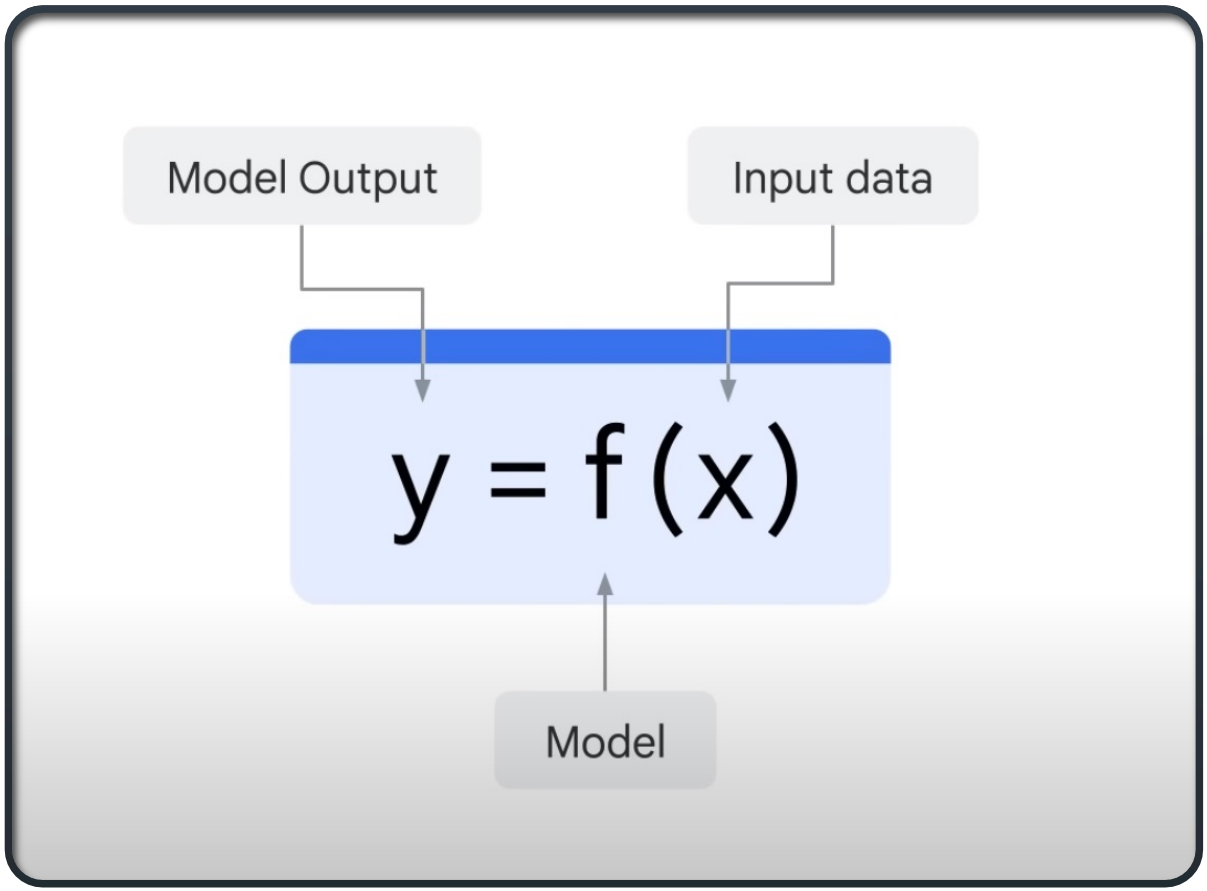
Introduction to Supervised Machine Learning

Soumya Banerjee

Supervised learning



Linear regression

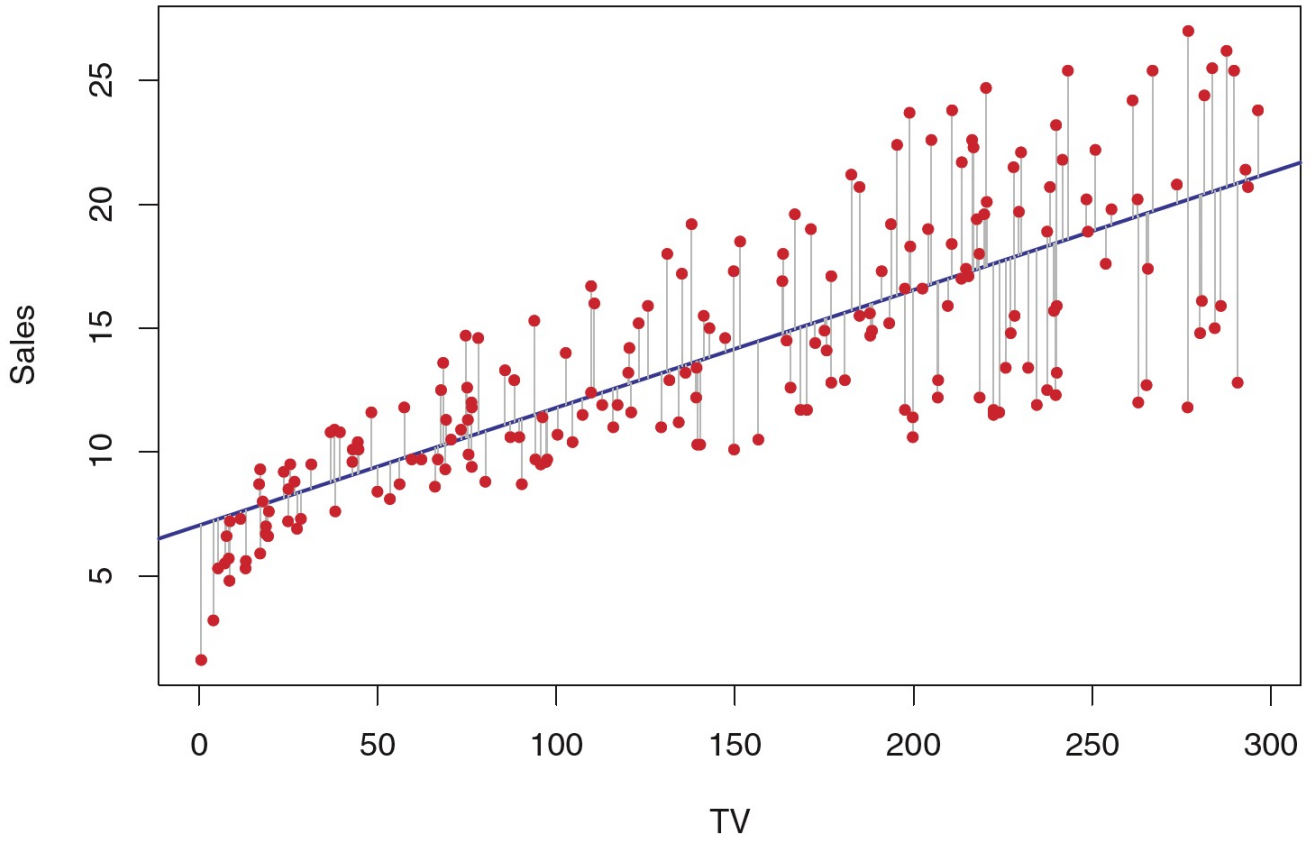


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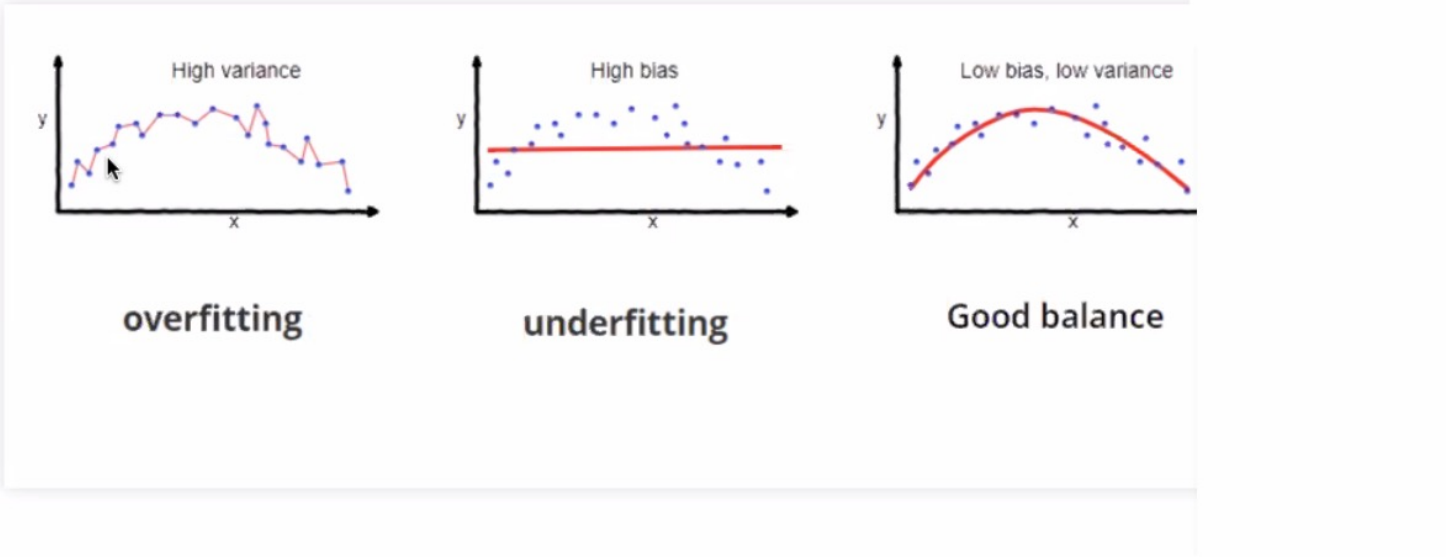
FIGURE 3.1. *For the* `Advertising` *data, the least squares fit for the regression of* `sales` *onto* `TV` *is shown. The fit is found by minimizing the sum of squared errors. Each grey line segment represents an error, and the fit makes a compromise by averaging their squares. In this case a linear fit captures the essence of the relationship, although it is somewhat deficient in the left of the plot.*

A fundamental concept in machine learning

Bias-variance tradeoff



- Bias is residual error from fitting the Training data
- Variance is generalization error when applying the model fit to

A fundamental concept in machine learning

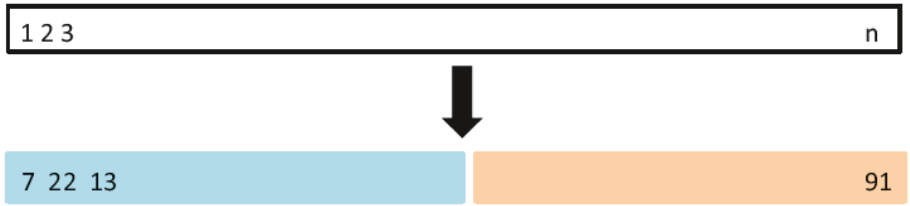


FIGURE 5.1. *A schematic display of the validation set approach. A set of n observations are randomly split into a training set (shown in blue, containing observations 7, 22, and 13, among others) and a validation set (shown in beige, and containing observation 91, among others). The statistical learning method is fit on the training set, and its performance is evaluated on the validation set.*

Leave one out cross-validation

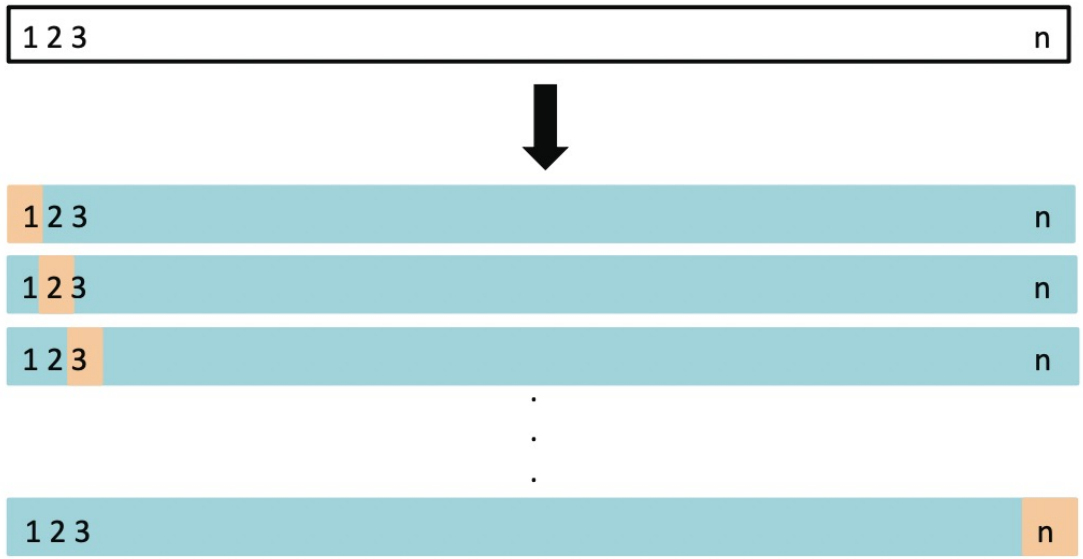


FIGURE 5.3. *A schematic display of LOOCV. A set of* n *data points is repeatedly split into a training set (shown in blue) containing all but one observation, and a validation set that contains only that observation (shown in beige). The test error is then estimated by averaging the* n *resulting MSEs. The first training set contains all but observation 1, the second training set contains all but observation 2, and so forth.*

K-fold cross-validation

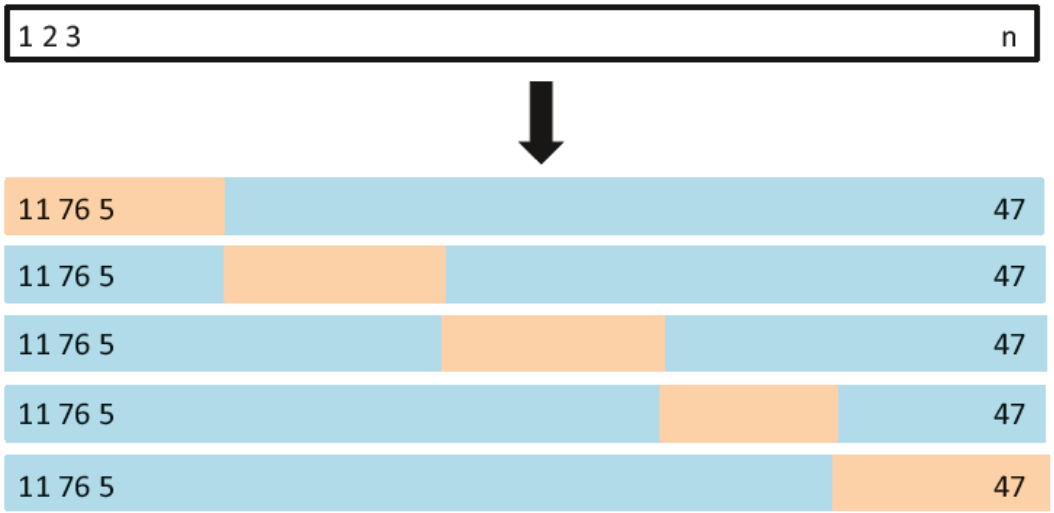


FIGURE 5.5. *A schematic display of 5-fold CV. A set of n observations is randomly split into five non-overlapping groups. Each of these fifths acts as a validation set (shown in beige), and the remainder as a training set (shown in blue). The test error is estimated by averaging the five resulting MSE estimates.*

chapters. The magic formula (5.2) does not hold in general, in which case the model has to be refit n times.

Cross-validation

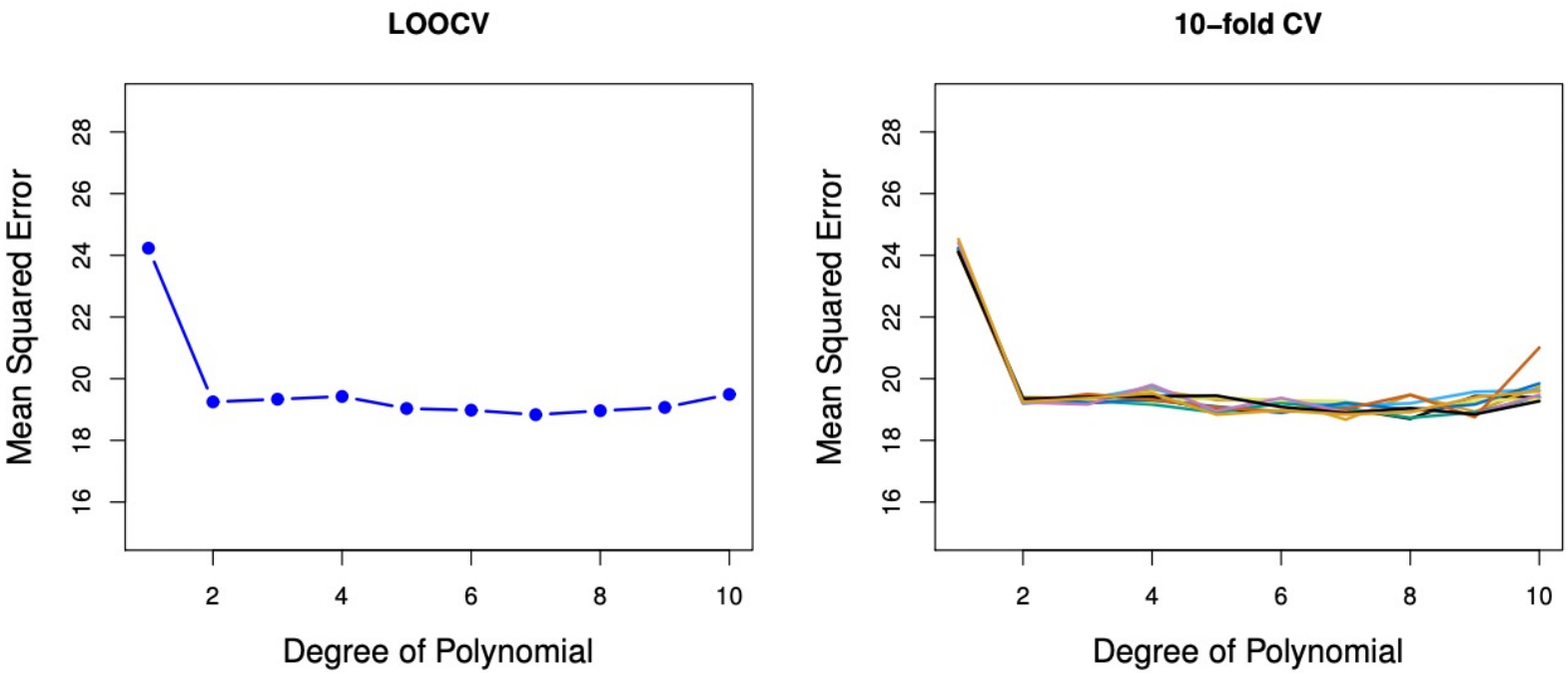
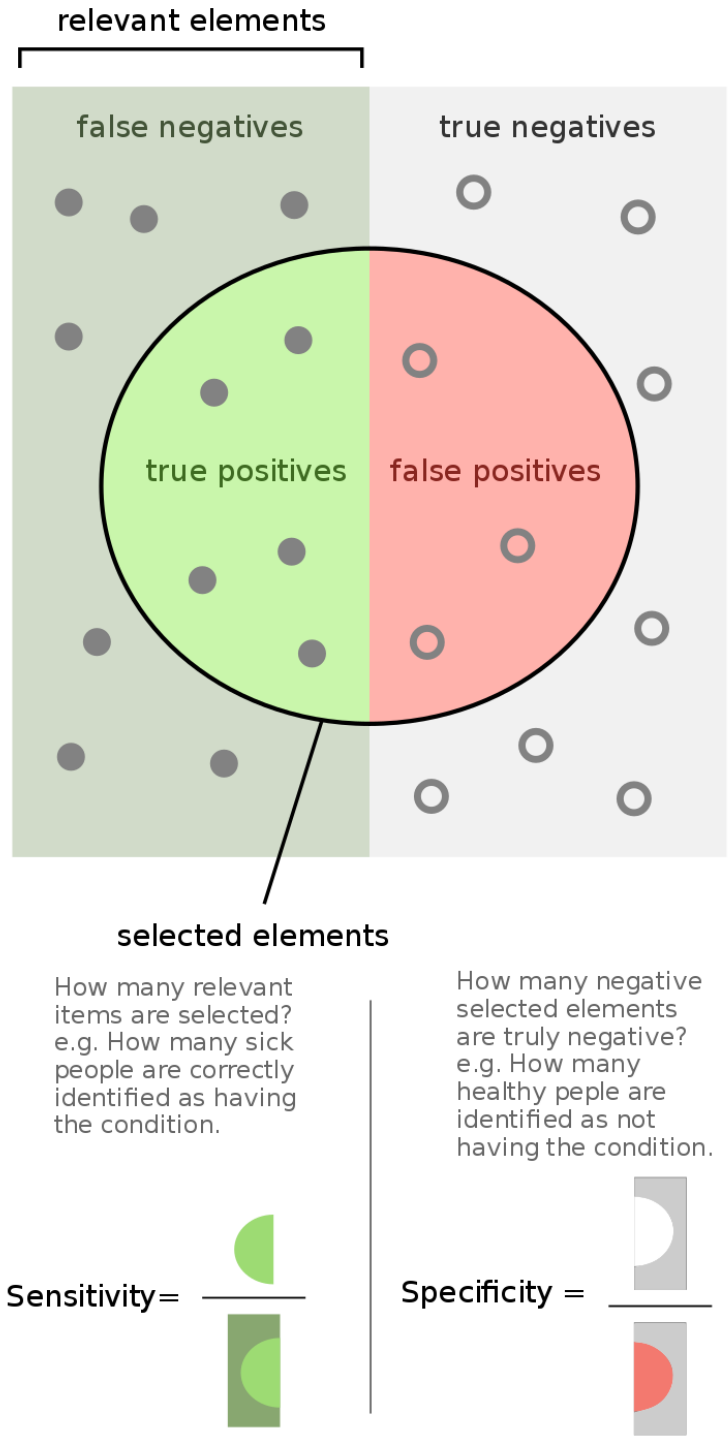
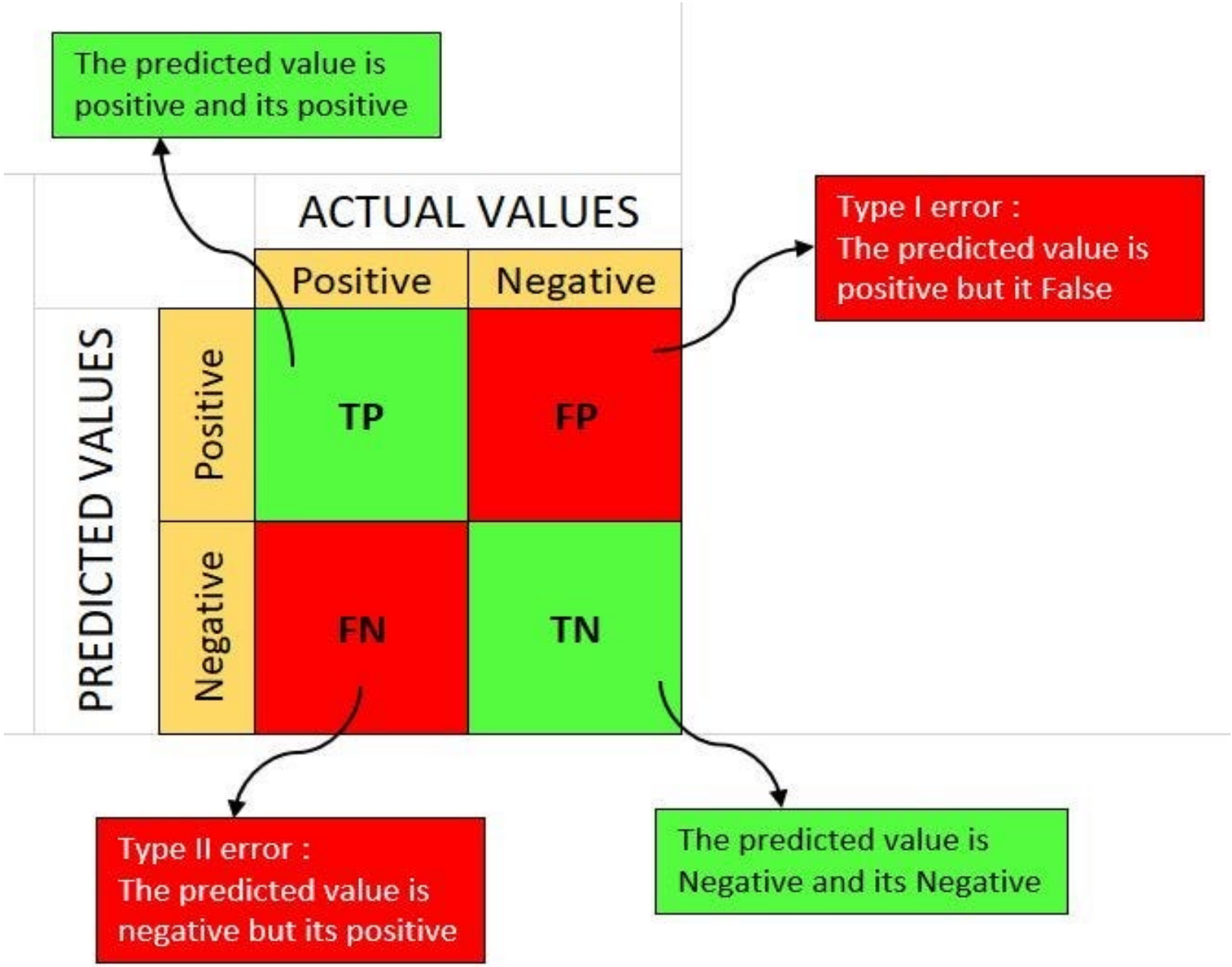


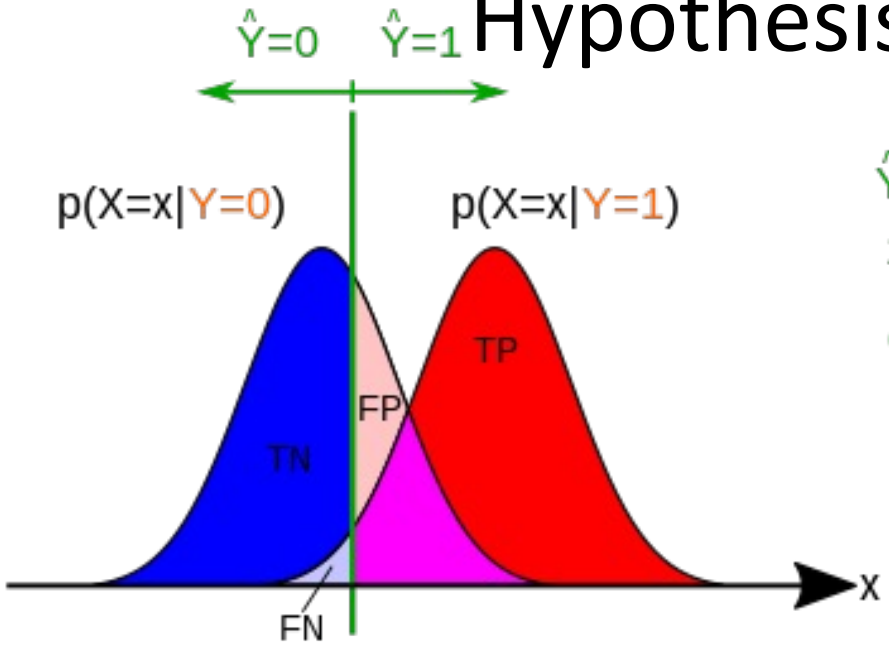
FIGURE 5.4. *Cross-validation was used on the* `Auto` *data set in order to estimate the test error that results from predicting* `mpg` *using polynomial functions of* `horsepower`. Left: *The LOOCV error curve.* Right: 10-*fold CV was run nine separate times, each with a different random split of the data into ten parts. The figure shows the nine slightly different CV error curves.*


relevant elements
false negatives
true negatives
true positives
false positives
selected elements
How many relevant items are selected? e.g. How many sick people are correctly identified as having the condition.
Sensitivity=
How many negative selected elements are truly negative? e.g. How many healthy peple are identified as not having the condition.
Specificity =

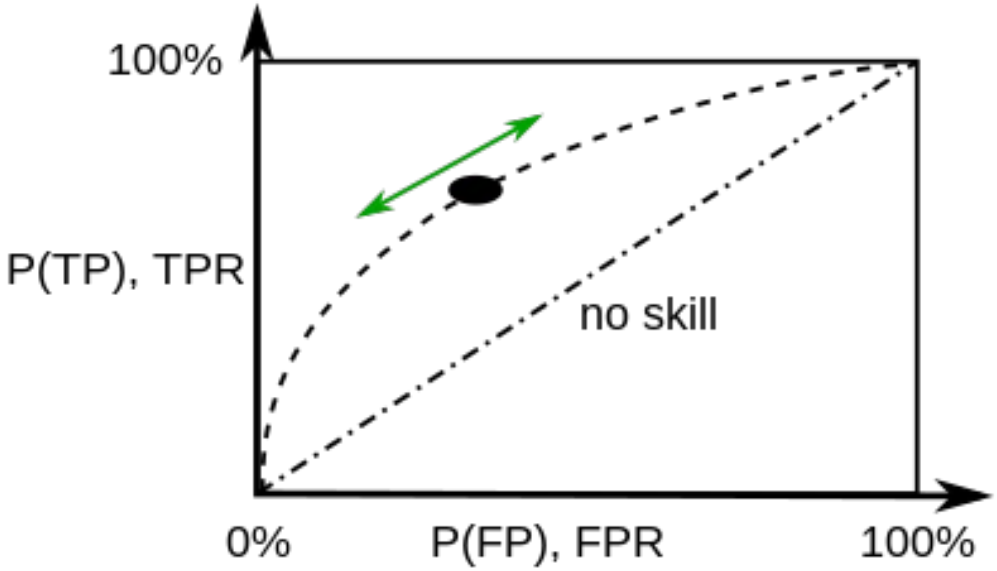
Confusion matrix



Hypothesis



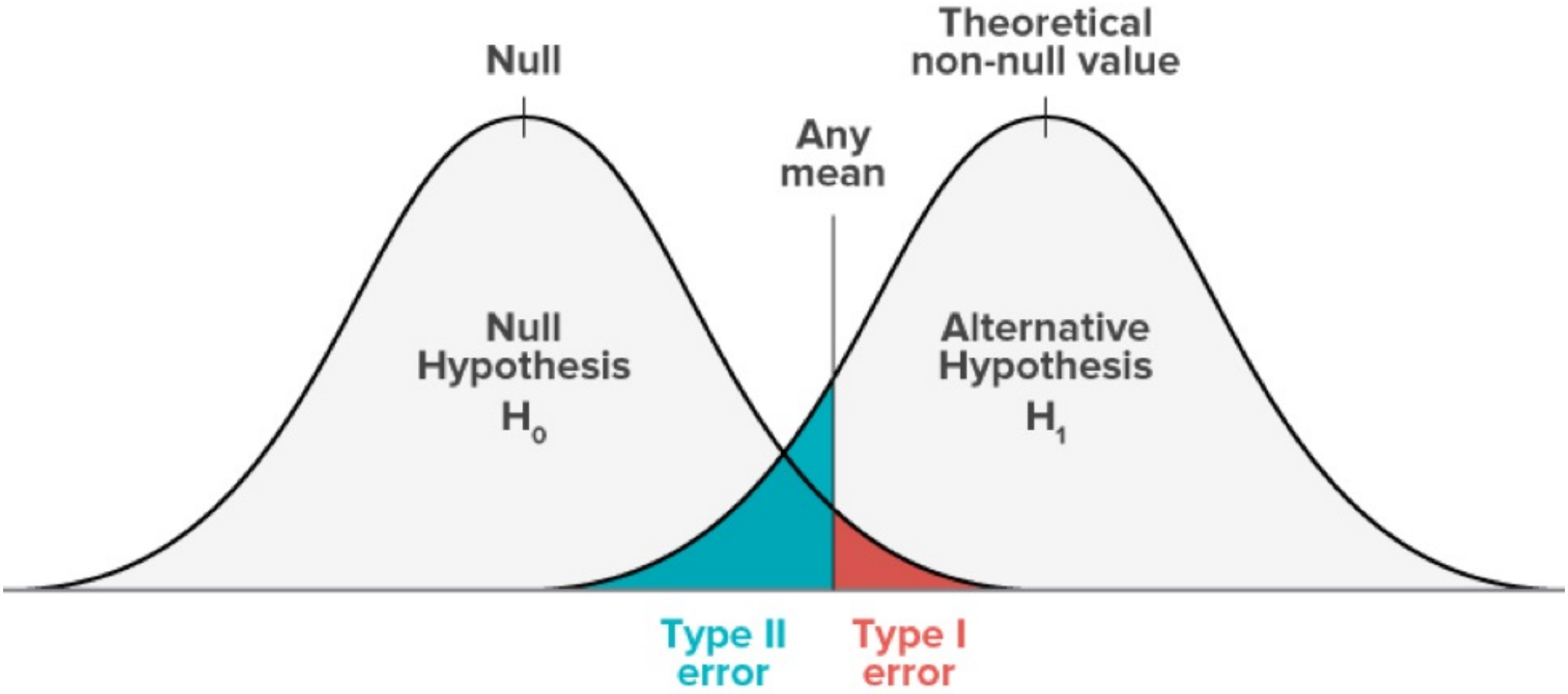
Ŷ \ Y	1	0
1	TP	FP
0	FN	TN



The probability of a Type 1 error is the significance level (0.05)

https://en.wikipedia.org/wiki/Type_I_and_type_II_errors

Hypothesis



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https://www.abtasty.com/blog/type-1-and-type-2-errors/

Question

What happens if we use a simple classifier that just predicts randomly on a disease?

For example, say you are trying to predict a particular disease.

1. Assume you have features like age, gender and medications.
2. You have to predict whether this patient will get a disease or not.
3. Assume the disease occurs in 90% of the population.

4. How should you build your algorithm? What metric should you look at?

Question

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4. How should you build your algorithm? What metric should you look at?

5. **Answer**: You should look at class-specific error (sensitivity/specificity).
    a. This is unbalanced data.
    b. Even an algorithm that randomly outputs 1 [the person has disease], (regardless of the input features), would give 90% accuracy on the data.

Decision Trees

How to pack groceries?

- Tomatoes, soft vegetables
- Wine, fragile items
- Bread
- Toiletries, shampoo
- Meat, fish

Decision Trees

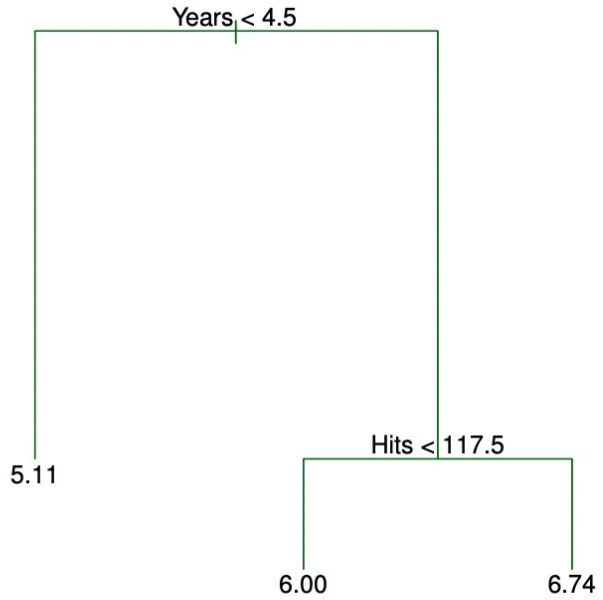


FIGURE 8.1. *For the* `Hitters` *data, a regression tree for predicting the log salary of a baseball player, based on the number of years that he has played in the major leagues and the number of hits that he made in the previous year. At a given internal node, the label (of the form* $X_j < t_k$*) indicates the left-hand branch emanating from that split, and the right-hand branch corresponds to* $X_j \geq t_k$*. For instance, the split at the top of the tree results in two large branches. The left-hand branch corresponds to* `Years<4.5`*, and the right-hand branch corresponds to* `Years>=4.5`*. The tree has two internal nodes and three terminal nodes, or leaves. The number in each leaf is the mean of the response for the observations that fall there.*

Decision Trees

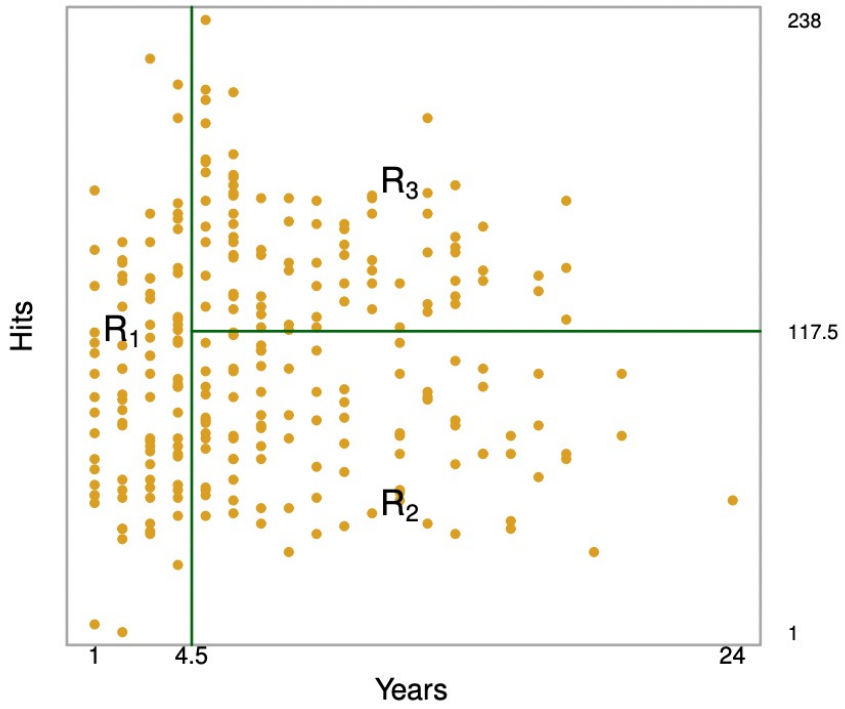


FIGURE 8.2. *The three-region partition for the* `Hitters` *data set from the regression tree illustrated in Figure 8.1.*

Decision Trees

We now elaborate on Step 1 above. How do we construct the regions $R_1, \ldots, R_J$? In theory, the regions could have any shape. However, we choose to divide the predictor space into high-dimensional rectangles, or *boxes*, for simplicity and for ease of interpretation of the resulting predictive model. The goal is to find boxes $R_1, \ldots, R_J$ that minimize the RSS, given by

$$\sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2, \tag{8.1}$$

where $\hat{y}_{R_j}$ is the mean response for the training observations within the jth box. Unfortunately, it is computationally infeasible to consider every possible partition of the feature space into J boxes. For this reason, we take a *top-down*, *greedy* approach that is known as *recursive binary splitting*. The approach is *top-down* because it begins at the top of the tree (at which point all observations belong to a single region) and then successively splits the predictor space; each split is indicated via two new branches further down on the tree. It is *greedy* because at each step of the tree-building process, the *best* split is made at that particular step, rather than looking ahead and picking a split that will lead to a better tree in some future step.

recursive binary splitting

Decision Trees. Splitting decision

Information Gain

The more homogenous something is the less information is needed to describe it and hence it has gained information. Information theory has a measure to define this degree of disorganization in a system and it is known as Entropy. If a sample is completely homogeneous, then the entropy is zero and if it is equally divided (50% – 50%), it has entropy of one.

Entropy can be calculated using formula

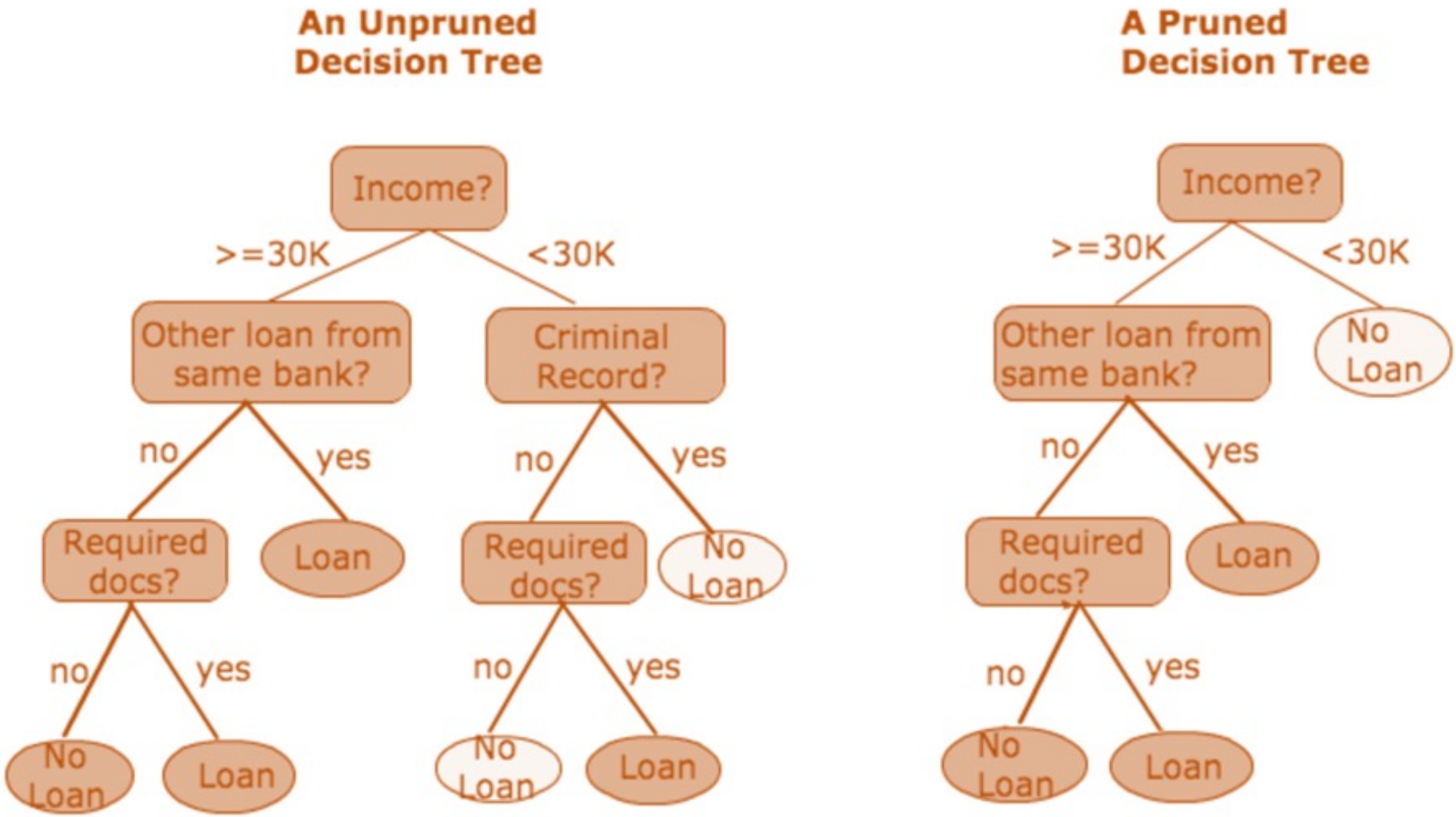
$$Entropy = -plog_2p - qlog_2q$$

Where p and q are probablity of success and failure

Reduction in Variance

Reduction in variance is an algorithm used for continuous target variables (regression problems). This algorithm uses the standard formula of variance to choose the best split. The split with lower variance is selected as the criteria to split the population:

Decision Trees: how to get smaller trees



https://medium.com/@ompramod9921/decision-trees-8e2391f93fa7

Decision Trees: how to get smaller trees

Cost complexity pruning—also known as *weakest link pruning*—gives us a way to do just this. Rather than considering every possible subtree, we consider a sequence of trees indexed by a nonnegative tuning parameter α. For each value of α there corresponds a subtree $T \subset T_0$ such that

cost complexity pruning

weakest link pruning

$$\sum_{m=1}^{|T|} \sum_{i:\, x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T| \qquad (8.4)$$

Decision Trees

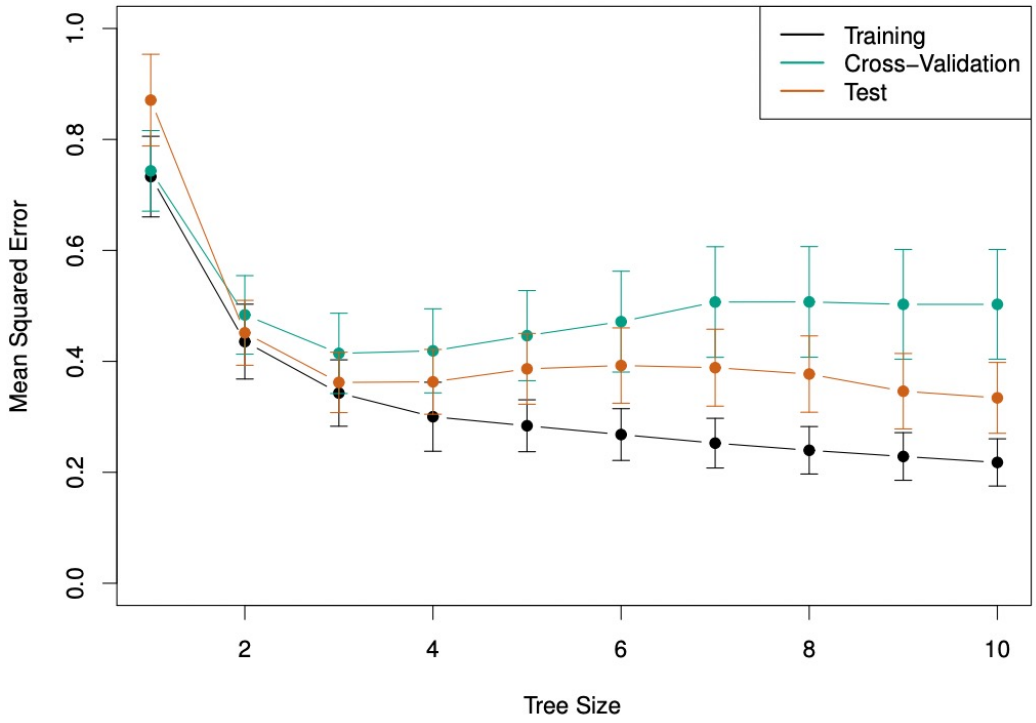


FIGURE 8.5. *Regression tree analysis for the* `Hitters` *data. The training, cross-validation, and test MSE are shown as a function of the number of terminal nodes in the pruned tree. Standard error bands are displayed. The minimum cross-validation error occurs at a tree size of three.*

Pros and cons of trees

8.1.4 Advantages and Disadvantages of Trees

Decision trees for regression and classification have a number of advantages over the more classical approaches seen in Chapters 3 and 4:

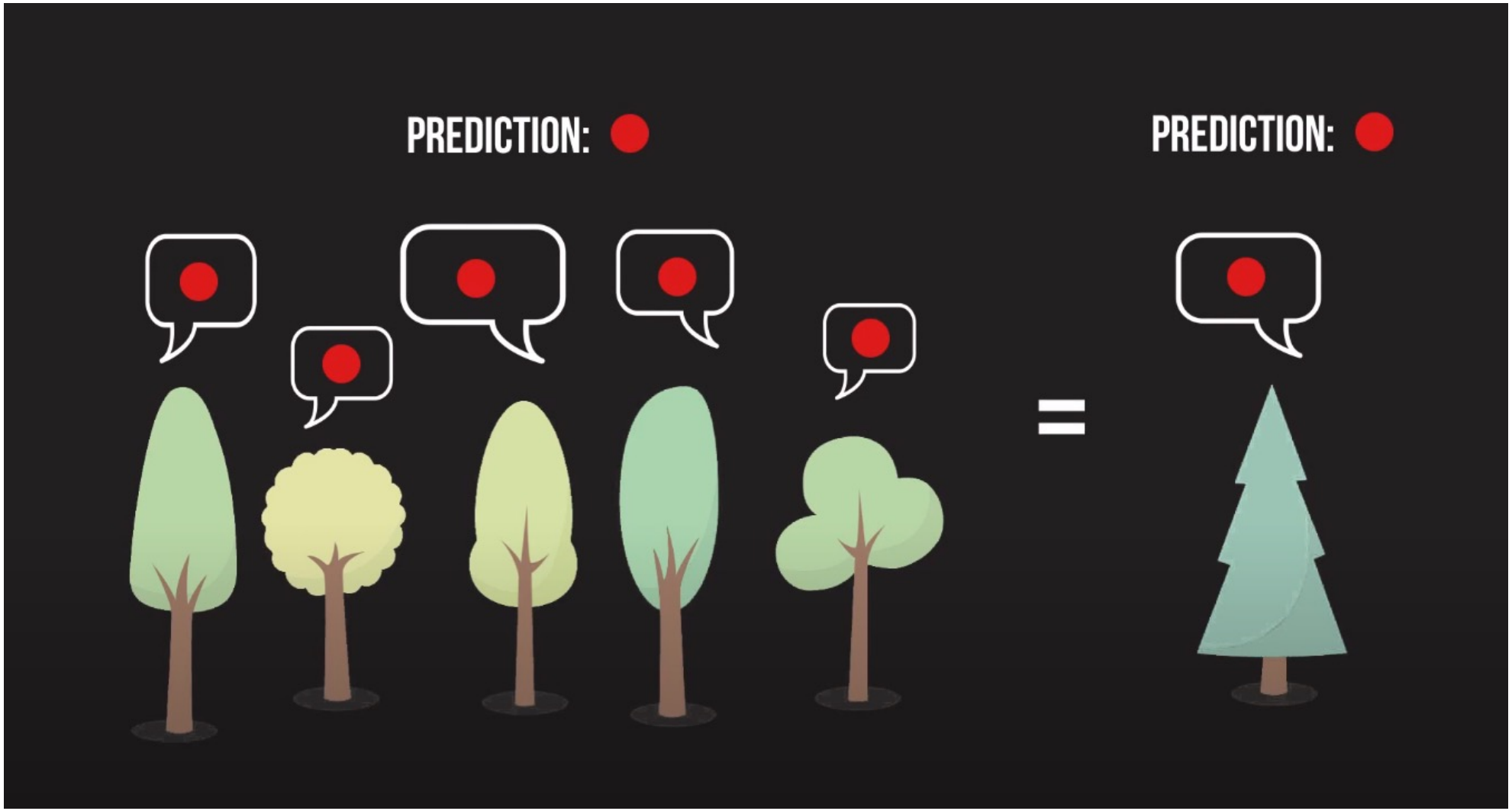
- Trees are very easy to explain to people. In fact, they are even easier to explain than linear regression!
- Some people believe that decision trees more closely mirror human decision-making than do the regression and classification approaches seen in previous chapters.
- Trees can be displayed graphically, and are easily interpreted even by a non-expert (especially if they are small).
- Trees can easily handle qualitative predictors without the need to create dummy variables.

Pros and cons of trees

- Unfortunately, trees generally do not have the same level of predictive accuracy as some of the other regression and classification approaches seen in this book.
- Additionally, trees can be very non-robust. In other words, a small change in the data can cause a large change in the final estimated tree.

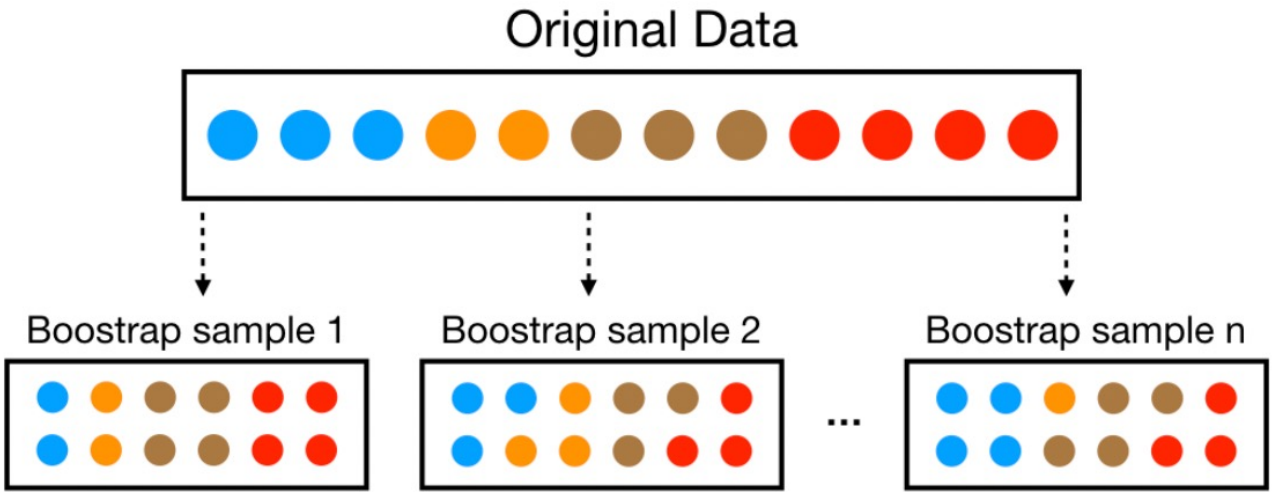
However, by aggregating many decision trees, using methods like *bagging*, *random forests*, and *boosting*, the predictive performance of trees can be substantially improved. We introduce these concepts in the next section.

Random Forests



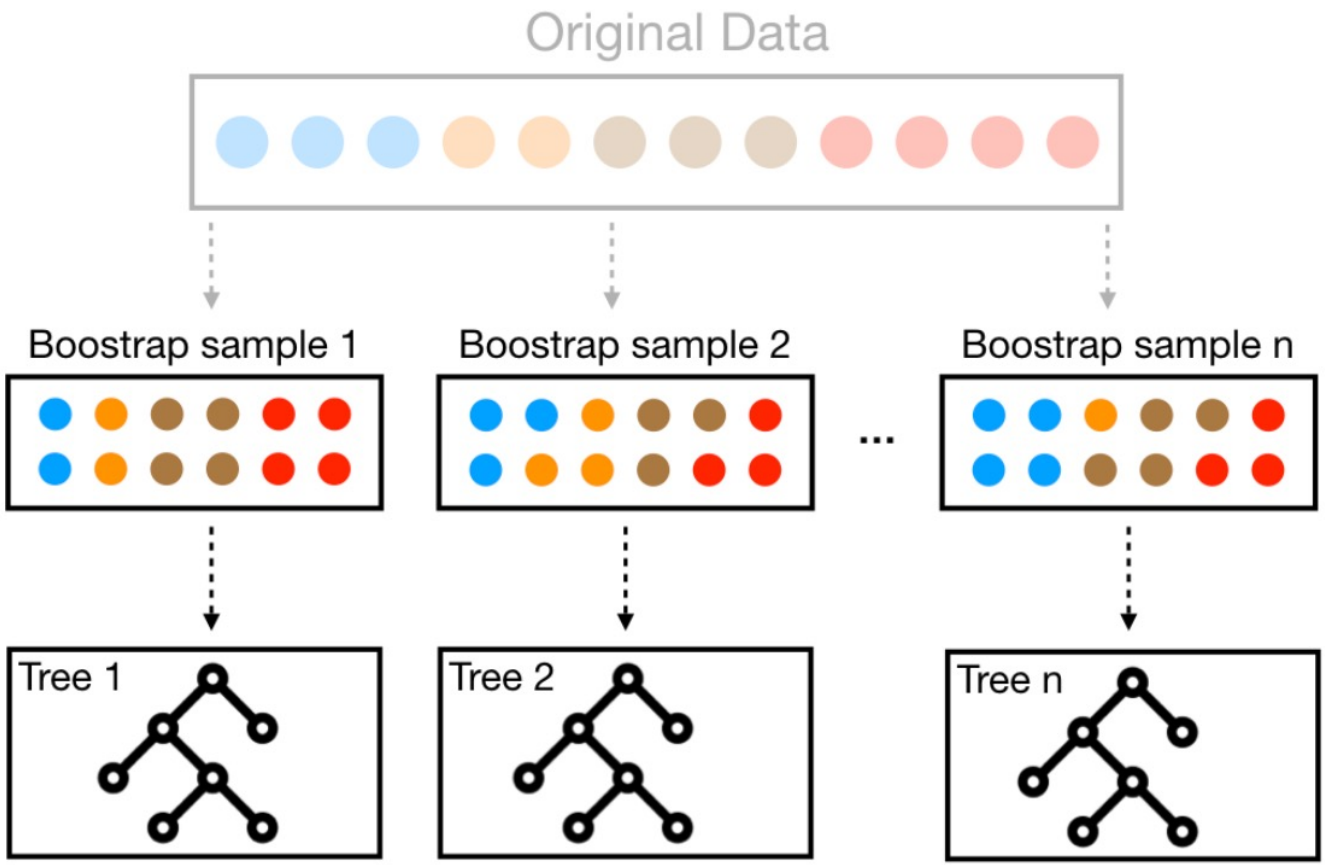
https://towardsdatascience.com/a-visual-guide-to-random-forests-b3965f453135

Bagging



https://bradleyboehmke.github.io/random-forest-training/slides-source.html#33

Bagging



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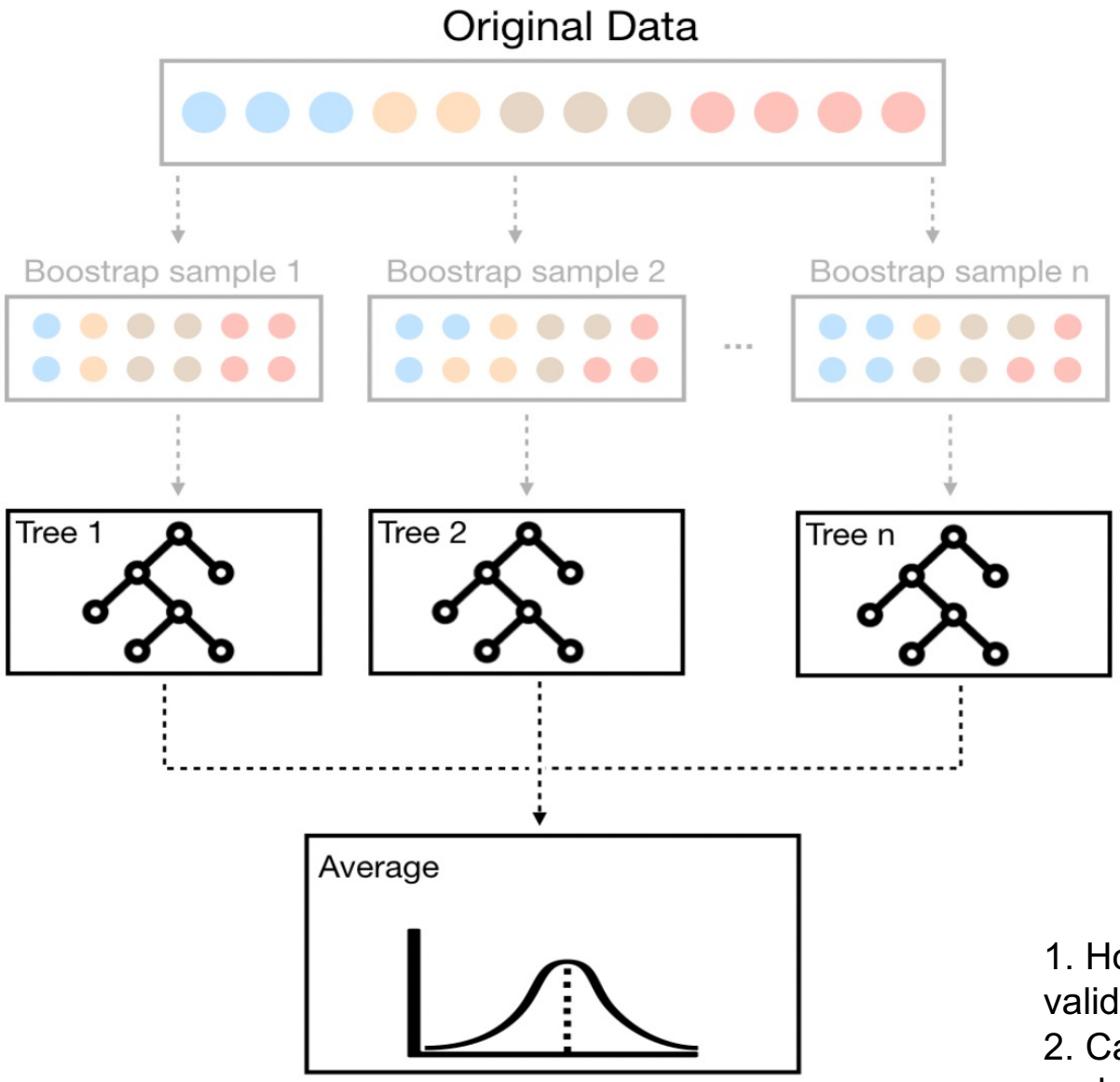
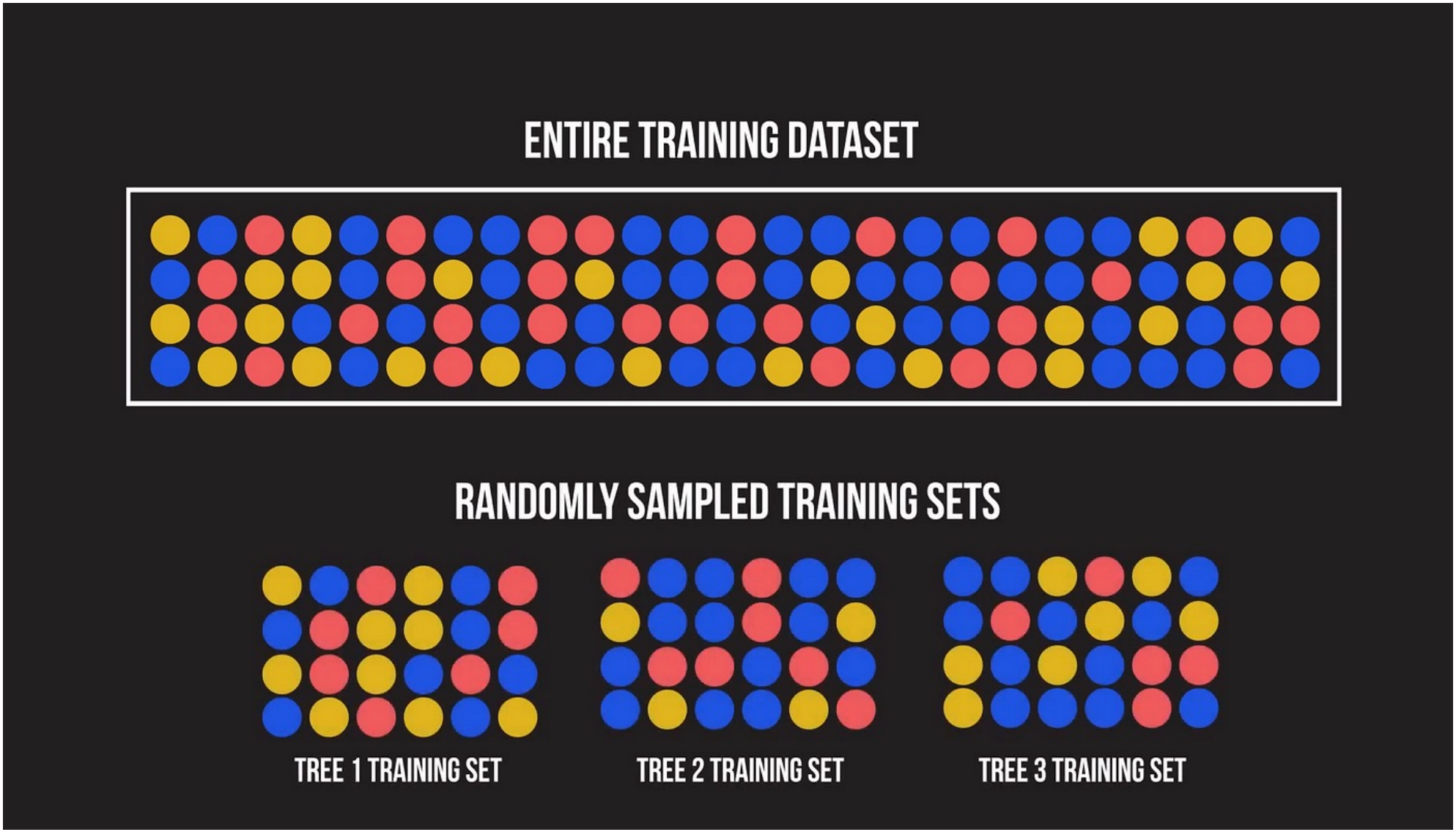
Bagging



1. How would you cross-validate?
2. Can this lead to any problems?

Correlated trees



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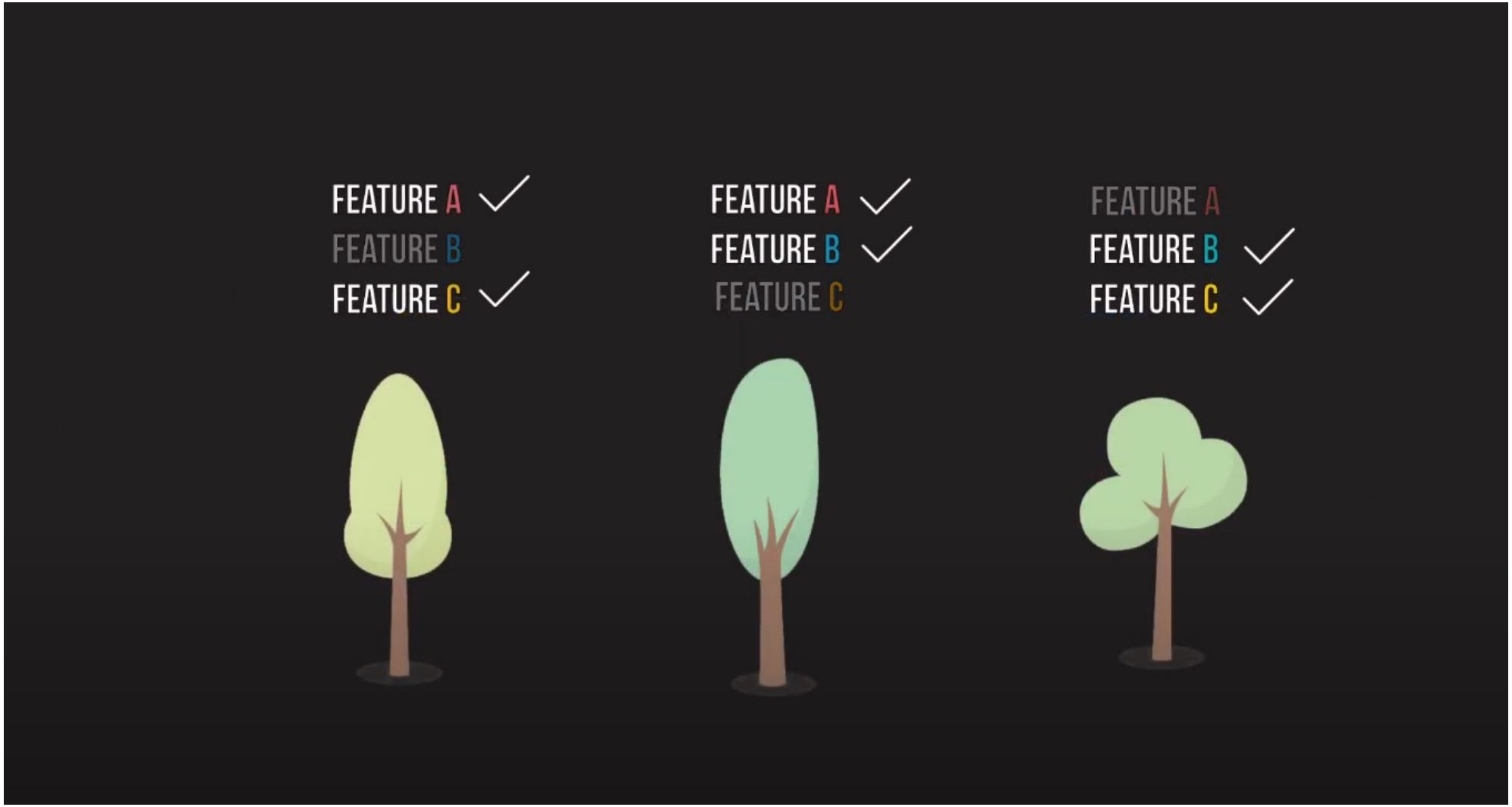
Solution



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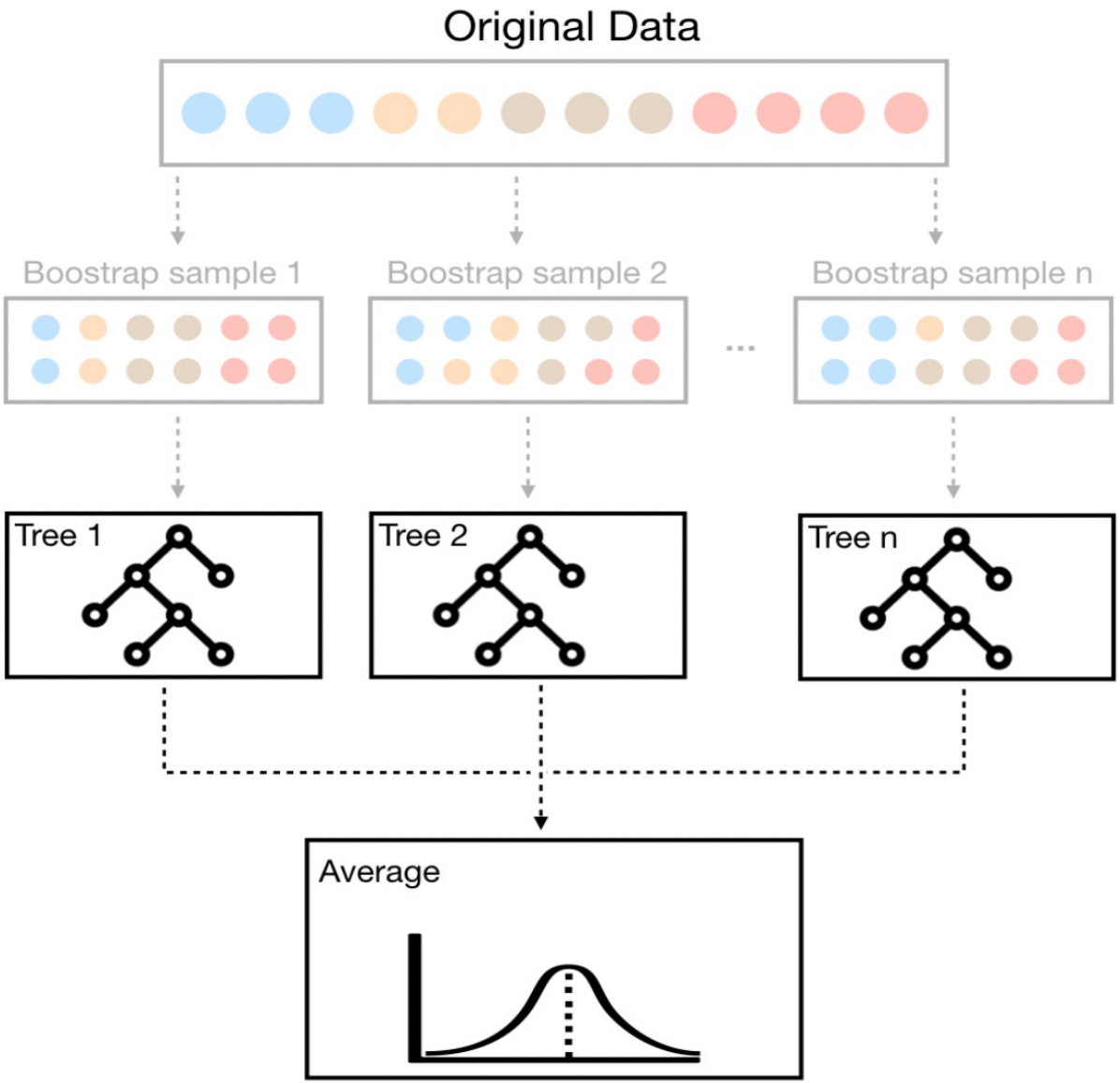
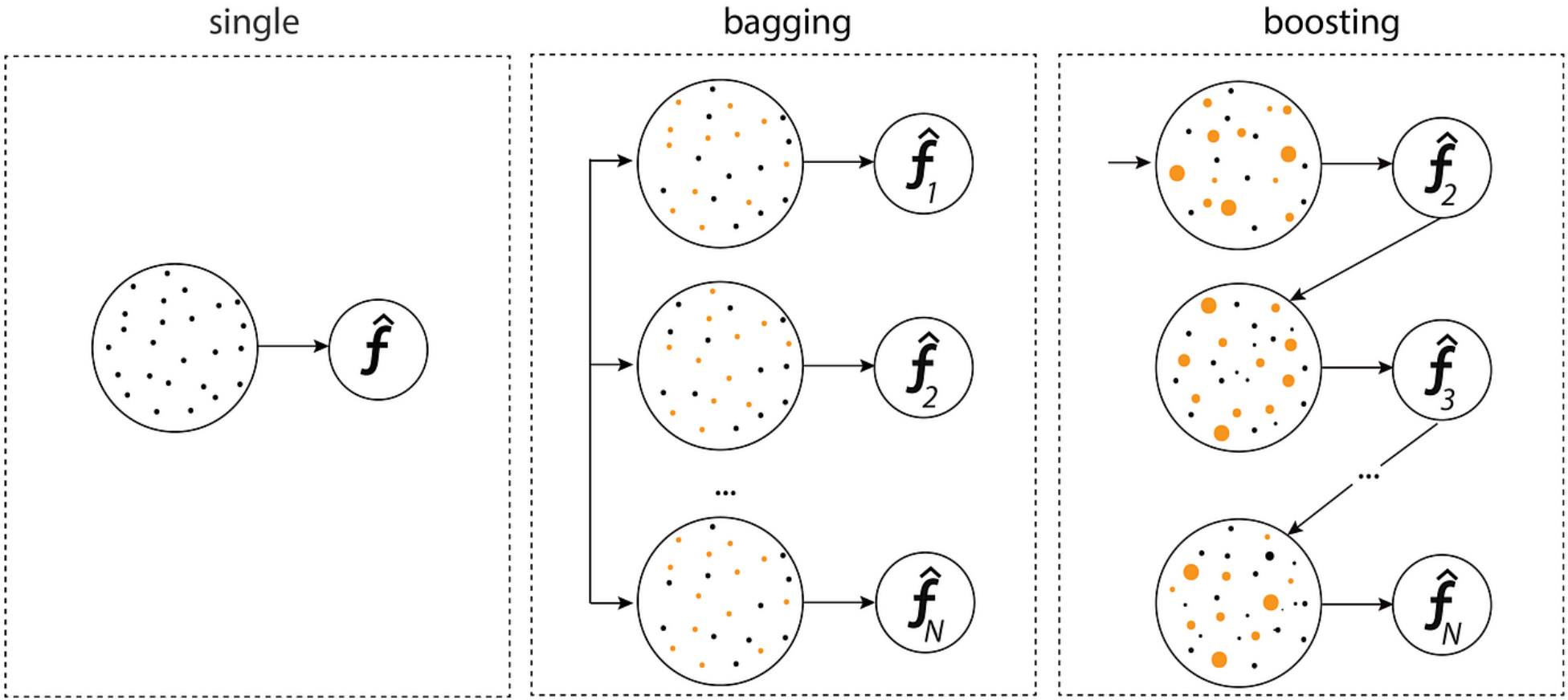
Random forests + Bagging



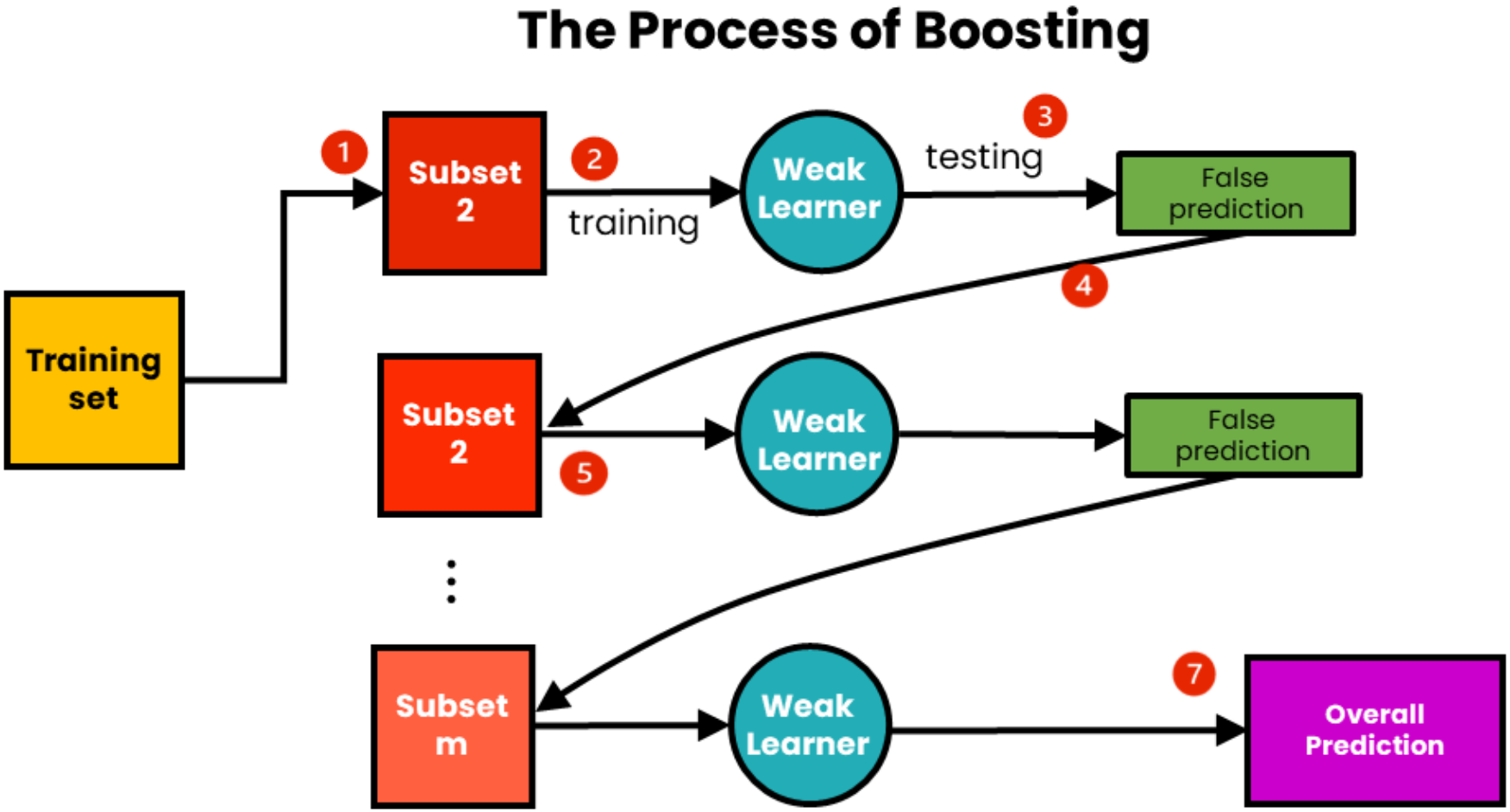
1. Decorrelate trees
2. When deciding on a split, a random sample of features is taken
3. Each tree is built on a different random sample of features!

Bagging and Boosting



https://medium.com/@senozanAleyna/ensemble-boosting-bagging-and-stacking-machine-learning-6a09c31df778

Boosting



https://medium.com/@brijesh_soni/understanding-boosting-in-machine-learning-a-comprehensive-guide-bdeaa1167a6

Random Forests (PRACTICAL)

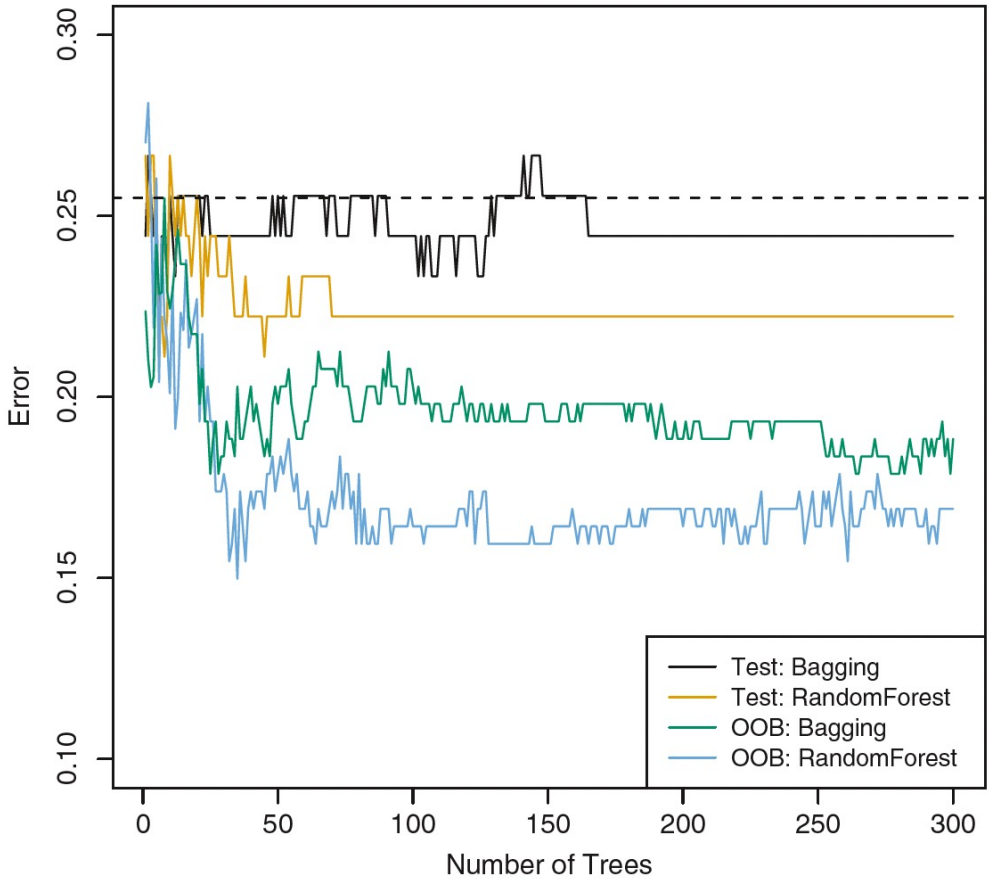
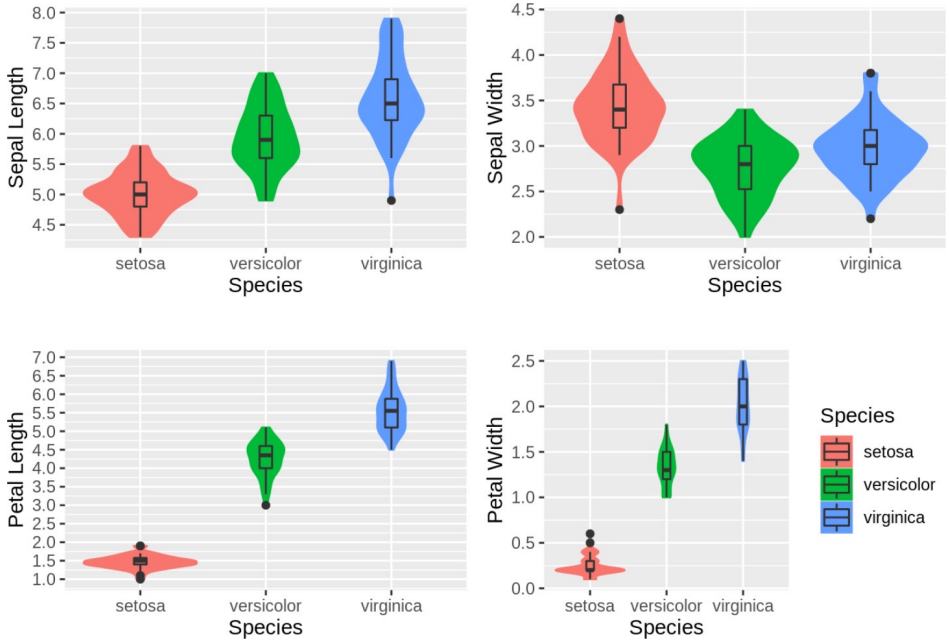
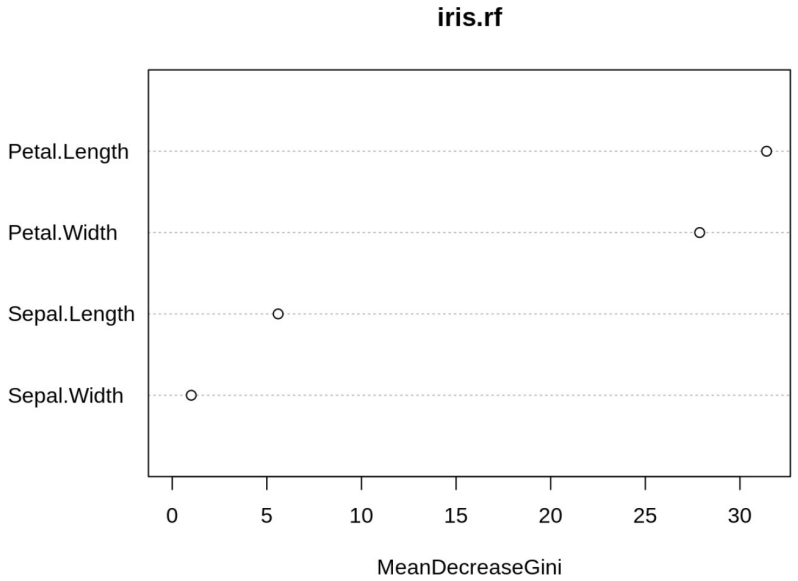


FIGURE 8.8. *Bagging and random forest results for the* `Heart` *data. The test error (black and orange) is shown as a function of* B*, the number of bootstrapped training sets used. Random forests were applied with* $m = \sqrt{p}$*. The dashed line indicates the test error resulting from a single classification tree. The green and blue traces show the OOB error, which in this case is considerably lower.*

Random Forests: Variable Importance (PRACTICAL)

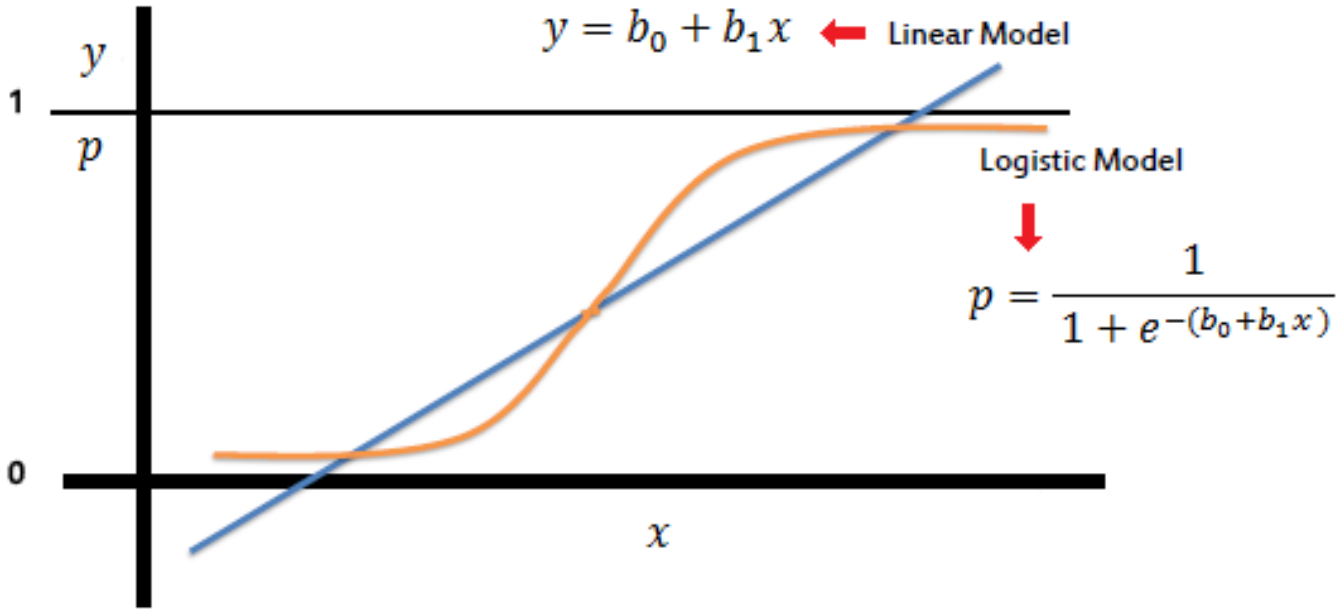




Slide courtesy Irina Mohorianu

Artificial Neural Networks

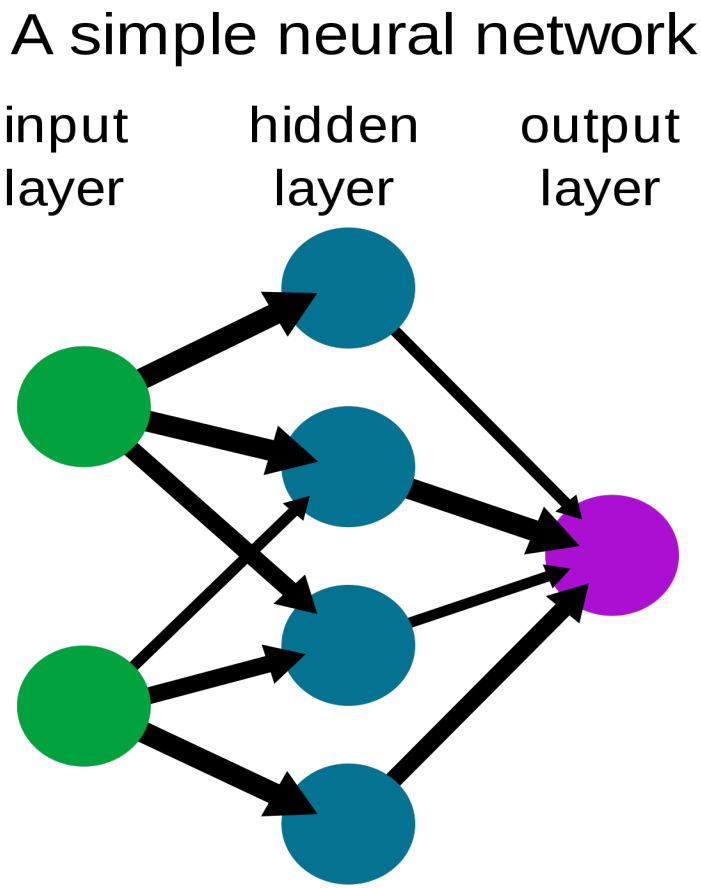
Iterated logistic regression



https://saedsayad.com/logistic_regression.htm

Artificial Neural Networks

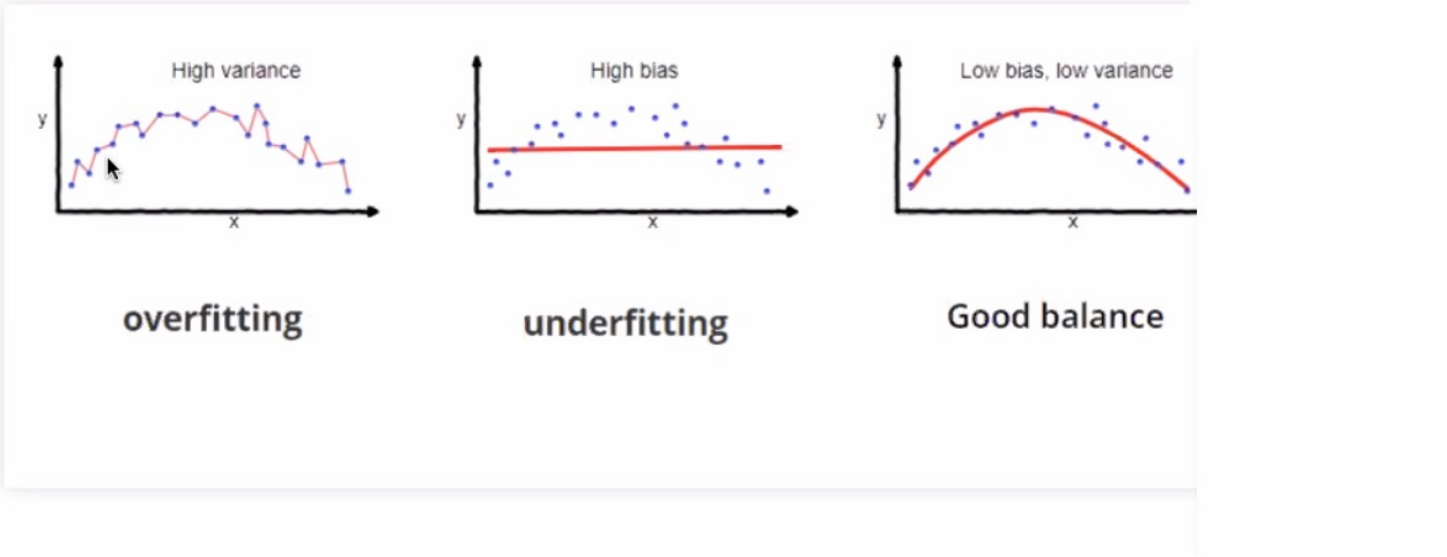
Iterated logistic regression



https://en.wikipedia.org/wiki/Neural_network#/media/File:Neural_network_example.svg

A fundamental concept in machine learning

Bias-variance tradeoff



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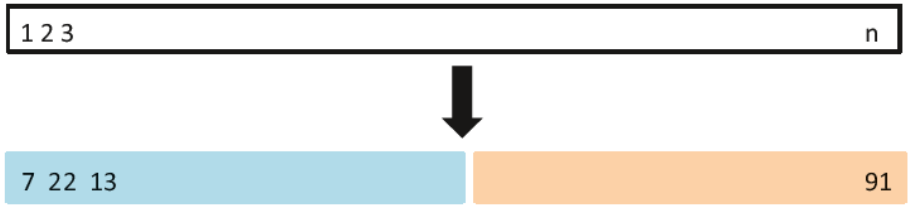
- Variance is generalization error when applying the model fit to

A fundamental concept in machine learning



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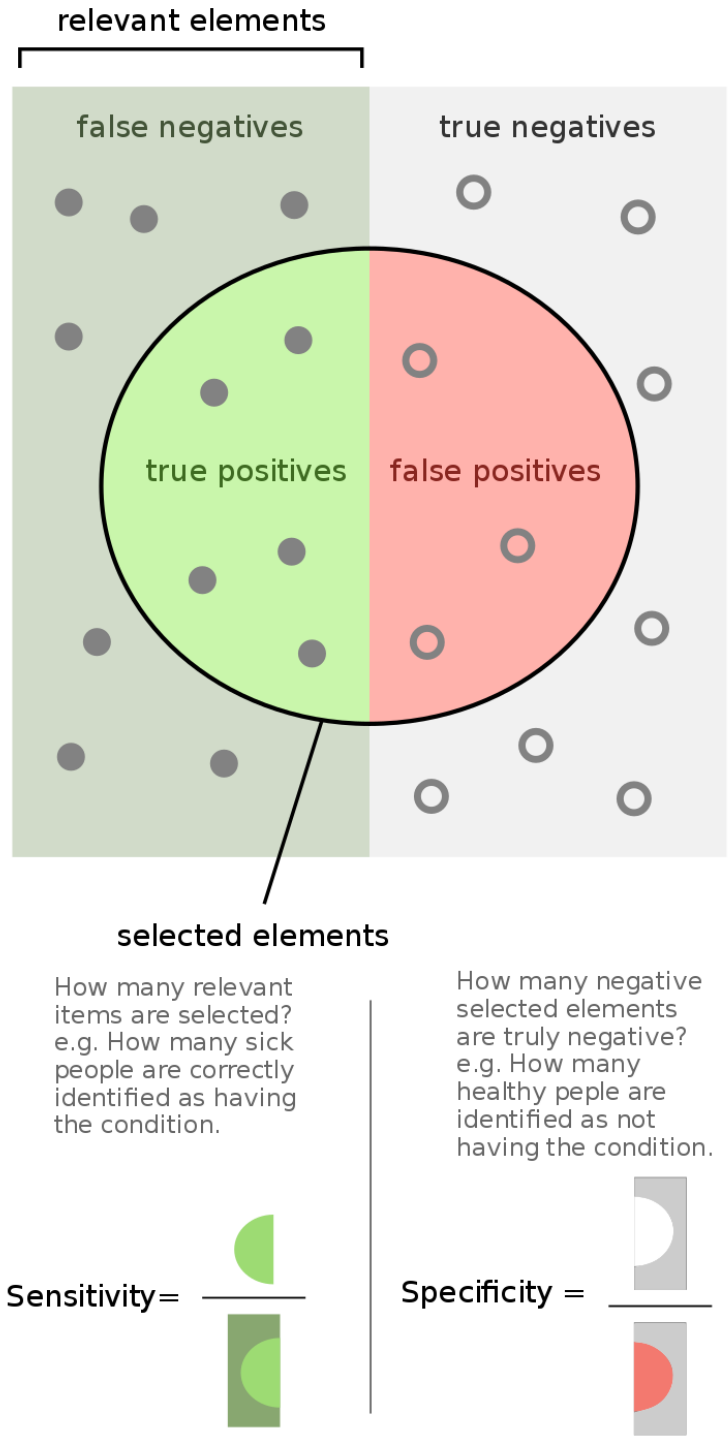
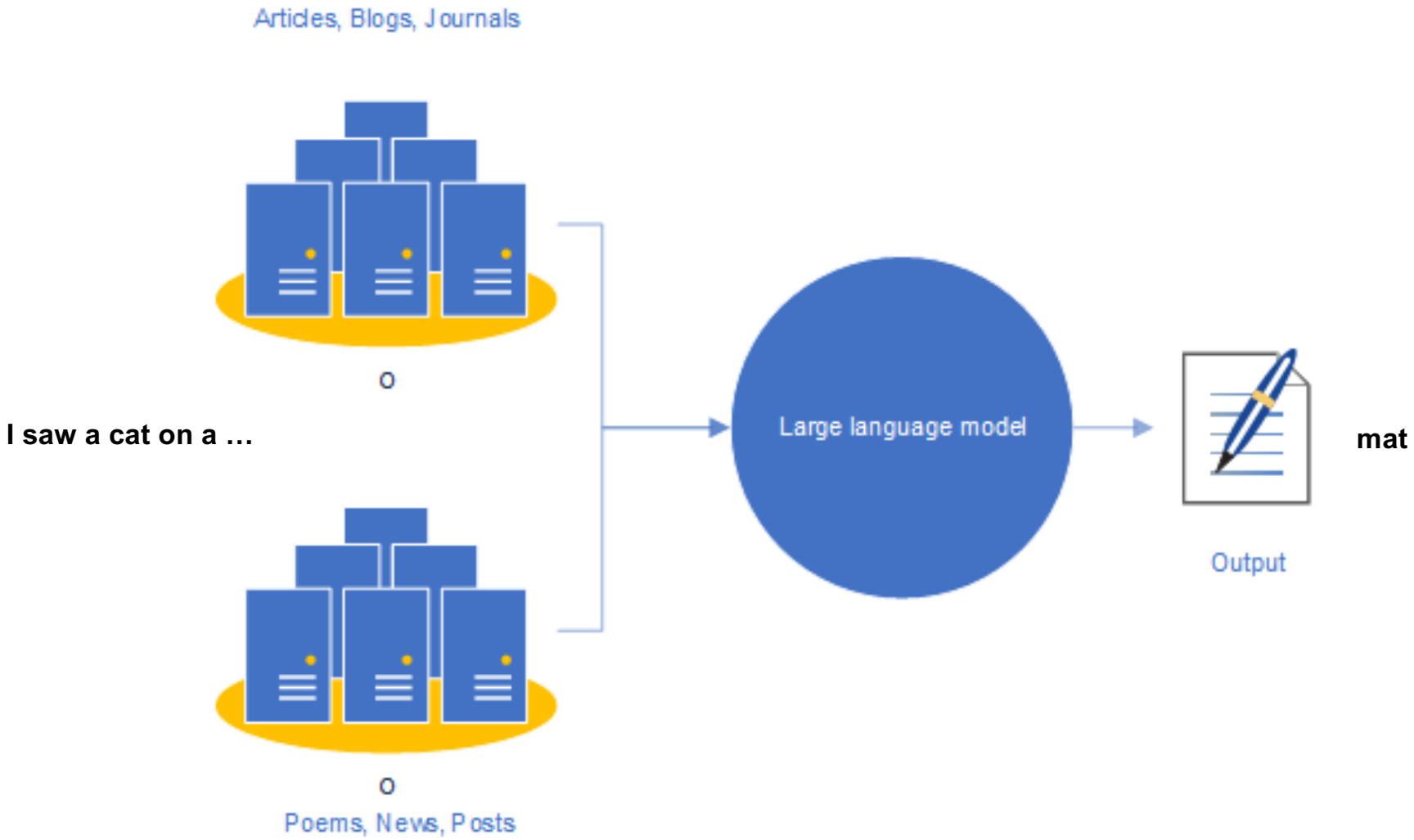
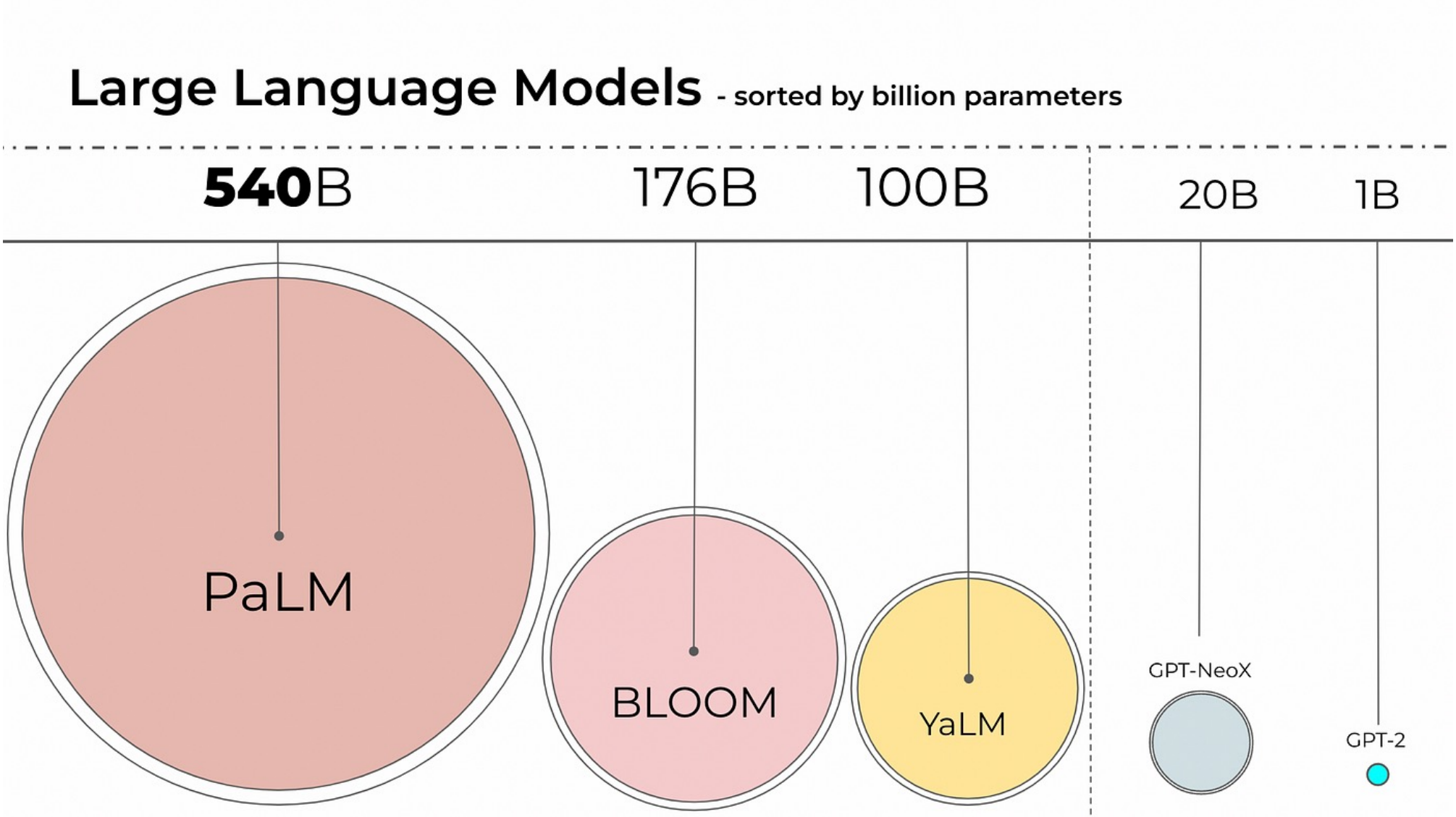

relevant elements
false negatives
true negatives
true positives
false positives
selected elements
How many relevant items are selected? e.g. How many sick people are correctly identified as having the condition.
Sensitivity=
How many negative selected elements are truly negative? e.g. How many healthy peple are identified as not having the condition.
Specificity =

Applications of this concept



https://becominghuman.ai/a-quick-introduction-to-the-large-language-model-chatgpt-a2f5f54b4d5e

Applications of this concept



https://ashukumar27.medium.com/decoding-large-language-models-quantization-ff58964c0f31

Resources

- Code, practicals and talk (recorded)
- https://github.com/neelsoumya/public_supervised_machine_learning

- https://github.com/neelsoumya/practical_supervised_machine_learning

- Free PDF of book and R code

- https://www.statlearning.com/resources-second-edition

- More practical tutorials and R code

- https://cambiotraining.github.io/intro-machine-learning/

Questions