Topics in Data Science

(Lecture 3)

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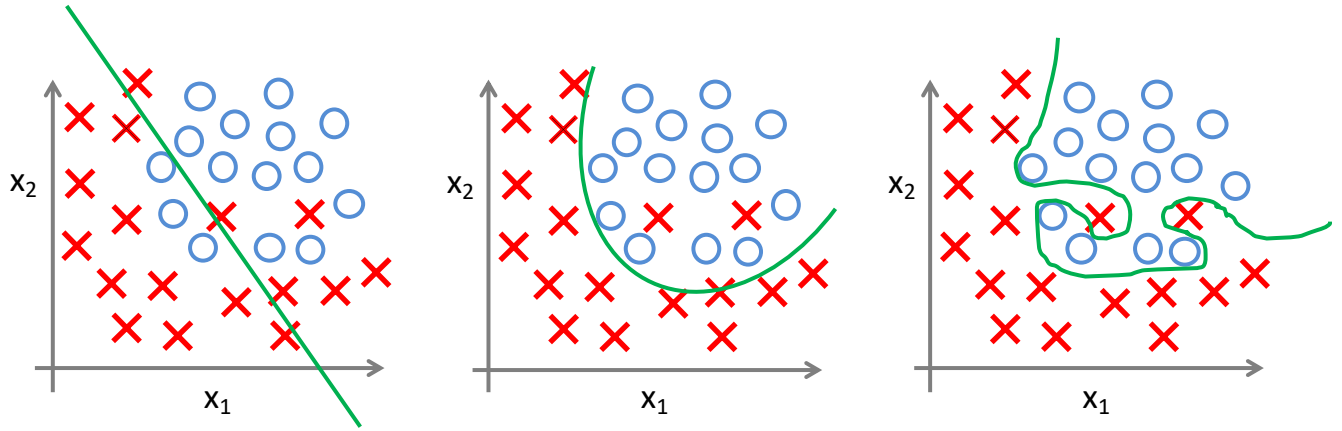
The Problem of Overfitting

- **Overfitting** happens when the predictive model (classification model or regression model) **fits too much** with the **training samples** so that it starts capturing, learning, and representing the **noise and randomness or outlier samples** of the training dataset.
- Overfitting provides excellent accuracy for training data, but poor results for future data samples (testing set)!



Under-fit (High Bias) **Ideal fit** **Over-fit (High Variance)**

Ensemble Learning:

Bagging, Boosting, and Random Forests

Ensemble Learning

- **Ensemble Learning** is a popular and effective approach to improve the accuracy and performance of a machine learning problem.
- **Ensemble Learning** uses a **group of machine learning algorithms** (called **base** learners), and then combine the results of them to achieve higher accuracy.

Ensemble Learning

- **Example**: Construct a Strong Classifier by combining several Weak Classifiers!

- Each learner (e.g. classifier) alone may have very poor performance. But, a group of them together can achieve very accurate results.

- For the sake of simplicity (or other reasons), each classifier may make some assumptions, which might be or not be valid for the problem!

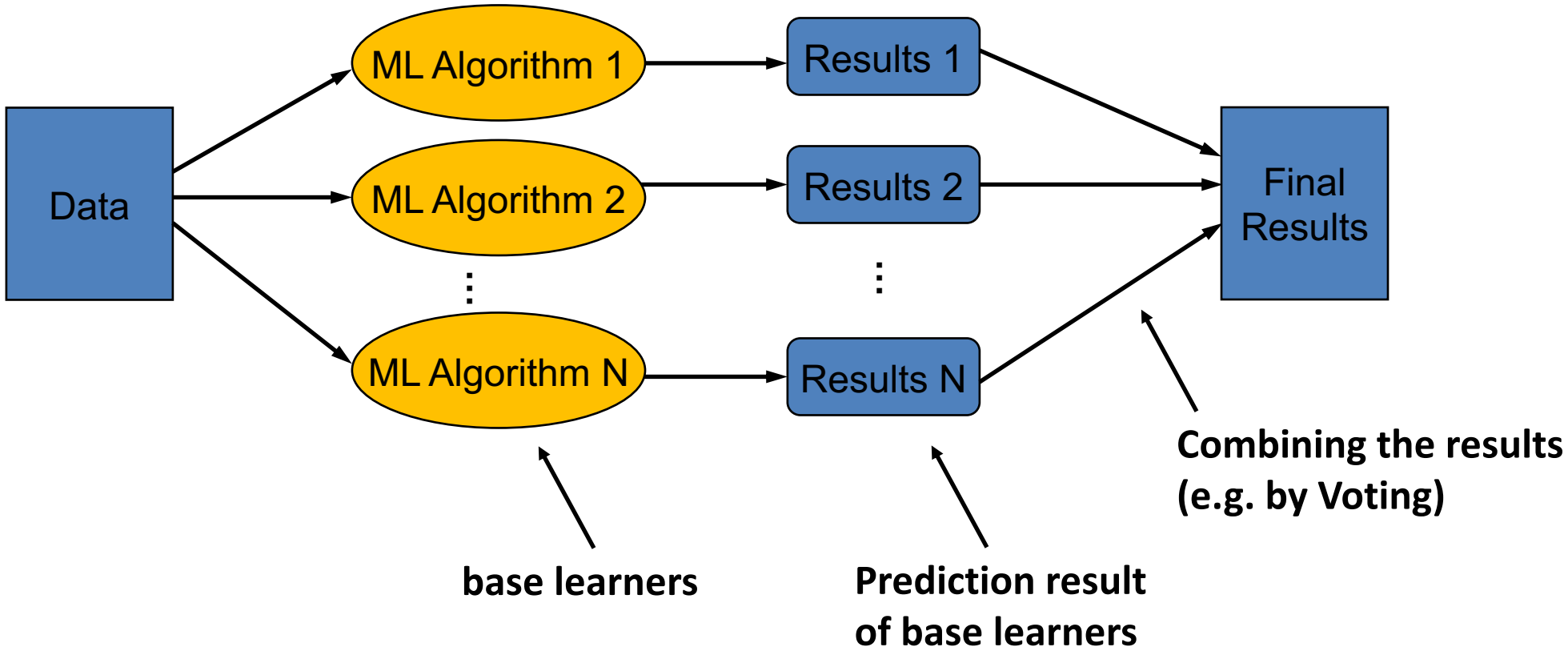
Different types of Ensemble Learning

- **Different learners of the Ensemble Learning may use:**

1. **Different learning Algorithms**
   - E.g. Combination of decision tree, KNN, and logistic regression
2. **Different choice of learning Parameters**
   - E.g. Several KNNs with various K's
3. **Different Features**
   - E.g. Several decision trees, each for a set of features
4. **Different Data Subsets**
   - E.g. Several decision trees, each for a section of the dataset
5. **Different Subproblems**
   - E.g. Several logistic regression classifiers, each for a part of the problem

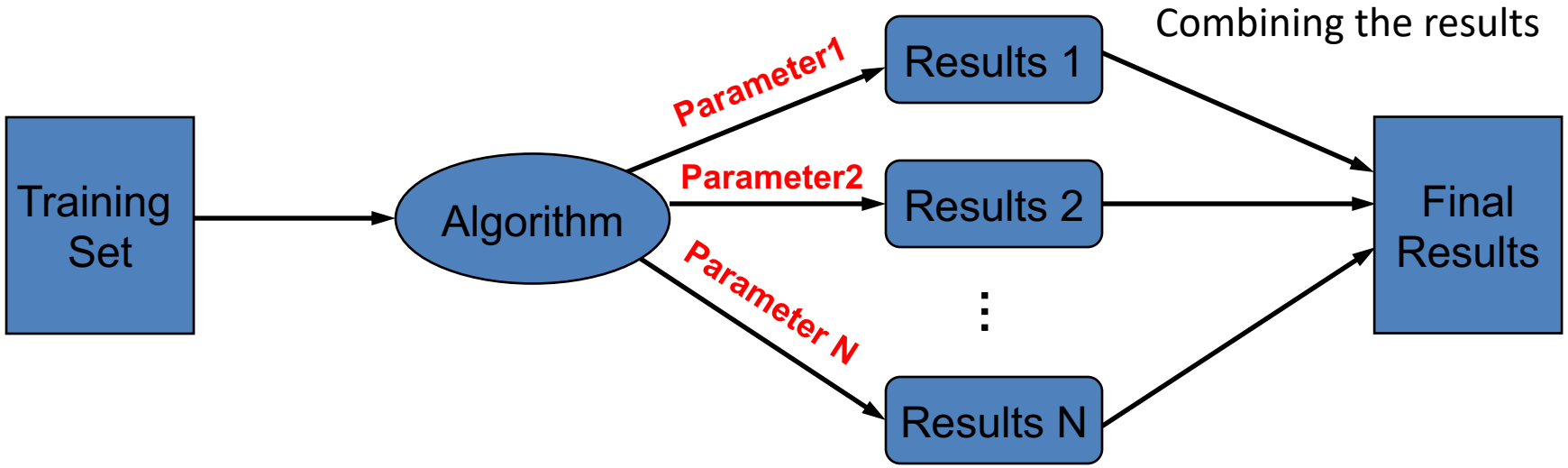
Different types of Ensemble Learning

1. **Different learning Algorithms:**



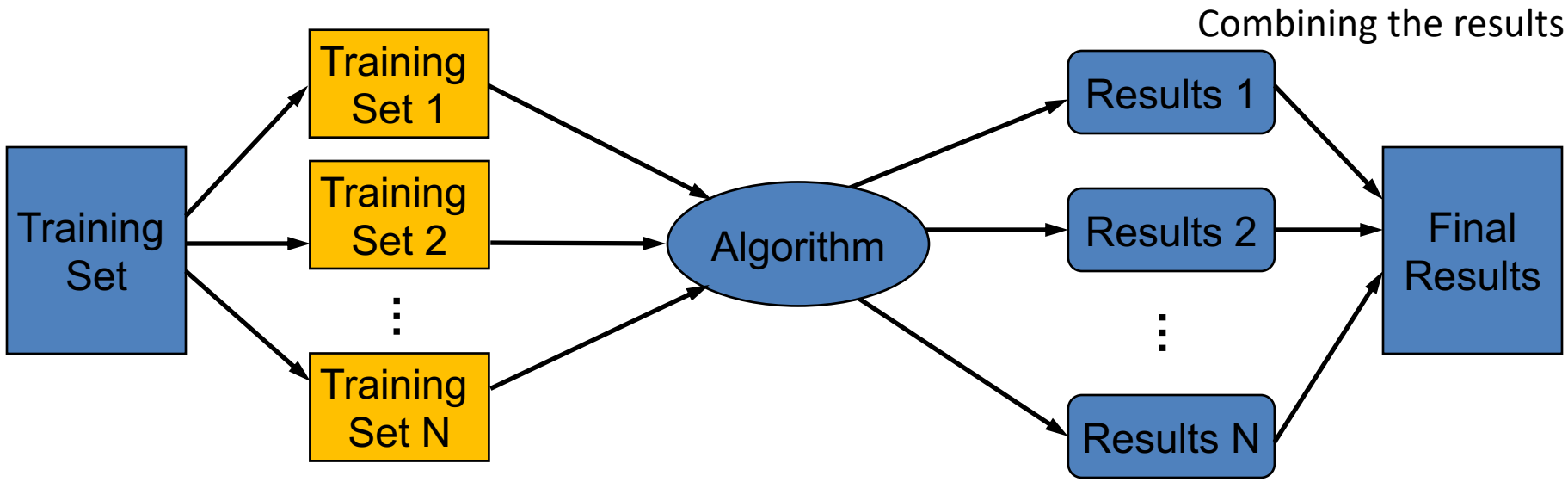
Different types of Ensemble Learning

2. Different choice of learning Parameters:



Different types of Ensemble Learning

3. Different Features
4. Different Subsets



An Important Note about Ensemble Learning

- The key in designing ensembles is **diversity** and **not necessarily high accuracy** of the base classifiers.

- Members of an ensemble group **should vary in the examples they misclassify, so that they cover each other's mistakes!**

- In other word, if we have several classifiers that are pretty accurate but they all misclassify the **same samples**, then ensemble learning will not achieve any better results! Therefore, most ensemble approaches, seek to promote diversity among the models they combine.

Combining the Results of Base Learners

- There are 3 main approaches for **combining** the results in Ensemble Learning:
  1. **Voting**
  2. **Stacking**
  3. **Cascading**

Combining the Results: Voting

- **Voting:**
  - Classifiers are combined in a **static** way.
  - Each base-level classifier gives a vote for its prediction.
  - **Plurality vote**: The final decision for each data sample (each prediction) is made based on the majority of votes.
    - E.g: Suppose we use 9 different decision tree classifiers for weather forecasting. 5 of them predict Rain for tomorrow, and 4 of them predict sunny. Thus, the final decision will be Rainy!
  - **Note**: Depending on the problem, some votes can be **weighted**. In this approach, the better base classifiers get higher voting weight.

Combining the Results: Stacking

- **Stacking:**
  - Classifiers are combined in a data-driven **dynamic** way.
  - An **upper level** machine learning method is used to learn how to combine the prediction results of the **base-level** classifiers.
  - The **upper level** classifier is used to make final decision from the predictions of the **base-level** classifiers.

Combining the Results: Cascading

- **Cascading:**
  - Classifiers are combined in an **iterative** way.
  - At each iteration, the training dataset is extended or modified based on the prediction results obtained in the previous iterations.
  - We will talk more about it later!

Intuitions: Why Does Ensemble Learning work?

- Suppose we have 3 completely Independent Classifiers, each one with prediction accuracy of 70%, and we want to use Voting Method for making a prediction:
  - For a positive sample, the final prediction is positive if **at least 2 out of 3** classifiers vote for positive:

$$0.7^3 + 0.7\times0.7\times0.3 + 0.7\times0.3\times0.7 + 0.3\times0.7\times0.7 = 0.78$$

  - Thus, combining 3 classifiers with accuracy of 70% each, using just a simple voting method can improve the accuracy to 78%.
  - **In theory**, If we use 101 independent classifiers, then the final voting accuracy will be 99.9%!!!!
  - But, can we always achieve this accuracy **in practice**? Why not?

Intuitions: Why Does Ensemble Learning work?

- **Note:** Making decision based on Independent Binary Classifiers, using Voting Method has Binomial Probability Distribution:
- **Binomial Distribution:** The probability that ***x*** out of ***n*** independent classifiers vote correctly, where each classifier predicts correctly with probability of ***p***, is

$$P(X = x|p, n) = \frac{n!}{r!(n-x)!}p^x(1-p)^{n-x}$$

  - In theory, If we use 101 independent classifiers, then the final voting accuracy will be 99.9%.
  - In practice, the accuracy is usually lower than theory because the classifiers are **NOT** completely independent and random!

Advantages and Disadvantages of Ensemble Learning

- **Advantages of Ensemble Learning:**
  - Improve prediction performance and accuracy
  - Robust to Overfitting

- **Disadvantages of Ensemble Learning:**
  - The combined classifier is not so transparent (black box)
  - Not a compact representation

Three Popular Approaches for Ensemble Learning

- **Bagging**: Bagging (stands for **B**ootstrap **Agg**regating) was first proposed by ***Leo Breiman*** to improve the classifier results by combining classifications of randomly generated training sets.

- **Boosting:** Originally proposed by ***Robert Schapire*** to build a strong classifier using a set of extremely weak base classifiers (with accuracy of slightly better than random guess).

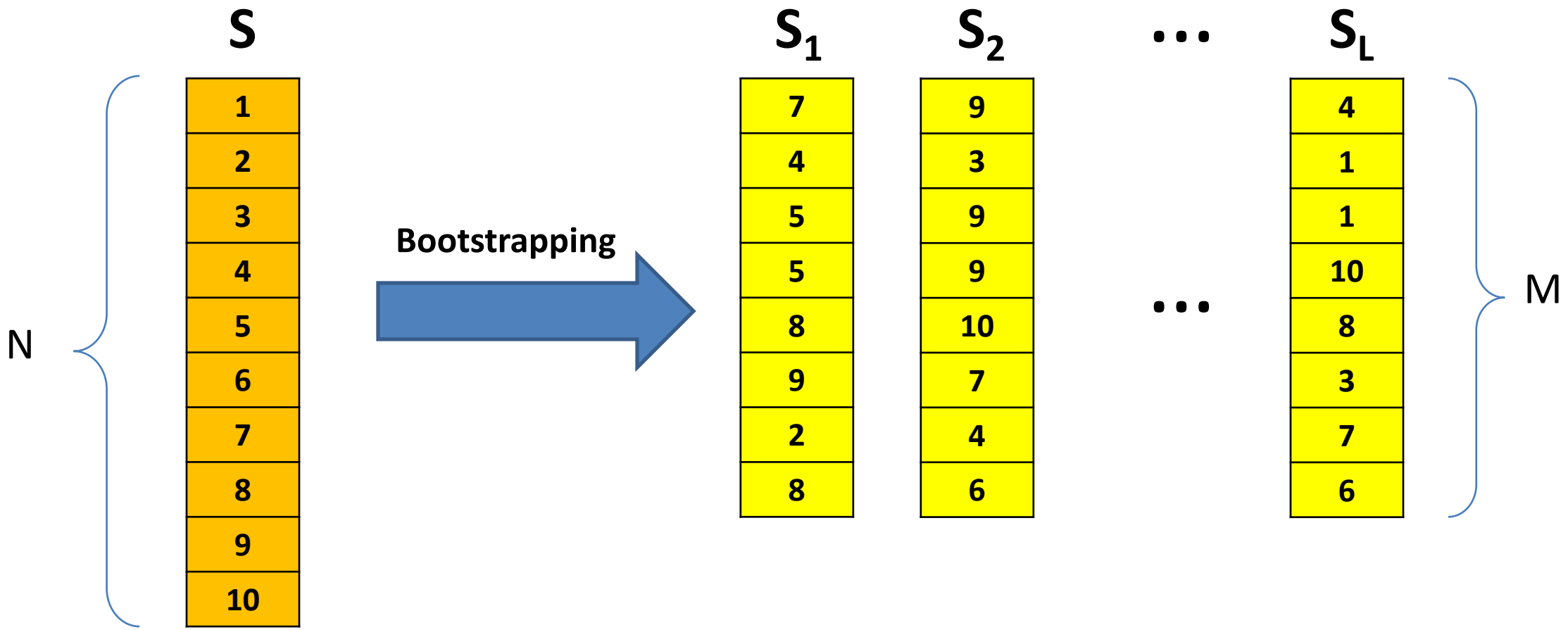
- **Random SubSpace (Random Forest):** First proposed by ***Leo Breiman*** to improve the accuracy of decision tree classifiers and address the overfitting problem.

Bagging
(Bootstrap Aggregation)

Bagging (Bootstrap Aggregation)

- Here are the main 4 steps for Bagging method:
- **Step1: Bootstrapping**: Suppose we have a **Training Dataset S** of **size N**. Bootstrapping generates **L** new training sets $\mathbf{S_1, S_2, \ldots, S_L}$ each of **size M**, by sampling from the original dataset **S** randomly and **with replacement.**
  - This type of sampling is called **Bootstrapping** or **Bootstrap Sampling.**
  - The bootstrap training sets $\mathbf{S_1, S_2, \ldots, S_L}$ may have overlap with each other.
  - By sampling with **replacement**, some data sample may be repeated in **each** $\mathbf{S_i}$.

Example for Bootstrap Sampling



Bagging (Bootstrap Aggregation)

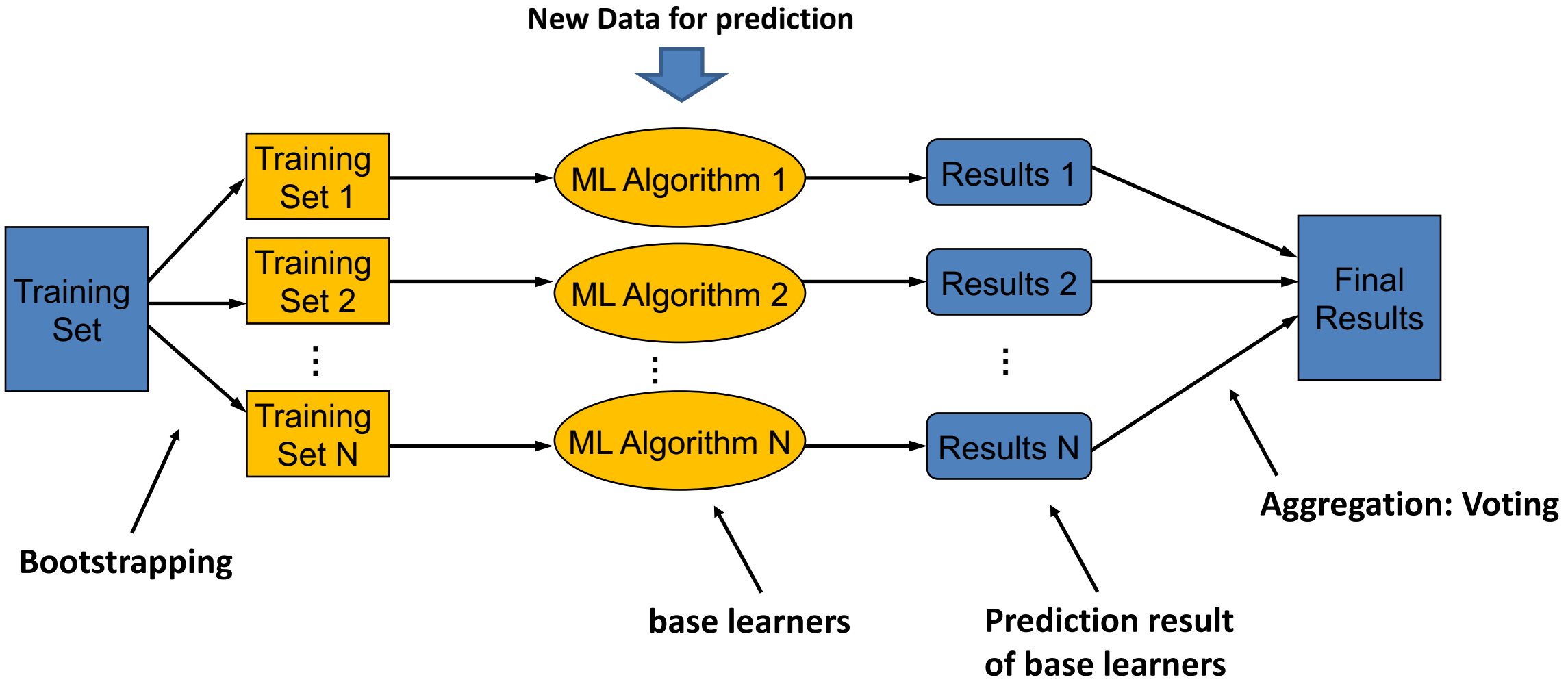
- **Step2: Training stage**: The **L** new training sets $S_1, S_2, \ldots, S_L$ will be used to train **L** learners (can be either **L** classifiers $C_1, C_2, \ldots, C_L$ or **L** regression models $R_1, R_2, \ldots, R_L$).
  - E.g. Training L decision trees for classification, or L linear regression models for regression.

- **Step3: Testing Stage:** Given a new unknown data sample, The **L** trained models will be used to make prediction for the new sample. In other word, Each classifier C_i or regressor R_i returns its prediction.

Bagging (Bootstrap Aggregation)

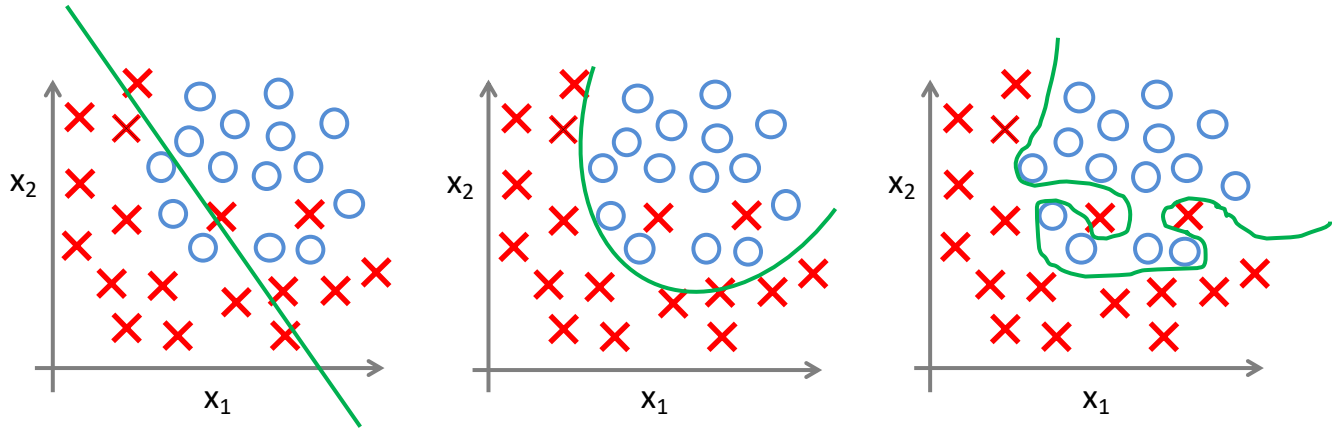
- **Step4: Combining the results:**
  - For Classification, we use **Voting** method. The final prediction is based on the majority vote of the **L** classifiers.
  - For Regression, we use **Averaging** method. The final prediction is the average of L predictions.
  - For Regression, depending on the application, sometimes we may prefer to use **Median** rather than average to get rid of outliers.

Bagging (Bootstrap Aggregation)



Important Notes

- For any machine learning method, there are two main sources of error:
  - **Bias**: Expected error due to inaccurate model in the learning algorithm that may cause to miss the relations between features and outputs (**underfit model**).
  - **Variance**: Expected error due to particular training sets, and high sensitivity of the system to small fluctuations in the training set (**overfit models**).



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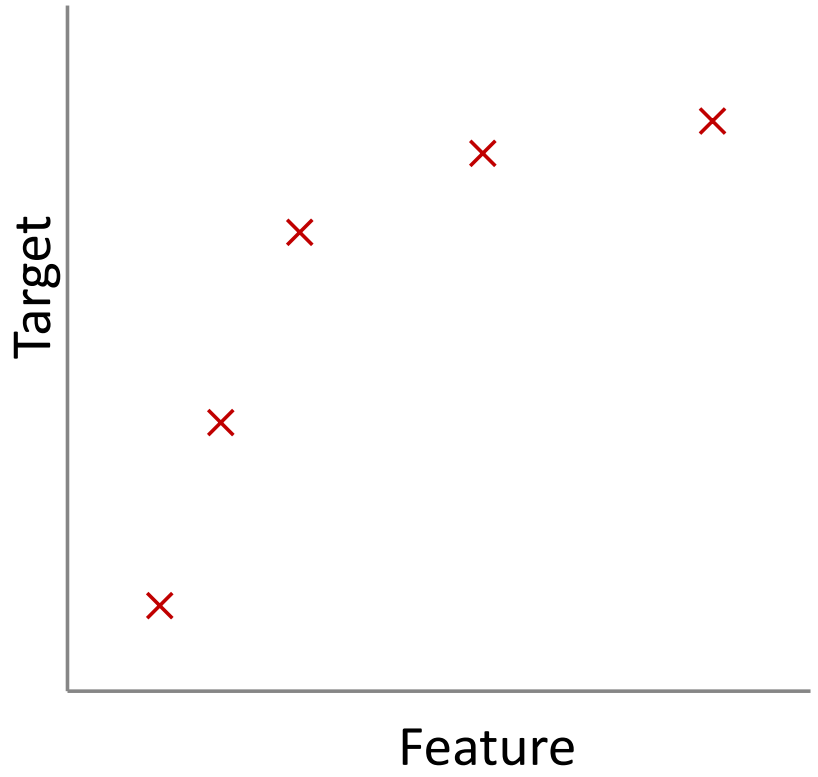
- Bagging works because it **reduces variance**. In other word, we don't suffer from random errors made by a single classifier. Thus, it is a good approach **to deal with overfitting**.

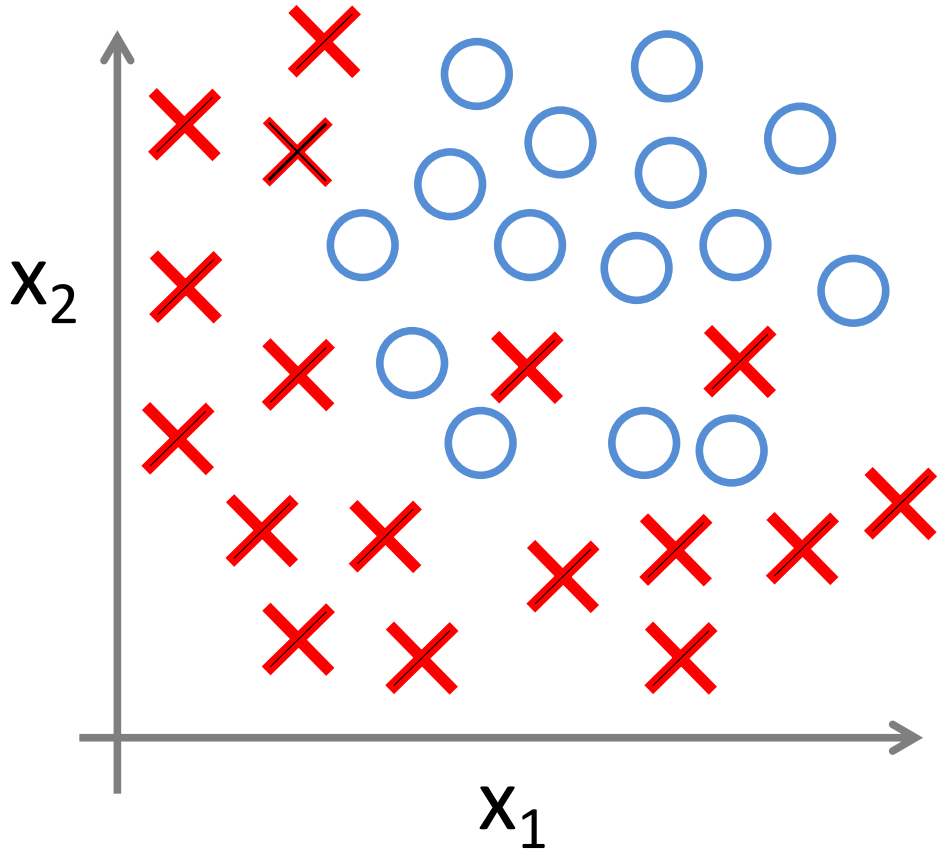
Important Notes

- Bagging has the best performance when the Learning Algorithm is **unstable (high variance)**: if small changes to the training set cause large changes in the prediction results.
  - Some candidates for Bagging: Decision Tree, Neural Networks, Linear Regression.

- In some rare cases, when the learning algorithm is **very stable** (low variance), Bagging may degrade the accuracy. But, it is easy to find out and avoid it.

How Can Bagging Resolve Overfitting?





Final Project!

Final Project!

- **Step 0:** Find your teammates! **3-5 students can team up** (if you *really* have difficulties in finding teammates, let me know!).
- **Step 1:** You have this option to select your own project. However, the TA should approve it!
  - A great source including hundreds of interesting projects is www.kaggle.com. Feel free to visit this website and pick one of the projects. Make sure that you select a doable project w.r.t the time and due dates!
- **Step 2:** The team should see the TA (**time/location: TBA on CSNS**) to describe the project details and get your project confirmed **(Due Date: Fri, Feb. 15)**.
- **Step 3:** Design your own project plan and schedule, assign the tasks to team members, and start the project!

Next

Final Project!

- **Step 4:** Make sure that the team have meetings on timely basis (e.g. weekly meetings) to evaluate the project progress! Don't leave everything for last days!
- **Step 5:** By end of the semester, each team should **either** give a 10 min presentation to the class, **or** come to my office to present their results, describe their project, the developed methods and algorithms, and the RESULTS (As time permits!).
- **Step 6:** By end of the semester, Each team should submit a **project report** including project details, the developed methods, algorithms, and codes to address the projects requirements, and the responsibility of EACH TEAM MEMBER. A big part of your grade depends on the quality of your report!

Next

Final Project: Some Tips!

- **AN IMPORTANT RECOMMENDATION:** Select a project that sounds **interesting, exciting** and **fun** to you, NOT something that looks just easy to do! Let's enjoy this project and this class. I don't expect you to get "record breaking" results! I just care about your effort and how you deal with challenges! So, try to work on an exciting project that pleases you, try to have a lot of fun, and enjoy your work!

- The due dates for report and presentation will be announced later.
- Your work including algorithms, codes, and reports **must be your original work!** The teams are not allowed to use other people's work from kaggle website or any other resources!
- Some of the outstanding class projects can form the basis of future **paper publications**. Let me know if you are interested in such an opportunity!

Thank You!

Questions?