

STAT406- Methods of Statistical Learning Lecture 12

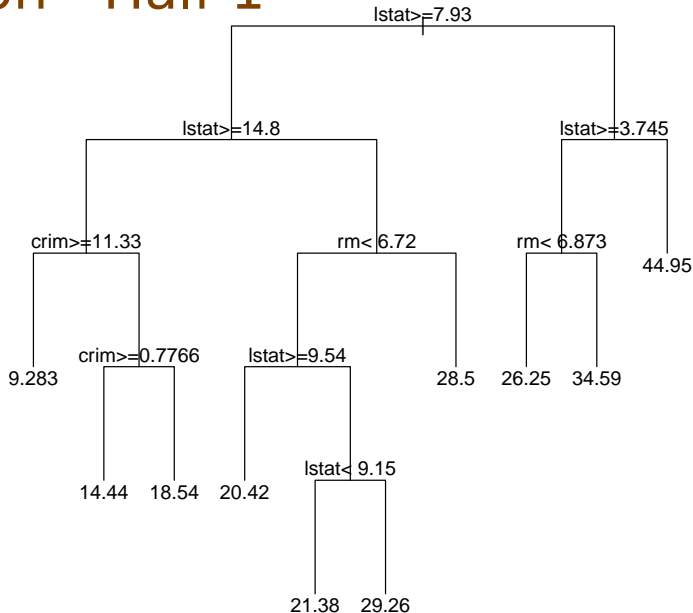
Matias Salibian-Barrera

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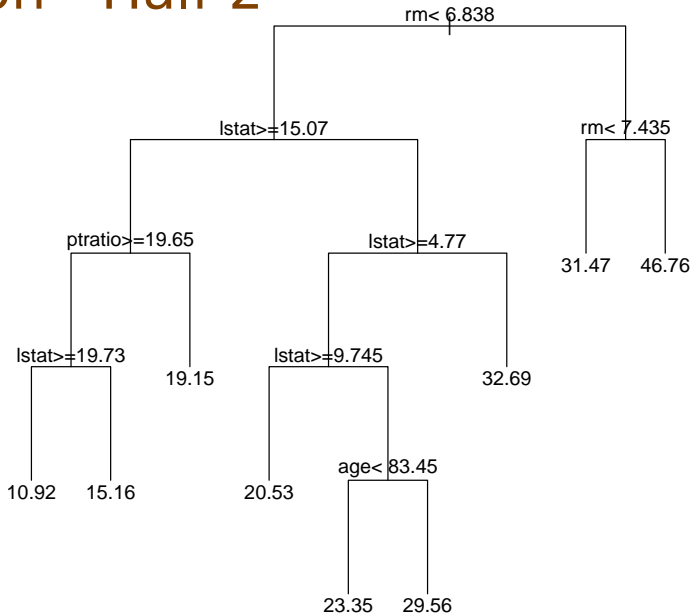
Bagging

- Trees can be highly variable
- Trees computed on samples from the sample population can be quite different from each other
- For example, we split the Boston data in two...

Boston - Half 1



Boston - Half 2



Bagging

- Linear regression, for example, is not so variable
- Estimated coefficients computed on the same two halves

```
      (Intercept)   crim    zn indus chas
[1,]          39.21 -0.13  0.04  0.04  2.72
[2,]          33.12 -0.10  0.05 -0.01  2.80
      nox    rm age    dis   rad    tax
[1,]   -20.07  3.45  0 -1.44  0.28 -0.01
[2,]   -14.18  4.15  0 -1.46  0.34 -0.02
      ptratio black lstat
[1,]   -1.01   0.01 -0.56
[2,]   -0.90   0.01 -0.50
```

Bagging

- If we could average many trees trained on independent samples from the same population, we would obtain a predictor with lower variance
- If $\hat{f}_1, \hat{f}_2, \dots, \hat{f}_B$ are B regression trees, then their average is

$$\hat{f}_{\text{av}}(\mathbf{x}) = \frac{1}{B} \sum_{j=1}^B \hat{f}_j(\mathbf{x})$$

Bagging

- However, we generally do not have B training sets...
- We can **bootstrap** the training set to obtain B pseudo-new-training sets
- Let $(Y_1, \mathbf{X}_1), (Y_2, \mathbf{X}_2), \dots, (Y_n, \mathbf{X}_n)$ be the training sample, where

$$(Y_j, \mathbf{X}_j) \sim F_0$$

Bagging

- If we knew F_0 , then we could generate / simulate new training sets, and average the resulting trees...
- We do not know F_0 , but we have an estimate for it
- Let F_n be the empirical distribution of our only training set $(Y_1, \mathbf{X}_1), (Y_2, \mathbf{X}_2), \dots, (Y_n, \mathbf{X}_n)$

Bagging

- We know that

$$F_n \xrightarrow{n \rightarrow \infty} F_0$$

(in what sense?)

- Bootstrap generates / simulates samples from F_n
- Taking a sample of size n from F_n is the same as sampling with replacement from the training set $(Y_1, \mathbf{X}_1), (Y_2, \mathbf{X}_2), \dots, (Y_n, \mathbf{X}_n)$

Bagging

- To apply bagging to a regression tree, take B independent samples (with replacement) from the training set
- Obtain the B trees: $\hat{f}_1^*, \hat{f}_2^*, \dots, \hat{f}_B^*$
- and average their predictions

$$\hat{f}_{\text{bag}}(\mathbf{x}) = \frac{1}{B} \sum_{j=1}^B \hat{f}_j^*(\mathbf{x})$$

Bagging

- Generally, we apply bagging on “large” trees, without pruning them (try to retain their low-bias and reduce their variance by averaging)
- With the Boston data set, if we apply bagging to the regression tree computed on the training set, and then use it to predict on the test set, we obtain:

Bagging

- $B = 1$

```
> mean((dat.te$medv - pr.ba)^2)
[1] 16.44972
```

- $B = 5$

```
> mean((dat.te$medv - pr.ba)^2)
[1] 15.12332
```

- $B = 100$

```
> mean((dat.te$medv - pr.ba)^2)
[1] 12.30543
```

- $B = 500$

```
> mean((dat.te$medv - pr.ba)^2)
[1] 12.32504
```

Bagging

- $B = 2000$

```
> mean((dat.te$medv - pr.ba)^2)
[1] 11.8116
```

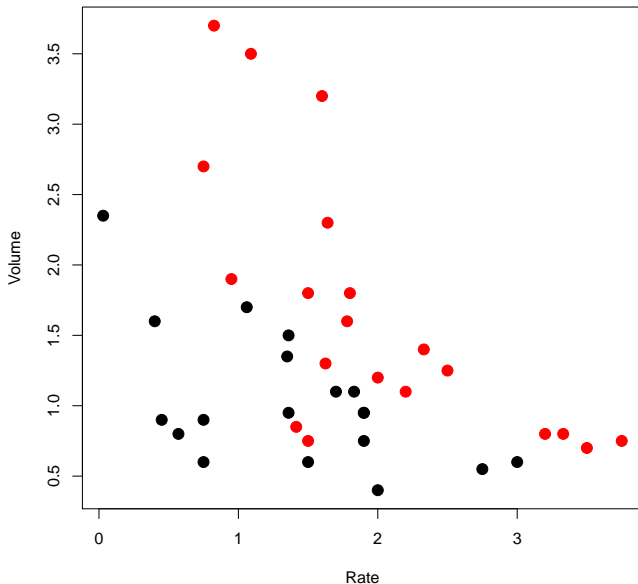
- $B = 5000$

```
> mean((dat.te$medv - pr.ba)^2)
[1] 11.85943
```

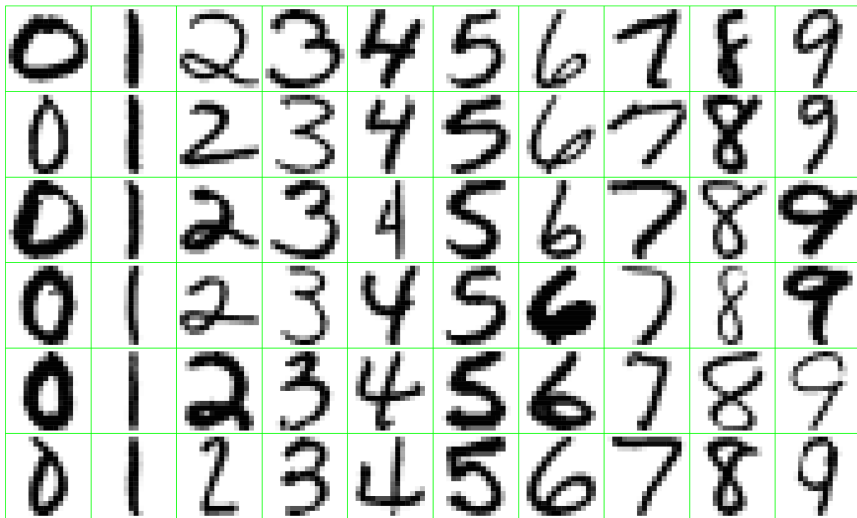
Bagging

- This approach applies to any predictor (not only trees)
- It will be particularly useful for low-bias / high-variance predictors

Classification



Predict hand-written digits



Classification as prediction

- In general, we have n observations (training)
- $(g_1, \mathbf{x}_1), (g_2, \mathbf{x}_2), \dots, (g_n, \mathbf{x}_n)$
- we would like to build a classifier, a function $\hat{g}(\mathbf{x})$ to predict the true class g of a future observation (g, \mathbf{x}) (for which g is unknown)

Classification as prediction

- In general, there are K possible classes, c_1, c_2, \dots, c_K . In other words $g \in \{c_1, c_2, \dots, c_K\}$
- Consider the following loss function

$$L(a, b) = \begin{cases} 0 & \text{if } a = b \\ 1 & \text{if } a \neq b \end{cases}$$

Classification as prediction

- Find a classifier $\hat{g}(\mathbf{x})$ such that

$$E_{(G,\mathbf{x})} [L (G, \hat{g}(\mathbf{x}))] \leq E_{(G,\mathbf{x})} [L (G, h(\mathbf{x}))]$$

for any other function h

$$\begin{aligned} E_{(G,\mathbf{x})} [L (G, \hat{g}(\mathbf{x}))] &= E_{\mathbf{x}} \{ E_{G|\mathbf{x}} [L (G, \hat{g}(\mathbf{x}))] \} \\ &= E_{\mathbf{x}} \left\{ \sum_{j=1}^K L (c_j, \hat{g}(\mathbf{x})) P (G = c_j | \mathbf{x}) \right\} \end{aligned}$$

Classification as prediction

- It is sufficient to find $\hat{g}(\mathbf{X})$ that minimizes

$$\begin{aligned} \sum_{j=1}^K L(c_j, \hat{g}(\mathbf{X})) P(G = c_j | \mathbf{X}) \\ = \sum_{c_j \neq \hat{g}(\mathbf{X})} P(G = c_j | \mathbf{X}) \\ = 1 - P(G = \hat{g}(\mathbf{X}) | \mathbf{X}) \end{aligned}$$

- Hence, the optimal classifier satisfies

$$P(G = \hat{g}(\mathbf{X}) | \mathbf{X}) \geq P(G = c_j | \mathbf{X}) \quad \text{for all } c_j$$

More than 2 groups

- In other words, $\hat{g}(\mathbf{X})$ should be the class with the highest probability

$$\hat{g}(\mathbf{X}) = \arg \max_{\mathbf{g} \in \{c_1, \dots, c_K\}} P(G = \mathbf{g} | \mathbf{X})$$

- “Assign \mathbf{X} to the class with largest conditional (posterior) probability given \mathbf{X} ”