MY474: Applied Machine Learning for Social Science

Lecture 8: Ensemble Methods, Bagging, Random Forests, Boosting

15 March 2023

Part II: Weeks 9 - 11

1. **Bagging, random forests, and boosting**
2. Neural networks
3. Unsupervised learning

Before we start

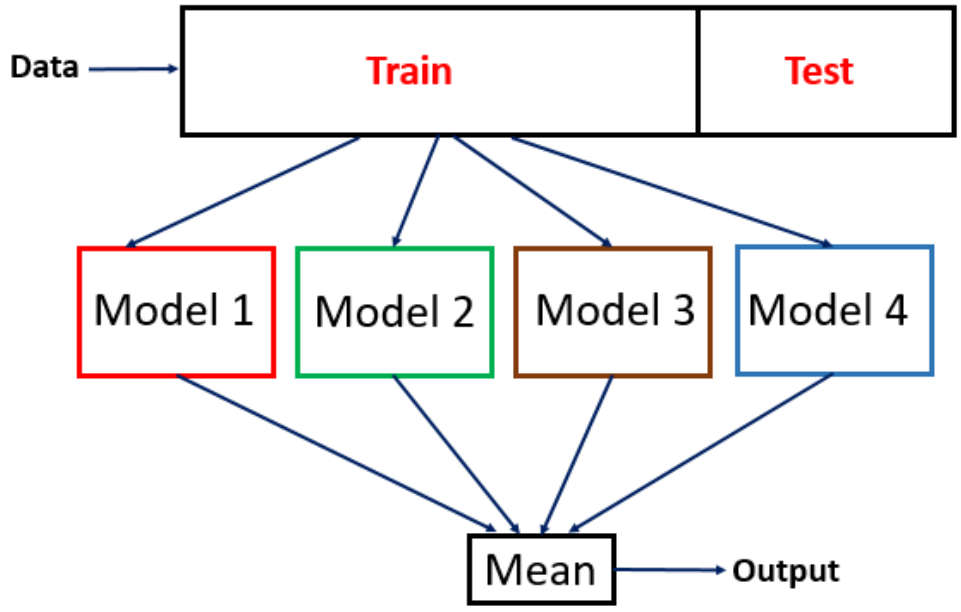
- Next week's lecture will be an introduction to neural networks and deep learning.
- As it covers a lot of content for one week, please do the following homework before:
- Watch videos one to three, the fourth one is optional https://www.youtube.com/playlist?list=PLZHQObOWTQDNU6R1_67000Dx_ZCJB-3pi
- These videos from the channel 3Blue1Brown are exceptionally well made and build key visual intuition before we start with the lecture.

Today

1. Ensembles
2. Bagging
3. Random Forests
4. Boosting
5. Guided coding

Ensembles

Simple Ensembles



- The idea of ensemble learning is to build a prediction model by combining the strengths of a collection of simpler base models.
- Ensembles are constructed using a **committee** of learners whose output are combined to formulate a decision
- For a regression task, this might involve taking the **mean** of each learner's output $\hat{y}_1 \ldots \hat{y}_L$
- For a classification task, we would take the **majority vote** of each learner's output

Ensemble Applied to Trees

- Classification trees are simple but often unstable (i.e. have very high variance and do not generalise well to new data). Solution: Combine many trees.
- Bagging (Breiman 1996): Fit many large trees to bootstrap resampled versions of the training data.
- Random forests (Breiman 1999): Improvements over bagging with some randomisation on features.
- Boosting (Freund & Schapire 1996; also see Friedman 2001 on gradient boosting machines): Sequentially fit many typically small trees to reweighted versions of the training data.

Bagging

Bagging

- **Bootstrap aggregation**, or **bagging**, is a general-purpose procedure for reducing the variance of a statistical learning method; we introduce it here because it is particularly useful and frequently used in the context of decision trees.
- Recall that given a set of n independent observations $Z_1, \ldots, Z_n$, each with variance σ^2, the variance of the mean $\bar{Z}$ of the observations is given by σ^2/n.
- In other words, **averaging a set of observations reduces variance**. Of course, this is not practical because we generally do not have access to multiple training sets.

Bagging— continued

- Instead, we can bootstrap, by taking repeated samples from the (single) training data set.
- In this approach we generate B different bootstrapped training data sets. We then train our method on each of the b bootstrapped training set in order to get $\hat{f}^{*b}(x)$, the prediction at a point x. For regression, we then average all the predictions to obtain

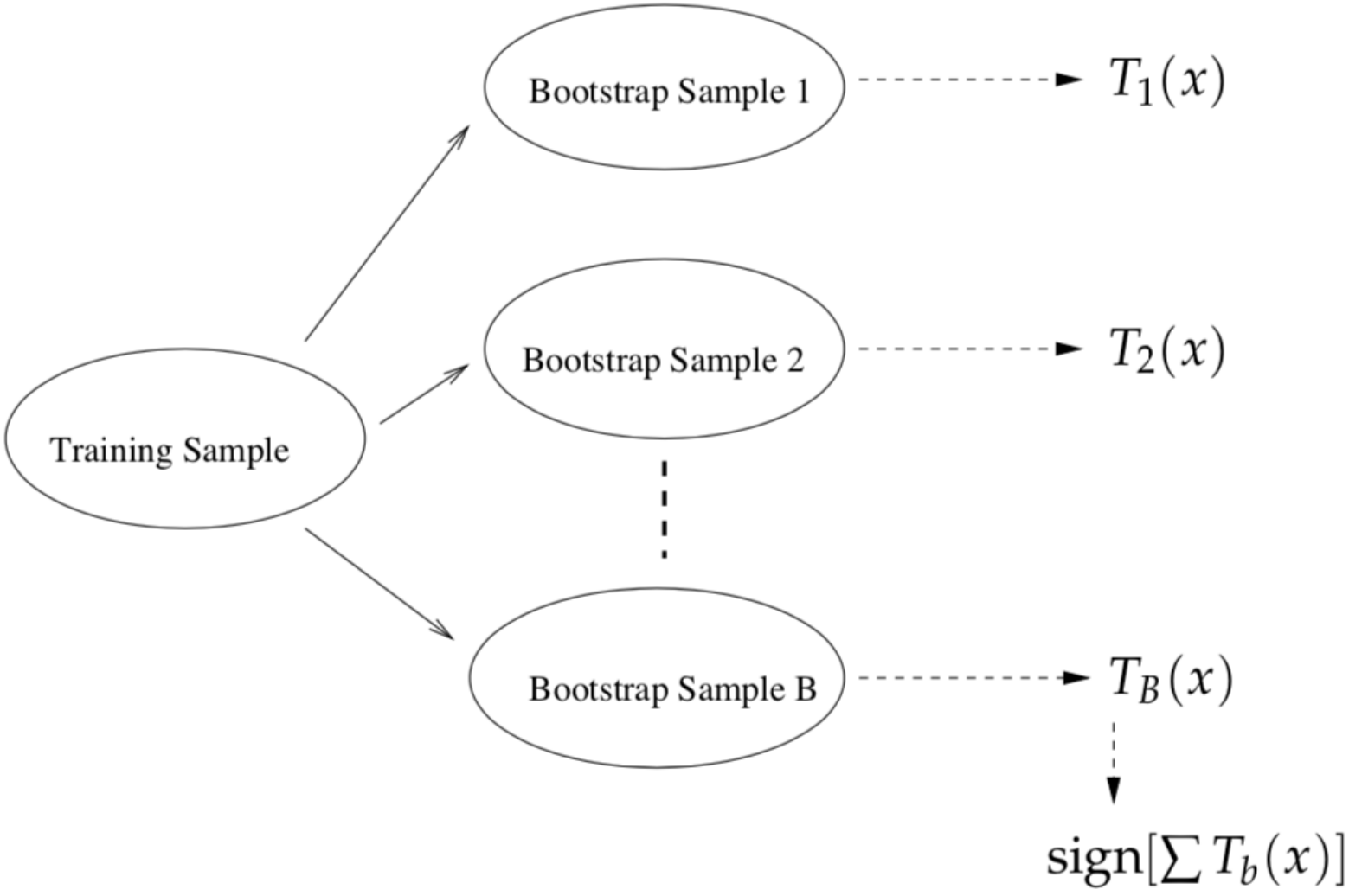
$$\hat{f}_{bag}(x) = \frac{1}{B}\sum_{b=1}^{B}\hat{f}^{*b}(x)$$

- For classification we take majority vote.

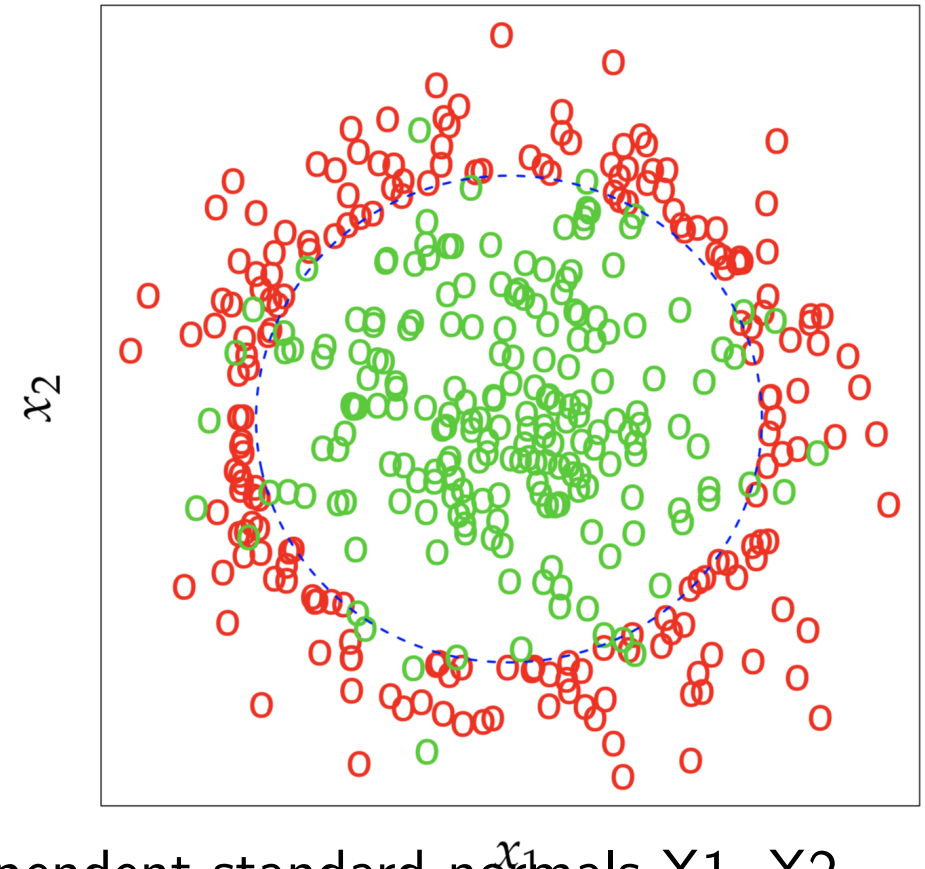
Schematics of Bagging with Trees

- Sample with replacement from the training data $(x_1, y_1), \ldots, (x_n, y_n)$ to obtain a bootstrap sample $(x_1^*, y_1^*), \ldots, (x_n^*, y_n^*)$.
- Construct a new tree T_1^*.
- Repeat everything B times, obtaining B trees $T_1^*, \ldots, T_B^*$.
- Given a new point x, predict average or classify by majority vote among $T_1^*(x), \ldots, T_B^*(x)$.
- Each individual tree is not pruned, so has high variance. Averaging the B trees reduces the variance.

Schematics of Bagging with Trees

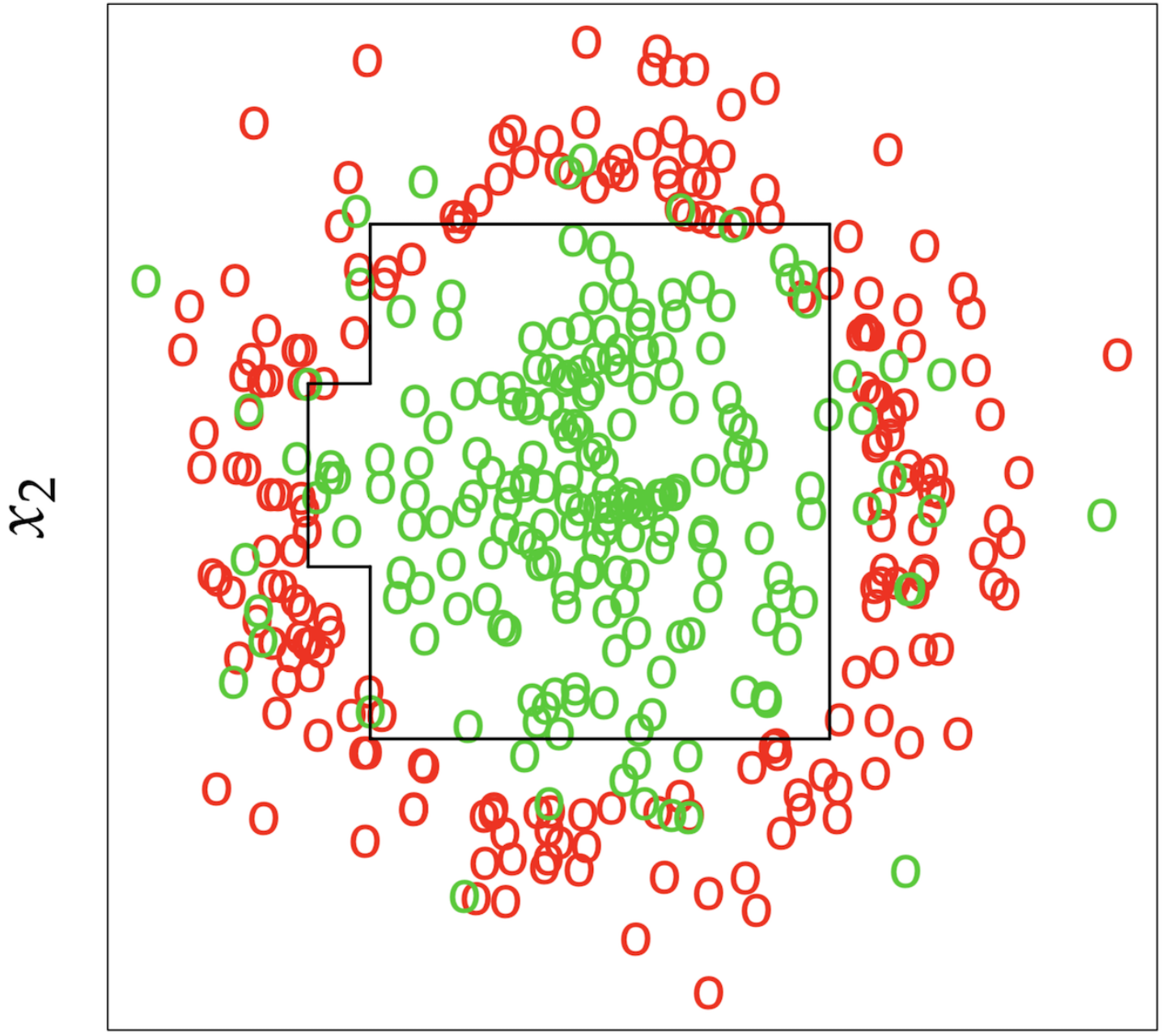


Example: Donut Data

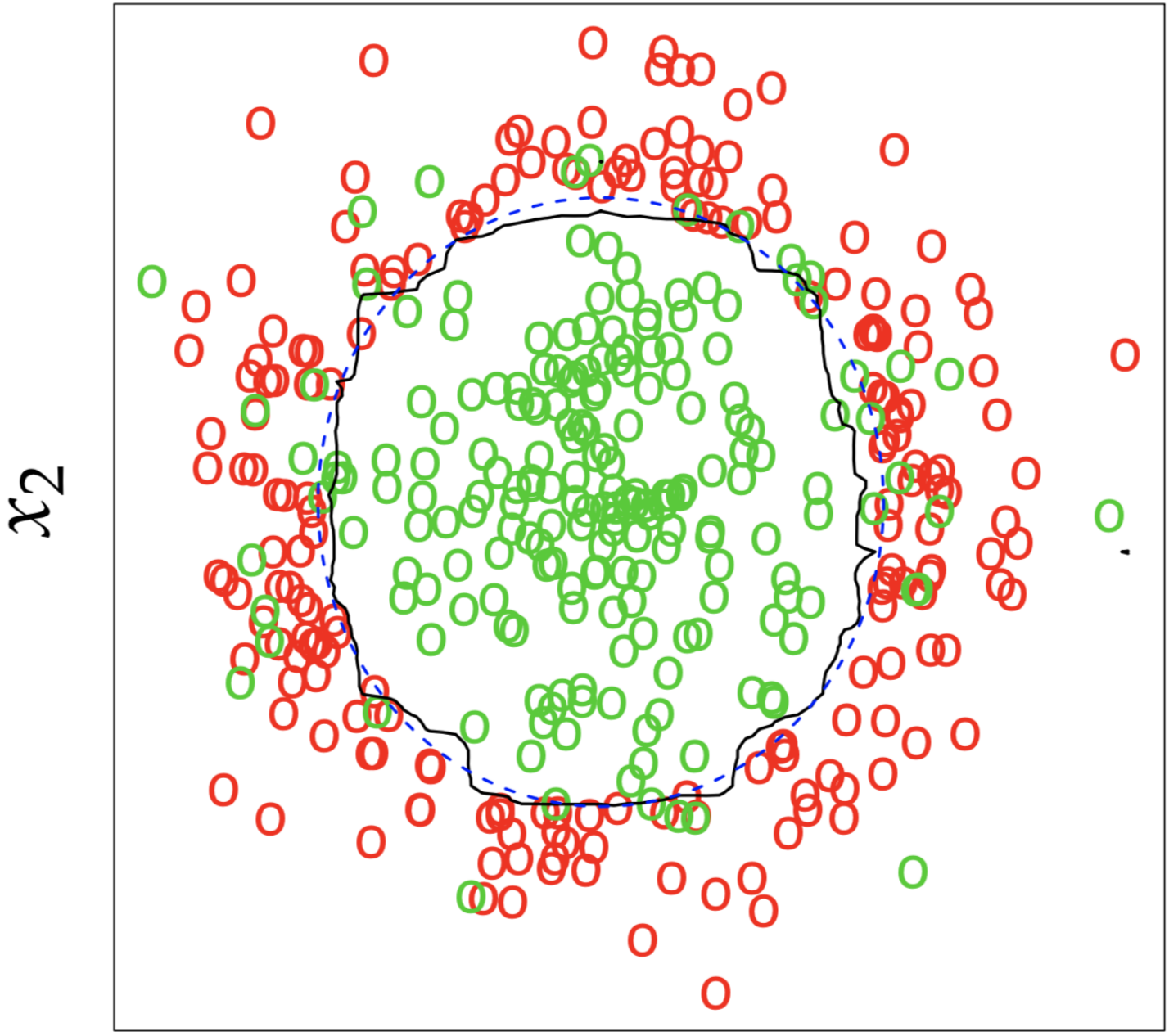


- Two independent standard normals X1, X2
- Green class: $X_1^2 + X_2^2 < 4.6$
- Red class: $X_1^2 + X_2^2 \geq 4.6$
- Plus some noise

Donut Data: Single tree decision boundary



Donut Data: Bagging decision boundary



Bagging the heart data

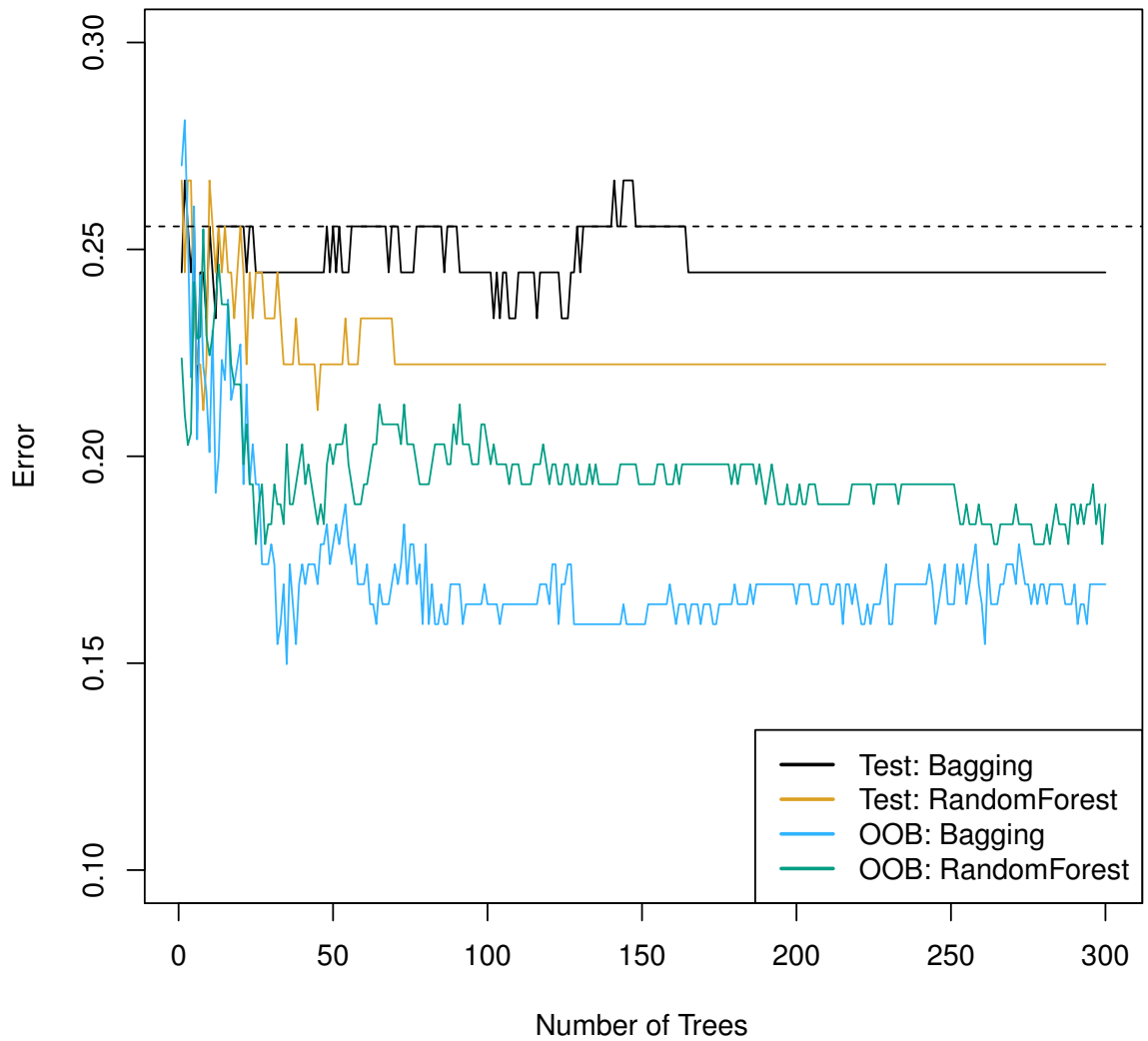


Figure 1: Bagging and random forest results for the Heart data.

Details of previous figure

- The test error (black and orange) is shown as a function of B, the number of bootstrapped training sets used.
- More about random forests in a bit.
- 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.

Out-of-Bag Error Estimation (1/2)

- It turns out that there is a convenient way to estimate the test error of a bagged model.
- Recall that trees are repeatedly fit to bootstrapped subsets of the observations. One can show that on average, each bagged tree makes use of around two-thirds of the observations.
- Why? Because the probability of an observation i not being in bootstrap sample b is: $Pr(i \notin sample_b) = (1 - \frac{1}{n})^n$ and $\lim_{n\to\infty}(1 - \frac{1}{n})^n = e^{-1} \approx 0.3679 \approx \frac{1}{3}$.
- These remaining one-third of observations are referred to as the **out-of-bag (OOB)** observations.

Out-of-Bag Error Estimation (2/2)

- So the probability of the *ith* observation not being in a given bootstrap sample b is approximately $1/3$ for large numbers of observations n.
- Thus, we have approximately $B/3$ trees whose predictions we can average to obtain an OOB prediction for the *ith* observation.
- This estimate is essentially the LOO cross-validation error for bagging if B is large.
- Why? When B is large, the $B/3$ trees used to predict observation i out of sample will most likely contain all other observations except i to some degree, and also behave/predict similarly to the full model which is averaged over all B trees.

Remarks on Bagging

- Bagging reduces the variance of individual high variance classifiers such as decision trees.
- Interpretability of individual classifiers is impeded.

Random forests

Random forests: Main idea

- Create B boostrapped training sets as in bagging.
- Grow a decision tree on each bootstrapped training data set, but consider a **random subset of variables** at each split. The trees are not pruned.

Random Forests

- **Random forests** can provide an improvement over bagged trees by way of a small tweak that further **decorrelates** the trees on the individual samples. This reduces the variance further when we average the trees.
- As in bagging, we build a number of decision trees on bootstrapped training samples.
- But when building these decision trees, each time a split in a tree is considered, **a random selection of m predictors** is chosen as split candidates from the full set of p predictors. The split is allowed to use only one of those m predictors. In other words, out of only a random subset m $<$ p predictors at each split, the algorithm chooses the best predictor.
- A fresh selection of m predictors is taken at each split.

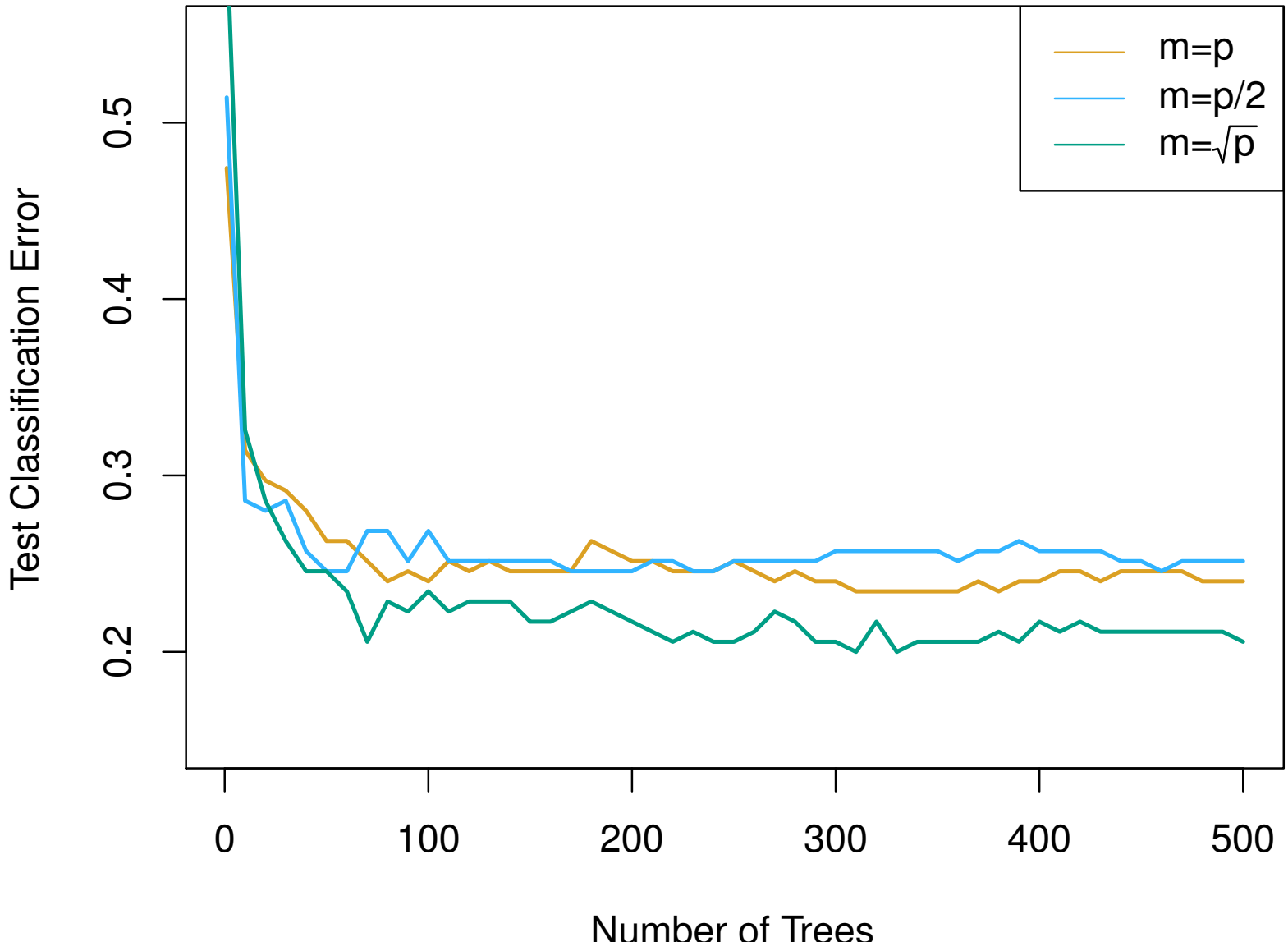
Choosing m

- Good baseline value for classification: choose $m \approx \sqrt{p}$ — that is, the number of predictors considered at each split is approximately equal to the square root of the total number of predictors (4 out of the 13 for the Heart data).
- Baseline for regression: $m \approx p/3$.
- Can also be chosen through cross validation.

Example: Gene expression data

- We applied random forests to a high-dimensional biological data set consisting of expression measurements of 4,718 genes measured on tissue samples from 349 patients.
- There are around 20,000 genes in humans, and individual genes have different levels of activity, or expression, in particular cells, tissues, and biological conditions.
- Each of the patient samples has a qualitative label with 15 different levels: either normal or one of 14 different types of cancer.
- We use random forests to predict cancer type based on the 500 genes that have the largest variance in the training set.
- We randomly divided the observations into a training and a test set, and applied random forests to the training set for three different values of the number of splitting variables m.

Results: gene expression data



Details of previous figure

- Results from random forests for the fifteen-class gene expression data set with $p = 500$ predictors.
- The test error is displayed as a function of the number of trees. Each colored line corresponds to a different value of m, the number of predictors available for splitting at each interior tree node.
- Random forests ($m < p$) lead to a slight improvement over bagging ($m = p$). A single classification tree has an error rate of 45.7%.

Feature/variable importance measures

- For bagged/RF regression trees, we can record the total amount that the RSS is decreased due to splits over a given predictor, averaged over all B trees.
- Similarly, for bagged/RF classification trees, we can add up the total amount that the criterion (e.g. Gini index or accuracy) is decreased by splits over a given predictor, averaged over all B trees.

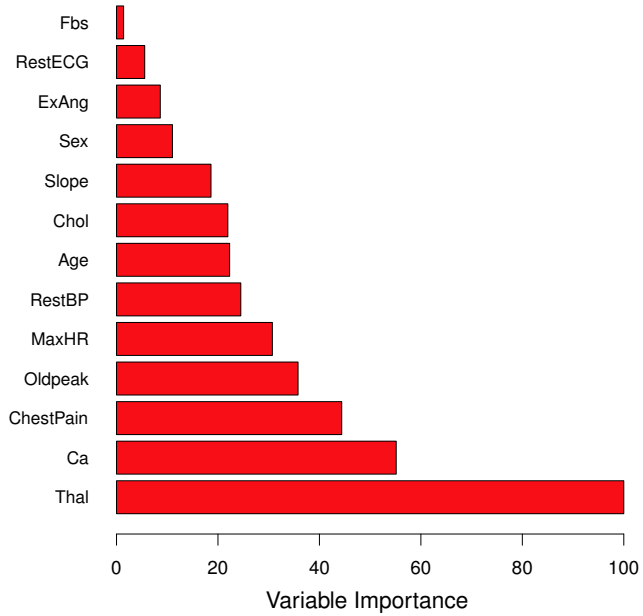


Figure 2: Variable importance plot for the Heart data

Excursus: A general feature importance measure (permutation importance)

A model-agnostic feature importance measure:

- Permute/shuffle the observations of first feature column in X.
- Make prediction with the new input $X_{permuted}$ but the old model (no re-estimation of model).
- Record the change in some metric such as RMSE for regression or accuracy for classification.
- Restore the feature's original observations and shuffle the next feature, make a prediction, and so on. Do this for all features and eventually compare how much shuffling each increased the error. The changes in error can be viewed as feature importances.

Some potential limitations

- One caveat for both tree specific and plain-vanilla permutation importance measures: Correlations between variables.
- For example, if two features are highly correlated, removing one would actually imply that the other one had picked up (part of) its task if the model had been re-estimated. Hence simple feature importance measure can overestimate the importance of variables.
- In general, take feature importance output as one guideline, but do not over-interpret rankings of features.

Further study on feature importance measures

- For a wide discussion of model interpretability and feature importance measures, see e.g. Molnar (2023) https://christophm.github.io/interpretable-ml-book/
- Shapley Values with SHAP by Lundberg (2017) is one of the most popular more advanced approaches currently used to explain behaviour of predictive models (can also generate feature importance measures).
- Molnar's book describes Shapley values as well (Chapters 9.5 and 9.6).

Remarks on random forests

- Random forests are considered one of the competitive classifiers and are popular.
- Random selection of variables further controls overfitting.
- For most data sets results seem not too sensitive to m, the number of variables used for splitting.
- While averaged models lack interpretability, features can be ranked by importance.
- However, importance rankings can be much more volatile than the classification results themselves.

Boosting

Boosting

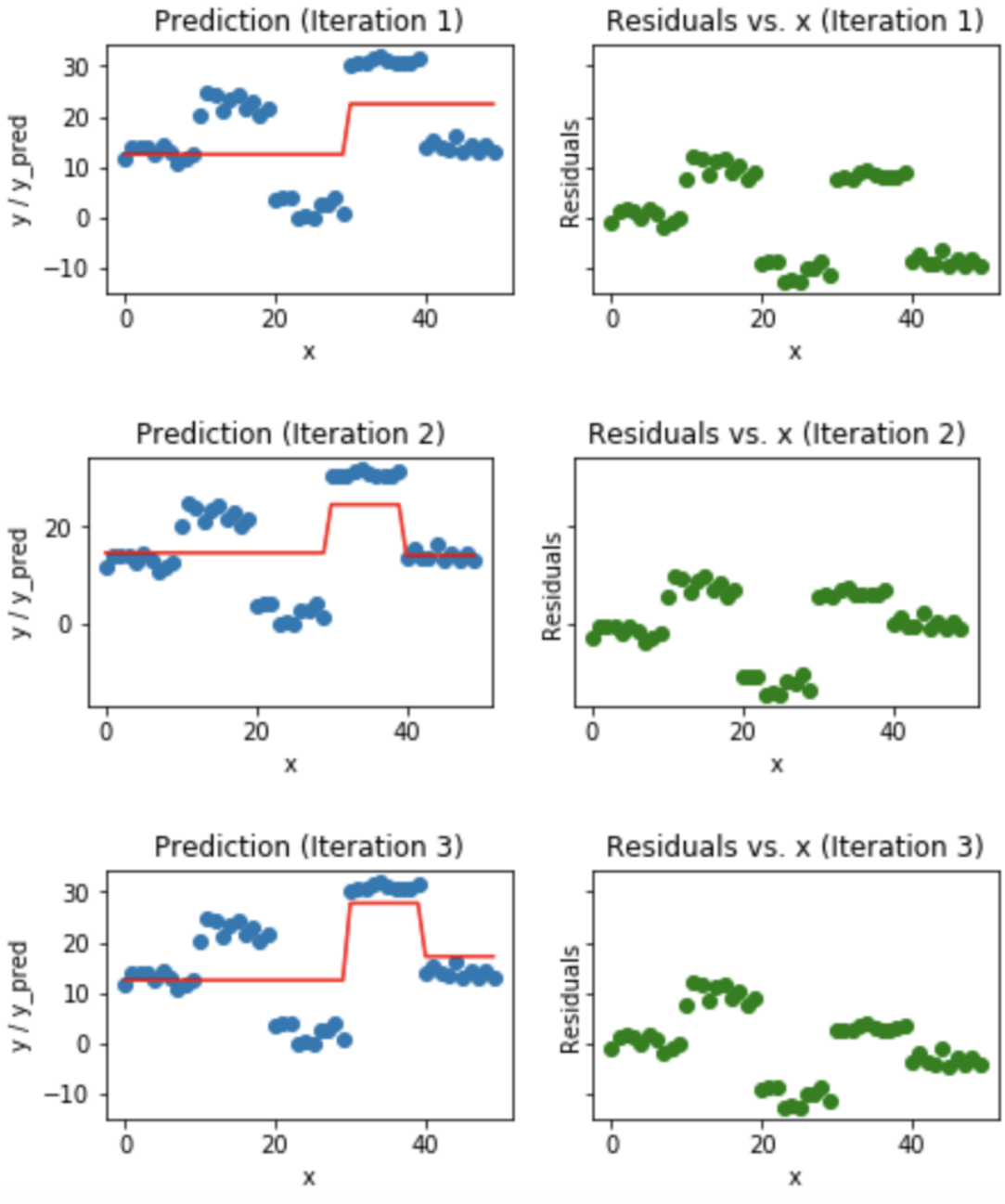
- Like bagging, boosting is a general approach that can be applied to many statistical learning methods for regression or classification. We only discuss boosting for decision trees.
- Recall that bagging and random forests involve creating multiple bootstrap samples of the original training data set, fitting a separate decision tree to each each of them, and then combining all of the trees in order to create a single predictive model.
- Notably, each tree is built on a separate bootstrap data set.
- In boosting trees are grown sequentially: Each tree is grown using information from previously grown trees.

Boosting algorithm for regression trees

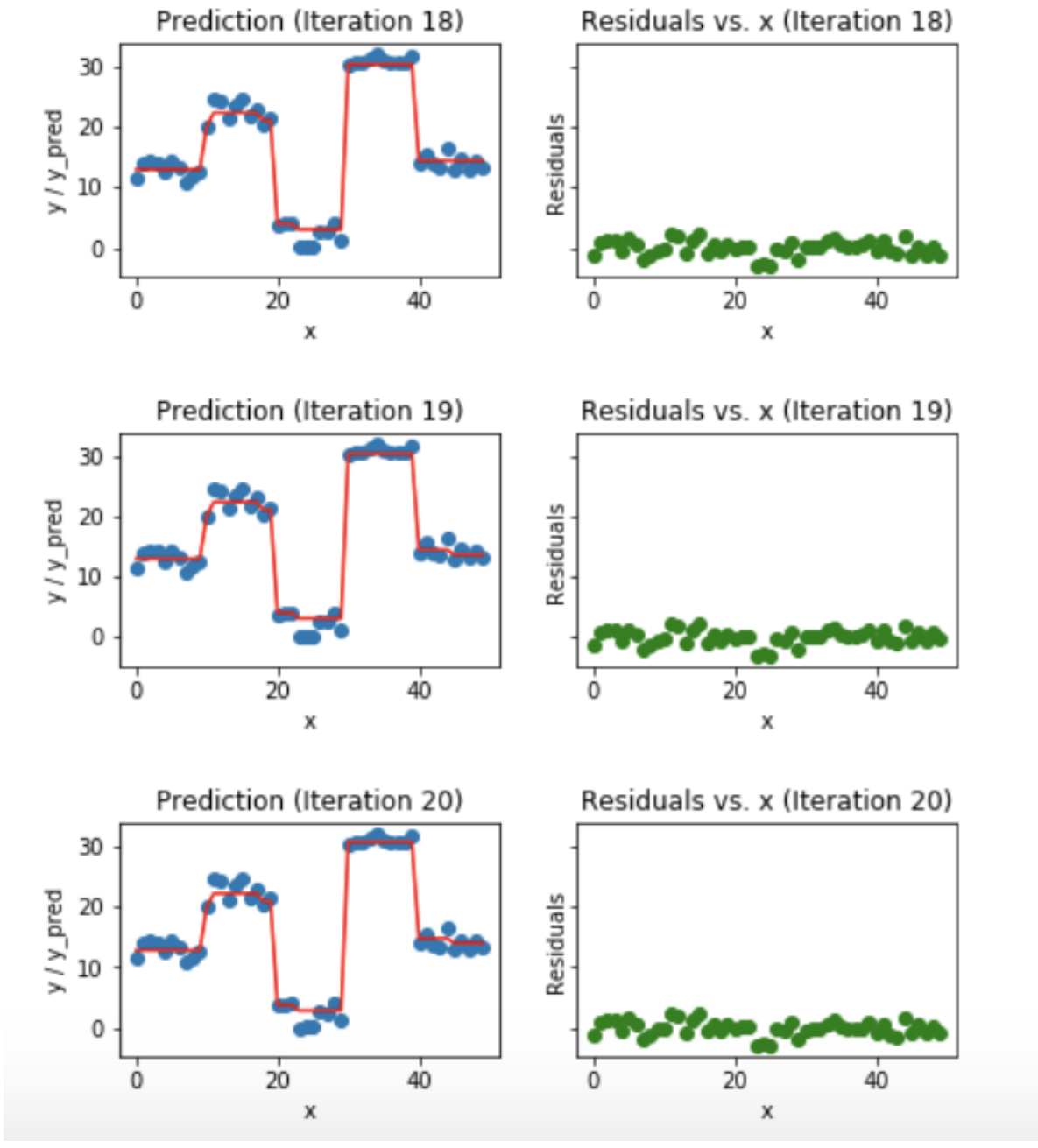
1. Set $\hat{f}(x) = 0$ and $r_i = y_i$ for all i in the training set.
2. For $b = 1, 2, \ldots, B$, repeat:
   - Fit a tree $\hat{f}_b$ with d splits ($d + 1$ terminal nodes) to the training data (X, r).
   - Update $\hat{f}$ by adding in a shrunken version of the new tree: $\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}_b(x)$.
   - Update the residuals, $r_i \leftarrow r_i - \lambda \hat{f}_b(x_i)$.
3. Output the boosted model,

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

Visualizing Boosting



Visualizing Boosting



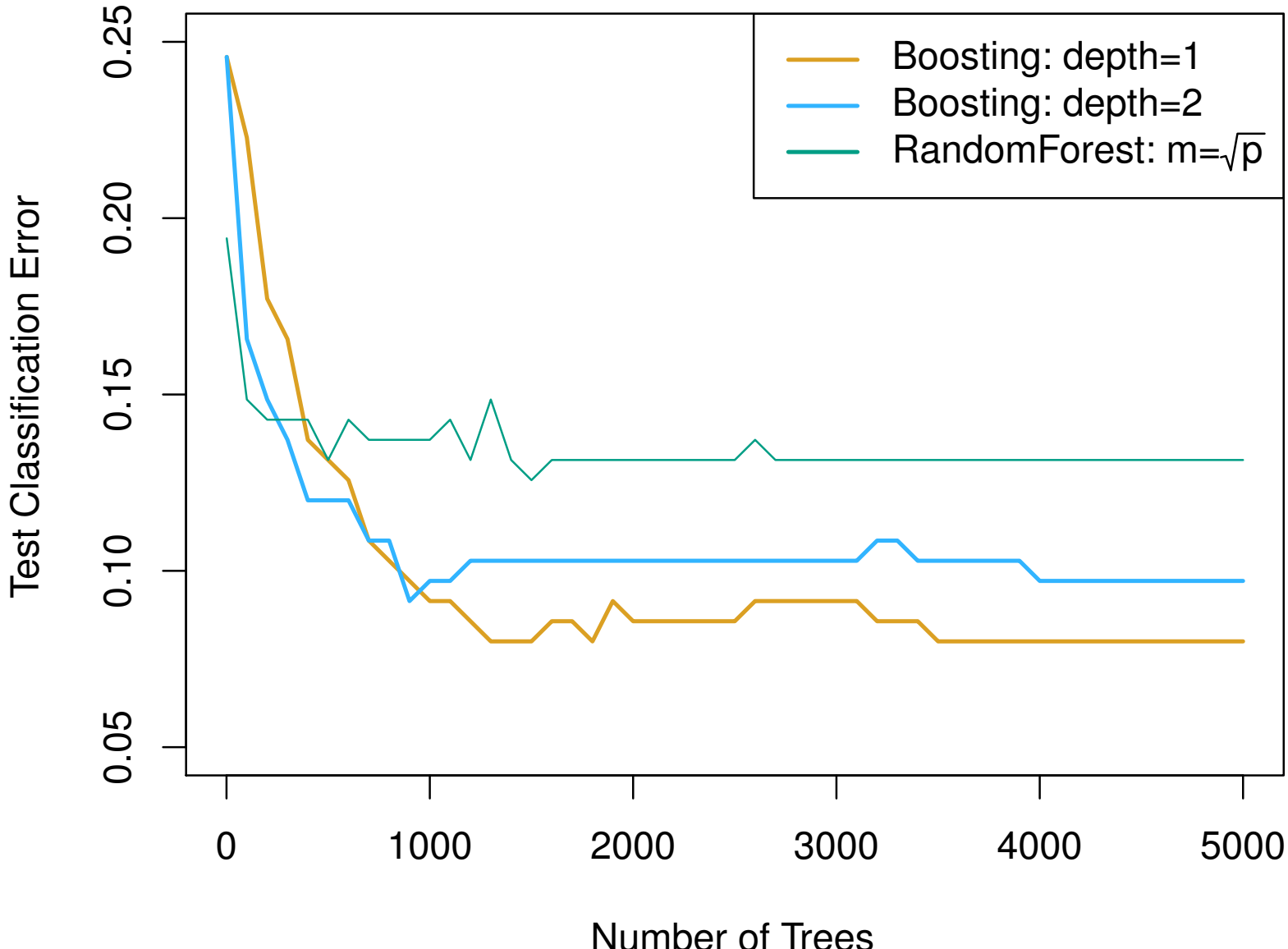
What is the idea behind this procedure?

- Unlike fitting a single large decision tree to the data, which can quickly overfit, the boosting approach instead **learns slowly**.
- Given the current model, we fit a decision tree to the residuals from the model. We then add this new decision tree into the fitted function in order to update the residuals.
- Each of these trees can be rather small, with just a few terminal nodes, determined by the parameter d in the algorithm.
- By fitting small trees to the residuals, we slowly improve $\hat{f}$ in areas where it does not perform well. The shrinkage parameter λ slows the process down even further, allowing more and different shaped trees to attack the residuals.
- Convert many "weak" learners into a complex predictor.

Boosting for classification

- Boosting for classification is similar in spirit to boosting for regression, but is a bit more complex. We will not go into detail here, nor does the ISL text book.
- Interested students can learn about the details in **Elements of Statistical Learning, Chapter 10**.
- In a nutshell, the key to modern boosting algorithms' generalisability is that they fit the gradient of a loss function w.r.t. the prediction, hence they are commonly referred to as **gradient boosting** (see Friedman 2001). Fitting the gradient of an MSE loss function in regression is just one case of this.
- The R package `gbm` (gradient boosted models) handles a variety of regression and classification problems, for more advanced boosting packages see the upcoming slides.

Gene expression data continued



Details of previous figure

- Results from performing boosting and random forests on the fifteen-class gene expression data set in order to predict cancer versus normal.
- The test error is displayed as a function of the number of trees. For the two boosted models, $\lambda = 0.01$. Depth-1 trees slightly outperform depth-2 trees, and both outperform the random forest, although the standard errors are around 0.02, making none of these differences significant.
- The test error rate for a single tree is 24%.

Tuning parameters for simple boosting model

1. The **number of trees** B. Unlike bagging and random forests, boosting can overfit if B is too large, although this overfitting tends to occur slowly if at all. We use cross-validation to select B.
2. The **shrinkage parameter** λ, a small positive number. This controls the rate at which boosting learns. Typical values are 0.01 or 0.001, and the right choice can depend on the problem. Very small λ can require using a very large value of B in order to achieve good performance.
3. The **number of splits** d in each tree, which controls the complexity of the boosted ensemble. Often $d = 1$ works well, in which case each tree is a **stump**, consisting of a single split and resulting in an additive model. More generally d is the **interaction depth**, and controls the interaction order of the boosted model, since d splits can involve at most d variables.

Boosting: Current algorithms

- Among the best algorithms from statistical machine learning today are some extensions of the simple benchmark boosting algorithm outlined above.
- Frequently win prediction competitions and are used for code in production.
- **Bold** words are links from here onwards.
- Prominent algorithms and packages are **XGBoost** and **LightGBM** which exist for R and Python (and other languages).
- Many options in regard to model flexibility, regularisation, loss functions, etc.

LightGBM key features

- Grows trees leaf-wise instead of level-wise (see e.g. the **documentation**).
- Very fast.
- **Very flexible**, for example:
  - Single and multi-class classification.
  - Regression with a range of loss functions (e.g. Huber loss which is more robust against outliers, or e.g. Gamma or Poisson for modeling some positive outcomes).
  - Can handle missing values.
  - Can be used in R, Python, and C.
- Full **paper** for technical details (NIPS, 2017).

Remarks on boosting

- Boosting works well with trees, but can in principle be applied to any classifier.
- Boosting can overfit, hyper parameter tuning is important.
- In more current libraries, there are many more tuning parameters.
- Interpretable structure of individual trees is largely lost.

Summary

- Decision trees are simple and interpretable models for regression and classification.
- However they are often not competitive with other methods in terms of prediction accuracy.
- Bagging, random forests and boosting are good methods for improving the prediction accuracy of trees. They work by growing many trees on the training data and then combining the predictions of the resulting ensemble of trees.
- In particular gradient boosting is among the state-of-the-art methods in statistical machine learning for tabular data. However, results can be difficult to interpret.

Guided coding

- 01-bagging-and-rf.Rmd
- 02-lightgbm.Rmd