MONASH University

ETC3250/5250: Introduction to Machine Learning

Regression Trees

Lecturer: *Professor Di Cook*

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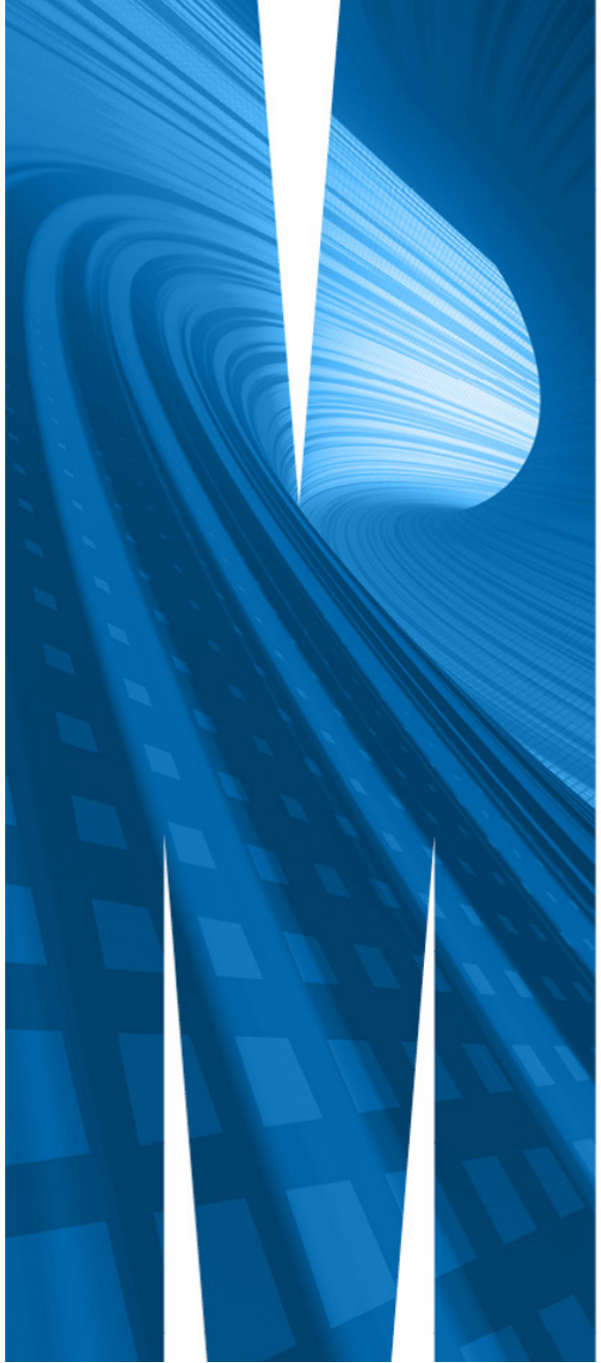
Week 6b



Difference with classification tree

The split criterion needs to use a quantitative response instead of categorical.

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

Split the data where combining MSE for left bucket (MSE_L) and right bucket (MSE_R), makes the biggest reduction from the overall MSE.

Note that, $\hat{y}_i = \bar{y}$ in regression trees.

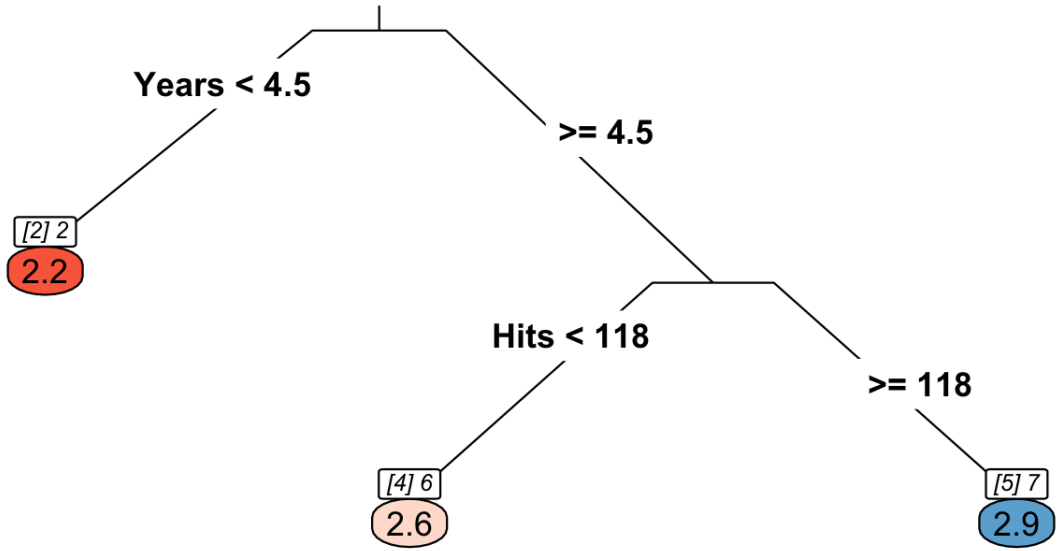
Predicting Salary

A regression tree to predict the `logSalary` of a baseball player, given their `Years` of playing and number of `Hits`.

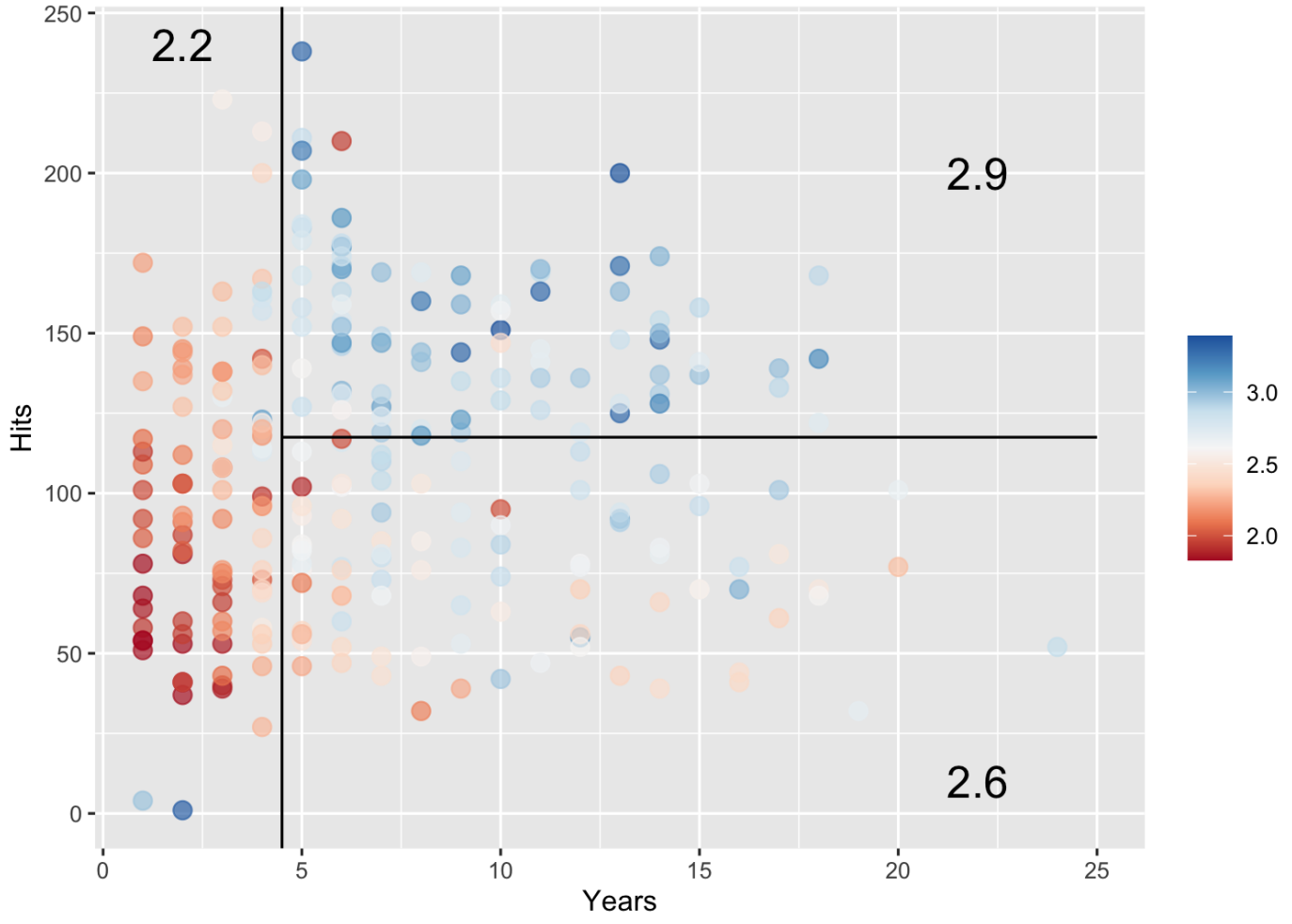
```
## parsnip model object
##
## n= 263
##
## node), split, n, deviance, yval
##       * denotes terminal node
##
## 1) root 263 39.071620 2.574160
##   2) Years< 4.5 90  7.988302 2.217851 *
##   3) Years>=4.5 173 13.713070 2.759523
##     6) Hits< 117.5 90  5.298802 2.605063 *
##     7) Hits>=117.5 83  3.938792 2.927009 *
```

Predicting Salary

Using the function `rpart`, we can build a regression tree to predict the `logSalary` of a baseball player, given their `Years` of playing and number of `Hits`.



Regions of the decision tree

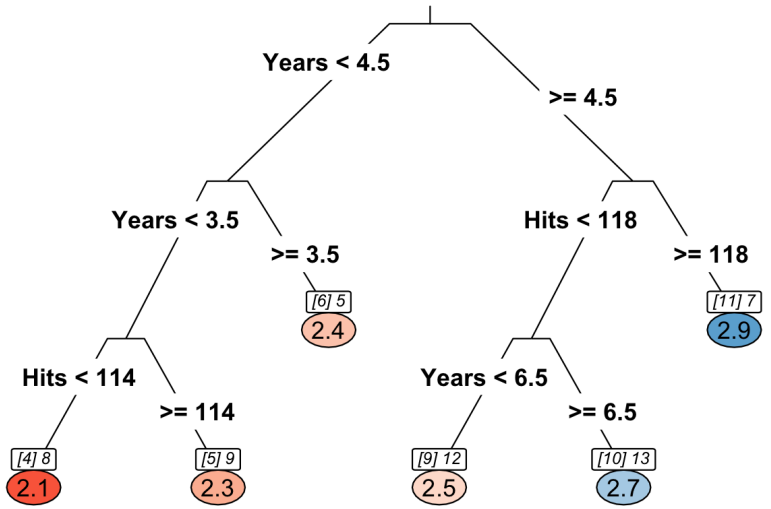


Deeper trees

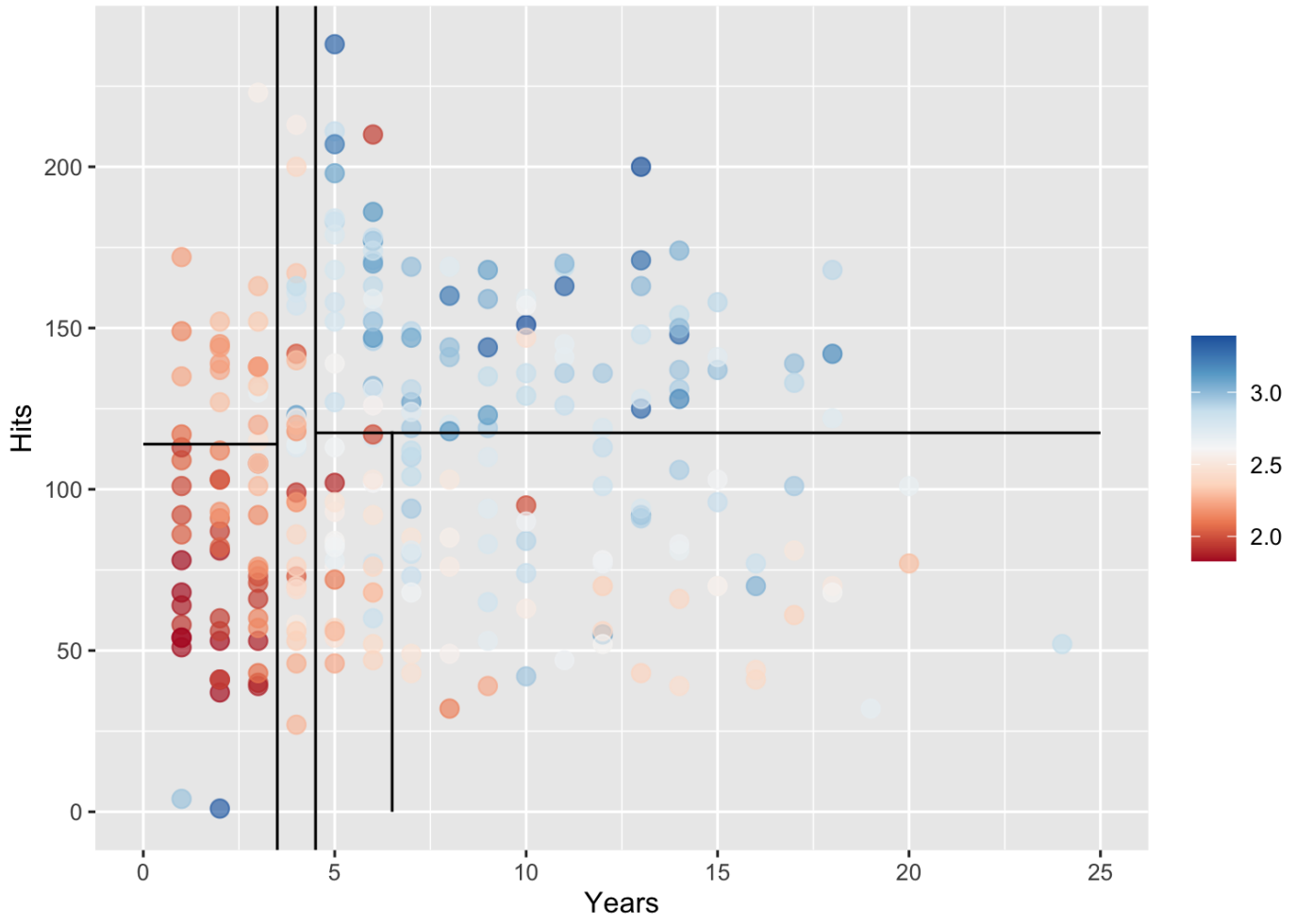
By decreasing the value of the complexity parameter cp, we can build deeper trees.

```
# Fit a regression tree
rpart_mod2 <-
  decision_tree(cost_complexity = 0.012) %>
  set_engine("rpart") %>%
  set_mode("regression") %>%
  translate()

hitters_fit2 <-
  rpart_mod2 %>%
  fit(lSalary ~ Hits+Years,
      data = Hitters)
```



Regions



Regression trees - construction

- We divide the predictor space - that is, the set of possible values for $X_1, X_2, \ldots, X_p$ into J distinct and non-overlapping regions, $R_1, R_2, \ldots, R_M$
- The regions could have any shape. However, for simplicity and for ease of interpretation, we divide the predictor space into high-dimensional rectangles.
- We model the response as a constant c_j in each region $f(x) = \sum_{j=1}^{J} c_j \, I(x \in R_m)$

e.g.

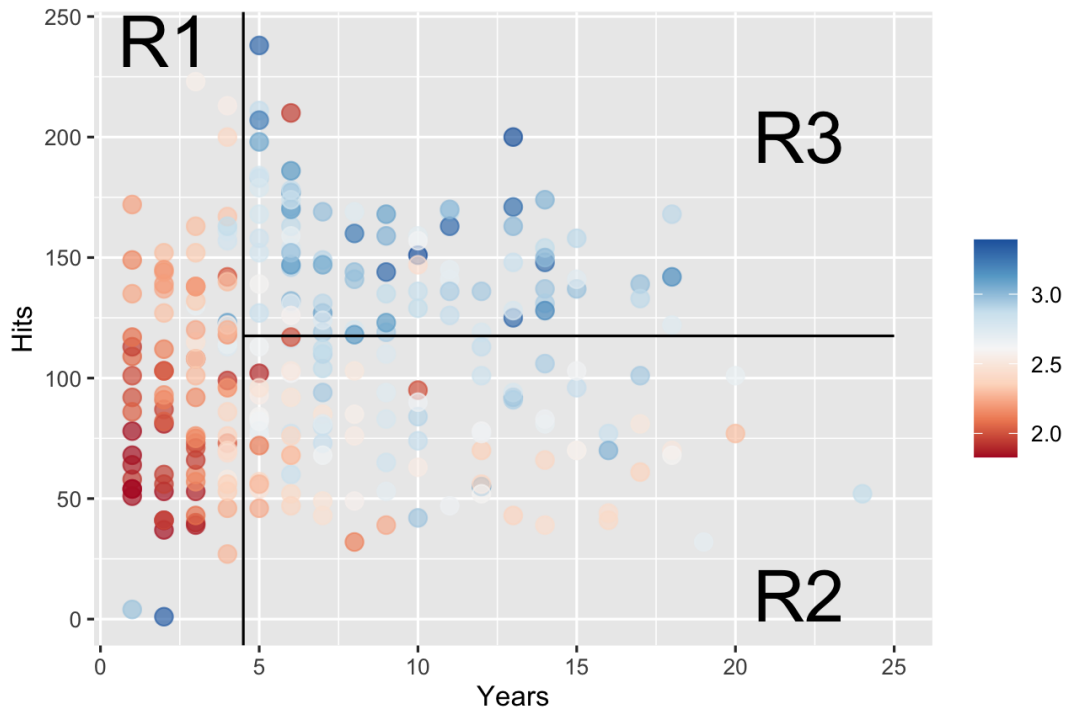
$$R_1 = \{X | \text{Years} < 4.5\}$$

$$R_2 = \{X | \text{Years} \geq 4.5, \text{Hits} < 117.5\}$$

$$R_3 = \{X | \text{Years} \geq 4.5, \text{Hits} \geq 117.5\}$$

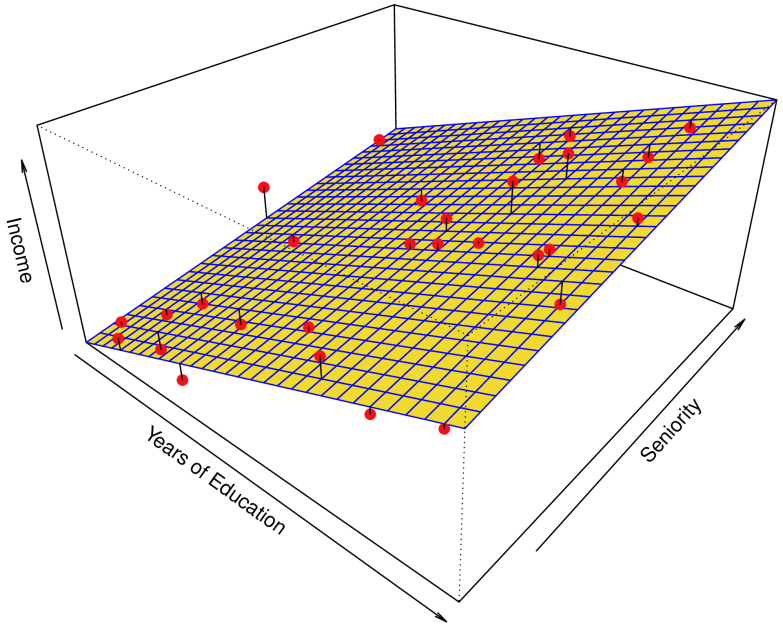
Leaves and Branches

- R_1, R_2 and R_3 are terminal nodes or leaves.
- The points where we split are internal nodes.
- The segments that connect the nodes are branches.



Linear regression

$$f(X) = \beta_0 + \sum_{j=1}^{p} X_j \beta_j$$



(Chapter 2/2.4)

Regression trees

$$f(X) = \sum_{m=1}^{M} c_m \, I(X \in R_m)$$

Strategy for finding good splits

- Top-down: it begins at the top of the tree (all observations belong to a single region) and then successively splits the predictor space; each split is indicated via two new branches further down on the tree.
- Greedy: at each step of the tree-building process, the best split is made at that particular step, rather than looking ahead and picking a split that will lead to a better tree in some future step.

Algorithm

1. Start with a single region R_1 (entire input space), and iterate:

   a. Select a region R_m, predictor X_j, and a splitting point s, such that splitting R_m with the criterion $X_j < s$ produces the largest decrease in RSS

   b. Redefine the regions with this additional split.

2. Continues until stopping criterion reached.

Stopping criterion

- Number of observations in R_m too small to further splitting (`minsplit`). (There is usually another control criteria, even if N_m large enough, you can't split it small number of observations off, e.g. 1 and $N_m - 1$ `minbucket`.)
- RSS : If $N_m < a$ reduction of error is too small to bother splitting further. (`cp` parameter in `rpart` measures this as a proportional drop - see earlier examples displaying the change in this parameter.)

Model fit

Residual Sum of Squared Error

$$\text{RSS}(T) = \sum_{m=1}^{|T|} \sum_{x_i \in R_m} (y_i - \hat{y}_m)^2$$

where $|T|$ the number of terminal nodes in T, and remember $\hat{y}_m = \bar{y}$. And MSE is obtained by dividing by n and RMSE takes the square root.

Size of tree

- It is possible to produce good predictions on the **training set**, but is likely to overfit the data (trees are very flexible).
- A smaller tree with fewer splits (that is, fewer regions) might lead to lower variance and better interpretation at the cost of a little bias.
- Tree size is a tuning parameter governing the **model's complexity**, and the optimal tree size should be adaptively chosen from the data
- Produce splits only if RSS decrease exceeds some **(high) threshold** can mean that a low gain split early on, might stop the fitting, even though there may be a very good split later.

Pruning

Grow a big tree, T_0, and then **prune** it back. The *pruning* procedure is:

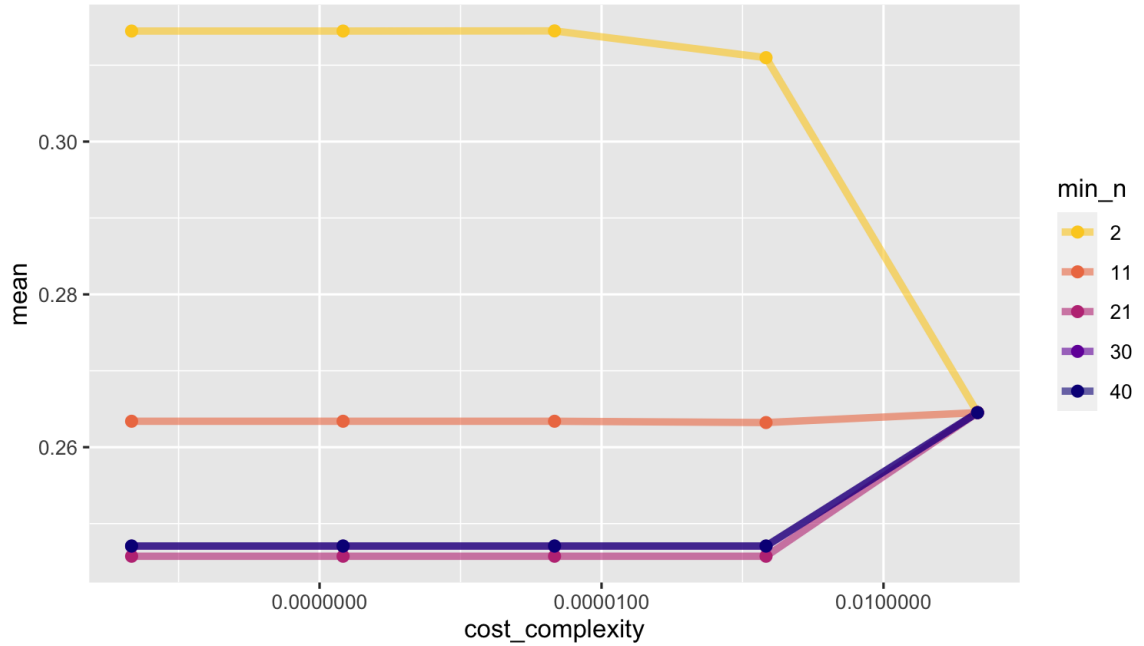
- Starting with with the initial full tree T_0, replace a subtree with a leaf node to obtain a new tree T_1. Select subtree to prune by minimizing

$$\frac{\text{RSS}(T_1) - \text{RSS}(T_0)}{|T_1| - |T_0|}$$

- Iteratively prune to obtain a sequence $T_0, T_1, T_2, \ldots, T_R$ where T_R is the tree with a single leaf node.
- Select the optimal tree T_m by cross validation

Model selection

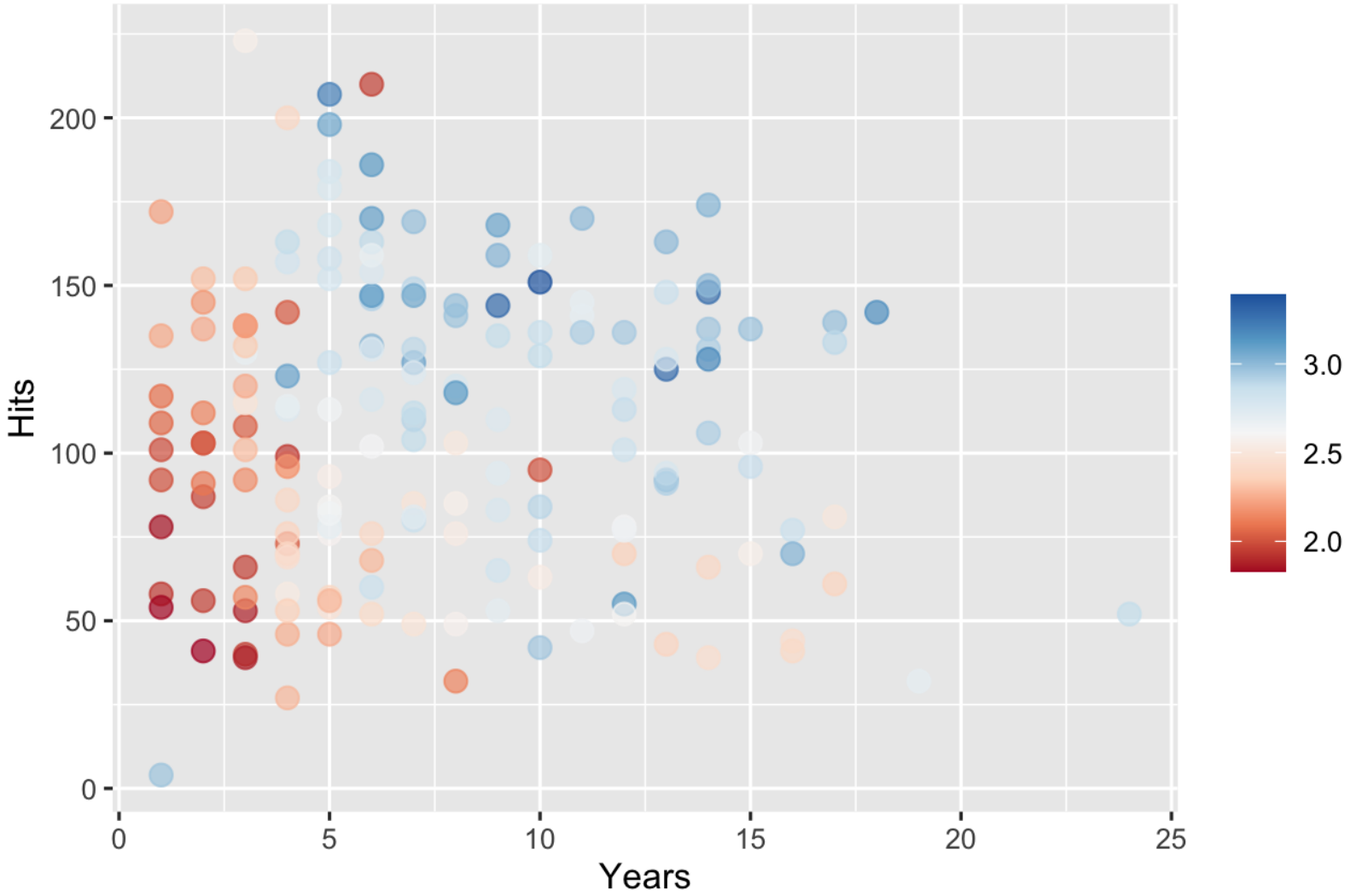
Using the `tune` package in tidymodels.




```
## # A tibble: 1 × 3
##   cost_complexity min_n .config
##             <dbl> <int> <chr>
## 1    0.0000000001    30 Preprocessor1_Model16
```

Yielding this model:

Reminder of what the training data looks like



Summary

Regression trees can provide a very flexible model.

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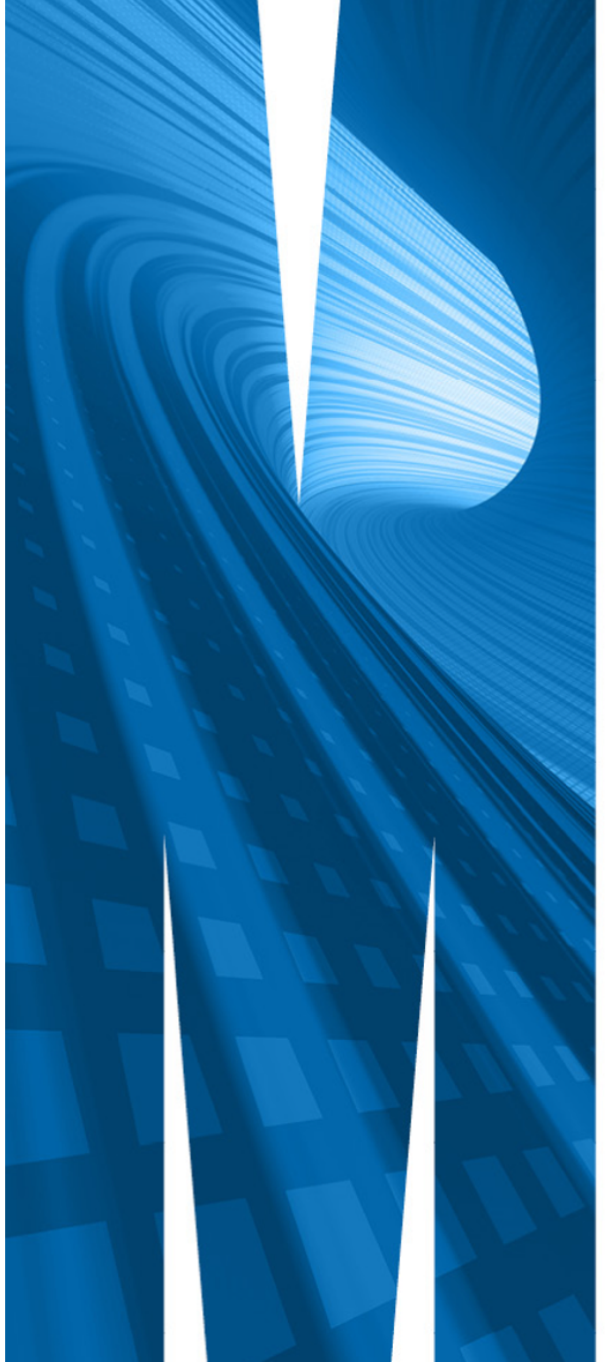

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Week 6b