STAT406- Methods of Statistical Learning Lecture 11

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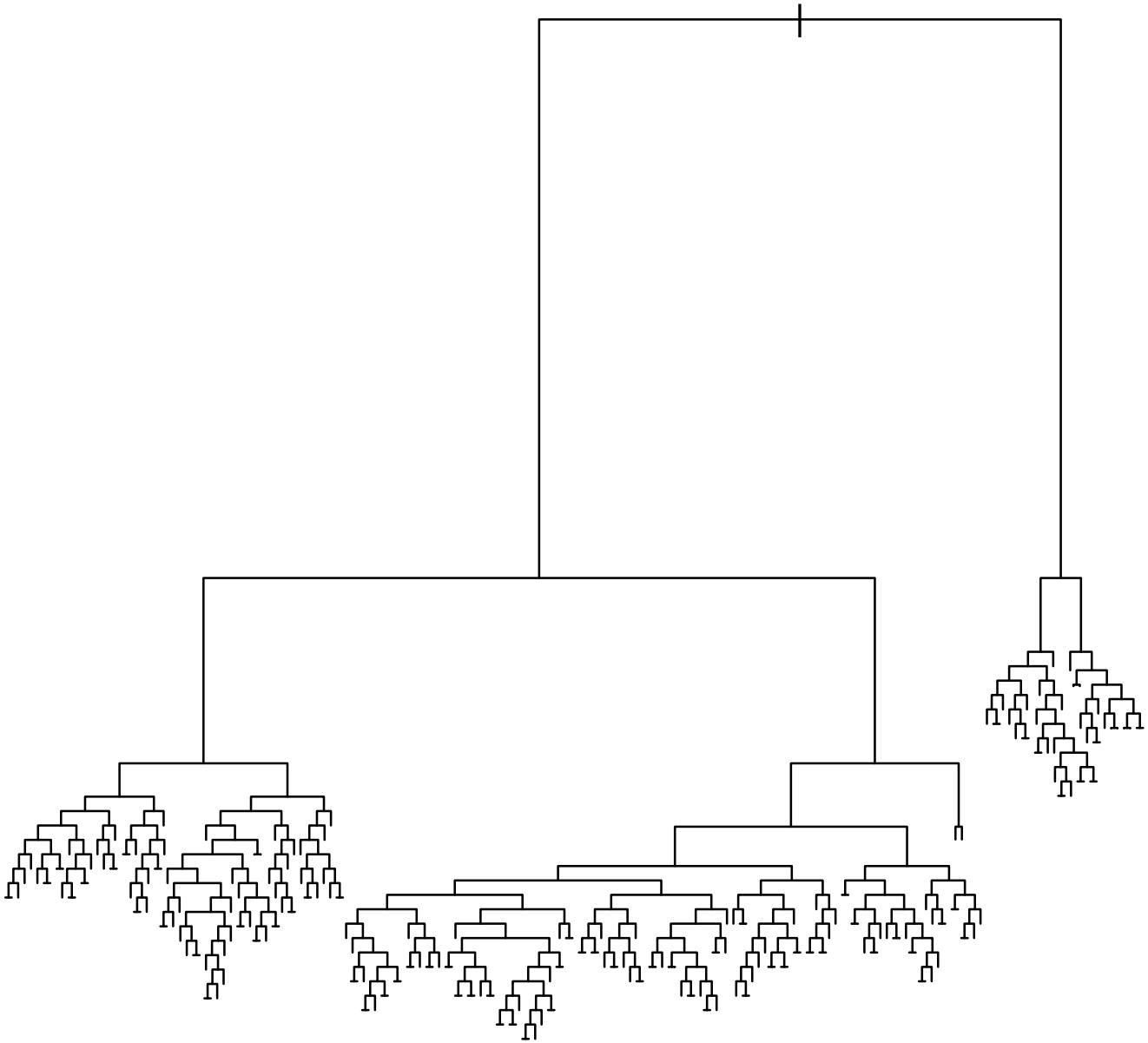
Overfitting...



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

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

- 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...

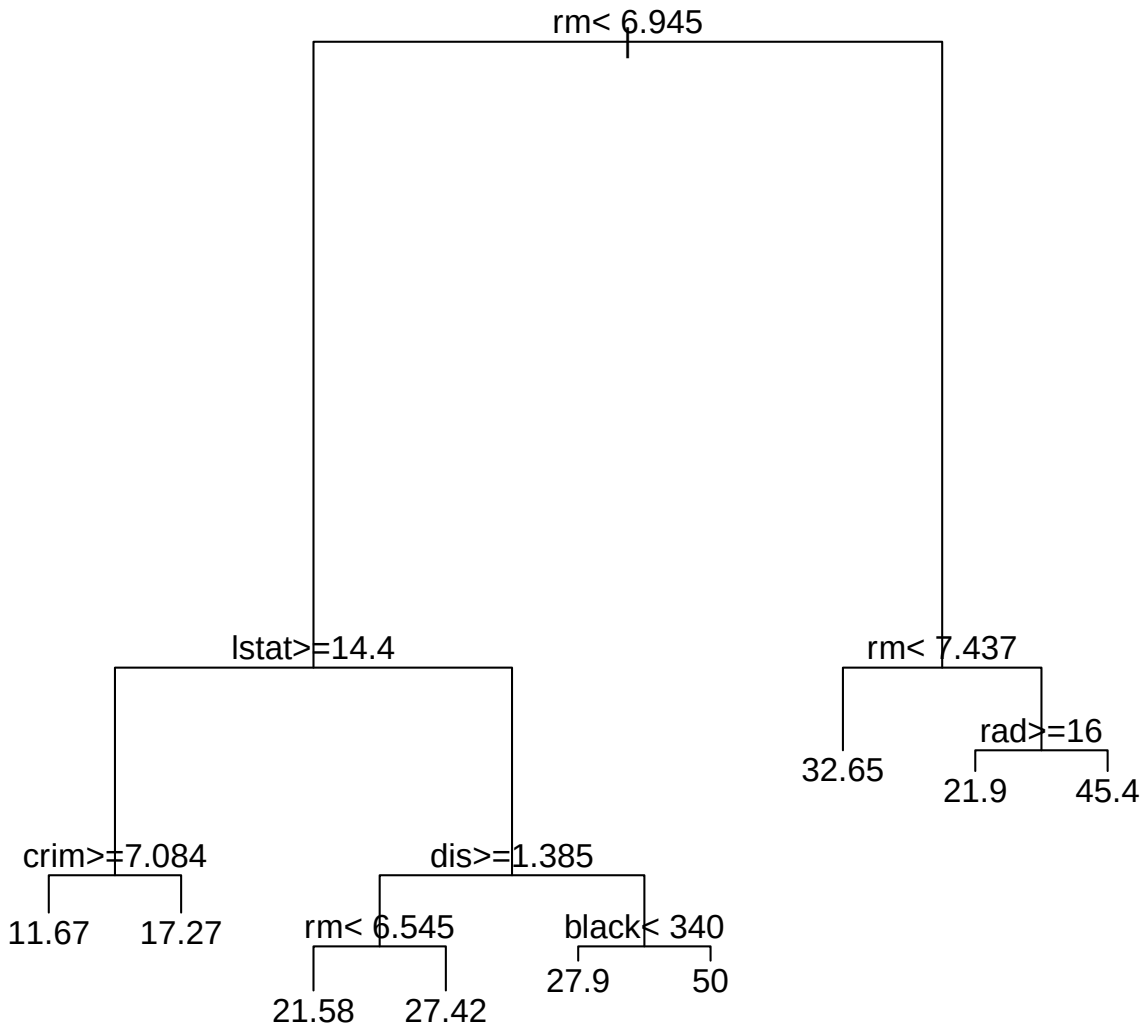
- Split the data into K folds
- For $j = 1, \ldots, K$
  - Build a tree without using the j-th fold
  - Prune it with penalties α_ℓ, $\ell = 1, \ldots, L$
  - Use these L trees to predict the j-th fold
  - Record the prediction errors.
- Sum or average over the folds.
- We obtain K-fold CV-estimated

Boston Example

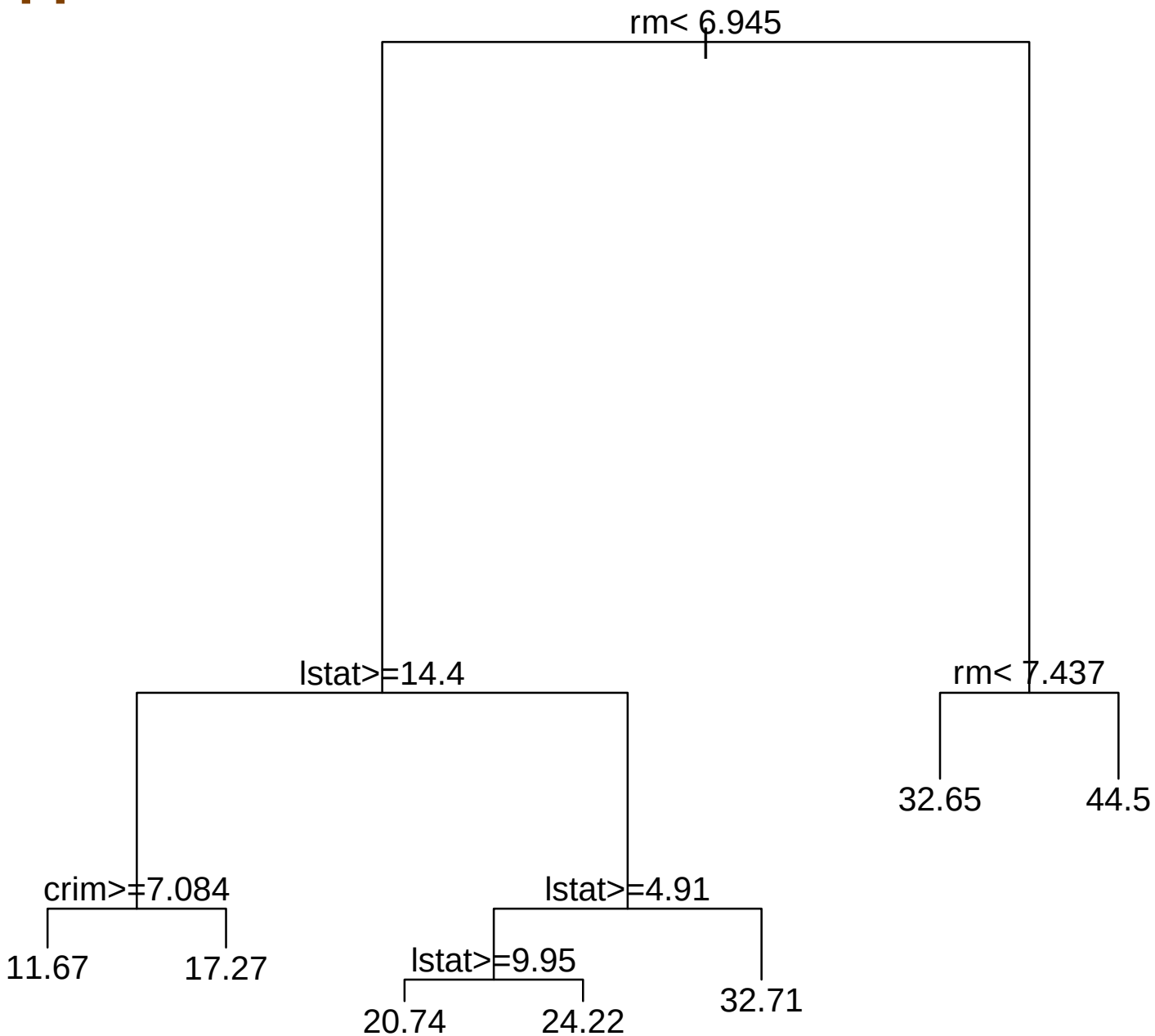
Pruning works...

```
> 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



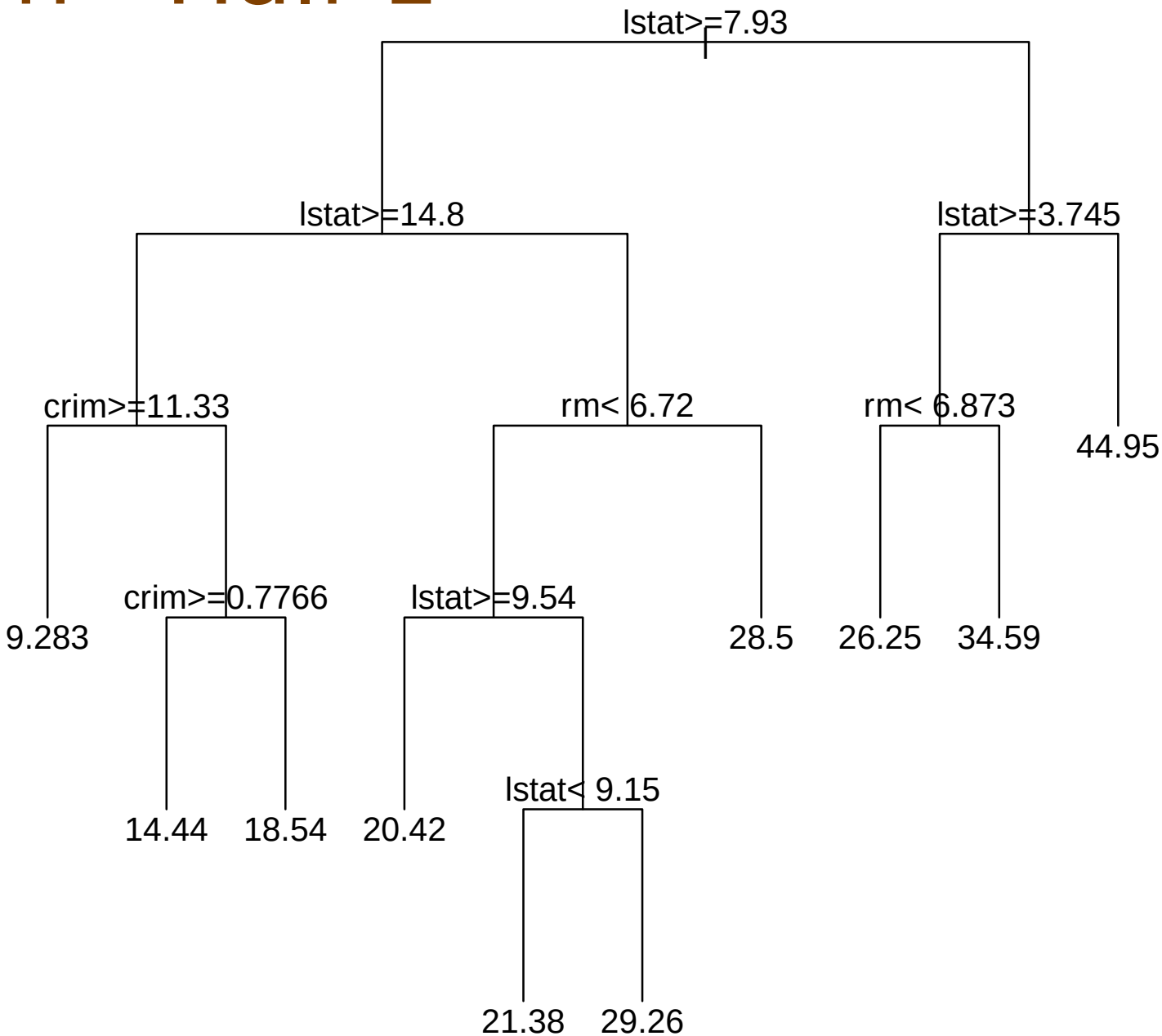
Boston



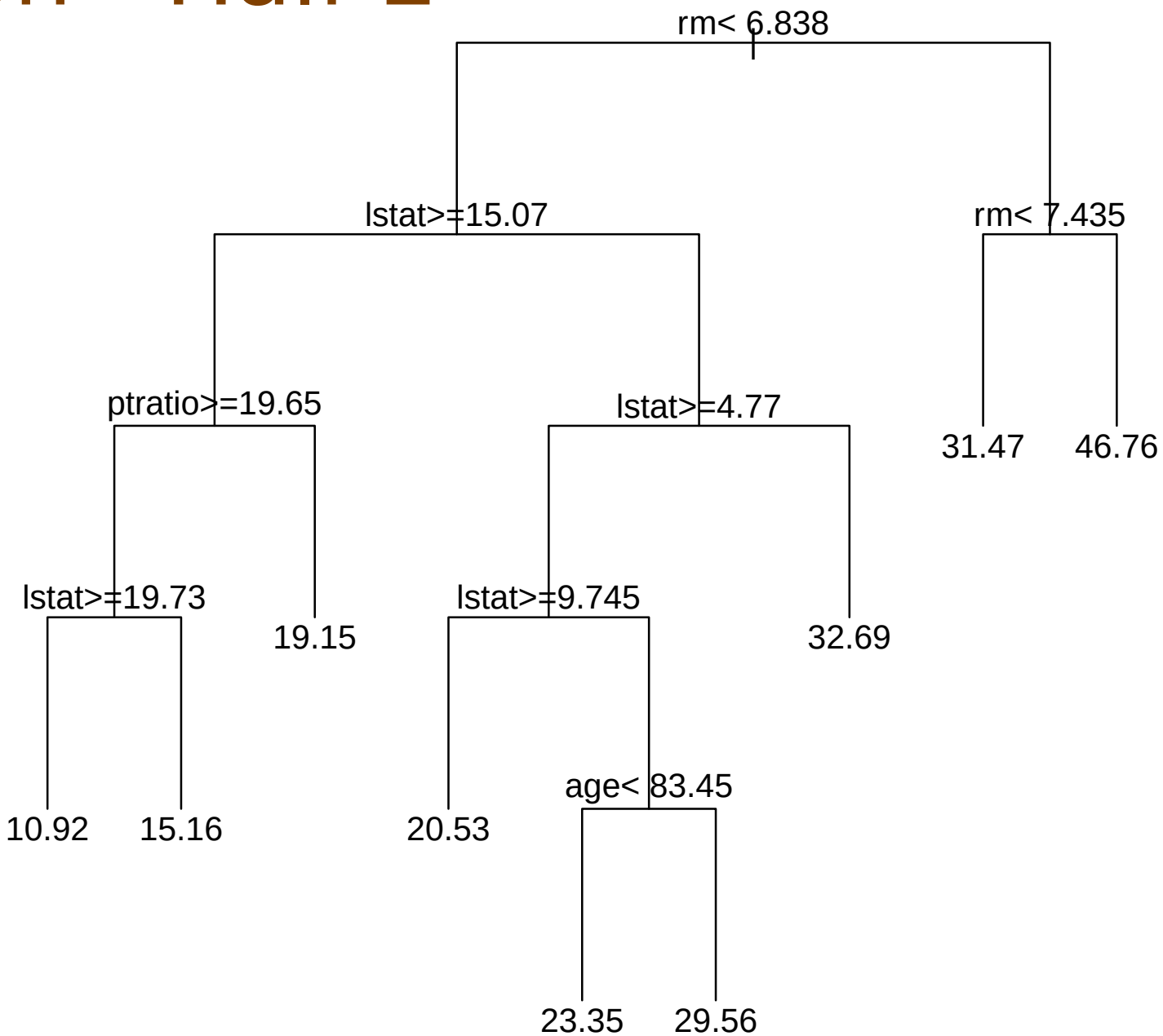
Bagging

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

Bagging

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