Machine Learning in R

Lecture 5 – Tree-based methods

Jean Feng – Epidemiology and Biostatistics

Today's Lecture

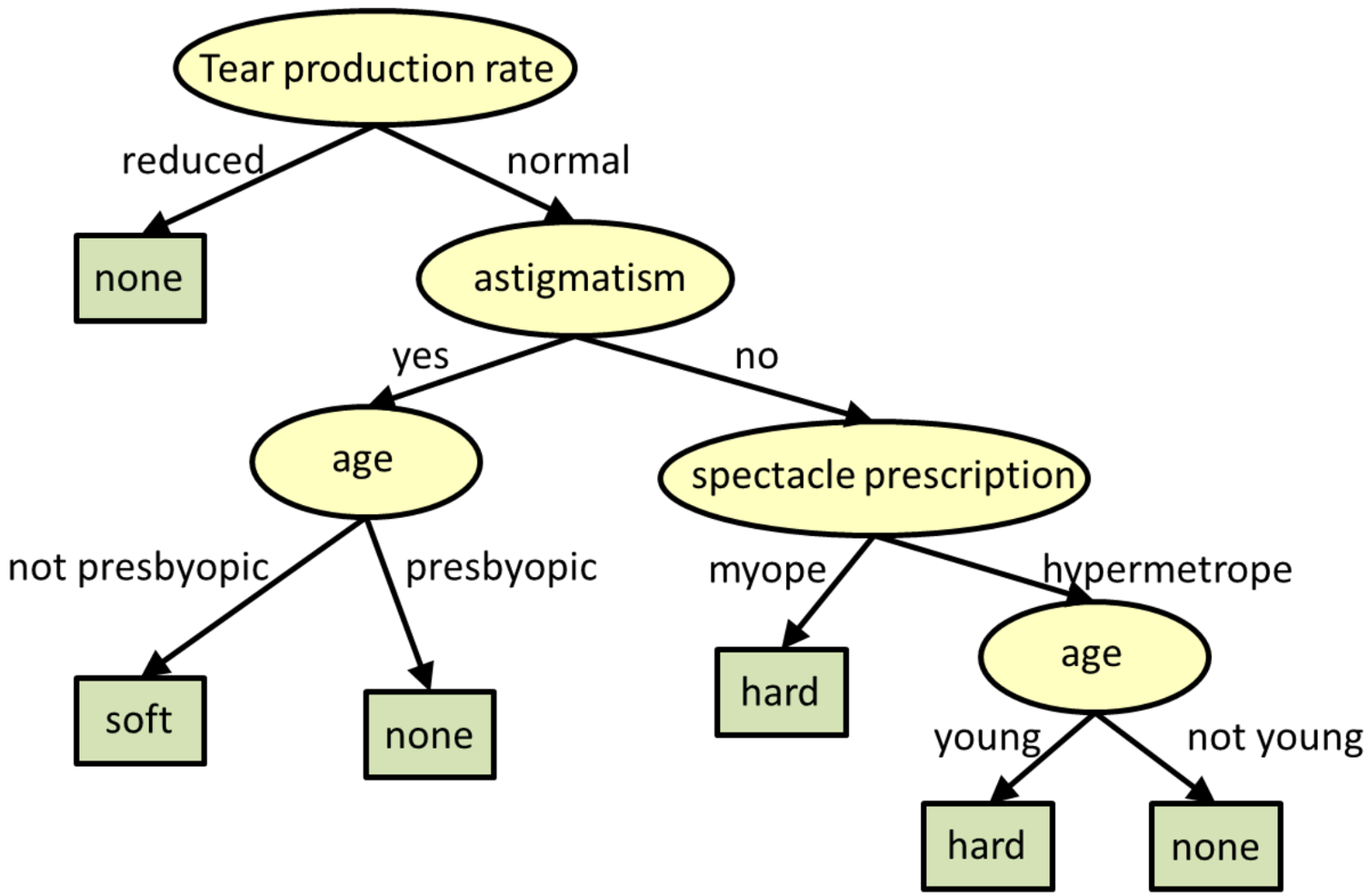
- Decision Trees
- Ensembling
  - Bagging
    - Random Forests
- Variable Importance

Today's Lecture

- **Decision Trees**
- Ensembling
    - Bagging
    - Random Forests
- Variable Importance

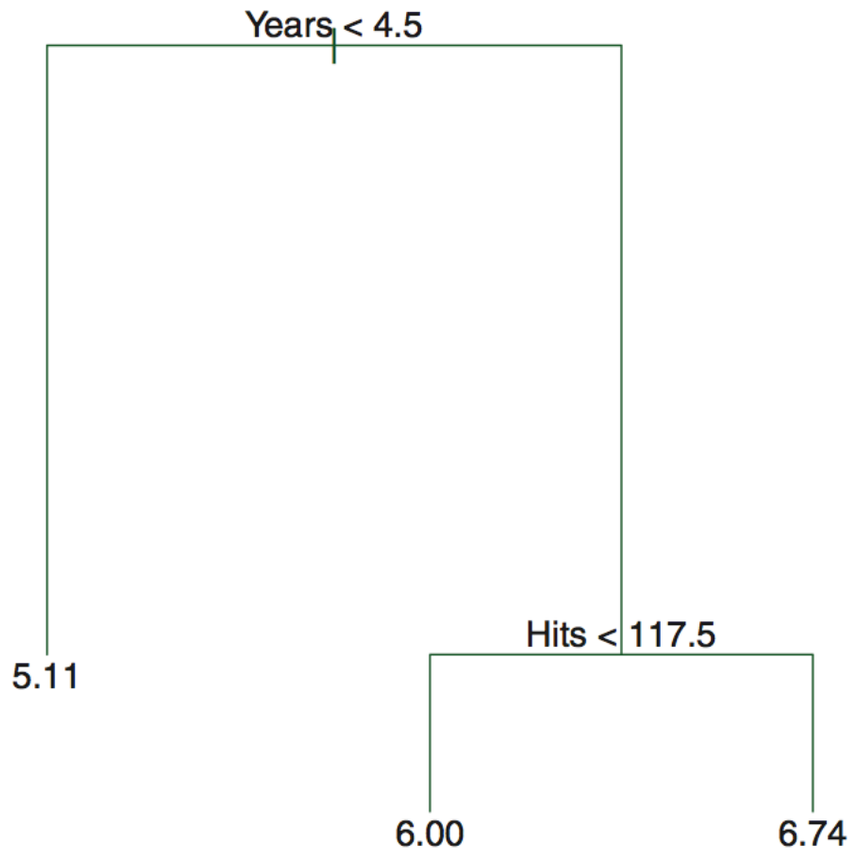
Tree-based methods

- An example tree for deciding what kind of contact lens a person should wear:



Toy Example: Predicting salaries of baseball players

- Outcome: Salary of baseball players (in millions)
- Two predictors: years of experience in MLB (Years) and number of hits made in the previous year (Hits)



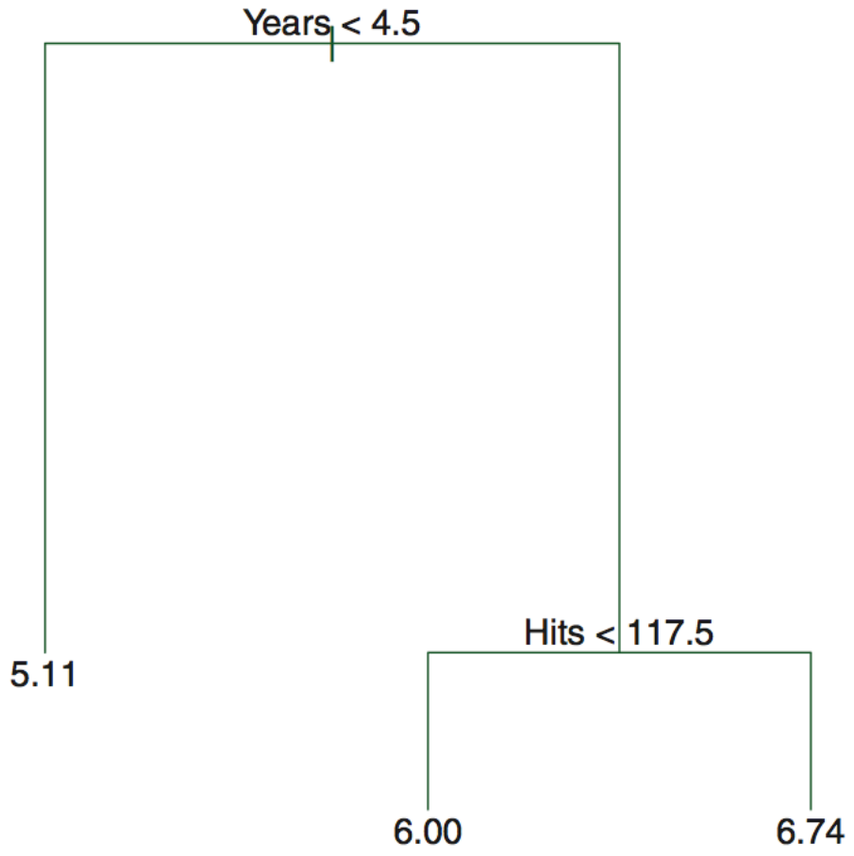
Toy Example: Predicting salaries of baseball players

- The top split predicts that baseball players having Years < 4.5 earn $5.11 million.

- Among players with > 4.5 Years of experience...

- For those with < 117.5 Hits, the predicted salary is $6.00 million.

- For those with > 117.5 Hits, the predicted salary is $6.74 million.



Decision Trees

- Decision trees — also known as **Classification and Regression Trees (CART)** — can be used in both regression and classification tasks.

    - They have also been extended for survival outcomes.

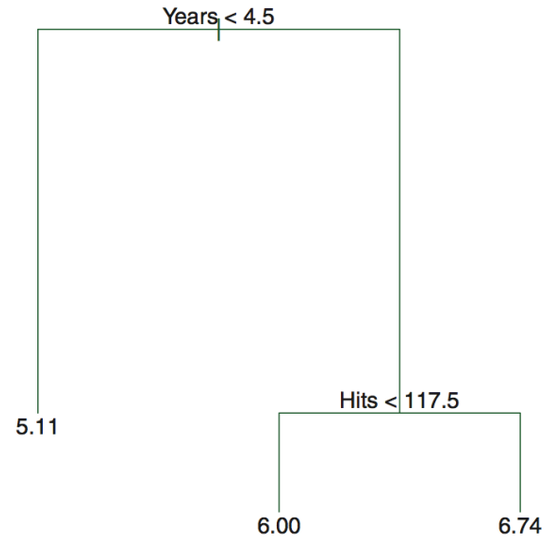
- Trees are able to model **non-linearities** and **interactions** between variables very naturally.

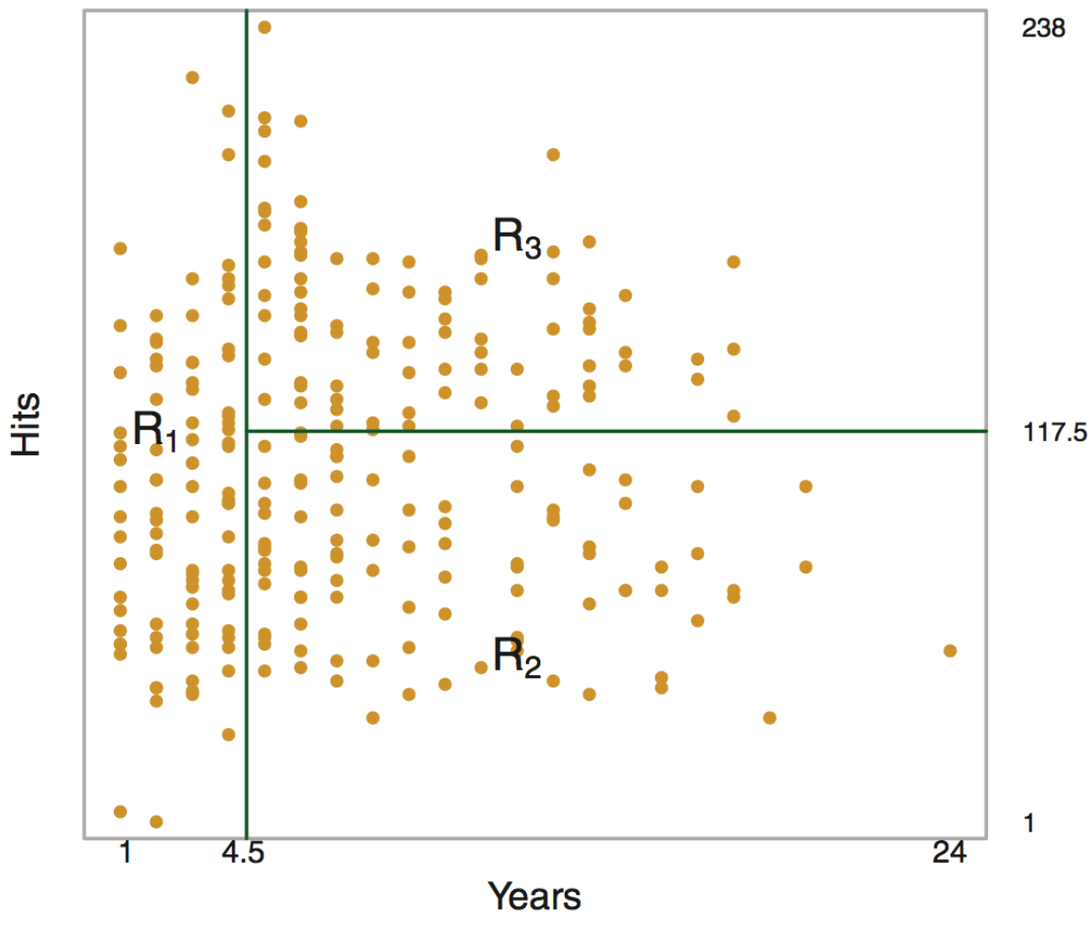
- Trees are probably an oversimplification of the true data, but they are very intuitive and interpretable.

A region-based view

1. **Stratify/Segment**: Partition the predictor space into *J* disjoint regions $R_1, \ldots, R_J$.
   - How should we construct the regions $R_1, \ldots, R_J$?
   - How many regions should there be? (How big should *J* be?)

2. **Prediction**: For observation X in region R_j, output the mean (regression) or mode (classification) of the observed outcomes for the training observations in region R_j



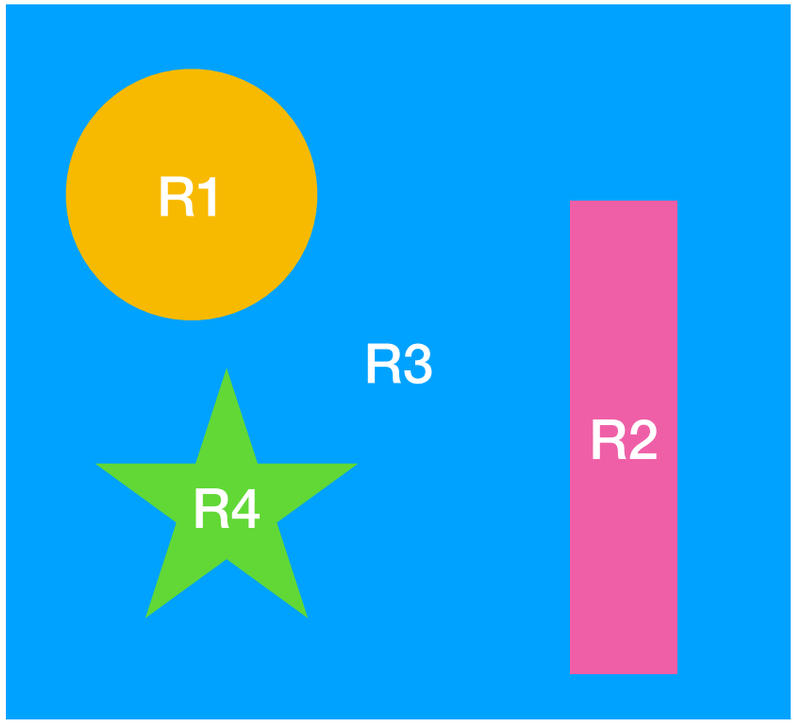


$$R_1 = \{X \mid Years < 4.5\}$$
$$R_2 = \{X \mid Years \geq 4.5, Hits < 117.5\}$$
$$R_3 = \{X \mid Years \geq 4.5, Hits \geq 117.5\}$$

Partitioning the Predictor Space

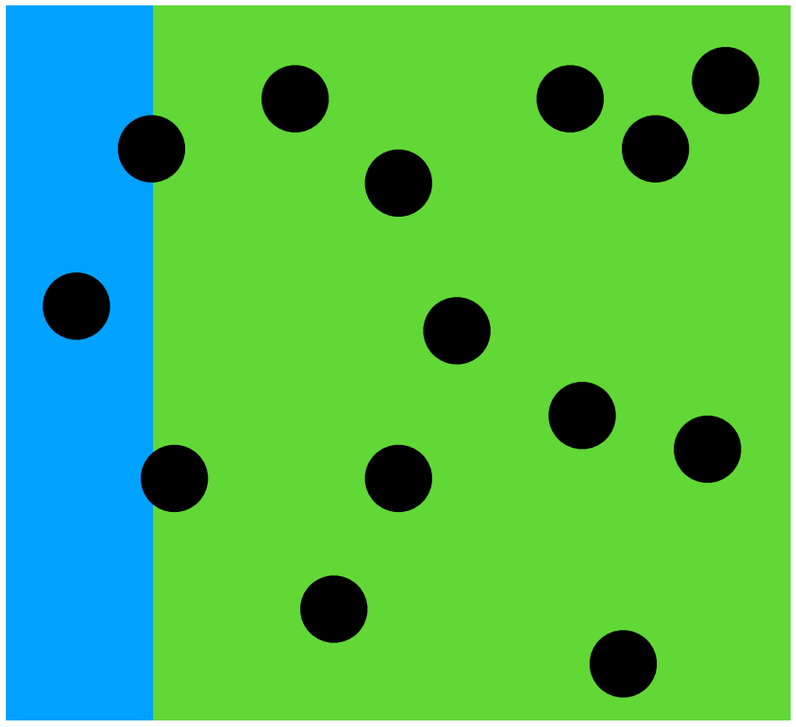
- For now assume J is known.
- Unfortunately, it is not possible to consider every possible partition of the space into J regions.
- We introduce two simplifications:

1. We will only split the region into rectangles/boxes in a hierarchical manner.
2. We'll create splits in a greedy fashion known as **recursive binary splitting**.



Recursive Binary Splitting

- Start with all the data.
- For all predictors X_j and cut points t:
  - Consider splitting the space into:
    $R_1(j,t) = \{X | X_j < t\}, R_2(j,t) = \{X | X_j \geq t\}$
  - Evaluate the quality of this candidate split according to some **split criterion function** (e.g. drop in mean squared error).
- Choose the best split according to this criterion function.
- Rinse and repeat the above process for each new region until there are J regions



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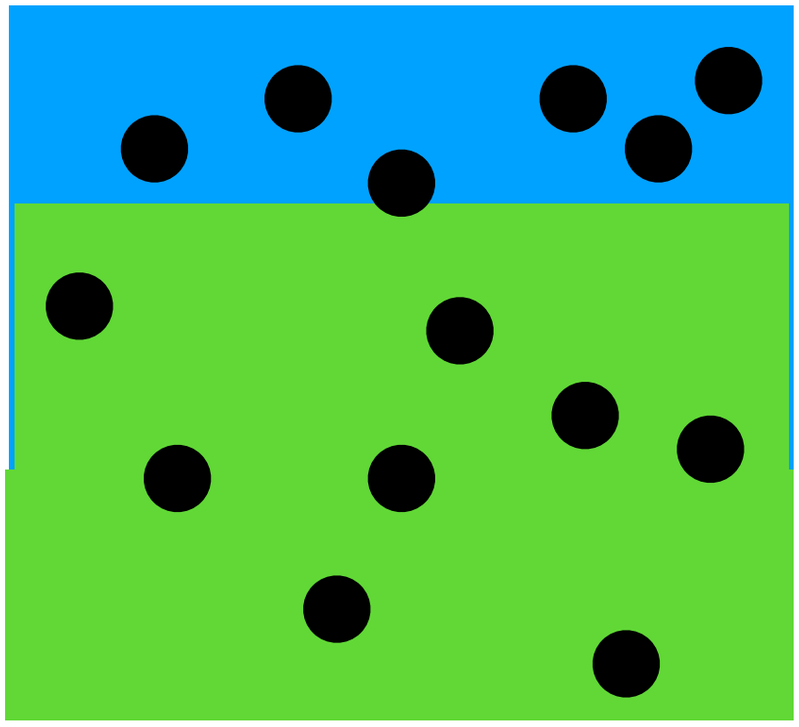

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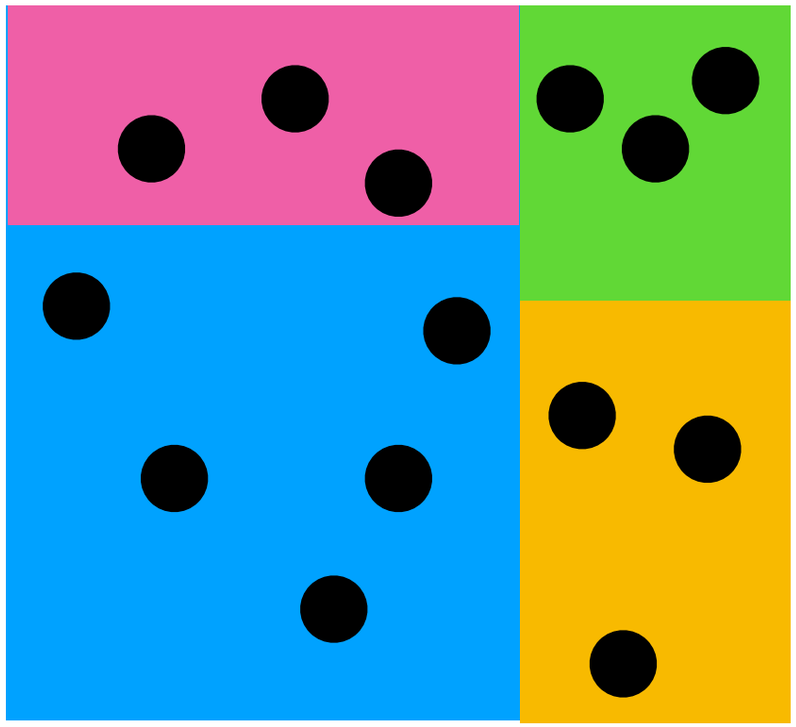
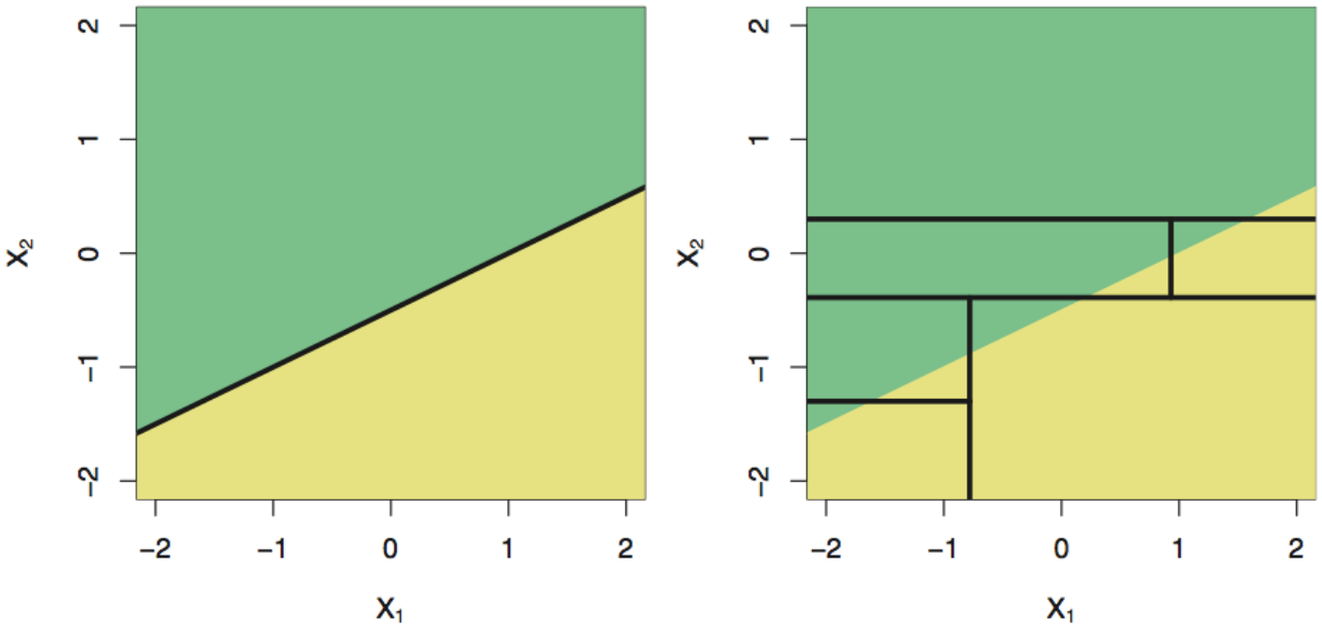


Tree versus Linear Models

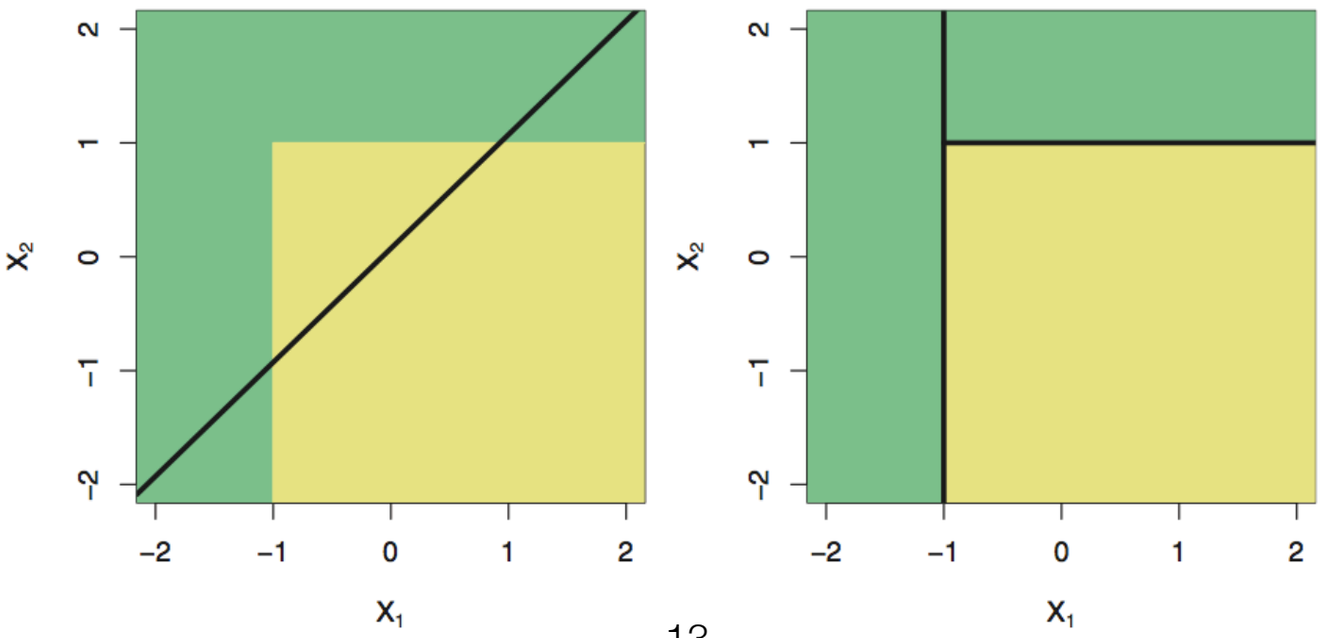
Linear model

Tree-based model

True linear boundary

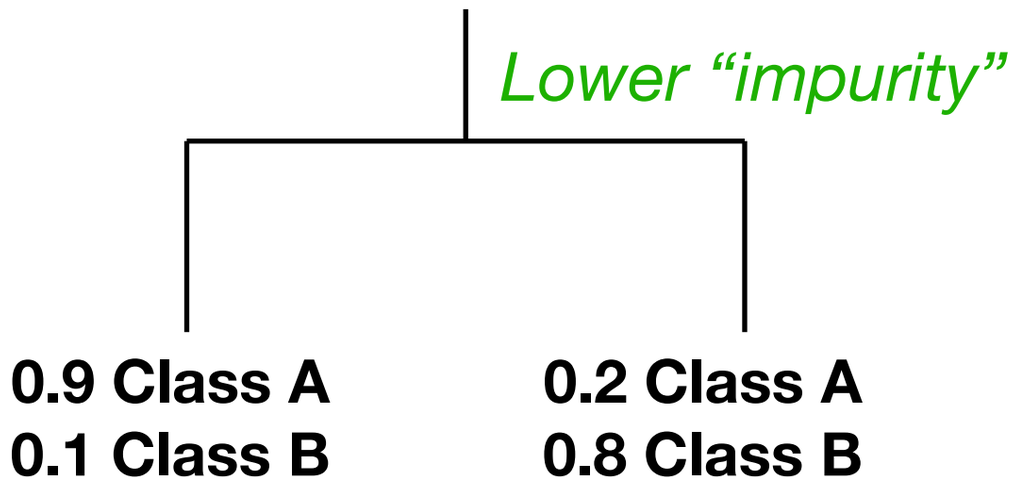


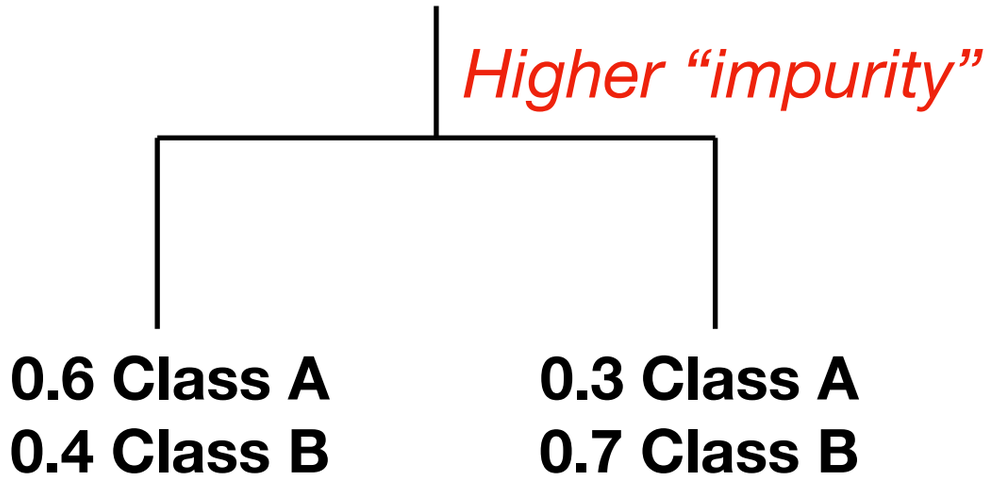
True non-linear boundary



Split Criterion Functions

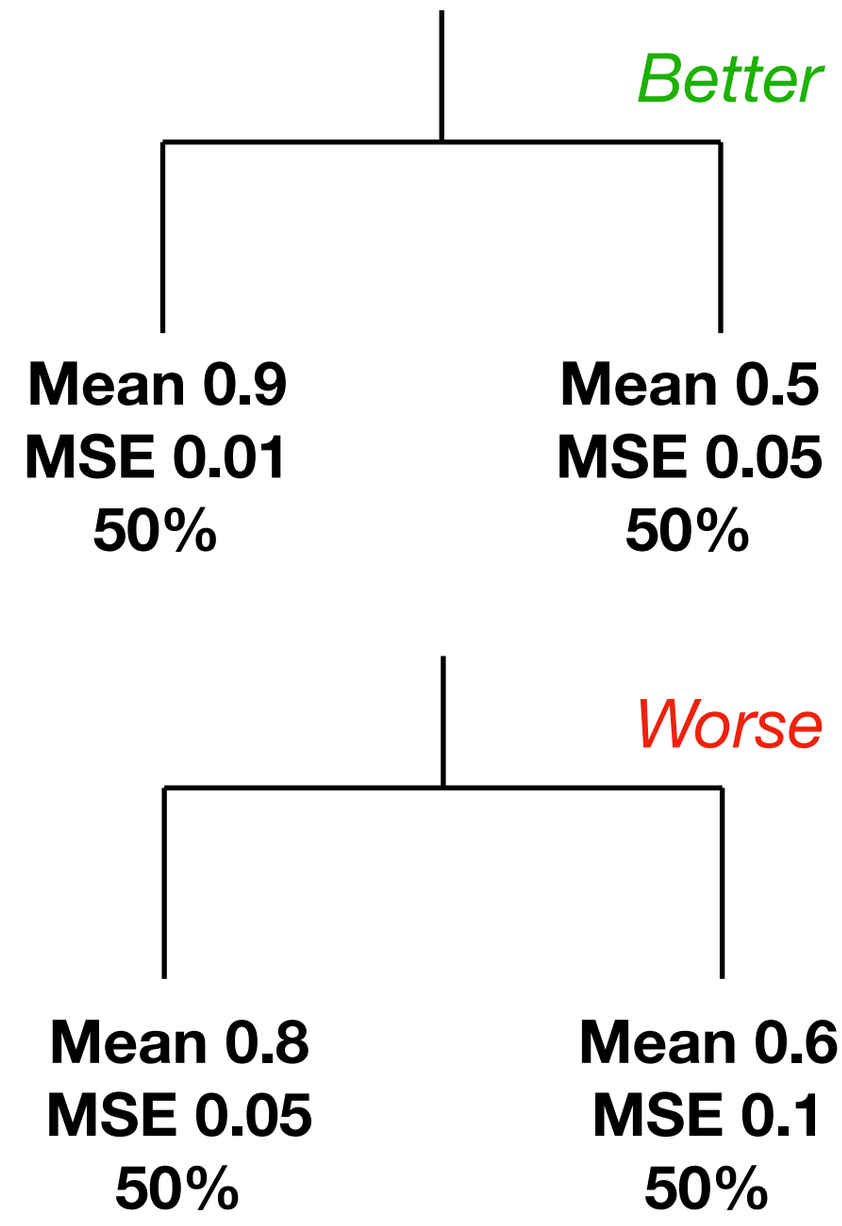
- **Classification**: Evaluate split by decrease in impurity. How often do outcomes differ from the mode for its split.
  - Gini index
  - Cross-entropy





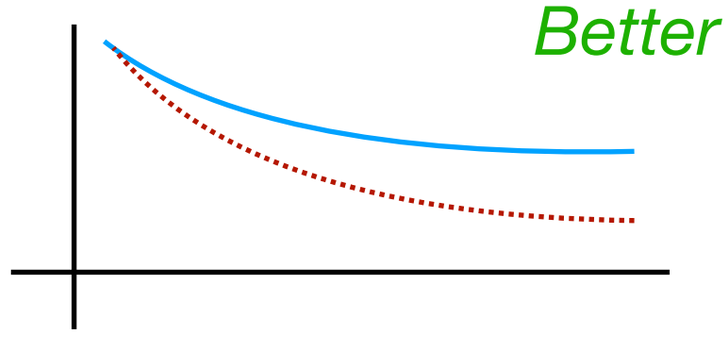
Split Criterion Functions

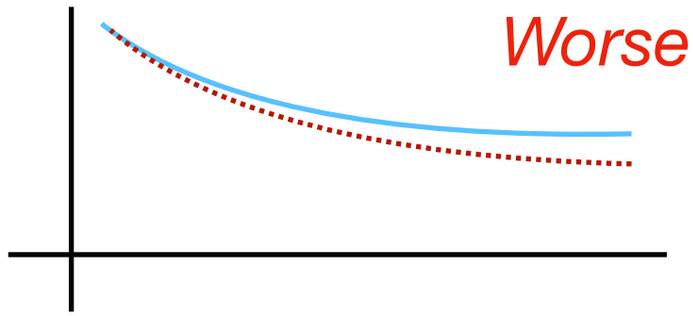
- **Regression:** Evaluate split by decrease in average deviation from the mean. How different are the outcomes from the mean for that split.
  - Squared-error deviations
  - Absolute deviations



Split Criterion Functions

- **Survival:** Evaluate split by how much we can separate the survival curves.
  - Log-rank statistic





How many candidate splits?

Q: Suppose we have a binary predictor $X_1 = \{0,1\}$ and a categorical predictor $X_2 = \{A, B, C\}$. How many candidate splits do we need to consider?

A. 2 splits

B. 4 splits

C. 8 splits

Candidate splits:

$$\{X_1 < 0.5\}, \{X_1 \geq 0.5\}$$
$$\{X_2 = A\}, \{X_2 \neq A\}$$
$$\{X_2 = B\}, \{X_2 \neq B\}$$
$$\{X_2 = C\}, \{X_2 \neq C\}$$

Categorical predictors

- If we have a categorical predictor, the splits have the form:

$R_1 = \{X : X_j \in S\}, R_2 = \{X : X_j \notin S\}$ where $S \subset \{1,...,q\}$.

- The software will search over all possible splits for binary or continuous predictors. For multi-class predictors, the software will do its best.

- **Note**: Recursive binary splitting will generally favor predictors with many levels because there are more chances for it to find a good split of the data.

A region-based view

1. **Stratify/Segment**: Partition the predictor space into *J* disjoint regions $R_1, \ldots, R_J$.
   - How should we construct the regions $R_1, \ldots, R_J$?
   - How many regions should there be? (How big should *J* be?)

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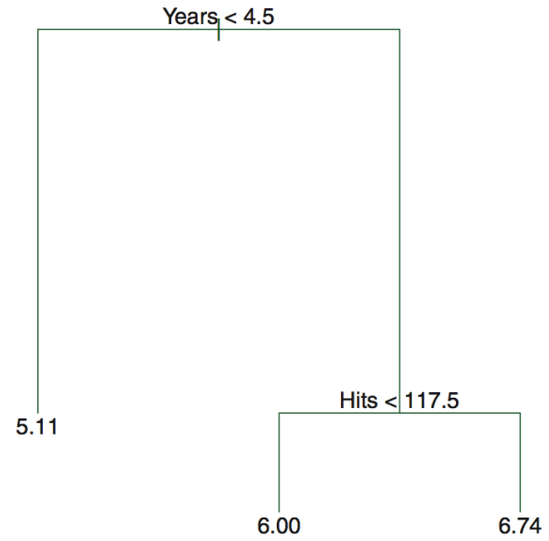

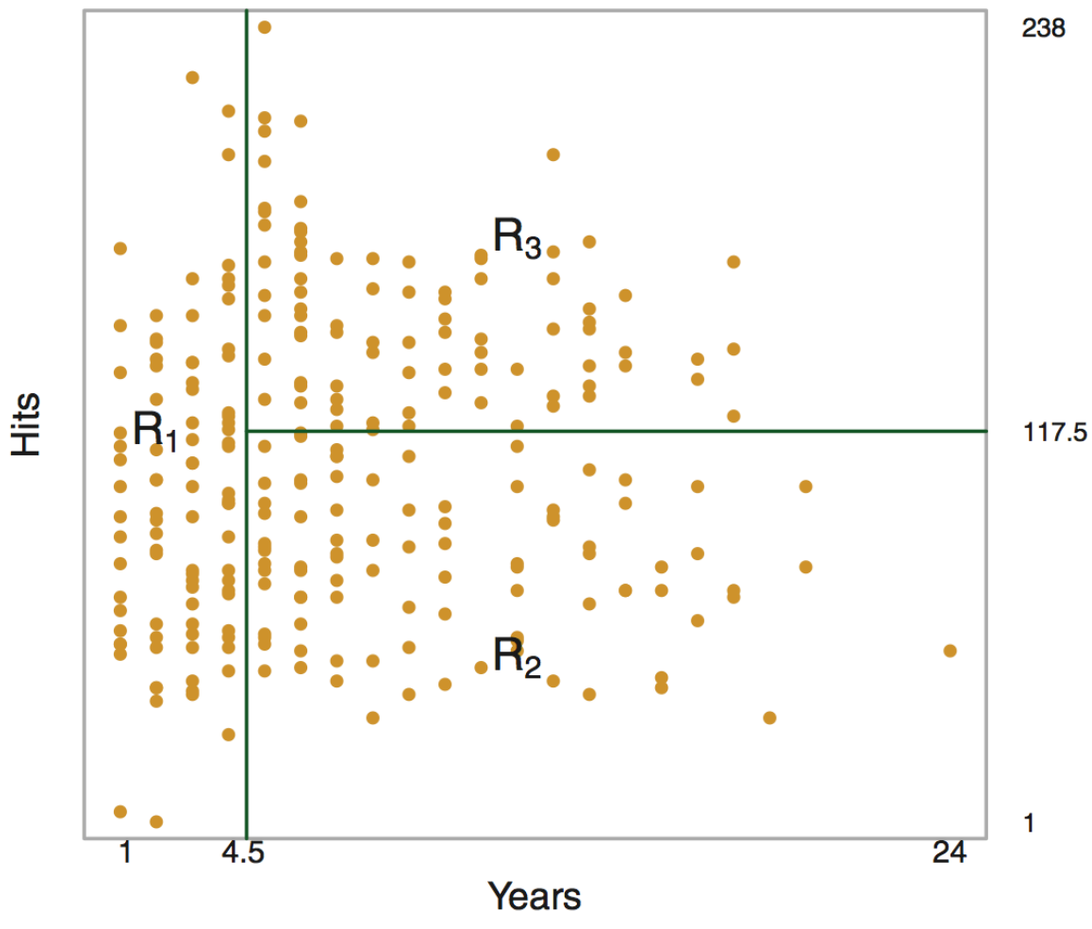

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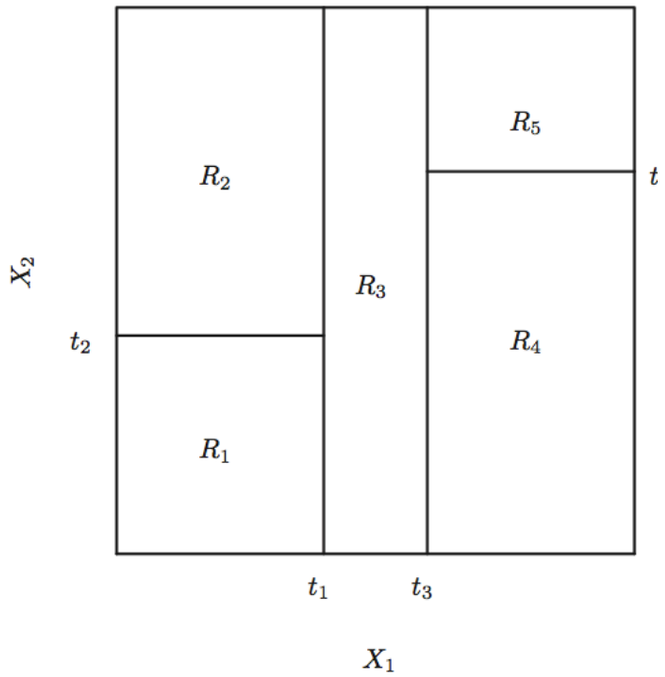
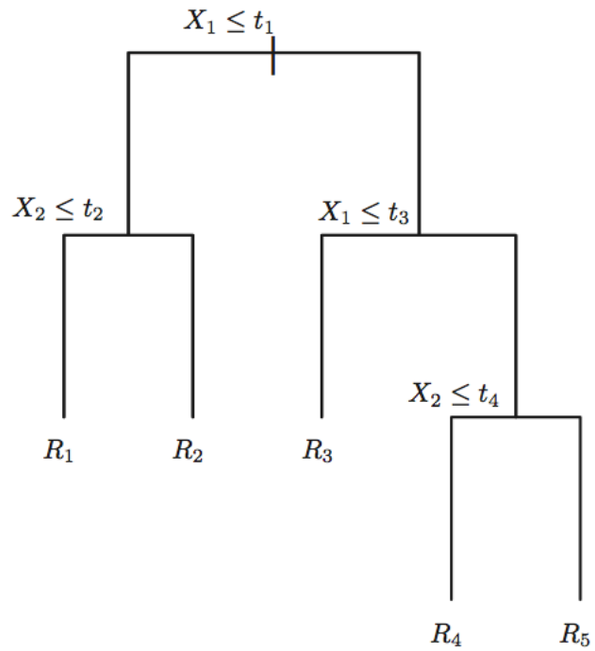
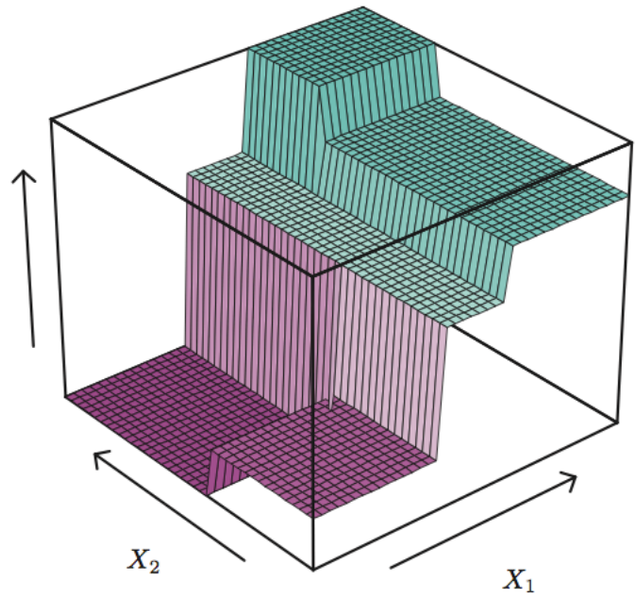
Interactions in a tree







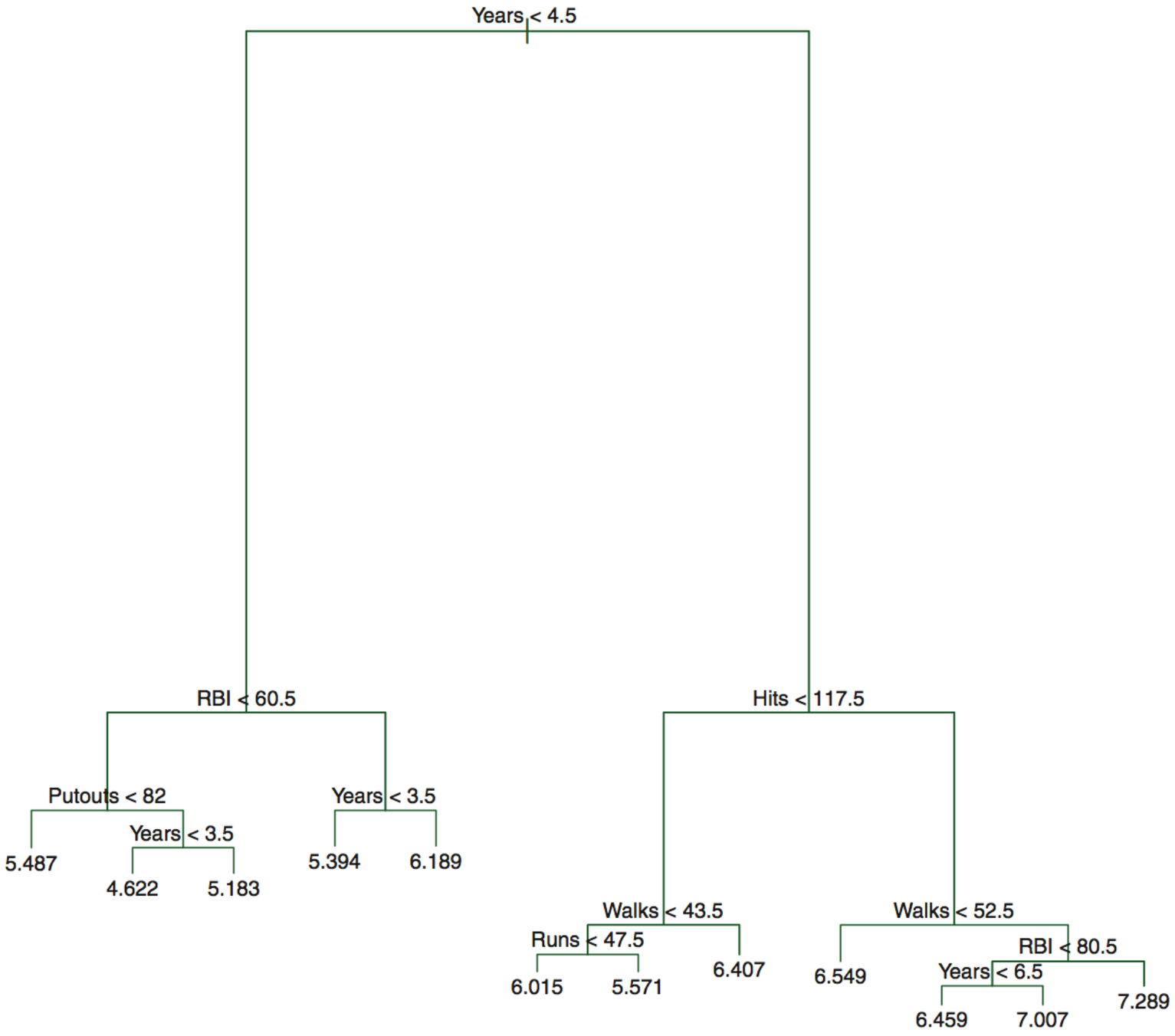
Question: The level of interaction between variables is controlled by the tree depth. For a tree of depth *J*, what is the maximum level of interaction between variables?

Answer: For tree depth *J*, there will be no interaction effects of level greater than *J*. In this example, the tree has depth *J*=3 and the level of interaction is 2.

Tuning the number of regions/tree size

- The **complexity** of the tree model is determined by the number of regions J.
- A tree with large J might overfit to the training data!
- A smaller tree with fewer splits might have lower **variance** (and better interpretability), at the cost of a little **bias**.
- To find a good small tree, a common approach is to:
    1. Grow a large tree, e.g. until no region has > 5 observations.
    2. Consider different subtrees by **pruning** the tree to different sizes.
    3. Use **cross-validation** to select J.

Full Tree for the baseball dataset

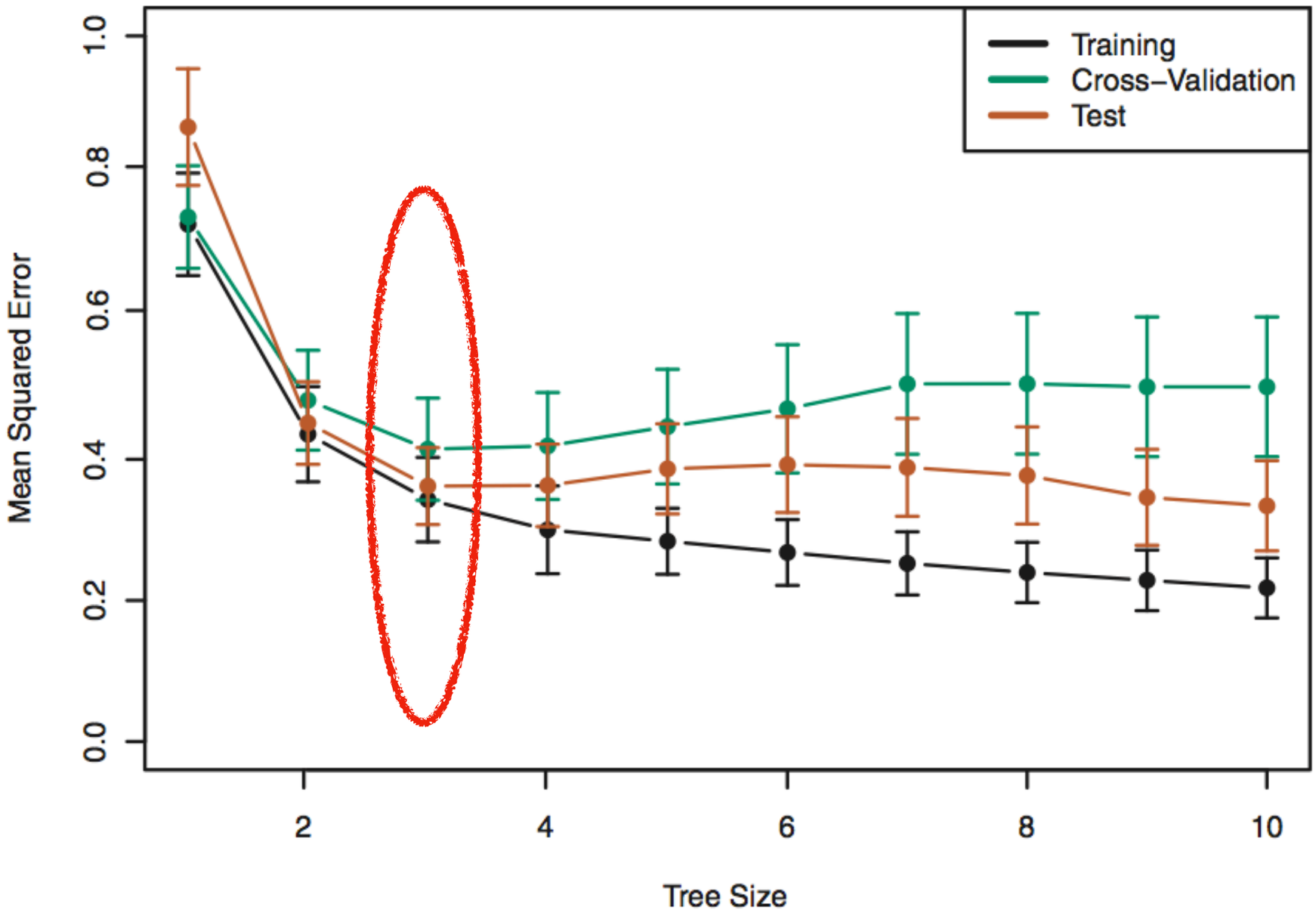


Cross-validation to determine tree size

- Split the data into K folds and fit K trees by holding out each of the folds for the candidate tree sizes.

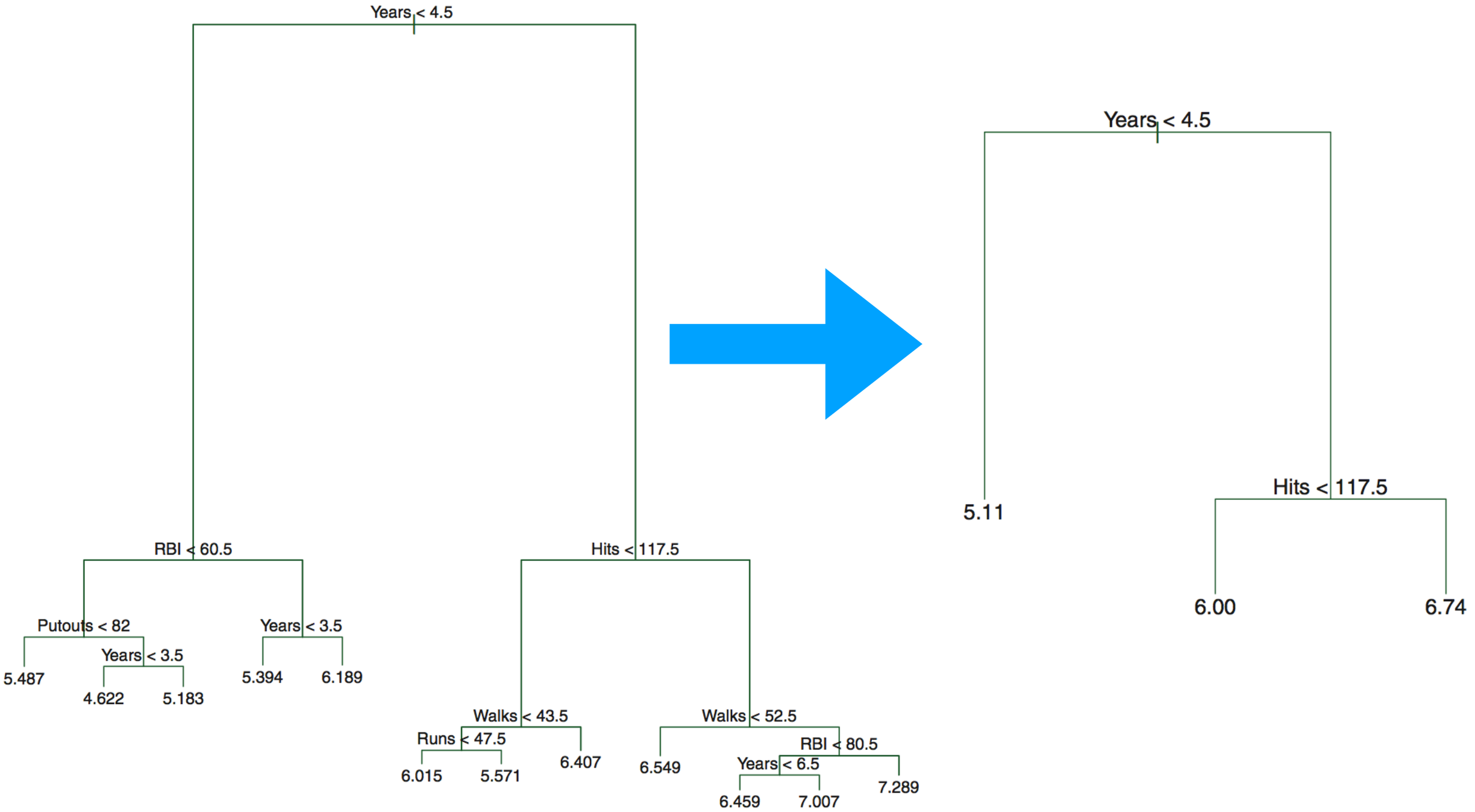
- Calculate the cross-validation error for the candidate tree sizes.

- Select the best tree size that minimizes the CV error (or use the 1-SE rule).



Note: The `rpart` package tunes a tree "complexity" parameter instead of tuning the tree size directly.

Pruned Tree for the baseball dataset

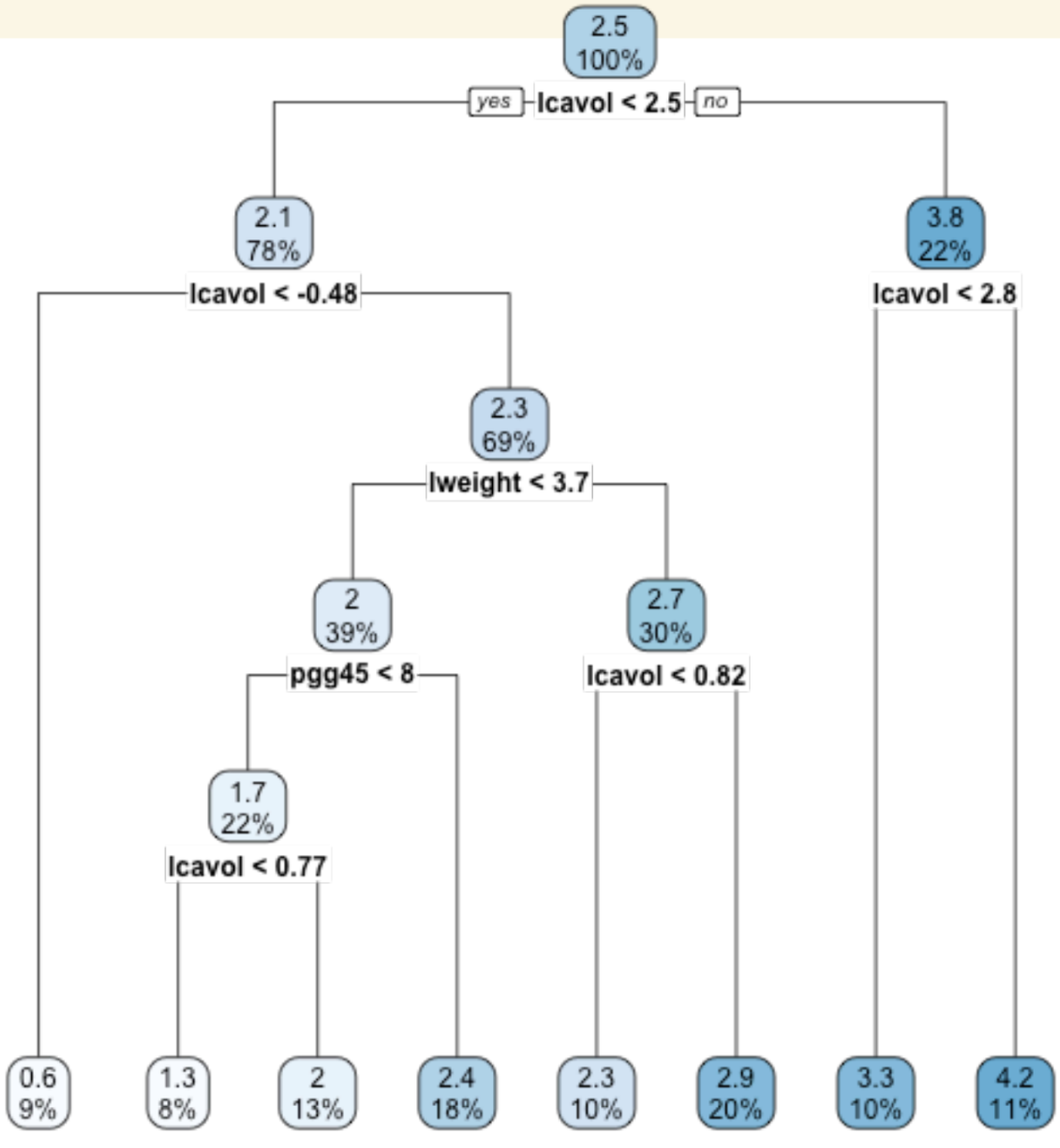


Example: Predicting log(PSA)

- Suppose we are studying the level of prostate-specific antigen (PSA), which is often elevated in men who have prostate cancer. We have $n = 97$ men with prostate cancer and $p = 8$ clinical measurements.

Example: Predicting log(PSA)

```
pros = read.table("http://statweb.stanford.edu/~tibs/ElemStatLearn/datasets/prostate.data")
psa_rpart <- rpart(lpsa ~ svi + lcavol + lweight + pgg45 + age + gleason, pros)
summary(psa_rpart)
rpart.plot(psa_rpart)
```



Missing Data

- Trees can easily handle data with missing predictor values. Two options are common:

    1. For categorical predictors, create a new category called “missing.”

    2. A more general approach is to create **surrogate splits**:

        - When considering a predictor for a split, use only observations for which that predictor is not missing.

        - After choosing the best **primary split**, then form a list of surrogate predictors and split points:

            - The first surrogate predictor is the best predictor and split point that best mimics the primary split.

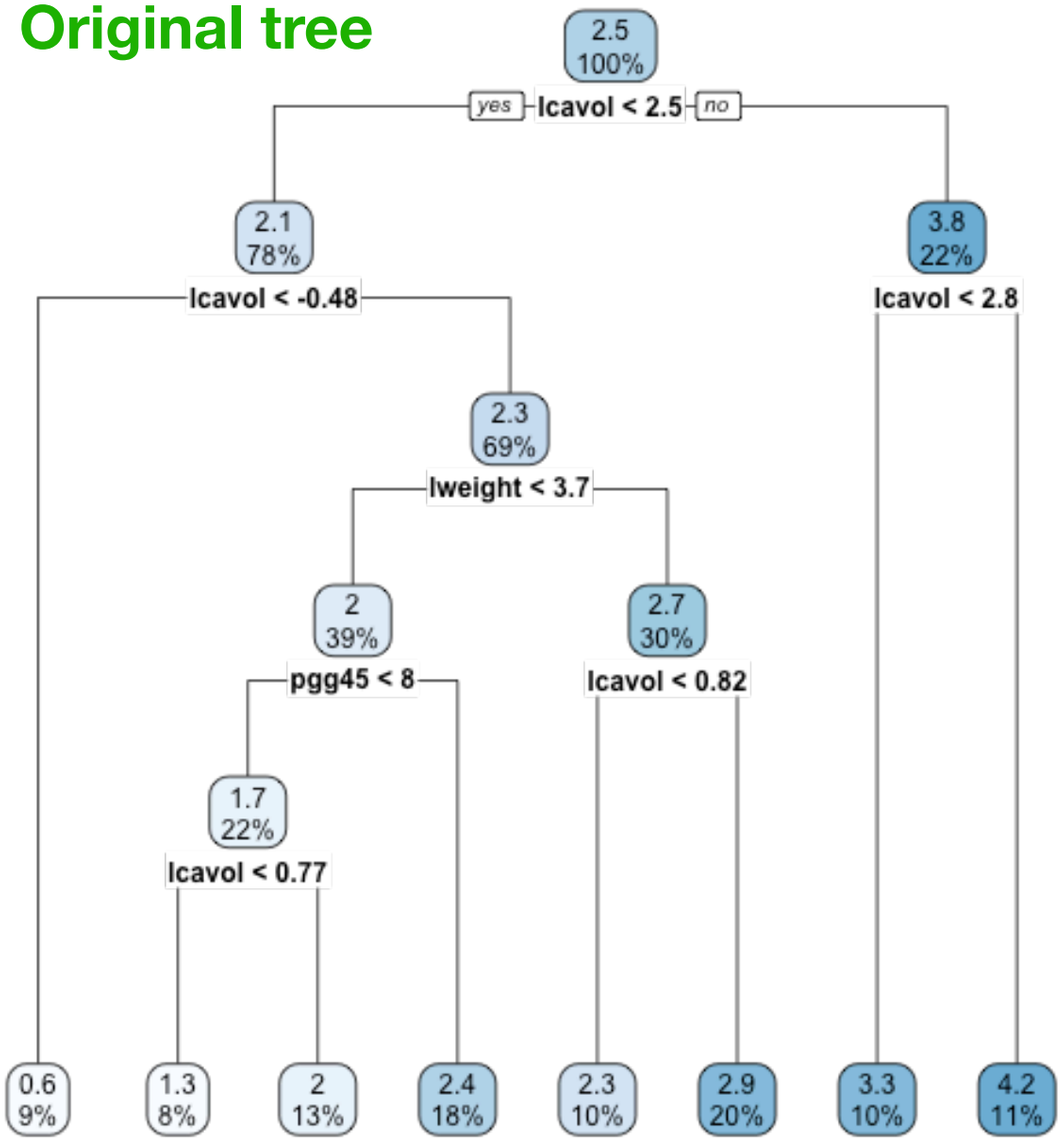
            - The second surrogate predictor is the predictor and split point that is second best at mimicking the primary split.

            - …

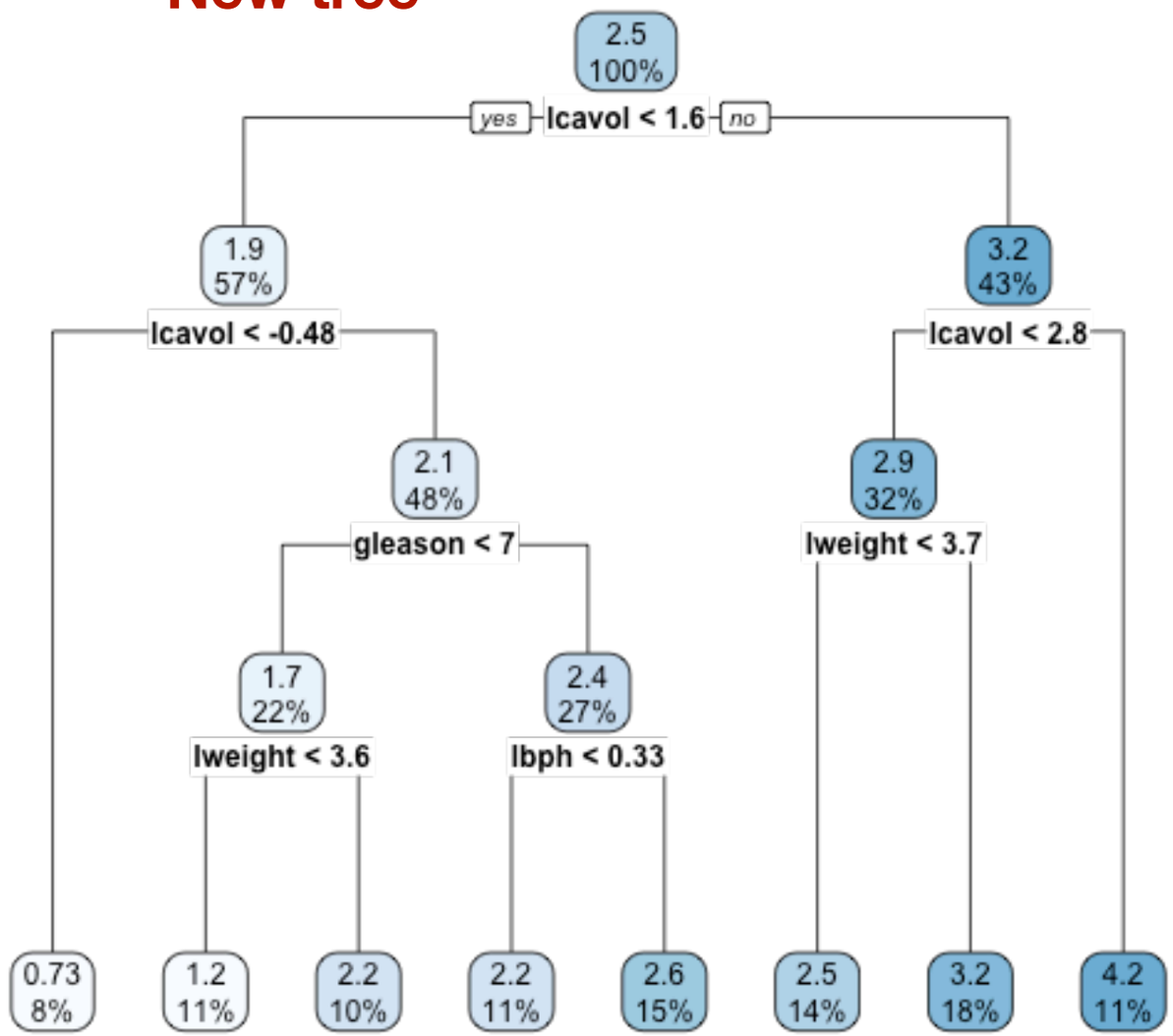
Example: Predicting log(PSA)

- Let's randomly remove some predictor values. For the variables age, gleason, and lcavol, I randomly selected 5 subjects and removed their values.

Original tree



New tree



Example: Predicting log(PSA)

- Let's look at the surrogate splits for the first node:

```
Node number 1: 97 observations,    complexity param=0.324024
  mean=2.478387, MSE=1.318739
  left son=2 (55 obs) right son=3 (42 obs)
  Primary splits:
      lcavol  < 1.551753    to the left,  improve=0.3232121, (5 missing)
      svi     < 0.5         to the left,  improve=0.3206031, (0 missing)
      lcp     < 0.1359669   to the left,  improve=0.2770979, (0 missing)
      pgg45   < 8           to the left,  improve=0.2519755, (0 missing)
      lweight < 3.672483    to the left,  improve=0.2254510, (0 missing)
  Surrogate splits:
      lcp     < 0.2616241   to the left,  agree=0.870, adj=0.707, (5 split)
      svi     < 0.5         to the left,  agree=0.761, adj=0.463, (0 split)
      pgg45   < 27.5        to the left,  agree=0.750, adj=0.439, (0 split)
      lweight < 3.446796    to the left,  agree=0.620, adj=0.146, (0 split)
      gleason < 6.5         to the left,  agree=0.609, adj=0.122, (0 split)
```

This is the primary split we chose for the first node.

This is the best split for mimicking the selected primary split.

Summary: Trees

- Pros:
    - Very easy to interpret and explain to others
    - Can easily handle both categorical and continuous predictors, as well as missing data
    - Invariant to monotonic transformations of the predictors
    - Fast to fit
- Cons:
    - Doesn’t model linear decision boundaries very well.
    - Decision trees have **high variance**. If we resample the training data, we may get a very different tree.

Today's Lecture

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- Ensembling
    - **Bagging**
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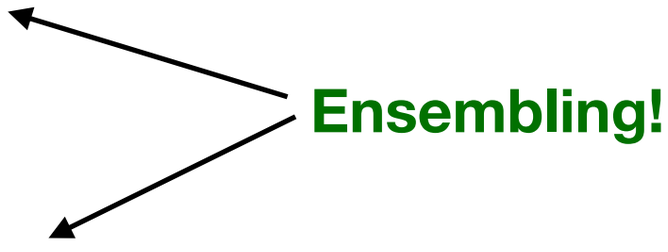


- Variable Importance

Bagging

- Bootstrap aggregation, or **bagging**, is a general-purpose procedure for reducing the variance of a statistical learning method by averaging.

- We know that **averaging reduces the variance**:

  - Specifically, if we take the average of *n* independent observations $Z_1, \cdots, Z_n$, each with variance σ^2, then

$$Var\left(\frac{1}{n}\sum_{i=1}^{n} Z_i\right) = \sigma^2/n.$$

- Idea: What if we can average models estimated on *B* datasets?

$$\hat{f}_{avg}(x) = \frac{1}{B}\sum_{b=1}^{B} \hat{f}^b(x)$$

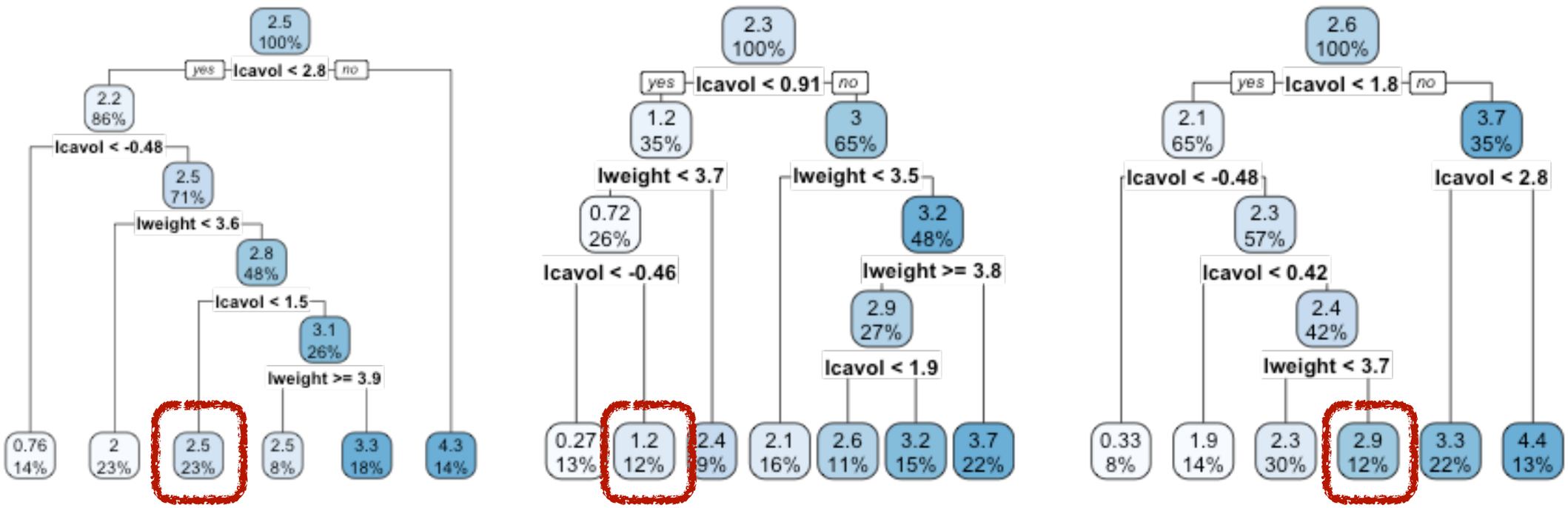
Bagging

- How do we make *B* datasets when we only have one dataset? We create bootstrap samples:
  - For $b = 1, \cdots, B$:
    - Randomly draw *n* observations with replacement.
    - Train model $\hat{f}^{*b}$ on the bootstrap sample.

- Bagging averages the models trained on *B* bootstrap samples:

$$\hat{f}_{bag}(x) = \frac{1}{B} \sum_{b=1}^{B} \hat{f}^{*b}(x)$$

Averaging the output from multiple trees



For a new observation with lcavol = 0.5, lweight = 3.8:

Tree 1 predicts 2.5
Tree 2 predicts 1.2
Tree 3 predicts 2.9

→ We average the predictions and output 2.2

- For classification trees, output the average as a probability or do majority voting.

Bagging

- The number of bootstrap samples *B* is a hyperparameter…

- But the procedure is not that sensitive to the value of *B:*

  - As *B* increases, the bagged model will converge.

  - In practice, *B* = 100 to *B* = 1000 work pretty well

An issue with Bagging

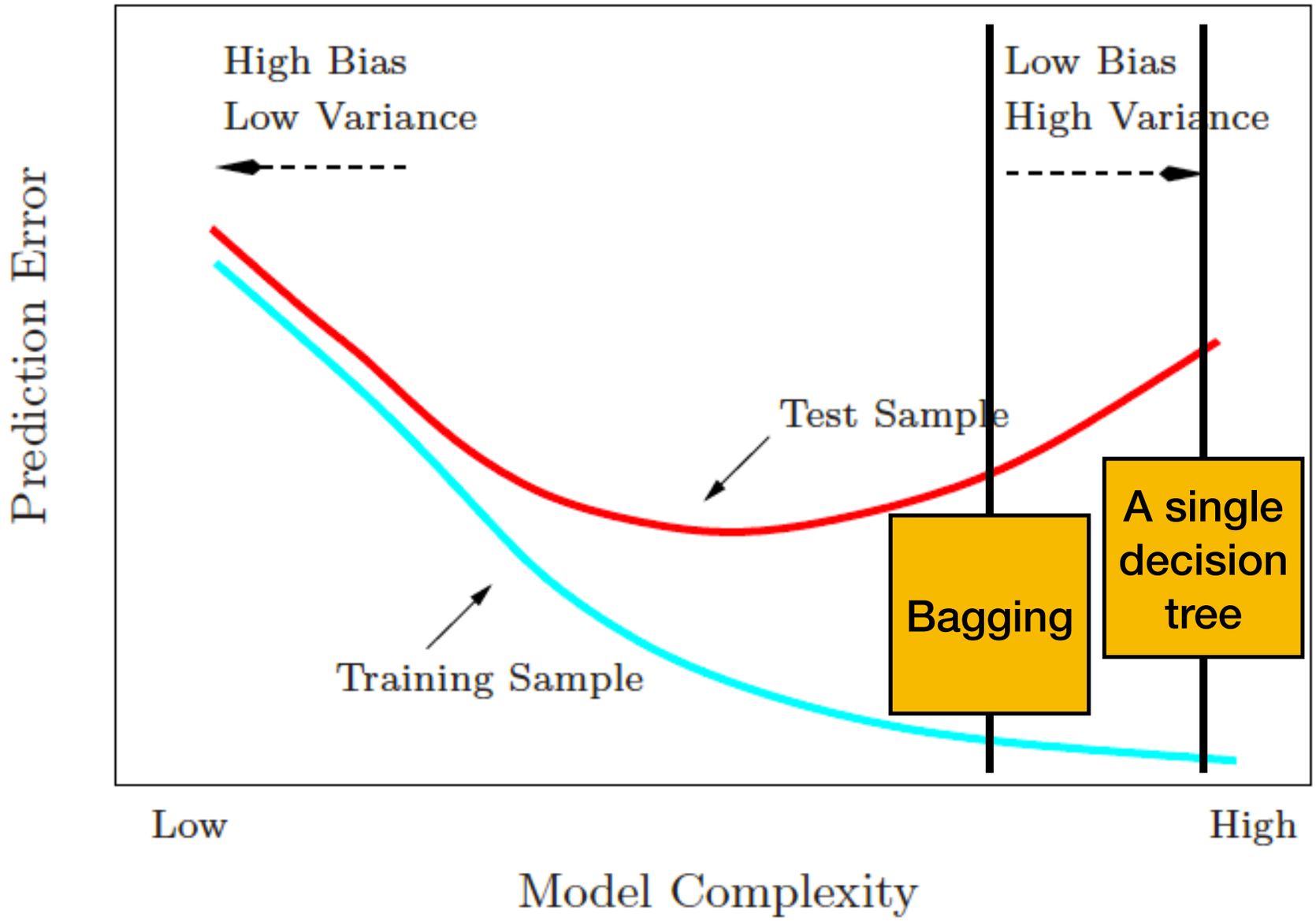
- Suppose that there is one very strong predictor in the data set, along with a number of moderately strong ones

- Then in the collection of bagged trees, most or all of the trees will **use this strong predictor in the top split**, and they all look somewhat similar

- This means that **predictions from the bagged trees can be highly correlated**.

- In this setting, bagging will only reduce the model variance slightly

Bias-variance trade-off



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    - **Random Forests**
- Variable Importance

Random Forests

- Goal: Make the trees less similar.

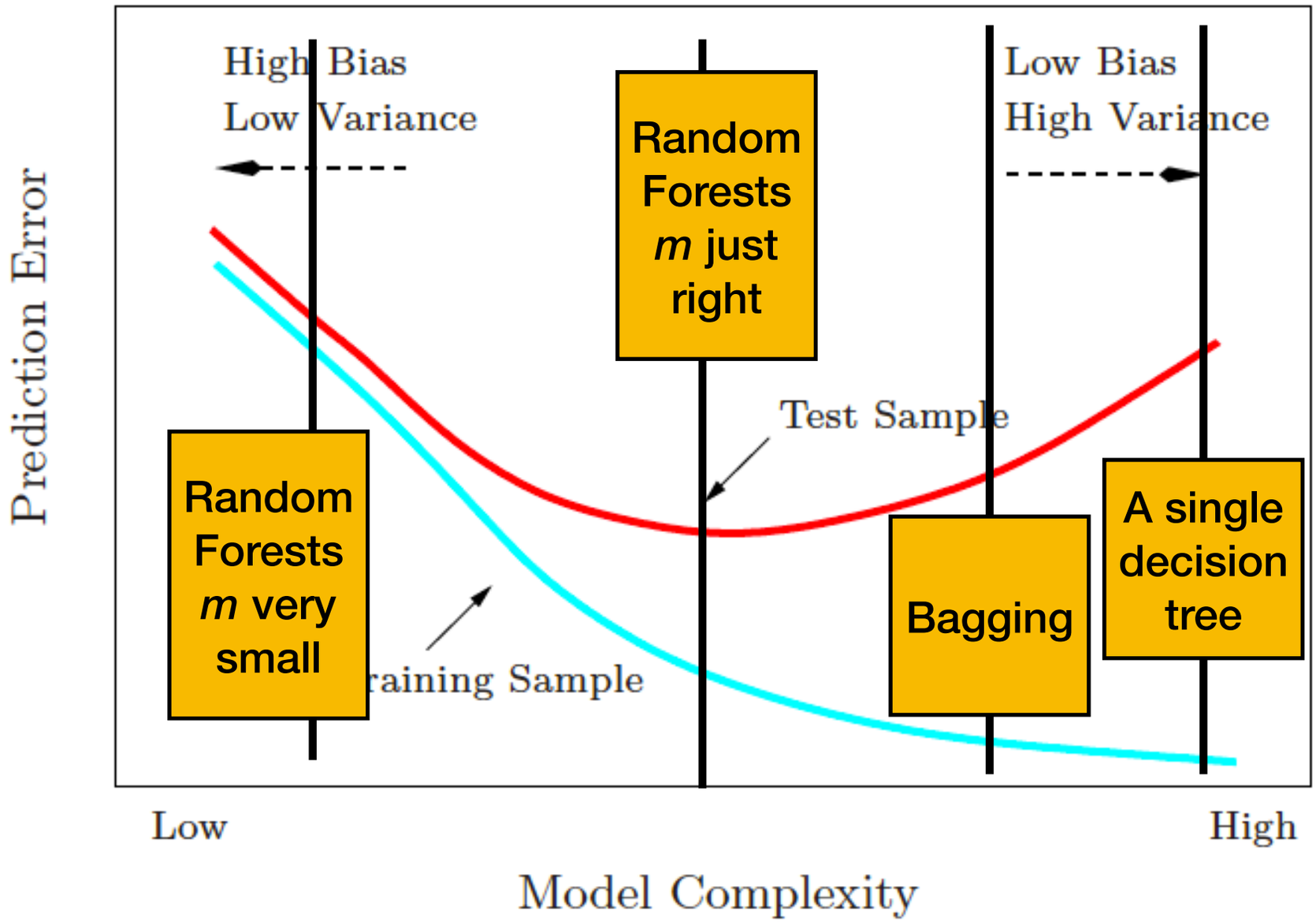
- Idea: When fitting a tree for each bootstrap sample, randomly pick m variables to consider at each split.

- By randomly selecting variables to use in each tree, we "**decorrelate**" the trees and achieve a larger reduction in variance.

Random Forests

- How many predictors should I pick at random?
  - As m increases, the trees become more similar.
  - If m is very small, the randomly selected variables will have very little predictive power and the trees will have higher bias.
- Typical choice is $m = \sqrt{p}$.

Bias-variance trade-off



Random Forests

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Do we Need Hundreds of Classifiers to Solve Real World Classification Problems?

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Abstract: We evaluate **179 classifiers** arising from **17 families**… We use 121 data sets, which represent the whole UCI data base and other own real problems… **The classifiers most likely to be the bests are the random forest (RF) versions**, the best of which… achieves 94.1% of the maximum accuracy over all the datasets…

Evaluating the test error of a random forest

- Every time we create a bootstrap sample to fit a tree, there will be leftover observations. These are referred to as **out-of-bag (OOB) observations**.

- We can use these to estimate the generalization error of the random forest:

  - For the *i*-th observation, predict its response using all the trees for which that observation was OOB.

  - We estimate the generalization error of the RF using the average error of the OOB predictions.

Example: Random Forest for Prostate data

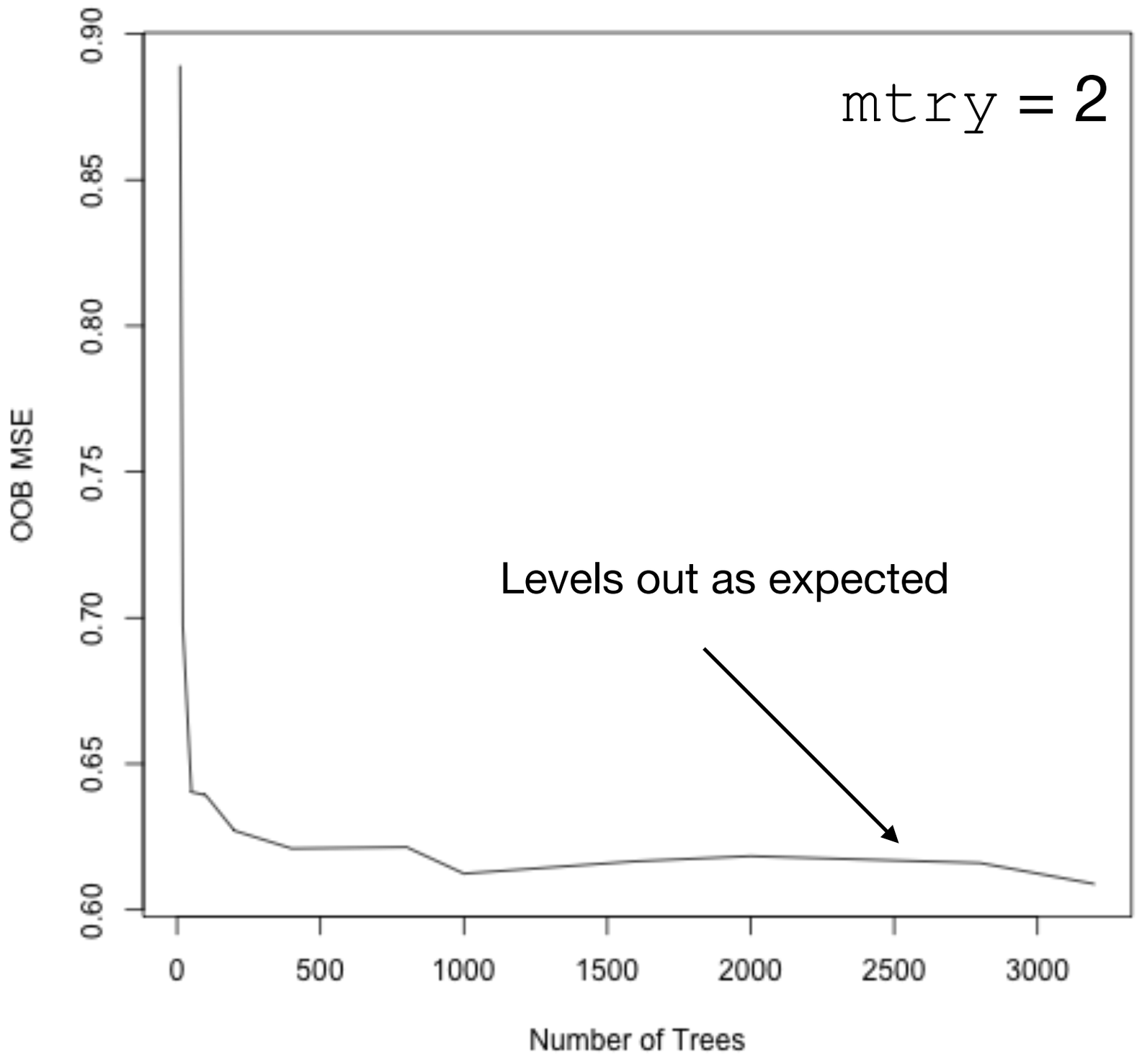
```
> psa_rf <- ranger(lpsa ~ svi + lcavol + lweight + pgg45 + age + gleason, pros
> psa_rf
Ranger result

Call:
 ranger(lpsa ~ svi + lcavol + lweight + pgg45 + age + gleason,

Type:                             Regression
Number of trees:                  500
Sample size:                      97
Number of independent variables:  6
Mtry:                             2
Target node size:                 5
Variable importance mode:         impurity
Splitrule:                        variance
OOB prediction error (MSE):       0.6197062
R squared (OOB):                  0.5349212
```

`mtry` is the number of covariates randomly sampled at each node

Example: Hyperparameters in the Random Forest



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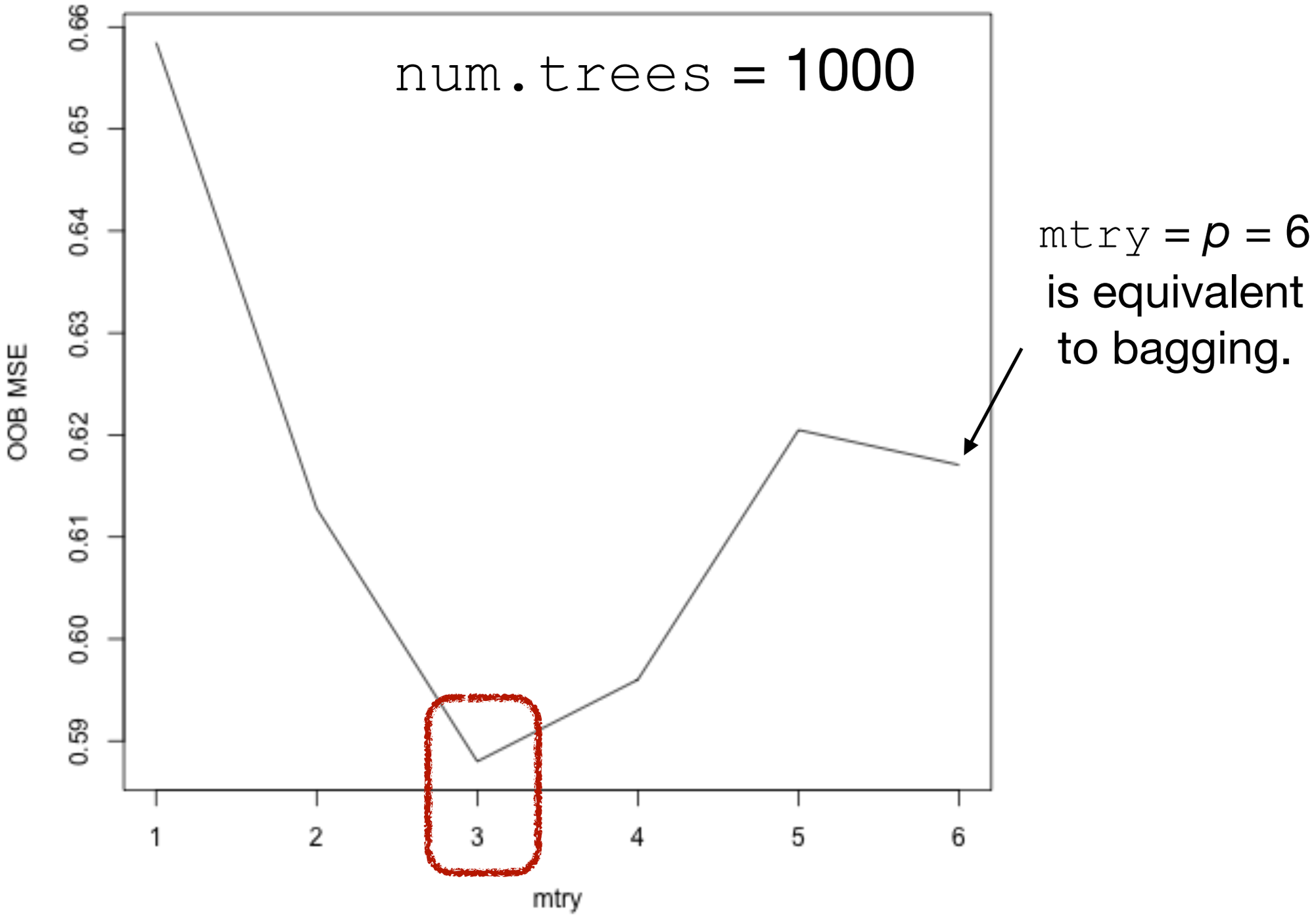


Random forests for high-dimensional data

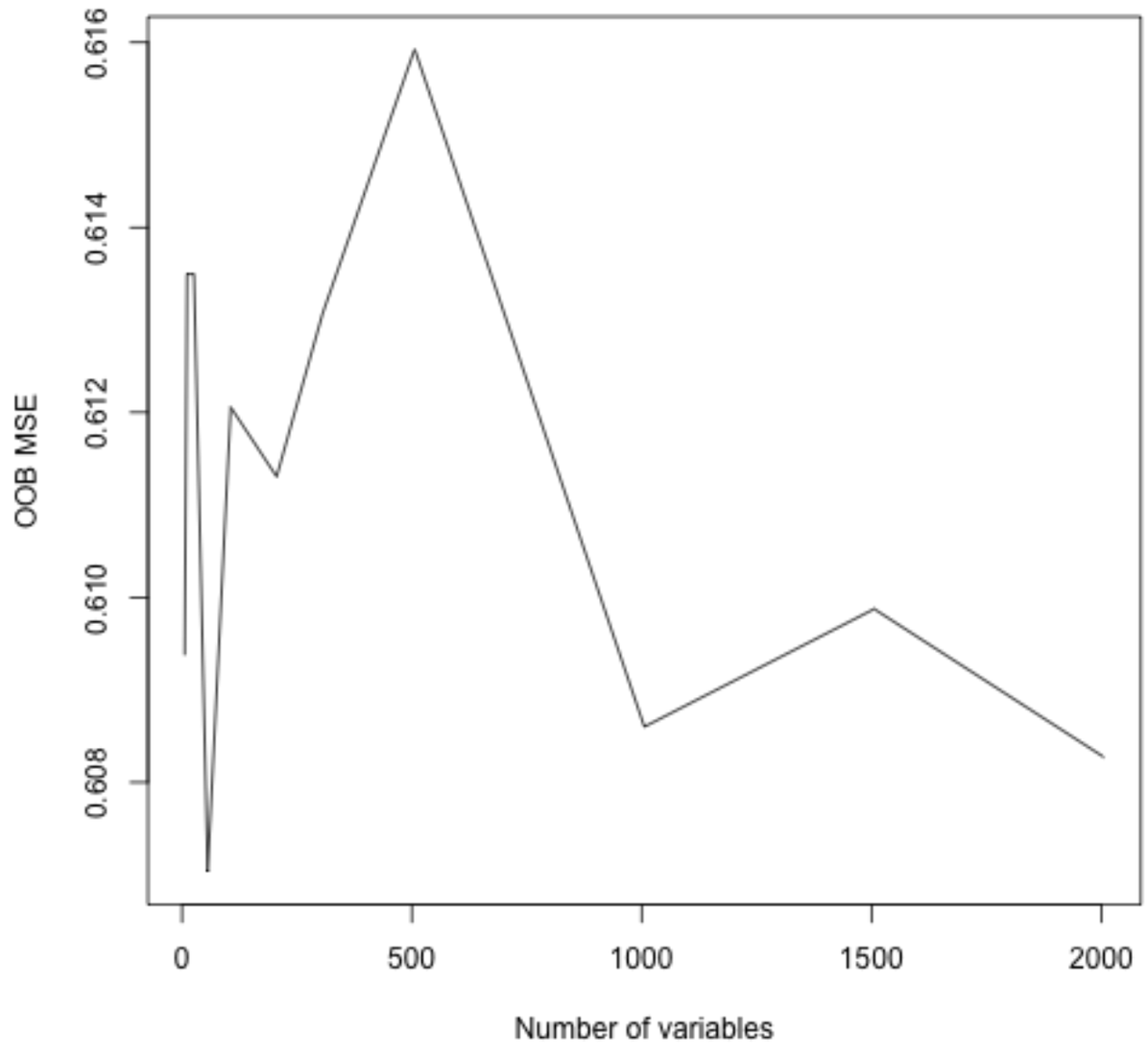
- **Q**: How do you think random forests will perform for high-dimensional data?

- **A**: Poorly. A random forest model will get confused by spurious correlations between the variables and the outcome.

- **B**: Random forests are naturally doing some sort of variable selection and this will help regularize the model. They'll probably do fine.

Example: RF for Prostate data with more variables

- Let's add many additional variables to the prostate data and see how this affects the OOB error.



Looks like RF is actually doing quite well in this high-dimensional example.

Today's Lecture

- Decision Trees
- **Ensembling**
    - Bagging
    - Random Forests
- Variable Importance

Ensemble methods

- Bagging and random forests are examples of ensemble methods.

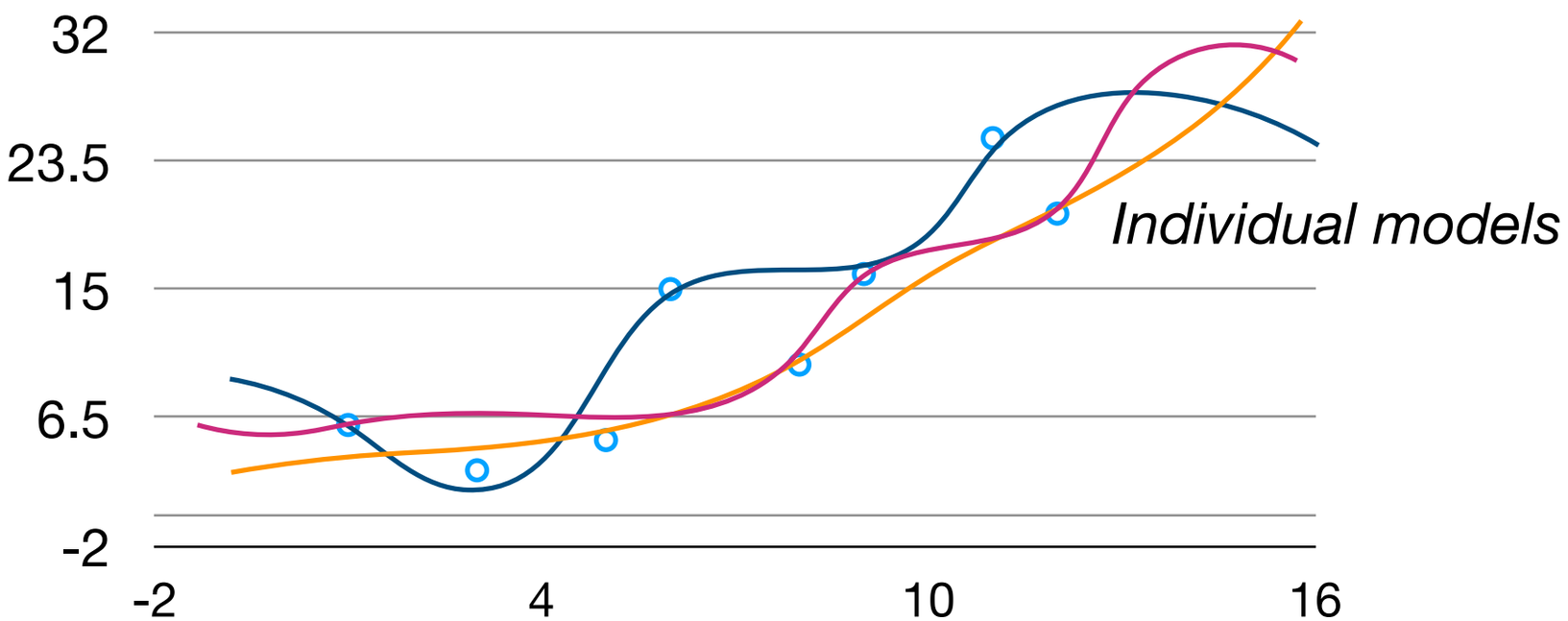
- Ensemble methods construct a set of prediction models and take a weighted average to make a final prediction.

- “Wisdom of the crowds”: Ensembles tend to be more accurate than the individual prediction models.

Benefits of ensembling

1. Protection against overfitting:

    - When the underlying models have low bias but high variance, ensemble methods reduce the variance and selects a more appropriate bias-variance tradeoff.
    - We can also get a sense of model uncertainty.



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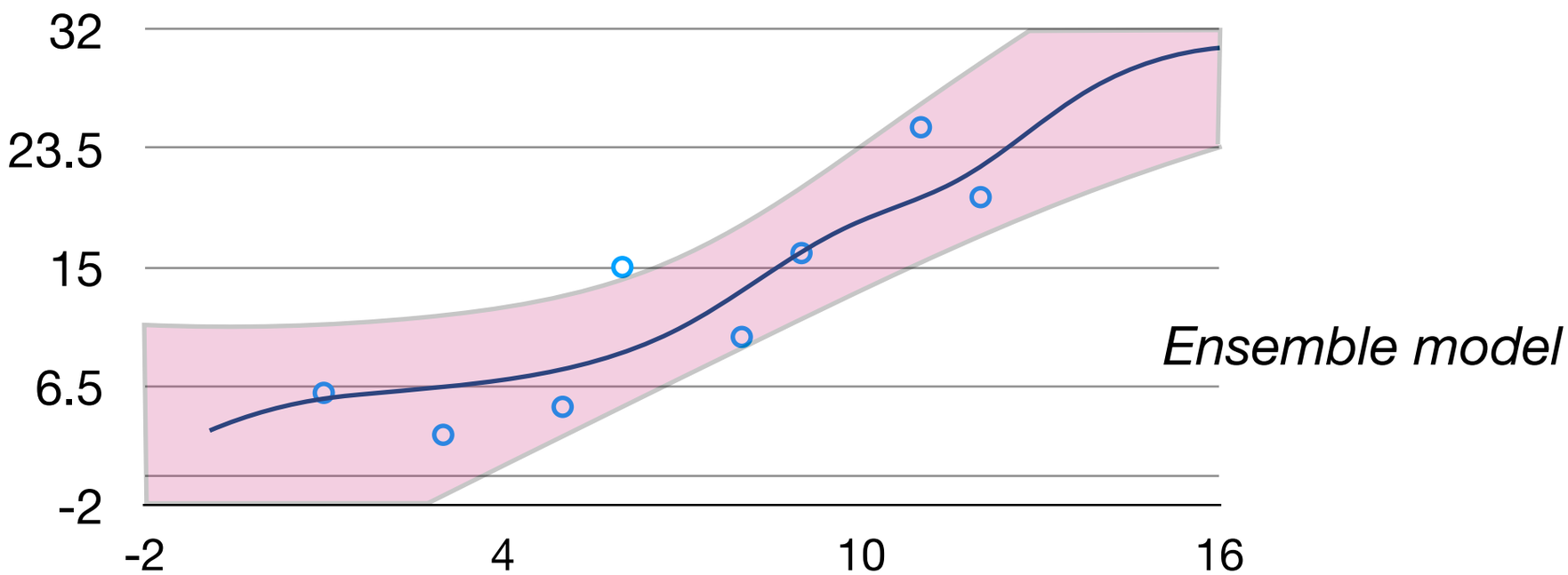
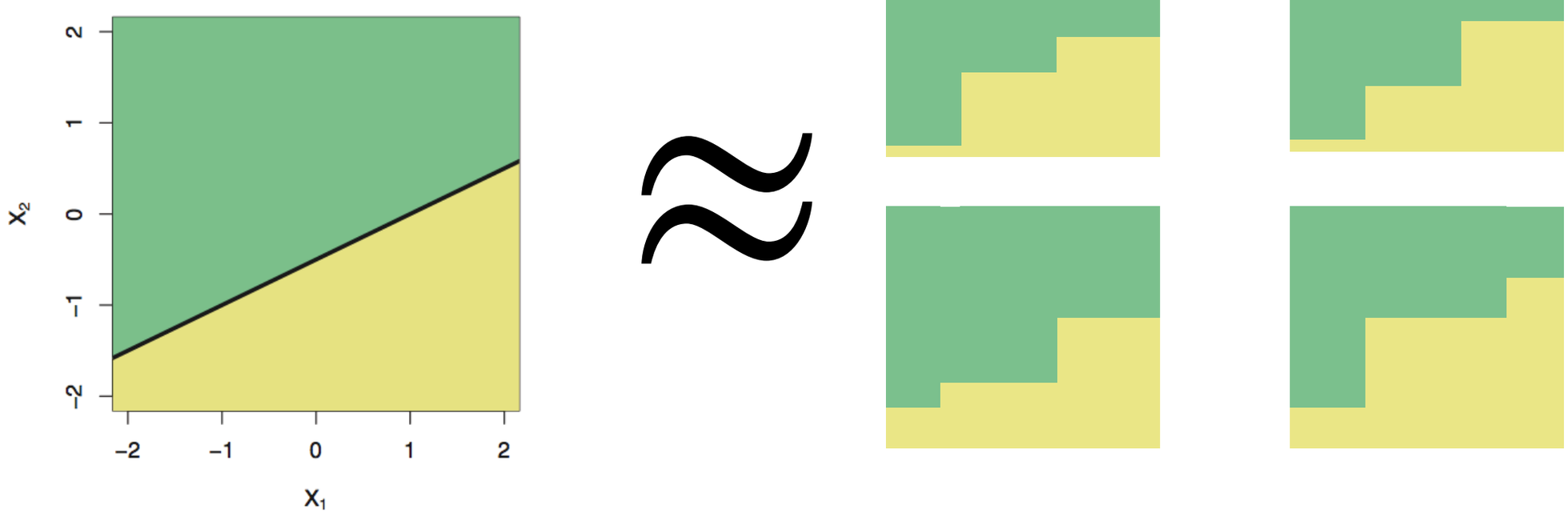


Benefits of ensembling

2. The model is misspecified, but their average is a good approximation:

- Even if the individual models are highly restricted and the true data cannot be fully represented by the individual models, we can expand the space of functions that we can estimate by taking an average of the individual models.

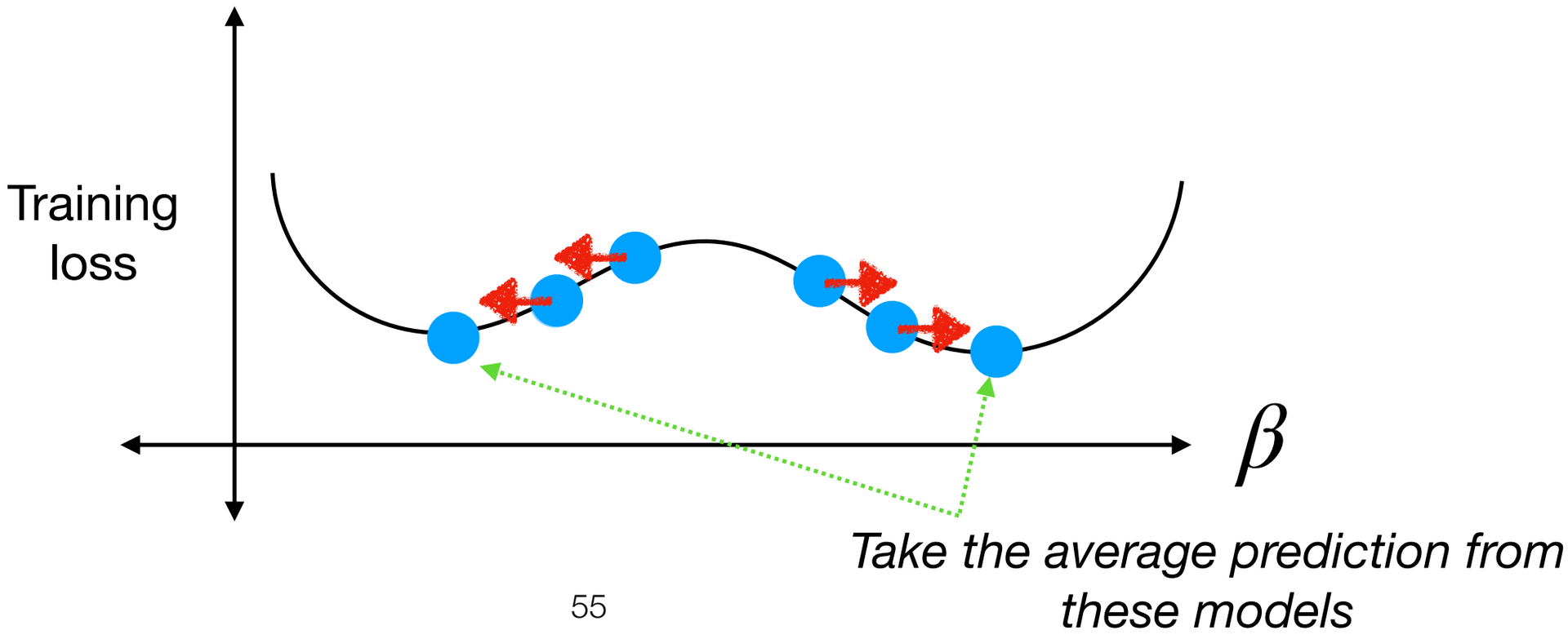


Benefits of ensembling

3. <u>Ensembling can help us overcome computational difficulties</u>:

- For ML algorithms like random forests and neural networks, the model is fit by attempting to solve a non-convex optimization problem.

- Because we are very likely to get stuck at a local optima, we should try multiple start points. For models that look equally good, taking an average can help.



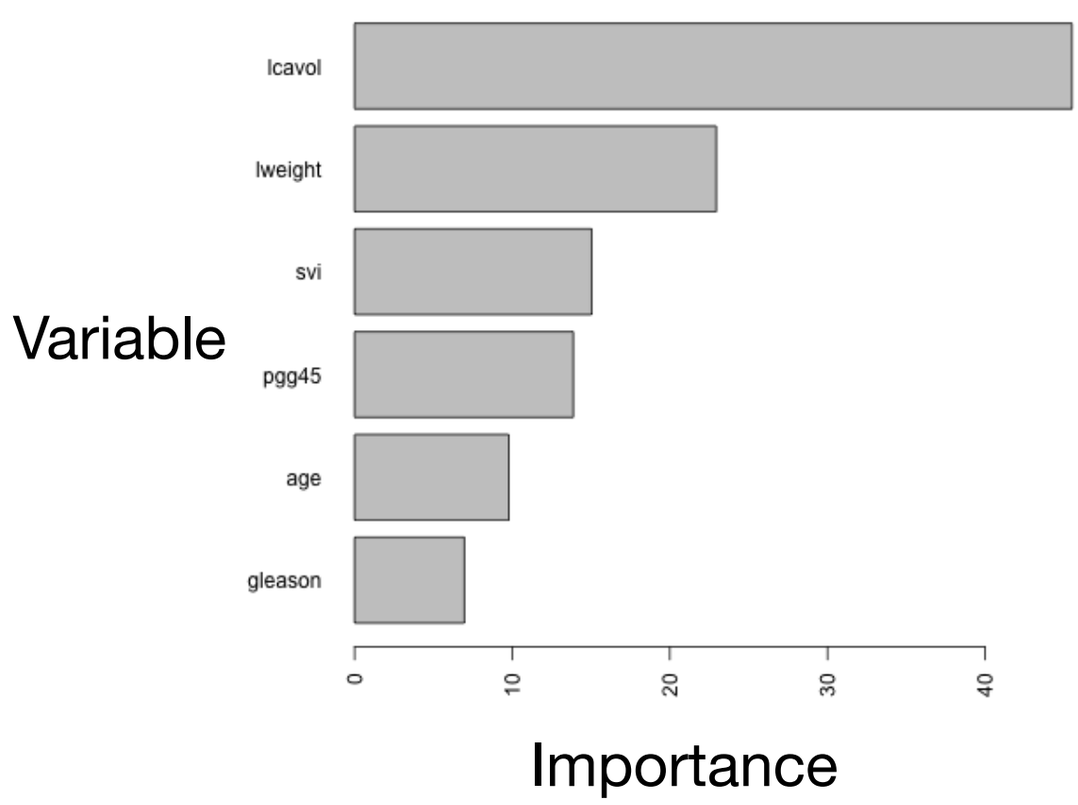
Today's Lecture

- Decision Trees
- Ensembling
    - Bagging
        - Random Forests
- **Variable Importance**

Interpreting random forests

- Interpreting random forests is tricky because we are averaging across trees with different structures.

- A very popular approach is to **estimate the importance of each variable**.



Permutation-based variable importance

- Fit the random forest.
- Compute the OOB error.
- For j = 1,…,p:
    - Permute the values of the j-th variable. Compute the OOB error of the fitted model for the permuted dataset.
- Compare the OOB error for the original dataset versus the permuted dataset.

Is this variable important?

- **Q**: Suppose I fit a random forest and it gets an AUC of 0.6. The plot of permutation variable importance is given below. Which of the following are true:

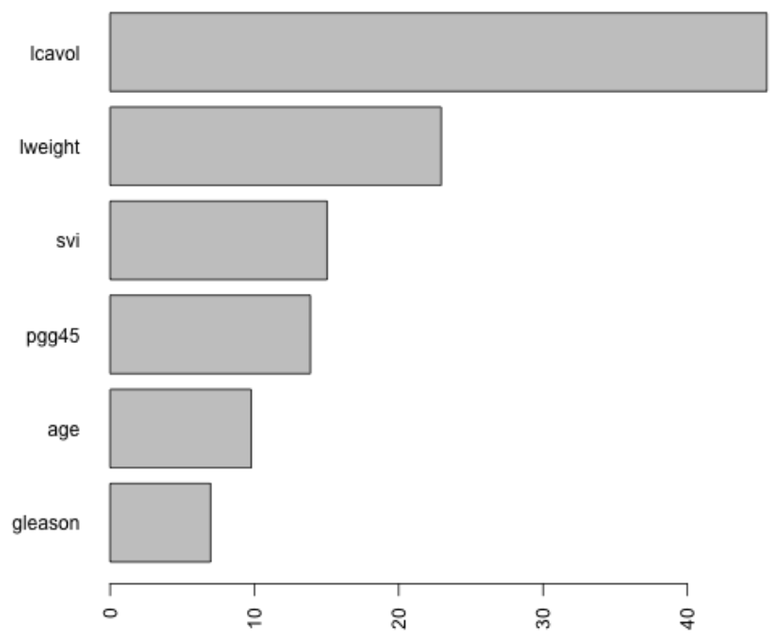
- **A**: The trained model assigned `lcavol` high importance.

- **B**: The variable `lcavol` is the most important variable for making accurate predictions.

- **C**: The trained model assigned `gleason` low importance.

- **D**: Suppose I was allowed to collect a larger training dataset for retraining the model, but I'm only allowed to collect data on 5 of 6 predictors. In this case, I should drop `gleason` from data collection because it has the lowest importance.

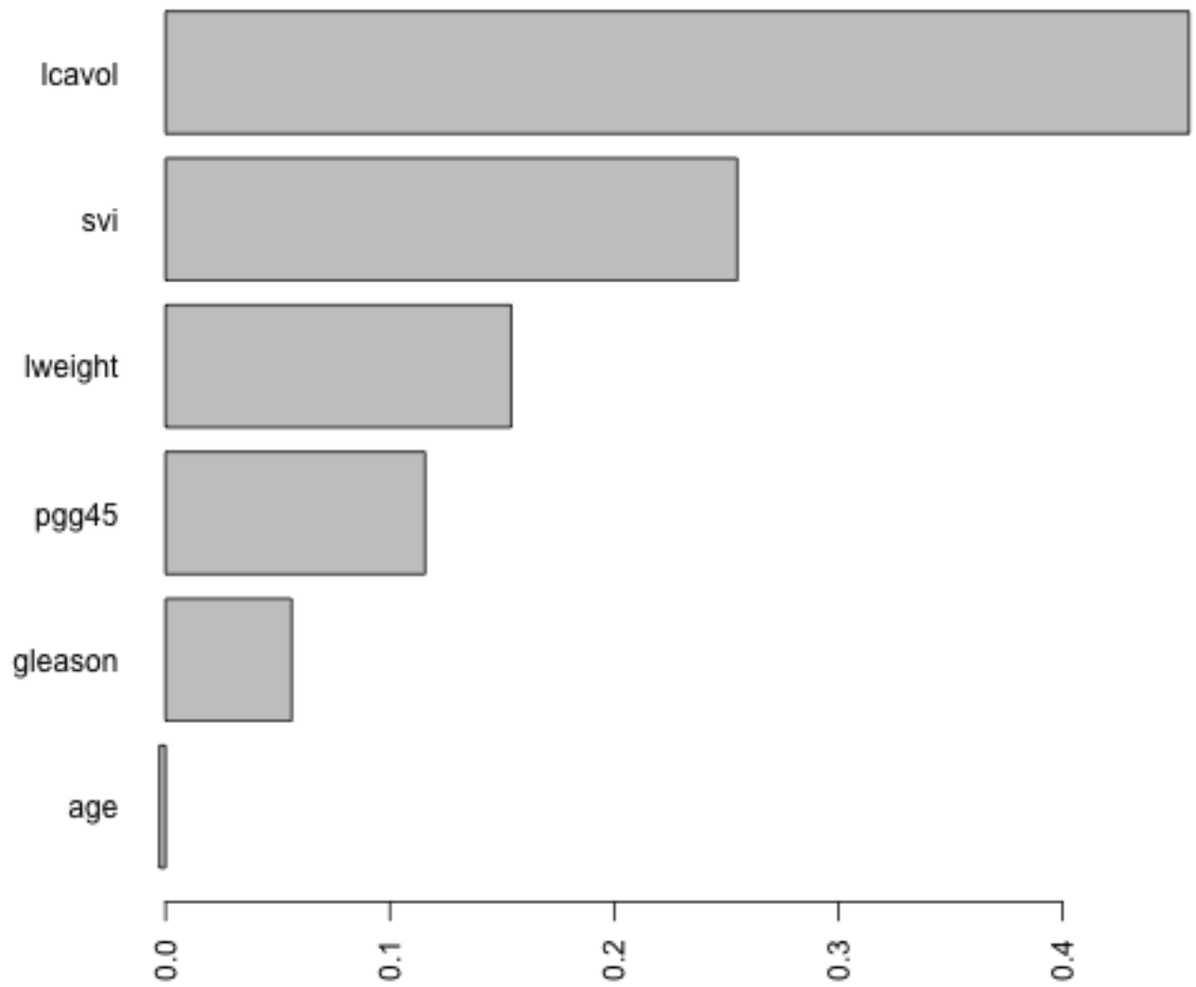
*Permutation variable importance describes the importance of a variable to the **fitted model**, not the importance of a variable in the **best possible model** for the target population.*



Example in R

```
> psa_rf <- ranger(lpsa ~ svi + lcavol + lweight + pgg45 + age + gleason, pros, importance = "permutation")
> importance(psa_rf)
         svi       lcavol      lweight        pgg45          age      gleason
 0.254875333  0.456267123  0.154121162  0.115708769 -0.002733986  0.056206880
```

- The importance of the *j*-th variable is the increase in OOB mean squared error when you permute the *j*-th variable.



A zoo of variable importance measures

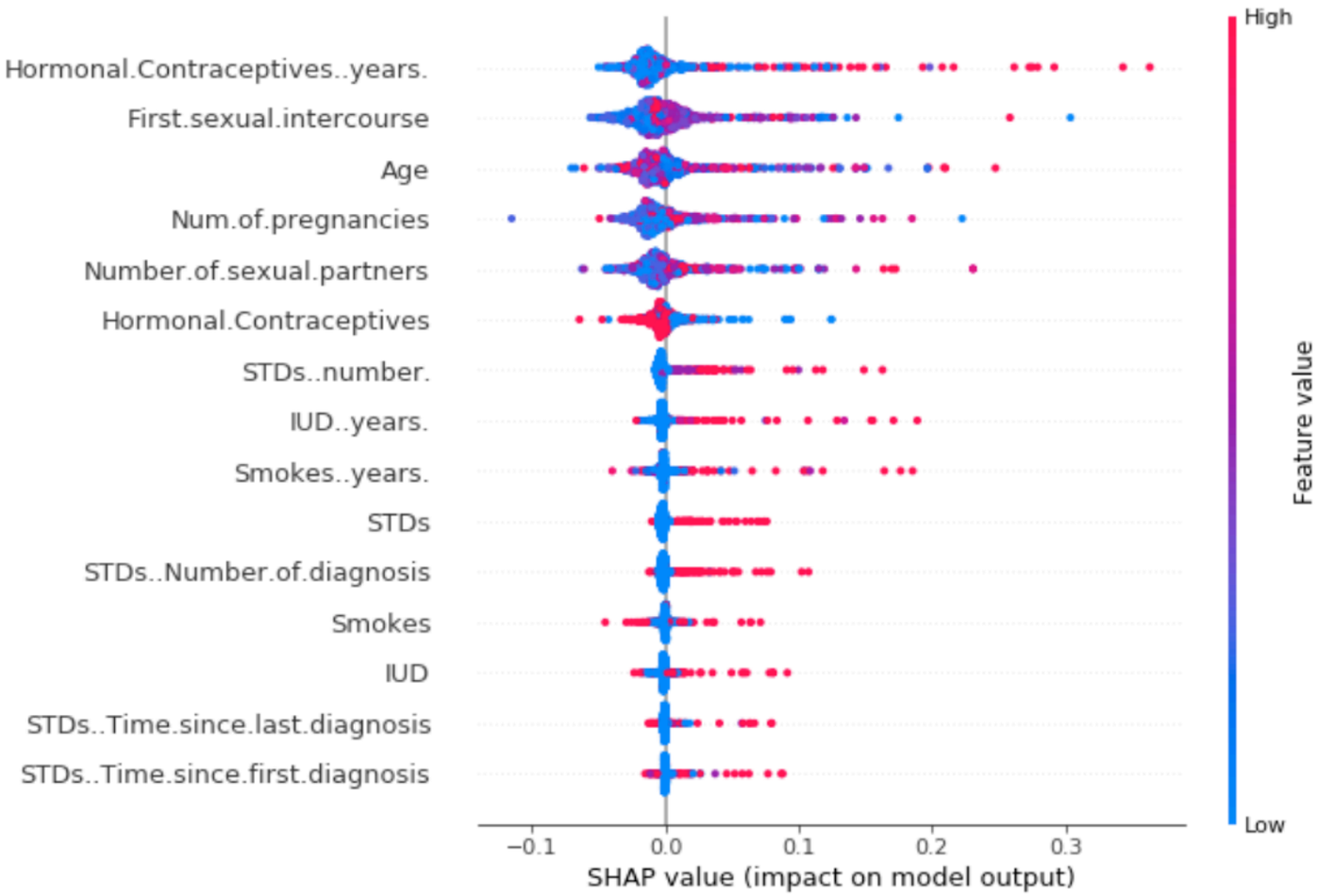
- There are now many variable importance measures in the machine learning literature. The major categories are…

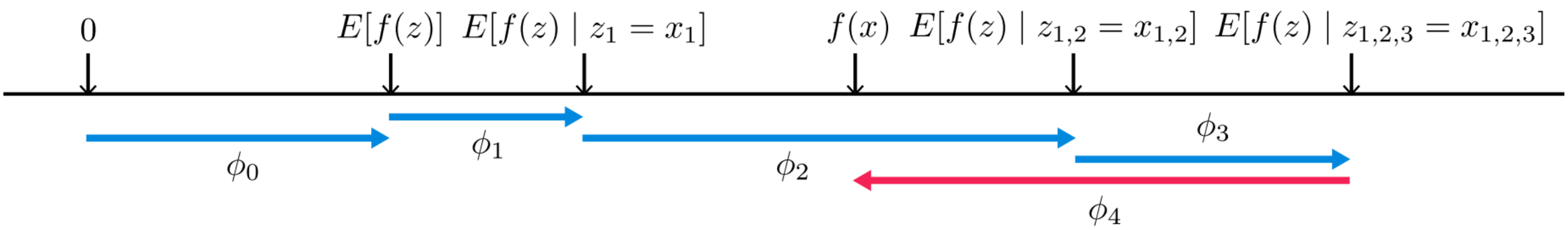
1. Explaining the importance of a variable in a fitted model
    1. The importance measure is specific to the particular model class
        - *e.g. Permutation variable importance in a random forest using OOB error*
    2. The importance measure is model agnostic
        - *e.g. Permutation feature importance using a training/test split*
2. Explaining the importance of a variable in the underlying population (This should also come with confidence intervals)
    1. Parametric model class (i.e. we assume the model is correctly specified)
        - *e.g. R^2 and ANOVA in linear/logistic regression*
    2. Nonparametric model class (i.e. we don't know what the true model is)
        - *Research!*
    3. Causal variable importance: How much will the patient outcome change if I modify this variable

SHAP values

- Shapley Additive exPlanation (SHAP) values summarize the variable importance **for a given prediction from a given model**.

- SHAP values measure how much the prediction changes when a feature is removed. Because there are many possible orders for removing the features, it averages over all possible orders.





SHAP values: calculations

Feature set	Prediction
{}	0.5
{1}	0.5
{2}	0.7
{3}	0.4
{1,2}	0.8
{1,3}	0.45
{2,3}	0.65
{1,2,3}	0.75

To calculate the SHAP value for X_1:

1. Determine how much X_1 changed our prediction with respect to possible feature subsets:
   - $\hat{f}(X_1) - \hat{f}(\{\}) = 0$
   - $f(X_1, X_2) - f(X_2) = 0.1$
   - $\hat{f}(X_1, X_3) - \hat{f}(X_3) = 0.05$
   - $\hat{f}(X_1, X_2, X_3) - \hat{f}(X_2, X_3) = 0.1$
2. Take a weighted average (for a special choice of weights) to get the SHAP value of X_1

Note: *In a linear model, the SHAP value for variable X_i is equal to $\beta_i x_i$.*

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