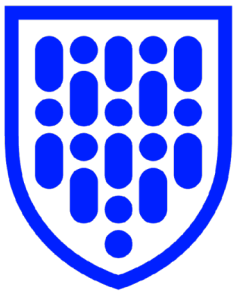


Institute of Data

2020

Data Science and AI

Module 8

Ensembles Methods

Agenda: Ensemble Methods

- Introduction
- **Bagging**
- **Boosting**
- **Stacking**

Introduction

- Overview
- Types of Ensembles methods
- Error in Ensembles (Variance vs. Bias)

Ensemble - Overview

- An Ensemble is a combination of a diverse set of learners (individual models) put together to improve on the stability and predictive power of the model.
- Each learner represents a hypothesis / model.
- Different set of learners can be established by having differing:
  - hypothesis
  - modelling technique
  - initial seed
  - population / sample

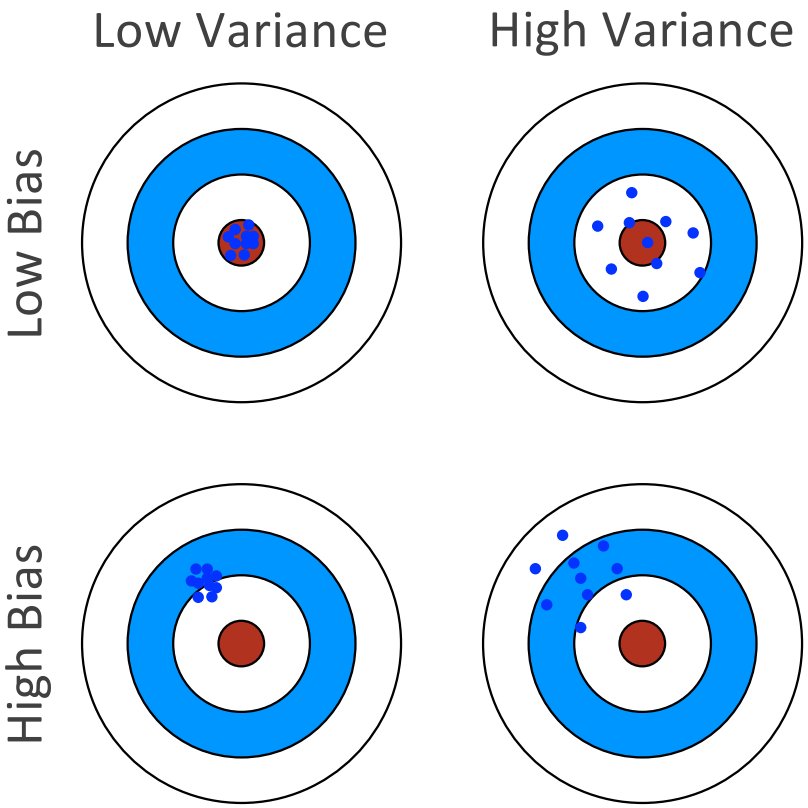
Ensemble - Overview

- In theory, ensembles tend to overfit on the training data.
- In practice, ensemble techniques (bagging mainly) tend to reduce issues related to overfitting of the training values.
- Ensemble techniques can be used for both supervised learning and unsupervised learning (consensus clustering or anomaly detection).

Types of Ensemble methods

- There are two types of Ensemble methods:
  - Sequential: where the learners are generated sequentially (e.g. AdaBoost)
    - The rationale is to benefit from the relationship between the learners.
    - The general performance can be boosted by penalising previously mislabeled examples with higher weight.
  - Parallel: where the learners are generated parallelly (e.g. Random Forest)
    - The motivation is to exploit independence between the learners since the error can be reduced dramatically by averaging.

Error in Ensembles (Variance vs. Bias)



- Bias measures the difference between the predicted and actual values on average.
- Variance quantifies how are the prediction made on same observation different from each other.

Error in Ensembles (Variance vs. Bias)

- Suppose we have a set of points $x_1, x_2, \ldots, x_n$ and a real values y_i
- Assume we have a function with some noise $y = f(x) + \in$ with zero mean and variance σ^2
- Assume we want to find a function $\hat{f}(x)$ that approximates the real function. We express the error of our function by measuring the 'mean squared error'. i.e. we want $(y - \hat{f}(x))^2$ to be minimum. Of course, we cannot do this perfectly, because the real function itself has noise.
- So, we can break down or 'expected' error to be:

$$Error(x) = Bias^2 + \text{Variance} + \text{Irreducible Error}$$

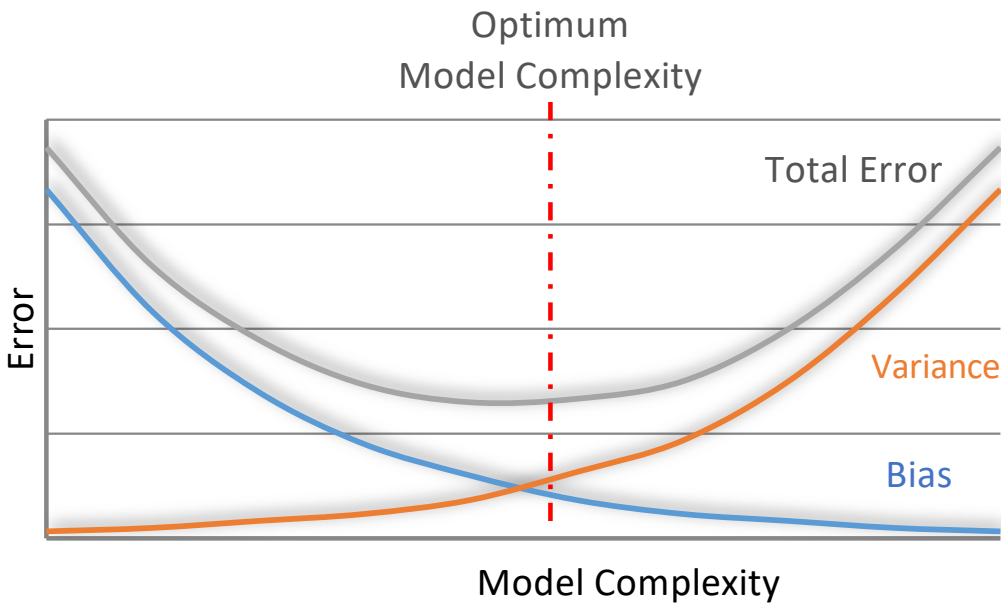
Where:

$$Bias\left[\hat{f}(x)\right] = E\left(\left[\hat{f}(x)\right]\right) - f(x)$$

$$Variance\left[\hat{f}(x)\right] = E\left[\left(\hat{f}(x)^2\right) - E\left[\hat{f}(x)\right]^2\right.$$

Irreducible Error = σ^2

Error in Ensembles (Variance vs. Bias)



- As the **complexity** of the model increases, there is a reduction in error due to **lower bias** in the model. However, this only happens up to a particular point.
- As the model becomes more complex, it becomes prone to **overfitting**, the model starts suffering from **high variance**.
- An ideal/optimal model should keep a **balance** between these bias and variance. This is known as the trade-off management of bias-variance errors.
- Ensemble learning can manage this **trade-off** analysis.

Error in Ensembles (Variance vs. Bias)

- Ensemble learning can manage this trade-off analysis.
- One way to reduce the variance of an estimate is to average together multiple estimates.
- For example, train M different trees on different subsets of the data (chosen randomly with replacement) and compute the ensemble output by averaging the output of the trees.

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Bagging

- Overview
- Algorithm
- Usage
- Methods
- Pros and Cons
- Example

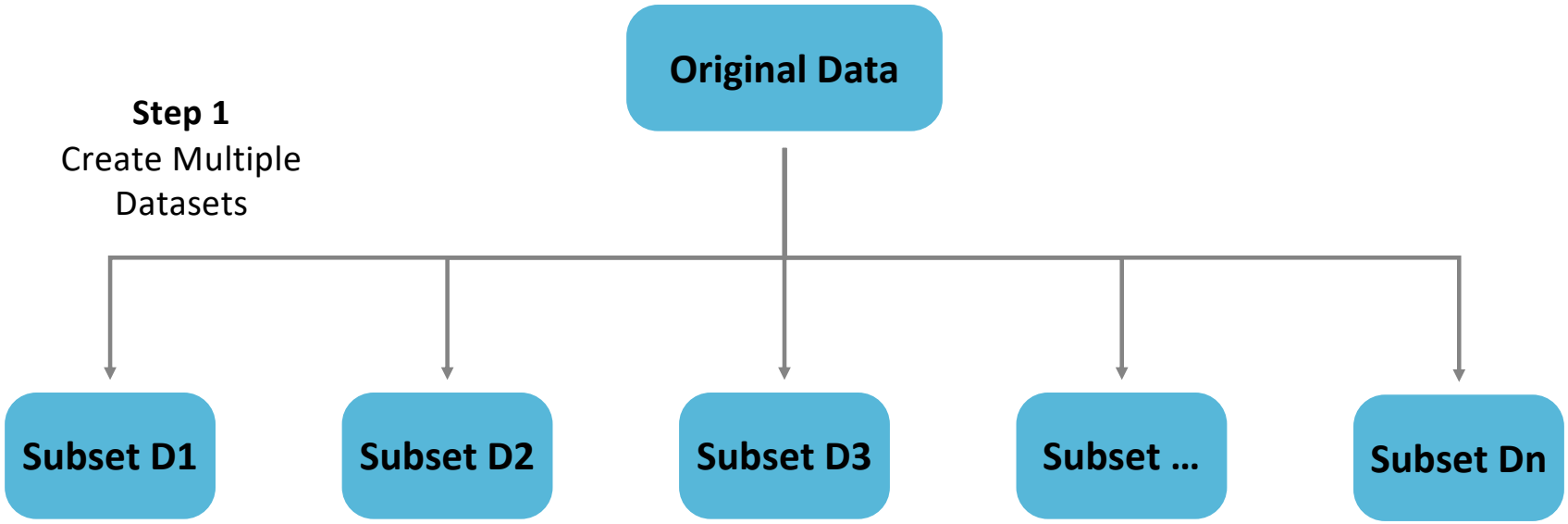
Bagging - Overview

- Different set of learners are using the same set of data and there is a high chance that these learners give the same result.
- One technique to solve this concern is with bootstrapping.
- Bootstrapping is a random sampling technique of creating subsets of observations from the original dataset with replacement (bootstrap sampling).
- Typically, the size of the subsets is the same size as the original set.

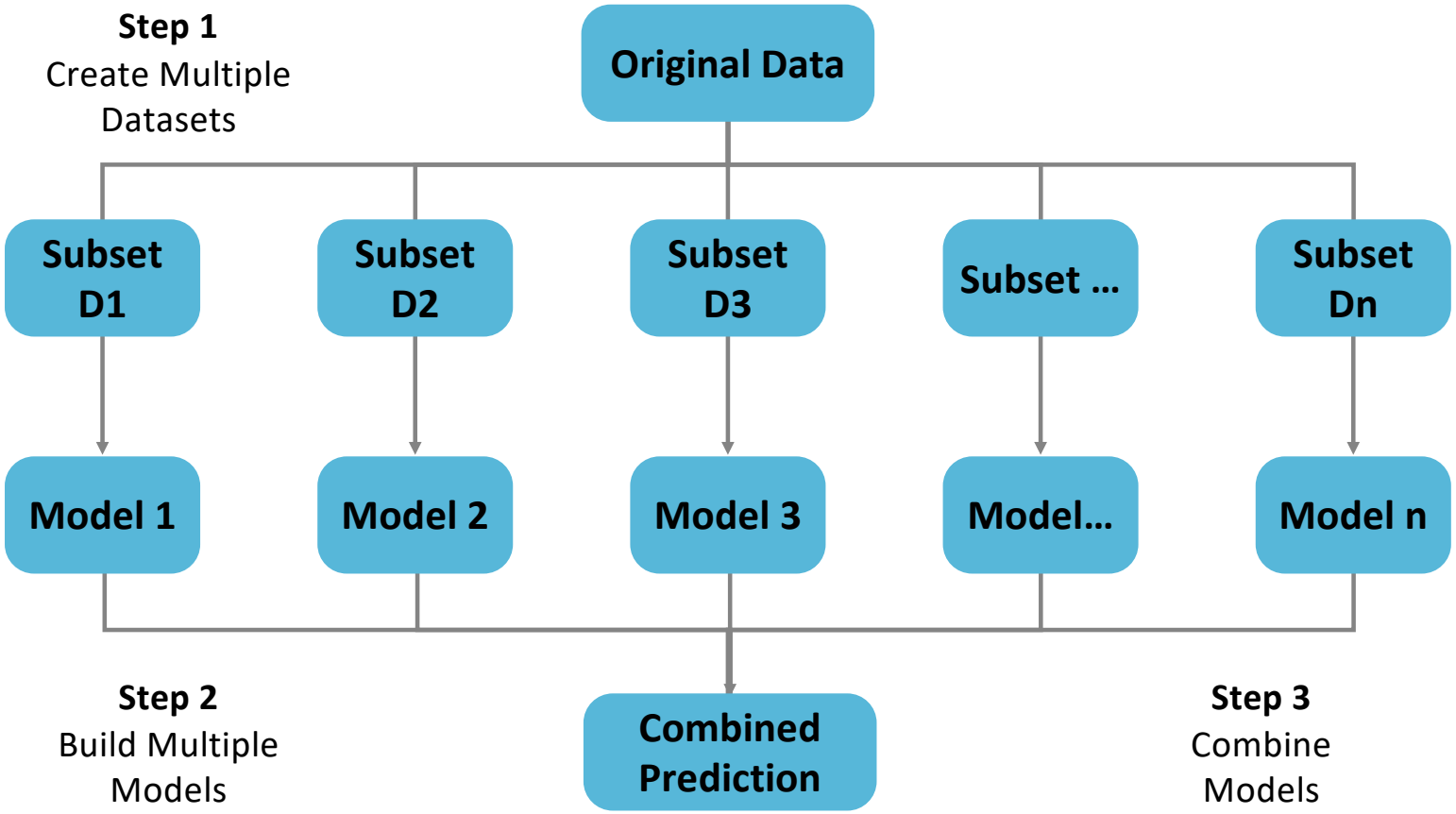
Bagging - Overview

- Bagging stands for Bootstrap Aggregation.
- Bagging uses subsets (bags) to get a fair idea of the distribution (complete set).
- The size of subsets created for bagging may be less than the original set.
- Bagging uses averaging for regression and voting for classification when aggregating the outputs of base learners.

Bagging Algorithm



Bagging Algorithm



Bagging Usage

- Forests of randomised trees are a type of ensemble algorithm
- In Random Forests, each tree is built by bootstrap sampling (drawn with replacement) from the training set
- Also, instead of using all the features, a random subset of features is selected, further randomising the tree
- The bias of the forest increases slightly as a consequence, but the variance decreases with the averaging of less correlated trees, producing an overall better model

Bagging Usage

- Algorithm randomness goes one step further in vastly randomised trees
  - The **splitting thresholds** are randomised
    - Thresholds are drawn at random for each available feature (opposed to the most discriminative threshold), and the best of these randomly-generated thresholds is picked as the splitting rule
  - This usually allows for an extra reduction of the variance of the model, with a slightly higher increase in bias

Bagging Methods

- Some Bagging algorithms
  - Bagging meta-estimator
  - Random forest

Bagging Pros

- Robust against **outliers and noise**
- Fast runtime
- **Reduces variance** and typically avoids overfitting
- Offers most of the **advantages of trees** like automatic selection of variable importance, handling missing values, and accommodating highly non-linear interactions
- Easy to use with limited well-established default parameters and works well off-the-shelf requiring **little additional tuning**

Bagging Cons

- The complexity of multiple trees **removes transparency** (**black box**)
- Can be slow to compute as complexity increases

Demo 8.2: Bagging

- Purpose
  - Understand the concept and potential of Bagging
- Resources
  - Sample data from SciKit-Learn
- Materials
  - Jupyter Notebook (Demo-8_2)

Lab 8.1: Bagging

- Purpose
  - Work with Bagging
  - Practice some coding in Python
- Resources
  - Sample data from SciKit-Learn
- Materials
  - Jupyter Notebook (Lab-8_1)

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Boosting

- Overview
- Algorithm
- Usage
- Methods
- Pros and Cons
- Example

Boosting Overview

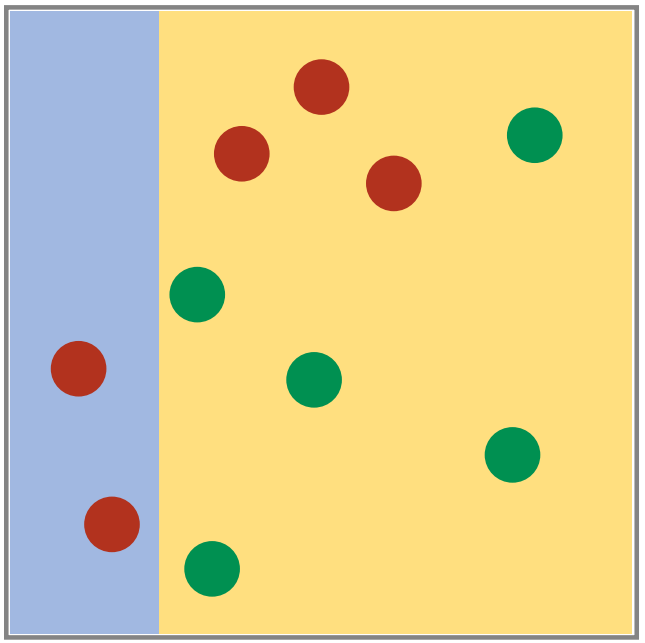
- Boosting refers to a category of algorithms that can convert weak learners to strong learners
  - The principle of boosting is to fit a sequence of weak learners **to weighted versions** of the data
  - Weak learners are models that are only slightly better than random guessing, such as small decision trees
  - **Examples that were misclassified by earlier rounds get more weight**

Boosting Overview

- The sequential training of base learners on **a weighted version** of the data is the main difference between boosting and committee methods (like bagging)
- The predictions are then **aggregated by a weighted sum** (regression) or weighted majority vote (classification) to produce the final prediction.
- Boosting is processed **in sequence**, so the next step's model attempts to **correct the errors** of the model form the previous step
- The following models are **dependent** on the previous model

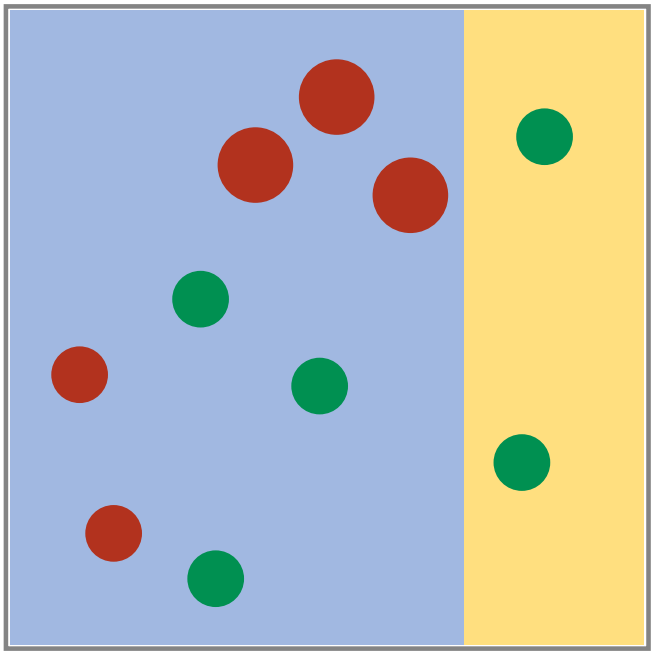
Boosting Algorithm

- The original dataset is the source of a subset
- Initially, the weights of all data points are equal
- A base model is created from this subset
- The base model serves to make predictions on the whole dataset



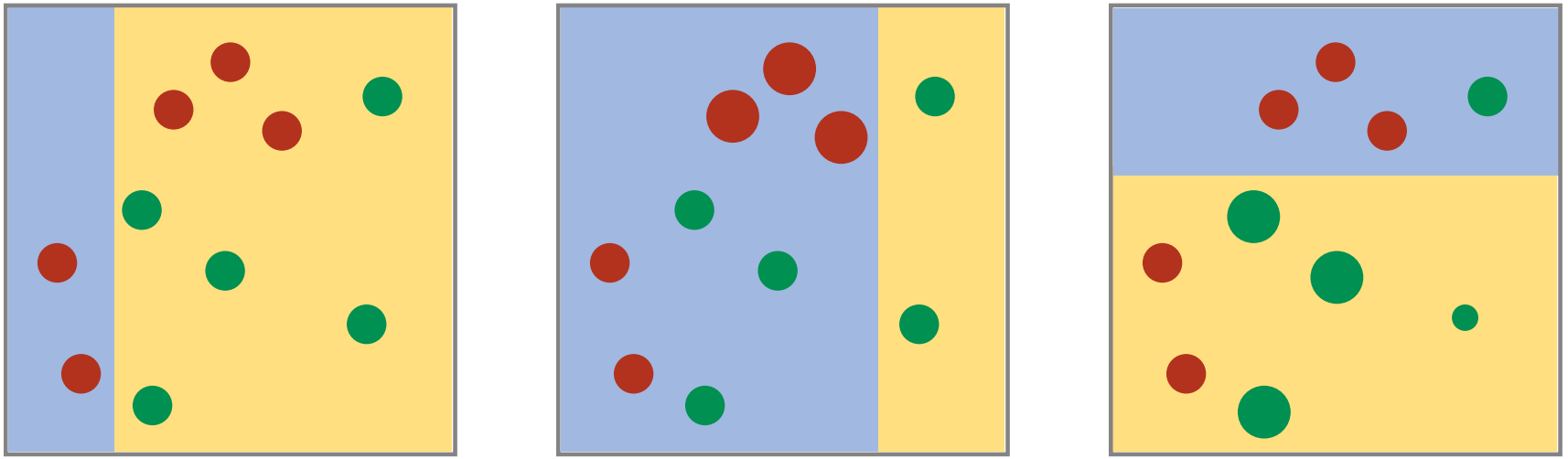
Boosting Algorithm

- The predicted and actual values are used to calculate the error
- The observations get higher weights if their predictions are incorrect
  - The three misclassified red points get bigger weights
- A new model is created producing predictions from the dataset
  - The model tries to correct the errors from the previous model



Boosting Algorithm

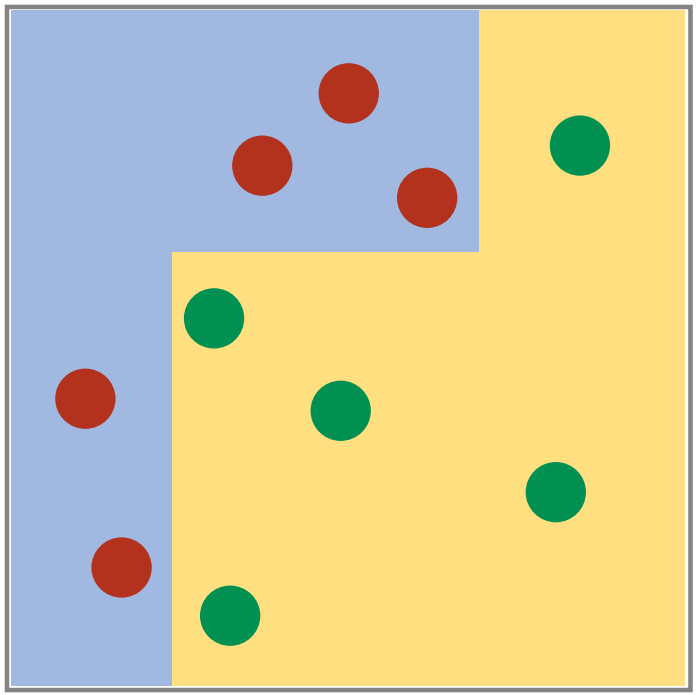
8. Each of multiple new models corrects the errors of the previous model



Boosting Algorithm

- The weighted mean of all the previous models (weak learners) create the finished model (strong learner)

- The separate models would not have a great performance on the entire dataset, but combined they work well for parts of the dataset, so each model boosts the performance of the ensemble



Boosting Algorithm (AdaBoost)

- AdaBoost (Adaptive Boosting)
- The **base classifier $y_1(x)$** is trained using equal weighted coefficients
- The weighted coefficients in subsequent rounds are
  - **Increased** for data points that are classified **incorrectly**, and
  - **Decreased** for data points that were classified **correctly**
- Each of the base classifiers has an epsilon quantity that represents a **weighted error rate**
- The weighting coefficients alpha attributes **bigger weight** to the **more accurate** classifiers

Boosting Usage

- Gradient Tree Boosting is a generalisation of boosting to arbitrary differentiable loss functions
- It can solve both regression and classification problems
- Gradient Boosting builds the model in a sequential way

$$F_m(x) = F_{m-1}(x) + \gamma_m h_m$$

Boosting Usage

- The decision tree $h_m(x)$ is chosen at each stage to minimise a loss function L given the current model $F_{m-1}(x)$

$$F_m(x) = F_{m-1}(x) + argmin_h \sum_{i-1}^{n} L(y_i, F_{m-1}(x_i) +$$

- The type of loss function used is the difference between classification and regression algorithms

Boosting Methods

- Some Boosting algorithms
  - AdaBoost (Adaptive boosting
  - GBM (Gradient boosting): uses differentiable loss function.
  - XGBoost ((eXtreme Gradient Boosting)
  - Light GBM

Boosting Pros

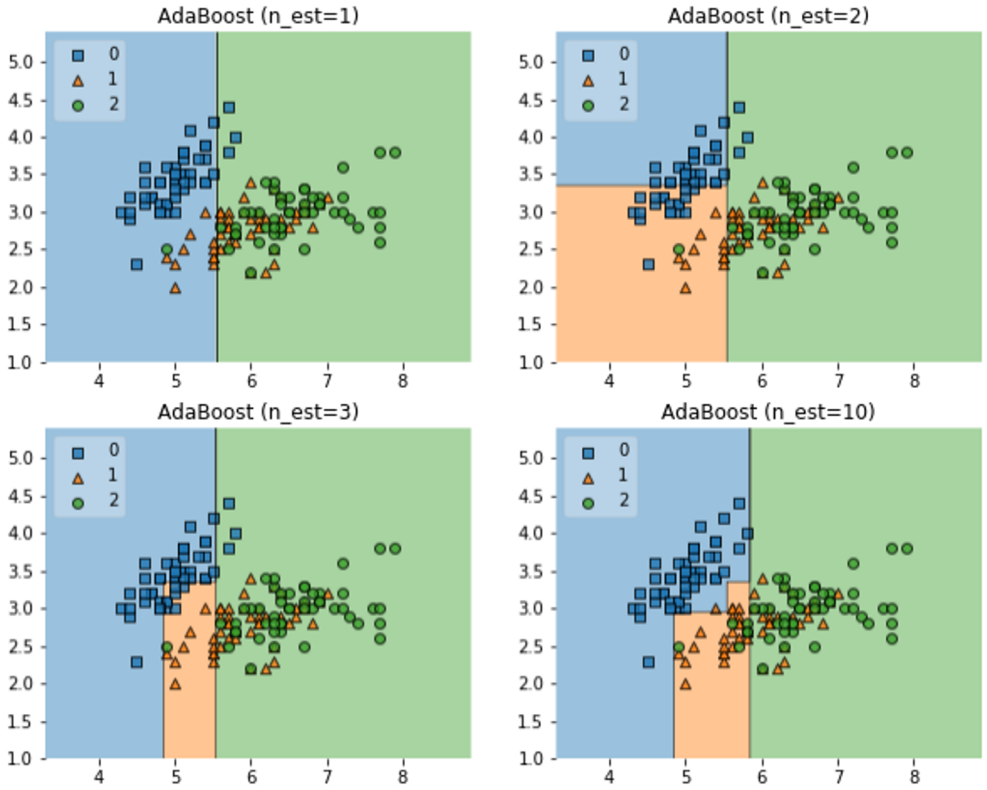
- Often the best possible model
- Directly optimises the cost function

Boosting Cons

- Not **robust** against **outliers and noise**
- Can overfit
- Need to find a proper stopping point
- Several **hyper-parameters**
- The complexity of multiple trees lacks transparency (**black box**)

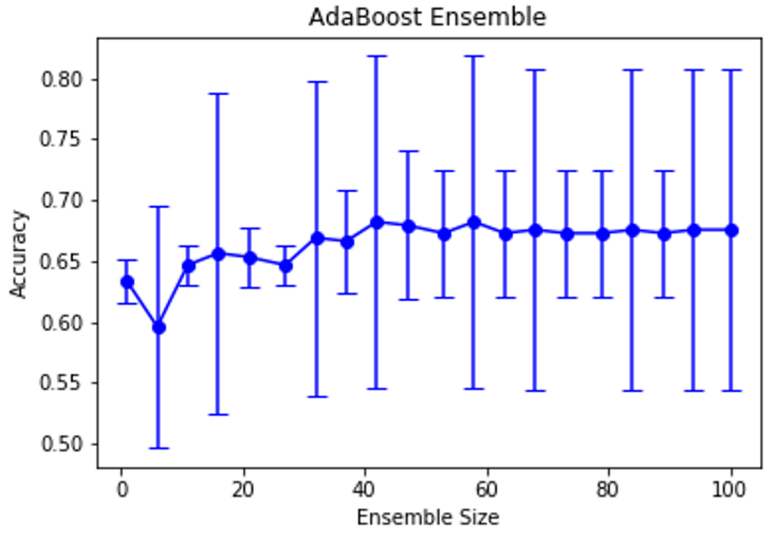
Boosting Example

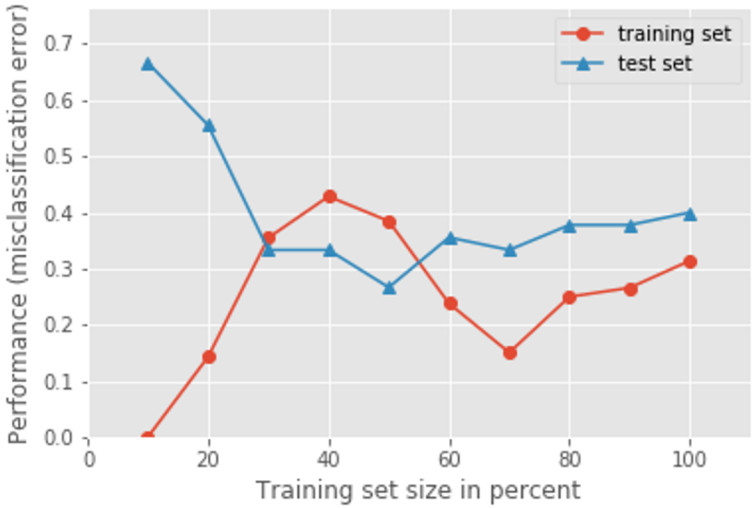
- Each base learner is a depth 1 decision tree which separates the space into two regions based on a feature threshold that partitions separated by a linear decision surface that is parallel to one of the axes



Boosting Example

- The test accuracy grows, up to a point, with the size of the ensemble (on the left)
- The figure on the right shows the learning curves for training and testing data





Demo 8.3: Boosting

- Purpose
  - Understand the concept and potential of Boosting
- Resources
  - Sample data from SciKit-Learn
- Materials
  - Jupyter Notebook (Demo-8_3)

Lab 8.2: Boosting

- Purpose
  - Work with Boosting
  - Practice some coding in Python
- Resources
  - Sample data from SciKit-Learn
- Materials
  - Jupyter Notebook (Lab-8_2)

Stacking

- Overview
- Algorithm
- Pseudocode
- Example

Stacking Overview

- Stacking is an ensemble learning approach that combines multiple regression or classifications models via a meta-regressor or a meta-classifier
- The **outputs of the base level model serve as features to train the meta-model**
- The base level models are trained based on **a complete training set**
- The base level often consists of **different learning algorithms** and therefore stacking ensembles are often heterogeneous

Stacking overview in other words

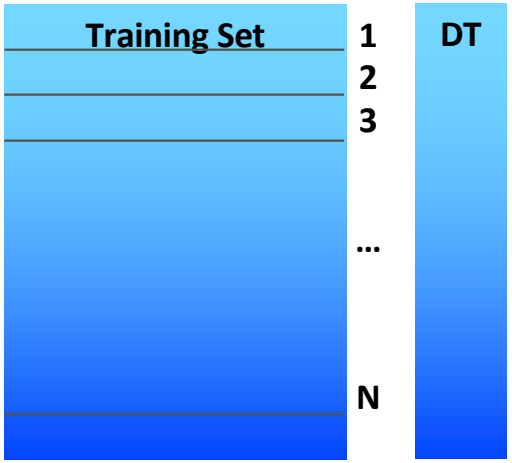
- Stacking is an ensemble learning approach that **uses predictions from various models to construct a new model**
  - A base model such as Decision Tree, K-NN or SVM
- The new model can then make predictions on the test set

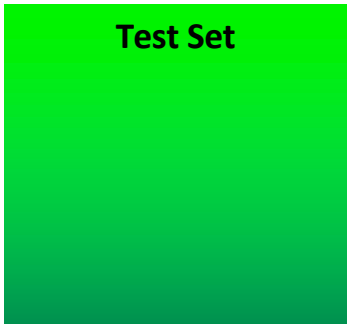
Stacking Algorithm

1. The train set is split into ***N*** parts

Stacking Algorithm

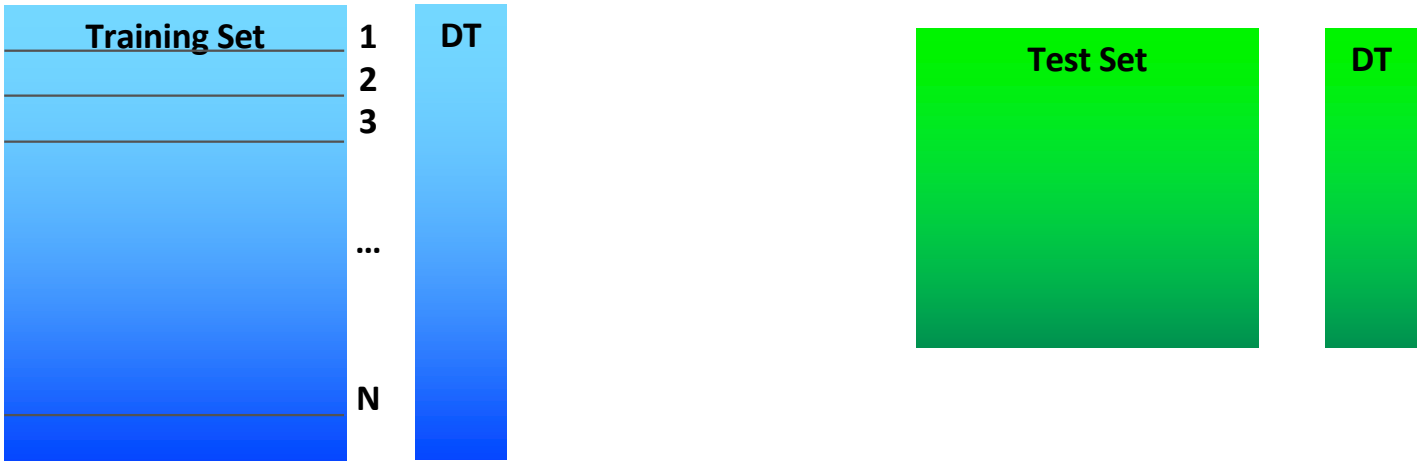
2. A base model (like CART) is fitted on ***N-1*** parts, and predictions are made for the ***N*** part
   - This applies to each part of the train set





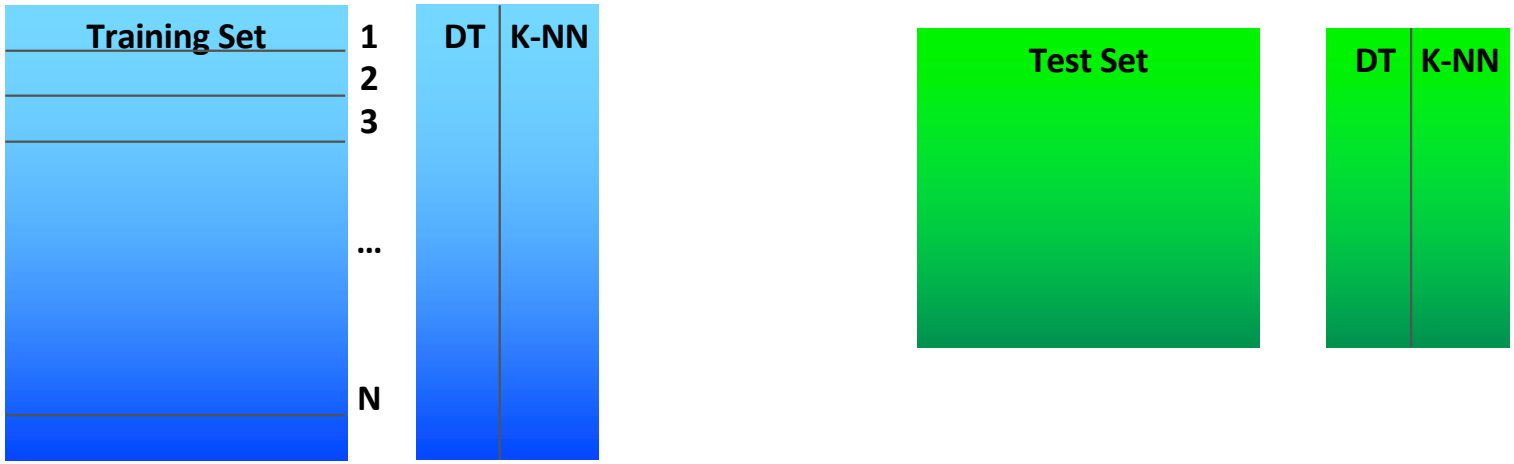
Stacking Algorithm

3. The base model (decision tree) is then fitted on the whole train dataset
4. Predictions are made on the test dataset using this model



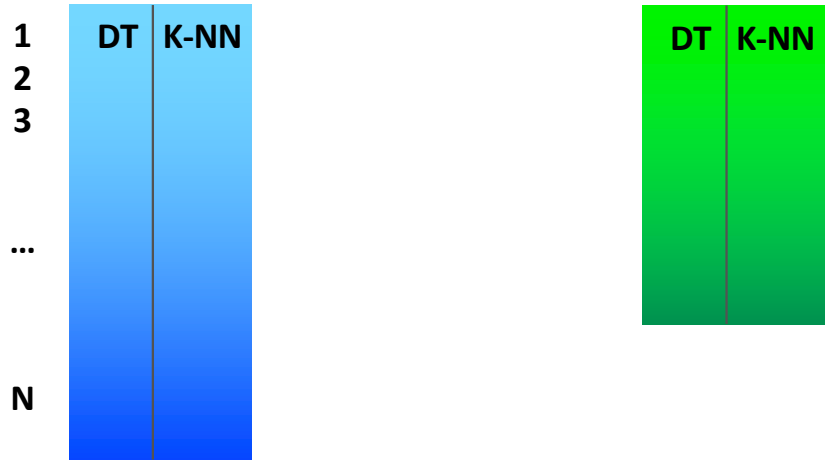
Stacking Algorithm

5. All other base models repeat steps 2 to 4 resulting in another set of predictions for both the train set and test set



Stacking Algorithm

6. The predictions from the train dataset serves as features to build a new model
7. The new model is used to make final predictions on the test prediction set



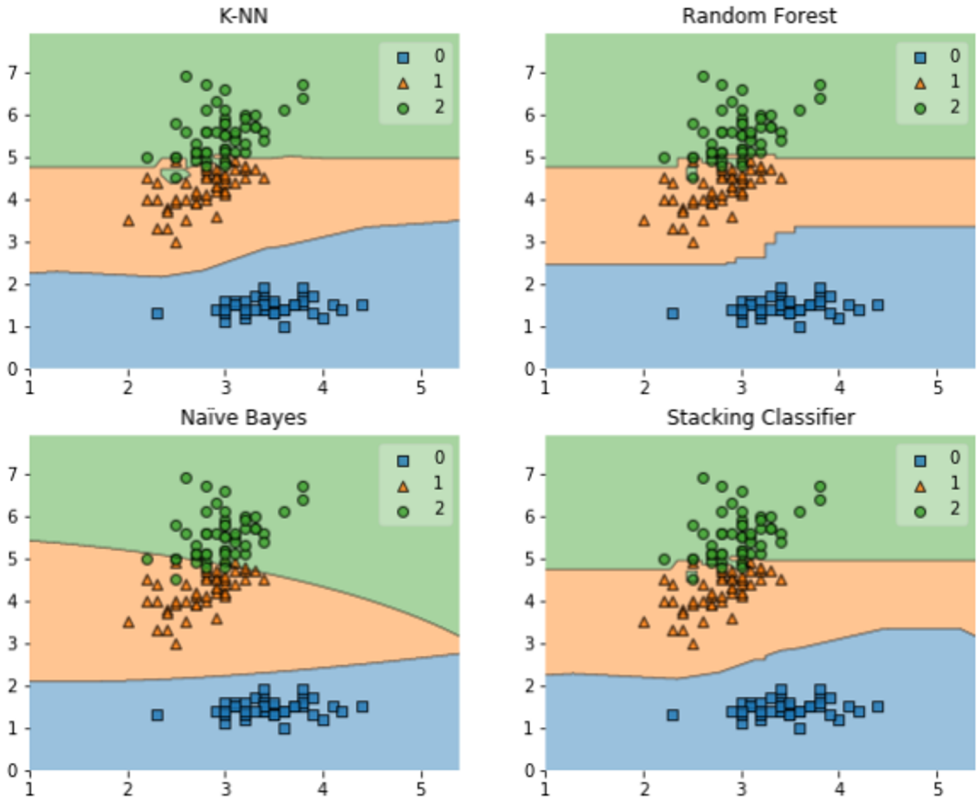
Stacking Algorithm

1: $Input: training data D = \{x_i, y_i\}_{i=1}^{m}$
2: $Output: ensemble classifier H$
3: $\#Step1: learn\ base\ level\ classifier$
4: $for\ t = 1 to T$
5: $learn\ h_t based\ on\ D$
6: $\#Step2: construct\ new\ dataset\ of\ predictions$
7: $for\ i = 1\ to\ m$
8: $D_h = \{x_i', y_i\}, where x_i' = \{h_1(x_i), \cdots, h_T(x_i)\}$
9: $\#Step3: learn\ a\ meta\ classifier$
10: $learn\ H\ based\ on\ D_h$
11: $return\ H$

Stacking Example

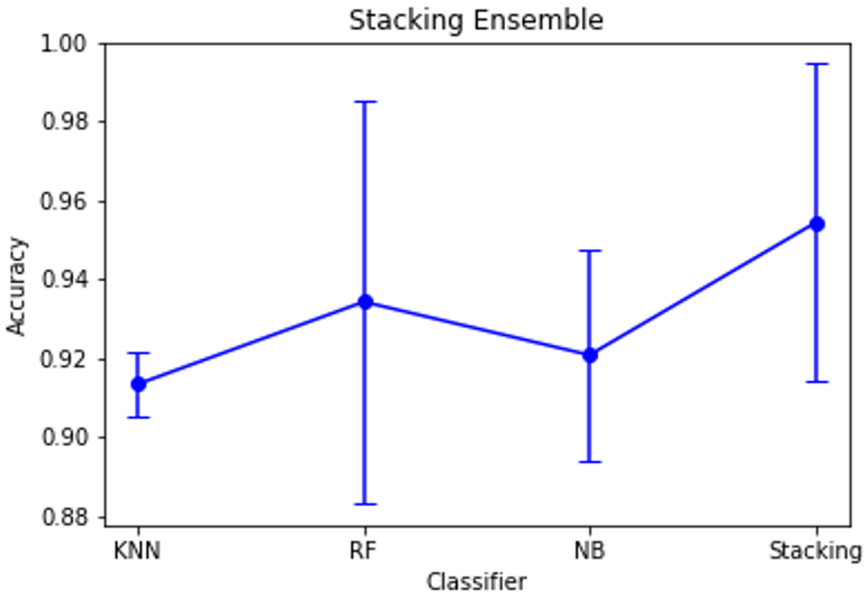
- The decision boundaries blend by the effect of the stacking classifier
- The stacking achieves higher accuracy than individual classifiers

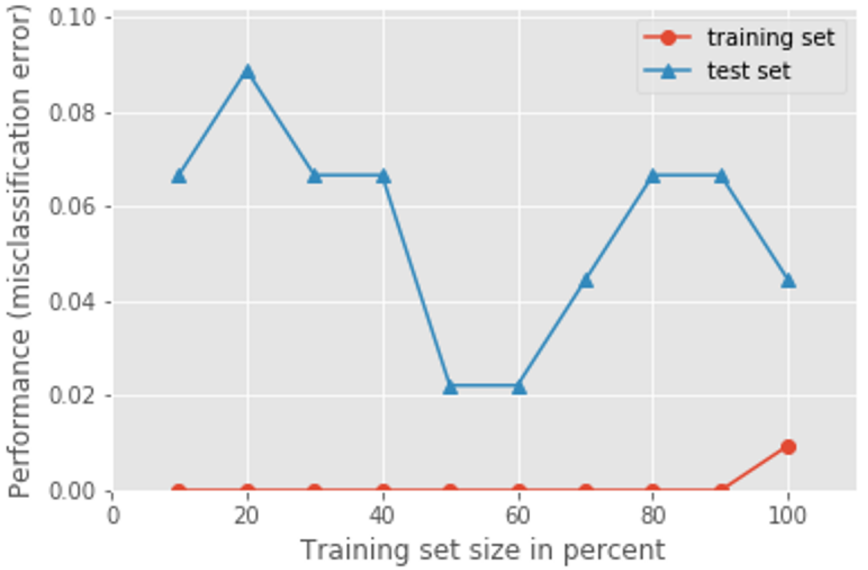
	Accuracy	
	Mean	Standard Deviation
N-NN	0.91	±0.01
Random Forest	0.93	±0.05
Naïve Bayes	0.92	±0.03
Stacking	0.95	±0.04



Stacking Example

- The learning curves show no signs of overfitting





Demo 8.4: Stacking

- Purpose
  - Understand the concept and potential of Stacking
- Resources
  - Sample data from SciKit-Learn
- Materials
  - Jupyter Notebook (Demo-8_4)

Lab 8.3: Stacking

- Purpose
  - Work with Stacking
  - Practice some coding in Python
- Resources
  - Sample data from SciKit-Learn
- Materials
  - Jupyter Notebook (Lab-8_3)

End of Presentation!