Dauphine UNIVERSITÉ PARIS | PSL

→ COMPUTER SCIENCE, DECISION-MAKING, AND DATA

Algorithmic and advanced Programming in Python

Eric Benhamou eric.benhamou@dauphine.eu
Remy Belmonte remy.belmonte@dauphine.eu

Masterclass 8

Outline

1. Introduction to Ensemble
2. Bagging
3. Boosting
4. Discussion around XGBoost and LightGBM

Reminder of the objective of this course

- People often learn about data structures out of context
- But in this course you will learn foundational concepts by building a real application with python and Flask

- To learn the ins and outs of the essential data structure, experiencing in practice has proved to be a much more powerful way to learn data structures

Reminder of previous session

In Master class 7, we discuss about graph traversal

Question: can you summarize the various algorithms seen?

Three major sections for classification

- We can divide the large variety of classification approaches into roughly three major types

1. Discriminative
   directly estimate a decision rule/boundary
   e.g., support vector machine, decision tree, logistic regression,
   e.g. neural networks (NN), deep NN

2. Generative:
   build a generative statistical model
   e.g., Bayesian networks, Naïve Bayes classifier

3. Instance based classifiers
   - Use observation directly (no models)
   - e.g. K nearest neighbors

Ensemble methods principle

In statistics and machine learning, **ensemble methods** use
- multiple learning algorithms
- to obtain better predictive performance than could be obtained from any of the constituent learning algorithms alone.

Its core principle: Together is better than alone as the majority vote cannot go wrong. Averaging over multiple experts should give a better answer!

Three major sections for classification

- We can divide the large variety of classification approaches into roughly three major types

1. Discriminative
   directly estimate a decision rule/boundary
   e.g., support vector machine, decision tree, logistic regression,
   e.g. neural networks (NN), deep NN

2. Generative:
   build a generative statistical model
   e.g., Bayesian networks, Naïve Bayes classifier

3. Instance based classifiers
   - Use observation directly (no models)
   - e.g. K nearest neighbors

Ensemble Core principles

- Framework of Ensemble:
  - 1. Get a set of classifiers $f_1(x), f_2(x), f_3(x), \ldots\ldots$

    They should be diverse.

    How to have different training data sets
    - Re-sampling your training data to form a new set
    - Re-weighting your training data to form a new set

  - 2. Aggregate the classifiers (*properly*)

The different type of Ensemble methods

- Bagging — reduce Variance
  - Bagged Decision Tree
  - Random forests:
- Boosting — reduce bias, reduce variance
  - Adaboost
  - Xgboost — Gradient Boosting
- Stacking

Bagging

- Bagging or *bootstrap aggregation*
  - a technique for reducing the variance of an estimated prediction function.

- For instance, for classification, a *committee* of decision trees
  - Each tree casts a vote for the predicted class.

Bootstrap

The basic idea:

randomly draw datasets *with replacement (i.e. allows duplicates)* from the training data, each samples *the same size as the original training set*

$f_1, f_2 \dots, f_B$ $\#|Tr|$

① change training set $\{S_1, S_2, \dots, S_B\}$

With Replacement

- Bootstrap with replacement can keep the sampling size the same as the original size for every repeated sampling. The sampled data groups are independent on each other.

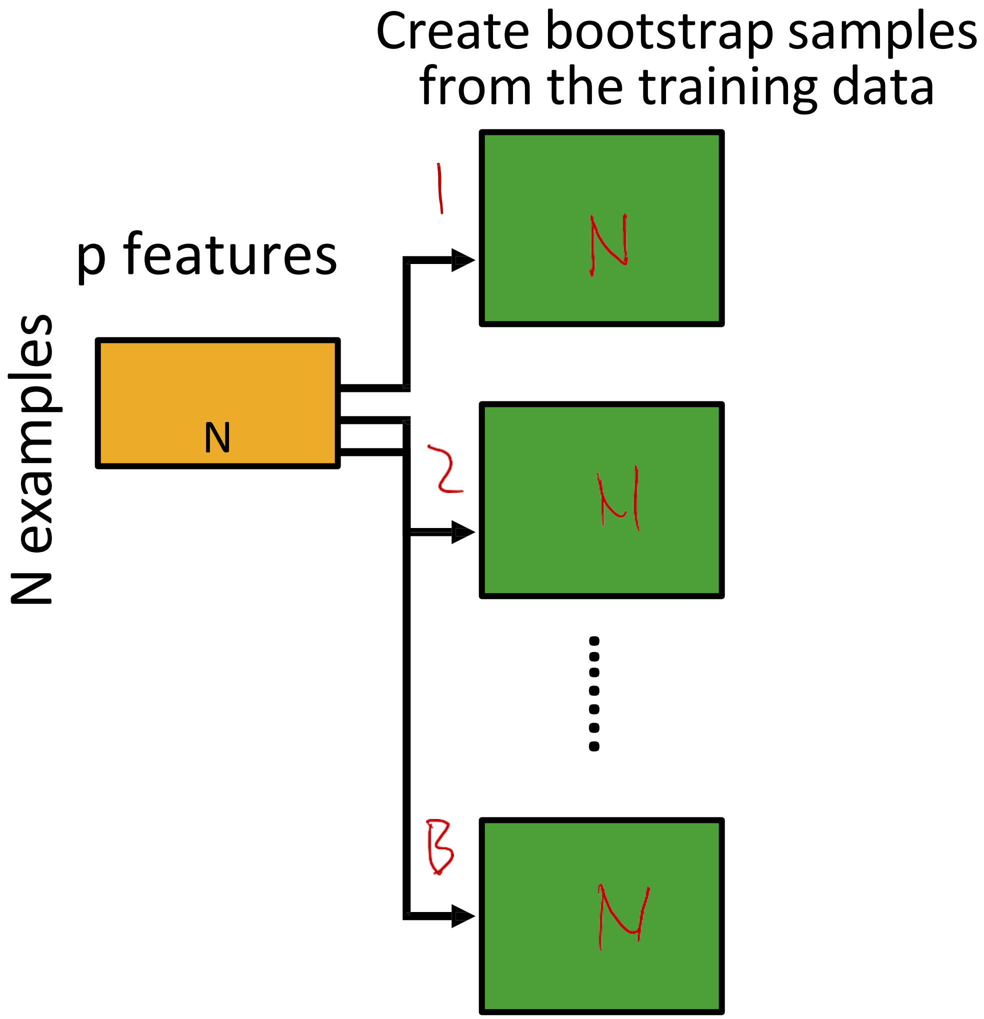
$S_1, S_2, \cdots, S_B$

Or Without Replacement

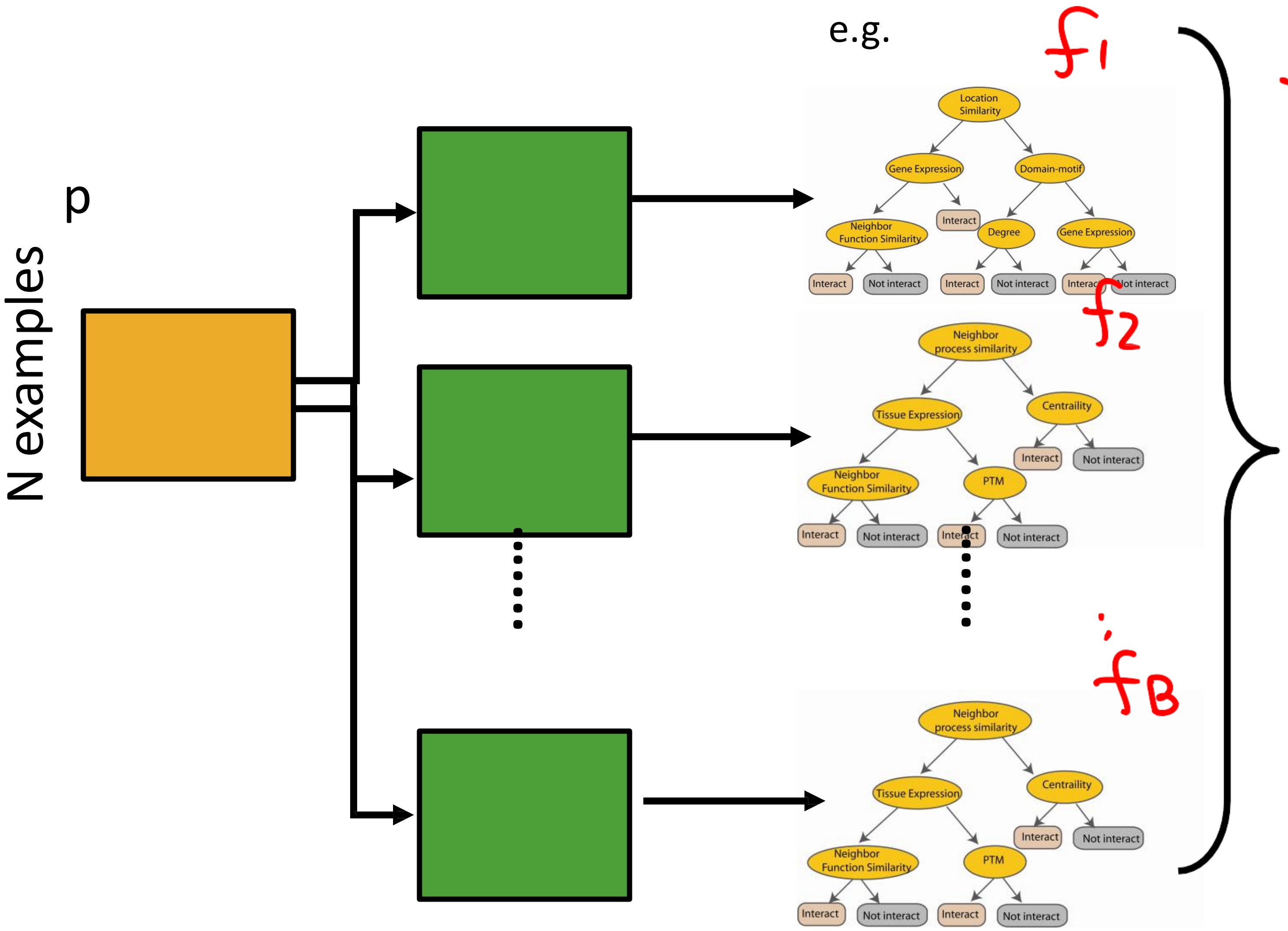
- Bootstrap without replacement cannot keep the sampling size the same as the original size for every repeated sampling. The sampled data groups are dependent on each other.

$S_1, S_2, \dots, S_B$

Bagging with simple graphs



Bagging of DT Classifiers

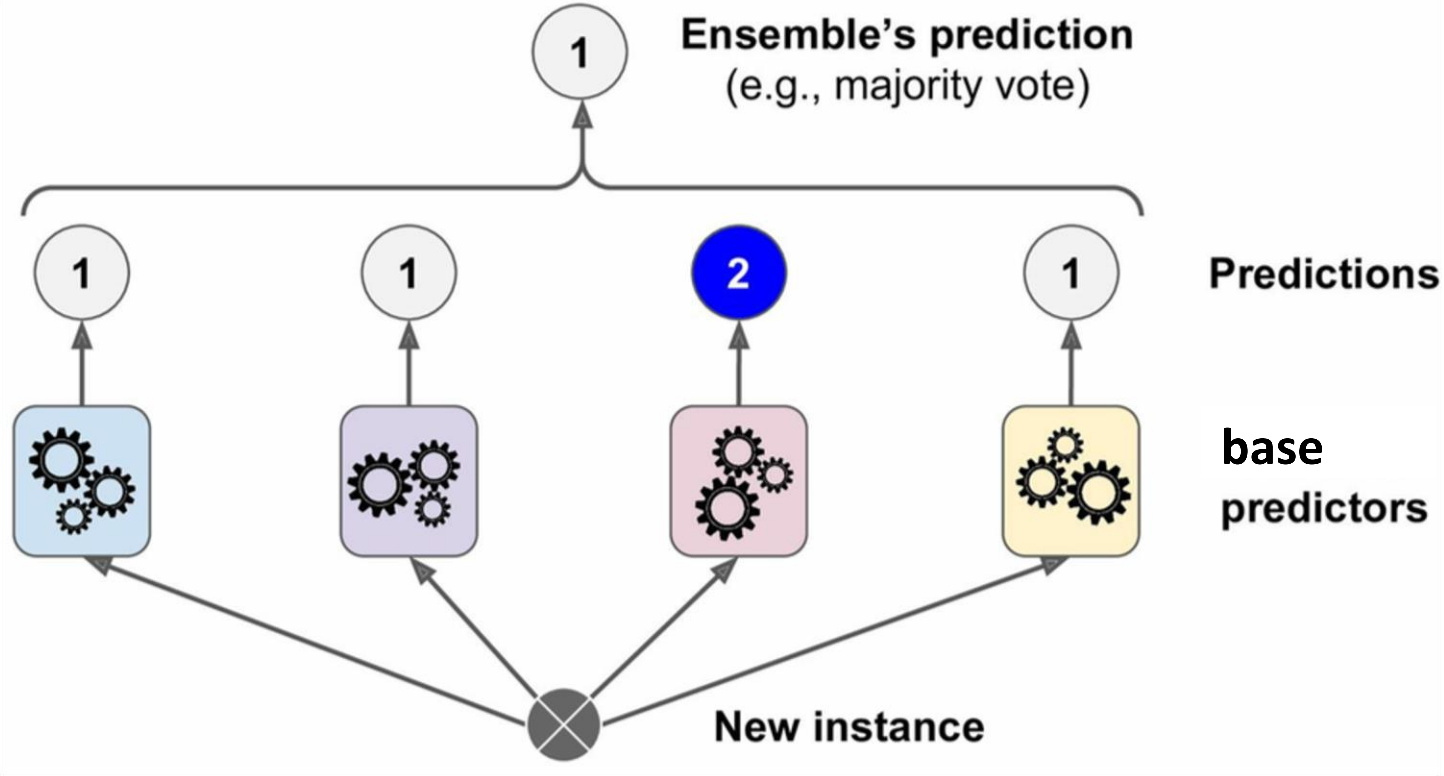


$$f_E = \frac{1}{B}\sum_{i=1}^{B} f_i$$

Take the majority vote

i.e. Refit the model to each bootstrap dataset, and then examine the behavior over the B replications.

E.g., Predict by Hard voting



Decision Boundary Comparison

$Var(f_i)$ vs $Var\left(\frac{1}{B}\sum_{i=1}^{B} f_i\right)$

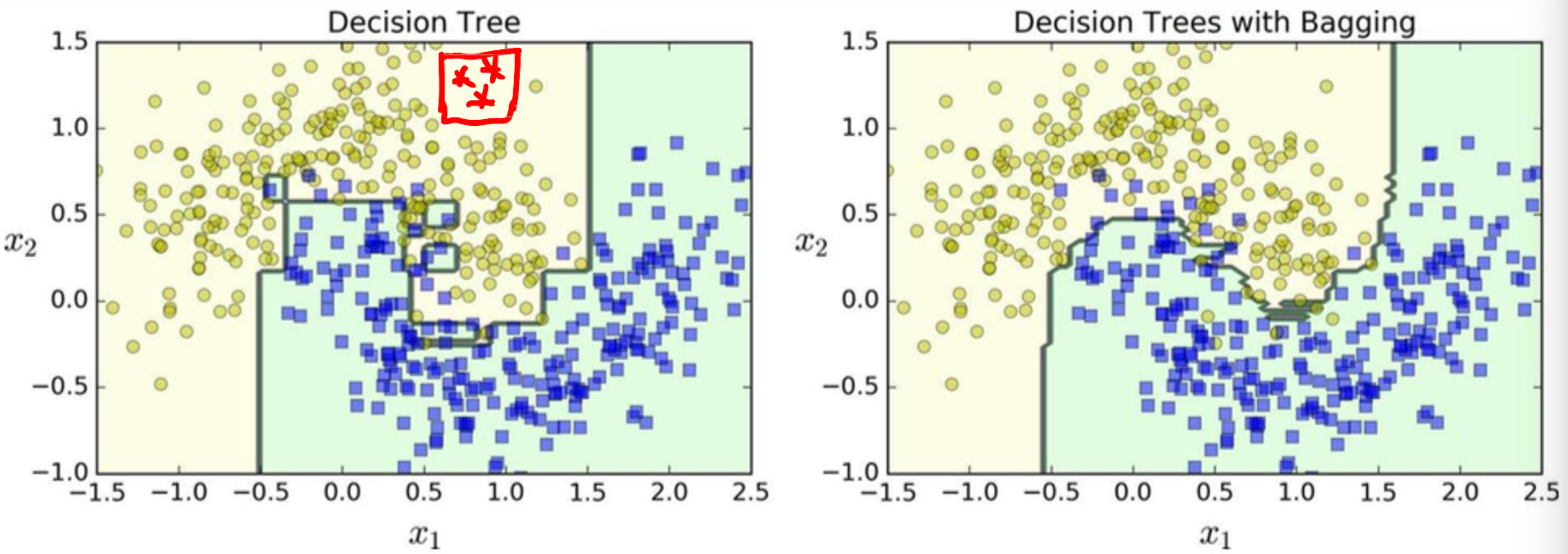
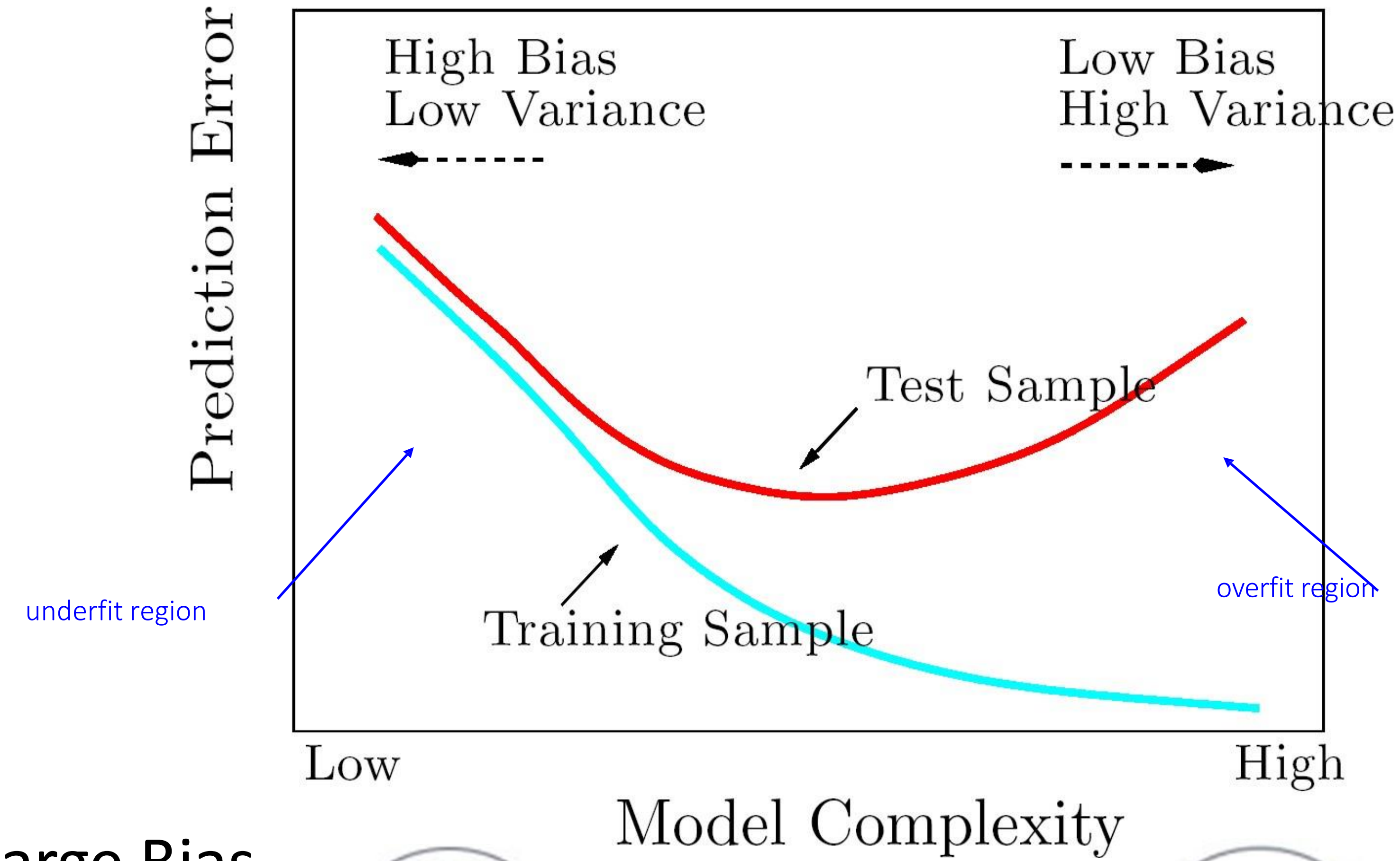


Figure 7-5. A single Decision Tree versus a bagging ensemble of 500 trees

Peculiarities of Bagging

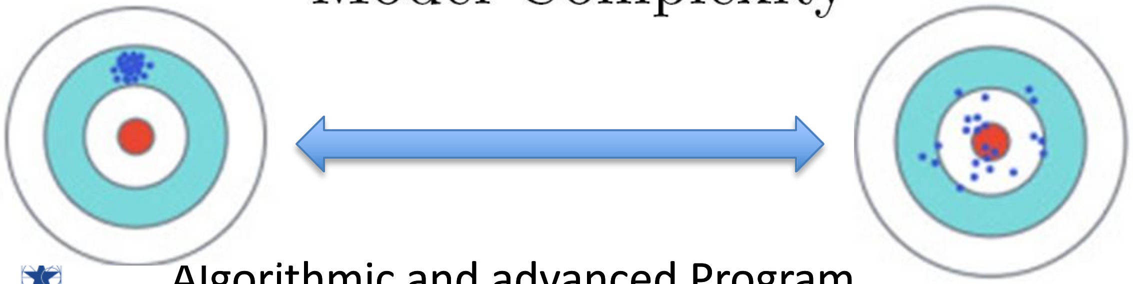
- Model Instability is good when bagging
  - The more variable (unstable) the basic model is, the more improvement can potentially be obtained
  - Low-Variability methods (e.g. LDA) improve less than High-Variability methods (e.g. decision trees)

Bias-Variance Tradeoff / Model Selection



Large Bias

Small Variance

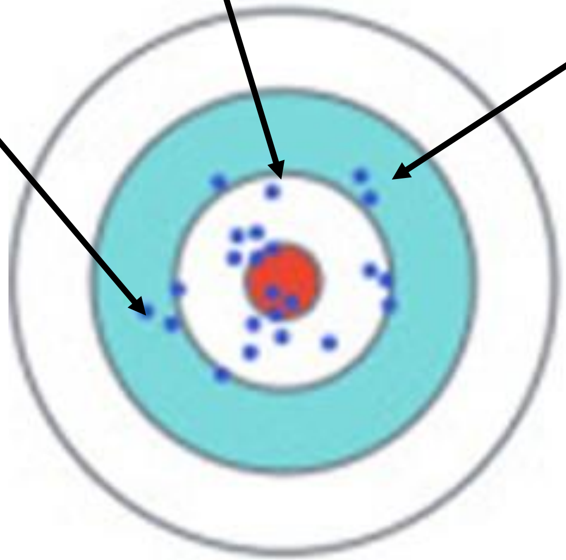


Small Bias Large Variance

In details

classifiers $f_1(x)$, $f_2(x)$, $f_3(x)$, …… $f_B(x)$

S_1 S_2 S_B



A complex model have large variance.

We can average complex models to reduce variance.

If we average all the f_i, is it close to f^*

$$E[f] = f^*$$

Algorithmic and advanced Programming in Python

$$\mathrm{Var}(aX + bY) = a^2\mathrm{Var}(X) + b^2\mathrm{Var}(Y) + 2ab\mathrm{Cov}(X, Y)$$

when $Cov(f_i, f_j) = 0$

$$Var(\hat{f}) = E((\hat{f} - \bar{f})^2) = Var(\frac{1}{B}\sum \hat{f}_i) = \frac{1}{B^2}\sum_{i=1}^{B} Var\ \hat{f}_i \quad (\ ) =$$

Base classifiers $f_1(x)$, $f_2(x)$, $f_3(x)$, …… $f_B(x)$

$$Var(\hat{f}) = Var\left(\frac{1}{B}\sum_{i=1}^{B}\hat{f}_i\right)$$

when $\forall i,j,\ Cov(f_i, f_j) = 0$

$$= \frac{1}{B^2}\sum_{i=1}^{B} Var(f_i)$$

, Because $|S_1| = |S_2| = \dots = |S_B|$

$$= \frac{1}{B} Var(f_i)$$

, $Var(f_i) \simeq Var(f_j)$

EXTRA

Bagging : an extreme case study using simulated data (with correlated features)

N = 300 training samples, $y \in \{0, 1\}$, $X_1, X_2, \dots, X_5$

Y: Two classes and X: p = 5 features,

Each feature N(0, 1) distribution and pairwise correlation .95

Response Y: generated according to:

$$\Pr(Y = 1 | x_1 \le 0.5) = 0.2 \qquad \Pr(Y = 1 | x_1 > 0.5) = 0.8$$

$y=0$ $y=1$

X_1

0.5

Test sample size of 2000

Fit classification trees to training set and bootstrap samples

B = 200

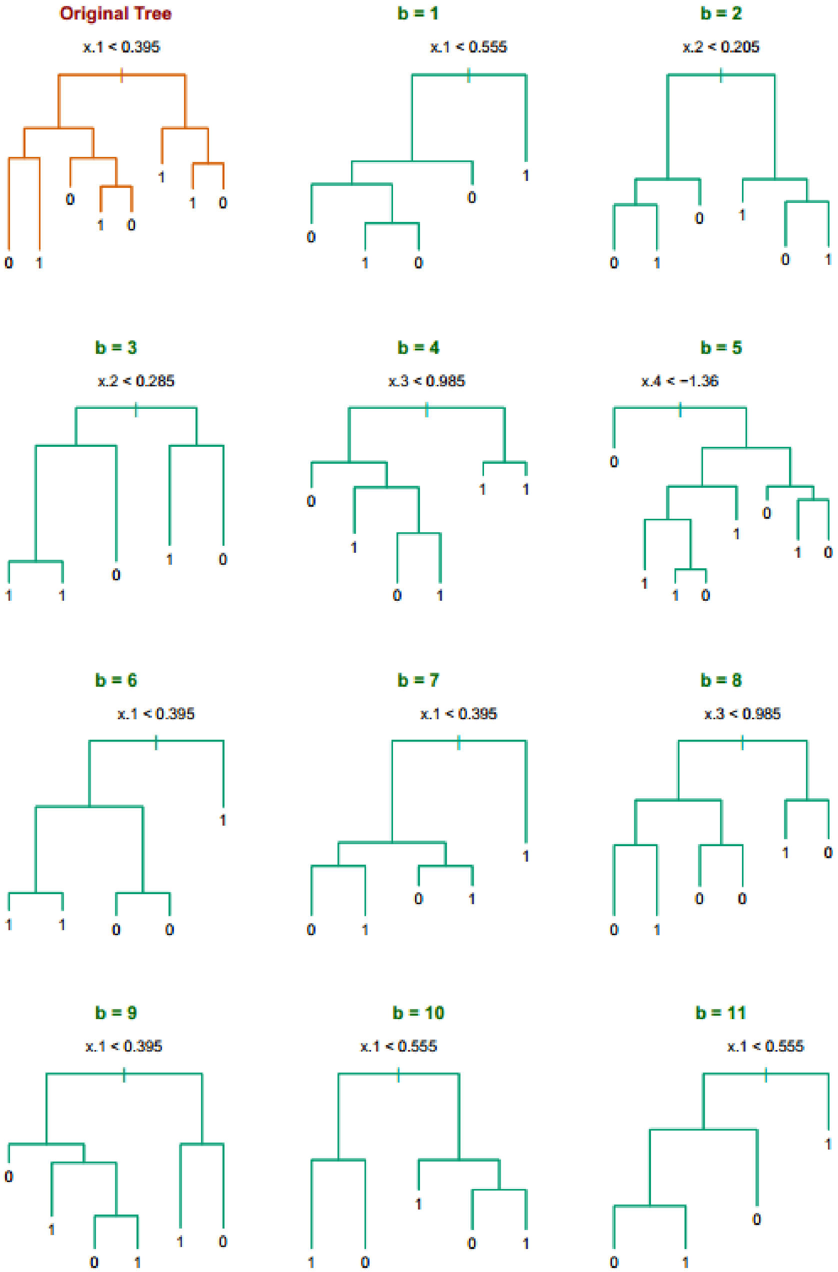
Notice the bootstrap trees look quite different from the original tree

$f_1(x)$

$f_2(x)$

$\vdots$

$f_B(x)$



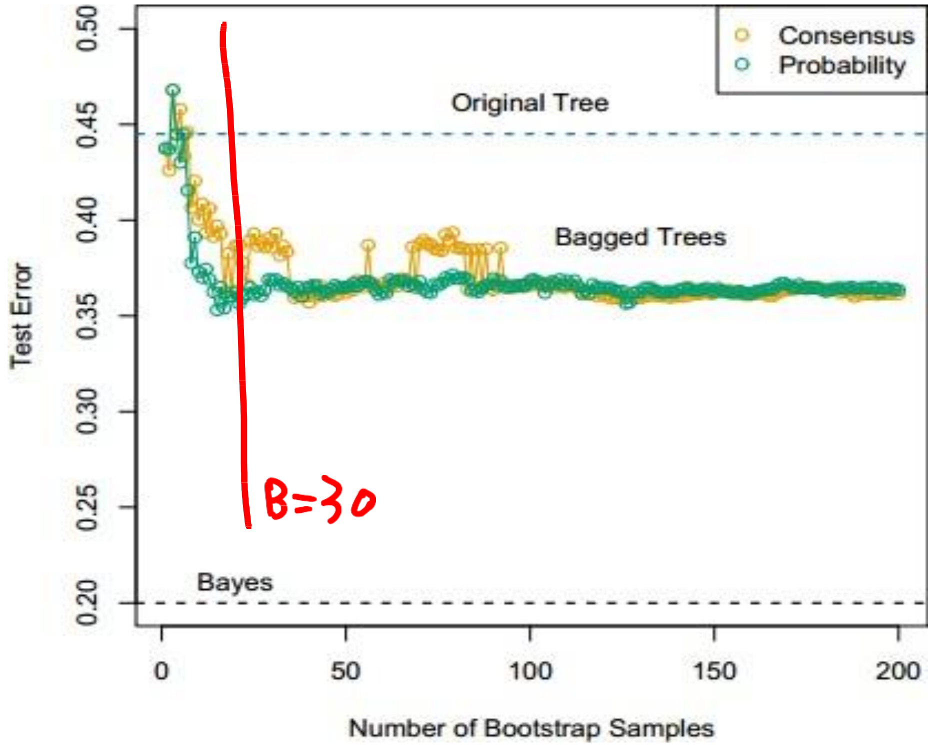
Five features highly correlated with each other

→ No clear difference with picking up which feature to split

→ Small changes in the training set will result in different tree

→ But these trees are actually quite similar wrt output classification

For B>30, more trees do not improve the bagging results



➔ Since the trees correlate highly to each other and give similar classifications

B $Var\left(\frac{1}{B}\sum f_i\right)$

Consensus: Majority vote

Probability: Average distribution at terminal nodes

Bagging

- Slightly increases model complexity
  - Cannot help when greater enlargement of model diversity is needed

- Bagged trees are correlated
  - Use random forest to reduce correlation between trees

$$\mathrm{Var}(aX + bY) = a^2\mathrm{Var}(X) + b^2\mathrm{Var}(Y) + \underline{2ab\mathrm{Cov}(X, Y)}$$

Bagged Decision Tree

Data
↓
Task
↓
Representation
↓
Score Function
↓
Search/Optimization
↓
Models, Parameters

Tabular
↓
Classification / Regression
↓
multiple (almost) full decision trees / bootstrap samples
↓
Split with Purity measure / e.g. IG / cross-entropy / Gini /
↓
Greedy like Decision Tree (e.g. GINI)
↓
Multiple Tree Model (s), i.e. space partition

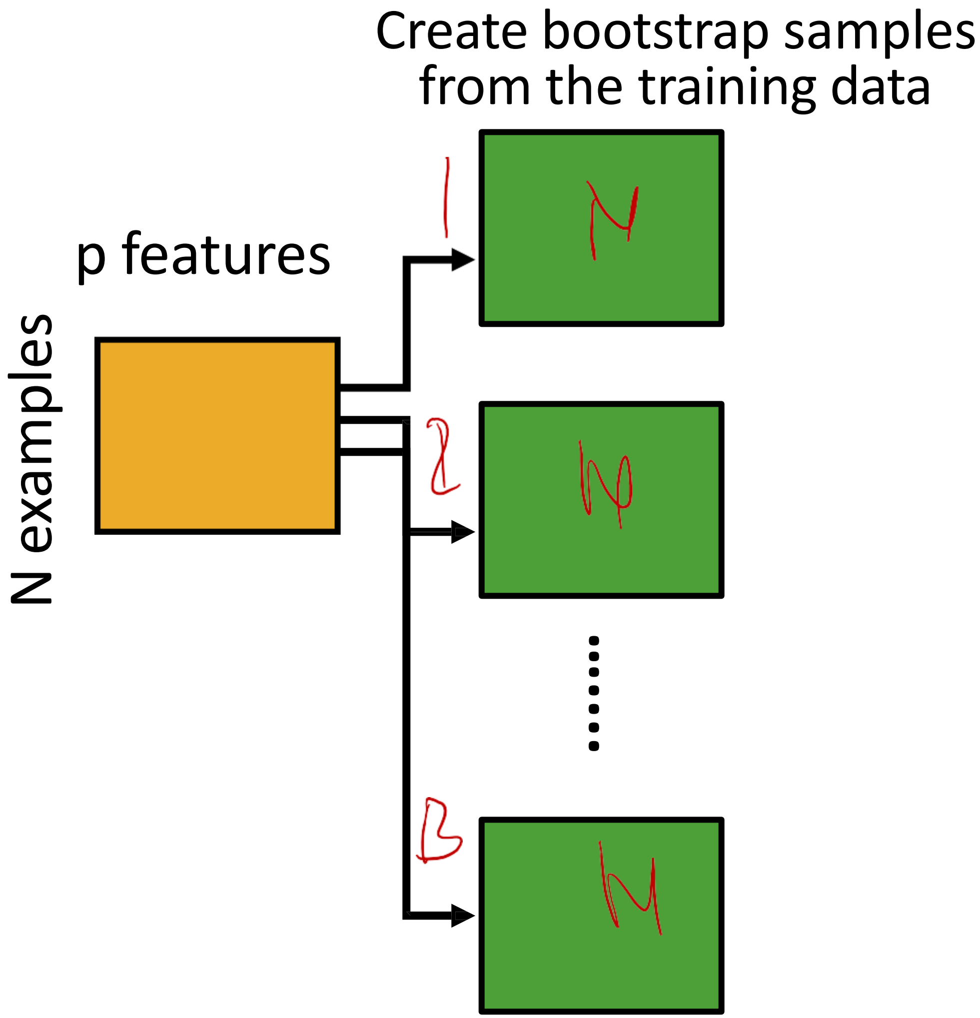
Let us discuss random forest

- Bagging
  - Bagged Decision Tree
  - Random forests
- Boosting
  - Adaboost
  - Xgboost
- Stacking

Random forest classifier

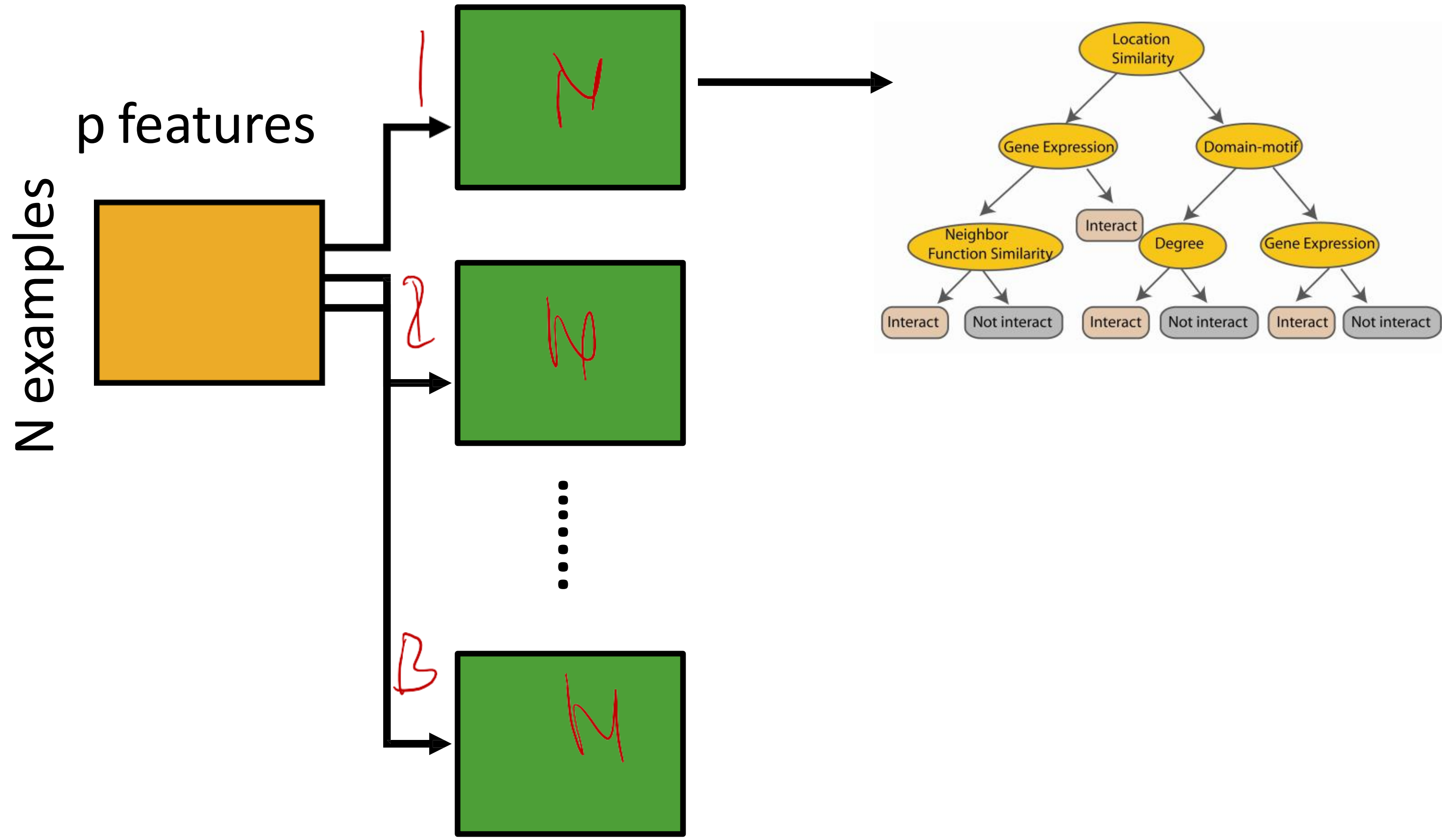
- Random forest classifier,
  - an extension to bagging
  - which uses *de-correlated* trees.

Random Forest Classifier



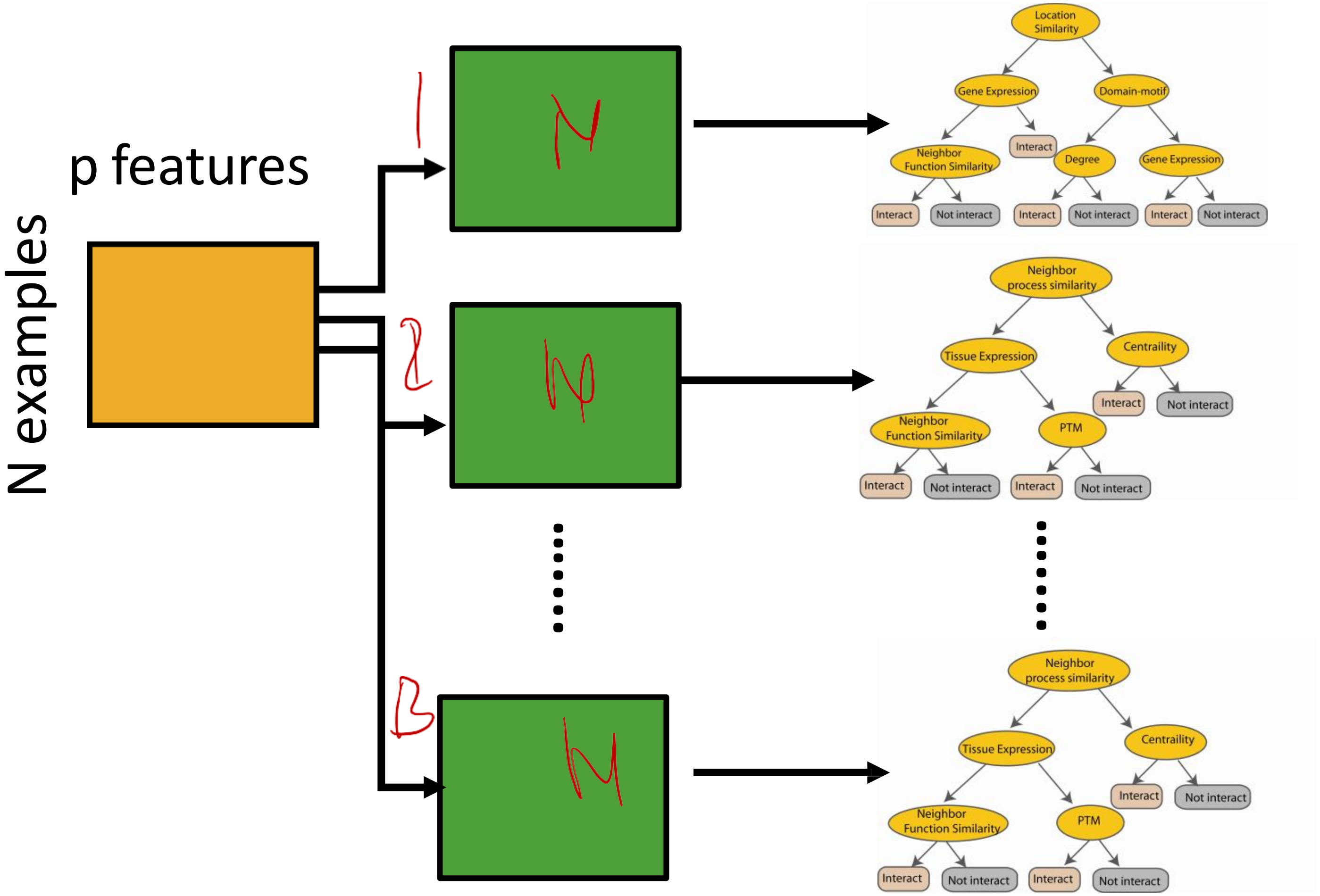
Random Forest Classifier

At each node when choosing the split feature
choose only among *m<p* features

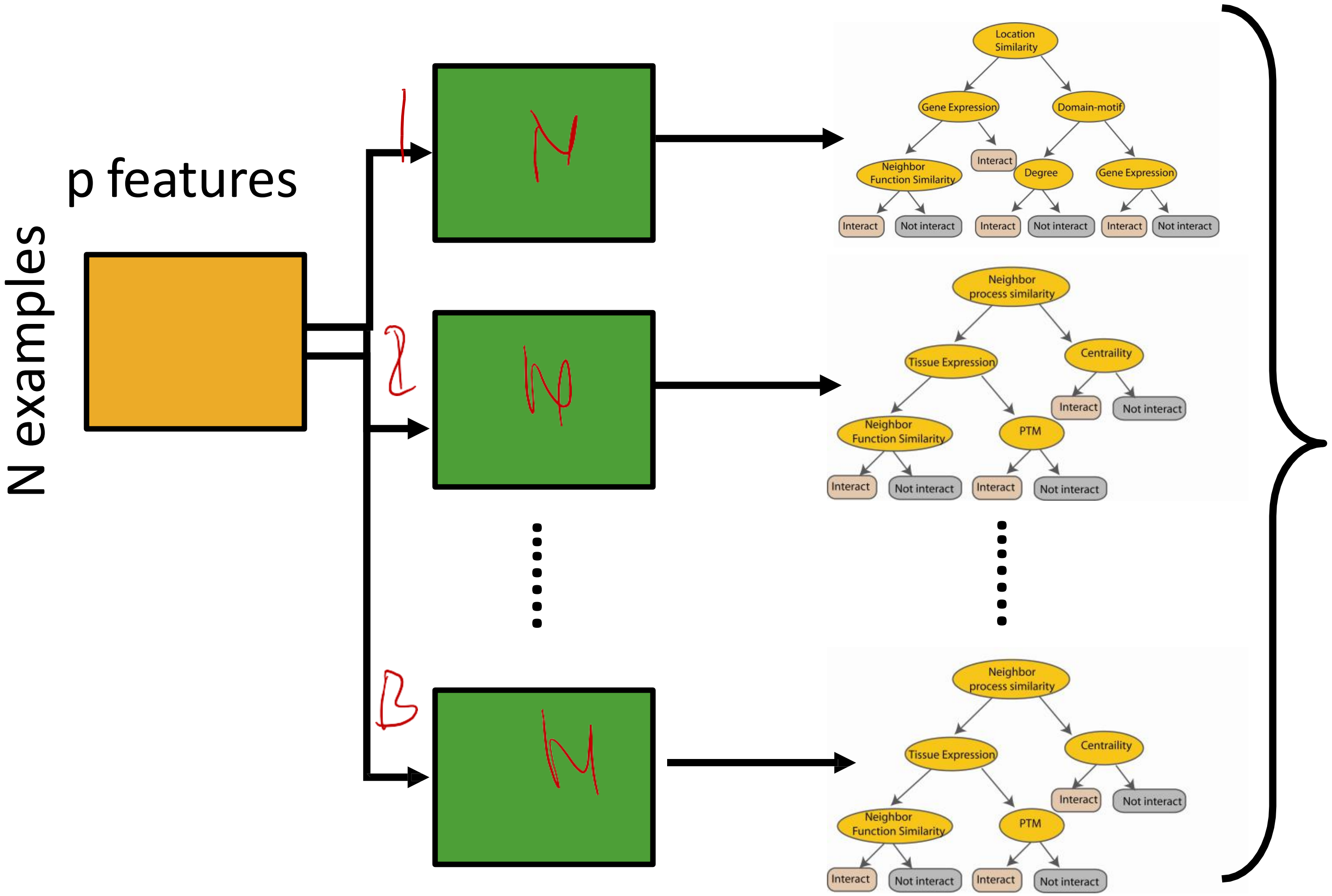


Random Forest Classifier

Create decision tree
from each bootstrap sample



Random Forest Classifier



Take he majority vote

Random Forests

For each of our *B* bootstrap samples

Form a tree in the following manner

i: Given *p* dimensions, pick *m* of them

ii: Split only according to these *m* dimensions

(we will NOT consider the other *p*-*m* dimensions)

Repeat the above steps i & ii for each split

Note: we pick a different set of *m* dimensions for each split on a single tree

$\rho = 0,06$

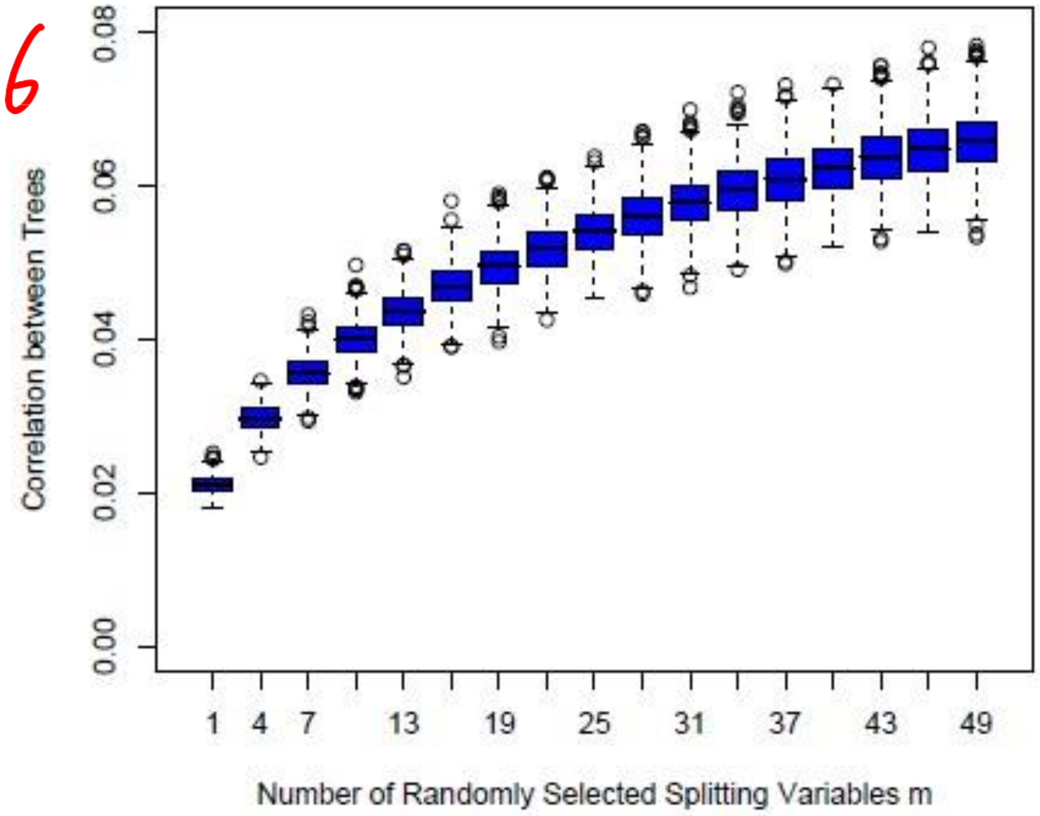


FIGURE 15.9. *Correlations between pairs of trees drawn by a random-forest regression algorithm, as a function of m. The boxplots represent the correlations at 600 randomly chosen prediction points x.*

Page 598-599 In ESL book

Random Forests

Random forest can be viewed as a refinement of bagging with a tweak of **decorrelating** the trees:

At each tree split, a random subset of **m** features out of all **p** features is drawn to be considered for splitting

Some guidelines provided by Breiman, but be careful to choose m based on specific problem:

m = p   amounts to bagging

m = p/3 or log2(p)   for regression

m = sqrt(p)   for classification

Why correlated trees are not ideal ?

Random Forests try to reduce correlation between the trees.

Why?

Why correlated trees are not ideal ?

Assuming each tree has variance σ^2

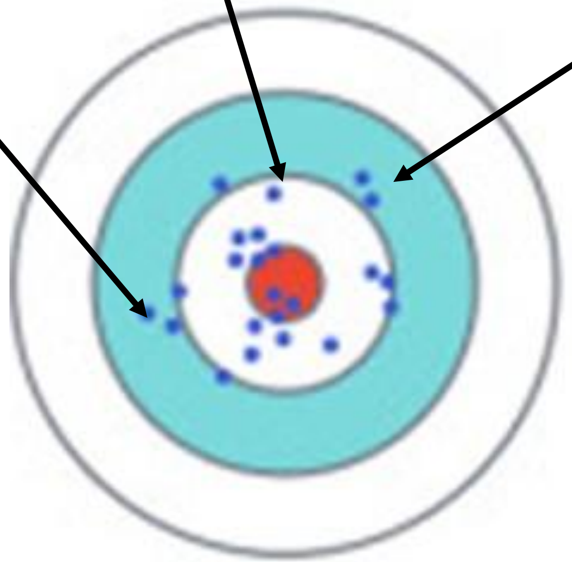
If trees are independently identically distributed, then average variance is σ^2/B

$$\mathrm{Var}(aX + bY) = a^2\mathrm{Var}(X) + b^2\mathrm{Var}(Y) + 2ab\mathrm{Cov}(X, Y)$$

$$Var(\bar{f}) = E((\bar{f} - f\$^{2}) = Var(\frac{1}{B}2\ \bar{f}_i) = \frac{1}{B^2}2\ \overbrace{Var\ \bar{f}_i}^{B\sigma^2} = \frac{1}{B}\sigma^2$$

classifiers $f_1(x)$, $f_\$(x)$, $f_3(x)$, ... $f_B(x)$

A complex model will have large variance.



If we average all the f_i, is it close to f^*

$$E[\bar{f}] = f^*$$

We can average complex models to reduce variance

Why correlated trees are not ideal ?

Assuming each tree has variance σ^2

If simply identically distributed, then average variance is

$\rho_{ij} = \mathrm{Corr}(f_i, f_j) = \rho$

$$\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2$$

As B → ∞, second term → 0

Thus, the pairwise correlation always affects the variance

Why correlated trees are not ideal ?

Assuming each tree has variance σ^2

If simply identically distributed, then average variance is

$$\Rightarrow \rho\sigma^2 + \cancel{\frac{1-\rho}{B}}\sigma^2$$

RAM $\times B$
trainTim $\times B$
testTime $\times B$

As B → ∞, second term → 0

Thus, the pairwise correlation always affects the variance

Why correlated trees are not ideal ?

How to deal?

If we reduce *m* (the number of dimensions we actually consider in each splitting),

then we reduce the pairwise tree correlation

Thus, variance will be reduced.

More about Random Forests

1. Construct subset $(x_1^*, y_1^*), \ldots, (x_n^*, y_n^*)$ by sampling original training set with replacement.
2. Build tree-structured learners $h(x, \Theta_k)$, where at each node, m predictors at random are selected before finding the best split.
   - Gini Criterion.
   - No pruning.
3. Combine the predictions (average or majority vote) to get the final result.

Random Forest

Task
↓
Representation
↓
Score Function
↓
Search/Optimization
↓
Models, Parameters

Classification / Regression
↓
multiple (almost) full decision trees / bootstrap samples / sample features
↓
Split with Purity measure / e.g. IG / cross-entropy / Gini /
↓
Greedy like Decision Tree (e.g. GINI)
↓
Multiple Tree Model (s), i.e. space partition

Let us discuss Boosting

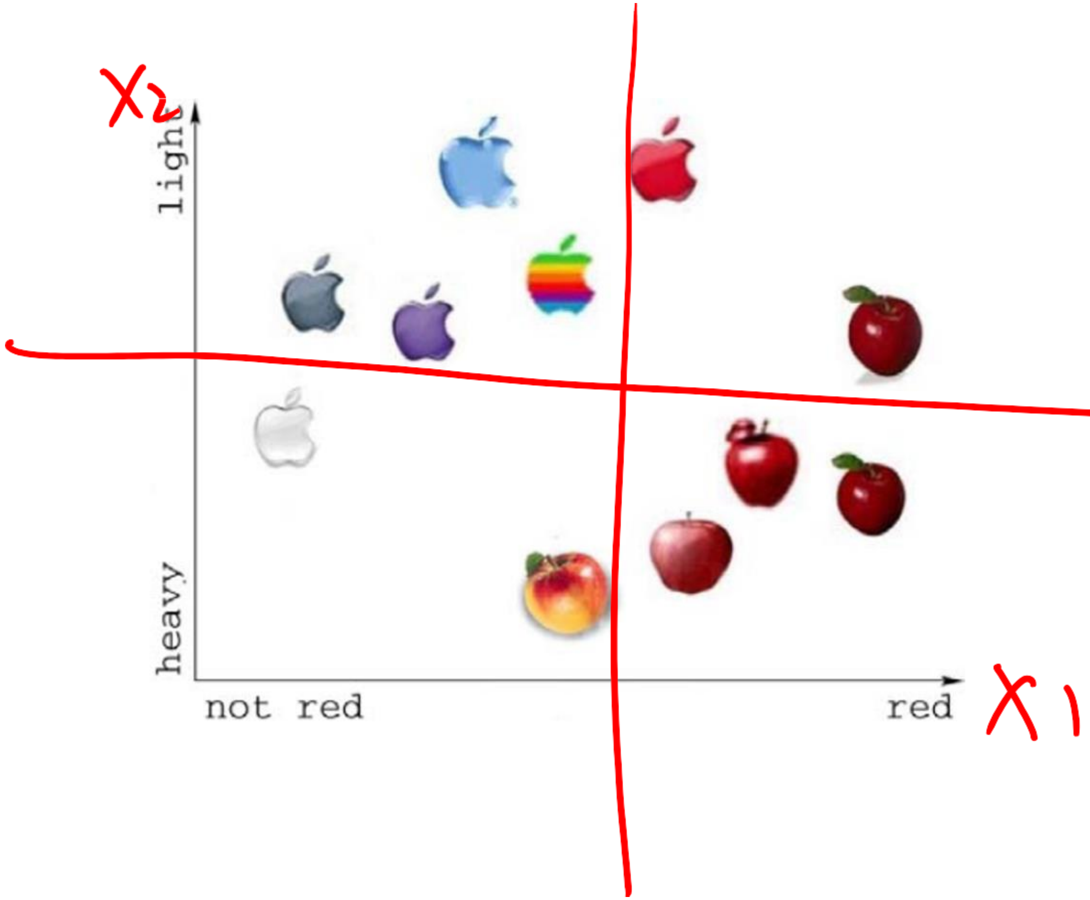
- Bagging
  - Bagged Decision Tree
  - Random forests:
- Boosting
  - Adaboost
  - Xgboost
- Stacking

Boosting Strategies

base learners : shallow DT
High bias

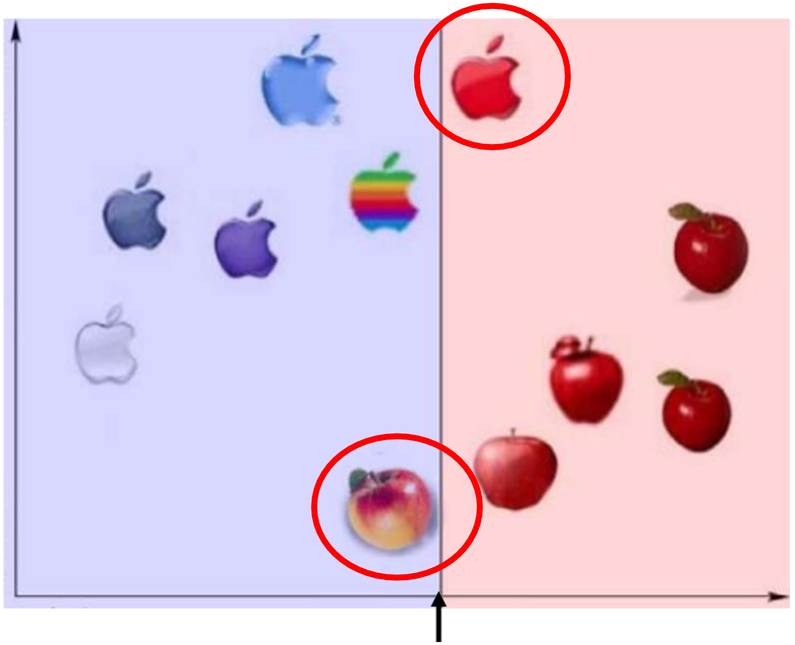
1. Have many rules (base classifiers) to **vote** on the decision
2. Sequentially train base classifiers that **corrects** mistakes of previous → focus on **hard** examples
3. Give higher **weight** to better rules

- Recognizing apples:
- (1) Collect a set of real apples and plastic apples
- (2) Observe some rules to tell them apart based on their characteristics



1. Have many rules (base classifiers) to vote on the decision

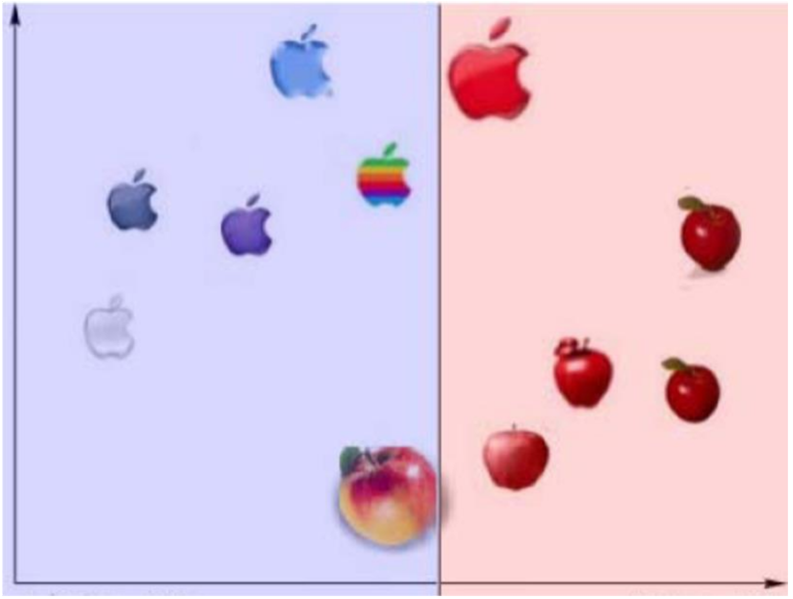
2. Sequentially train base classifiers that **corrects** mistakes of previous → focus on **hard** examples
3. Give higher **weight** to better rules



1st Simple Rule

1. Have many rules (base classifiers) to vote on the decision

2. Sequentially train base classifiers that **corrects** mistakes of previous → focus on **hard** examples
3. Give higher **weight** to better rules



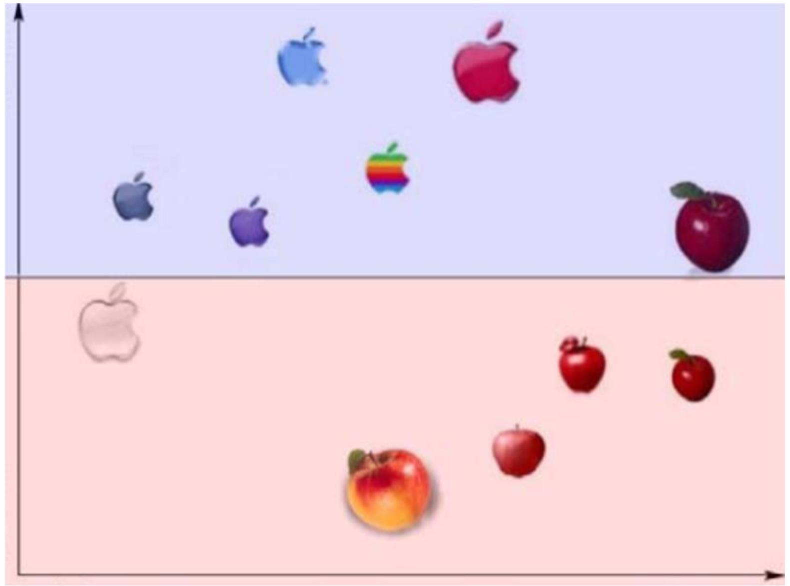
1. Have many rules (base classifiers) to vote on the decision

2. Sequentially train base classifiers that **corrects** mistakes of previous → focus on **hard** examples
3. Give higher **weight** to better rules

2nd Rule

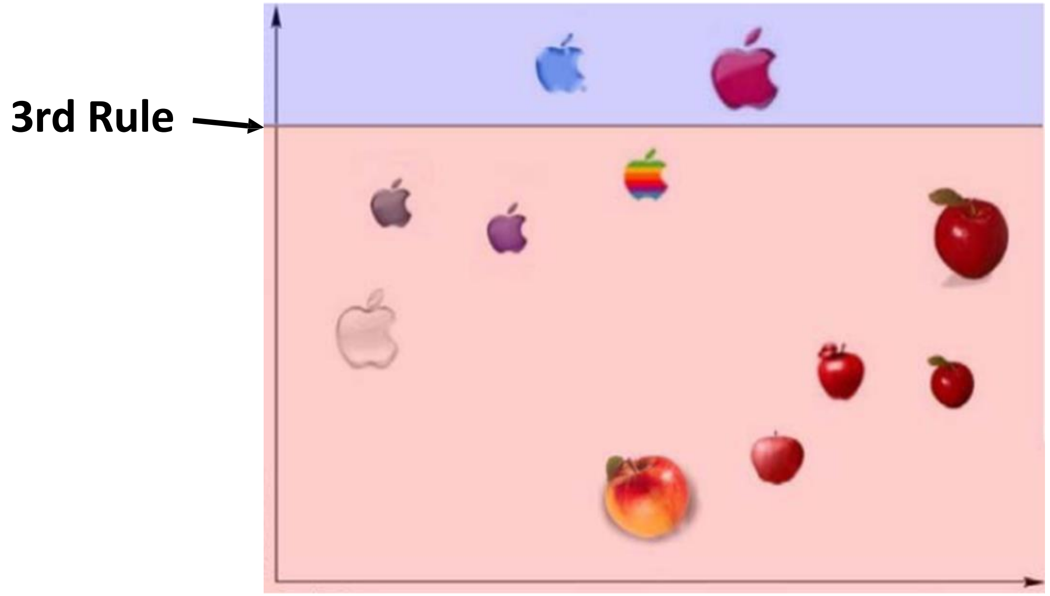
1. Have many rules (base classifiers) to vote on the decision

2. Sequentially train base classifiers that **corrects** mistakes of previous → focus on **hard** examples
3. Give higher **weight** to better rules



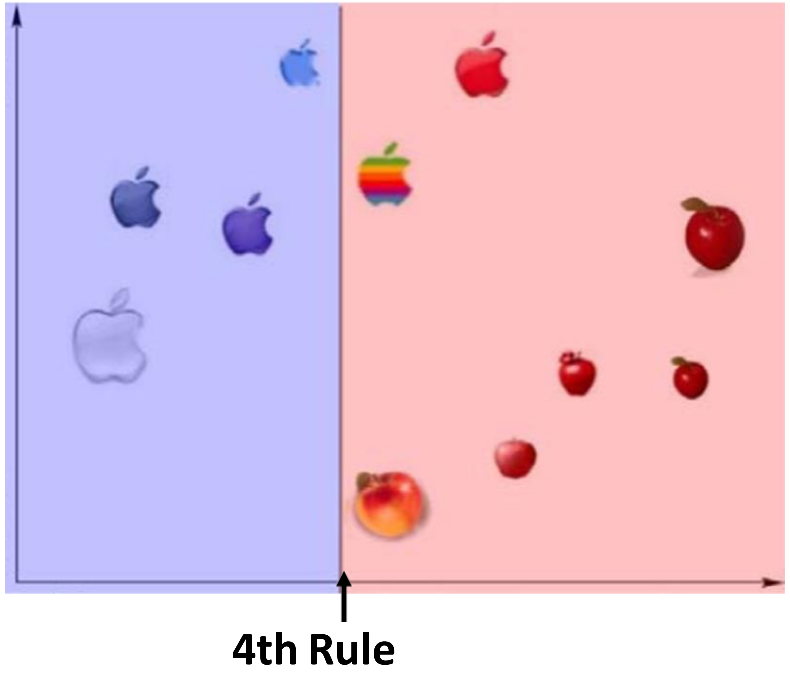
1. Have many rules (base classifiers) to vote on the decision

2. Sequentially train base classifiers that **corrects** mistakes of previous → focus on **hard** examples
3. Give higher **weight** to better rules



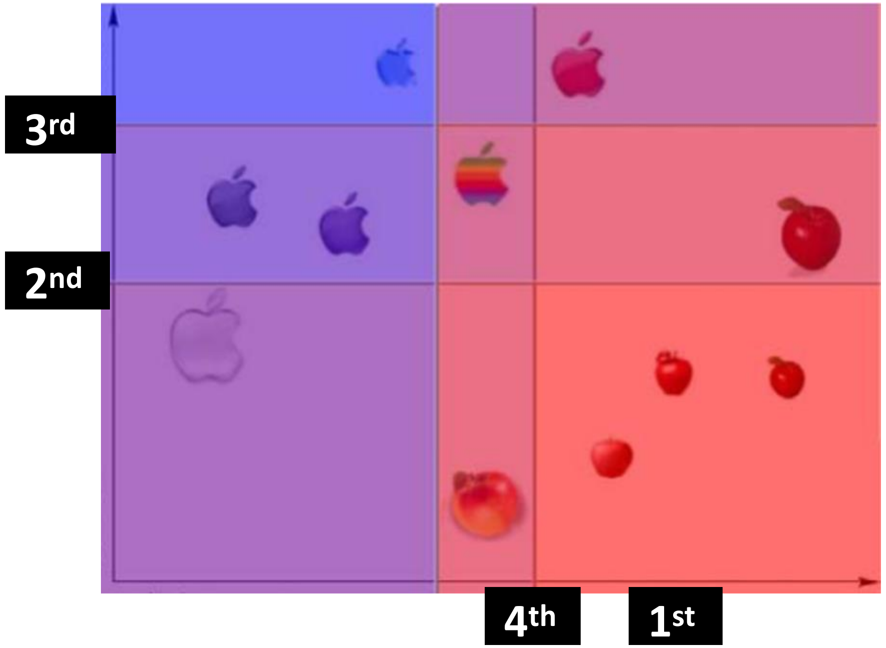
1. Have many rules (base classifiers) to vote on the decision

2. Sequentially train base classifiers that **corrects** mistakes of previous → focus on **hard** examples
3. Give higher **weight** to better rules



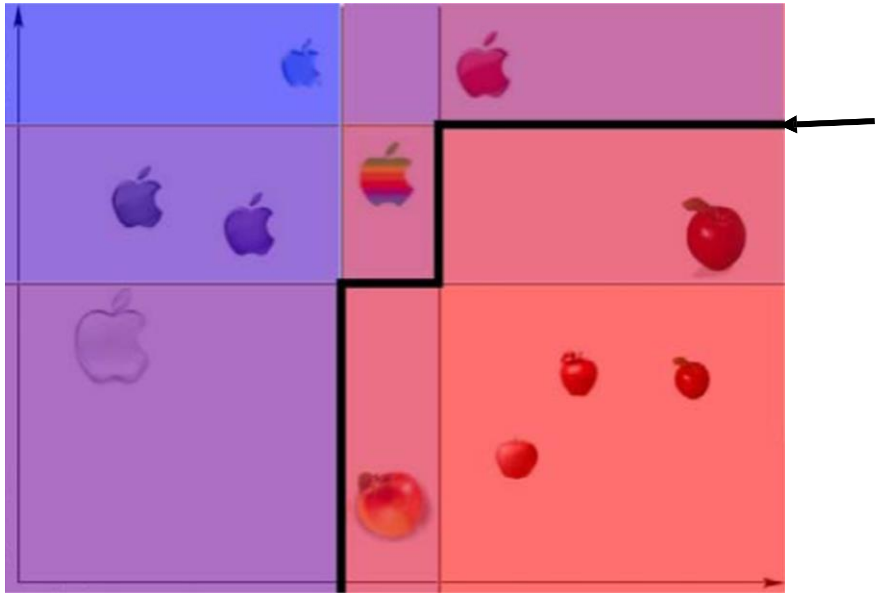
1. Have many rules (base classifiers) to vote on the decision

2. Sequentially train base classifiers that **corrects** mistakes of previous → focus on **hard** examples
3. Give higher **weight** to better rules



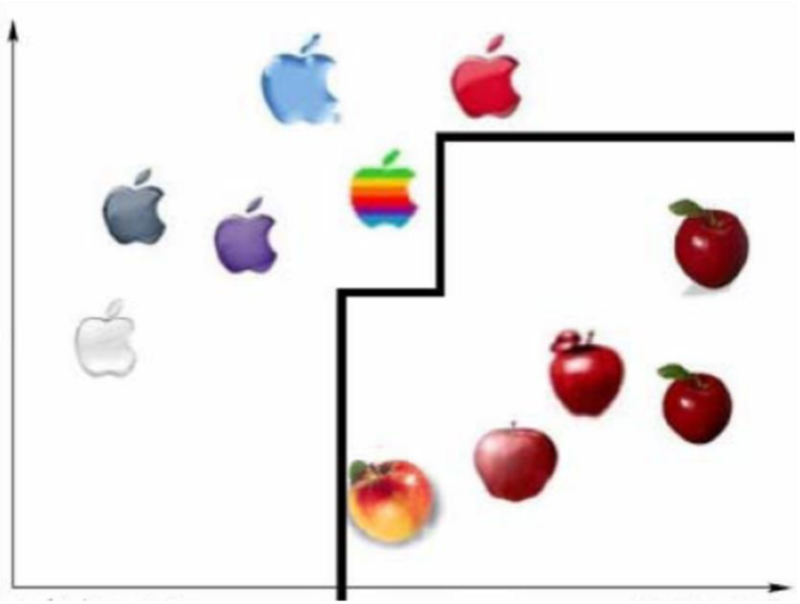
1. Have many rules (base classifiers) to vote on the decision

2. Sequentially train base classifiers that **corrects** mistakes of previous → focus on **hard** examples
3. Give higher **weight** to better rules



A More Complex Rule

Final Classifier is the additive combination of base rules:



Adaboost Algorithm (Proposed by Robert Schapire)

Training Data: $\mathbf{D} = \{(\mathbf{x}_i, y_i) | \mathbf{x}_i \in \mathcal{R}^n, y_i \in \{-1, 1\}, 1 \le i \le m\}$

Set uniform example weight $w_i, 1 \le i \le m$

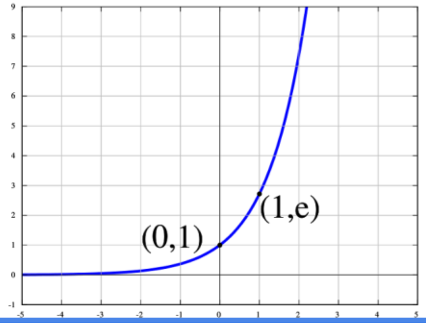
For t = 1 **to** T **iterations:**

Select a base classifier: $h_t(\mathbf{x}_i) = \arg\min(\epsilon_t)$

$$\epsilon_t = \sum_{i=1}^{m} w_i [y_i \neq h_t(\mathbf{x}_i)]$$

Set classifier weight: $\alpha_t = \frac{1}{2} \ln \frac{1-\epsilon_t}{\epsilon_t}$

Update example weight: $w_i = w_i e^{-\alpha_t y_i h_t(\mathbf{x}_i)}$



Final Classifier: $\hat{f} = \text{sign}\,(\sum_{t=1}^{T} \alpha_t h_t(\mathbf{x}_i))$

Boosting vs. Bagging

- Similar to bagging, boosting combines a weighted sum of many classifiers, thus **it reduces variance**.

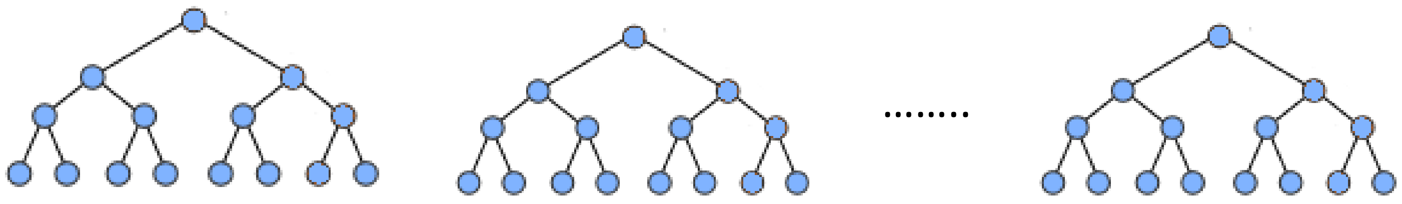
- One key difference: unlike bagging, boosting fit the tree to the entire training set, and adaptively weight the examples.

- Boosting tries to do better at each iteration, (by making model a bit more complex), thus

XGBoost

- Additive tree model: add new trees that complement the already-built ones
- Response is the optimal linear combination of all decision trees
- Popular in Kaggle Competitions for efficiency and accuracy

Additive tree model



More in 18c-extraBoosting Slides

Greedy Algorithm

XGBoost

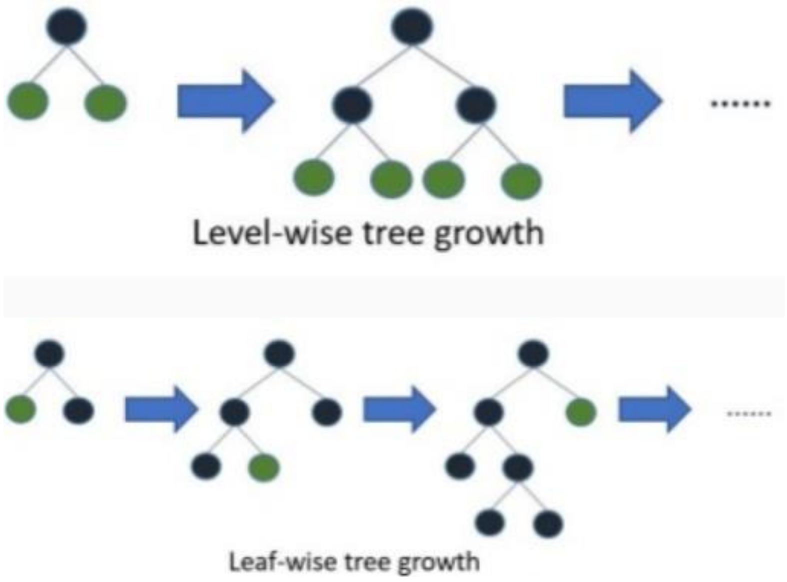
- XGBoost is a very efficient Gradient Boosting Decision Tree implementation with some interesting features:
- **Regularization:** Can use L1 or L2 regularization.
- **Handling sparse data:** Incorporates a sparsity-aware split finding algorithm to handle different types types of sparsity patterns in the data.
- **Weighted quantile sketch:** Uses distributed weighted quantile sketch algorithm to effectively handle weighted data.
- **Block structure for parallel learning:** Makes use of multiple cores on the CPU, possible because of a block structure in its system design. Block structure enables the data layout to be reused.
- **Cache awareness:** Allocates internal buffers in each thread, where the gradient statistics can be stored.
- **Out-of-core computing:** Optimizes the available disk space and maximizes its usage when handling huge datasets that do not fit into memory.

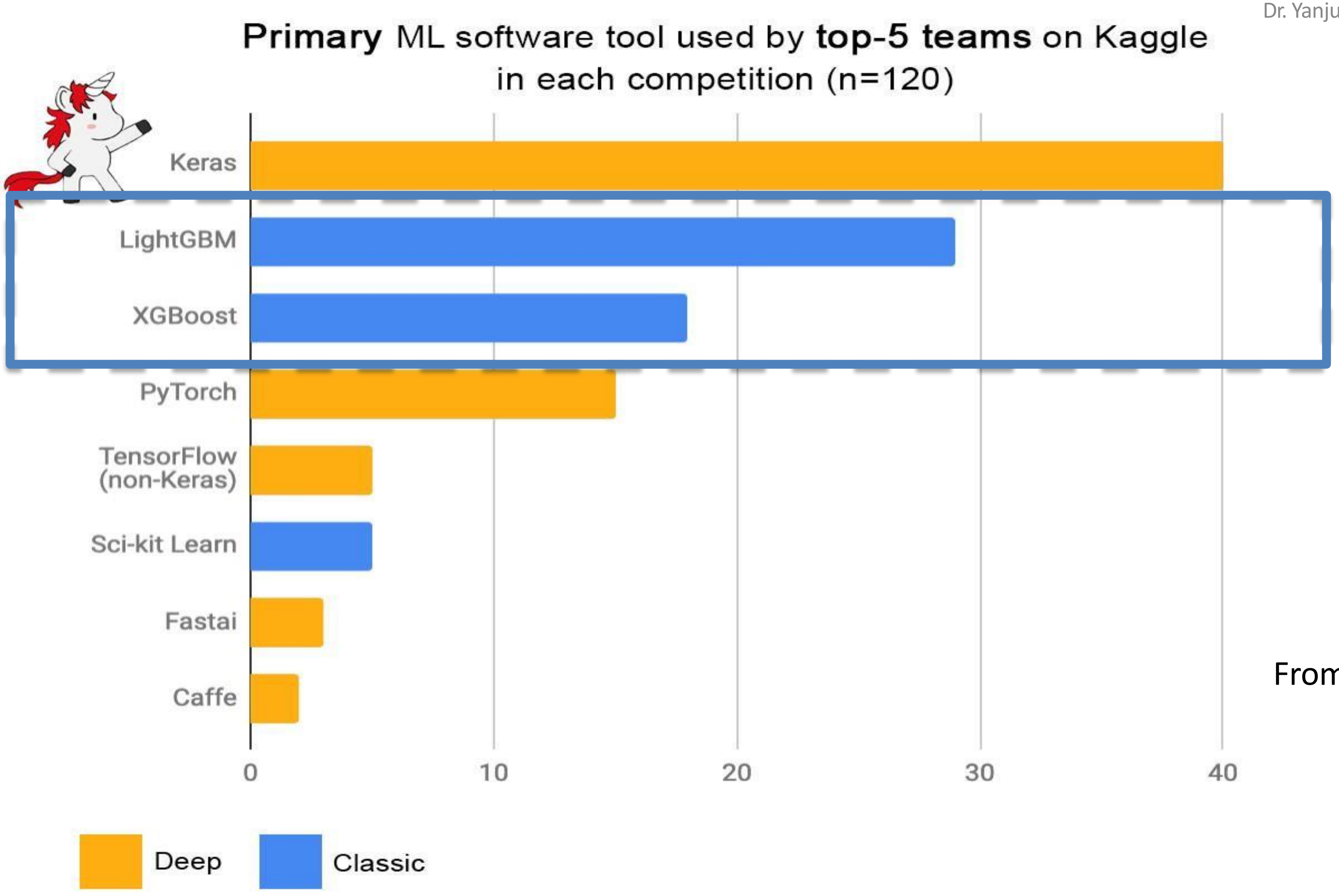
More about History …

- Introduction of Adaboost:
  - Freund; Schapire (1999). "A Short Introduction to Boosting“
- Multiclass/Regression
  - Y. Freund, R. Schapire, “A Decision-Theoretic Generalization of on-Line Learning and an Application to Boosting”, 1995.
  - Robert E. Schapire and Yoram Singer. Improved boosting algorithms using confidence-rated predictions. In Proceedings of the Eleventh Annual Conference on Computational Learning Theory, pages 80–91, 1998.
- Gentle Boost
  - Schapire, Robert; Singer, Yoram (1999). "Improved Boosting Algorithms Using Confidence-rated Predictions".

LGBM

- Stands for Light Gradient Boosted Machines. It is a library for training GBMs developed by Microsoft, and it competes with XGBoost.
- Extremely efficient implementation.
- Usually much faster than XGBoost with low hit on accuracy.
- Main contributions are two novel techniques to speed up split analysis: Gradient based one-side sampling and Exclusive Feature Building.
- Leaf-wise tree growth vs level-wise tree growth of XGBoost.





From: [François Chollet](#) 2019

Boosting

Data
↓
Task
↓
Representation
↓
Score Function
↓
Search/Optimization
↓
Models, Parameters

Tabular
↓
Classification / Regression
↓
Weighted sum of a series of shallow decision trees
↓
Exponential Loss
↓
Gradient based search of weights / DT split
↓
Multiple Trees + Tree Weights

Stacking

- Bagging
  - Bagged Decision Tree
  - Random forests
- Boosting
  - Adaboost
  - Xgboost
- Stacking

e.g. Ensembles in practice

Each rating/sample:
+ <user, movie, date of grade, grade>
Training set (100,480,507 ratings) Qualifying set (2,817,131 ratings)➔ winner

Oct 2006 - 2009

- Training data is a set of users and ratings (1,2,3,4,5 stars) those users have given to movies.
- Predict what rating a user would give to any movie

- $1 million prize for a 10% improvement over Netflix's current method (MSE = 0.9514)

Team “Bellkor's Pragmatic Chaos” defeated the team “ensemble” by submitting just 20 minutes earlier! 1 million dollar !

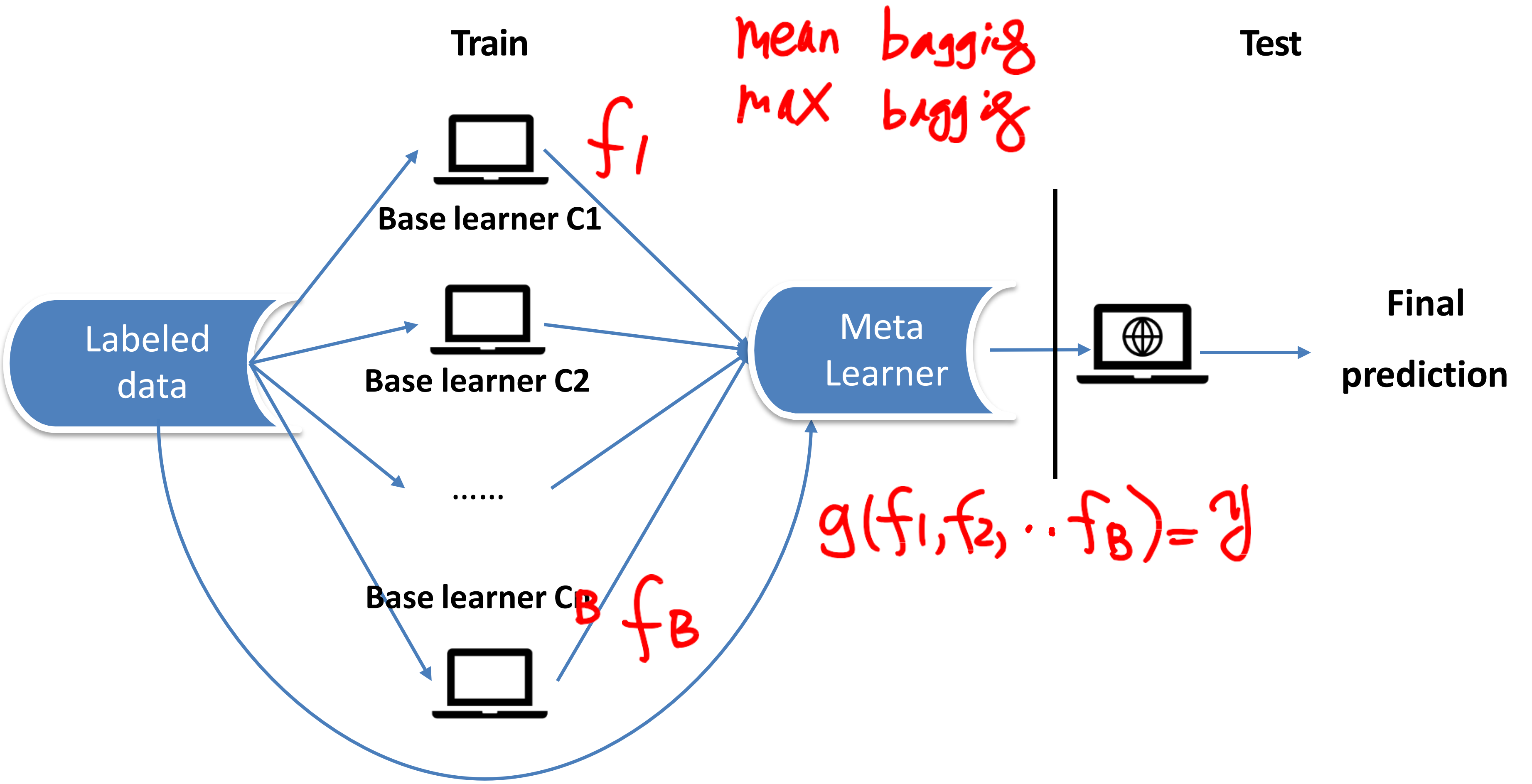
Ensemble in practice

Rank	Team Name	Best Test Score	% Improvement	Best Submit Time
Grand Prize - RMSE = 0.8567 - Winning Team: BellKor's Pragmatic Chaos				
1	BellKor's Pragmatic Chaos	0.8567	10.06	2009-07-26 18:18:28
2	The Ensemble	0.8567	10.06	2009-07-26 18:38:22
3	Grand Prize Team	0.8582	9.90	2009-07-10 21:24:40
4	Opera Solutions and Vandelay United	0.8588	9.84	2009-07-10 01:12:31
5	Vandelay Industries !	0.8591	9.81	2009-07-10 00:32:20
6	PragmaticTheory	0.8594	9.77	2009-06-24 12:06:56
7	BellKor in BigChaos	0.8601	9.70	2009-05-13 08:14:09
8	Dace_	0.8612	9.59	2009-07-24 17:18:43
9	Feeds2	0.8622	9.48	2009-07-12 13:11:51
10	BigChaos	0.8623	9.47	2009-04-07 12:33:59
11	Opera Solutions	0.8623	9.47	2009-07-24 00:34:07
12	BellKor	0.8624	9.46	2009-07-26 17:19:11

The ensemble team ➔ blenders of multiple different methods

Stacking

- Main Idea: Learn and combine multiple classifiers



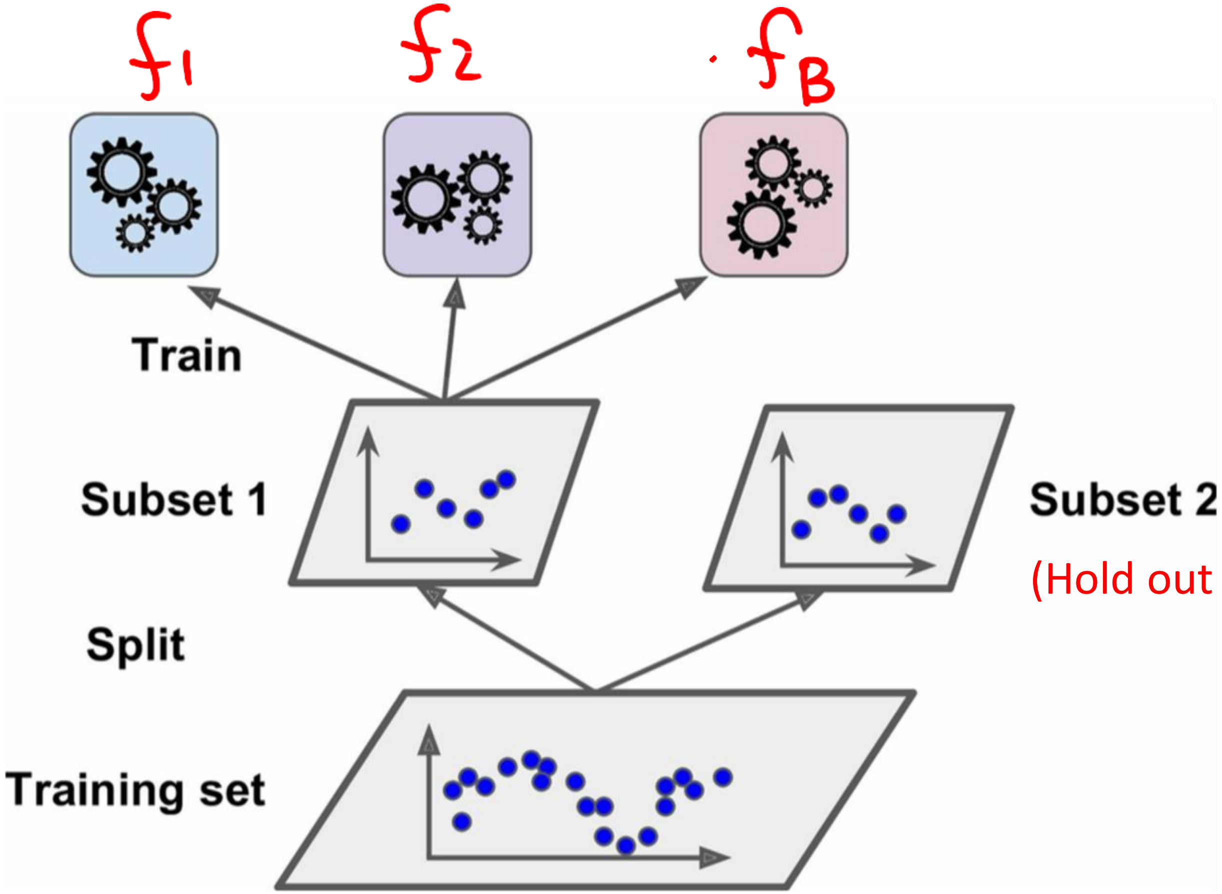
Generating Base and Meta Learners

- **Base model—efficiency, accuracy and diversity**
  - Sampling training examples
  - Sampling features
  - Using different learning models

- **Meta learner**
  - Majority voting
  - Weighted averaging
  - …..

  Unsupervised
  - Higher level classifier — Supervised (e.g. Xgboost as blender)

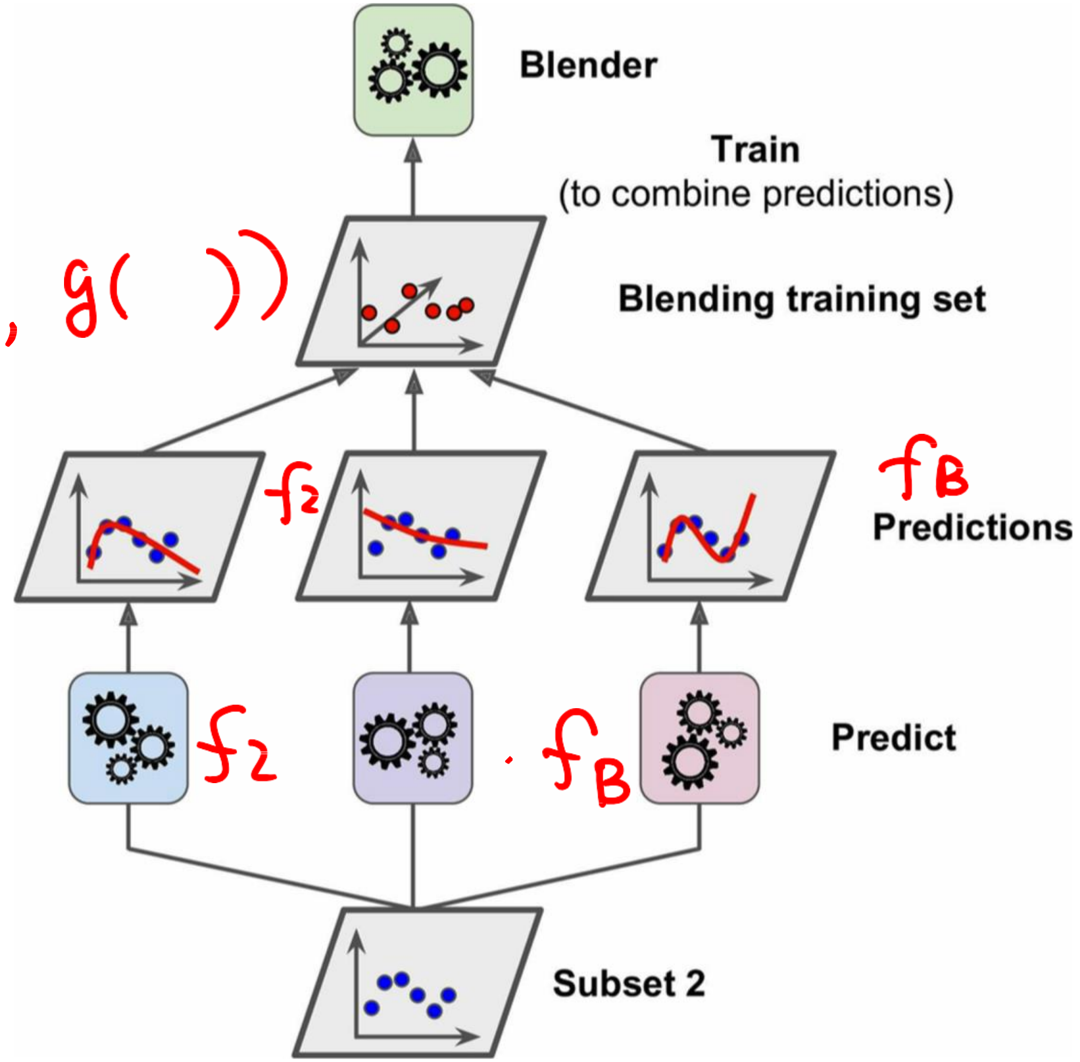
Training the base predictors



(Hold out for later)

Training the meta blender

loss (y , g( ))



In Lab session

You will see how to use XGBoost to do price prediction for houses in Boston
This can be useful for your **FINAL** project

Lab is done by Remy Belmonte