771A43 – Machine Learning for Social Science

Lecture 2

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2024-09-30

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- Beyond the standard linear paradigm
  - *Splines*, *GAMs*—enables $\hat{f}$ to pick up more patterns in data ($\downarrow$bias).
  - *Ridge*, *Lasso*—penalizes $\hat{f}$ that picks up too much of the patterns in data ($\downarrow$variance)
  - *Cross-validation*—helps find a good level of complexity/flexibility; helps us balancing bias- and variance trade-off.

This week

- Non-parametric supervised learning
- KNN
- Decision trees
- Ensembles
  - Bagging & Random Forest
  - Boosting
- Principles of prediction

Non-parametric SL

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Non-parametric models

- Does not make explicit assumptions about the parametric form of $\hat{f}$.
- Instead let's "data speak".

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Non-parametric methods is what we'll consider today!

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KNN

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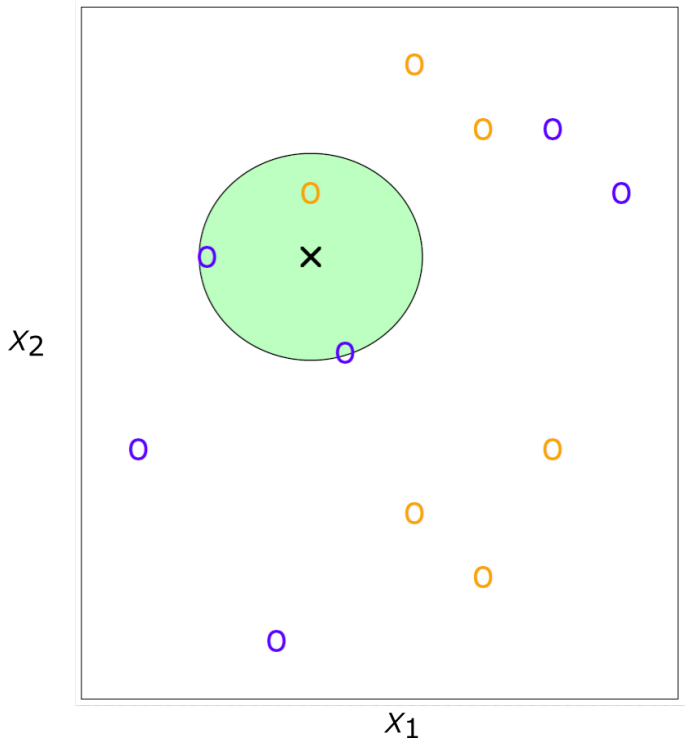
Let's consider a simple example to get some intuition!

Toy example

Data: suppose we have 12 observations, each described by:

- Two continuous input variables: X_1 and X_2.
- An outcome $Y \in \{\text{blue}, \text{orange}\}$.



KNN prediction

- Step 1: Identify the K (here: 3) closest *training observations*
- Step 2: Perform "majority-vote": 2/3 blue $\rightarrow \hat{y}_x =$ blue

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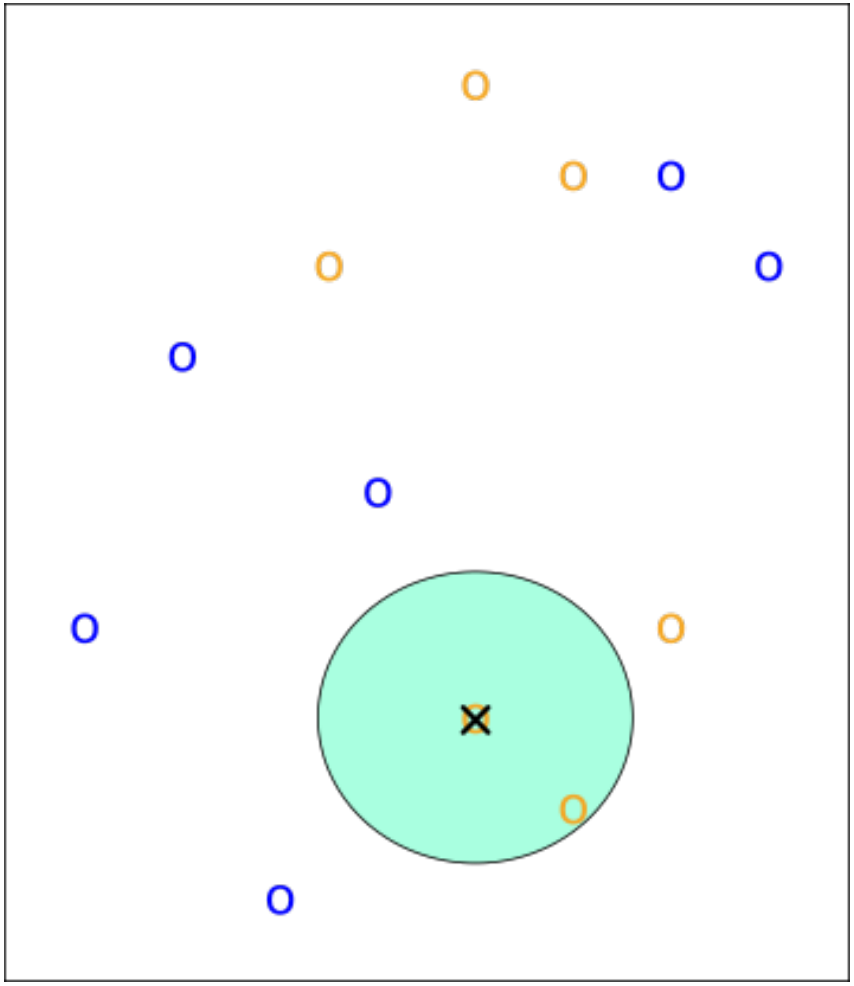
For demonstration, let's consider the toy example again!

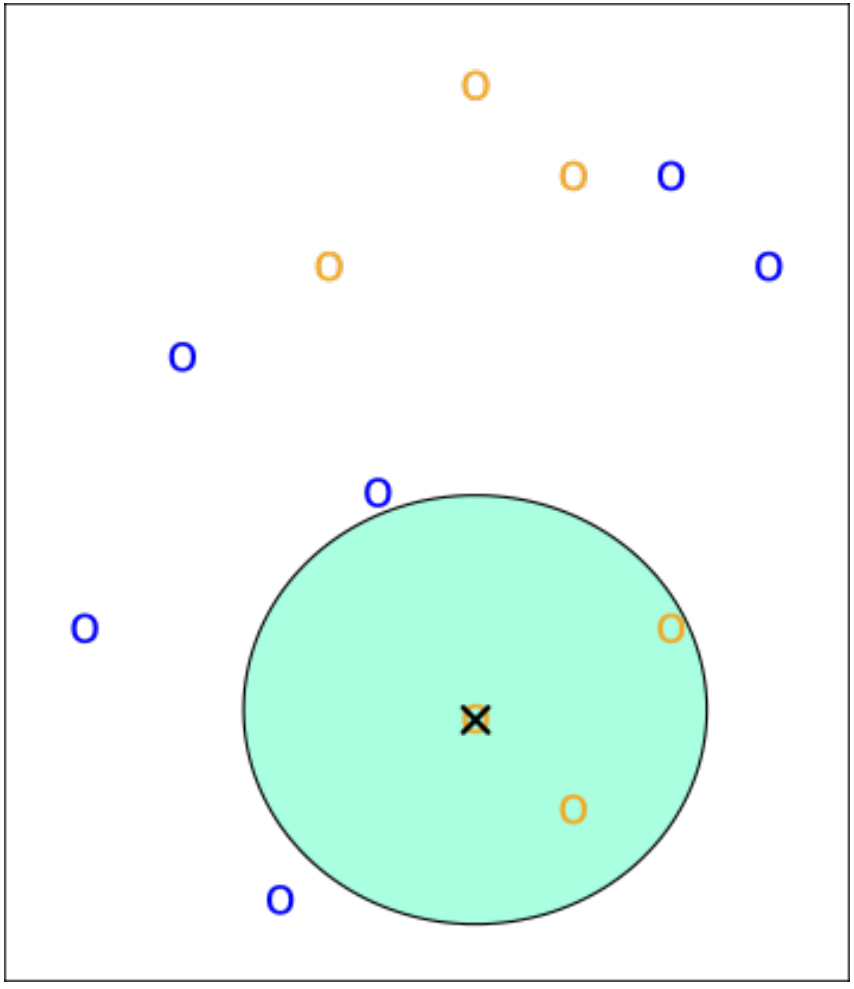
$K = 1$

Prediction: $1/1$ orange $\rightarrow \hat{y}_x =$ orange (correct)



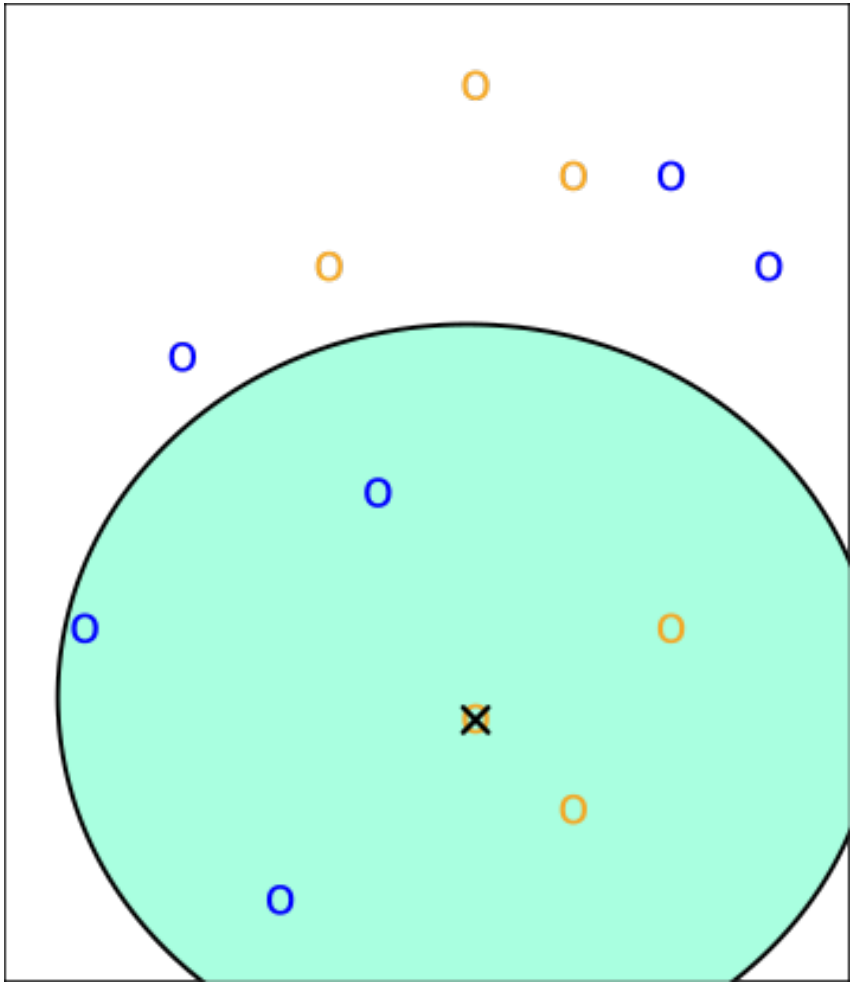
$K = 2$

Prediction: 2/2 orange $\rightarrow \hat{y}_x =$ orange (correct)



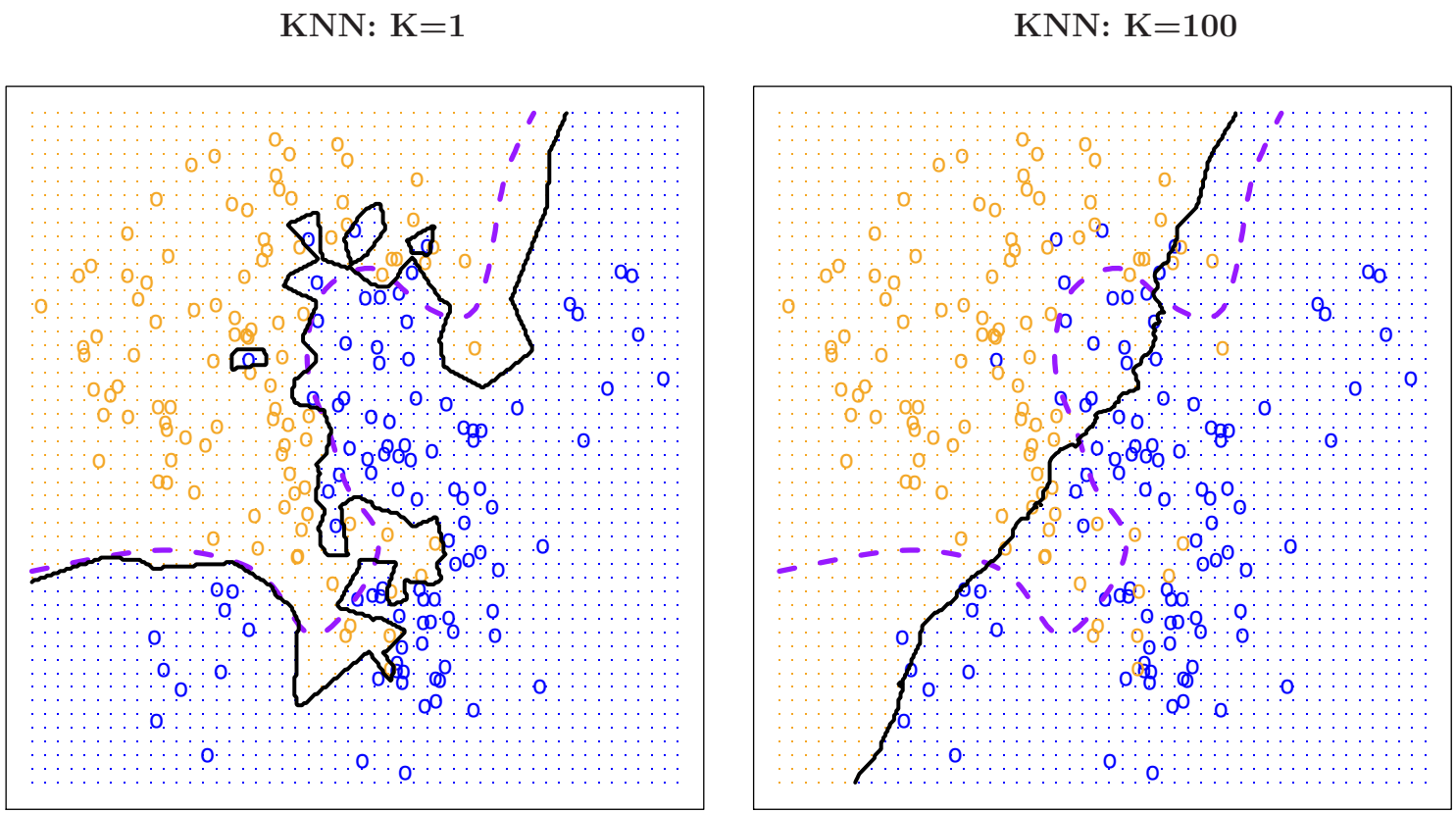
$K = 5$

Prediction: 3/5 blue $\rightarrow \hat{y}_x =$ blue (incorrect)



Applying this to all obs $\rightarrow$ *prediction boundary*

If we apply KNN-prediction to *all observations*, one by one—for different K (1 vs. 100)—we get the following *prediction boundary* (solid black line):



- Line for $K = 100$ is **not flexible enough**:
- Line for $K = 1$ is **overly flexible**.

Turns out: another case of *bias-variance trade-off*

- Too *small* $K \rightarrow$ low bias, high variance (overfitting)
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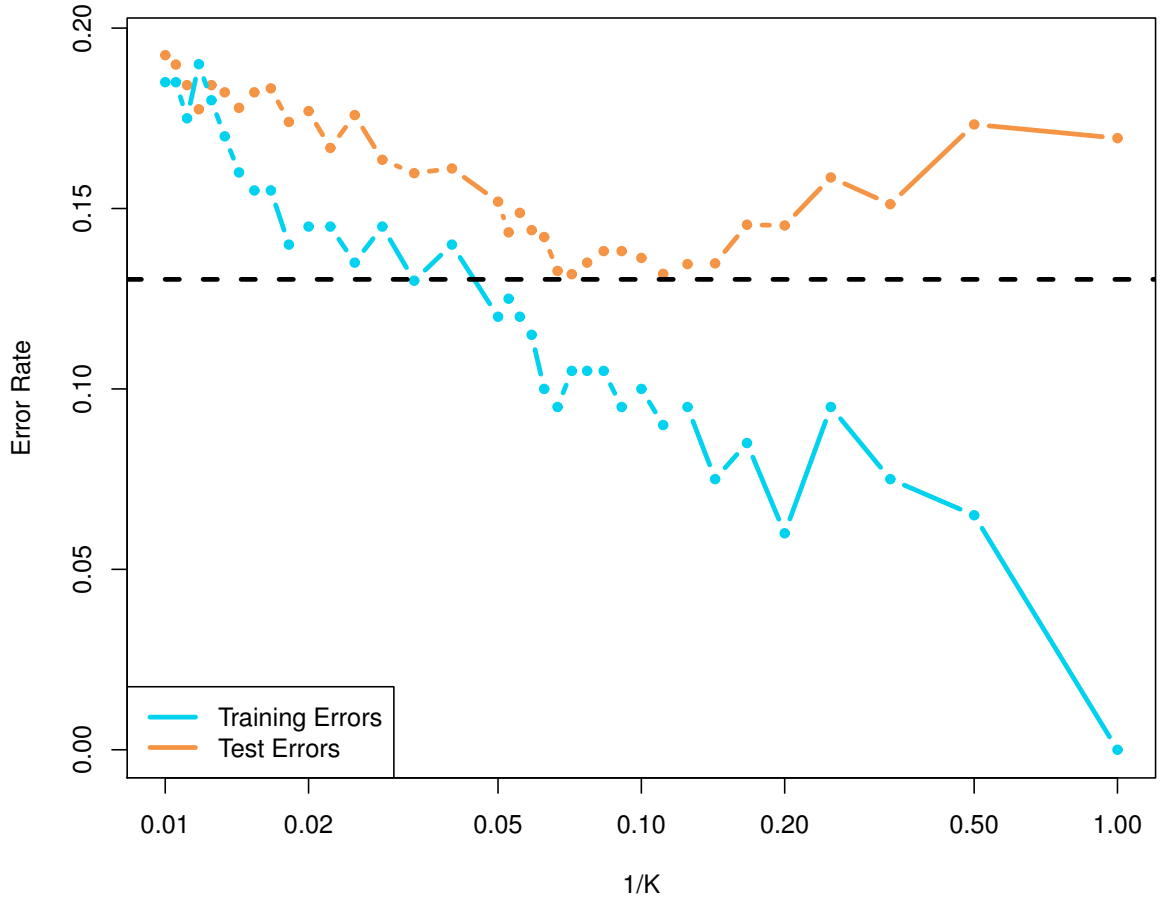

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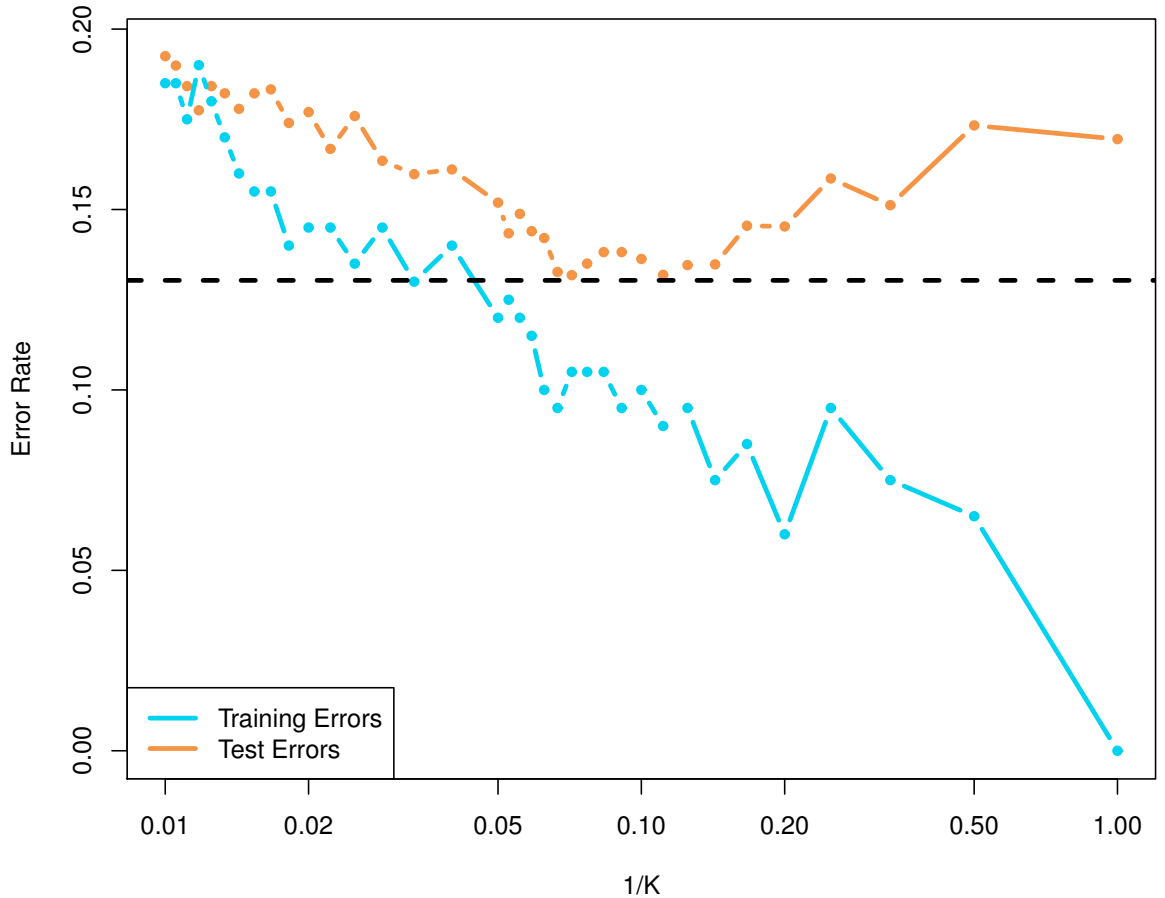

How to choose K? Surprise, surprise: **cross-validation**!

Pros and cons of KNN

Pros

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- One single parameter (K) that regulates smoothness—relatively easy to calibrate via cross-validation.
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Cons

- Lack of *interpretability*: no parameters to say why a given observation was classified the way it was.[4]
- Does not *weight* X_i's based on how predictive they are $\rightarrow$ even more sensitive to inclusion of noisy/less important features.
- Researcher cannot incorporate *domain knowledge*

[4] As is the case more generally for non-parametric methods; weak for *inference*.

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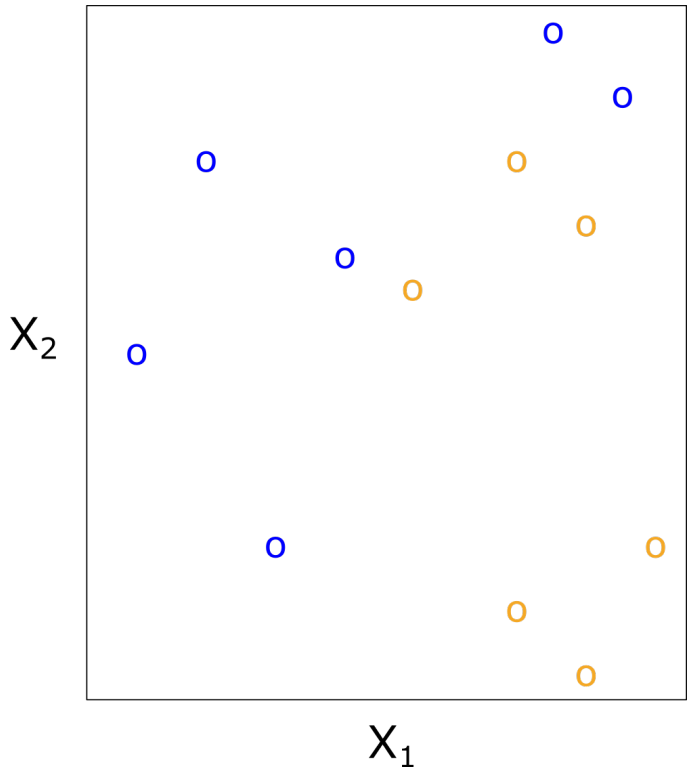
$$\underbrace{\sum_{j}^{J} \sum_{i \in R_j} (y_i - \bar{y}_{R_j})^2}_{\text{Summed error across regions}}$$

Toy example

Let's reconsider the toy example we used for KNN.



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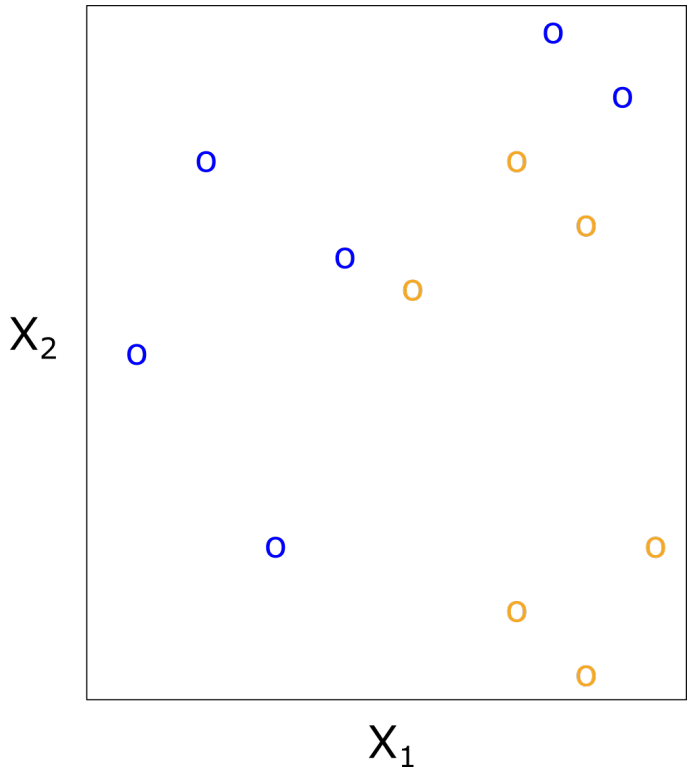

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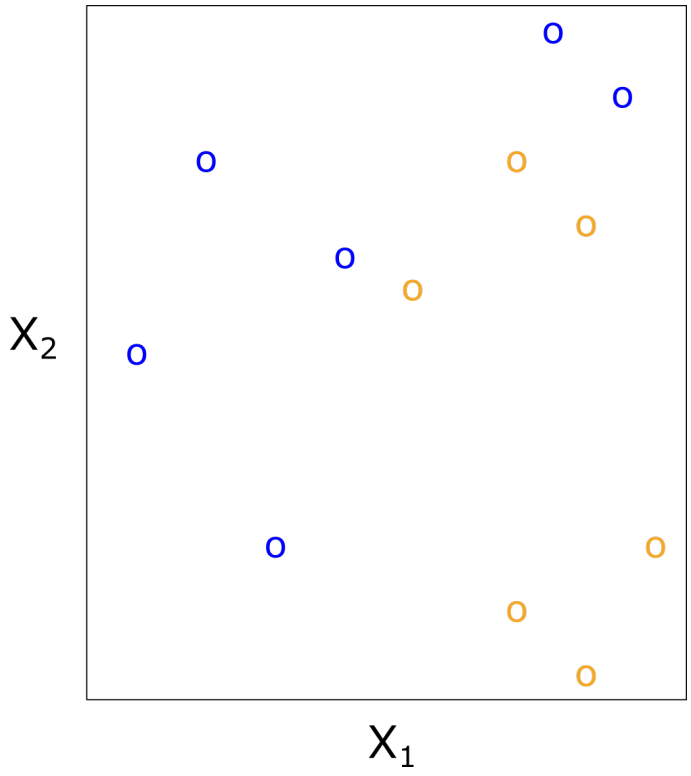

How can we partition this X_1,X_2 space so that:

- We get *homogeneous regions*—i.e., "blue" and "yellow" regions?

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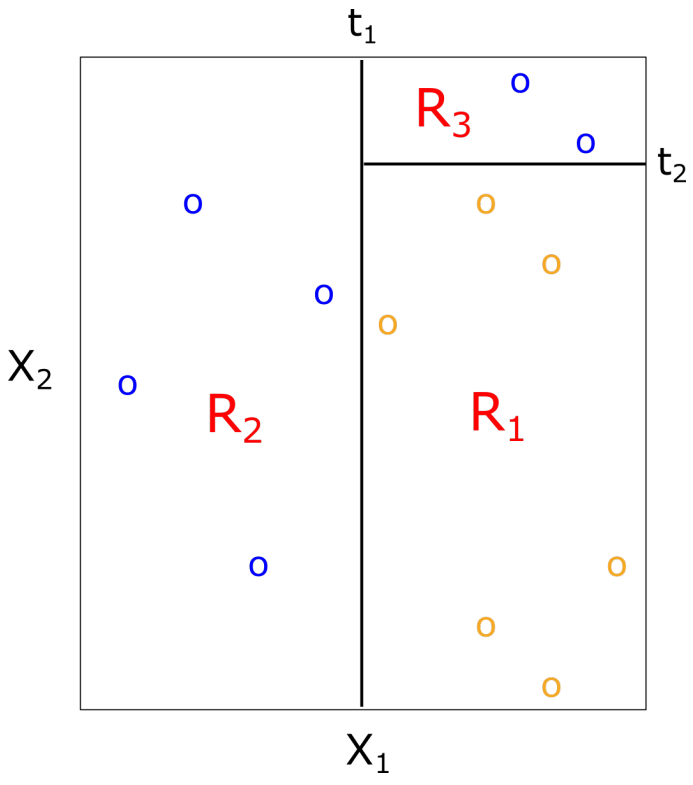

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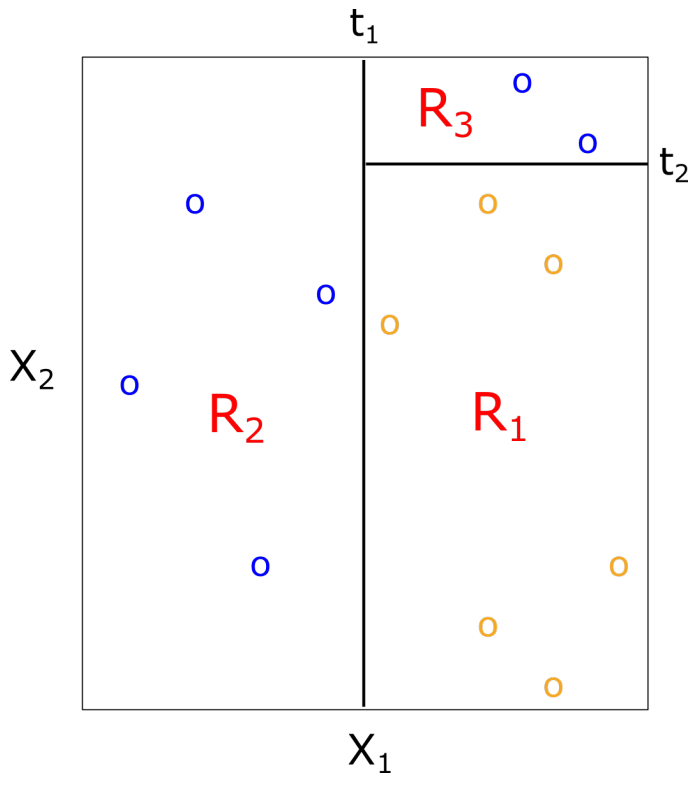

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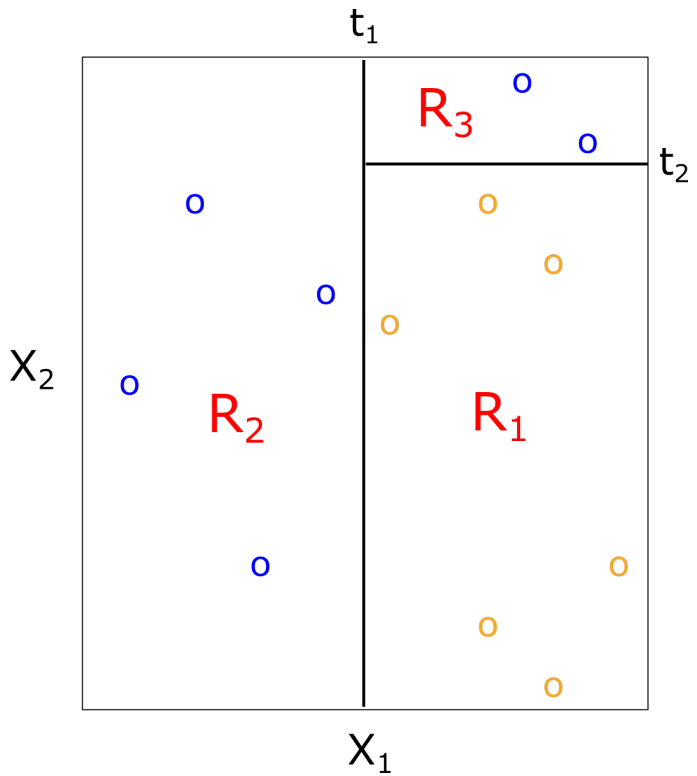

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Let's return to our toy example!

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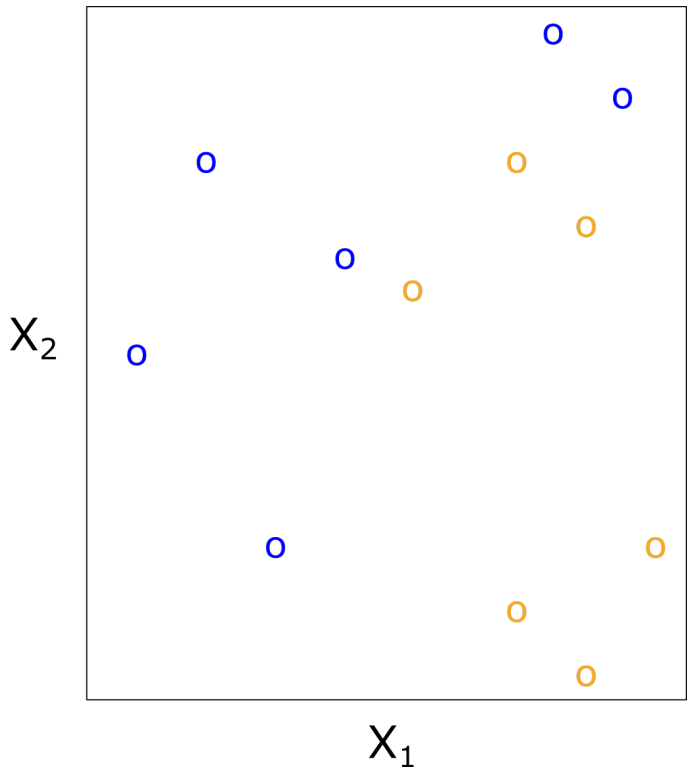

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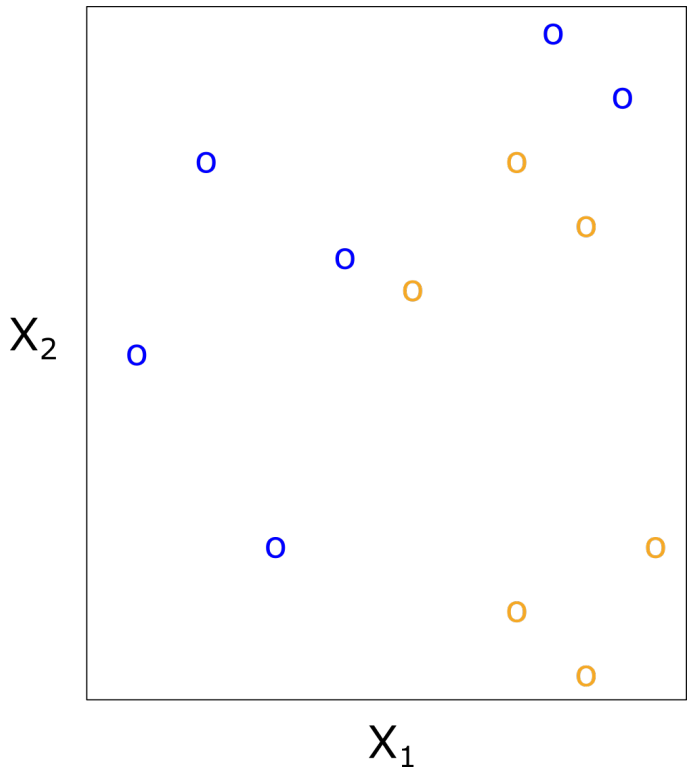
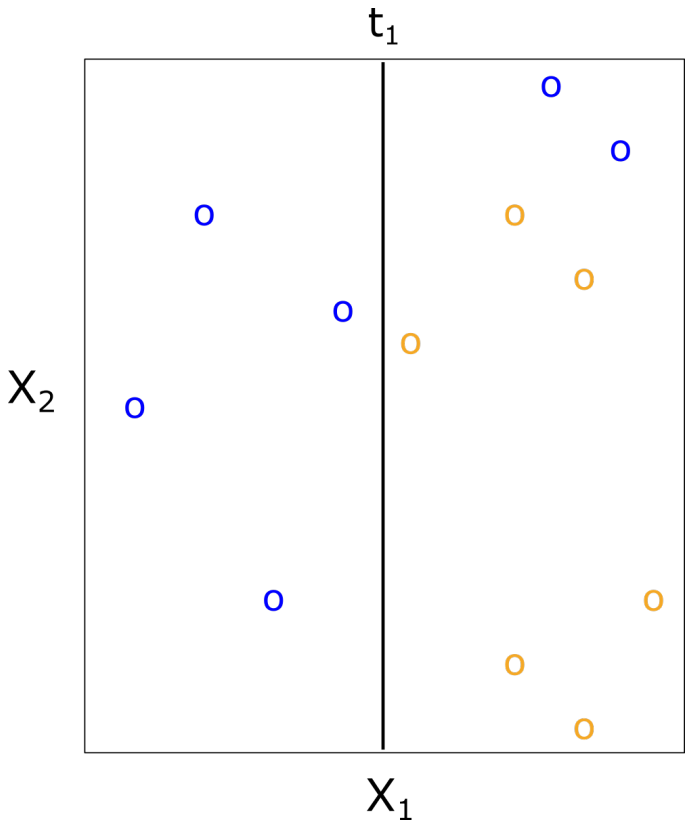


Then we ask—how can we insert a **vertical** (splitting on X_1) or **horizontal** (splitting on X_2) line such that the resulting two regions becomes *maximally more homogeneous*?

Split no. 1

In this example, it turns out that creating a split at *value* t_1 on *variable* X_1 is the split which results in the *biggest error reduction*.



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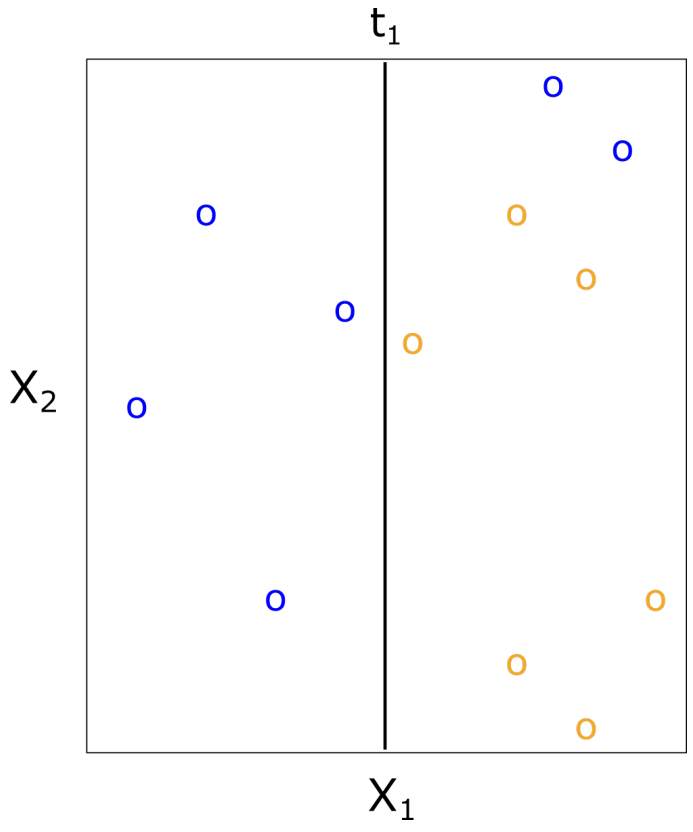

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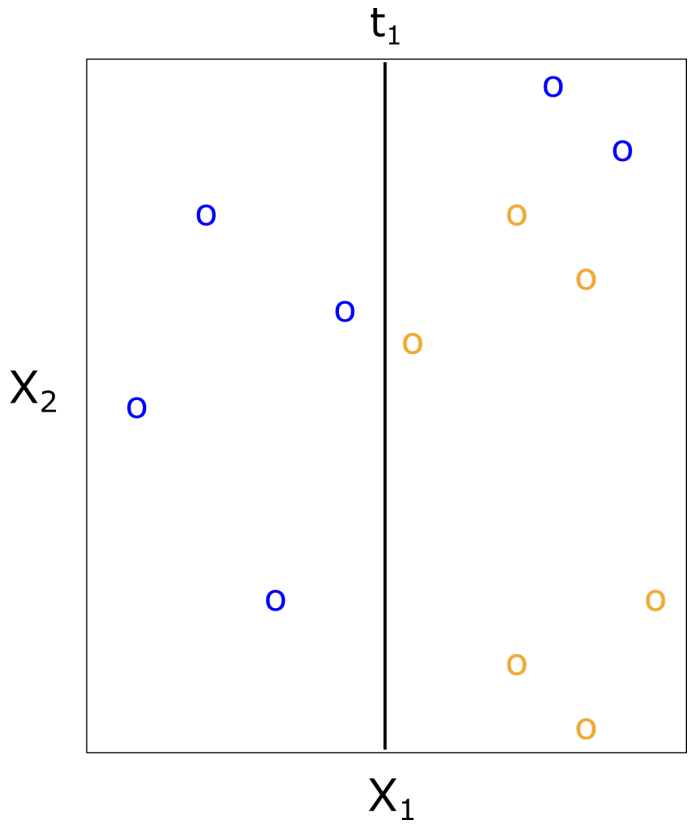

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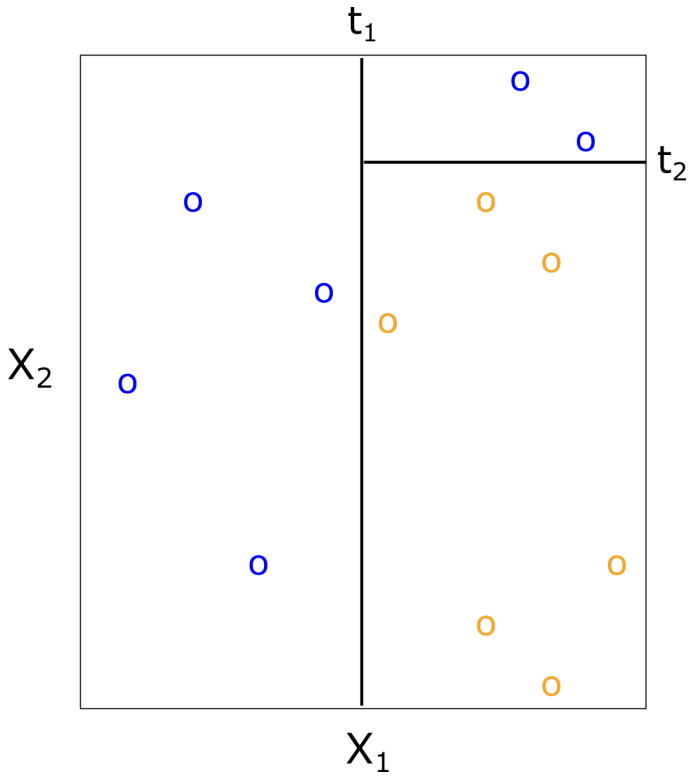
Q: Can we add additional splits that further reduces the error?

Split no. 2

Yes! Splitting the "right-region" at value t_2 on variable X_2 reduces error further.



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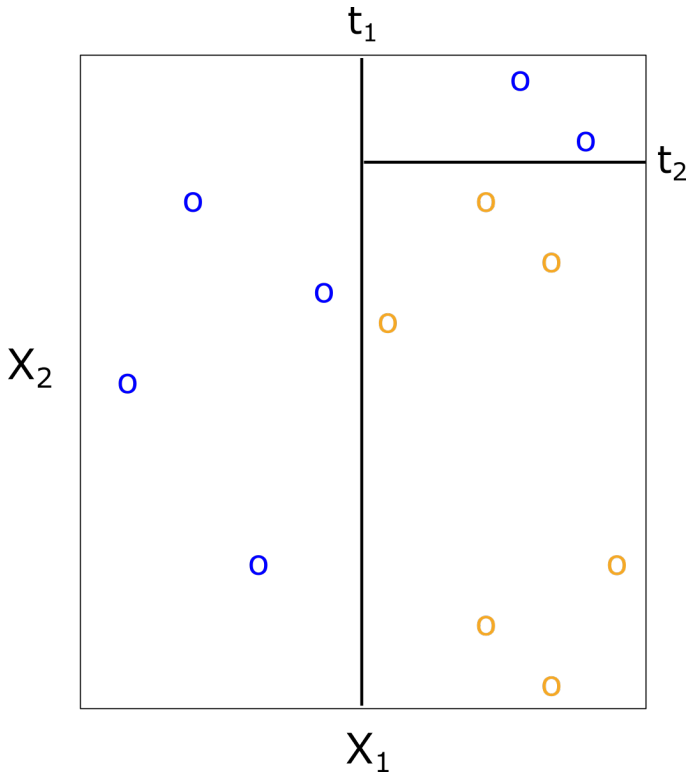
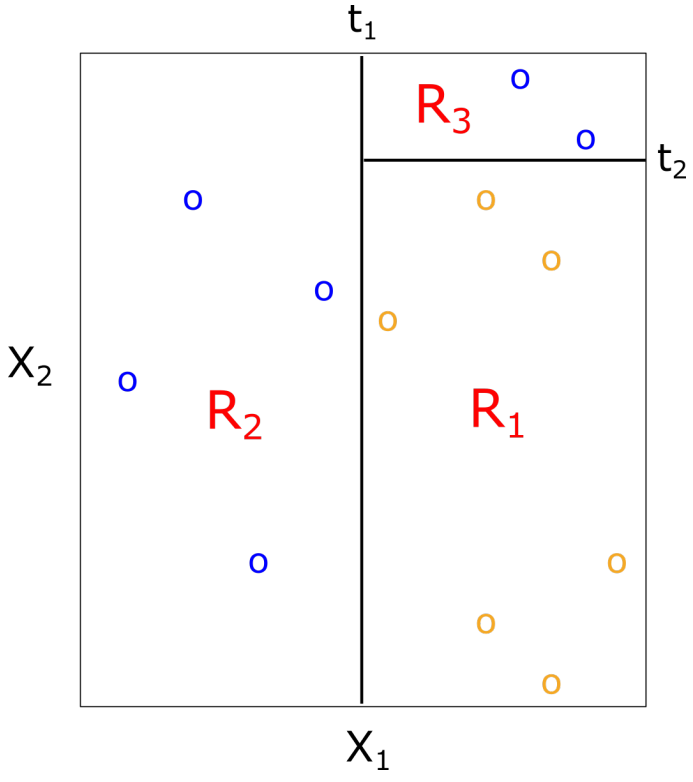


After this, no further improvements are possible, and we retain three regions.

Three-region solution



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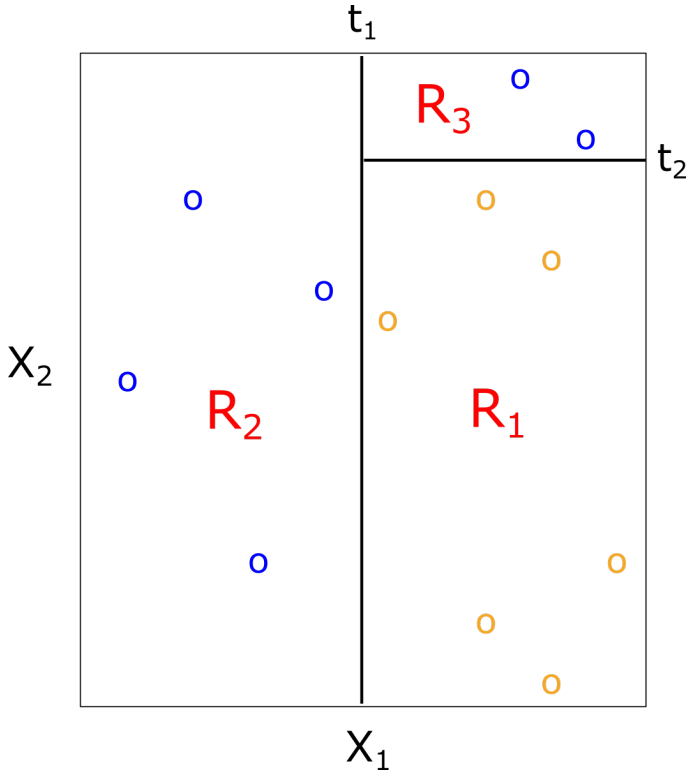

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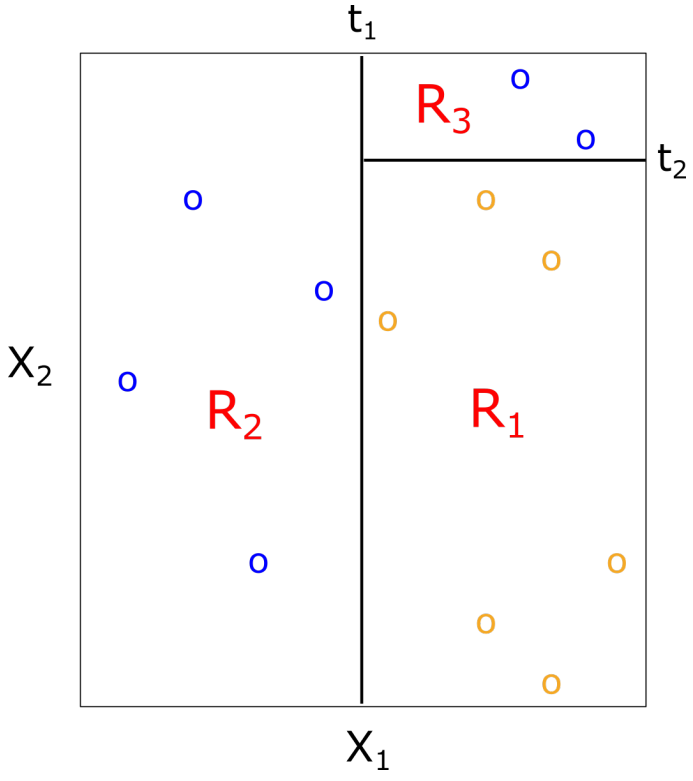
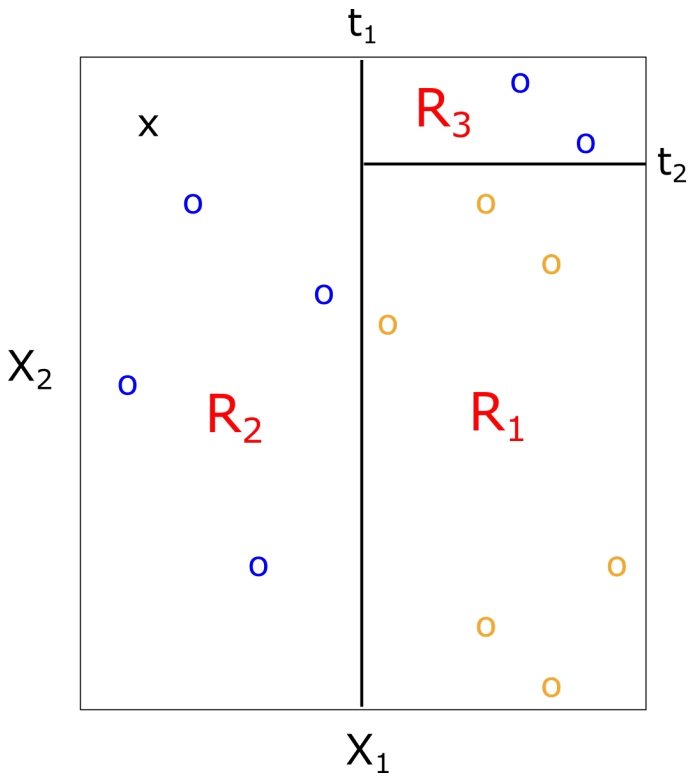


With these regions identified—how do we use them to make **predictions**? Again:

- *Categorical* Y: *majority vote* with each region.
- *Continuous* Y: *mean* within each region.

Example prediction

What would we predict for this *test* observation "x"?



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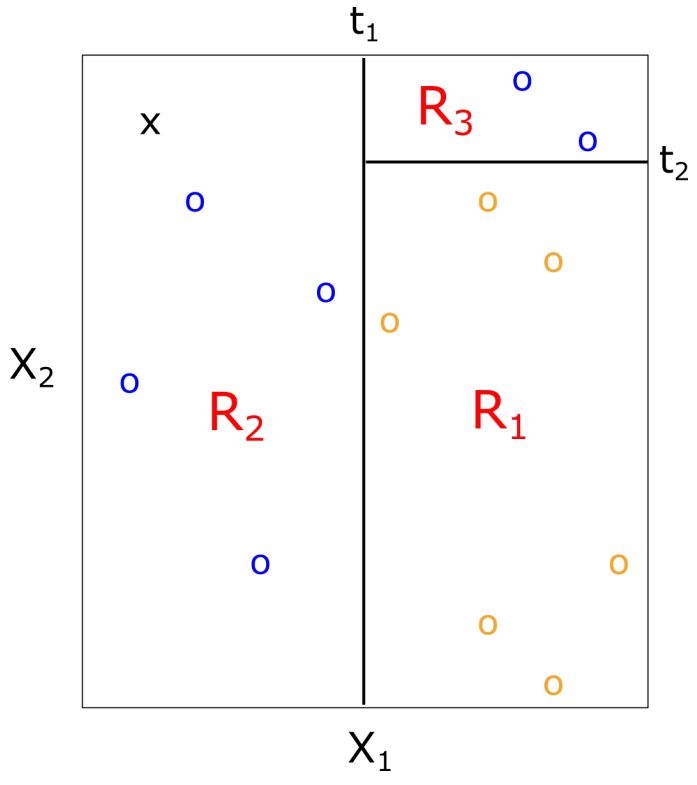

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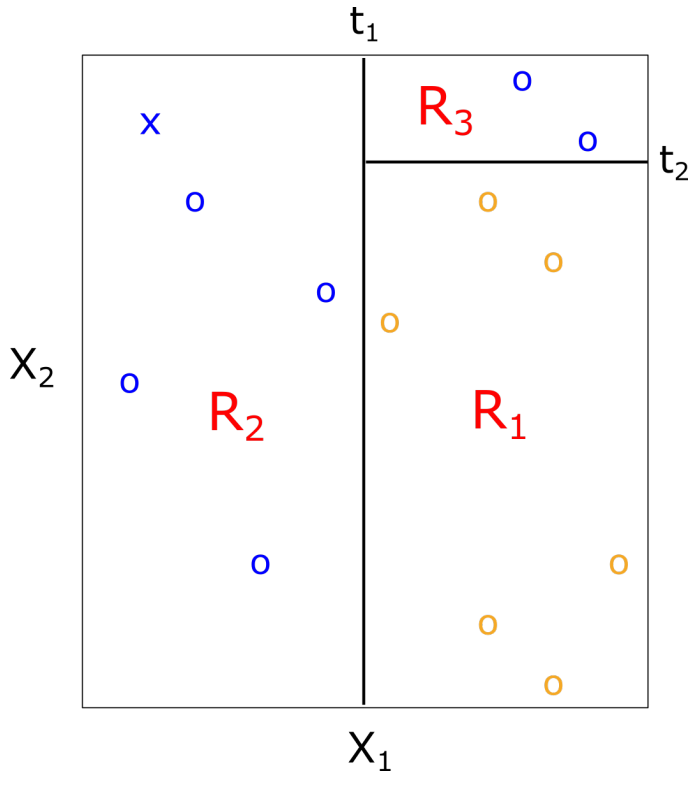

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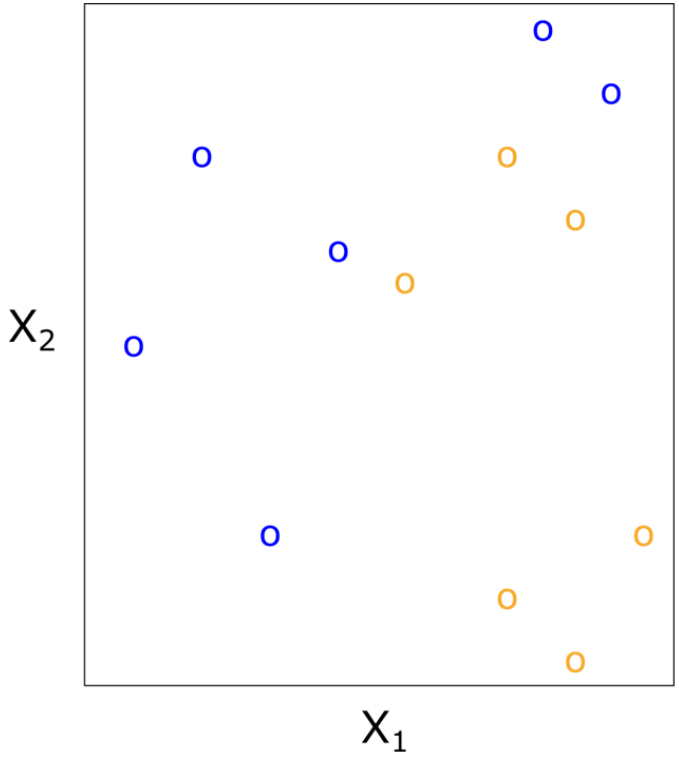

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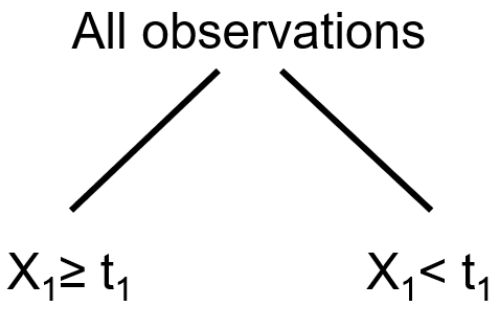

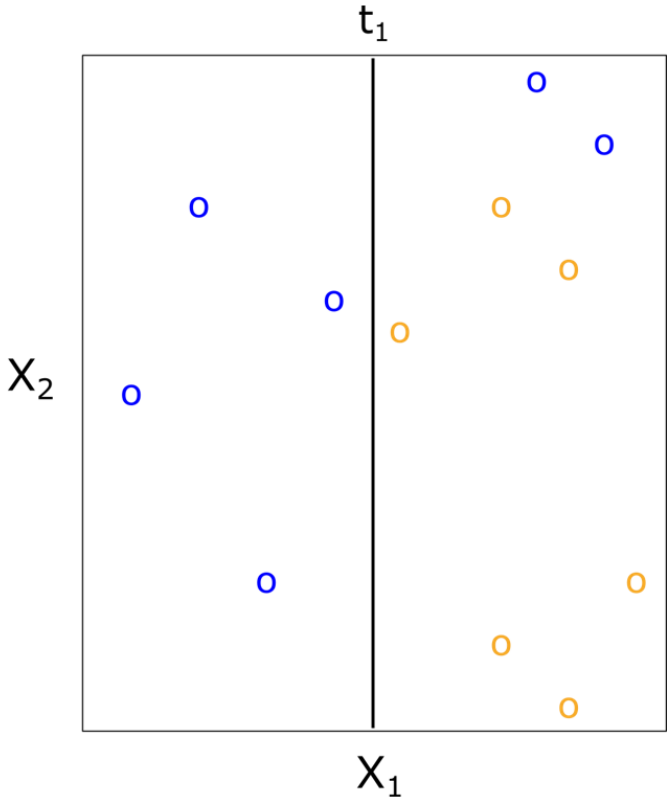

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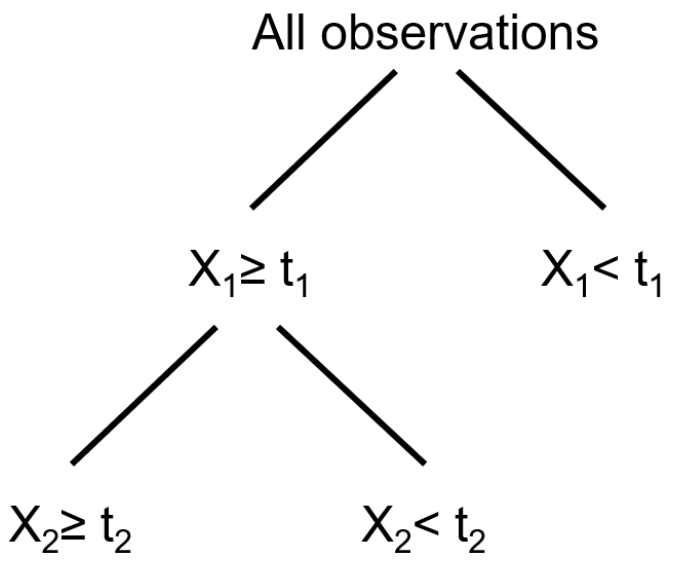

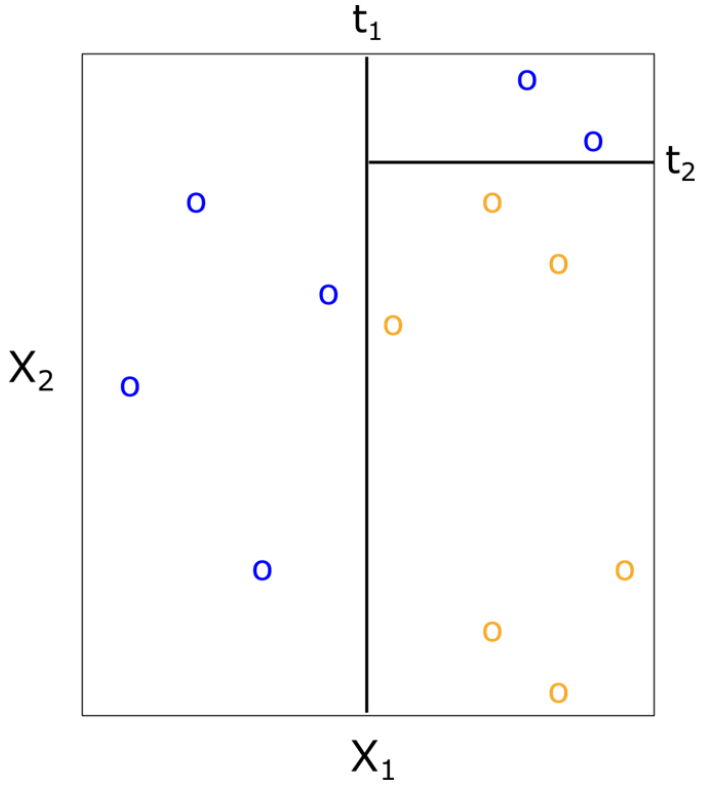

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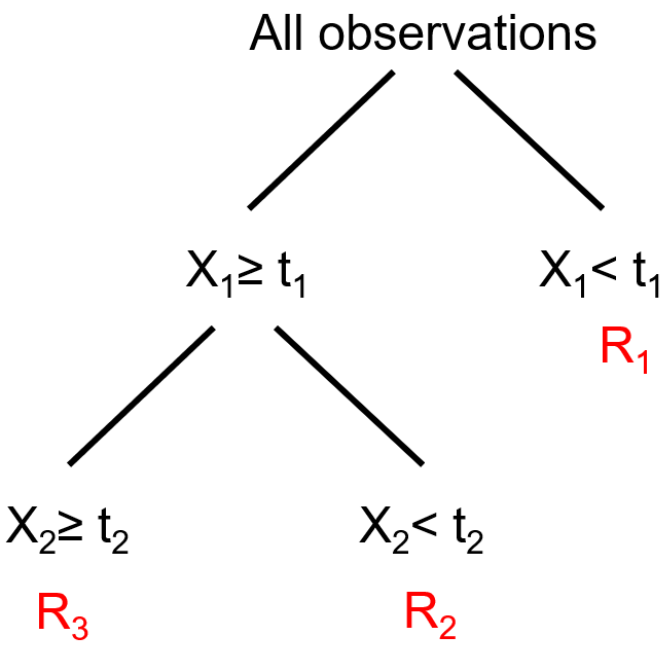

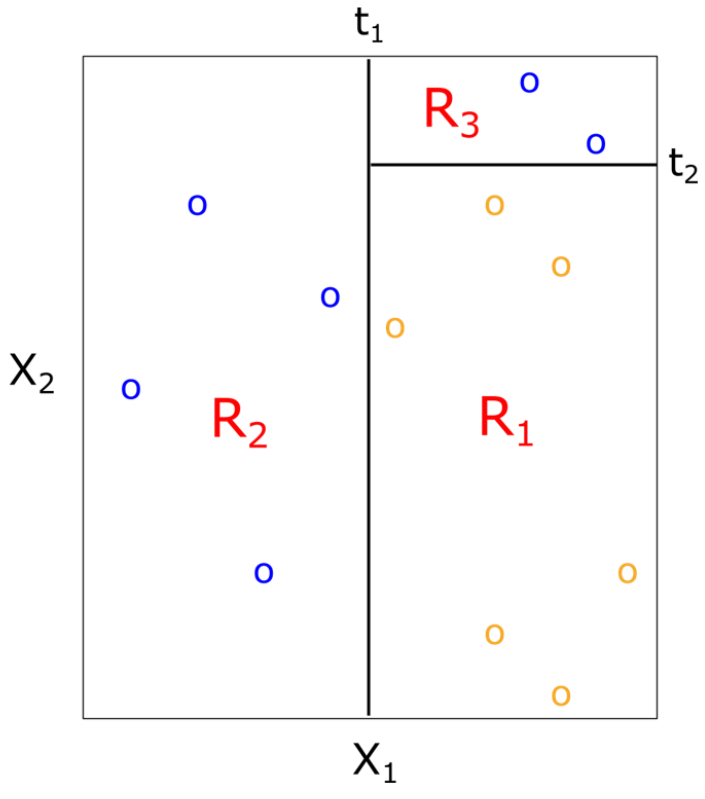

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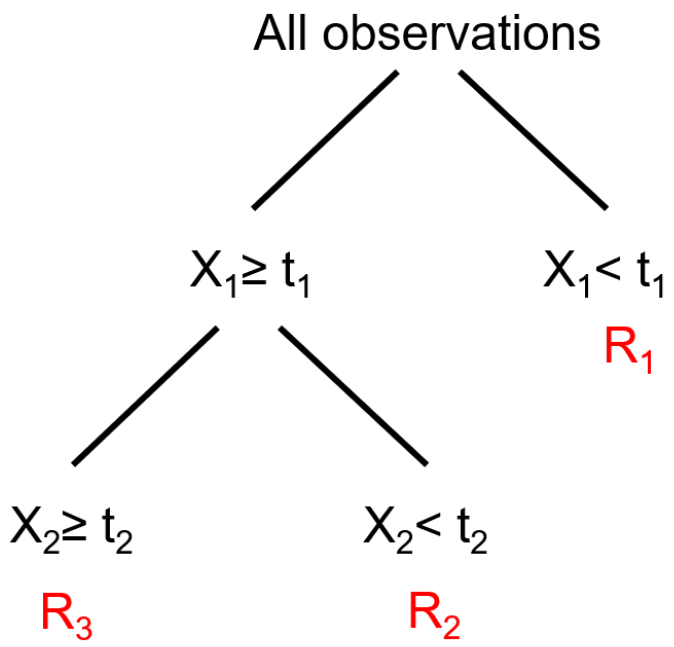

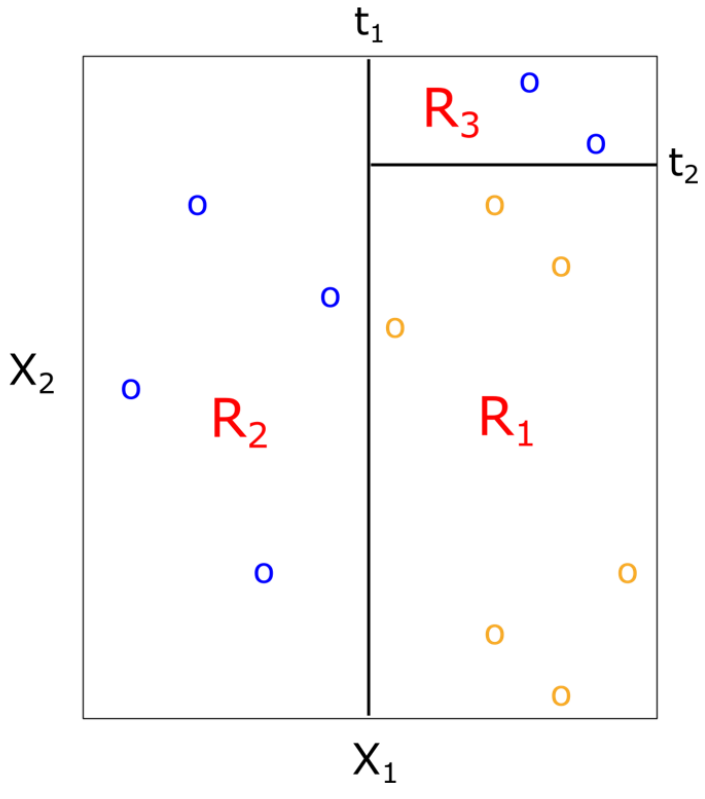

This is neat—our predictions become very interpretable!

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- Large X_1 & large $X_2 \rightarrow$ blue
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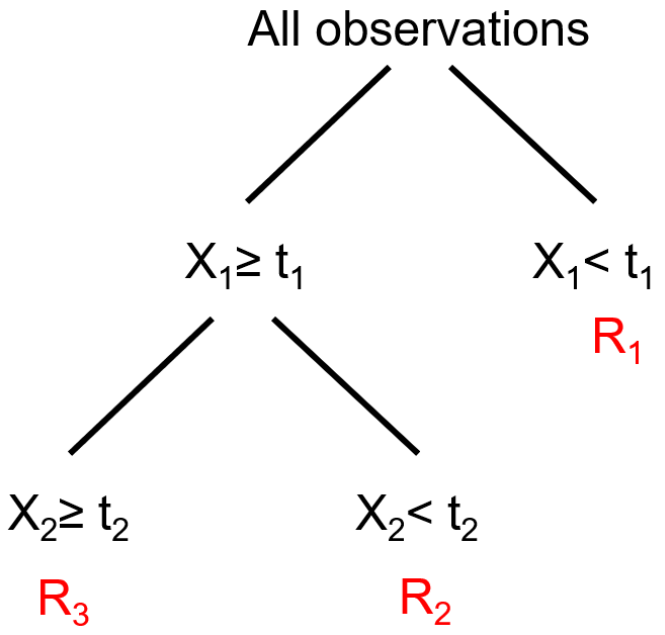

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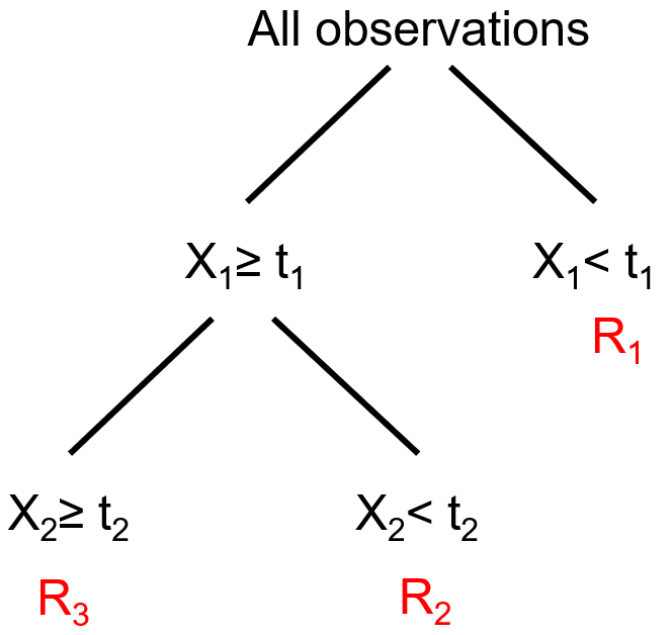

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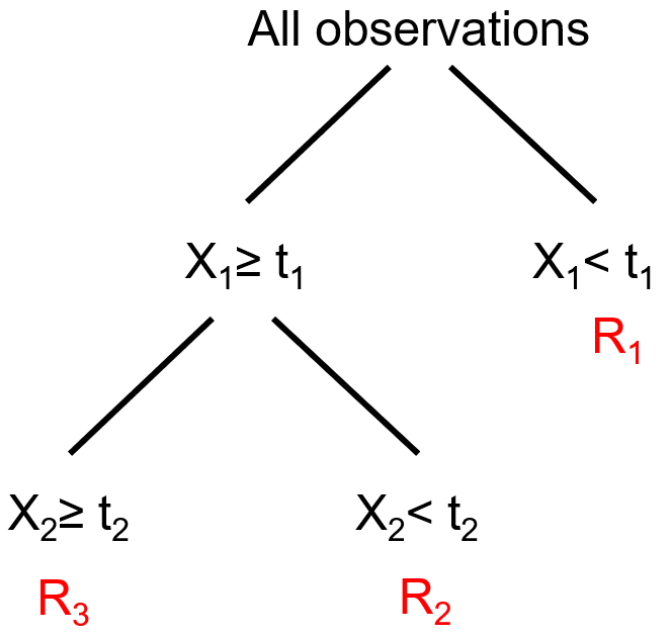

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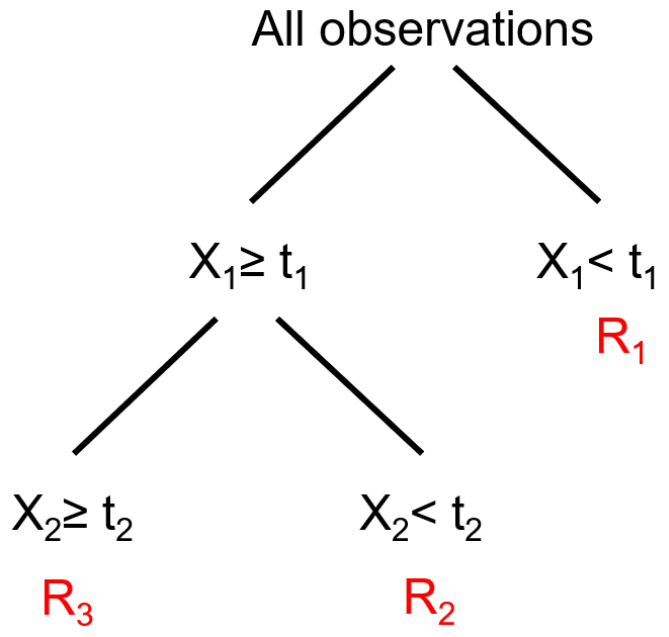

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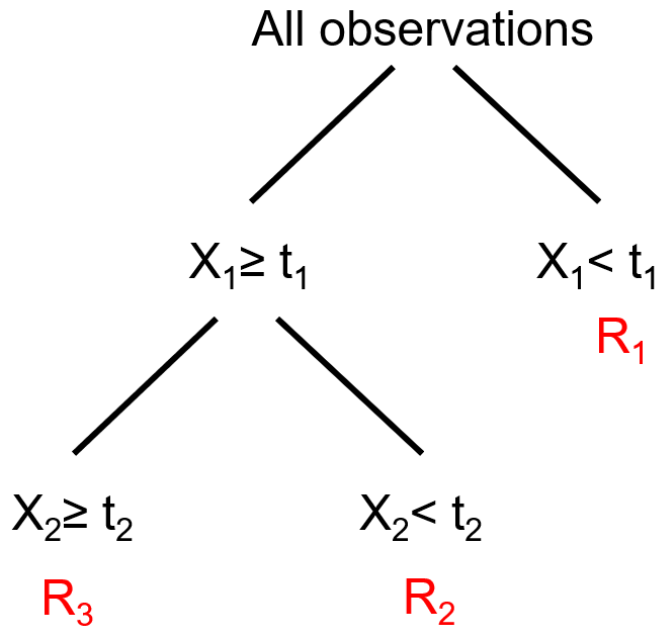

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4. Continue until you reach a *leaf node* of some *pre-specified size* (e.g., 10 observations).

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As we grow the **tree** *larger & larger* $\Rightarrow$ **error** becomes *smaller & smaller*.

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These ideas/concepts reemerge here as well, as we'll see.

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   - If the penalty $>$ error reduction $\rightarrow$ undo split.

More detail: the penalty

When **constructing** the *initial* (large) tree, we want to minimize:

$$\underbrace{\sum_{j}^{J} \sum_{i \in R_j} (y_i - \bar{y}_{R_j})^2}_{\text{Summed error across leaves}}$$

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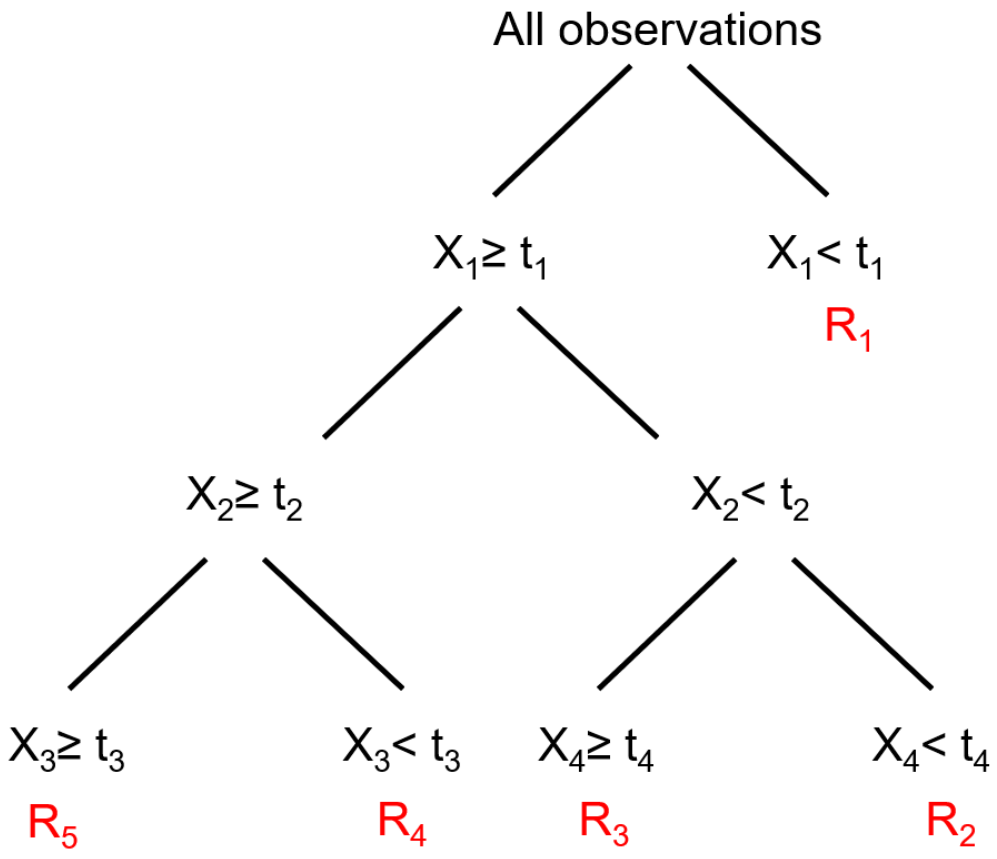
- Q—How do we set α?? Surprise, surprise: **cross-validation**!

Illustration of pruning (toy example)

Suppose this is our *fully grown tree* T_0:



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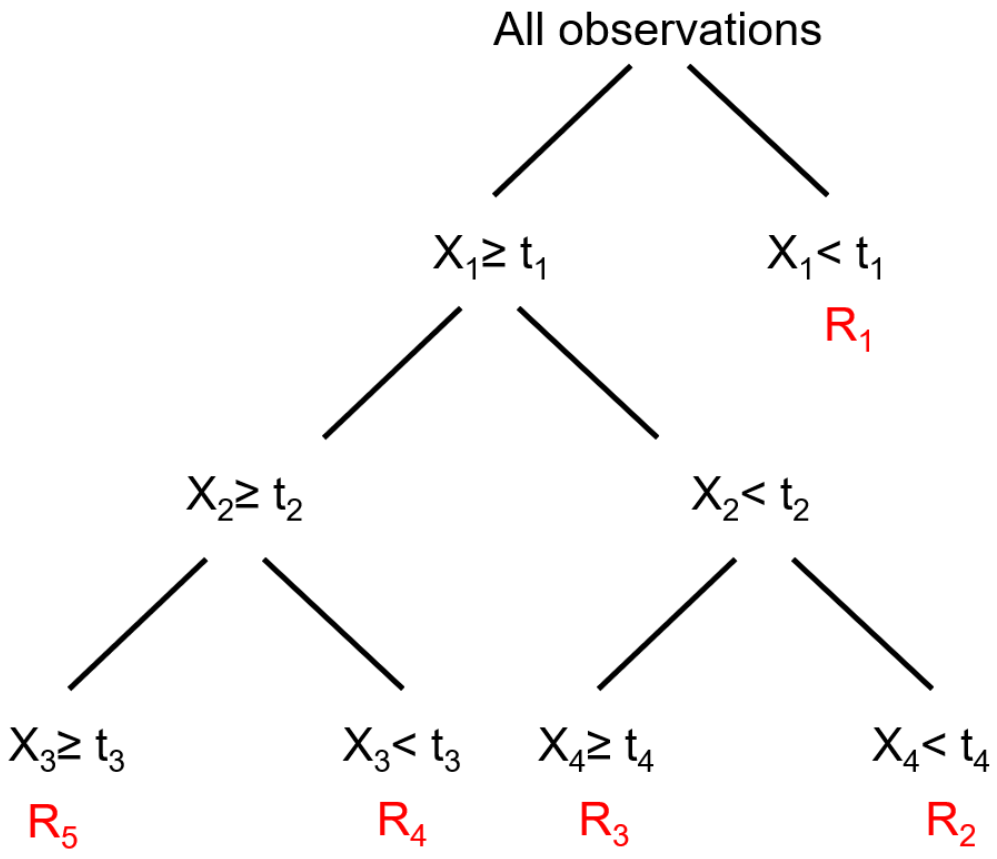

Then—to prune—we *reconsider* the last split.

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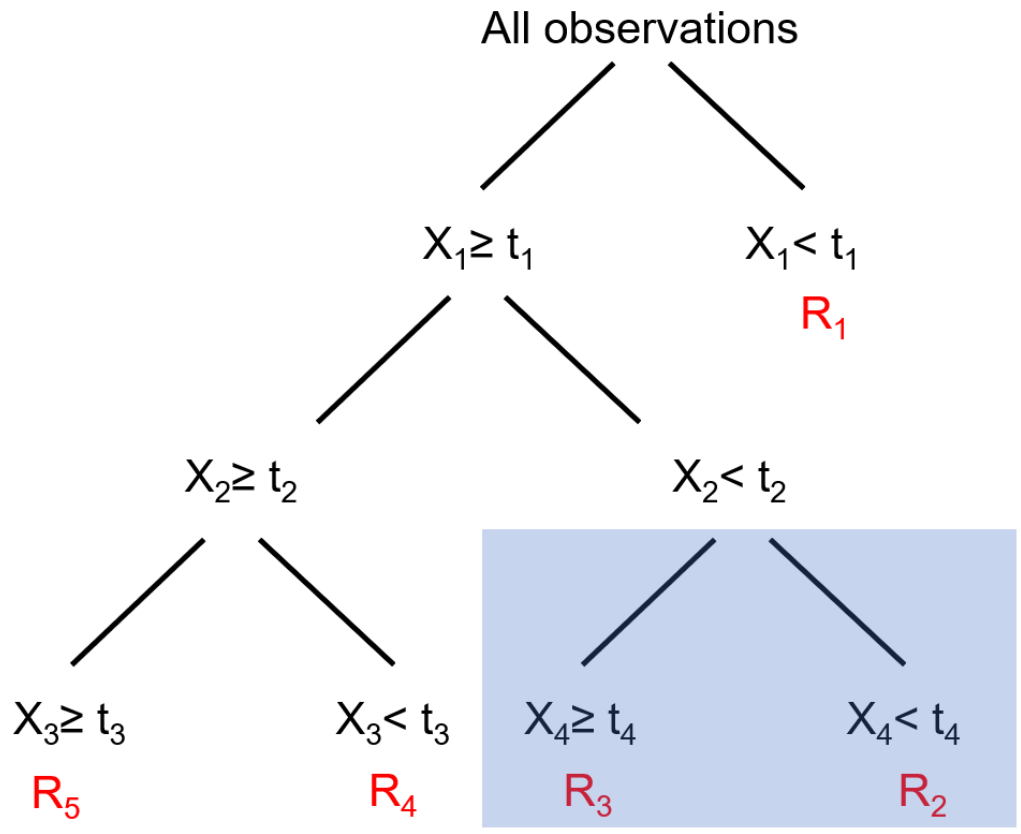

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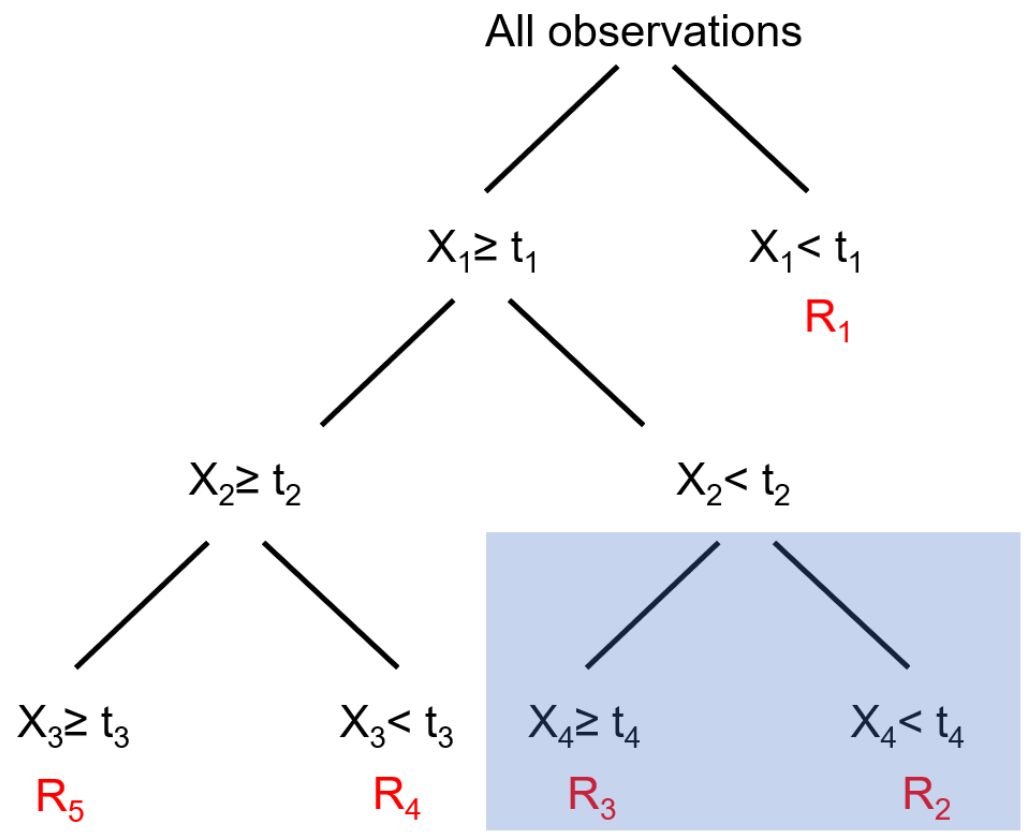

If the *error reduction* from splitting on X_4 is $< 2 \times \alpha$, then prune!

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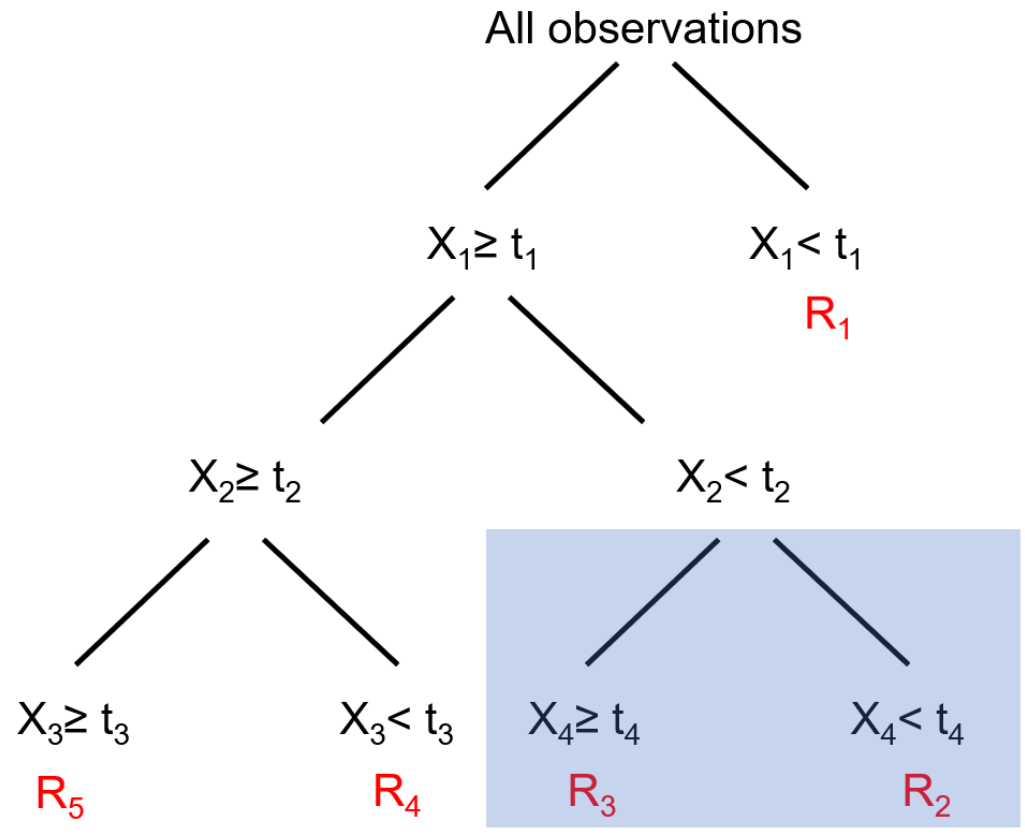

If the *error reduction* from splitting on X_4 is $< 2 \times \alpha$, then prune!

- It is $(\times 2)$ because we add *two extra nodes* in the split.

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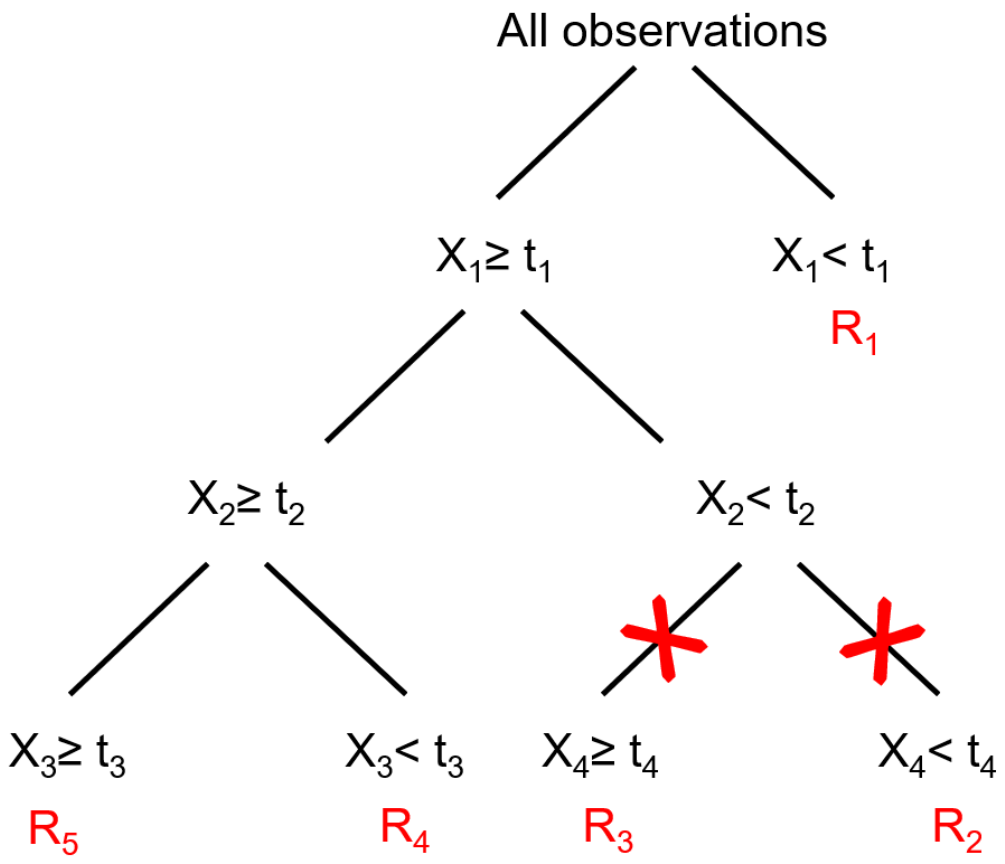

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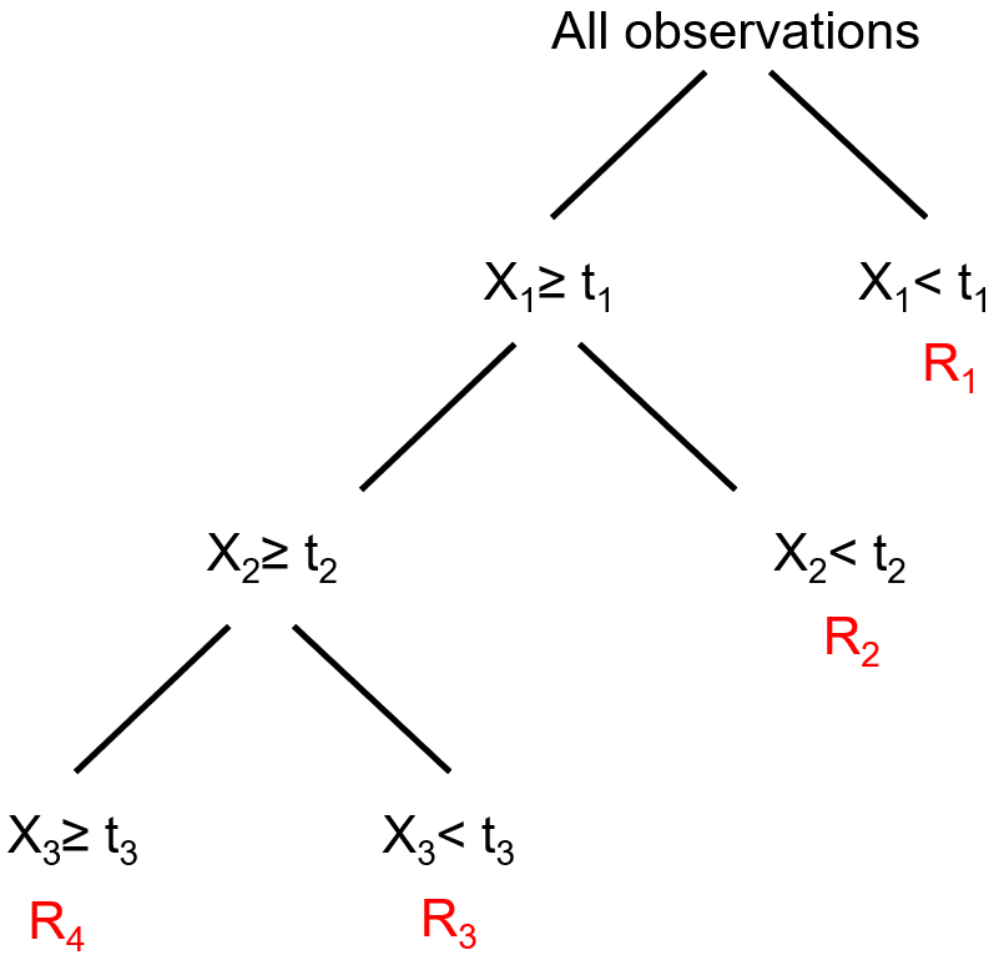

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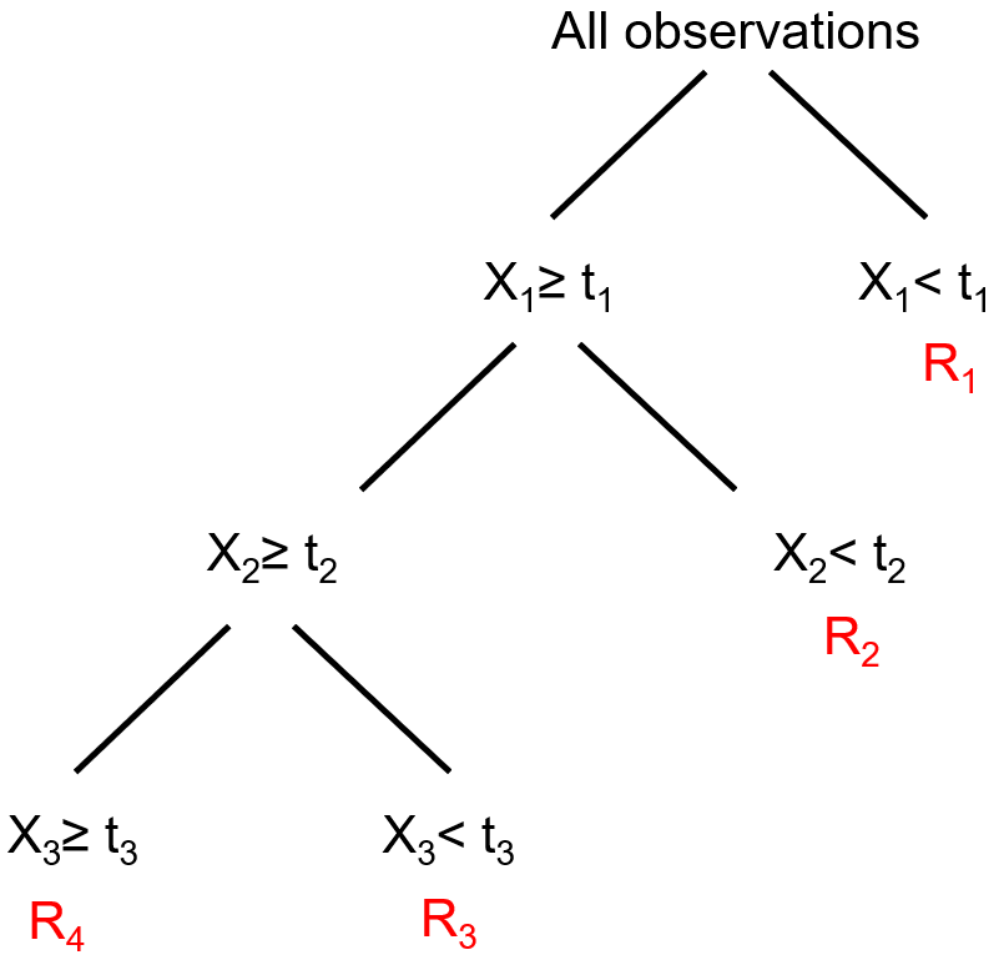
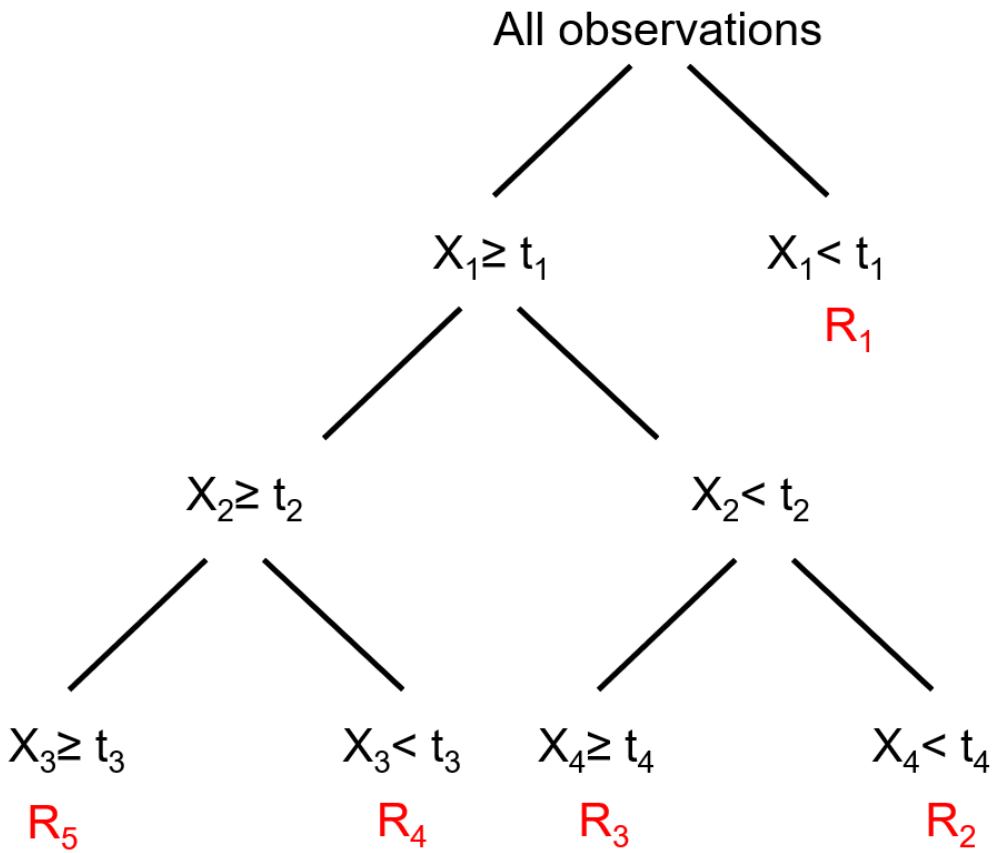


Now that we have some intuition for how *pruning* works—what is the effect of α?

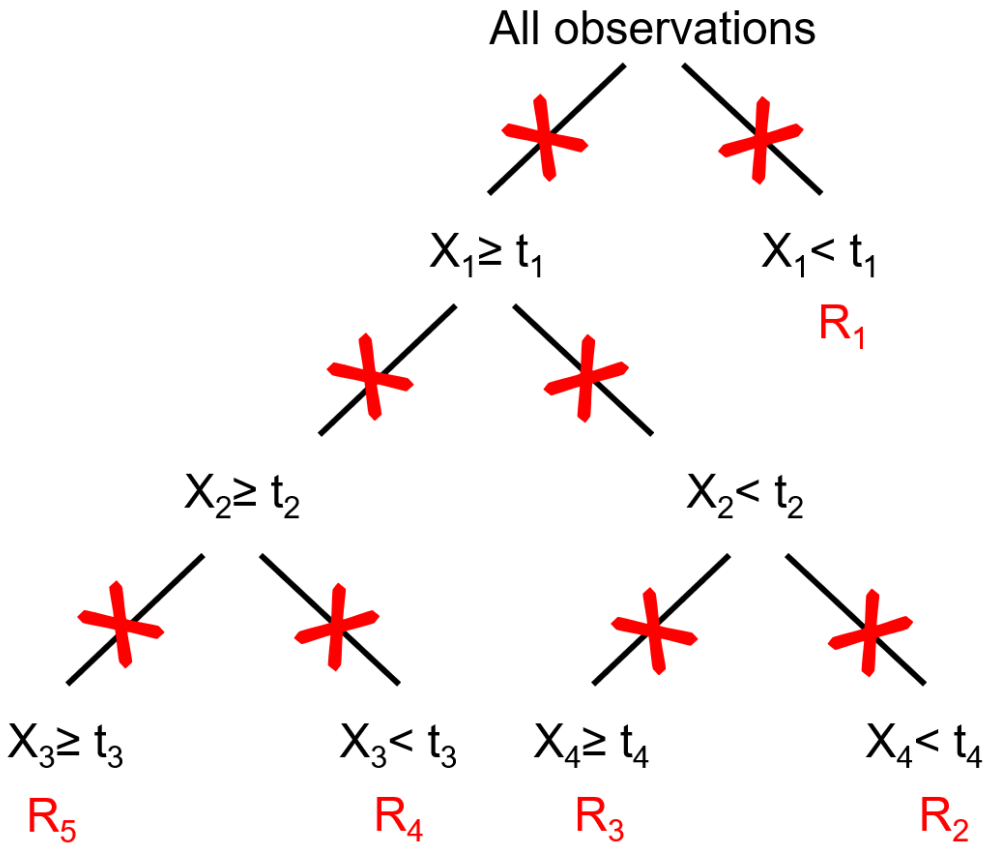
Effect of α? Extreme #1: $\alpha = 0$

Similar to lasso/ridge, when $\alpha = 0$, we retain the *full tree* (T_0).



Effect of α? Extreme #2: $\alpha = \infty$

Also similar to lasso/ridge, when $\alpha = \infty$, we retain the *NULL* model.



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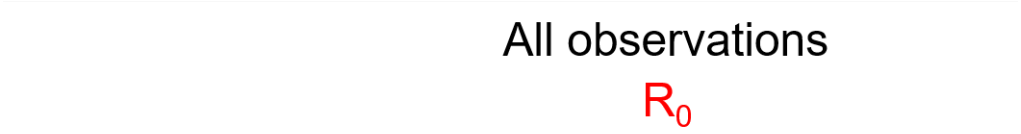
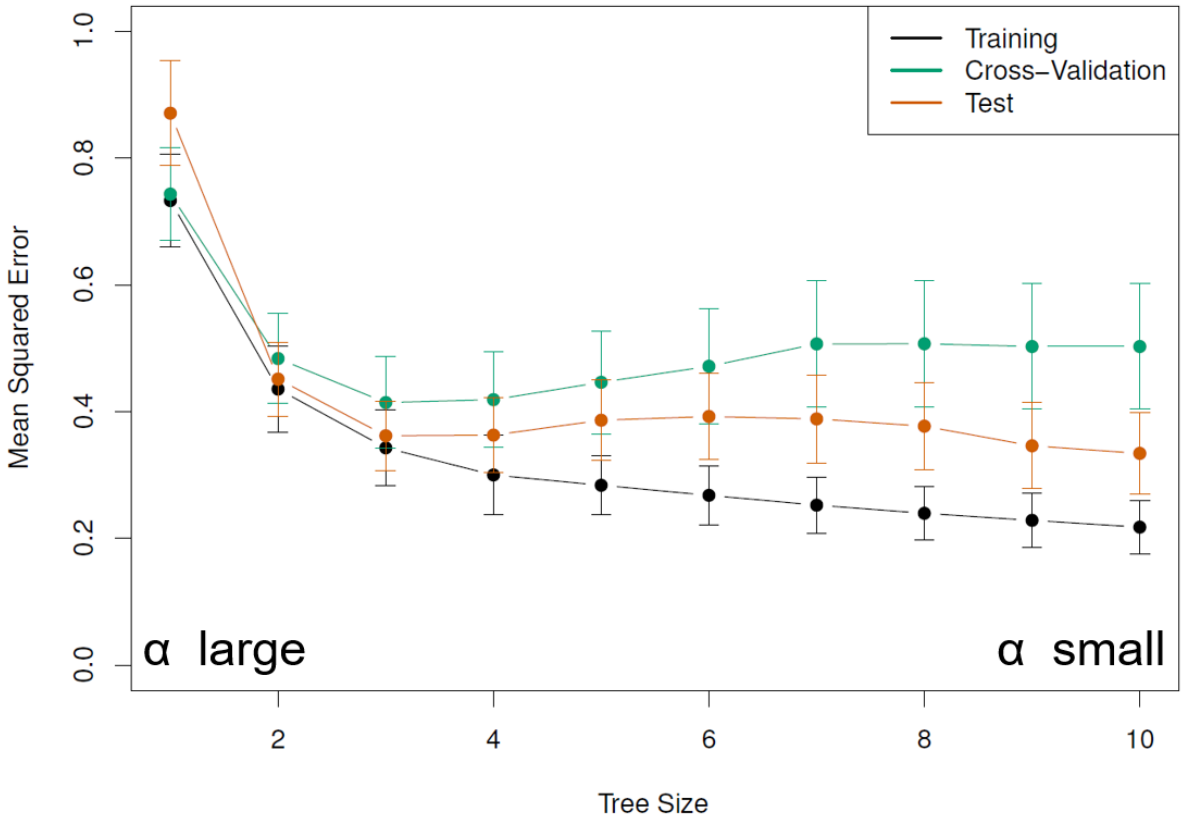


More generally: *tree-size* vs. *test error* (ISL, Fig. 8.5)



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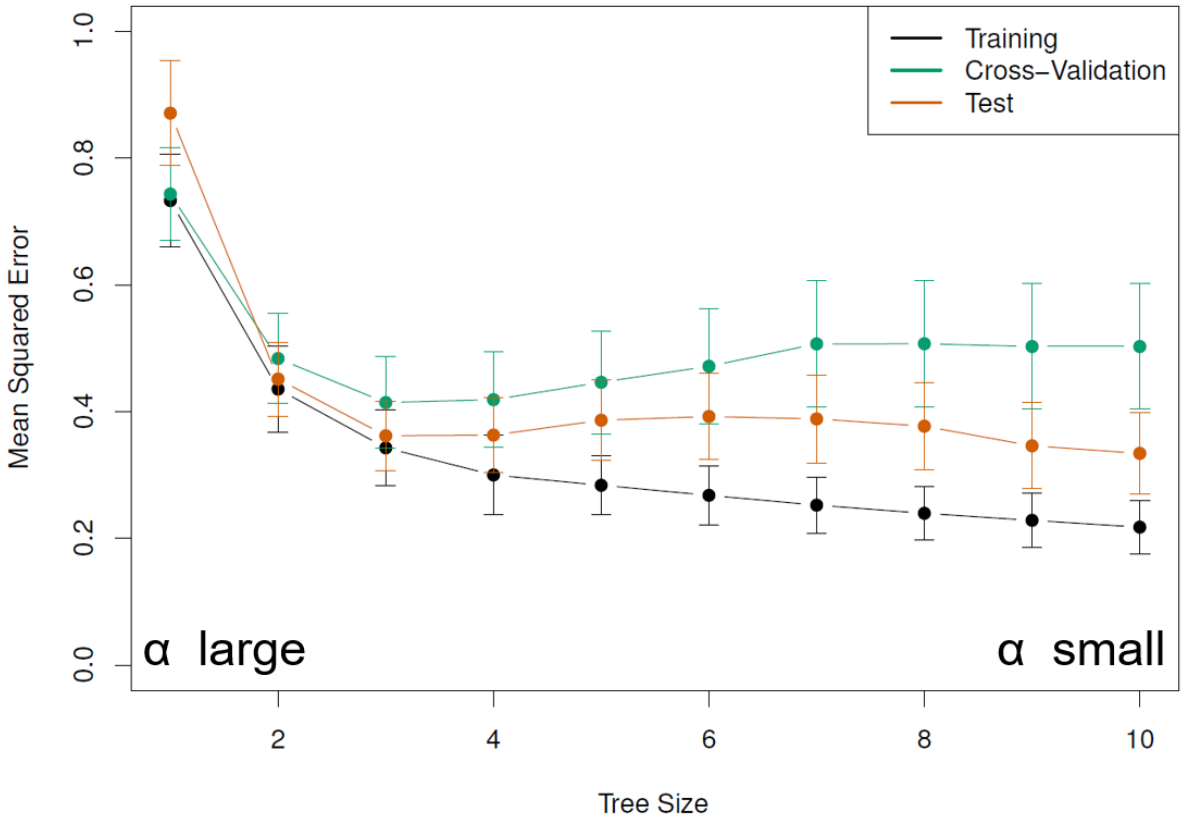

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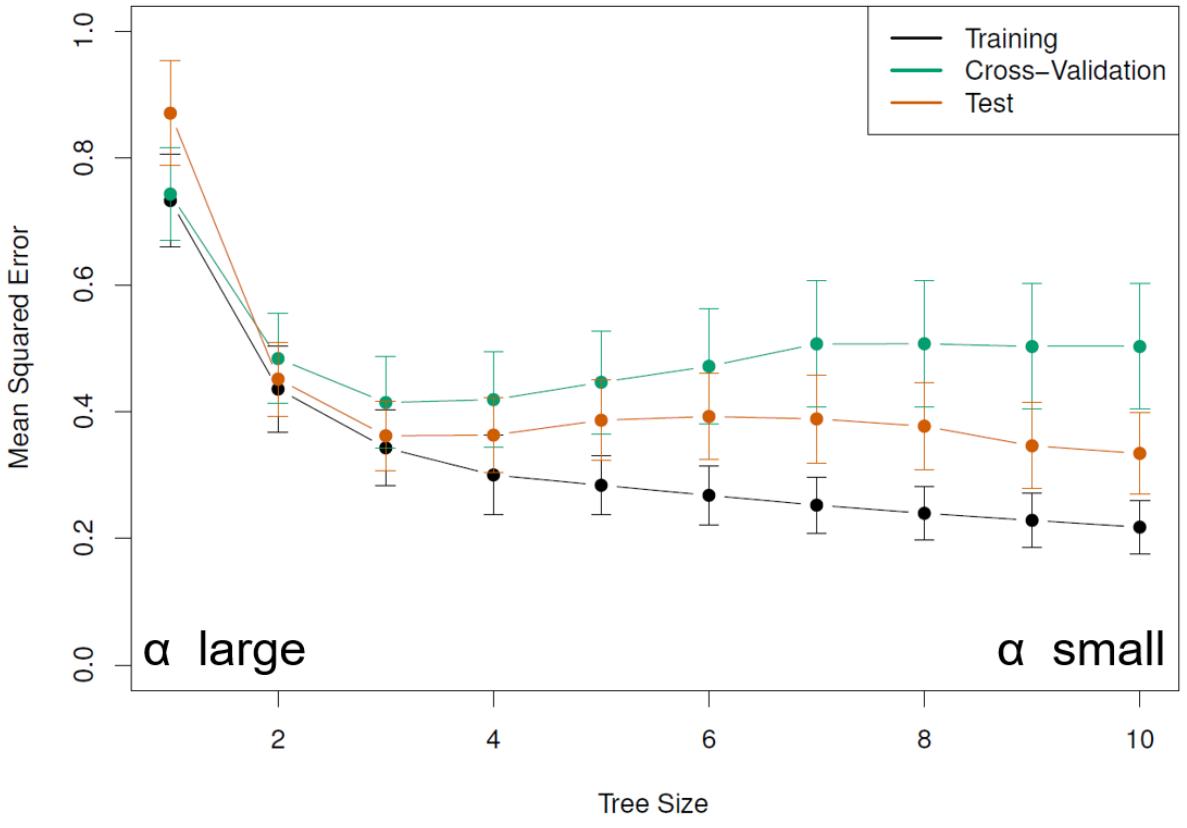

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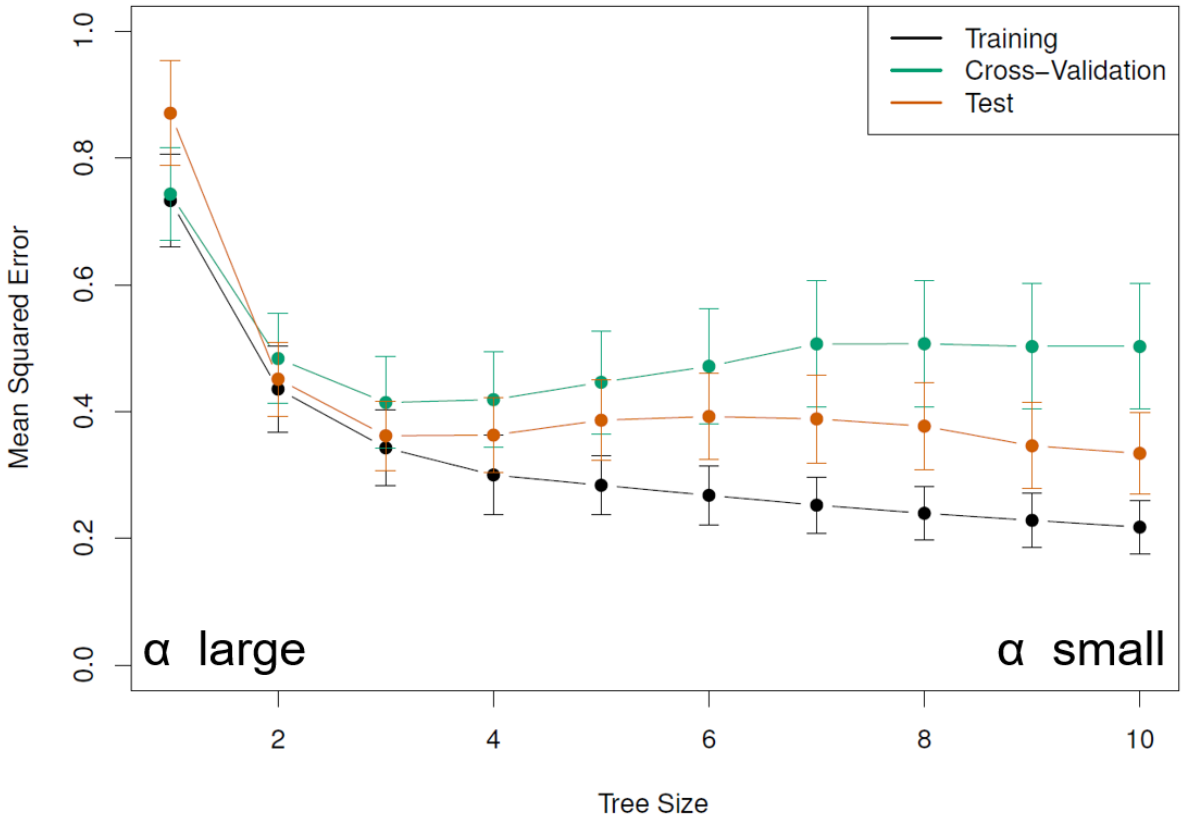

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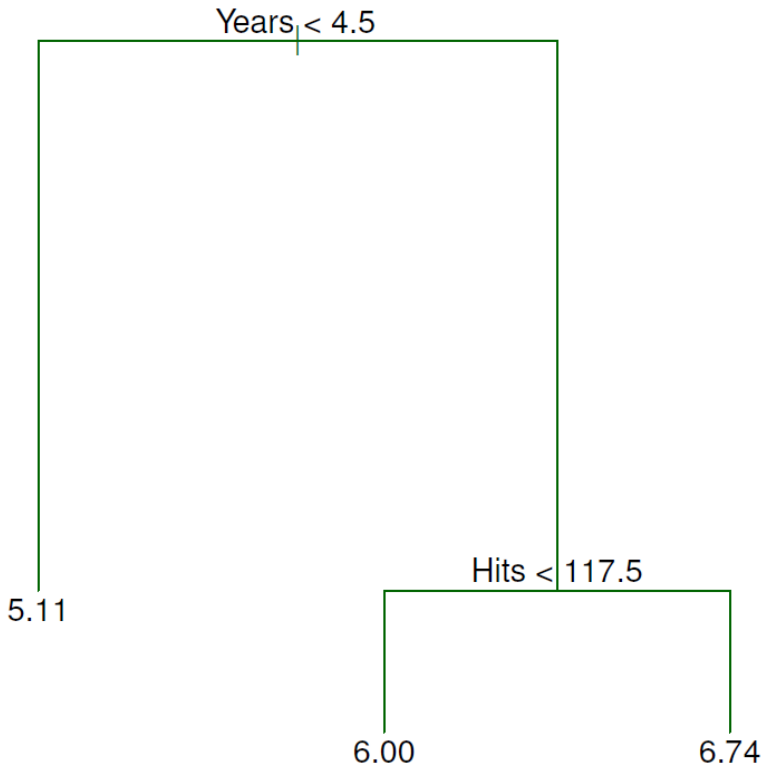
- But test error only improves initially, then it starts to worsen.
  - It improves *first* by *reducing bias*.
  - It starts to worsen because of *increased variance*.

Some additional applied concerns

Now that we have a pretty good understanding of the "inner-workings" of decision trees, we'll consider some *additional applied concerns*:

- Interpretability
- General strengths, weaknesses.

Re. interpretability



As noted earlier:

- Very interpretable because it provides simple depiction of how combinations of variables predict outcome.

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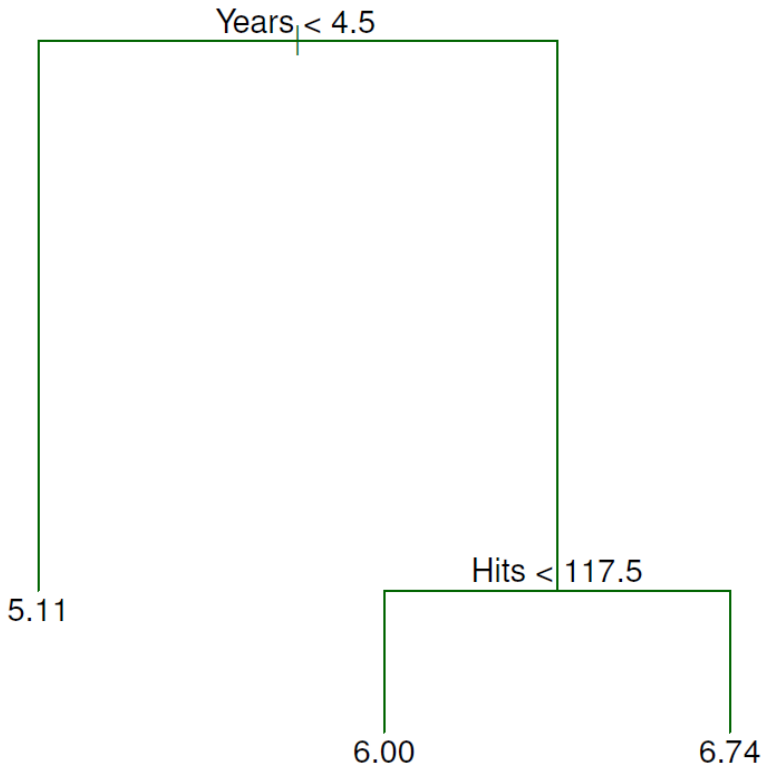

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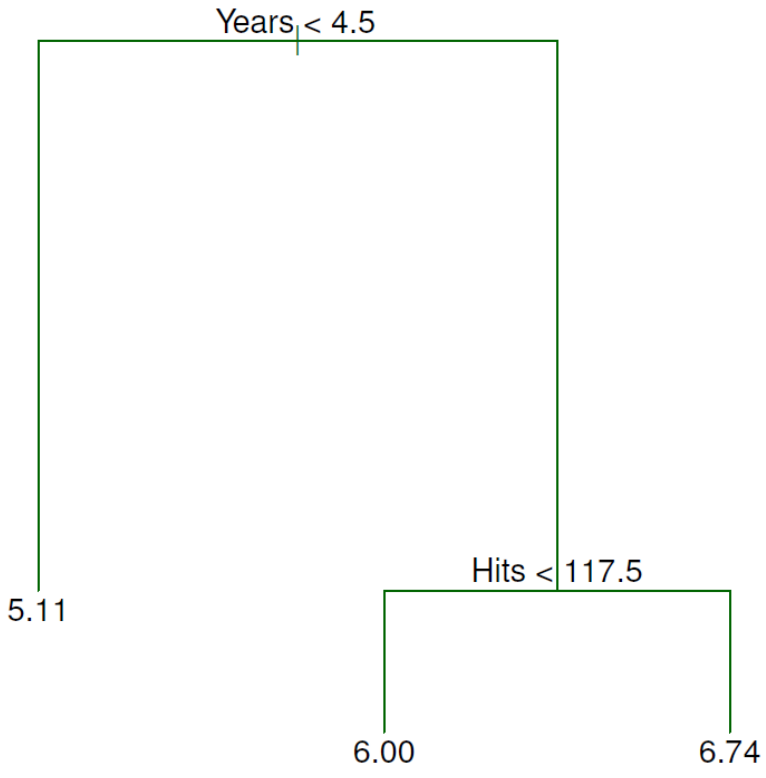

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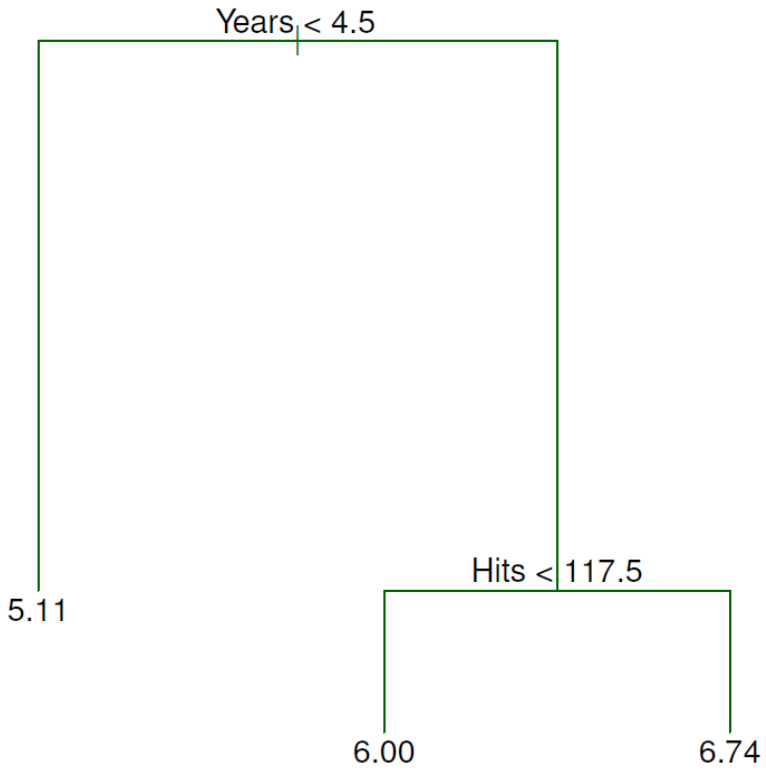

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- Additionally—variables that appear *higher-up* / *more often* in tree are more important.
  - Such variables contribute more to *reduction in RSS*.

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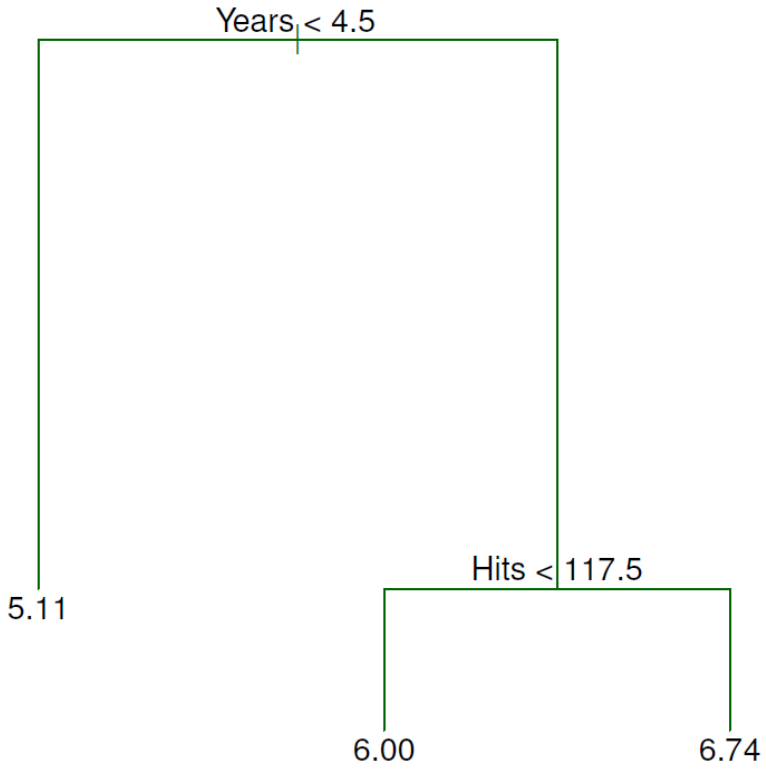
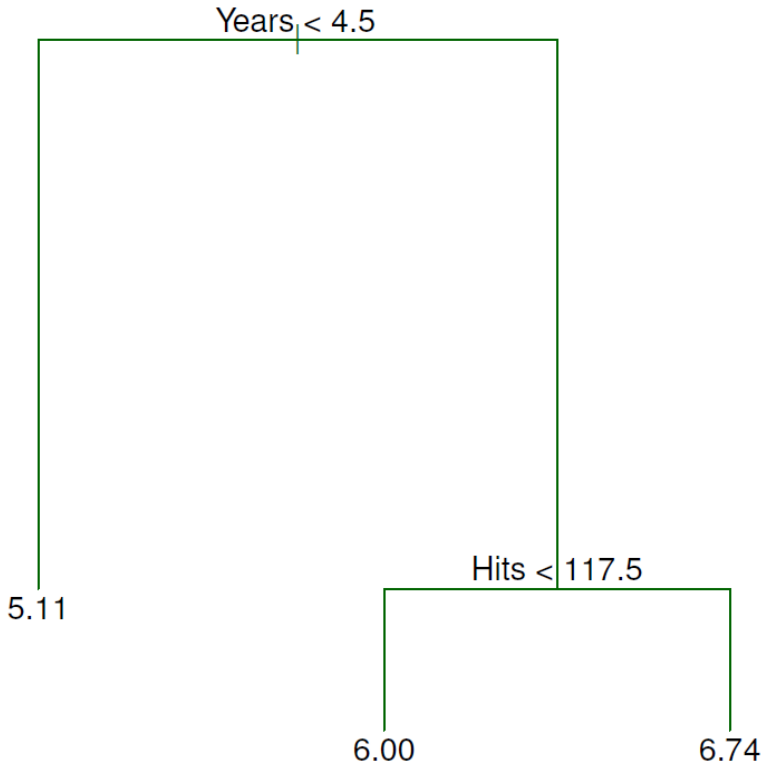


However, some caveats:

1. The structure does not reveal how X is associated with Y controlling for Z.
   - It simply finds splits that are predictive.
   - Thus—careful with interpretation.

Re. interpretability



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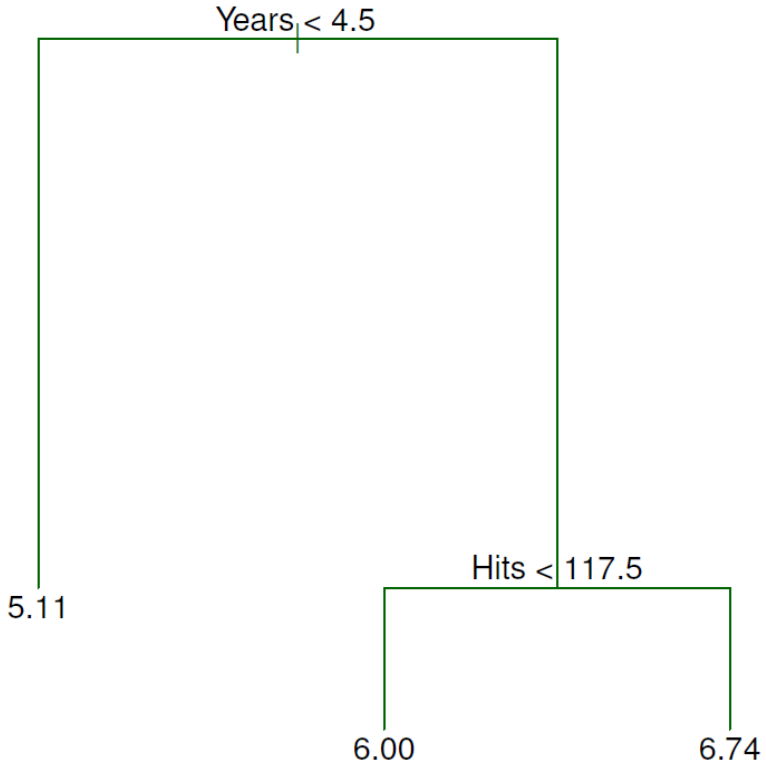
2. The structure is sometimes sensitive to observations used for training.
   - Does the branch you find interesting re-appear often or rarely?
   - Sensitivty analysis—bootstrap to examine this Q.

Re. interpretability



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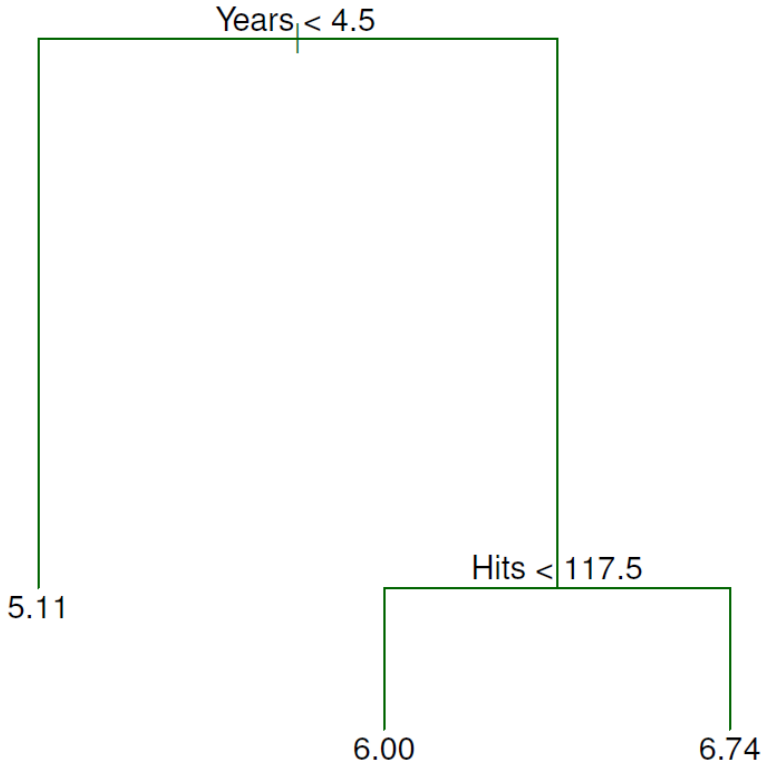

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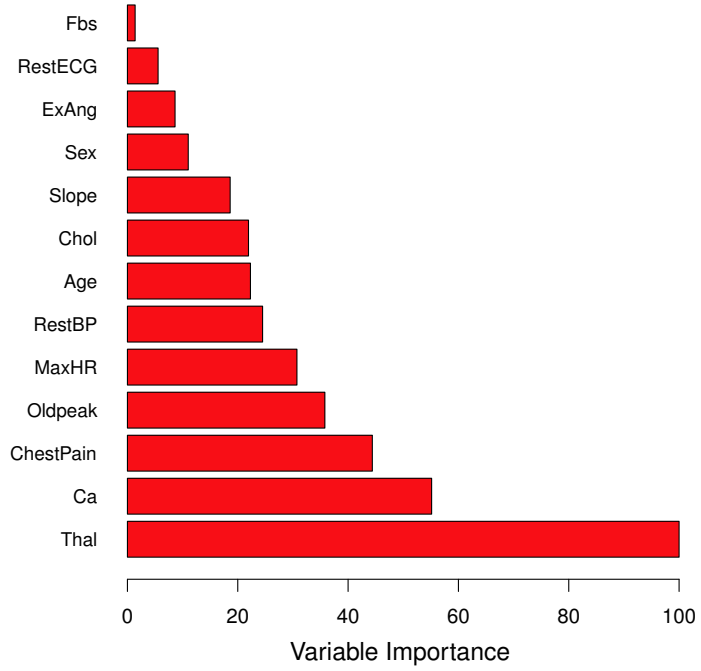
   - Note: *rpart* pkg provide function for calculating variable importance accounting for this ("surrogate splits").

Plotting variable importance (ISL, Fig 8.9)



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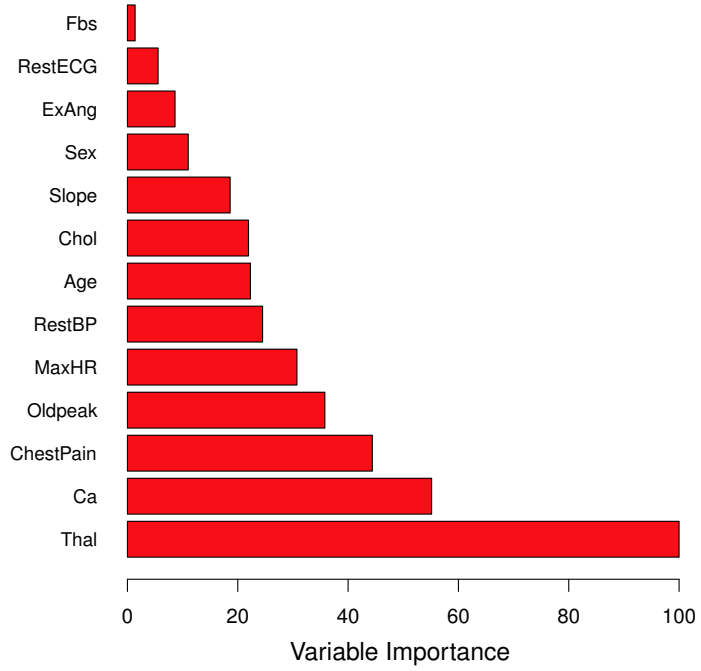

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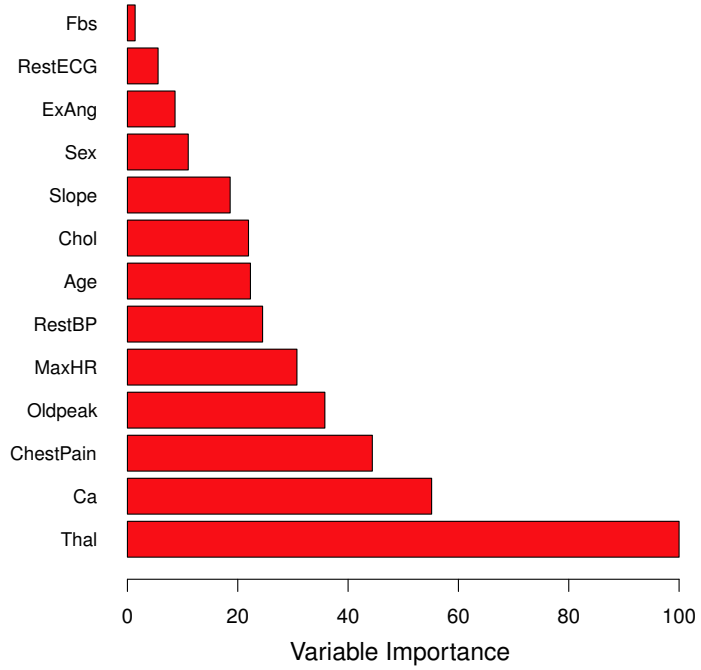

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In this example:

- The variables with the largest decrease in error are `Thal`, `Ca`, `ChestPain`.
- `Ca` reducing error about half as much as `Thal`.

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- Relatedly—can be very *non-robust*: small change in data $\rightarrow$ large change in tree structure.

Ensembles

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- We will soon see what this means.

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  3. Repeat 1–2 many times $\rightarrow$ *sampling distribution* of that statistic.

Why should this help to *reduce variance* of a model?

Classic statistics[5]: given a set of n independent variables $Z_1, \ldots, Z_n$, each with a *variance* σ^2, the *variance* of the *mean* $\bar{Z}$ is given by $\frac{\sigma^2}{n}$.

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Can we get some more *intuition* for why this should work? *Toy example*!

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Thus: averaging the three, we get an *expected accuracy* of:
$0.512 + 0.384 = \mathbf{0.896} > 0.8$!

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This is called **bagging**.

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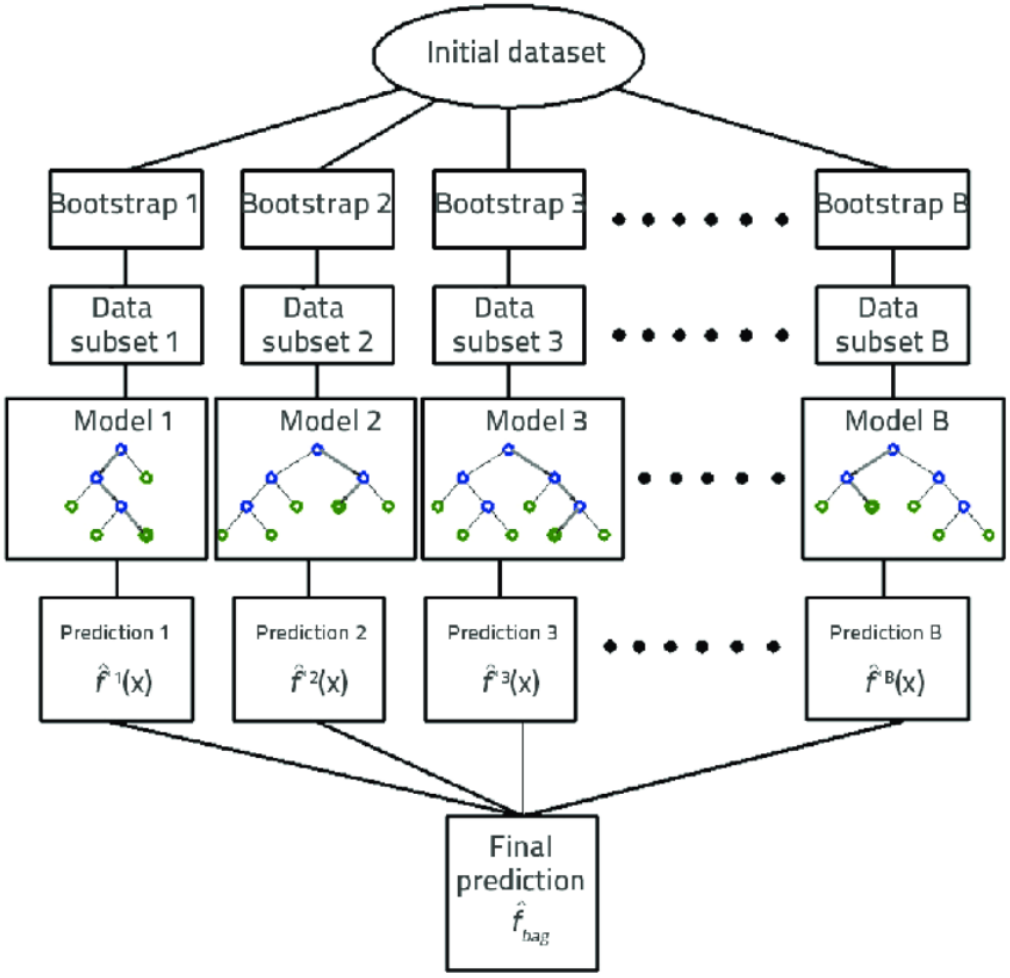
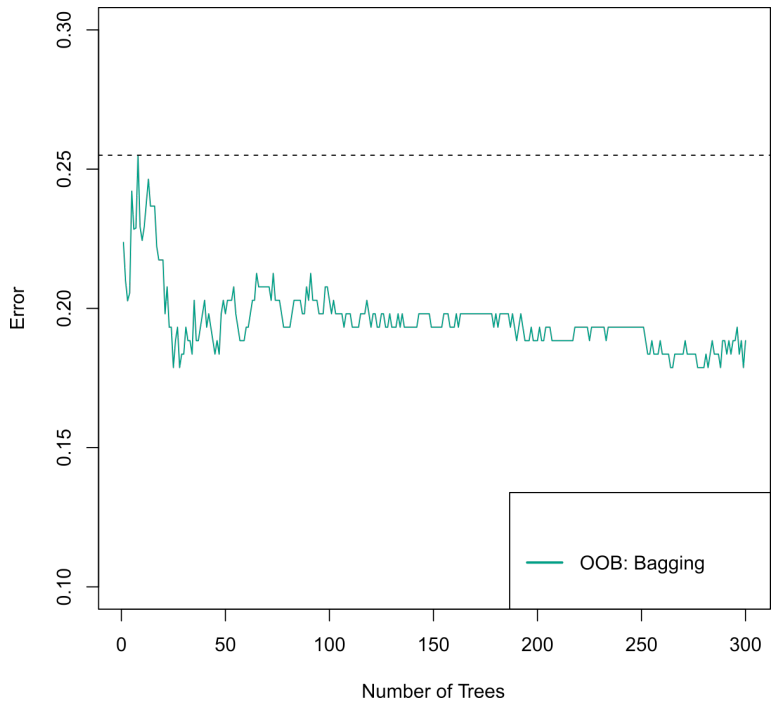
- Each tree is trained **deep** and *not pruned* $\rightarrow$ each tree has *low bias* and *high variance*.
- Averaging these B trees reduces the variance—in the hope to get the "best of both worlds" (low bias, low variance).

Illustration



One tree vs. many (ISL, Fig. 8.8)



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- *Averaging many trees* improves *test error* [6] compared to a single tree.

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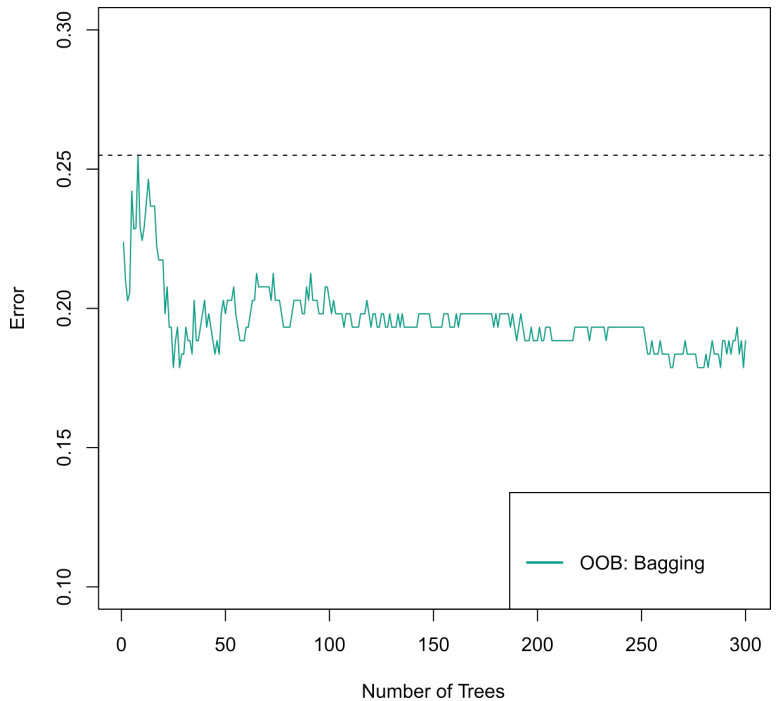

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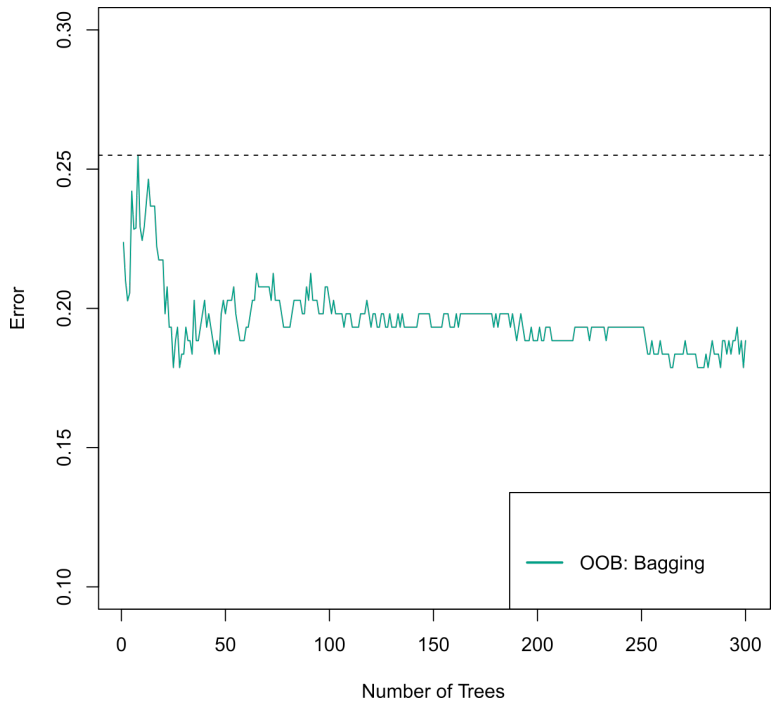

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- Results are robust to the *choice of no. of trees*. Typical choice $\approx$ 100.

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  - Same measure as for a single tree, just *averaged across all trees*.

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Can we make trees *less correlated*?

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  - E.g., if we have 36 predictors, only 6 will be considered at a given split.
  - Thus—each split does not even consider a majority of predictors.

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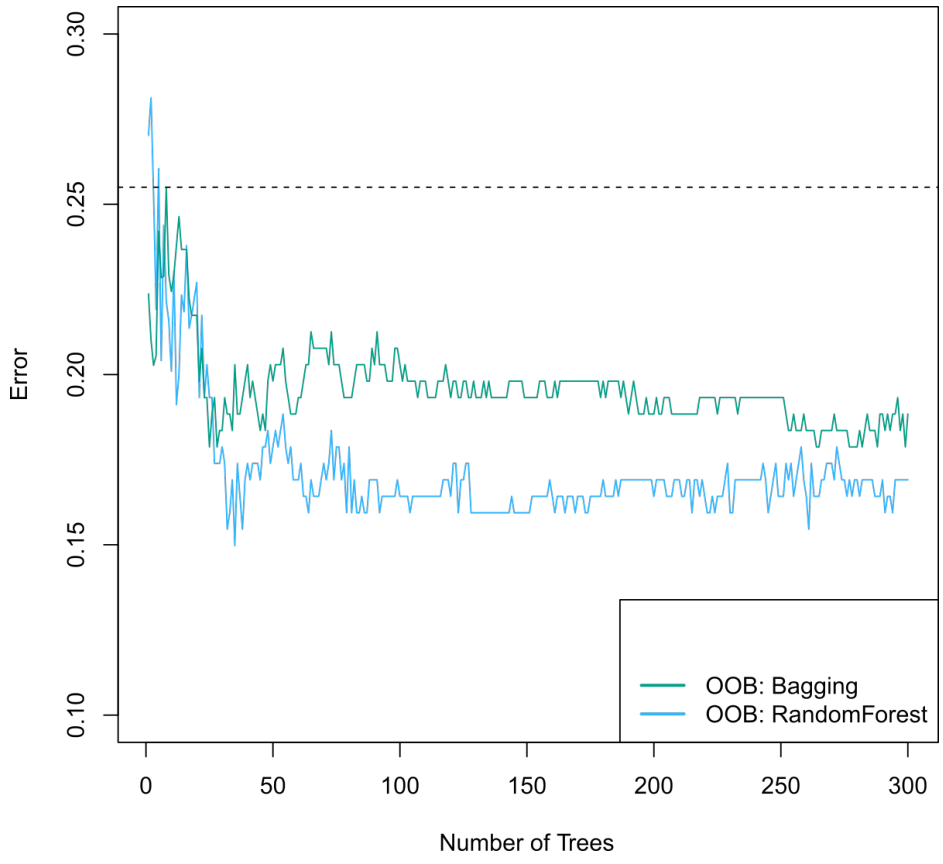
Imposing restrictions have the effect of reducing the power of any given tree, **but** when **pooling them**, they can together become **stronger**.

ISL example (Fig. 8.8)

Comparing *random forest* to *bagging*, we see that *random forest* here provides a substantial improvement!



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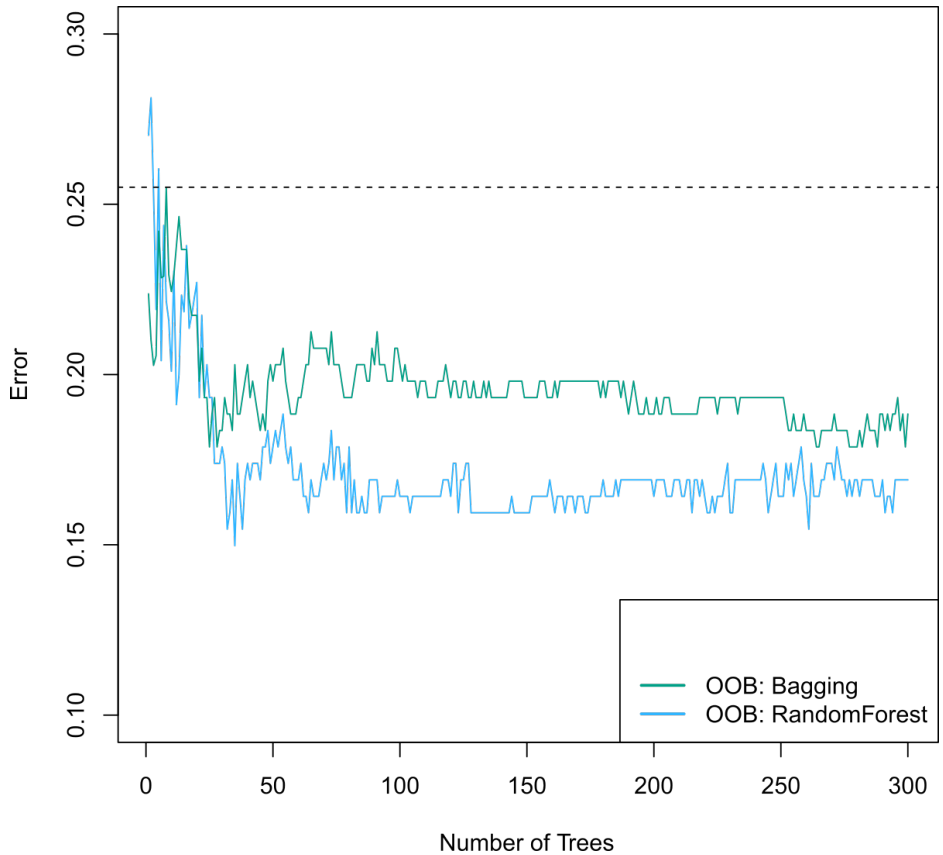
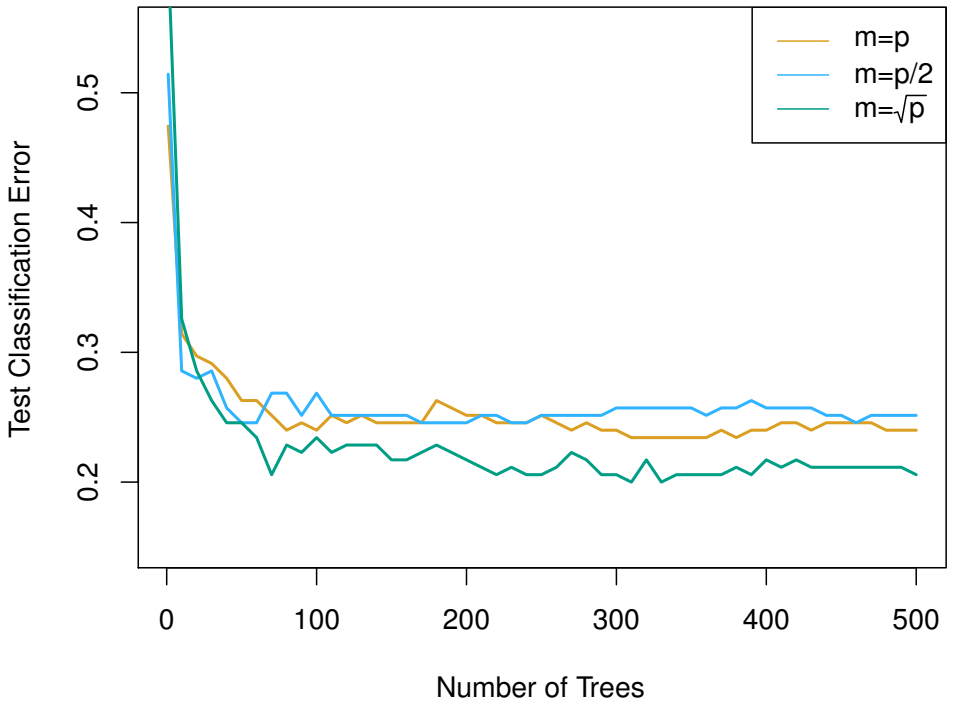


Note: as with bagging, the results are usually quite stable under different *number of trees used* (beyond a few hundred).

Effect of m (ISL, Fig. 8.10)



This example shows how *restricting the number of variables considered in every split* can improve performance.

Pros and cons of *random forest*

Pros

- Even *stronger performance* compared to *bagging*.

Cons

- In comparison to *standard decision tree*—less interpretable.

Boosting

Like bagging

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- That is: each tree is grown using information from previously grown trees.
- More specifically—the tree grown at the t'th iteration models the residuals of the combined predictions of the $(t-1)$ previous trees.

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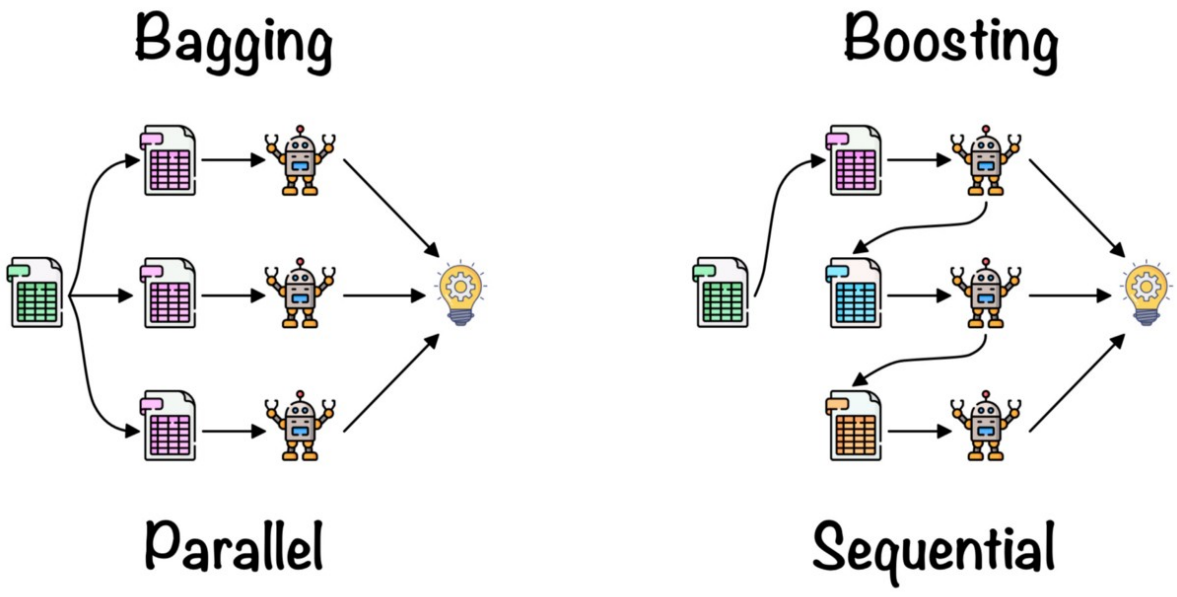
Illustration: *boosting* vs. *bagging*



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8. Fit a 3rd tree, $\hat{f}_3$, to *modified data*:
   - *Input* variables: X (the same)
   - *Output* variable: r (the residuals from step 7)
9. And so on.

Outputted model:

Boosting trees—the basic procedure

1. Fit 1st tree, $\hat{f}_1(x)$, to *original data*.
   - Input: X | Output: y
2. Apply *shrinking* to $\hat{f}_1$
3. Compute residuals: $r = (\hat{f}_1(x) - y)^2$
4. Fit 2nd tree, $\hat{f}_2(x)$, to *modified data*:
   - Input: X (the same as step 1)
   - Output: r (the residuals from step 3)
5. Apply *shrinking* to $\hat{f}_2$
6. Create a *joint prediction model* (average predictions from 1 and 2):
   - $\hat{f}(x) \leftarrow \hat{f}_1(x) + \hat{f}_2(x)$
7. Compute updated residuals $r = (\hat{f}(x) - y)^2$
8. Fit a 3rd tree, $\hat{f}_3$, to *modified data*:
   - *Input* variables: X (the same)
   - *Output* variable: r (the residuals from step 7)
9. And so on.

Outputted model:

$$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x)$$

Tunable parameters

- B—*number of trees* to grow. Unlike bagging and random forest, we can overfit as we increase B. How to select? **cross-validation**

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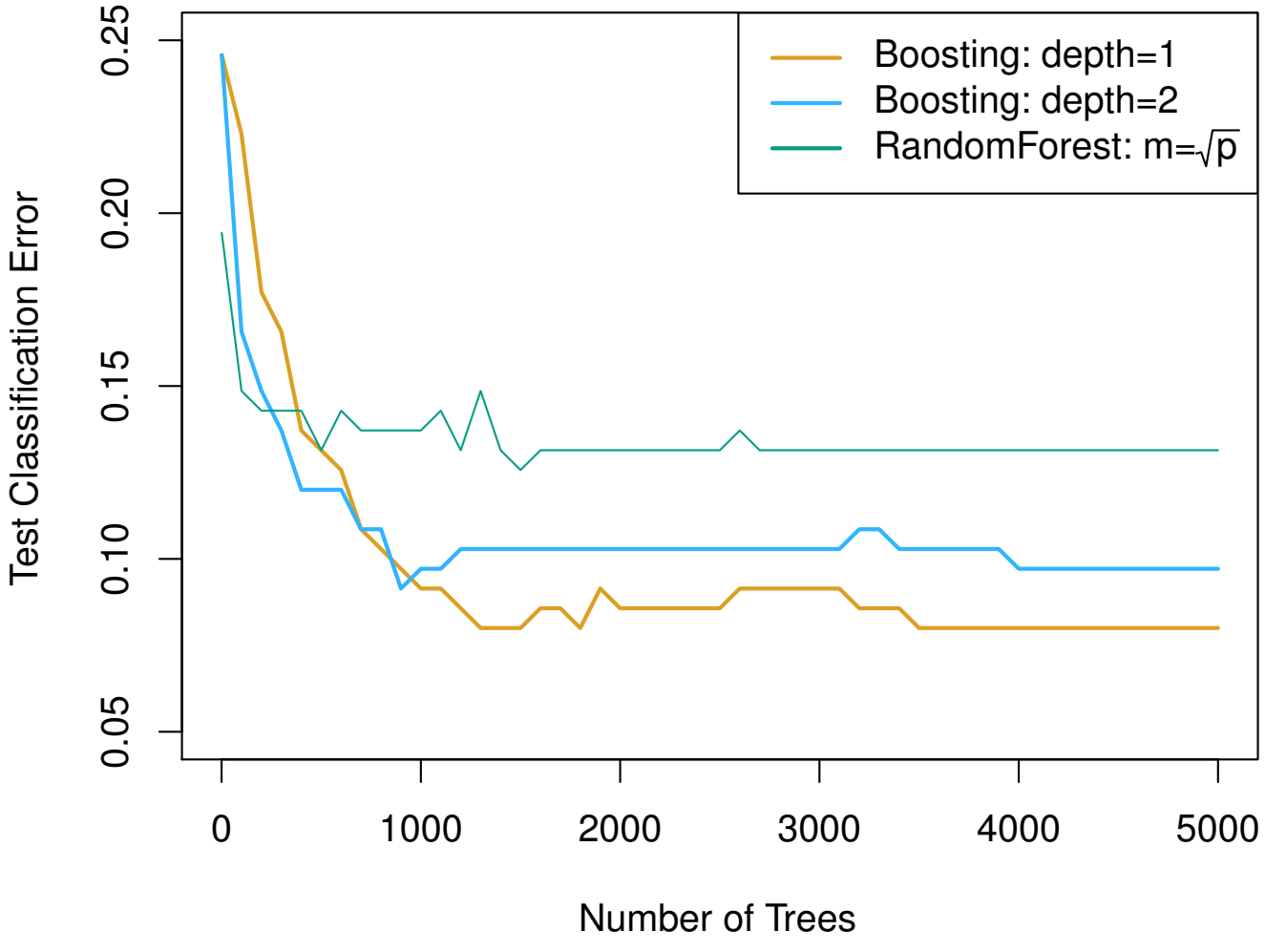
- d—the *number of splits per tree*; controlling the *complexity* of boosted ensemble.
  - Often, $d = 1$ works well—in which case each tree is a "stump" (just one split).

Performance comparison (random forest vs. boosting)



Pros and cons

Pros

- Have demonstrated even more competitive performance than random forest.
- In special case of $d = 1$, becomes an *additive model* (+ interpretability)

Cons

- Relative to *standard trees*, not as interpretable.
- More sensitive to specification of constants (B, λ, d).

Misc

Interpretable Machine Learning

Recent focus in machine learning literature (Molnar 2020)

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We will briefly consider two popular techniques:

- *Permutation variable importance* measure
- *Partial dependence* plots

Permutation variable importance

Very informative quote from Boelaert & Ollion (2018):

- Read when you get time.

BOX 3. – ***Permutation importance: which variables matter for prediction?***

As its name suggests, the *permutation importance* measure aims at assessing the relative (predictive) importance of the variables at hand, using permutation. It exploits the fact that once the model has been trained, it works as a prediction machine that can be fed any predictor data. Its principle is simple: using a subset of the population under study (preferably the test set), the values of a given variable are randomly permuted (rearranged in a random order), leaving all other variables intact. When these perturbed data are passed through the model, the prediction quality is degraded (when compared to prediction on the unperturbed data). This degradation in prediction quality is interpreted as an importance measure for the current variable: a variable that makes the model much worse when it is permuted is important, while a variable that can be permuted without affecting prediction quality is not important. The procedure is repeated for each variable in sequence, and may be repeated several times for each variable to improve robustness. The whole process thus offers a standardized, interpretable measure of variable importance that can be compared across predictors (both continuous or categorical), does not depend on the type of learning model used, and demands only a single trained model.[26]

Permutation variable importance

Basic procedure:

1. Estimate your $\hat{f}$.

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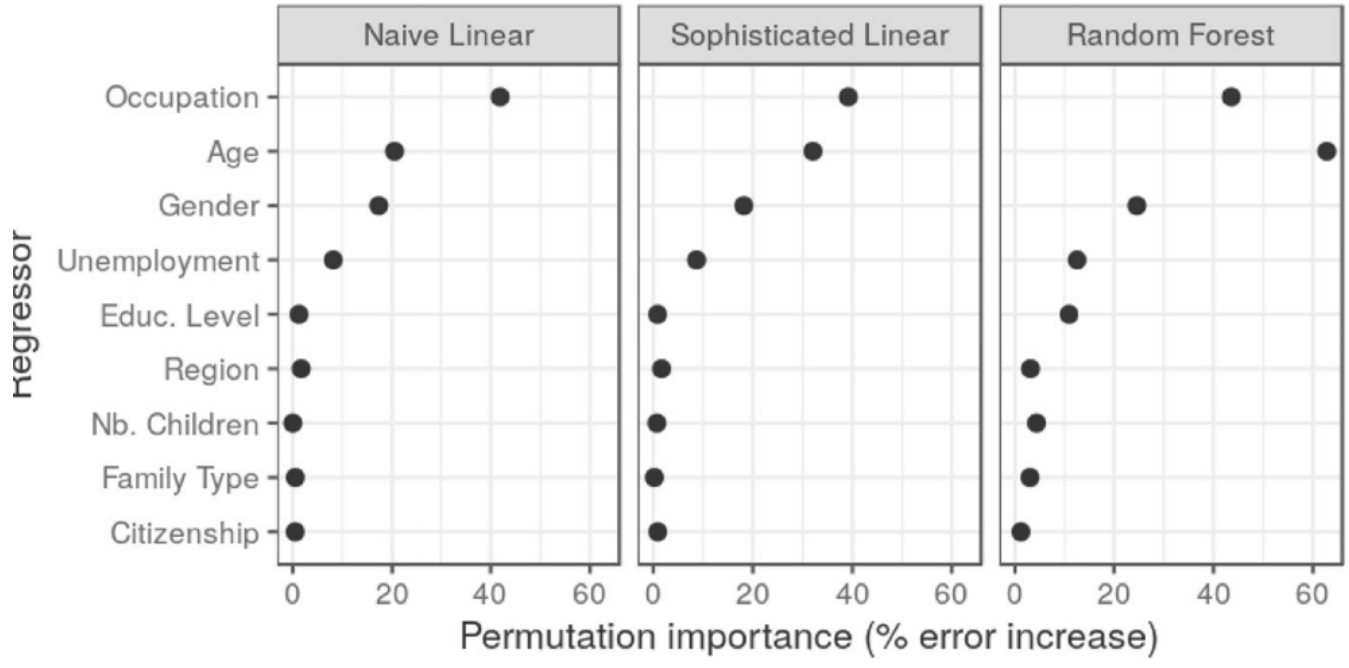
3. Permutate variable X_1.
4. Generate predictions from $\hat{f}$ on *modified data* and assess *accuracy*.
5. Difference in accuracy between step 2 and 4 = importance of variable X_1.

Example (Boelaert & Ollion 2018)



Partial dependence plot

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BOX 4. – ***Partial dependence: isolating the effect of a single variable in a complex model***

The intuition for partial dependence is that, if one is to study the association of a single variable with the outcome, the effects of all other predictors can be neutralized by *averaging them out*. Just as permutation importance, partial dependence combines predictive power and perturbations of the original dataset to produce interpretable measures. The partial dependence of the outcome variable on a given predictor X_1 is computed in the following way: for each value x that X_1 takes in the dataset (and preferably in its test-subsample), a new dataset is created in which all values of X_1 are replaced by this single value x. If X_1 is gender, for instance, two synthetic datasets are created, each one with as many observations (N) as the base dataset: in the first table all observations are assumed to be women (while all other variables are left untouched), in the other all are set to be men. Both these synthetic datasets are fed, in turn, to the predictive model, yielding N predicted wages for synthetic women, and another N for synthetic men. Finally, we compute the average prediction for the synthetic men and for the synthetic women, and these two average predictions make up the partial dependence plot.[28] In the case of age, 47 different synthetic datasets of size N are created: one where all individuals are set to be 18 years old, one for 19, and so on until 65 years old.

Partial dependence plot

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For some variable $X_1 \ldots$

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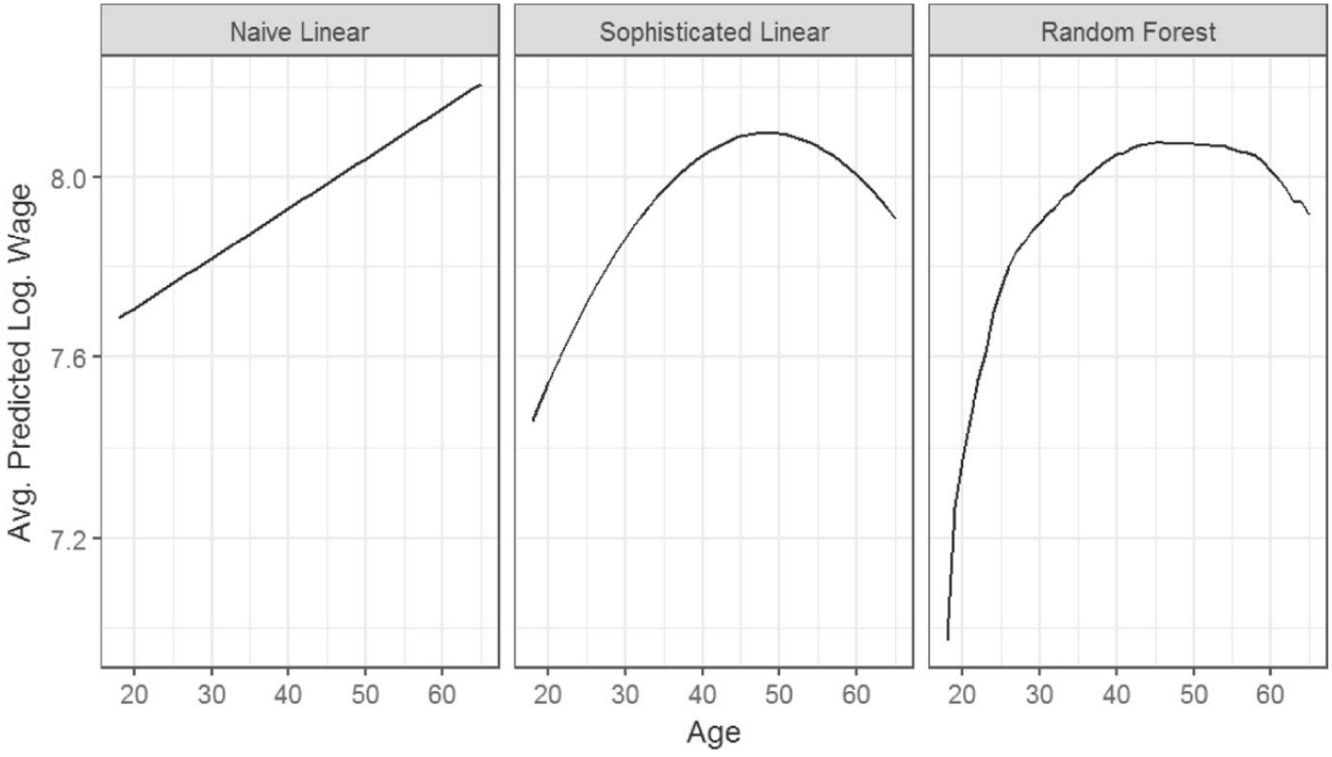
2. Generate predictions for data set from step 1.
3. Average predictions from step 2 into a single prediction.
4. Repeat step 1–3 for all unique values for X_1.

Example (Boelaert & Ollion 2018)



Principles of prediction (Grimmer et al. 2022)

1. Predictive features do not have to cause the outcome
   - Prediction: include all variables that help improve test accuracy.
   - Inference: if we are interested in the relation between X_1 and Y—only include variables measuring things prior to X_1; only include variables that are correlated with X_1 or Y; do not include "collider" variables.

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3. It's not always better to be more accurate on average
   - We discussed this in the last lecture (accuracy may vary within subgroups which we care about, and a certain class might be *rare*).
4. There can be practical value in interpreting models for prediction.[8]

[8] Note: they also include a firth principle. I exclude it here for brevity; it is not as crisp as the other points.

This week's reading

- ISL, Ch. 8: 8.1–8.2 (minus 8.2.4)
- TAD, Ch. 23: 23.3