STAT406- Methods of Statistical Learning Lecture 11

Matias Salibian-Barrera

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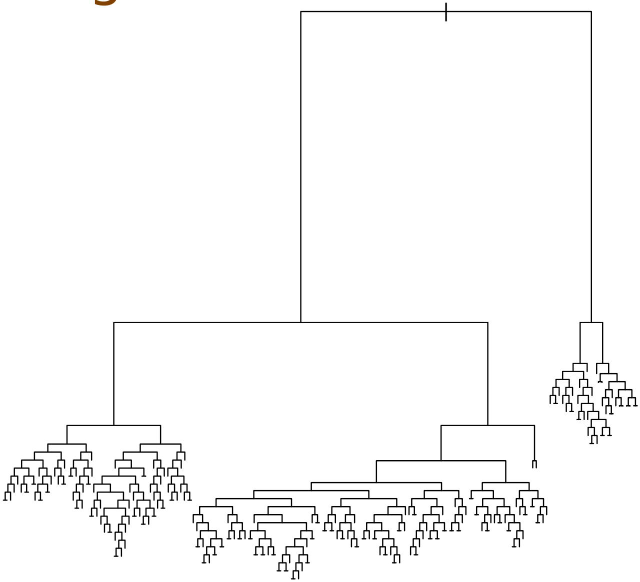
Overfitting...



Boston Example

Not surprisingly, when we overfit...

```
> pr.to <- predict(bos.to,
     newdata=dat.te,
     type='vector')
> with(dat.te, mean((medv - pr.to)^2))
[1] 36.51097
```

Pruning...

- Cost pruning

$$\min_{T \subset T_0} \sum_{m=1}^{|T|} \sum_{\mathbf{x}_i \in R_m} \left(y_i - \hat{\mu}_m \right)^2 + \alpha \, |T|$$

- We can compute the solution for all α
- Compare each subtree in this sequence using CV
- Pick the best subtree

Pruning...

- More specifically:
- Let $T_\ell \subset T_0$ be the solution to

$$\min_{T \subset T_0} \sum_{m=1}^{|T|} \sum_{\mathbf{x}_i \in R_m} (y_i - \hat{\mu}_m)^2 \ + \ \alpha \, |T|$$

when

$$\alpha \in [\alpha_\ell, \alpha_{\ell+1}) \subseteq [0, +\infty) \quad \ell = 1, 2, \ldots, L$$

Pruning...

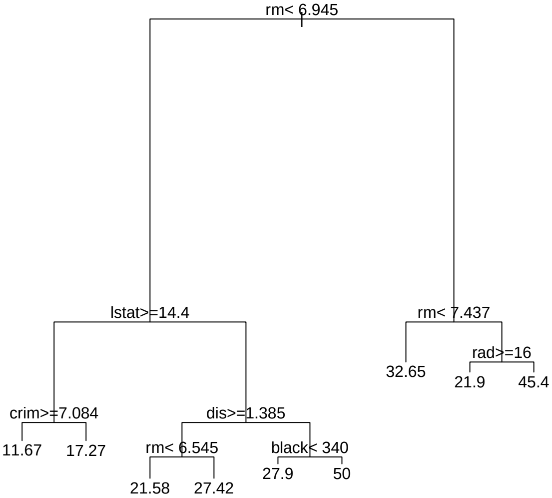
- Split the data into K folds
- For $j = 1, \ldots, K$
  - Build a tree without the j-th fold
  - Prune it with α_ℓ, $\ell = 1, \ldots, L$
  - Predict j-th fold with these L trees
  - Record the prediction errors.
- Average over the folds.
- We obtain K-fold CV-estimated prediction errors for the L trees corresponding to pruning with α_ℓ, $\ell = 1, \ldots, L$.

Boston Example

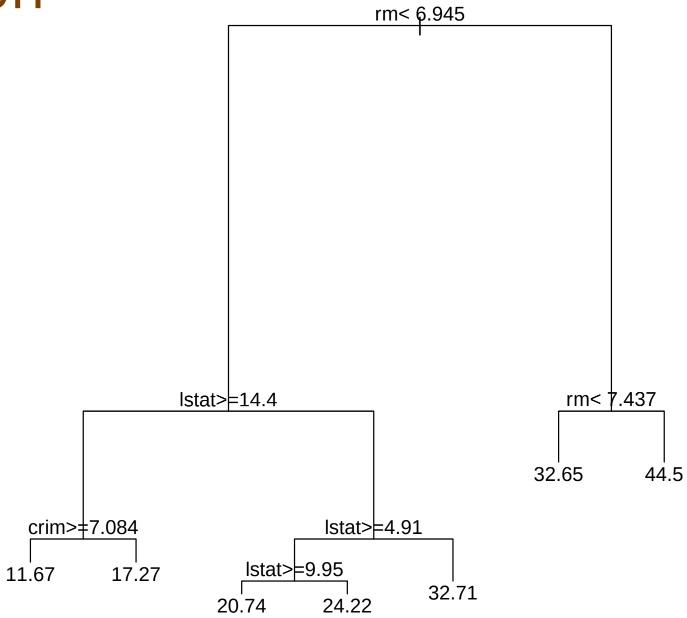
Pruning works...

```
> b <- ***cp with minimum xerror***
>
> bos.t3 <- prune(bos.to, cp=b)
> plot(bos.t3)
> pr.t3 <- predict(bos.t3,
        newdata=dat.te,
        type='vector')
> with(dat.te, mean((medv - pr.t3)^2))
[1] 18.96988
```

Pruned tree


rm< 6.945
lstat>=14.4
rm< 7.437
rad>=16
32.65
21.9
45.4
crim>=7.084
dis>=1.385
11.67
17.27
rm< 6.545
black< 340
27.9
50
21.58
27.42

Boston

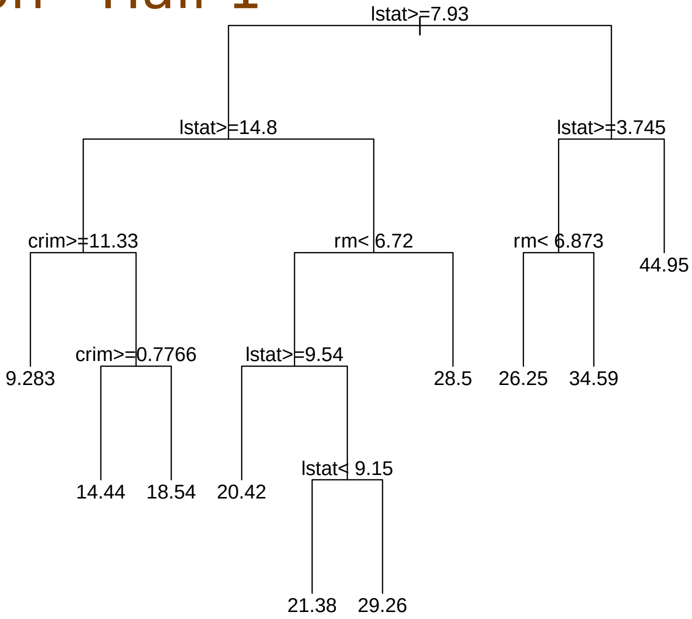


rm< 6.945
lstat>=14.4
rm< 7.437
32.65
44.5
crim>=7.084
lstat>=4.91
11.67
17.27
lstat>=9.95
20.74
24.22
32.71

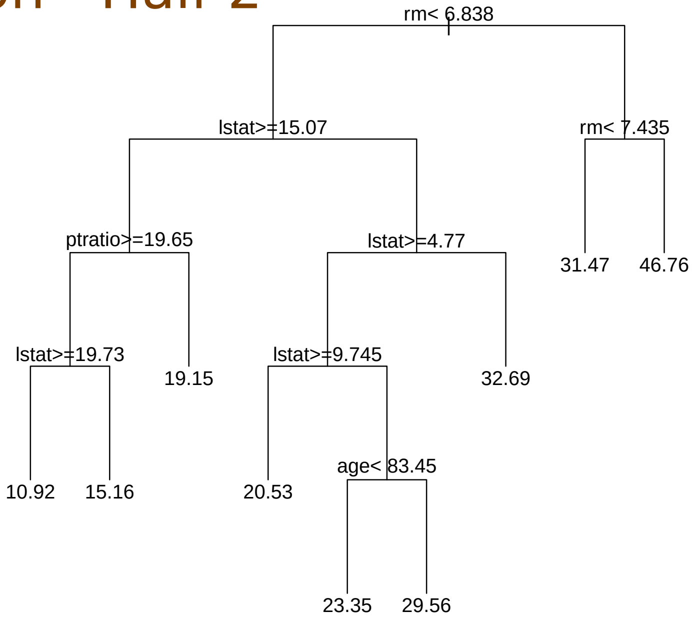
Bagging

- 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 halfs

```
     (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 $\hat{f}_1, \hat{f}_2, \ldots, \hat{f}_B$ 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 $(Y_1, \mathbf{X}_1)$, $(Y_2, \mathbf{X}_2)$, $\ldots$, $(Y_n, \mathbf{X}_n)$ 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 $(Y_1, \mathbf{X}_1)$, $(Y_2, \mathbf{X}_2)$, $\ldots$, $(Y_n, \mathbf{X}_n)$

Bagging

- We know that

$$F_n \xrightarrow[n \to \infty]{} F_0$$

  (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 $(Y_1, \mathbf{X}_1), (Y_2, \mathbf{X}_2), \ldots, (Y_n, \mathbf{X}_n)$