STAT406- Methods of Statistical Learning Lecture 16

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UBC - Sep / Dec 2018

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

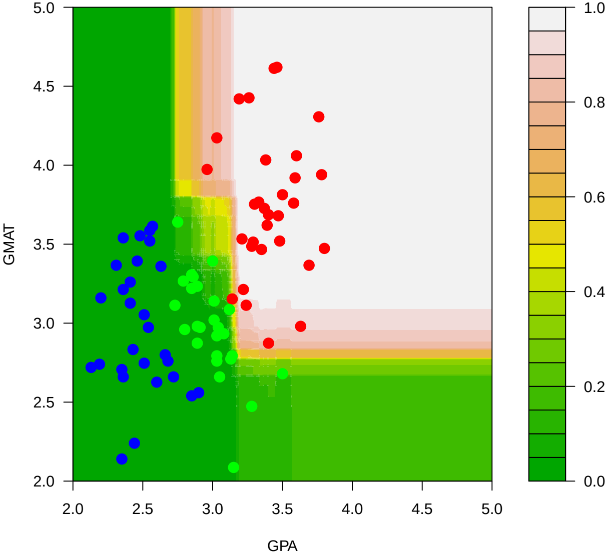
- Our aggregated classifier is

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

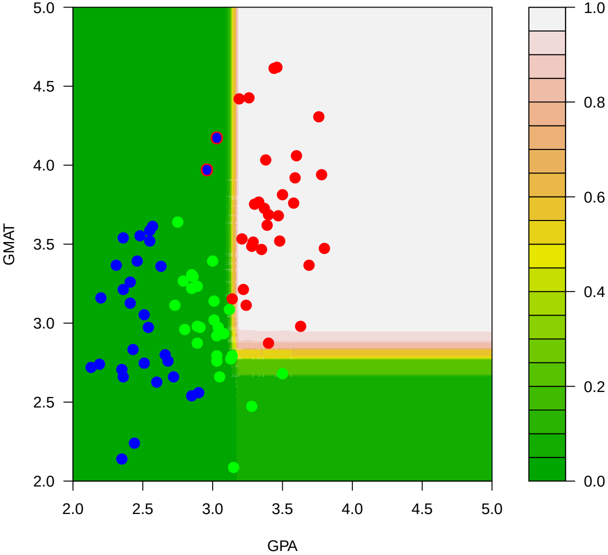
  where $\left(\bar{P}(g_1|\mathbf{X}), \ldots, \bar{P}(g_K|\mathbf{X})\right)$ are averaged conditional probabilities over the boostrap samples;

  $(n_1, n_2, \ldots, n_K)$ are the number of times each class was selected and $n_1 + n_2 + \cdots + n_K =$ number of bootstrap samples

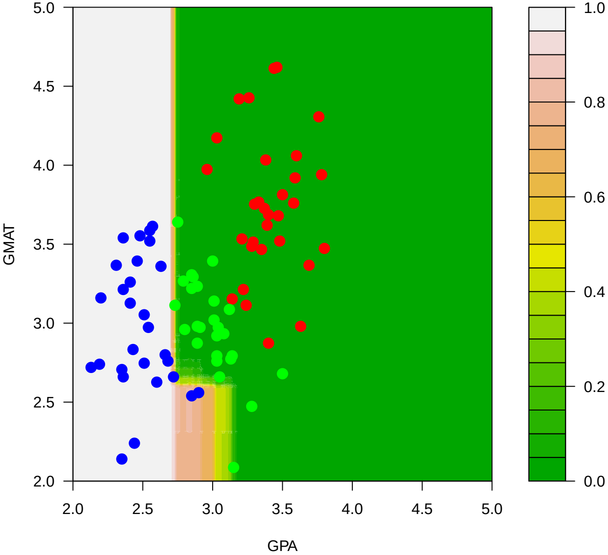
Bagged trees -original data



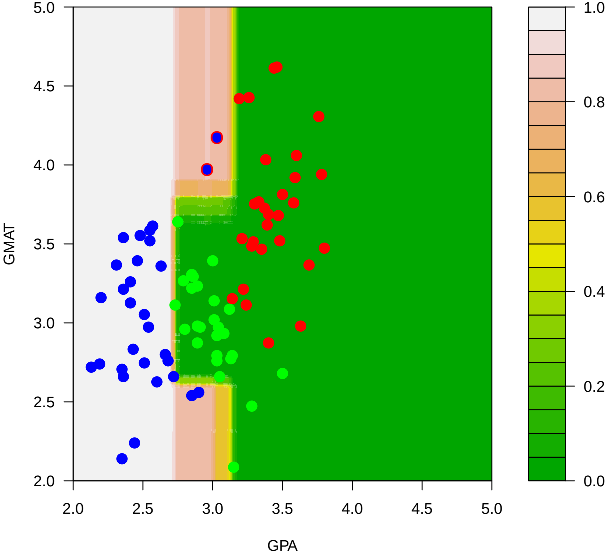
Bagged trees -modified data



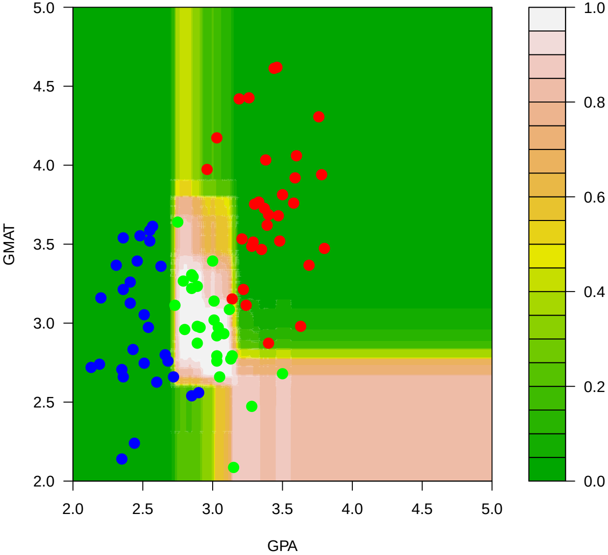
Bagged trees -original data



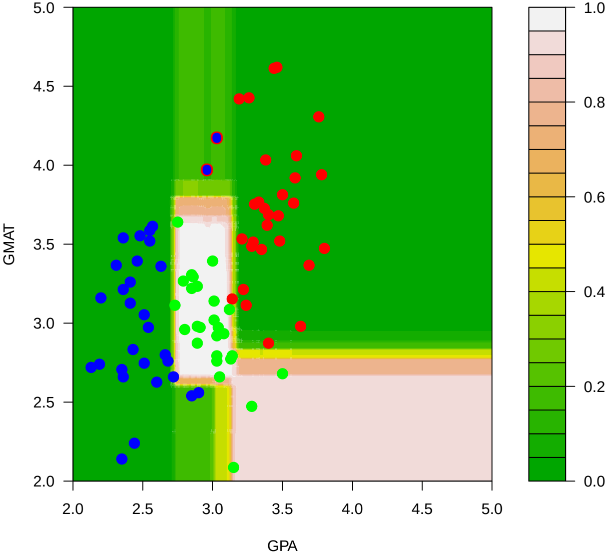
Bagged trees - modified data



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:

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

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

OOB example on GitHub