SIRCSS – Machine Learning for Social Science

Lecture 1 (cont.)

Martin Arvidsson
Institute of Analytical Sociology, Linköping University

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- Beyond the standard linear model
  - *Polynomials*—enable $\hat{f}$ to pick up more patterns in data ($\downarrow$bias).
  - *Ridge*—penalizes $\hat{f}$ that picks up too much patterns ($\downarrow$variance)
  - *Cross-validation*—helps find a good level of complexity; balancing bias- and variance trade-off.

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- Most common measure for classification: **accuracy** (% correct classifications).

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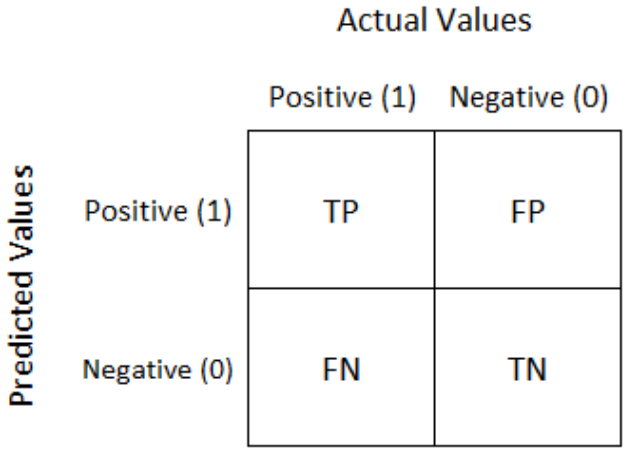
Depending on the setting — it can also be worth distinguishing between *false positives* and *false negatives* (*true positives* and *true negatives*).



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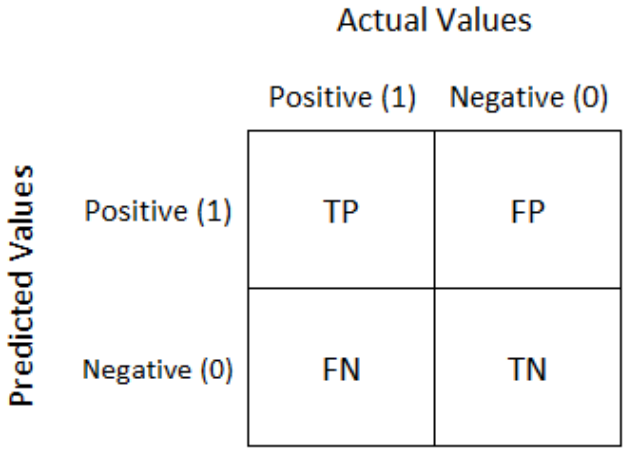

It may for example be that *certain errors are more important*. E.g.,

- Incorrectly classifying an individual with cancer as not having cancer (*false negative*) vs. incorrectly classifying an individual with no cancer as having cancer (*false positive*).

Remainder of lecture

Class of methods that 'learn' from data in more automatized ways.

- **Non-parametric** supervised learning
  - KNN
  - Decision trees
  - Random forest

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 now!

KNN

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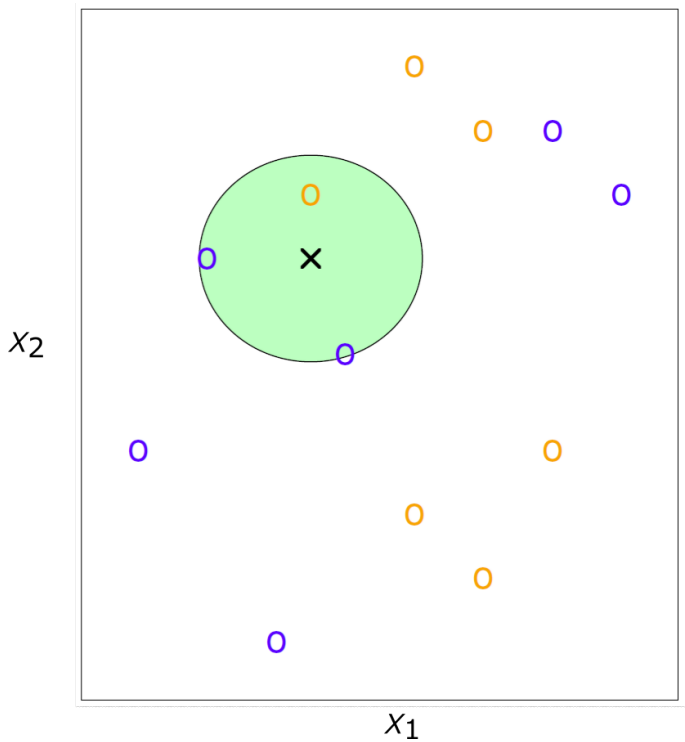
Let's consider a simple example to get some intuition!

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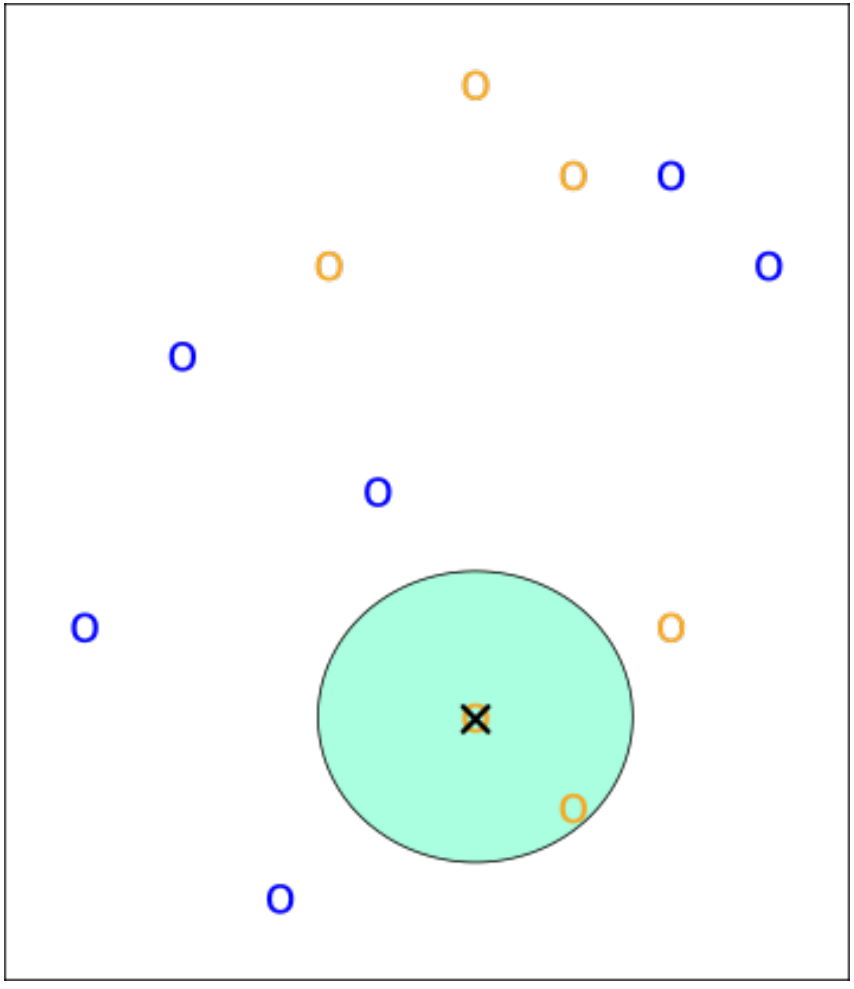
For demonstration, let's consider the toy example again!

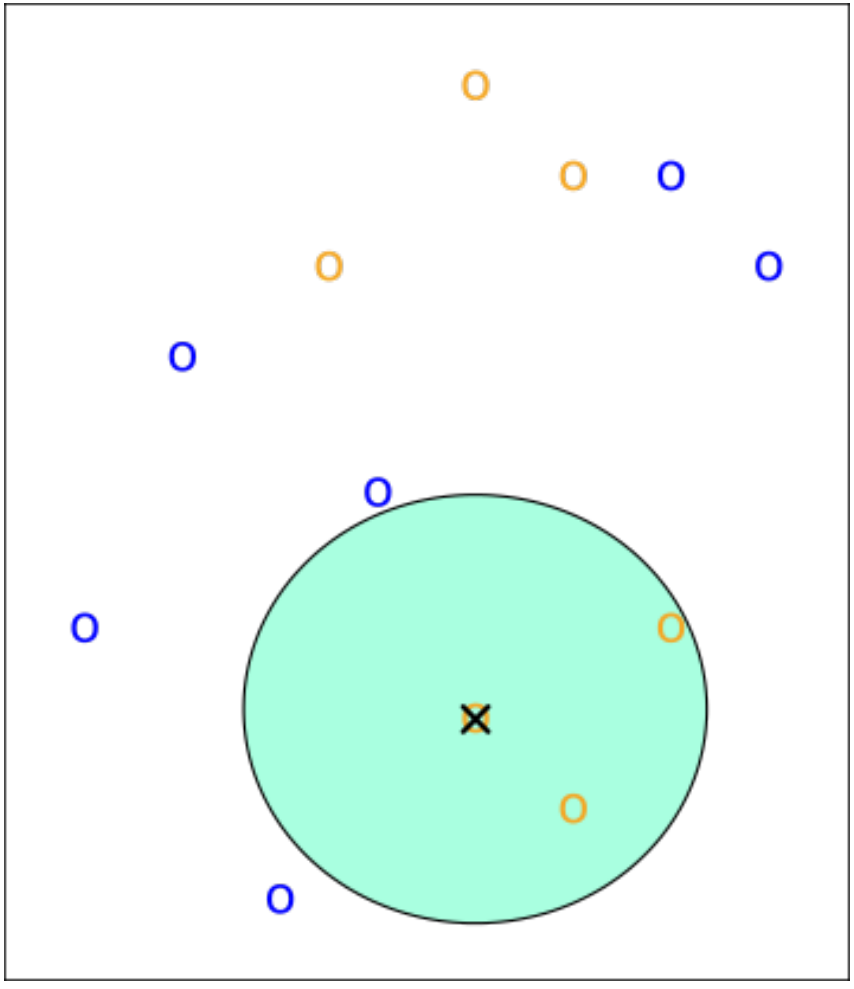
$K = 1$

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



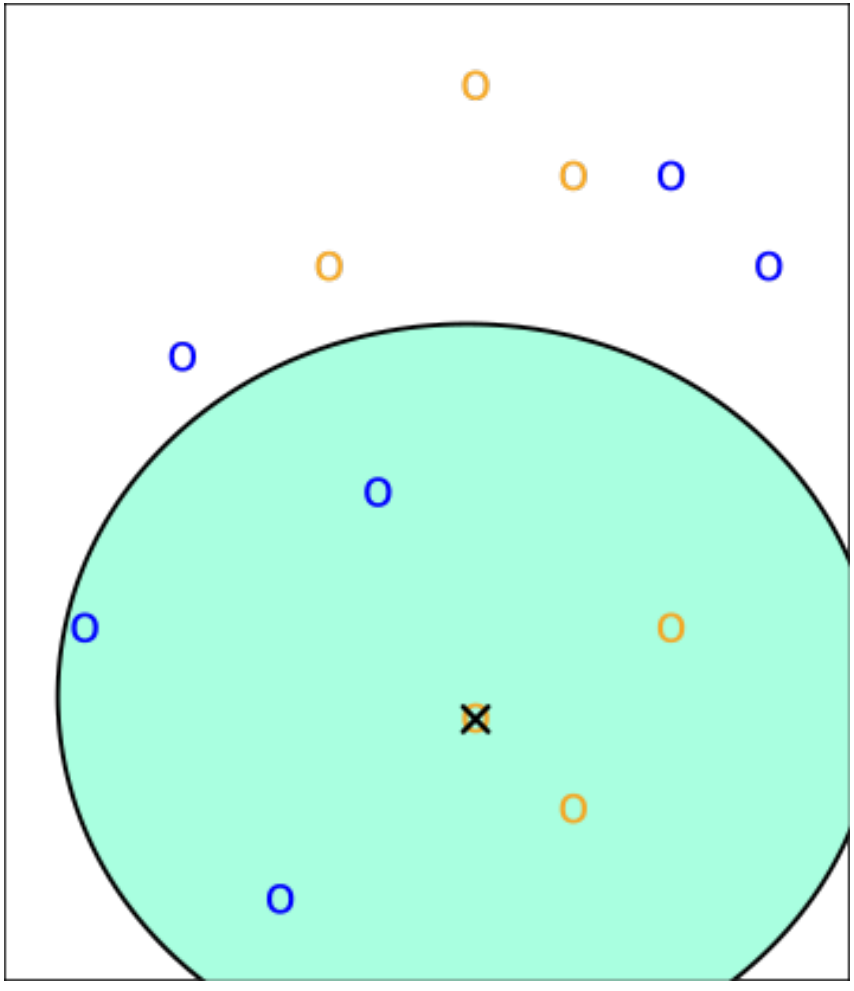
$K = 2$

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



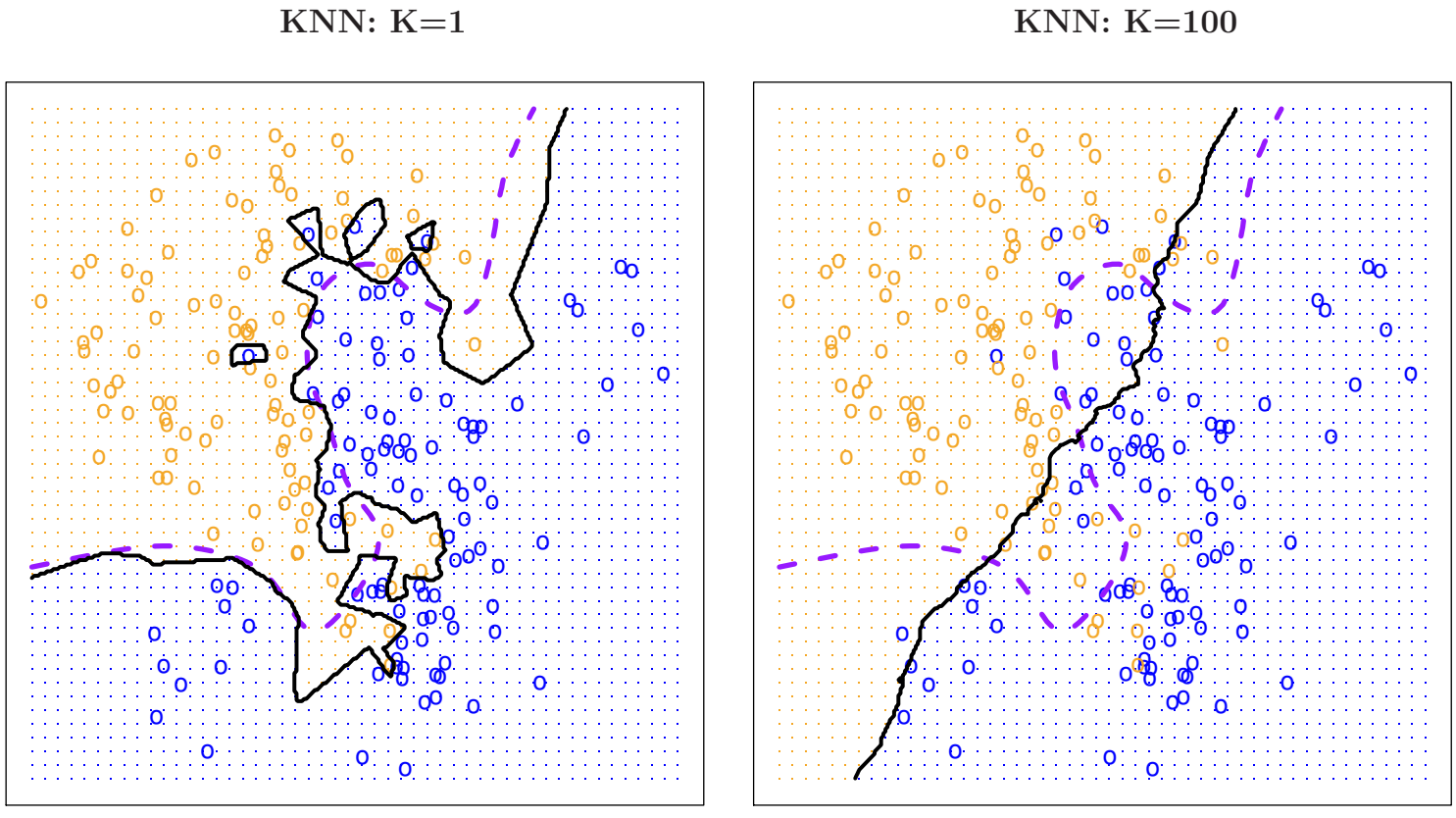
$K = 5$

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



Applying this to all obs → *prediction boundary*

If we apply KNN-prediction to *all training observations*, one by one—for different K—we get the following *prediction boundaries* (black lines):



- 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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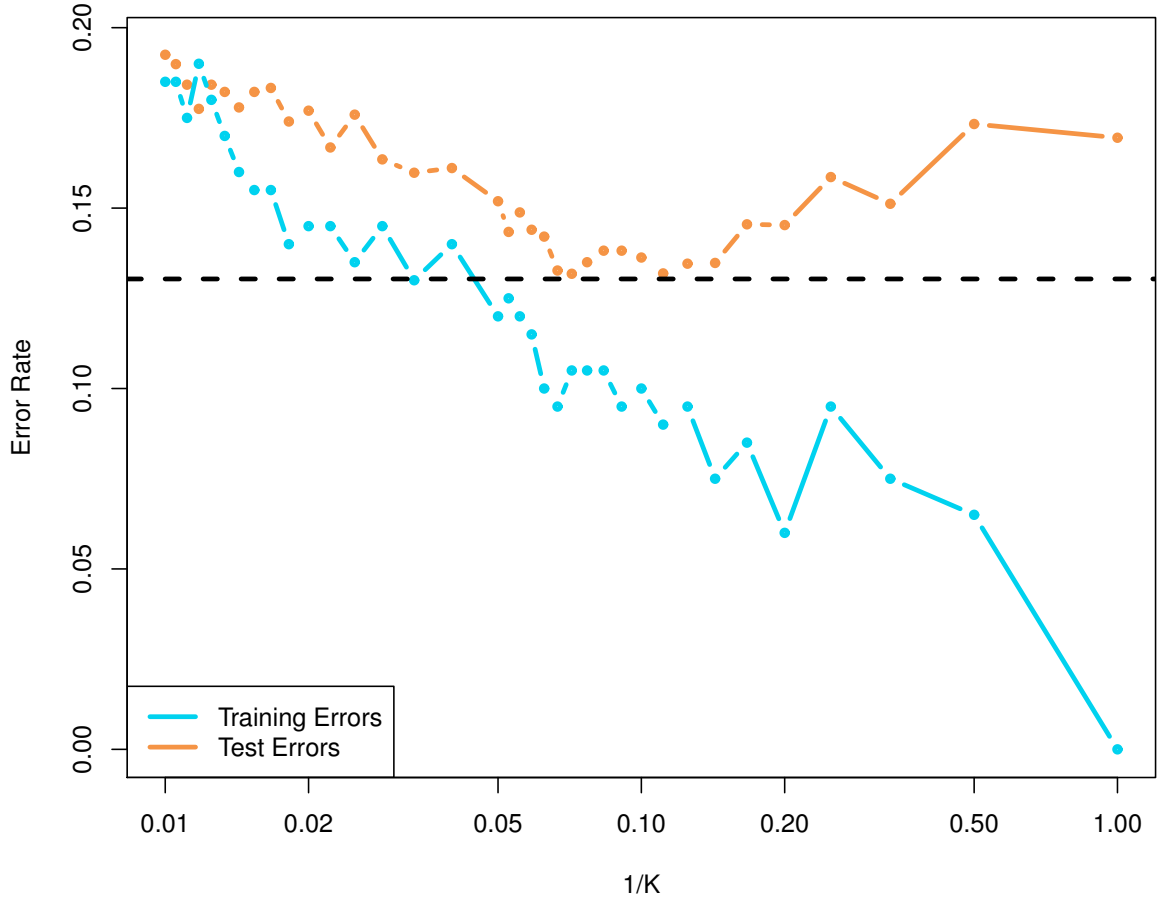

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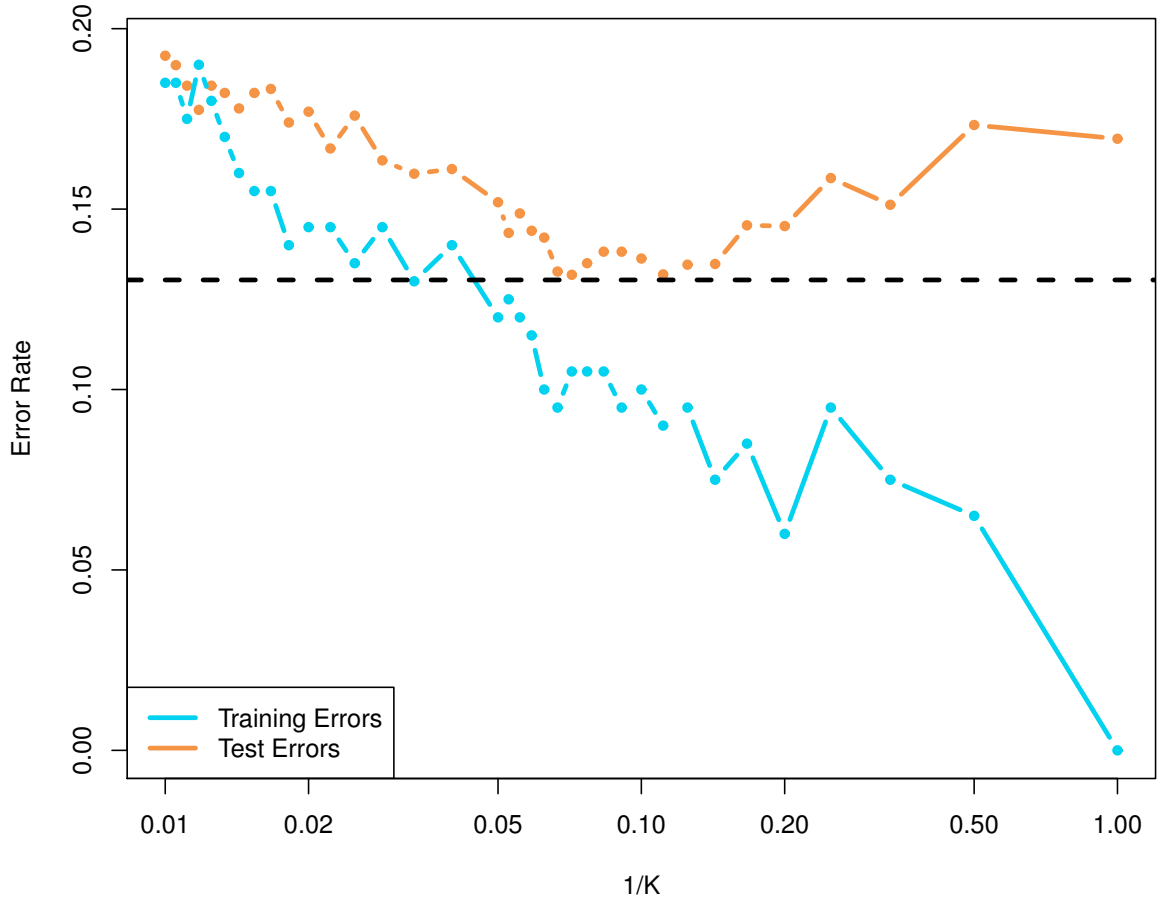

How to choose K? Surprise, surprise: **cross-validation**!

Pros and cons of KNN

Pros

- Highly flexible — can capture considerable *non-linearity*.
- One single parameter (K) that regulates smoothness — relatively easy to calibrate via cross-validation.
- Simple.

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

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

Cons

- Lack of interpretability — no parameters to say why a given observation was classified the way it was.[1]
- Does not *weight* X_i's based on how predictive they are $\rightarrow$ even more sensitive to inclusion of unimportant features.

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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

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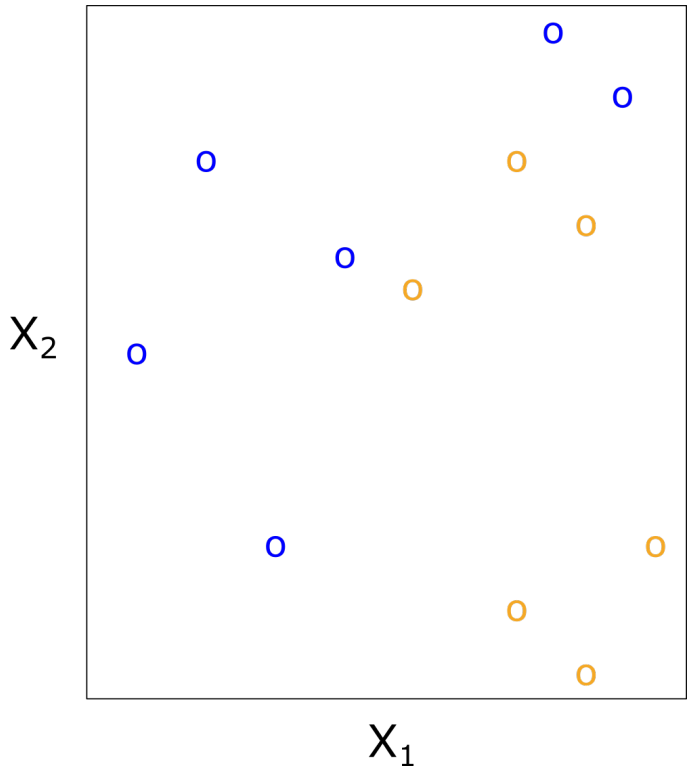

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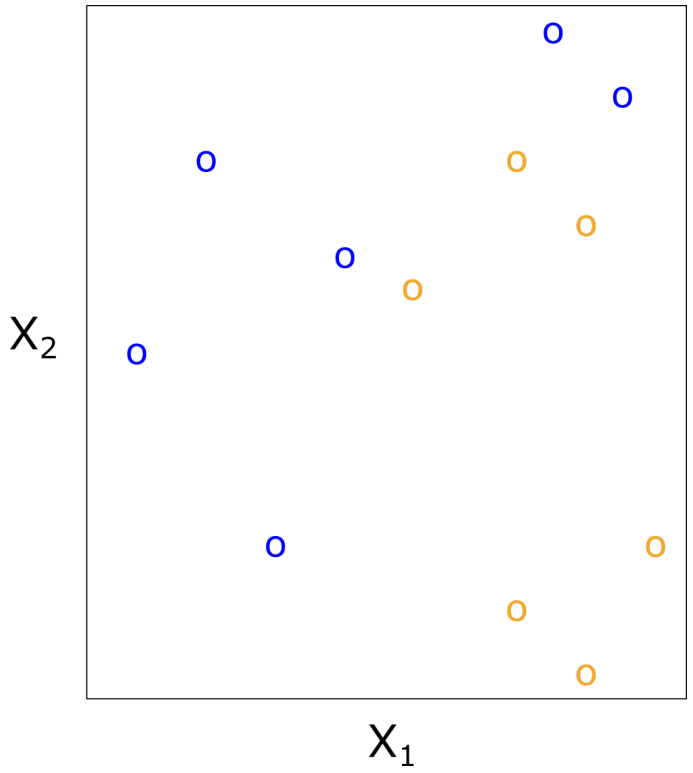

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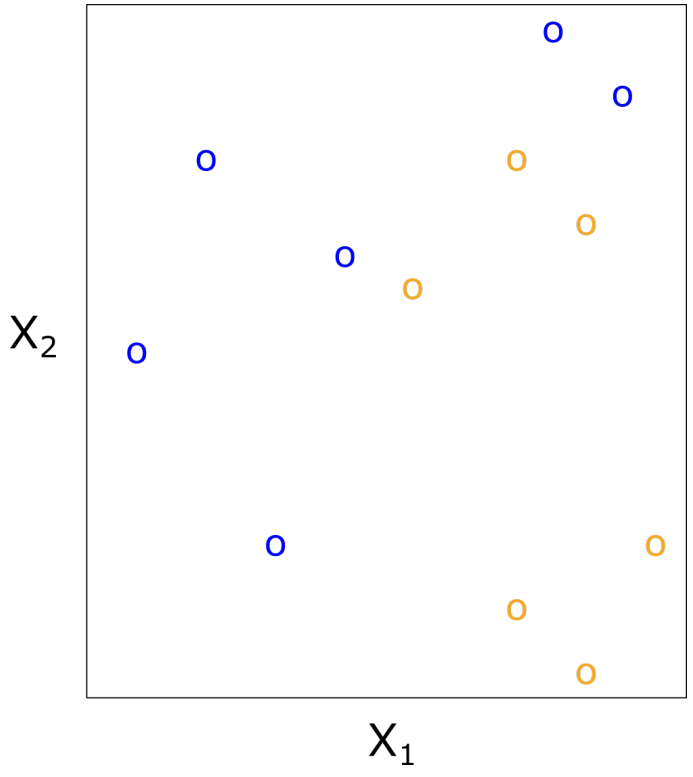

How can we partition this X_1,X_2 space so that:

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

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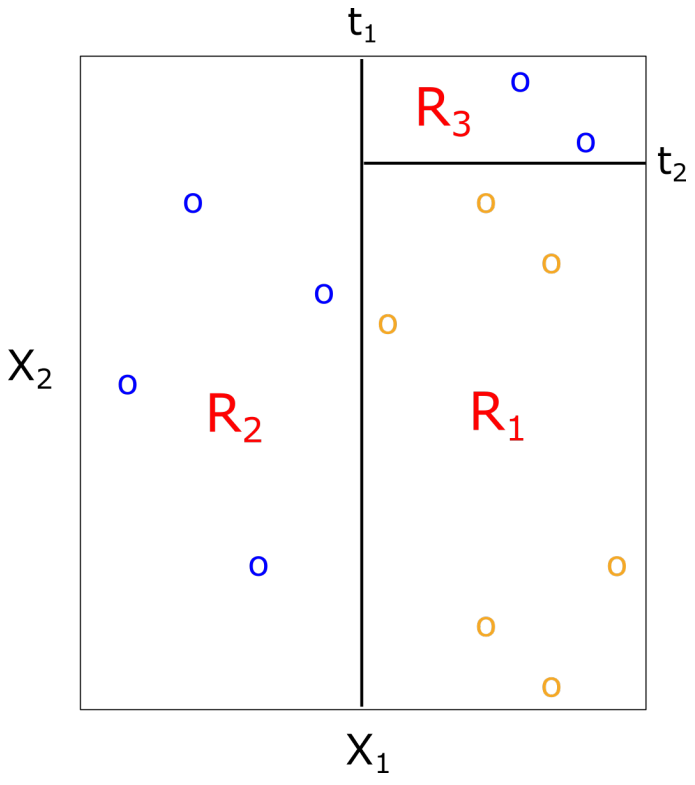

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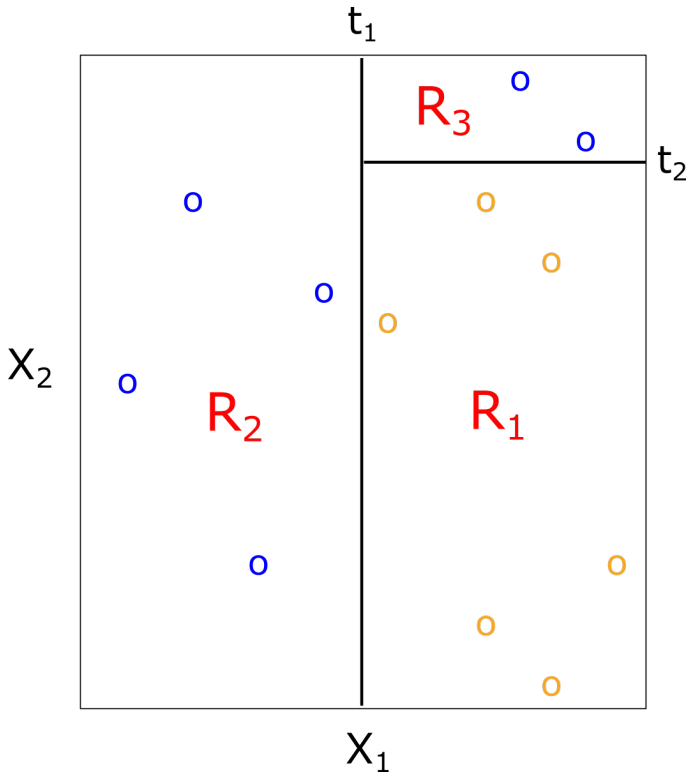

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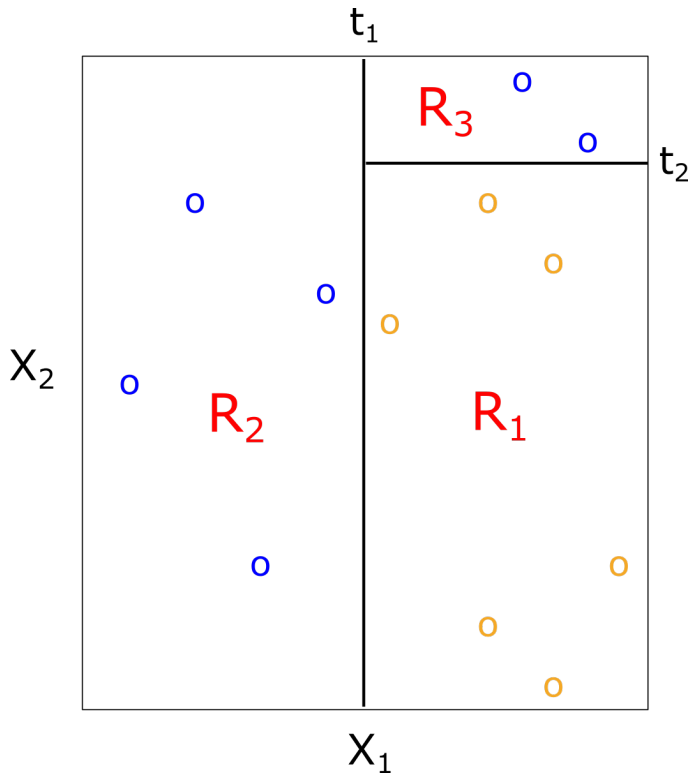

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Let's return to our toy example!

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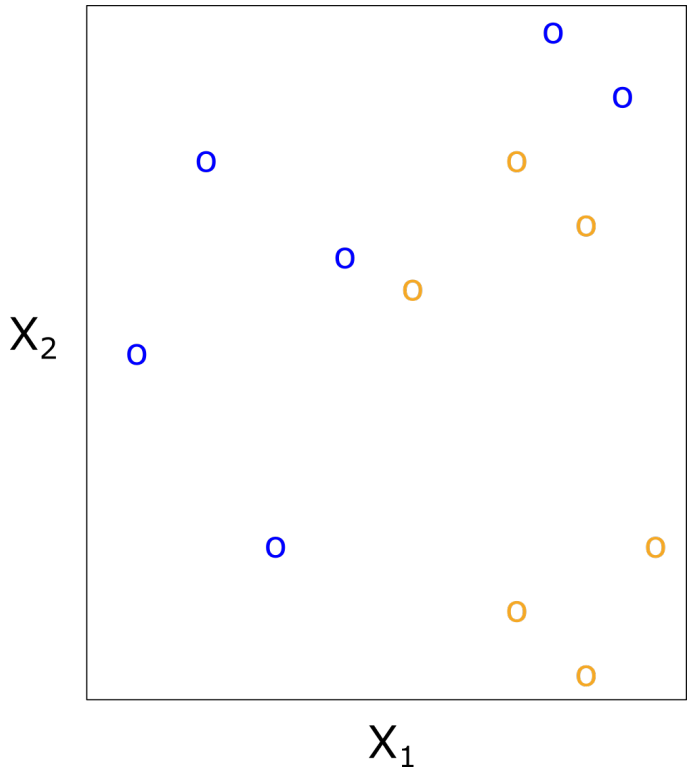

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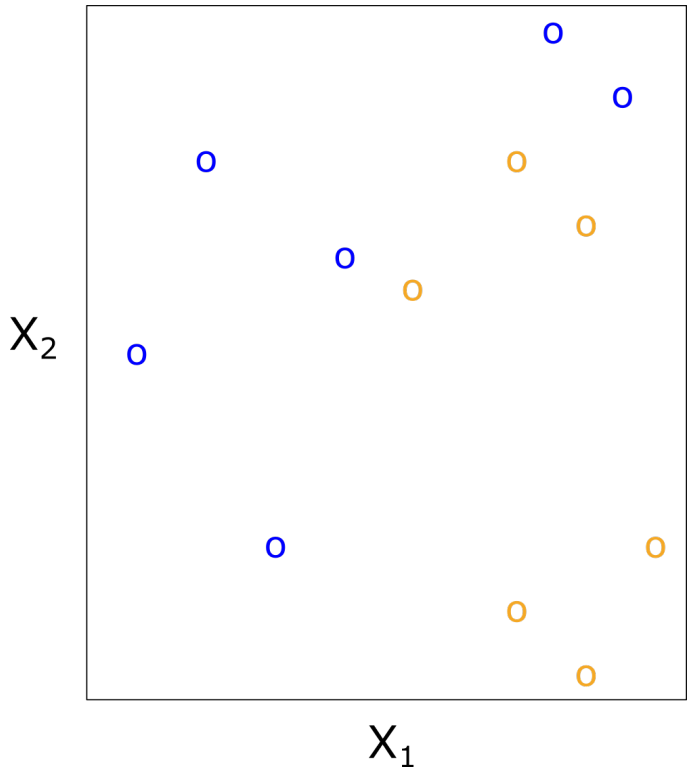
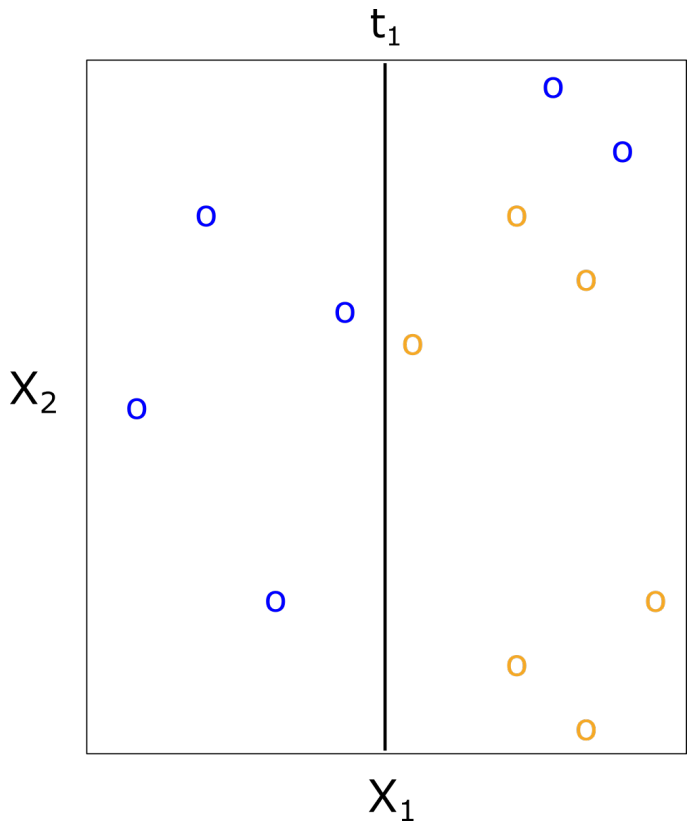


Then we ask—how can we insert a **vertical** (splitting on X_1) or **horizontal** (splitting on X_2) line such that the resulting two regions becomes *maximally more homogeneous*?

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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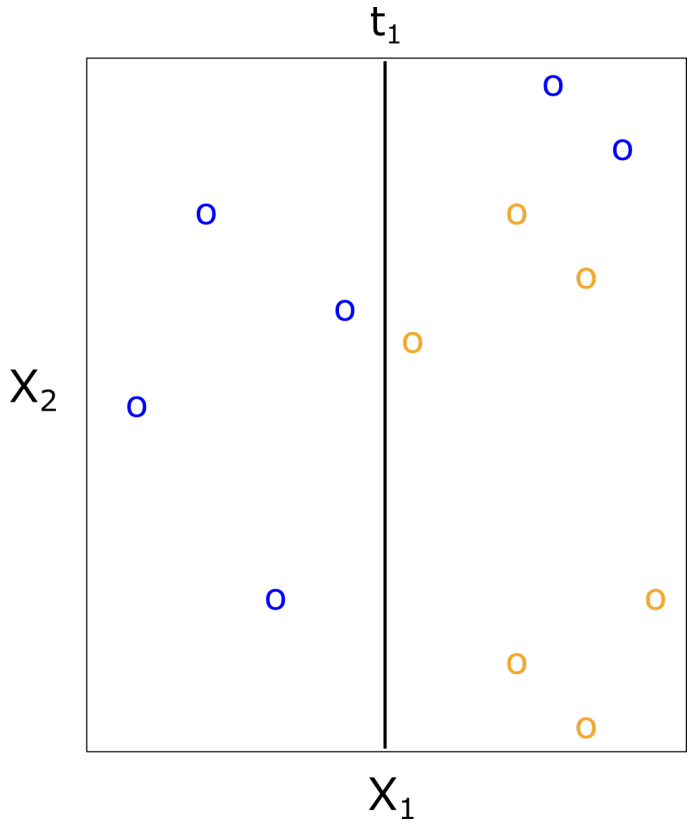

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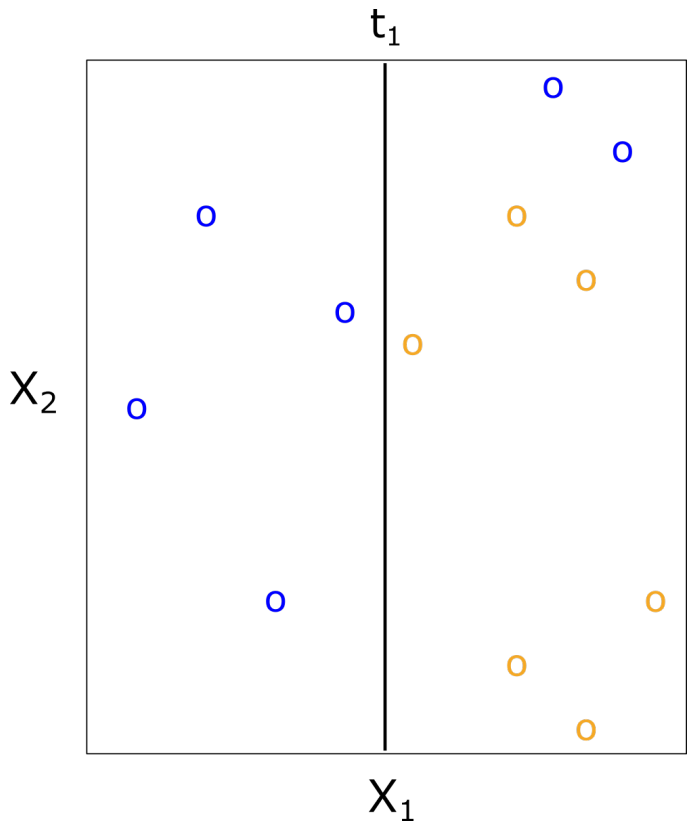

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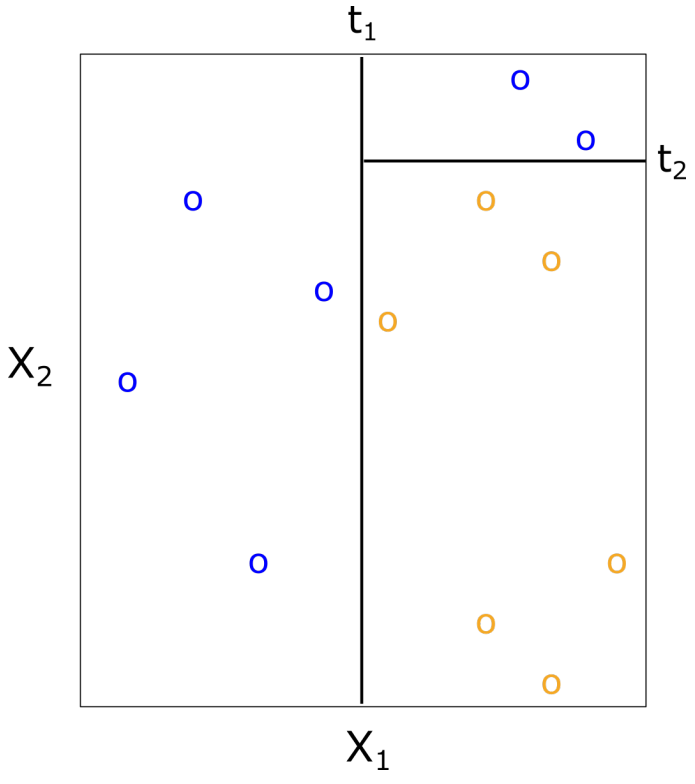
Q: Can we add additional splits that further reduces the error?

Split no. 2

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



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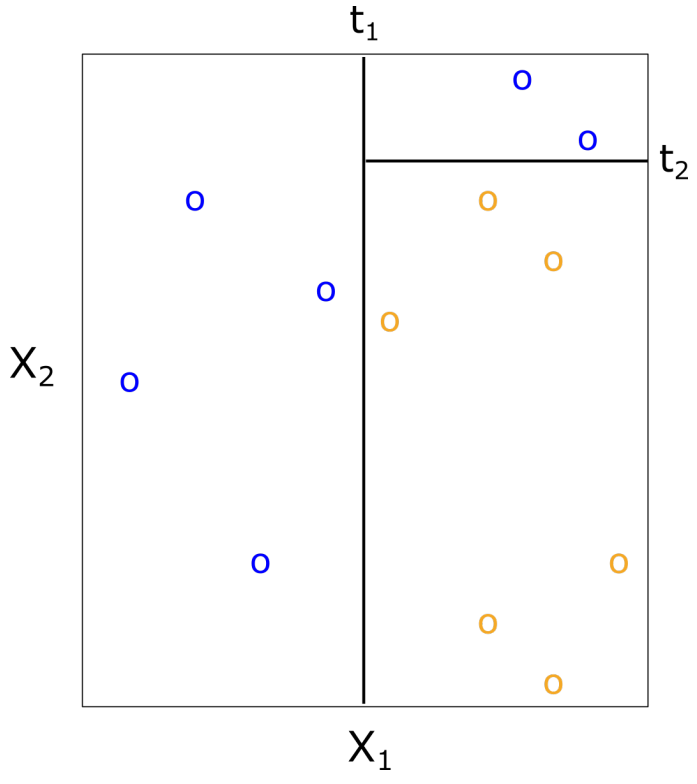
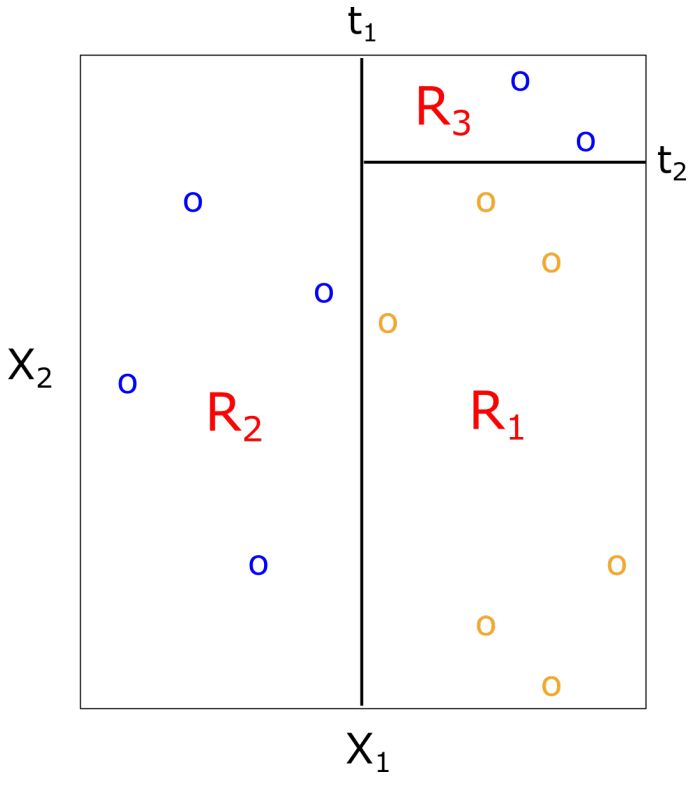


After this, no further improvements are possible, and we retain three regions.

Three-region solution



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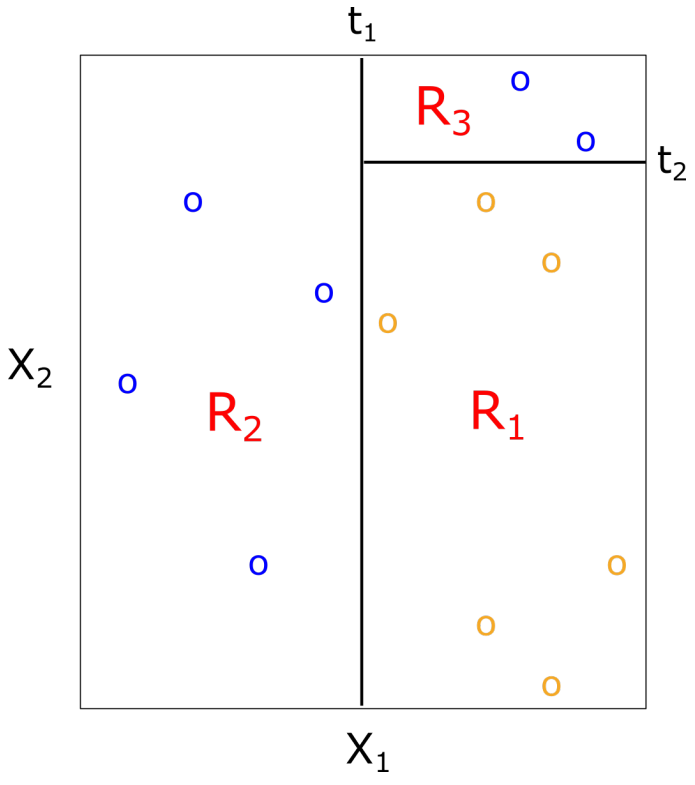

With these regions identified—how do we use them to make **predictions**?

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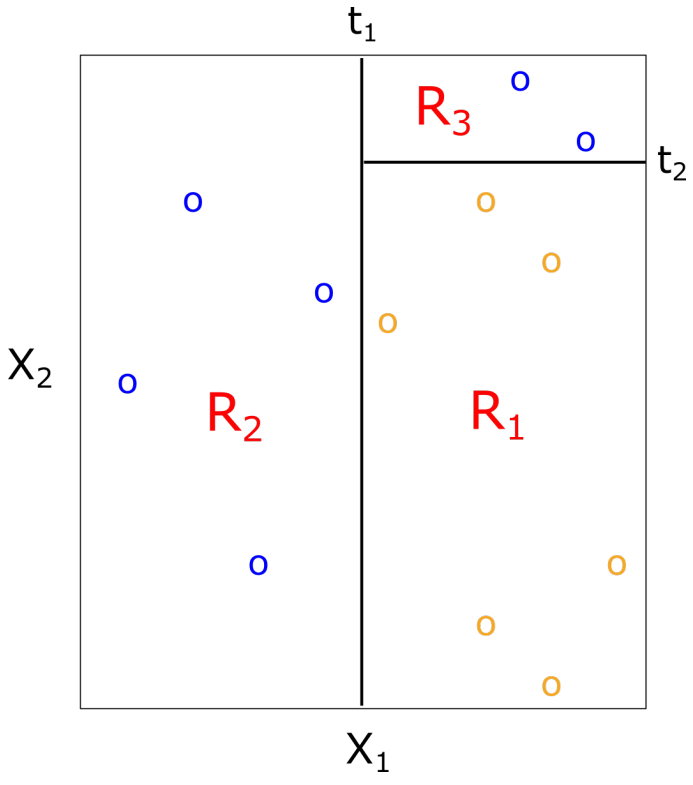
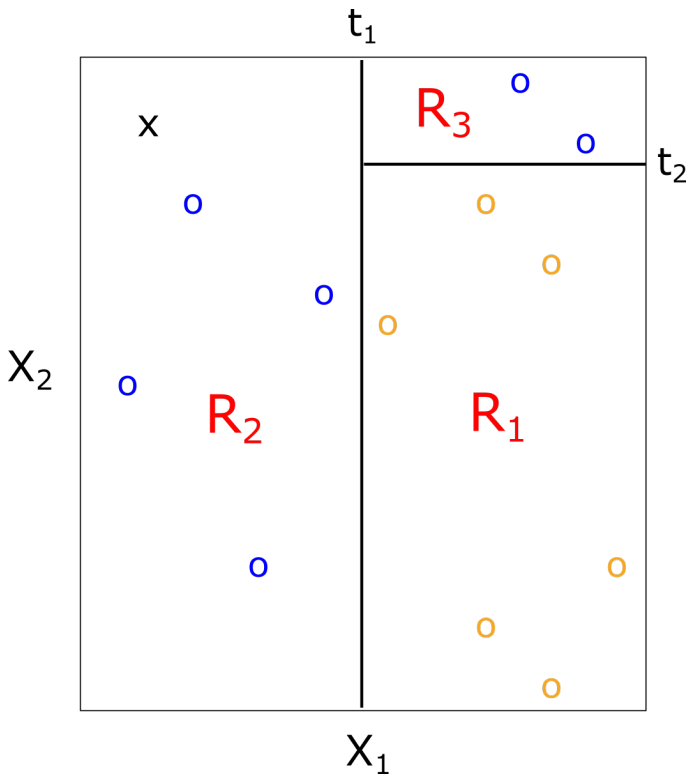


With these regions identified—how do we use them to make **predictions**? Again:

- *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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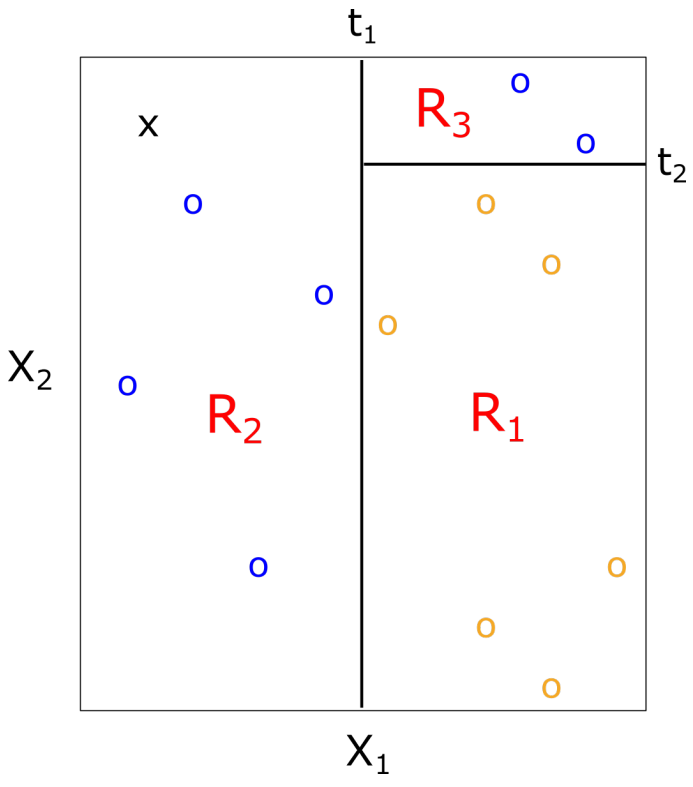

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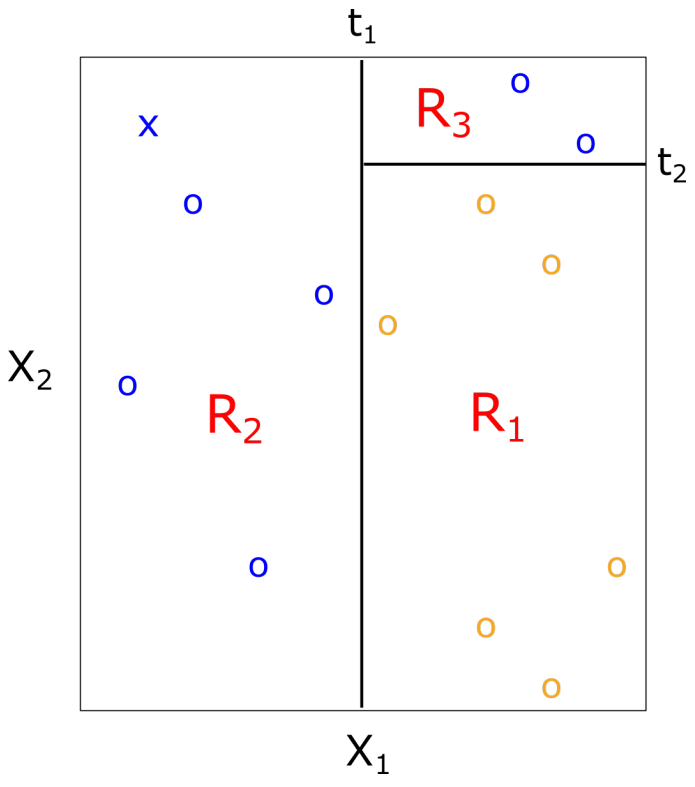

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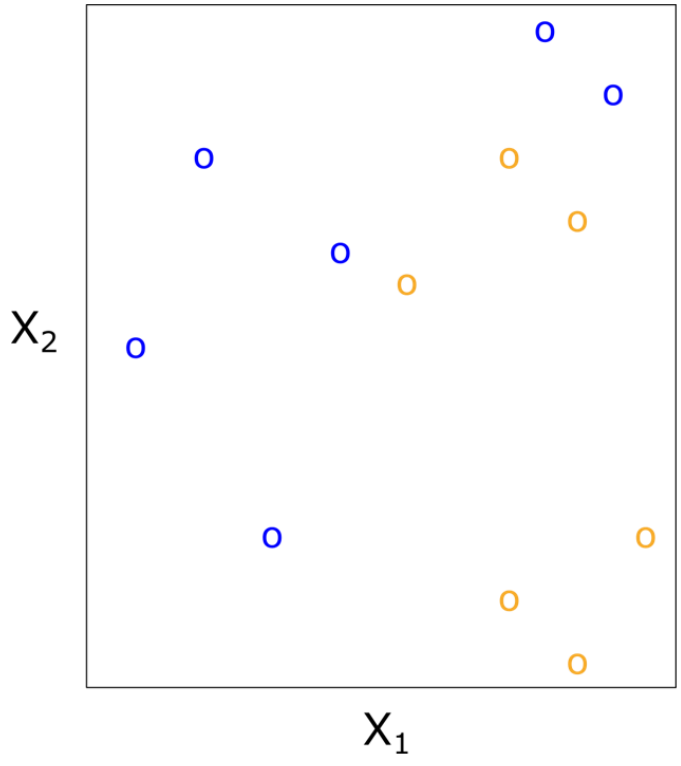

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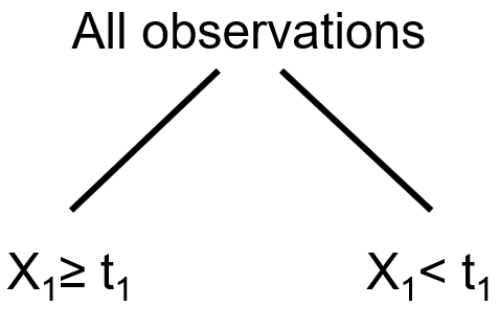
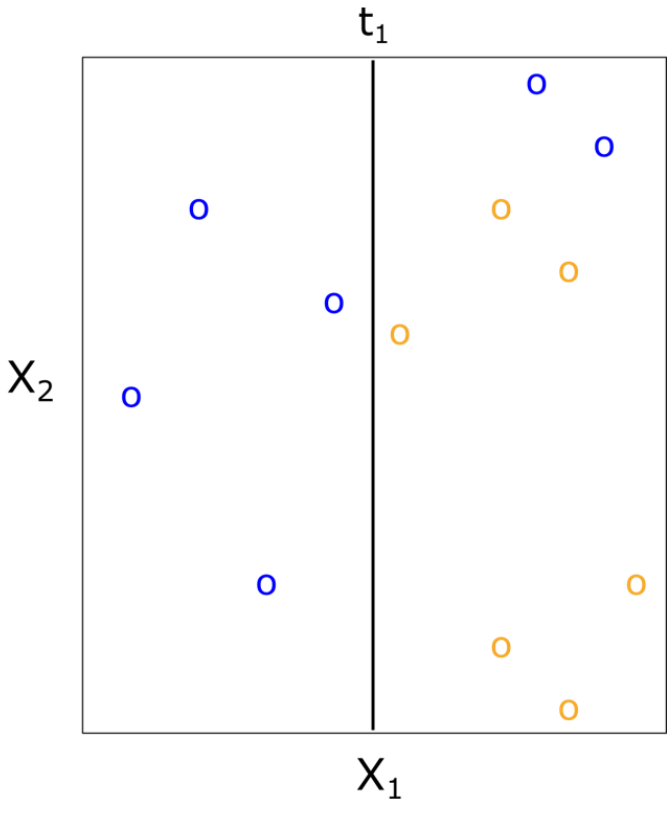
Saved to this PC





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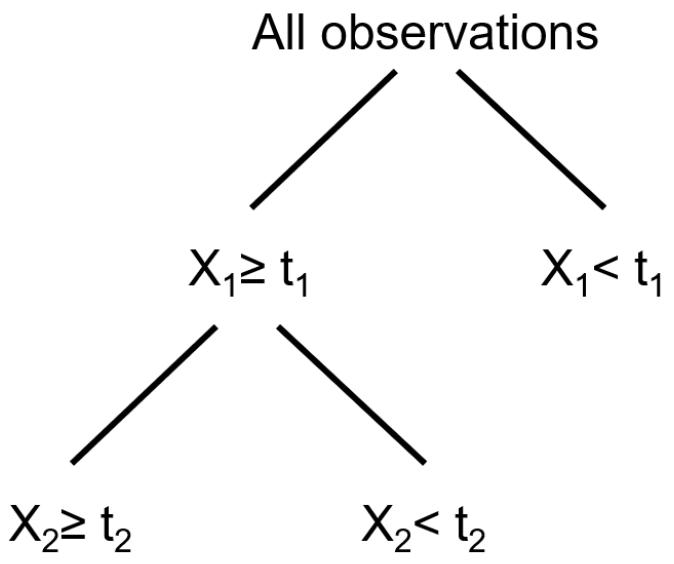

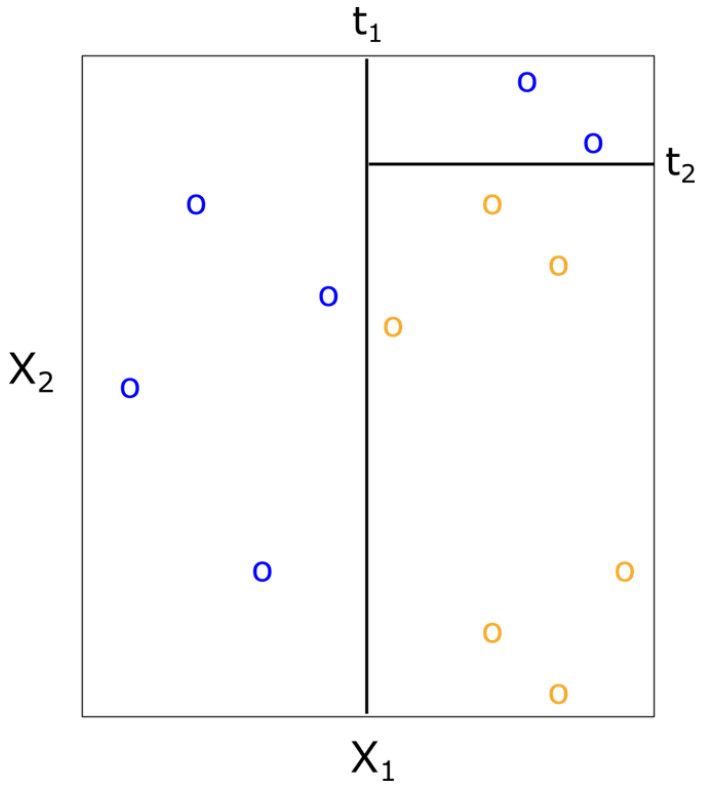

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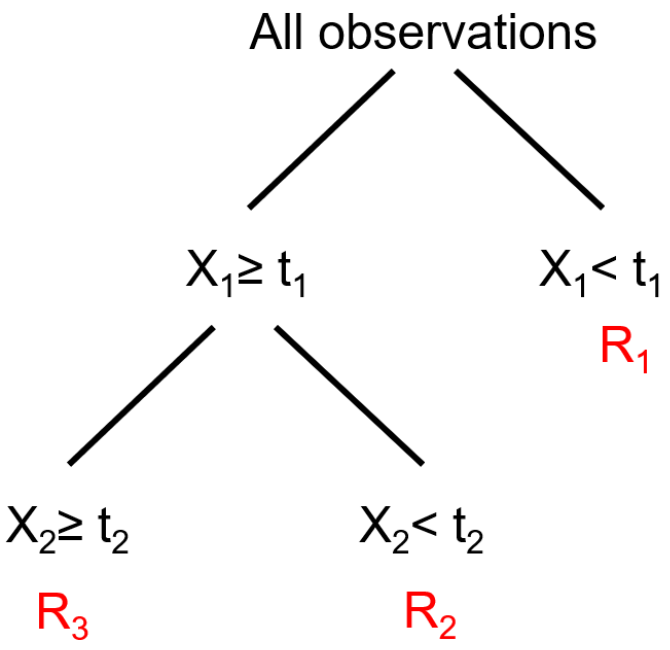

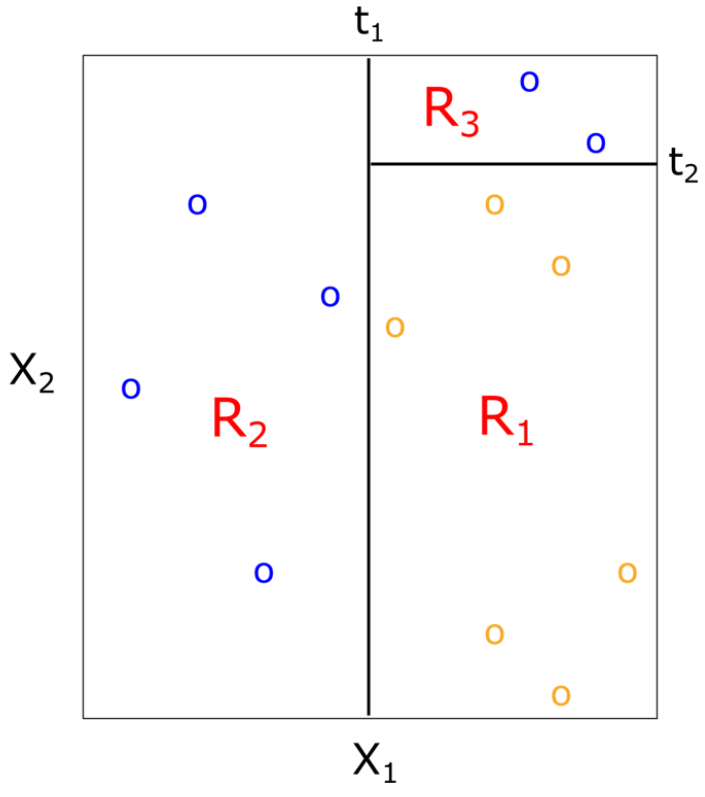

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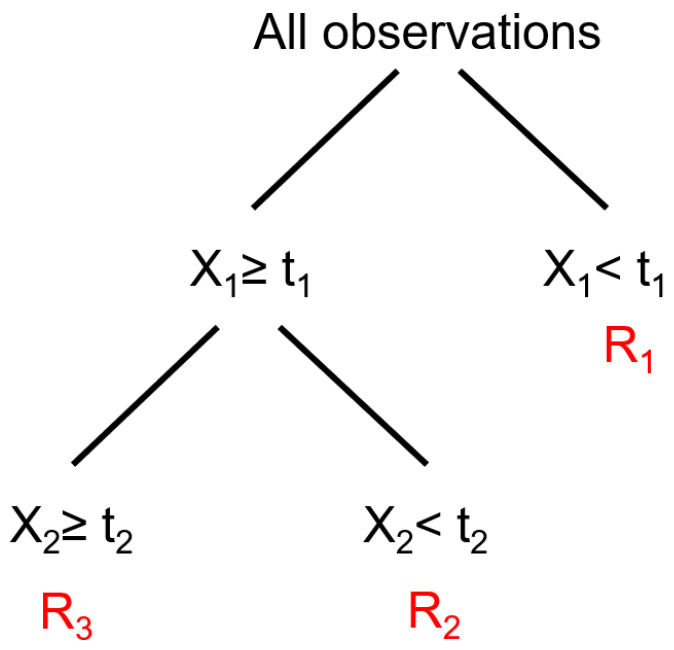

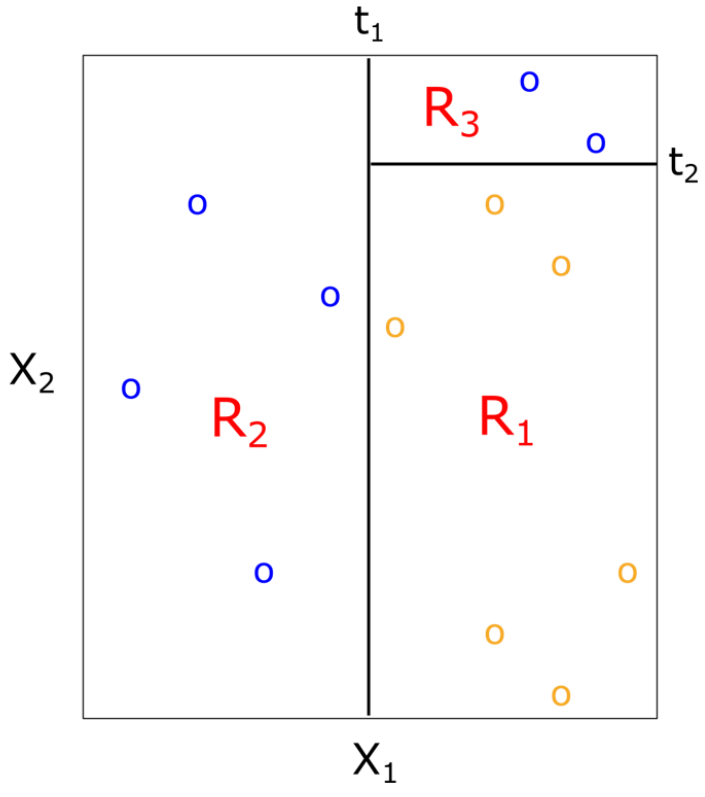

This is neat—our predictions become very interpretable!

Interpretation of toy example

- Small $X_1 \rightarrow$ blue
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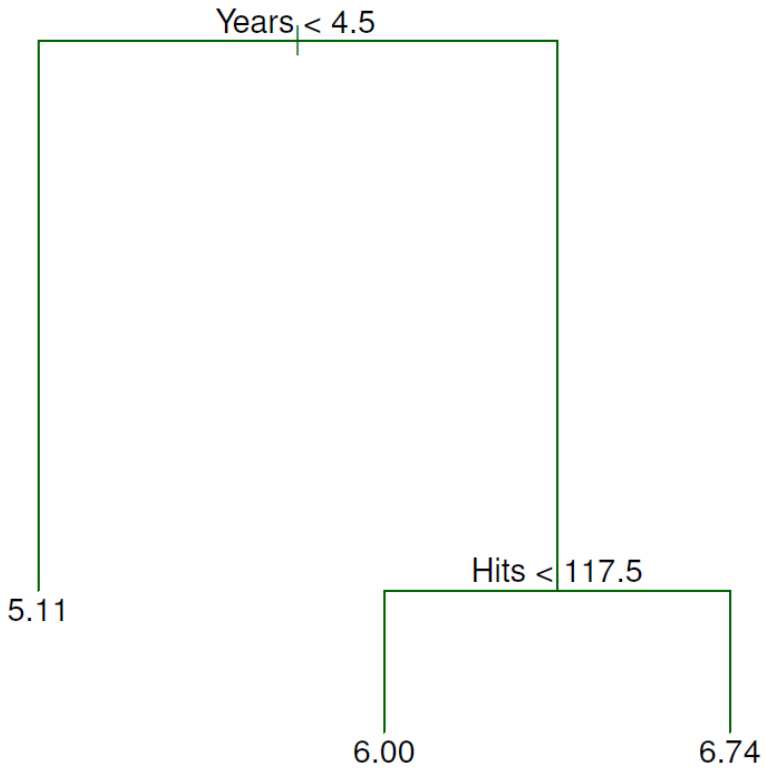
Here we see something else which is neat — the *automatic discovery* of important *non-linearities* & *interactions*!

ISL example



- A simple *regression tree* to predict baseball players' (log) salary, using two variables, *Years* and *Hits*.

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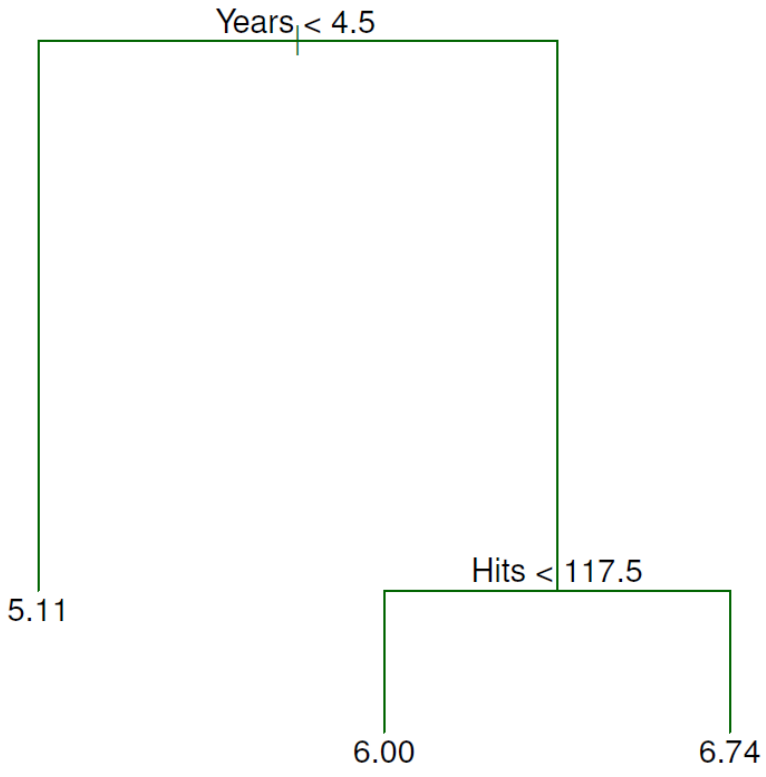

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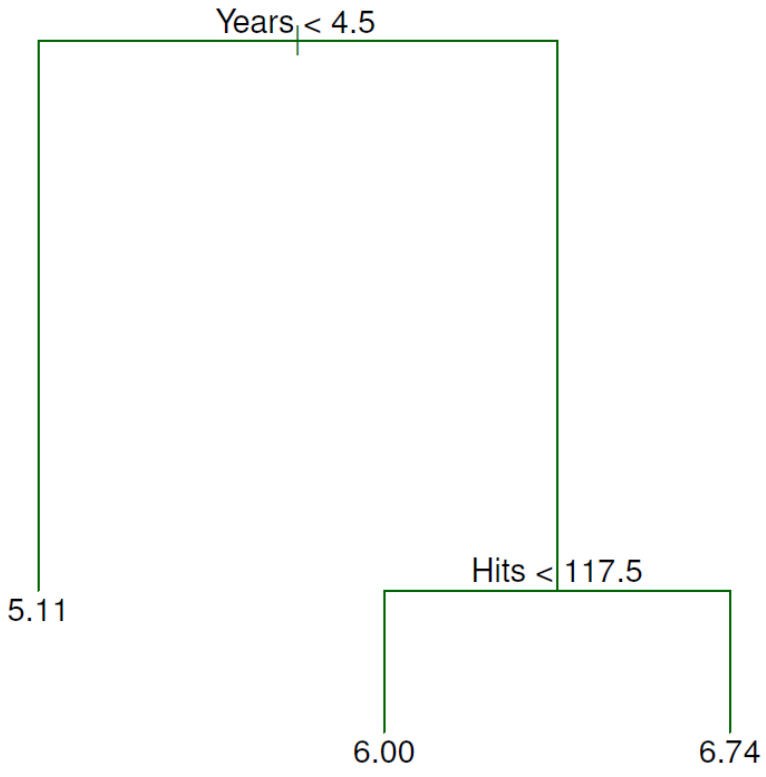

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Natural Q—how *deep* to grow the tree?

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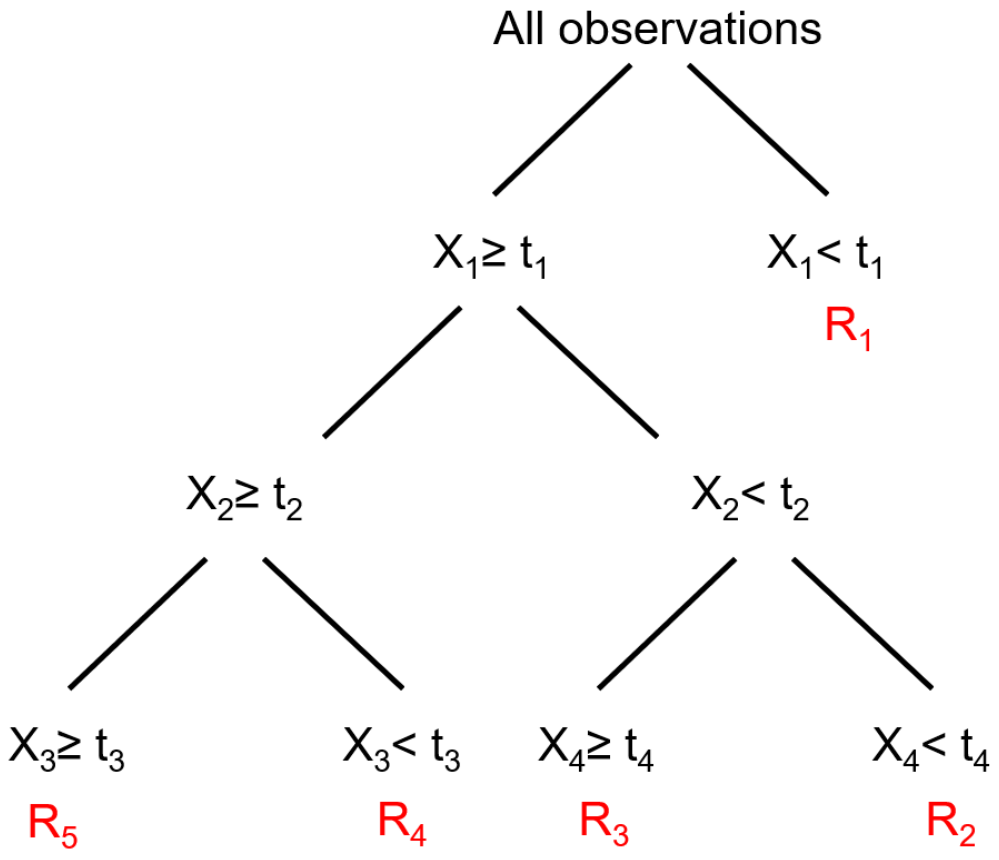
- Q—How do we set α?? Surprise, surprise: **cross-validation**!

Illustration of pruning (toy example)

Suppose this is our *fully grown tree* T_0:



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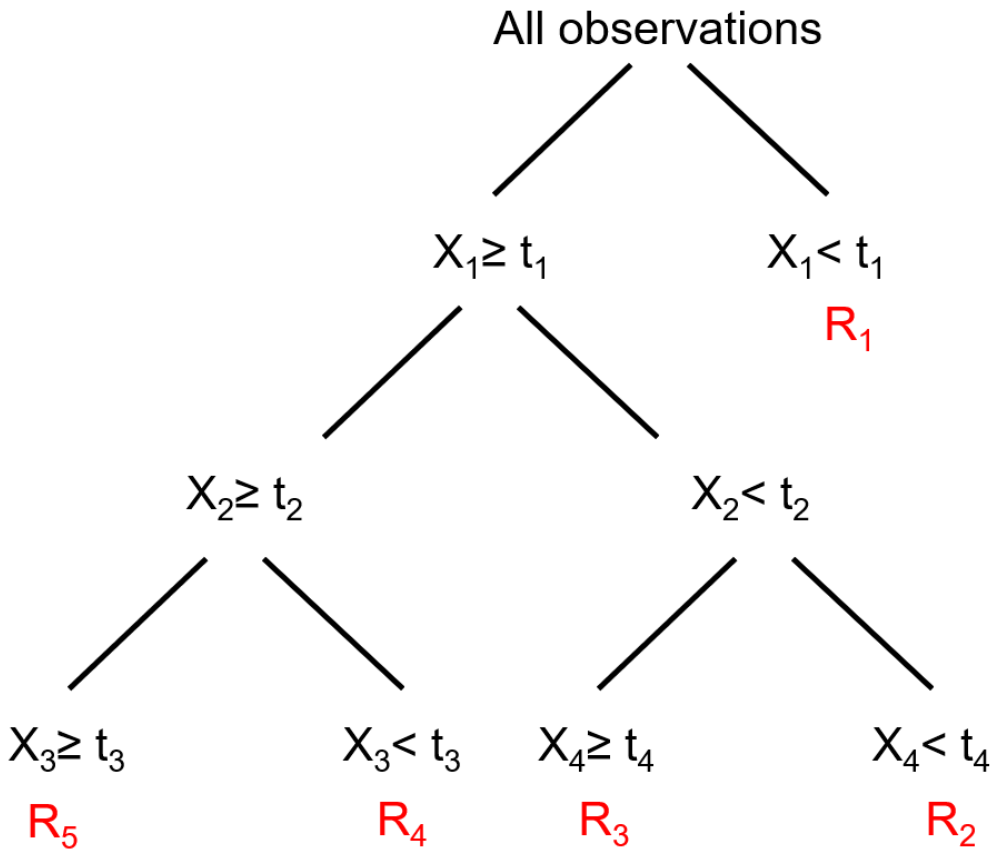

Then—to prune—we *reconsider* the last split.

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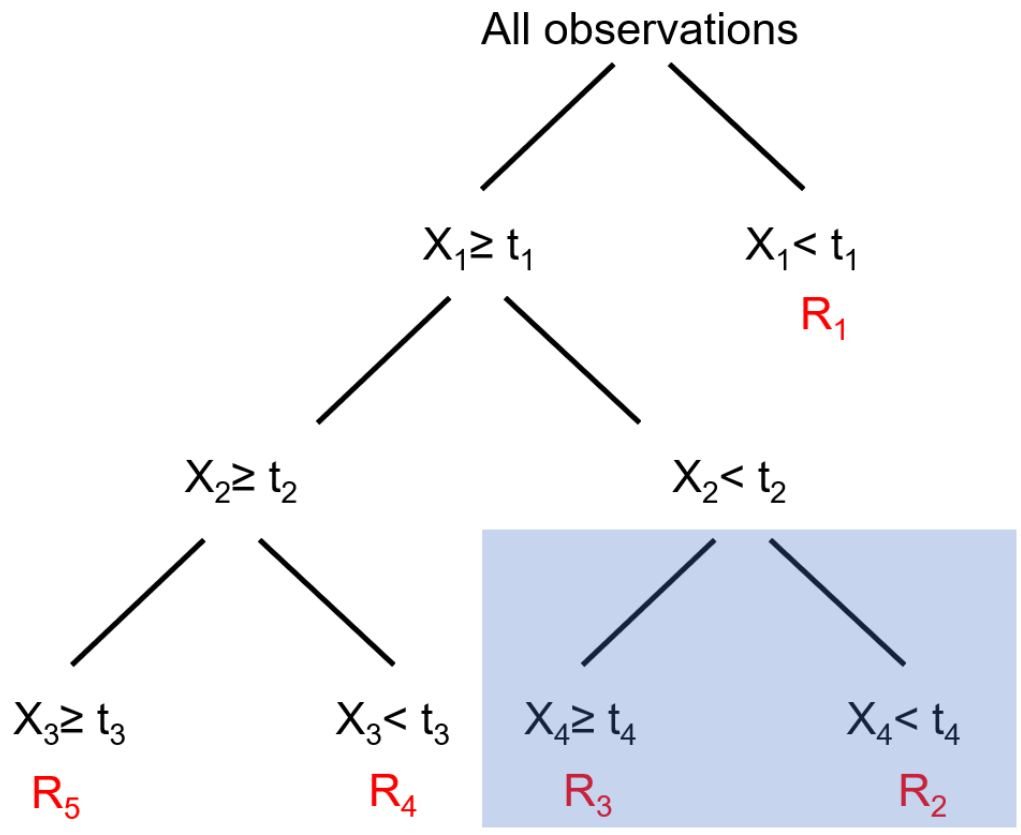

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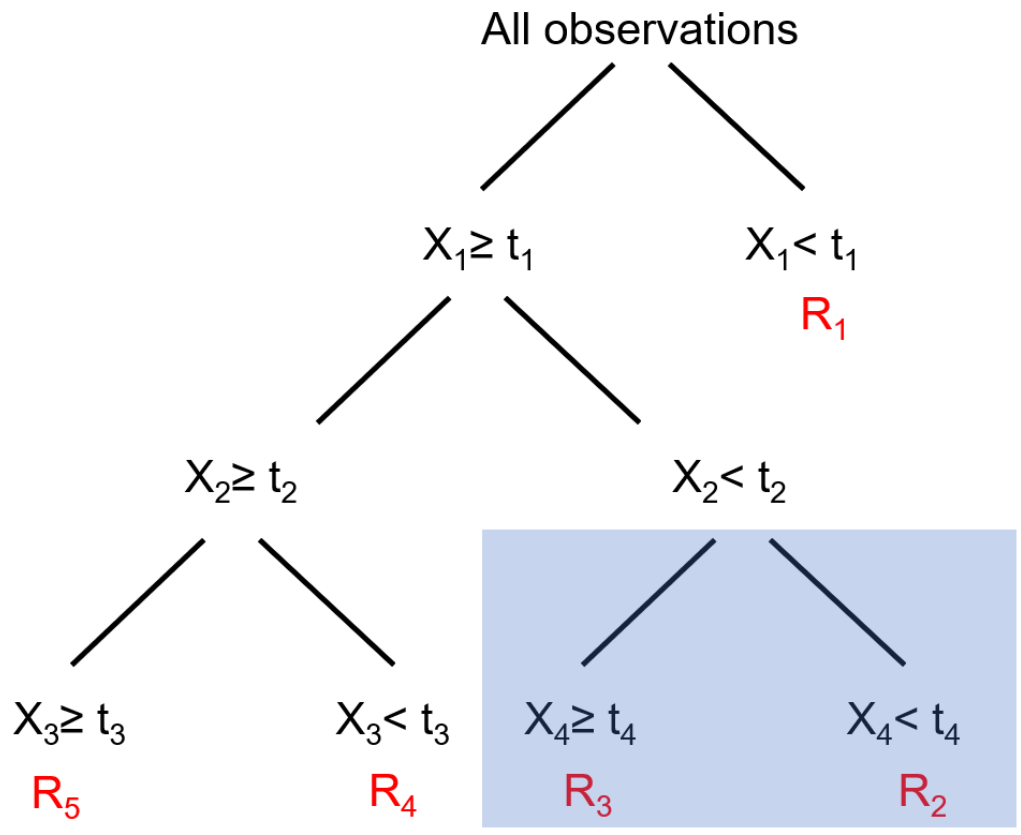

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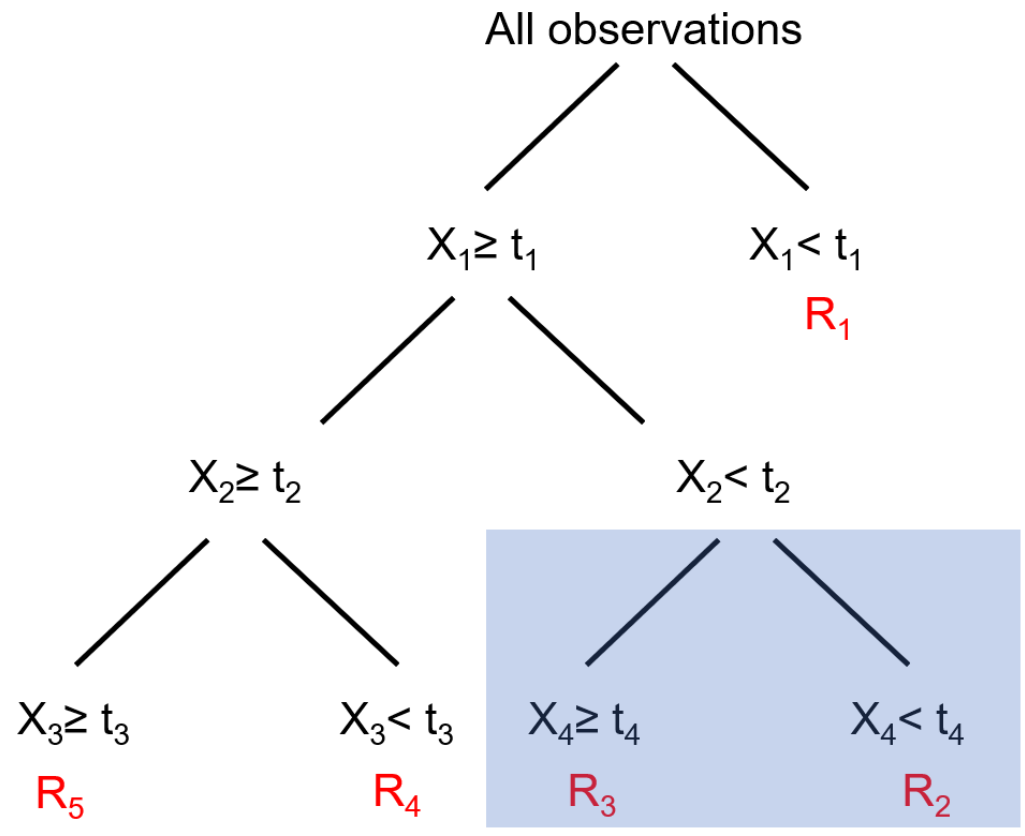

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- It is ($\times 2$) because we add *two extra nodes* in the split.

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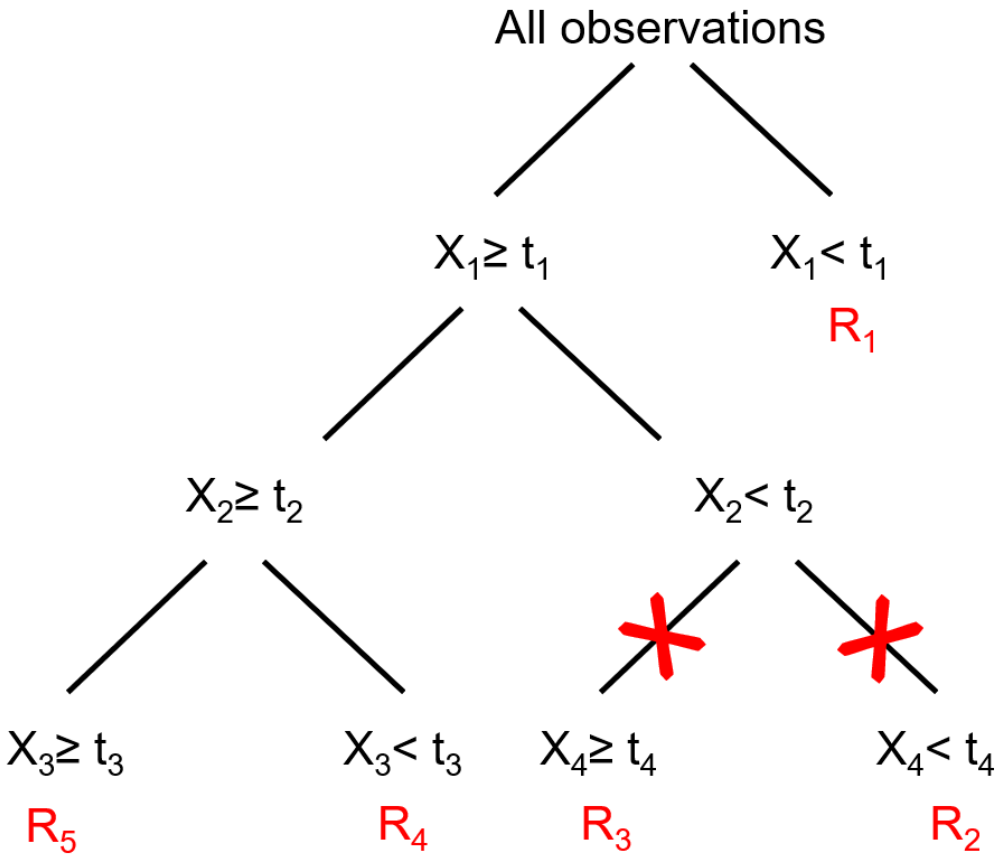

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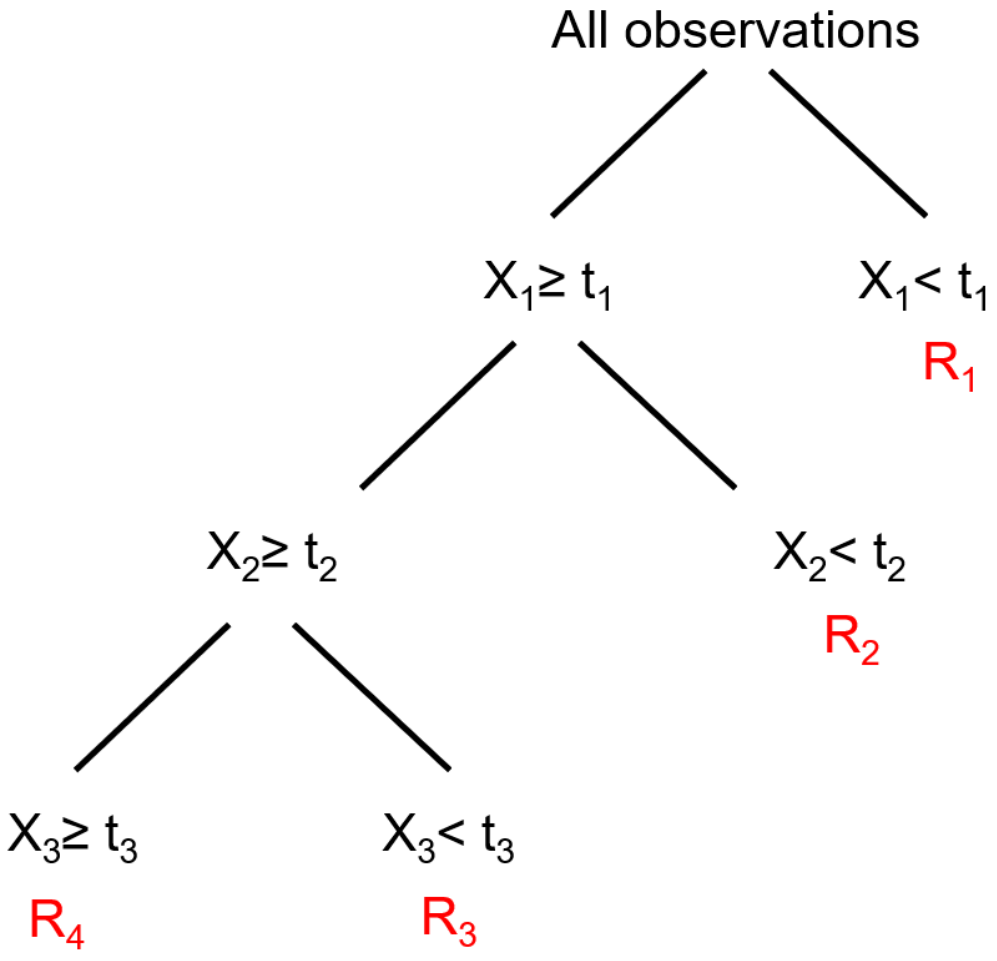

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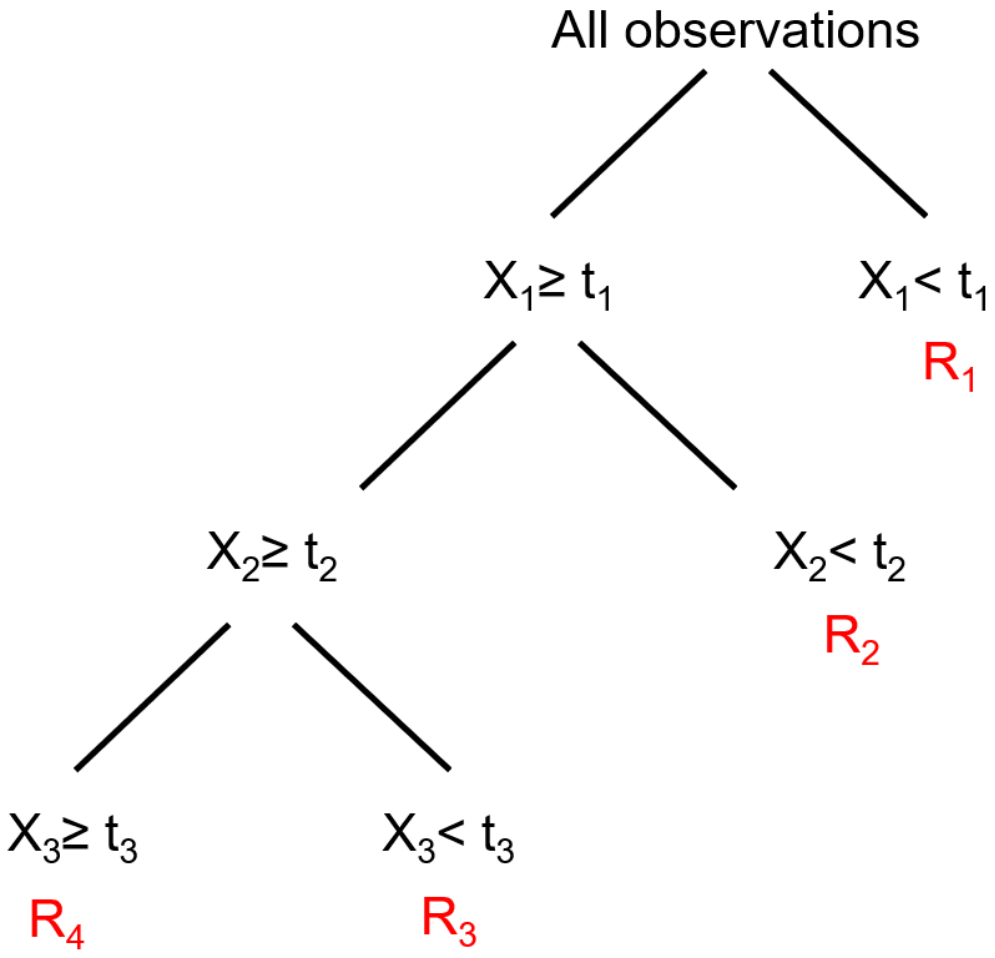
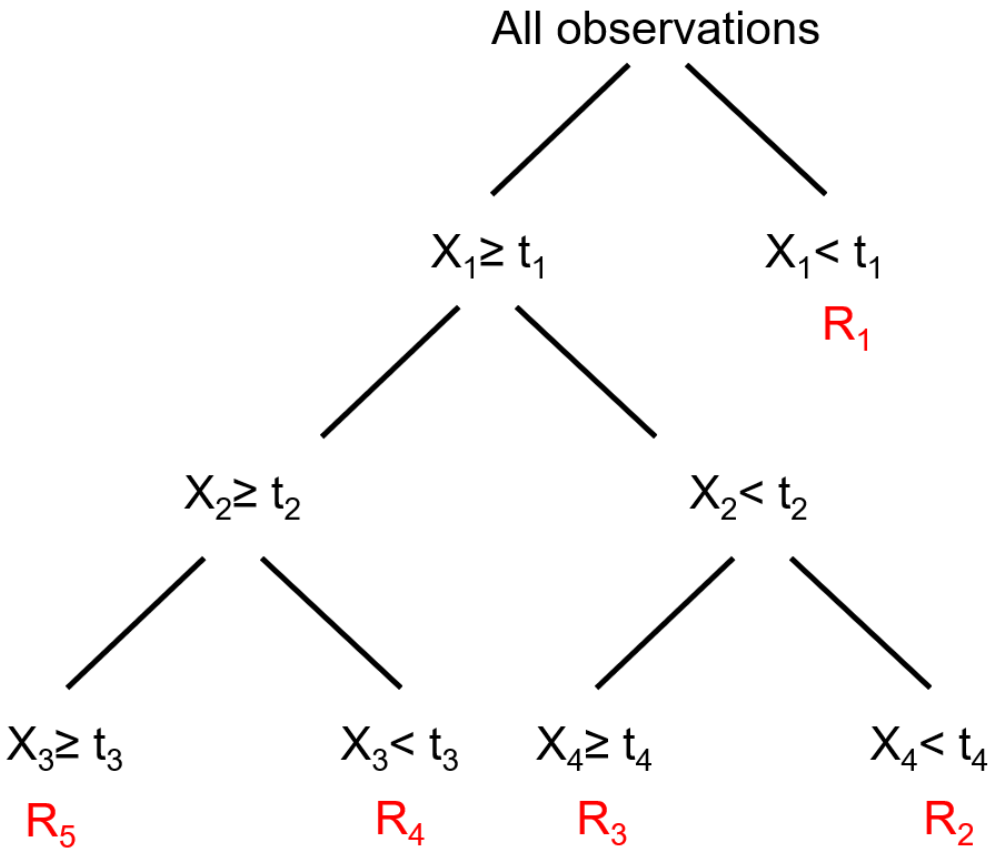


Now that we have some intuition for how *pruning* works—what is the effect of α?

Effect of α? Extreme #1: $\alpha = 0$

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



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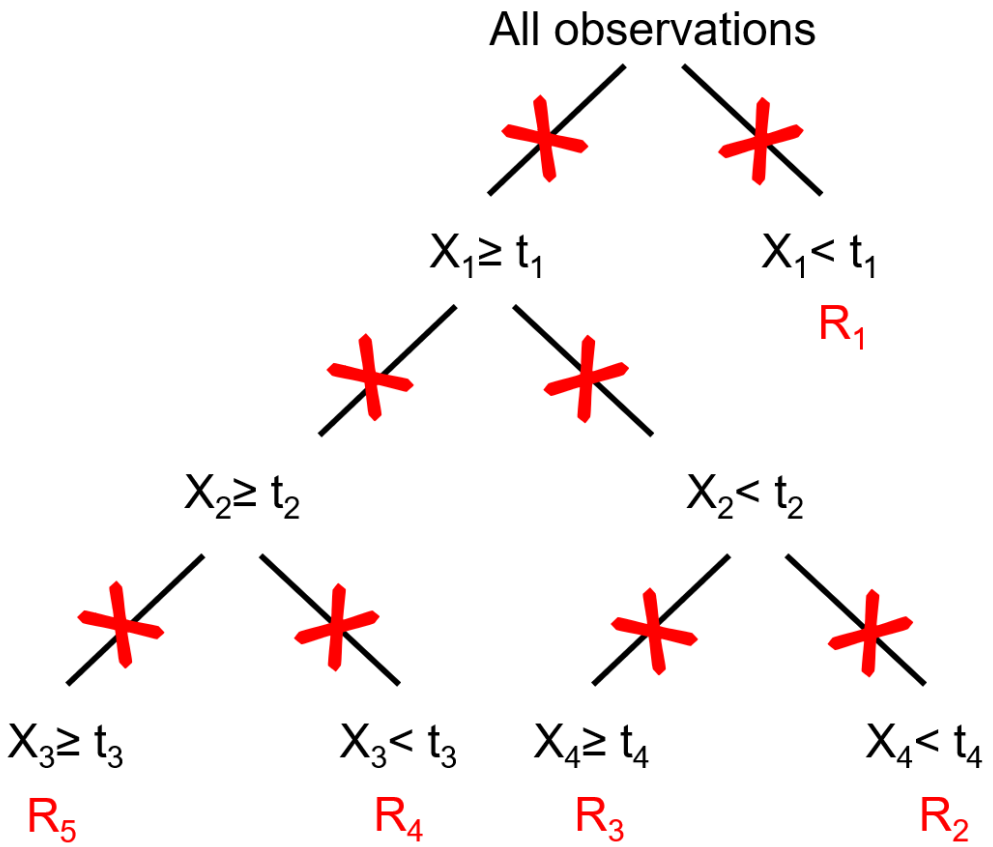

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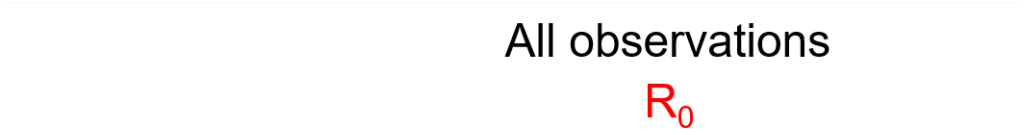
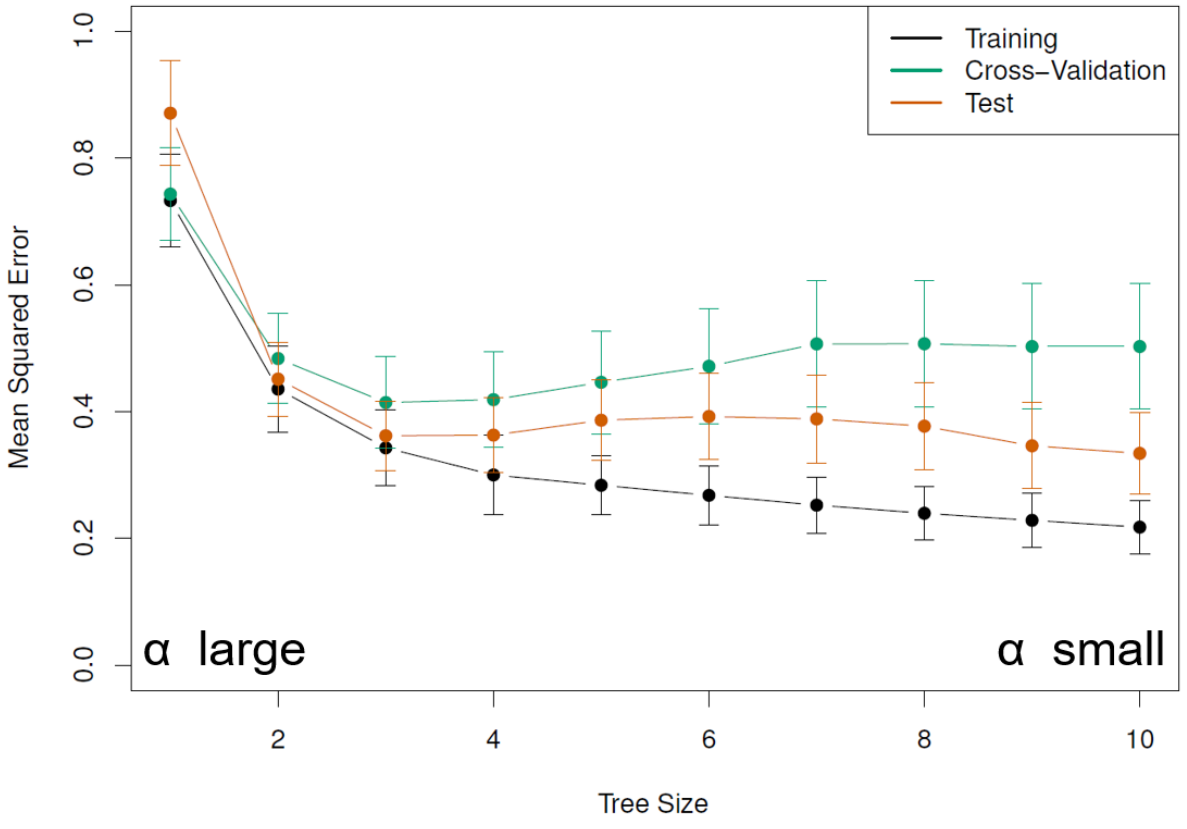


More generally: *tree-size* vs. *test error* (ISL, Fig. 8.5)



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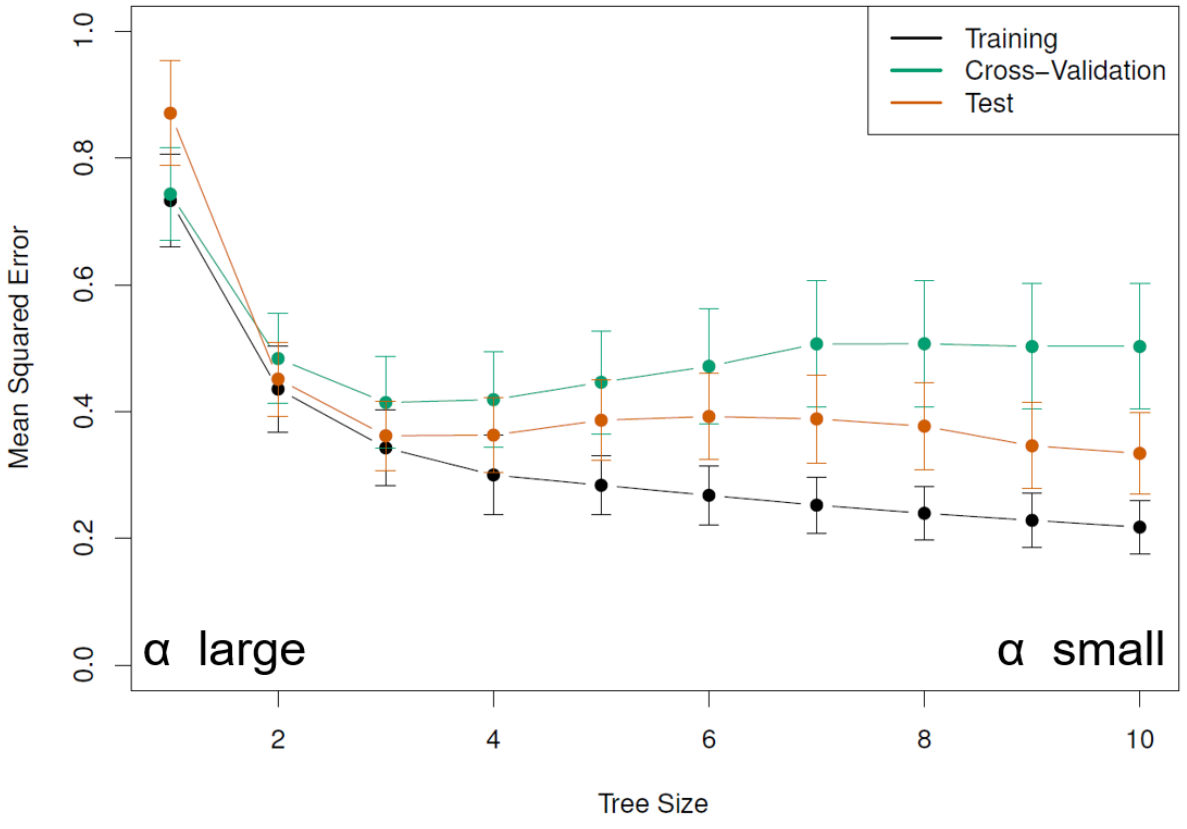

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- But test error only improves initially, then it starts to worsen.

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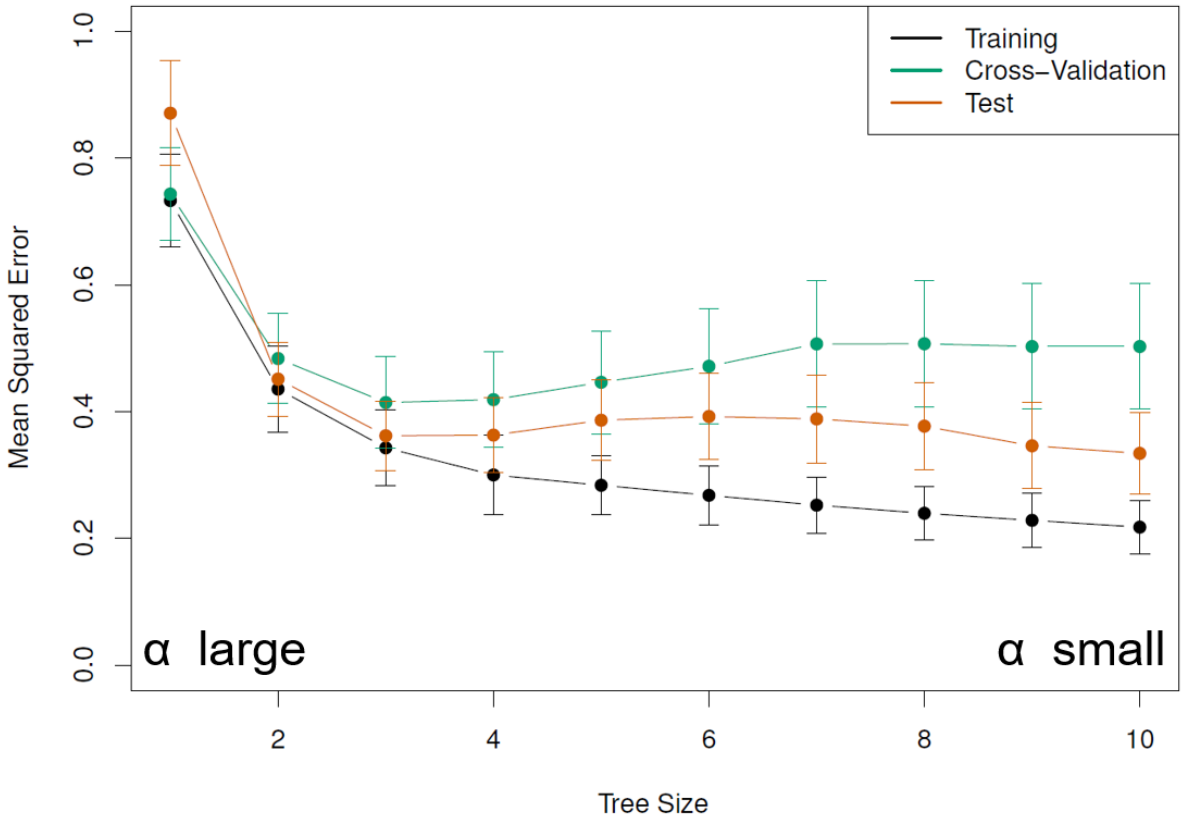

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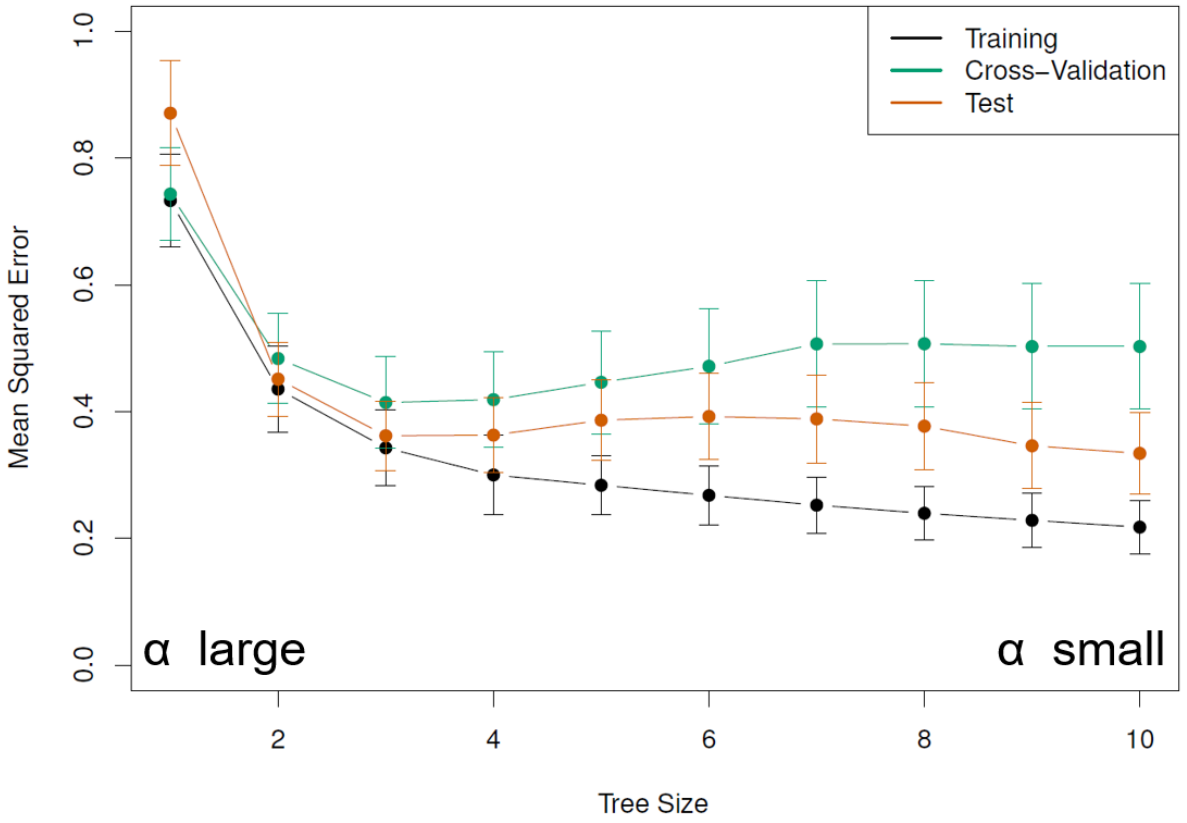
More generally: *tree-size* vs. *test error* (ISL, Fig. 8.5)



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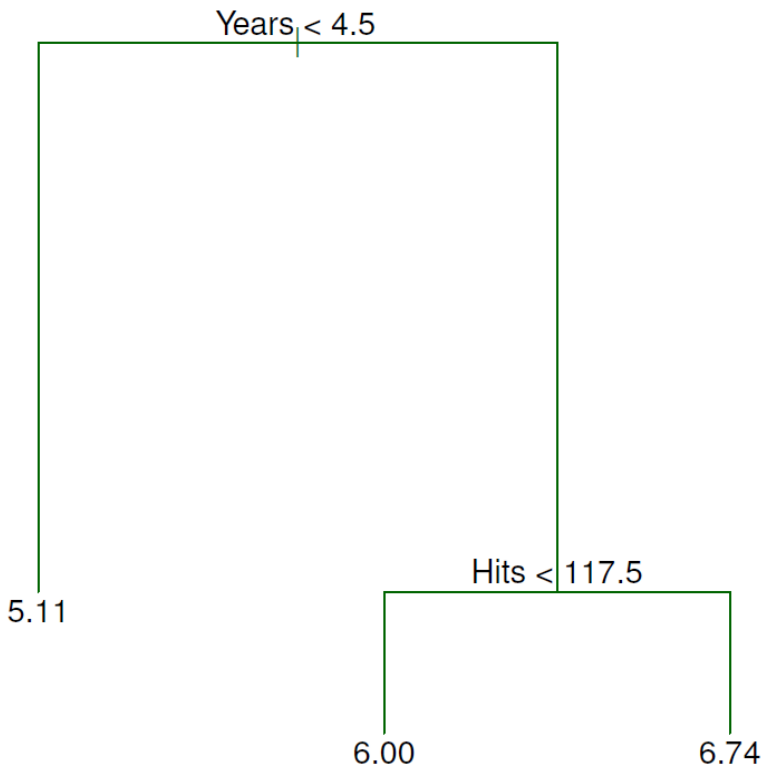
- Instead — until a minimum leaf size (in R, default: 10).
- Implies a baseline (weak) protection against *overfitting*.

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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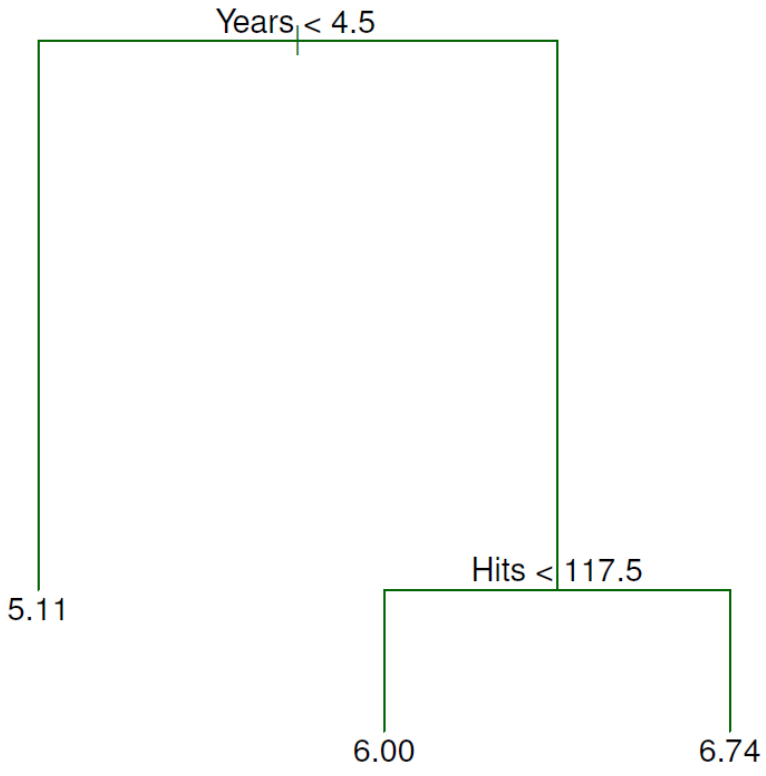

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- Measure 'variable importance' by *sum of error reduction* across splits.

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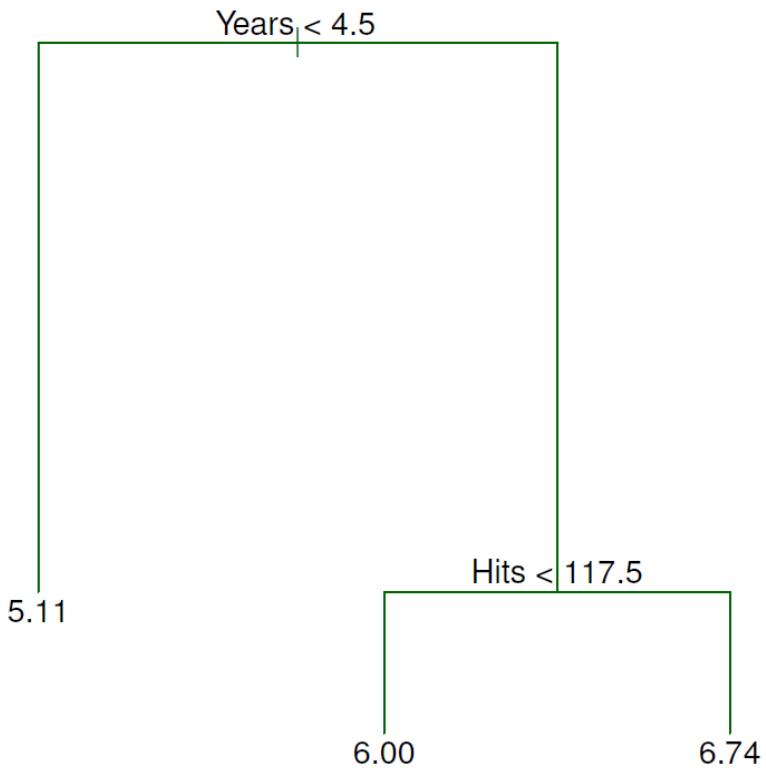

As noted earlier:

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

Additionally:

- Measure 'variable importance' by *sum of error reduction* across splits.
- Including splits evaluated but not realized.

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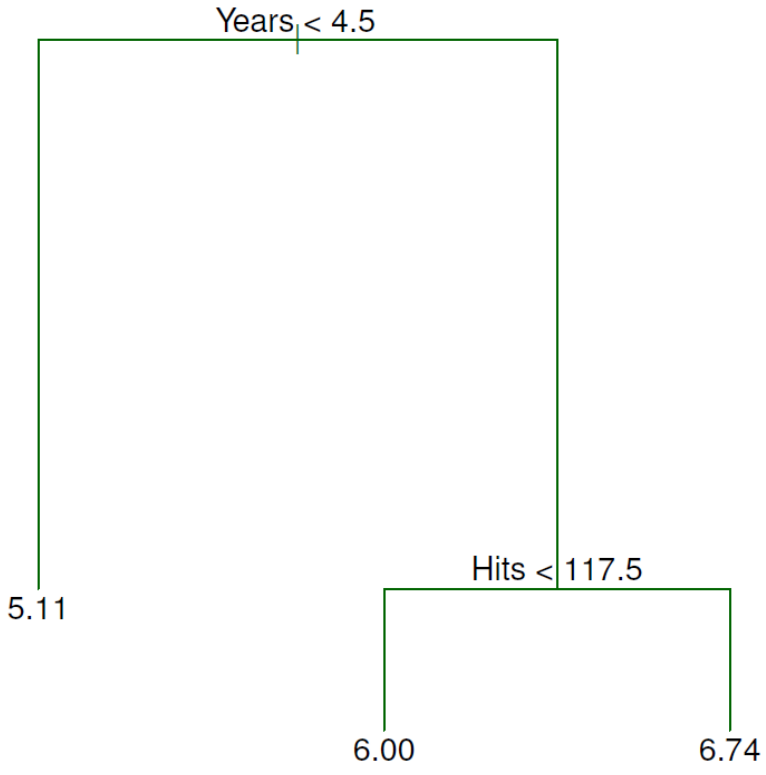


However, some caveats:

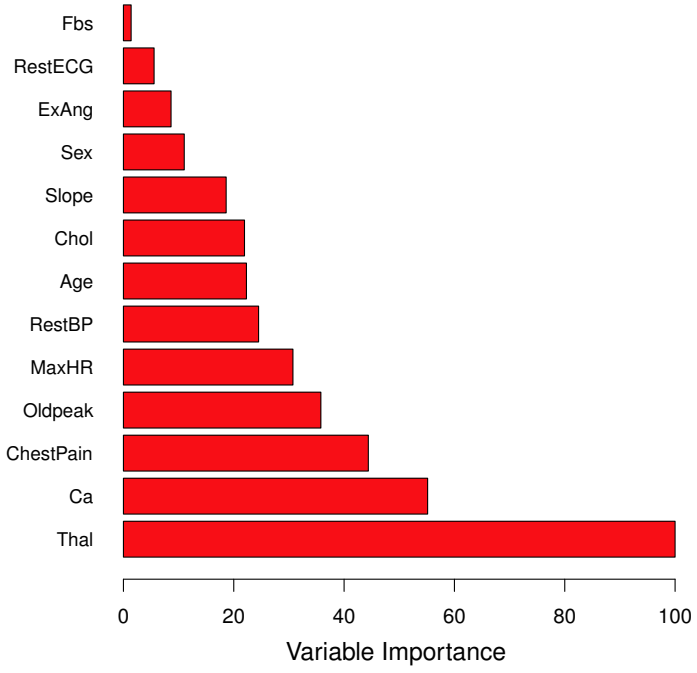
1. The structure does not reveal how X is associated with Y controlling for Z.
   - It simply finds splits that are predictive.
   - Thus—careful with interpretation.

Re. interpretability

However, some caveats:

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.

Plotting variable importance (ISL, Fig 8.9)



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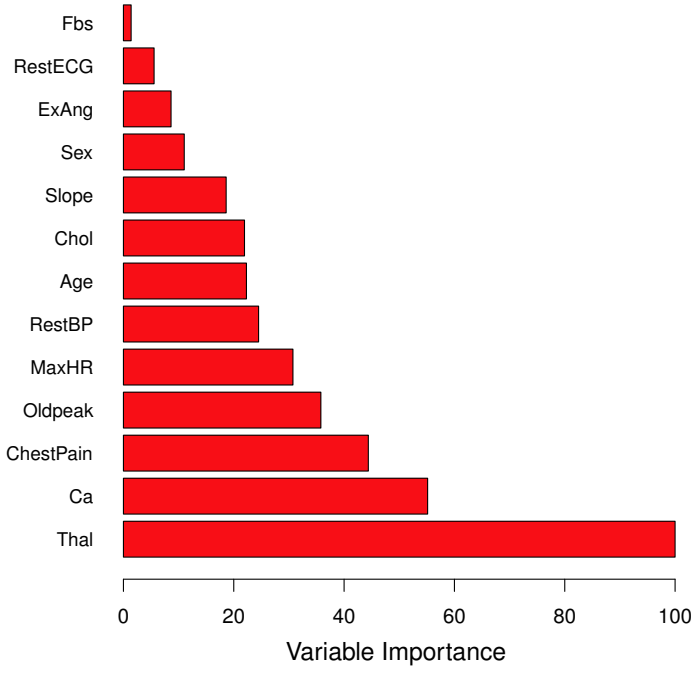

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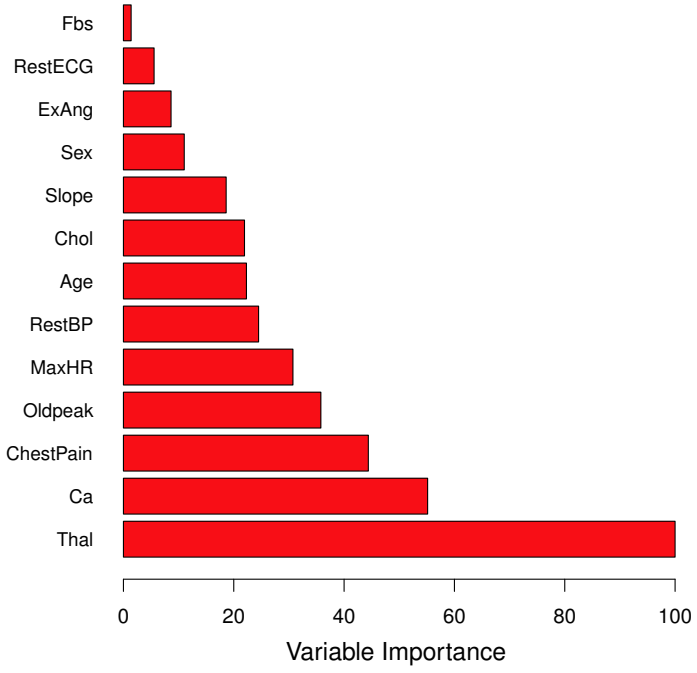

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- `Ca` reducing the error about half as much as `Thal`.

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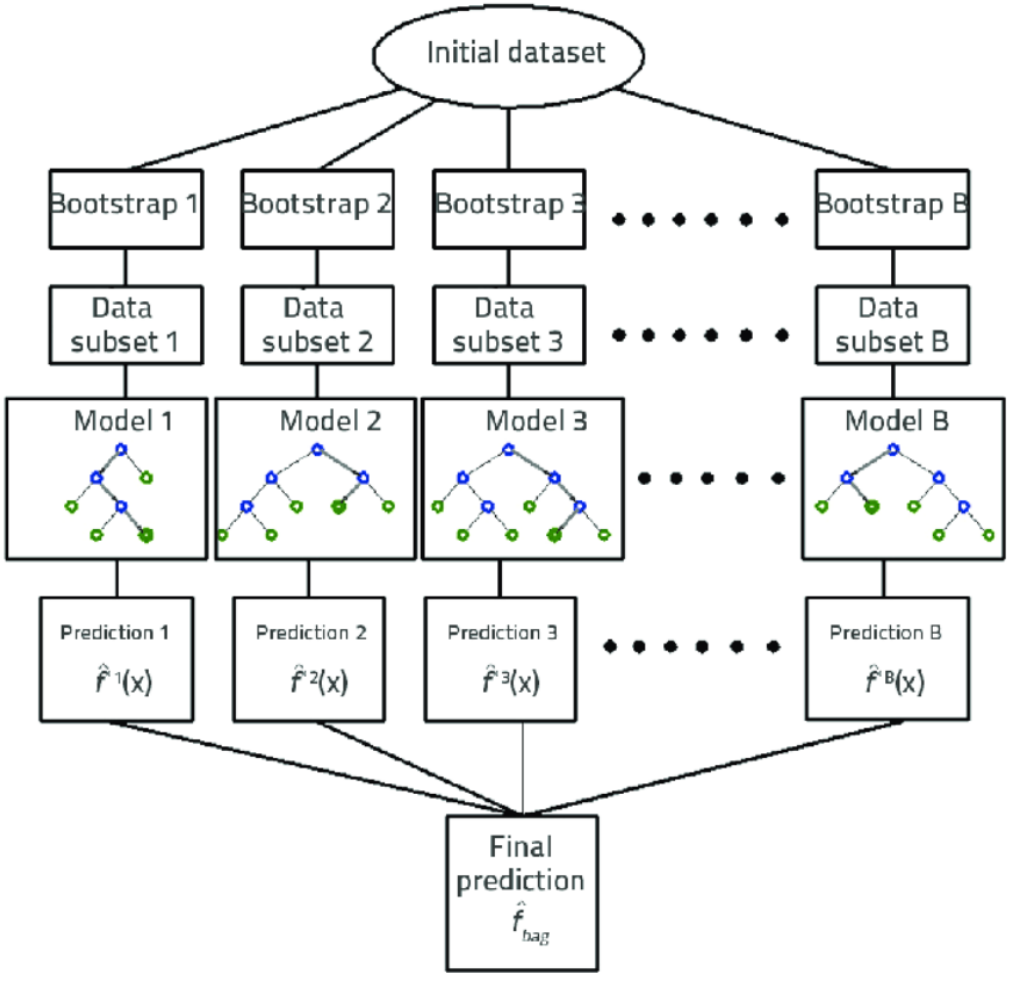
- Each tree is trained **deep** and *not pruned* $\rightarrow$ each tree has *low bias* and *high variance*.
- Averaging these B trees reduces the variance—in the hope to get the "best of both worlds" (low bias, low variance).

Illustration



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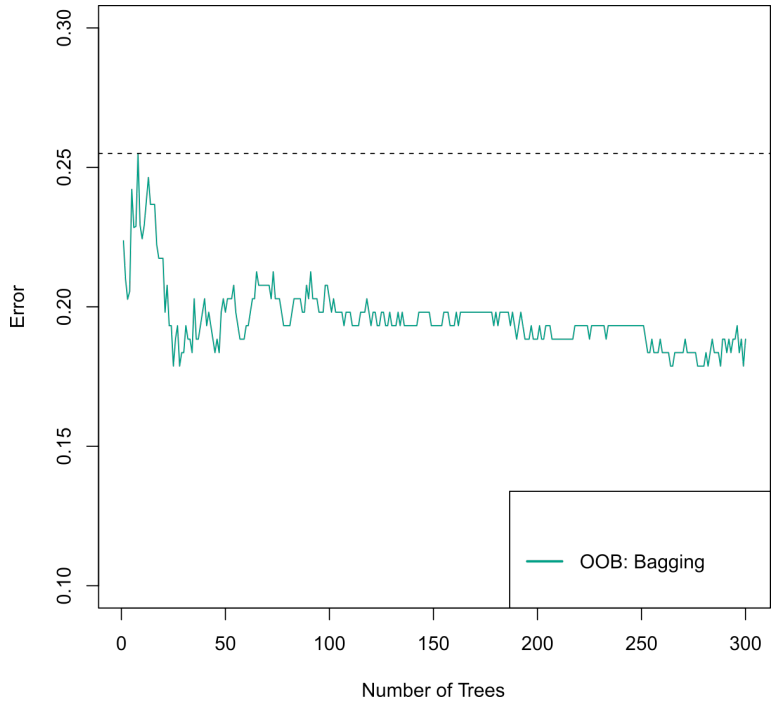

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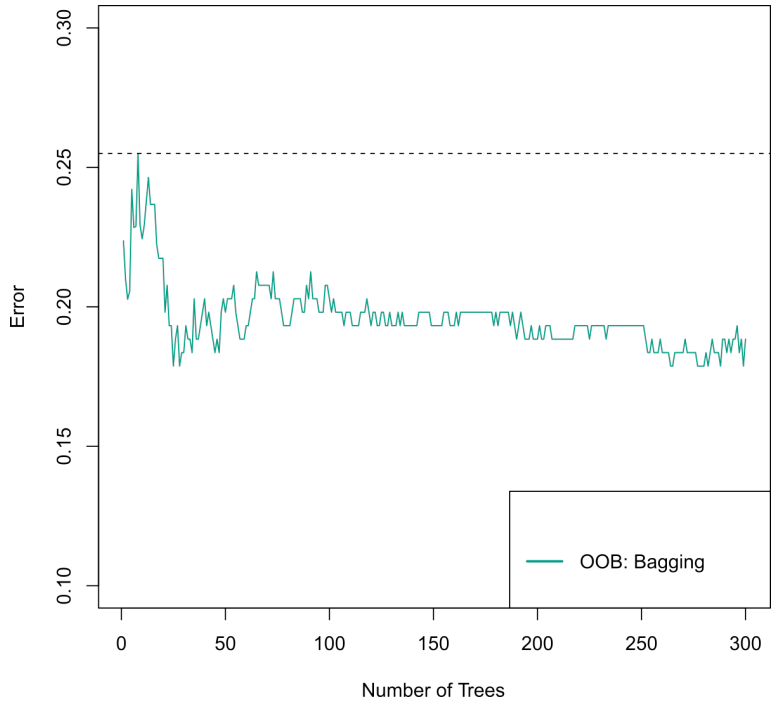

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- Results are robust to the *choice of no. of trees*. Typical choice: 100-1000.

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Can we make trees *less correlated*?

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  - Thus—each split does not even consider a majority of predictors.

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What is the rationale for such strong restrictions?

Counterintuitive: why exclude most important variables from some trees?

Basic answer: If we don't;

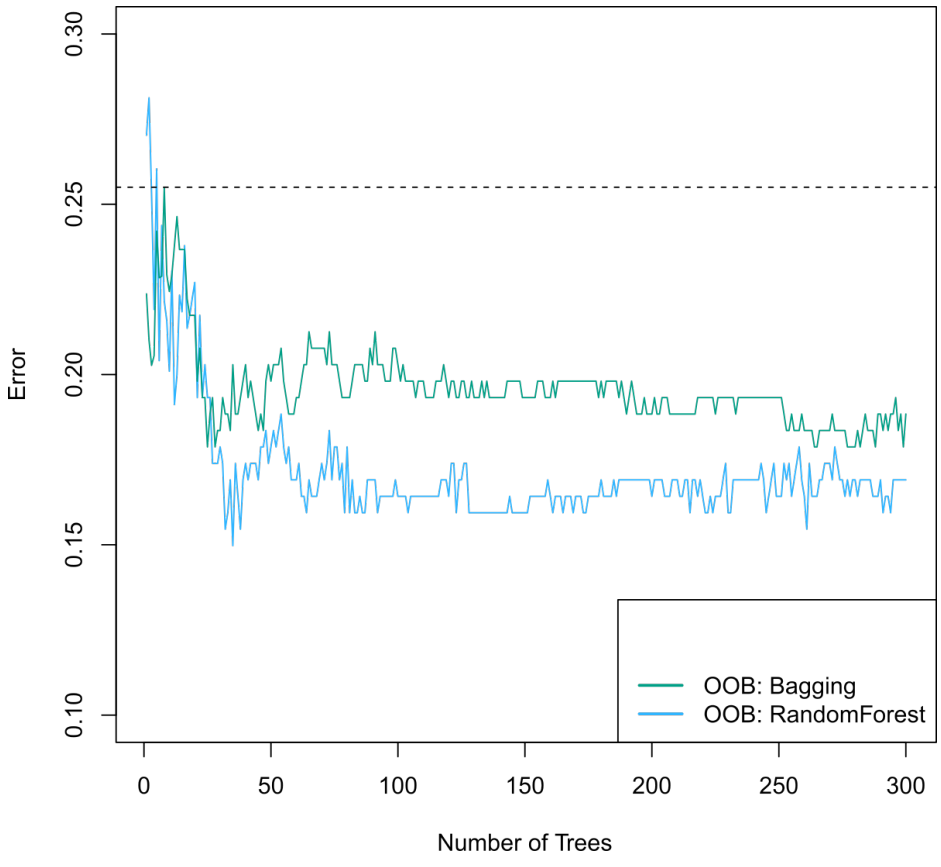
- They will dominate most trees.
- Thus create similarity (correlation) across trees.
- Averaging will not reduce variance as much.

In other words:

Imposing restrictions reduce the power of any given tree, but pooling them, they 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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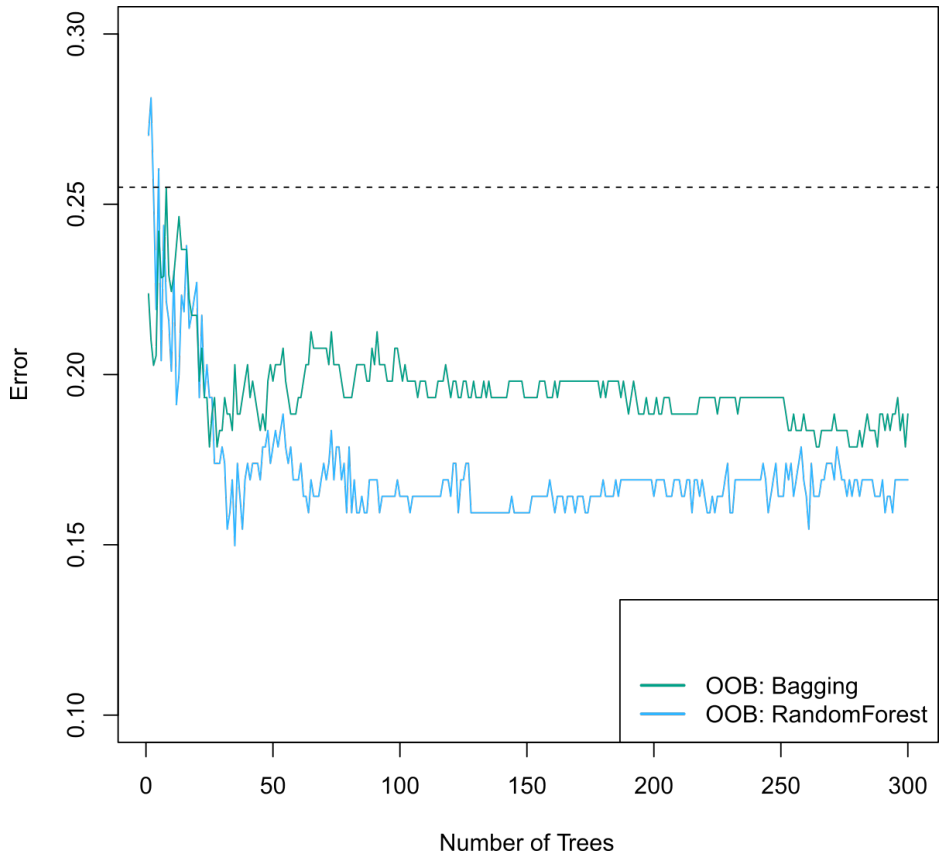
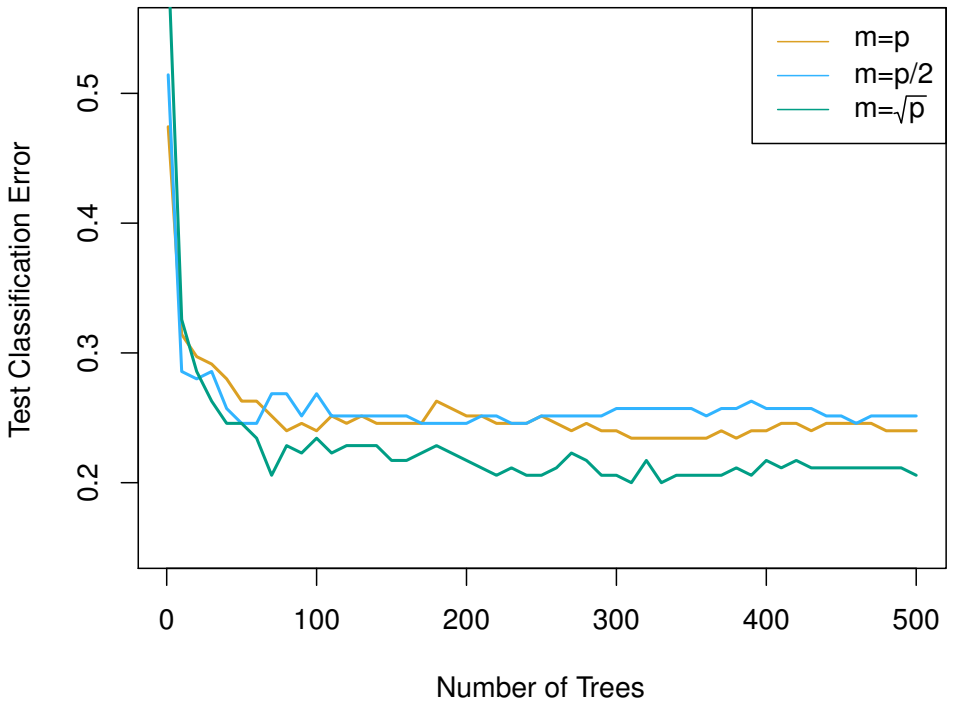


Note: as with bagging, the results are usually quite stable under different *number of trees used* (beyond a few hundred).

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.

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

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For both bagging and RFs:

- Better predictions — but less interpretability
- Would be very useful to understand why predictions improve!
- Maybe picked up novel pattern that is scientifically interesting?

Interpretable ML

Interpretable Machine Learning

Recent focus in machine learning literature (Molnar 2020)

- Develops **post-hoc techniques** to *extract* interpretability from *black-box methods*.

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- *Permutation variable importance* measure

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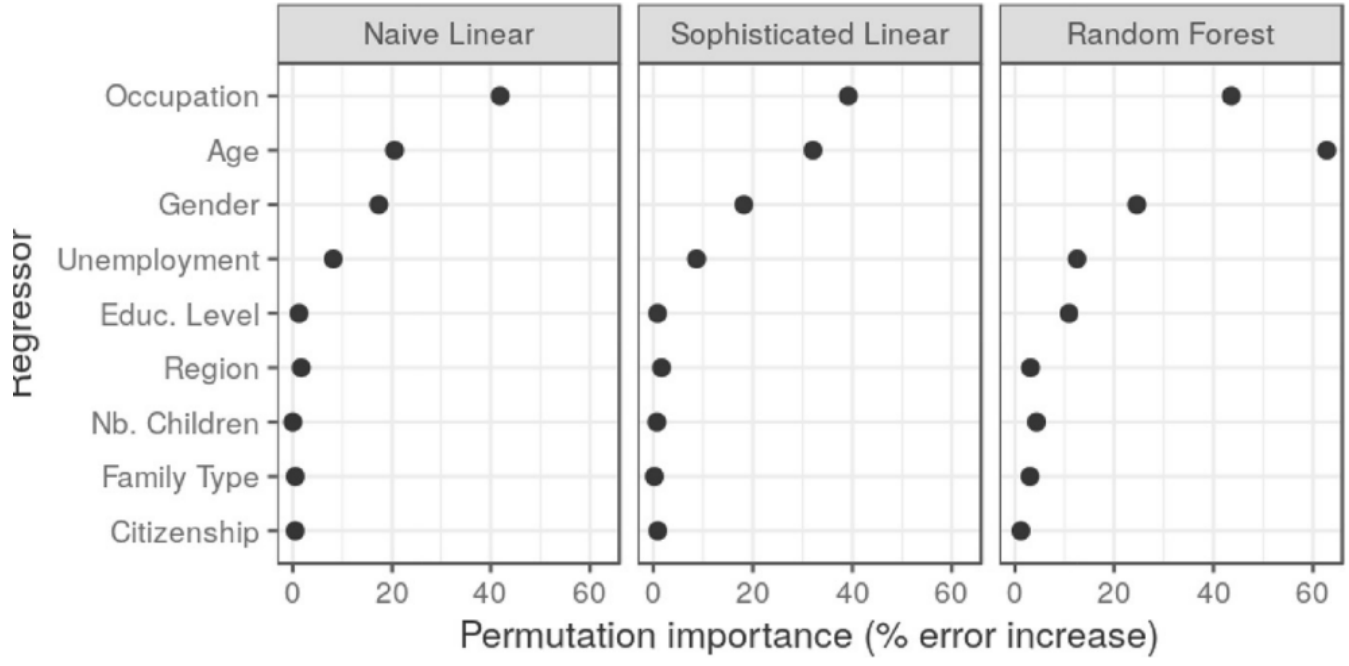
4. Generate predictions from $\hat{f}$ on *modified data* and assess *accuracy*.
5. Difference in accuracy between step 2 and 4 = importance of variable X_1.

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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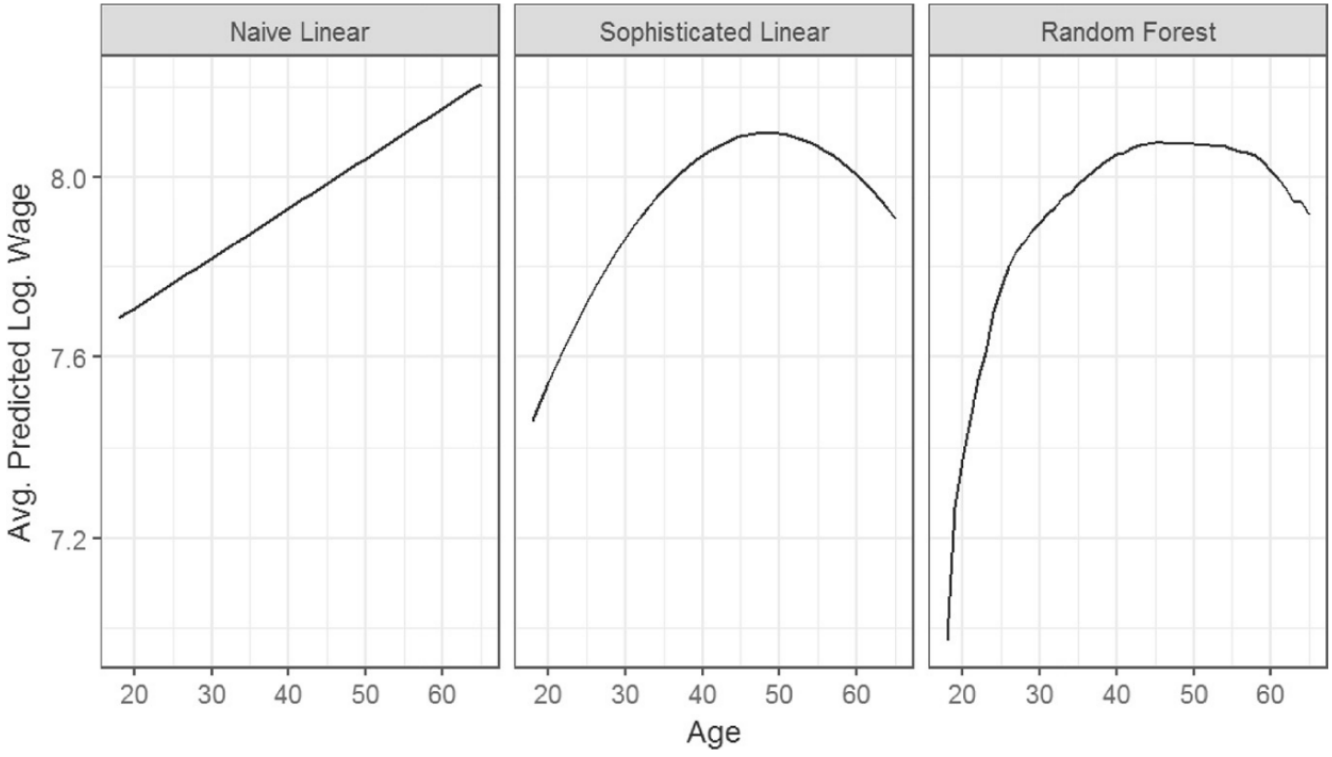
Basic procedure
For some variable $X_1 \ldots$

1. For a given value x that X_1 takes in the data, create a new synthethic data set in which all values of X_1 is replaced by this value.
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)



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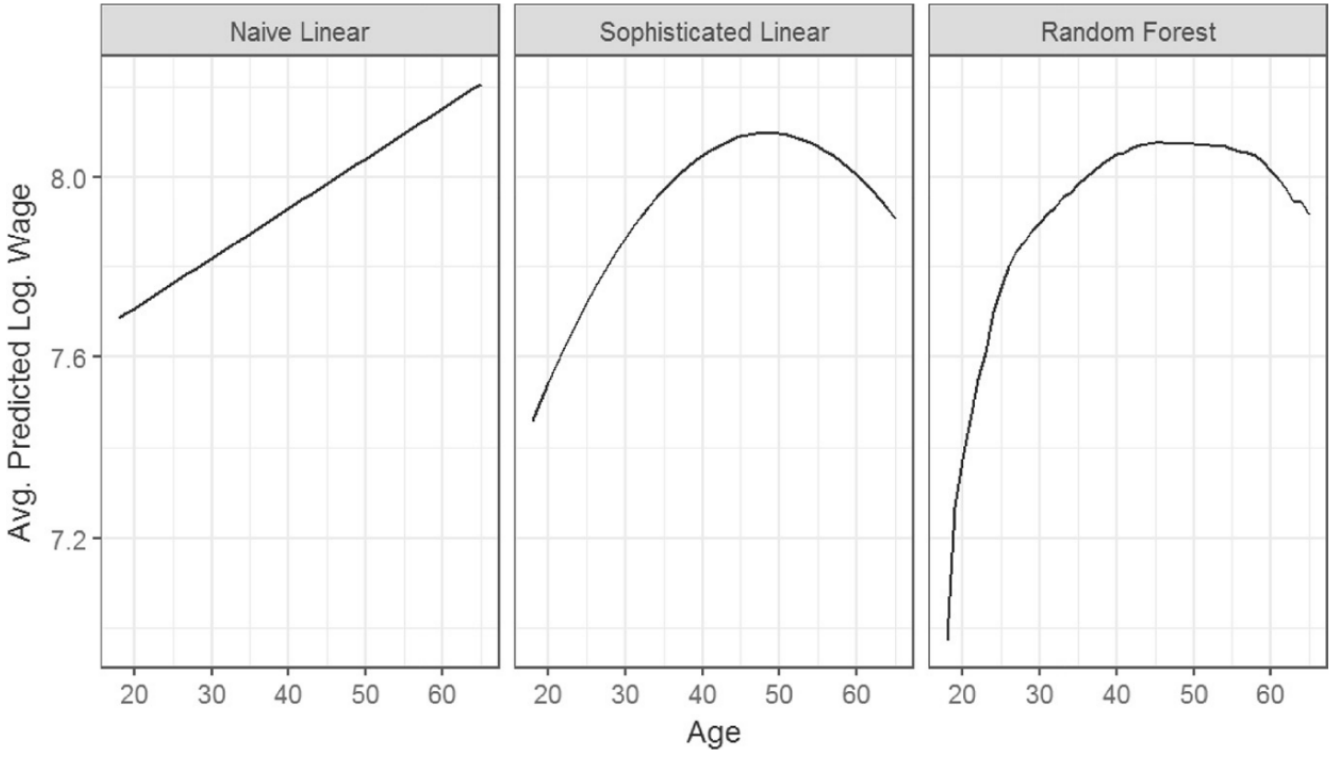

Here, variable/pattern not so-so interesting perhaps. But you could imagine a model revealing some non-linearity not previously considered in the literature.

Recapping this last part

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  - Parametric: makes strong assumptions about $\hat{f}$ (e.g., additive)
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- Interpretable machine learning

That is all — now break, then lab!