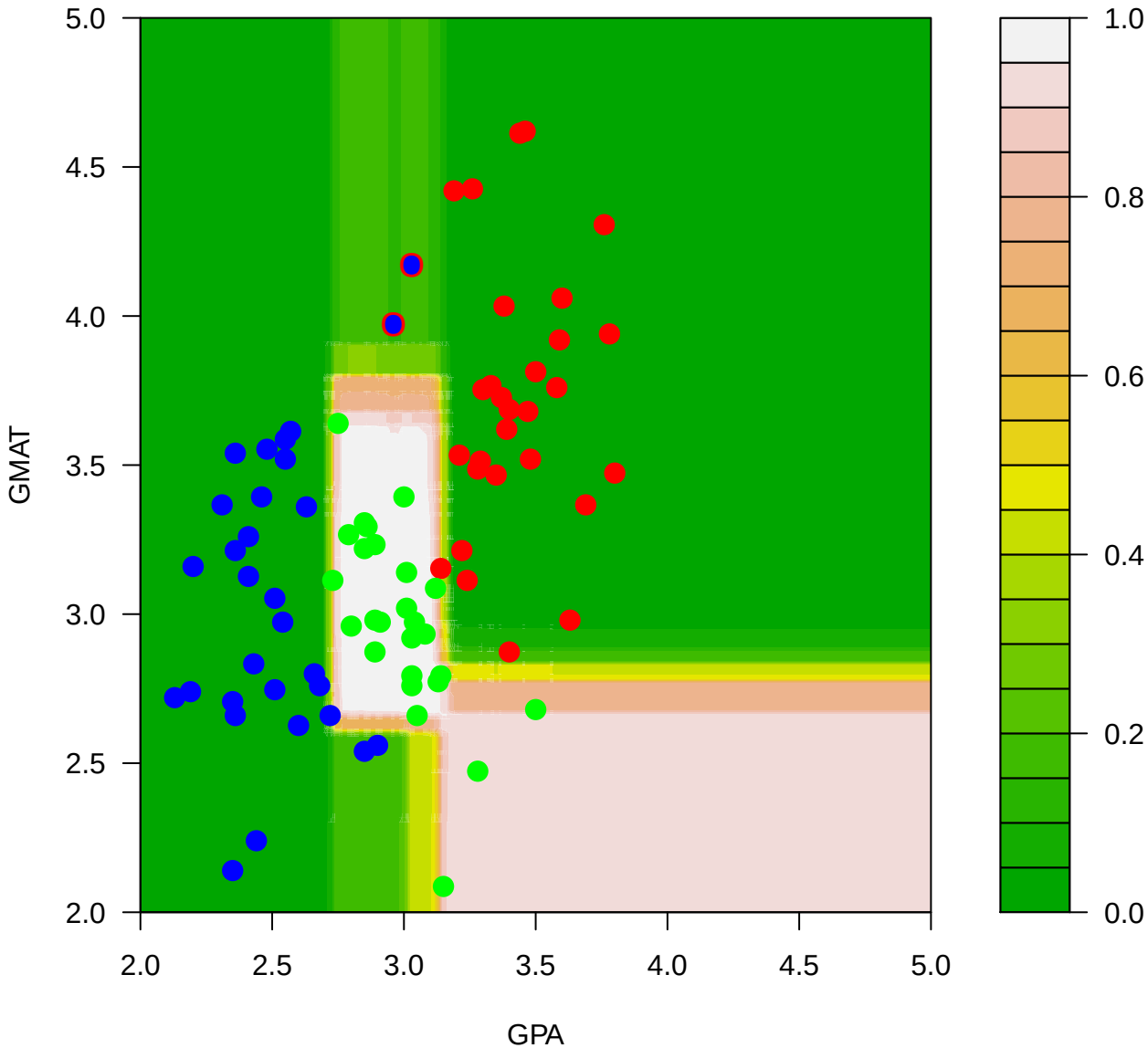
Bagged trees - modified data



Bagged trees -original data



Bagged trees - modified data



Random forests

- Bagging - averaging identically distributed trees (which may be correlated)

- Random forests - making the “bagged” trees less correlated
- The bootstrapped trees are de-correlated by making them use different features for the splits

Random forests

(1) `for(b in 1:B)`

  (a) Draw a bootstrap sample from the training data

  (b) Grow a “random forest tree” as follows: for each terminal node:

    (i) Randomly select `m` features

    (ii) Pick the best split among these

    (iii) Split the node into two children

  (c) Repeat (b) to grow a (very very) large tree

(2) Return the ensemble of trees $(T_b)_{1 \leq b \leq B}$

Random forests

- Given a new point $\mathbf{x}$, for regression we use

$$\hat{f}(\mathbf{x}) = \frac{1}{B}\sum_{b=1}^{B} T_b(\mathbf{x})$$

- For classification:

$$\hat{f}(\mathbf{x}) = \text{majority vote among} \left\{ T_b(\mathbf{x}), \; 1 \leq b \leq B \right\}$$

Q: why not average conditional prob's?

Out-of-bag error estimates

- Each bagged tree is trained on a bootstrap sample
- Predict the observations not in the bootstrap sample with that tree
- One will have "about" $B/3$ predictions for each point in the training set
- These can be used to estimate the prediction error (classification error rate) without having to use CV

Out-of-bag error estimates

- For each training observation $(y_i, \mathbf{x}_i)$, obtain a prediction using only those trees in which $(y_i, \mathbf{x}_i)$ was **NOT** used
- In other words, let $\mathcal{I}_i$ the set of trees (bootstrap samples) where $(y_i, \mathbf{x}_i)$ does not appear, then

$$\hat{y}_i = \frac{1}{|\mathcal{I}_i|} \sum_{j \in \mathcal{I}} T_j(\mathbf{x}_i)$$

Random forests

- This error estimate can be computed at the same time as the trees are being built
- When this error estimate is stabilized we can stop adding trees to the ensemble

Example

Example

Random forests

- Feature ranking - relative importance of each variable
- Given a single tree T, at each node t split we can compute the sum of reductions in sum of squares (or gini or deviance measures) m_t^2
- We assign this squared measure m_t^2 to the variable (feature) used in the split

Random forests

- To each feature, we assign the sum of "squared gains" attributed to it
- For the i-th variable X_i we have

$$\mathcal{I}_i^2(T) = \begin{cases} m_t^2 & \text{if split involved } X_i \\ 0 & \text{otherwise} \end{cases}$$

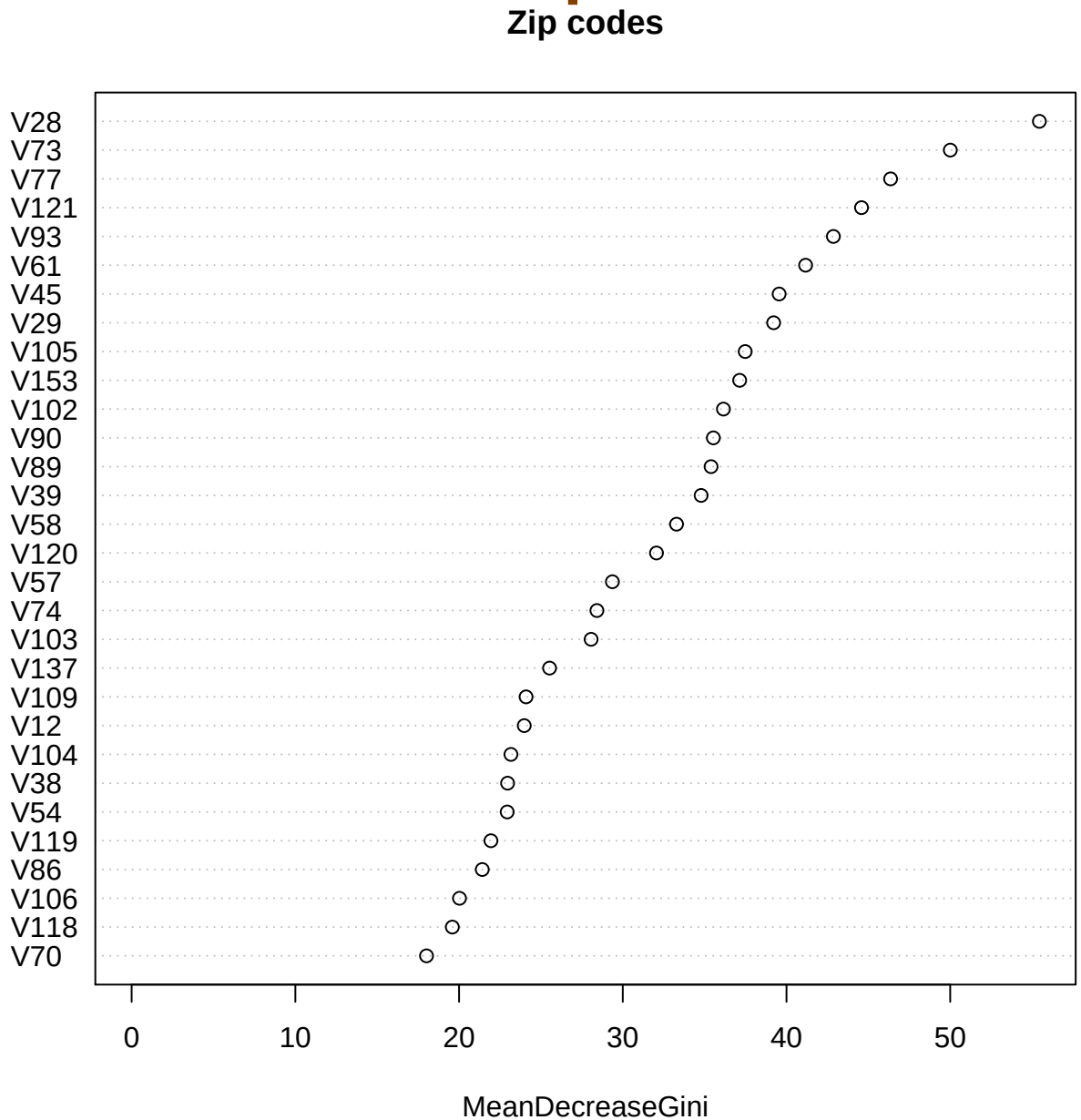
Random forests

- For a random forest we use

$$\mathcal{I}_i^2 = \sum_T \mathcal{I}_i^2(T)$$

- In other words, we sum (or average) the importance of the variable across the trees in the forest

Random Forest - plot



Ensembles

- Ensembles of classifiers
- Combine classifiers trained on the same (or similar [e.g. bootstrapped]) data
- Consensus is reached by (equally weighted) voting or averaged estimated probabilities.
- Bagging and Random Forests are examples of ensembles.

Boosting

- Originally proposed for classification
- Main idea: sequentially re-train a simple classifier assigning more importance to points that were previously misclassified

Boosting

- The end result is a weighted average of all the classifiers
- Interesting ideas:
  - Not all components of the ensemble are treated equally
  - Members of the ensemble use information about other members
  - The underlying loss function has a “margin” (unlike 0-1 losses)

Boosting - AdaBoost.M1

Algorithm. Data $(y_{\mathbf{i}}, \mathbf{x}_{\mathbf{i}})$, with $y_{\mathbf{i}} \in \{-1, 1\}$

- Set initial weights $w_{\mathbf{i}} = 1/n$, $1 \leq \mathbf{i} \leq n$
- For $\mathbf{j} = 1, \ldots, K$
- Build a classifier $T_{\mathbf{j}}(\mathbf{x})$ to the data using weights $w_{\mathbf{i}}$, $1 \leq \mathbf{i} \leq n$

Boosting - AdaBoost.M1

- Let

$$e_{\mathbf{j}} = \sum_{\mathbf{i}=1}^{n} w_{\mathbf{i}} I\left(y_{\mathbf{i}} \neq T_{\mathbf{j}}(\mathbf{x}_{\mathbf{i}})\right) \Big/ \sum_{\ell=1}^{n} w_{\ell}$$

- Let $\alpha_{\mathbf{j}} = \log\left((1 - e_{\mathbf{j}})/e_{\mathbf{j}}\right)$ and

$$w_{\mathbf{i}} = w_{\mathbf{i}} \exp\left(\alpha_{\mathbf{j}} I\left(y_{\mathbf{i}} \neq T_{\mathbf{j}}(\mathbf{x}_{\mathbf{i}})\right)\right), \mathbf{i} = 1, \ldots, n$$

- Final classifier:

$$T(\mathbf{x}) = \text{sign}\left(\sum_{\mathbf{j}=1}^{K} \alpha_{\mathbf{j}} T_{\mathbf{j}}(\mathbf{x})\right)$$