



Never Stand Still

Ensemble Learning

集成学习

COMP9417 Machine Learning & Data Mining

Term 3, 2019

Adapted from slides by Dr Michael Bain

Aims

This lecture will develop your understanding of ensemble methods in machine learning, based on analyses and algorithms covered previously. Following it you should be able to:

- Describe the framework of the bias-variance decomposition and some of its practical implications
- describe how ensembles might be used to address the bias and variance components of error
- outline the concept of the stability of a learning algorithm
- describe different ensemble methods of bagging, randomization, boosting, etc.

Introduction

In previous lectures, introduced some theoretical ideas about limits on machine learning. But do these have any practical impact ?

The answer is **yes** !

One of these theoretical tools is bias-variance decomposition:

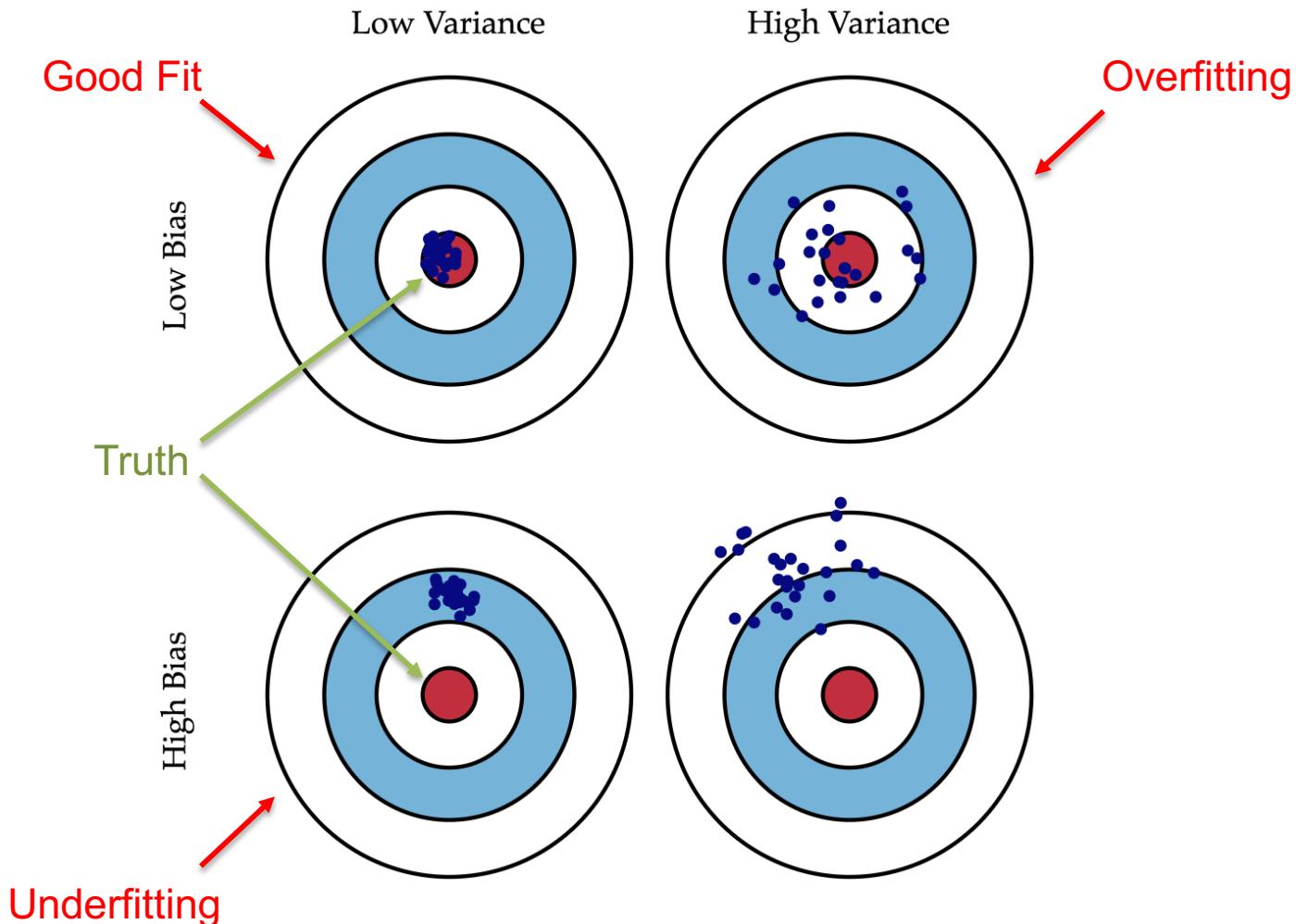
- The bias-variance decomposition of error can be a tool for thinking about how to reduce error in learning
- Take a learning algorithm and ask:
 - how can we reduce its bias ?
 - how can we reduce its variance ?
- Ensemble learning methods can be viewed in this light
- A form of *multi-level* learning: learning a number of base-level models from the data, and learning to combine these models as an ensemble

Review: bias-variance decomposition

- Theoretical tool for analyzing how much specific training set affects performance of classifier
- Assume we have an infinite number of classifiers built from different training sets all of the same size:
 - The *bias* of a learning scheme is the expected error due to the mismatch between the learner's hypothesis space (class of models) and the space of target concepts
 - The *variance* of a learning scheme is the expected error due to differences in the training sets used
 - The *variance* of a learning scheme is how much the predictions for a given point vary between different model.
 - Total expected error \approx bias² + variance

Bias-Variance

偏差-方差



Source: Scott-Fortmann, Understanding Bias-variance tradeoff

Bias-Variance

sort of expected value

- The inability of the learning algorithm to capture the true relationship between the output and the features/attributes is called **bias**.
- The learning algorithm difference in fits between datasets is called **variance**.

Three commonly used methods to find a good bias-variance tradeoff are:

- Regularization
- Bagging
- Boosting

Bias-variance: a trade-off

权衡

Easier to see with regression in the following figure¹(to see the details you will have to zoom in in your viewer):

- each column represents a different model class $g(x)$ shown in red
- each row represents a different set of $n = 6$ training points, D_i , randomly sampled from target function $F(x)$ with noise, shown in black
- probability functions of mean squared error E are shown

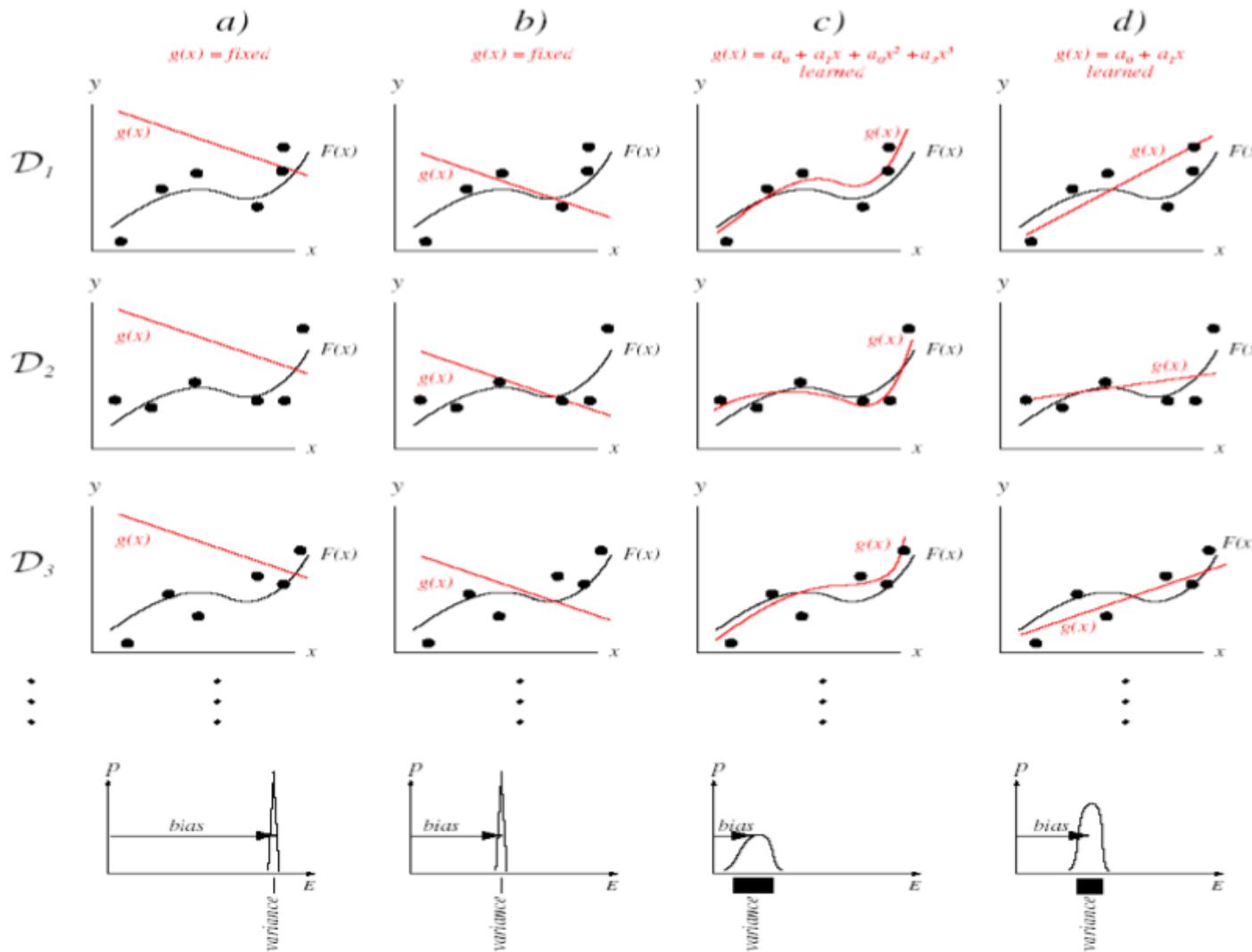
1- from: "Elements of Statistical Learning" by Hastie, Tibshirani and Friedman (2001)

Bias的对象是单个模型，是期望输出与真实标记的差别。它描述了模型对本训练集的拟合程度。

Variance的对象是多个模型，是相同分布的不同数据集训练出模型的输出值之间的差异。

它刻画的是数据扰动对模型的影响

Bias-variance: a trade-off



Bias-variance: a trade-off

- “ a ” is very poor: a linear model with fixed parameters independent of training data; high bias, zero variance
- “ b ” is better: a linear model with fixed parameters independent of training data; slightly lower bias, zero variance
- “ c ” is a cubic model with parameters trained by mean-square-error on training data; low bias, moderate variance
- “ d ” is a linear model with parameters adjusted to fit each training set; intermediate bias and variance
- training with data $n \rightarrow \infty$ would give
 - “ c ” with bias approaching small value due to noise
 - but not “ d ”
 - variance for all models would approach zero

Bias-variance in ensemble classification

- Recall that we derived the bias-variance decomposition for regression (squared-error loss function)
- Cannot apply same derivation for classification (zero-one loss can be used)
- Bias-variance decomposition used to analyze how much restriction to a single training set affects performance
- Can decompose expected error of any individual ensemble member as follows:
 - Bias = expected error of the ensemble classifier on new data
 - Variance = component of the expected error due to particular training set being used to build classifier

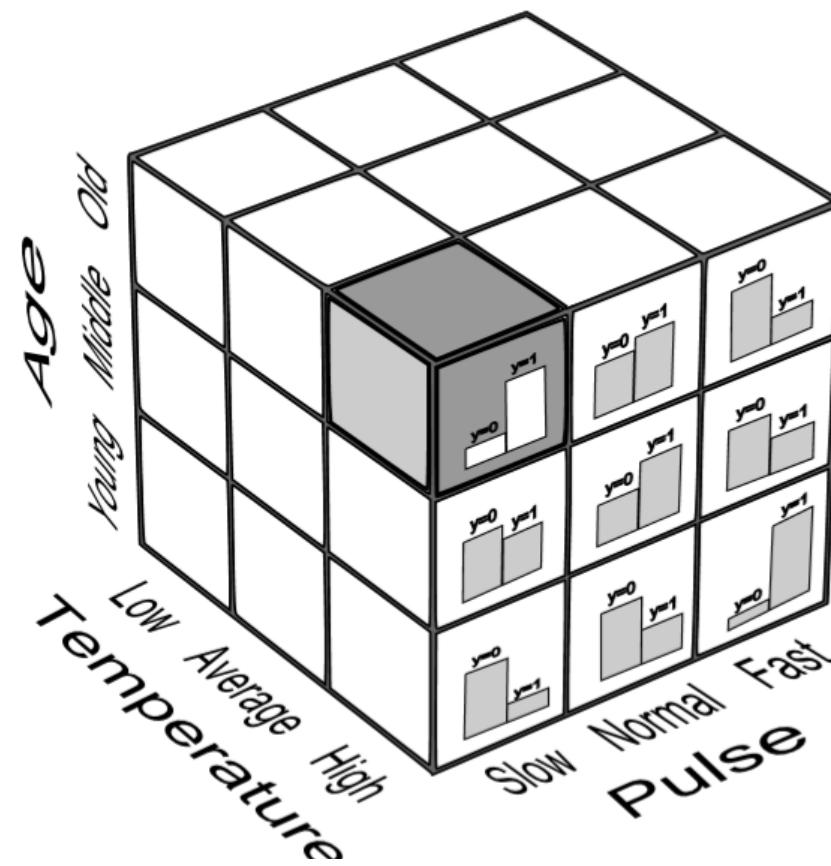
Bias-variance with “Big Data”

- high bias algorithms often used for efficiency
 - why ?
 - less complexity
 - usually simpler to compute
- big data can reduce variance
 - why ?
 - enough data to cover all features so that can predict more precisely

This slide and the following 3 slides are due to Prof. G. Webb, Monash U.

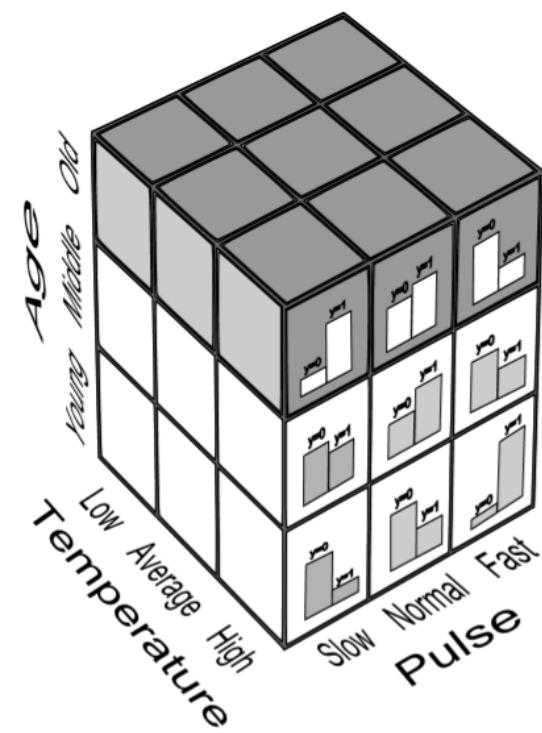
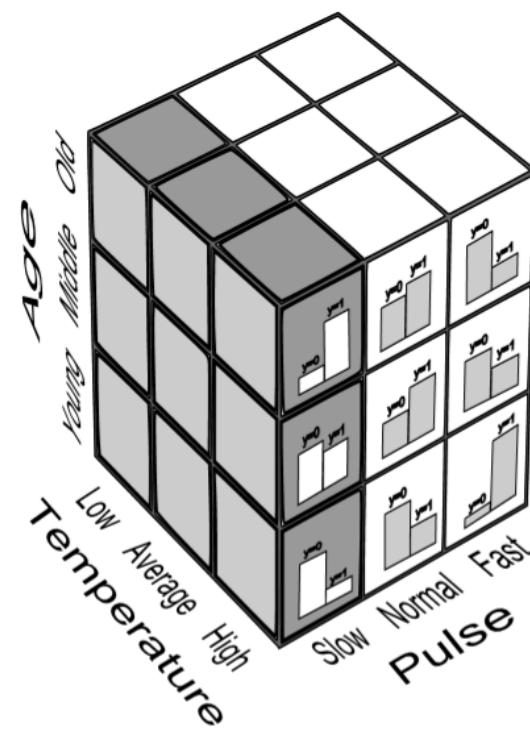
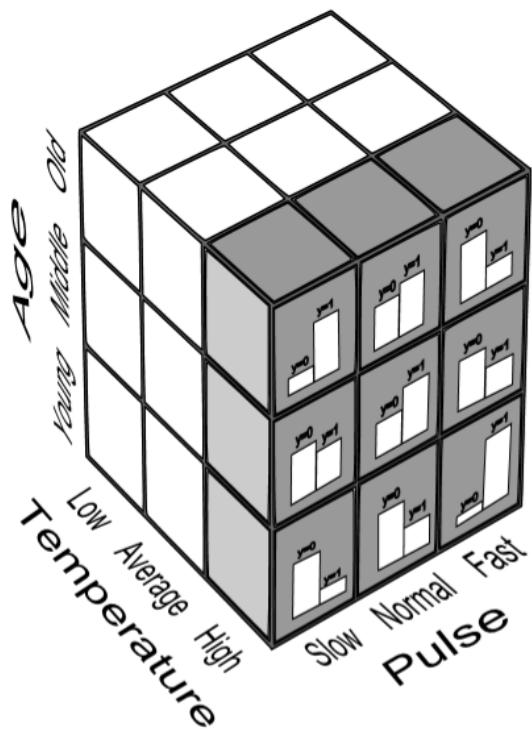
Bias-variance with “Big Data”

Suppose we have a low bias representation (e.g., all conjunctive concepts), but such concepts may not always occur frequently in small datasets:



Bias-variance with “Big Data”

So we can increase bias – e.g., by Naive Bayes-type conditional independence assumptions – but this forces averaging of class distributions over all “small concepts”:



Bias-variance with “Big Data”

“Big Data” may help to resolve the bias-variance dilemma:

- high bias algorithms are often used for efficiency
 - usually simpler to compute
- big data can reduce variance
 - “small” concepts will occur more frequently
 - low bias algorithms can find them in each sample
 - but: how to compute efficiently ?

This is still largely an open problem!

Bias-variance in “Real-world AI”

Imagine the following situation:

- Applications increasingly require machine-learning systems to perform at “human-level” (e.g., personal assistants, self-driving vehicles, etc.)
- Suppose you are developing an application and you know what “human-level” error would typically be on this task.
- You have sufficient data for training and validation datasets, and you are not restricted in terms of the models that you could learn (e.g., from linear regression or classification up to kernel methods, ensembles, deep networks, etc.)
- How can an understanding of the bias-variance decomposition help ?

Bias-variance in “Real-world AI”

The following scenarios can happen:

the model is not so complex

1. Training-set error is observed to be high compared to human-level – why ?
 - Bias is too high – solution: move to a more expressive (lower bias) model

2. Training-set error is observed to be similar to human-level, but validation set error is high compared to human-level – why ?
 - Variance is too high – solution: get more data (!), try regularization, ensembles, move to a different model architecture

These scenarios are often found in applications of deep learning²

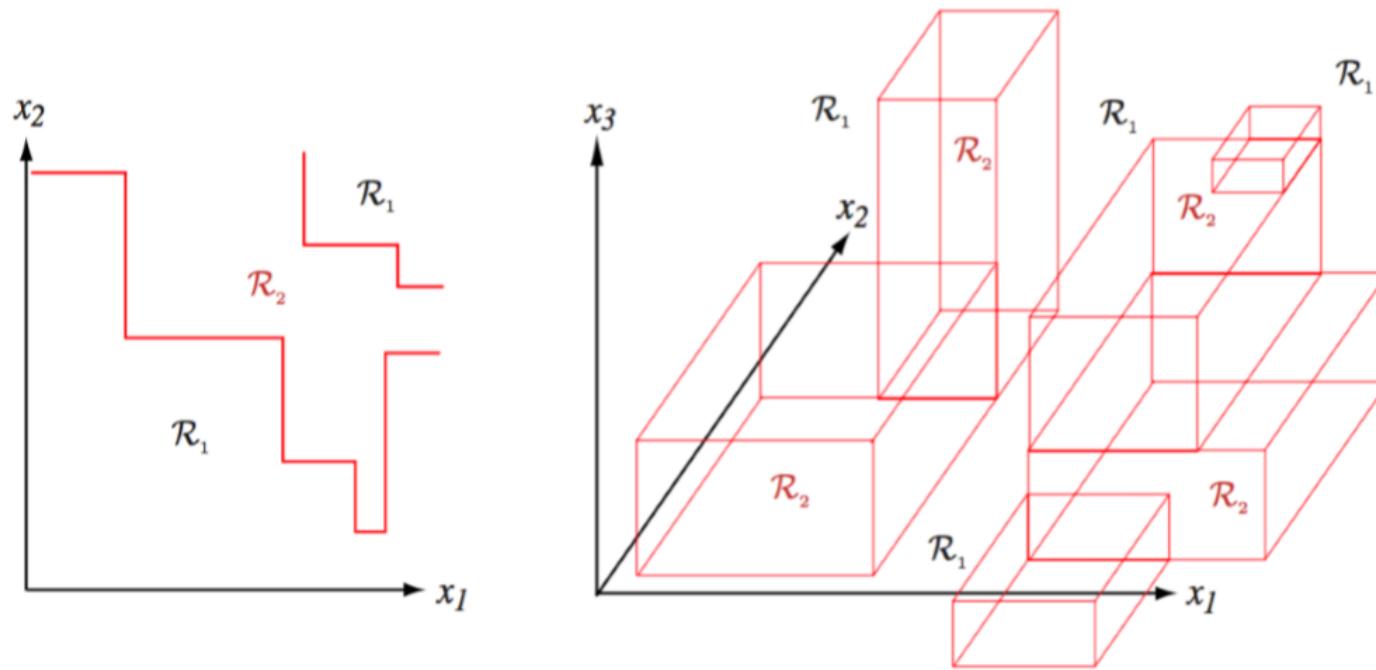
2-“Nuts and Bolts of Applying Deep Learning” by Andrew Ng
<http://www.youtube.com/watch?v=F1ka6a13S9I>

Stability

- for a given data distribution \mathcal{D}
- train algorithm L on training sets S_1, S_2 sampled from \mathcal{D}
- expect that the model from L should be the same (or very similar) on both S_1 and S_2
- if so, we say that L is a stable learning algorithm
- otherwise it is unstable
- typical stable algorithm: k NN (for some k)
- typical unstable algorithm: decision-tree learning
 - can cause overfit even do pruning

Turney, P. "Bias and the Quantification of Stability"

Decision boundaries in tree learning



Decision boundaries for monothetic two-class trees in two and three dimensions; arbitrarily fine decision regions for classes \mathcal{R}_1 , \mathcal{R}_2 can be learned by recursively partitioning the instance space.

Instability of tree learning

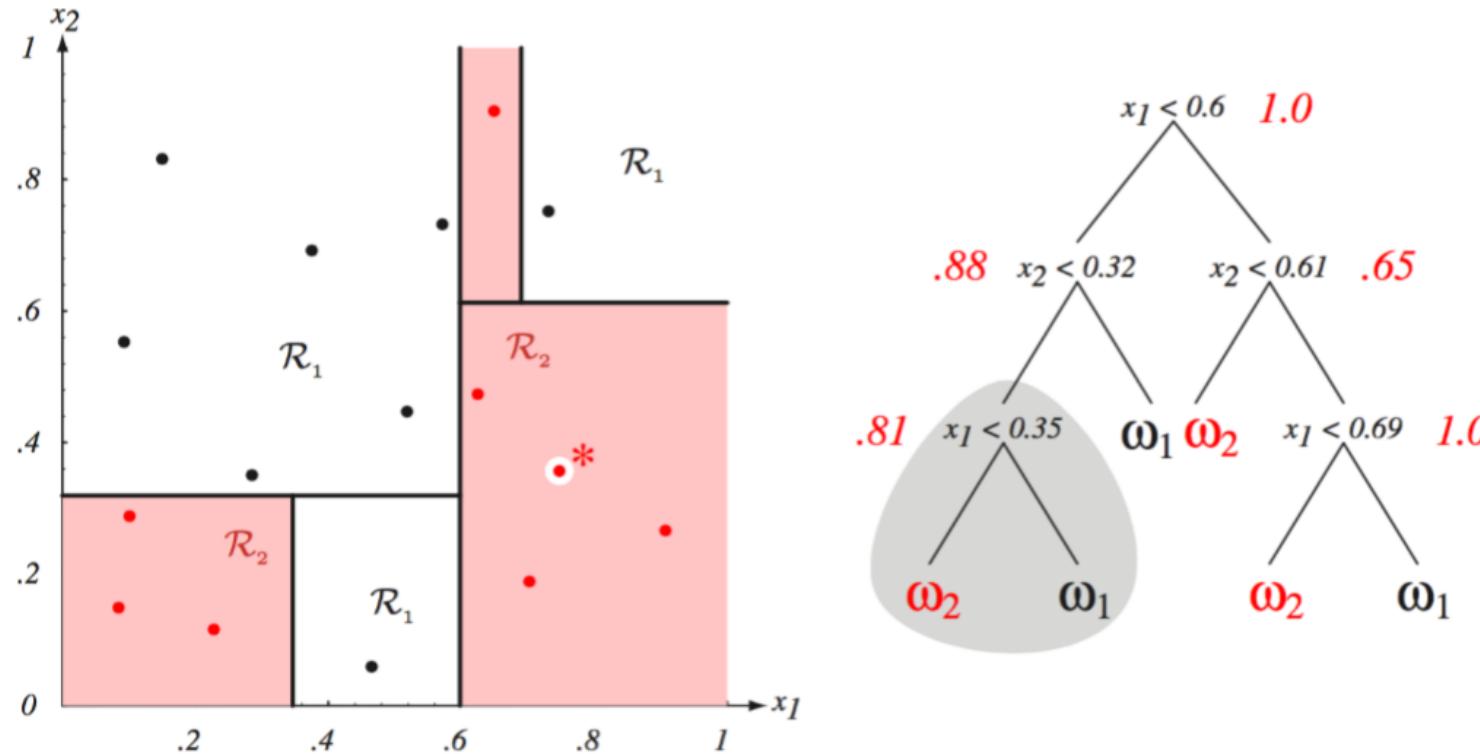
An example shows the effect of a small change in the training data on the structure of an unpruned binary tree learned by CART. The training set has 8 instances for each class:

ω_1 (black)		ω_2 (red)	
x_1	x_2	x_1	x_2
.15	.83	.10	.29
.09	.55	.08	.15
.29	.35	.23	.16
.38	.70	.70	.19
.52	.48	.62	.47
.57	.73	.91	.27
.73	.75	.65	.90
.47	.06	.75	.36* (.32 [†])

Note: for class ω_2 (red) the last instance has two values for feature x_2 . On the next slide is a tree learned from the data where this instance has value $x_2 = .36$ (marked *), and on the following slide we see the tree obtained when this value is changed to $x_2 = .32$ (marked [†]).

From: "Pattern Classification". R. Duda, P. Hart, and D. Stork (2001) Wiley.

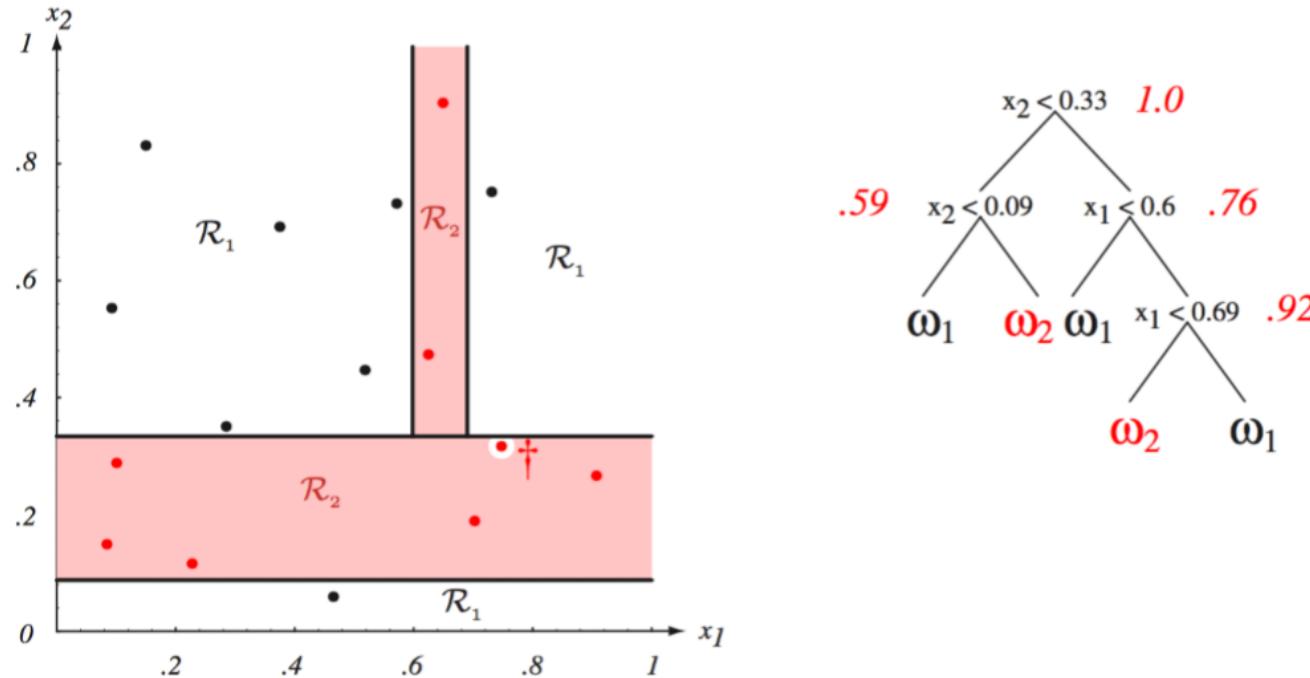
Instability of tree learning



The partitioned instance space (left) contains the instance marked * and corresponds to the decision tree (right).

From: "Pattern Classification". R. Duda, P. Hart, and D. Stork (2001) Wiley.

Instability of tree learning



The partitioned instance space (left) contains the instance marked \dagger and corresponds to the decision tree (right). Note that both the decision boundaries and the tree topology are considerably changed, for example, testing x_2 rather than x_1 at the tree root, although the change in data was very small.

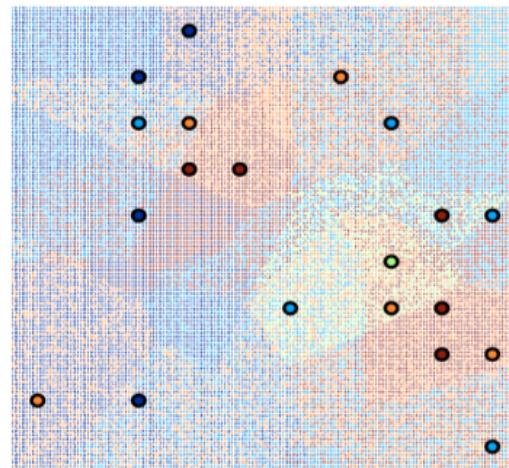
From: "Pattern Classification". R. Duda, P. Hart, and D. Stork (2001) Wiley.

Stability and Bias-Variance

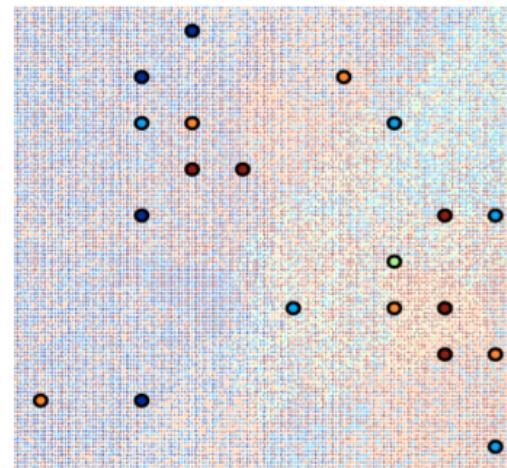
- stable algorithms typically have high bias
- unstable algorithms typically have high variance
- BUT: take care to consider effect of parameters on stability, e.g., in k NN:
 - 1NN perfectly separates training data, so low bias but high variance
 - By increasing the number of neighbors k we increase bias and decrease variance (what happens when $k = n$?)
 - Every test instance will have the same number of neighbors, and the class probability vectors will all be the same !

Three-, five- and seven-nearest neighbour

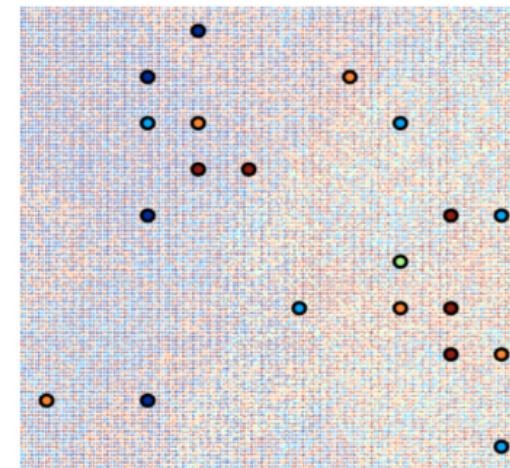
Decision regions of kNN classifiers; the shading represents the predicted probability distribution over the five classes.



3-nearest neighbour



5-nearest neighbour



7-nearest neighbour

Illustrates the effect of varying k on stability (i.e., bias and variance).

Ensemble Methods

Supervised learning

We have looked into different supervised methods:

- Basic linear classifier
- kNN
- Naïve Bayes
- Logistic regression
- Decision trees
- Perceptron
- Support vector machine
- ...

For a new problem, which method to pick?

Supervised learning

- We can test all different methods on a validation set and pick the one which gives the best performance
- Each learning method gives a different hypothesis,... but no hypothesis is perfect
- Maybe we can combine different hypotheses to build a better hypothesis (model) !?

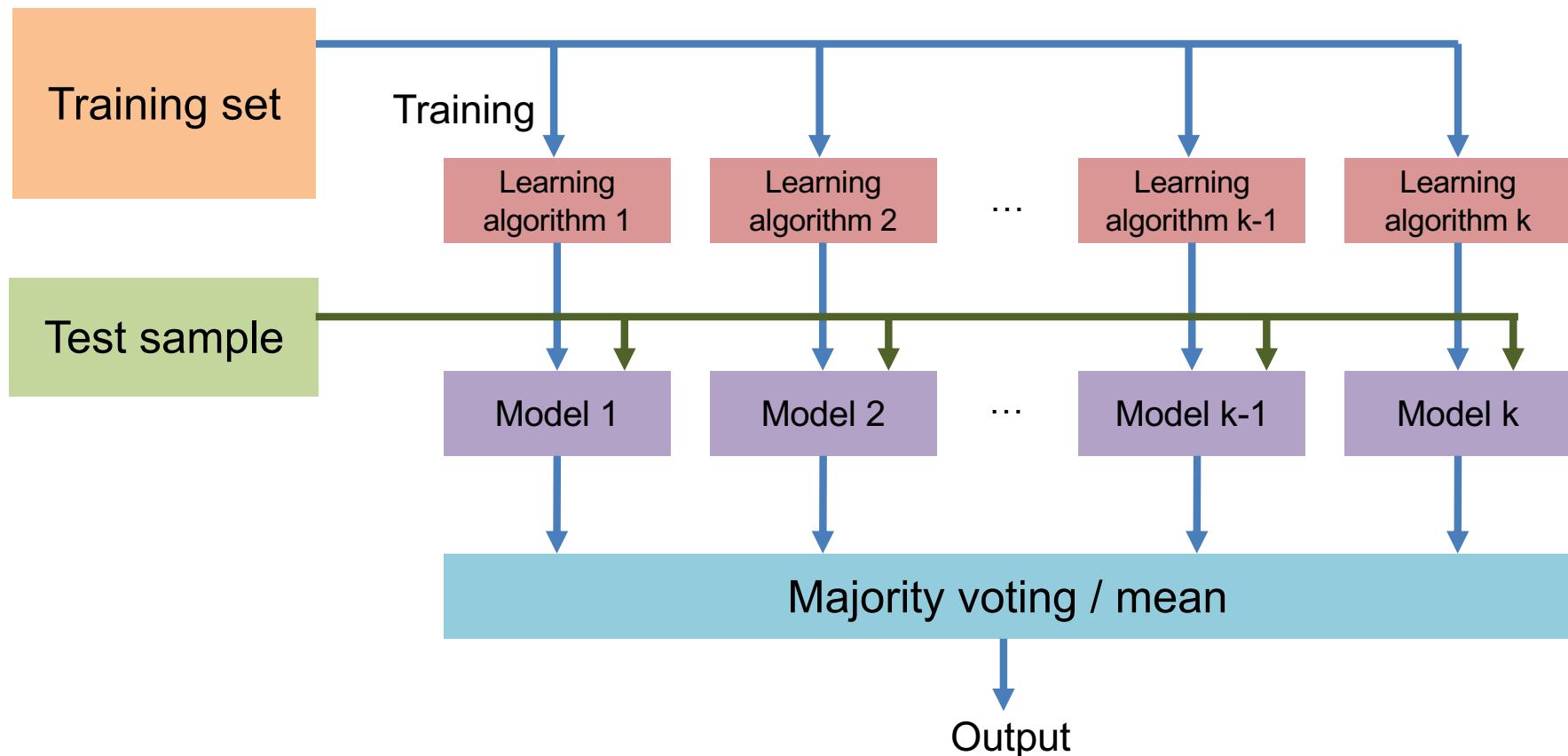
Ensemble methods

- Ensemble methods are meta-algorithms that combine different models into one model and they can:
 - Decrease variance
 - Decrease bias
 - Improve performance
- The idea relates to the “wisdom of crowd” phenomenon:
聚合
 - Aggregation of information in groups (by James Surowiecki, 1907)
 - Aggregation of independent estimate can be really effective for prediction
 - » Unweighted average (e.g. majority vote)
 - » Weighted average (e.g. committee of experts)

Simple ensembles

There are different ways of combining predictors:

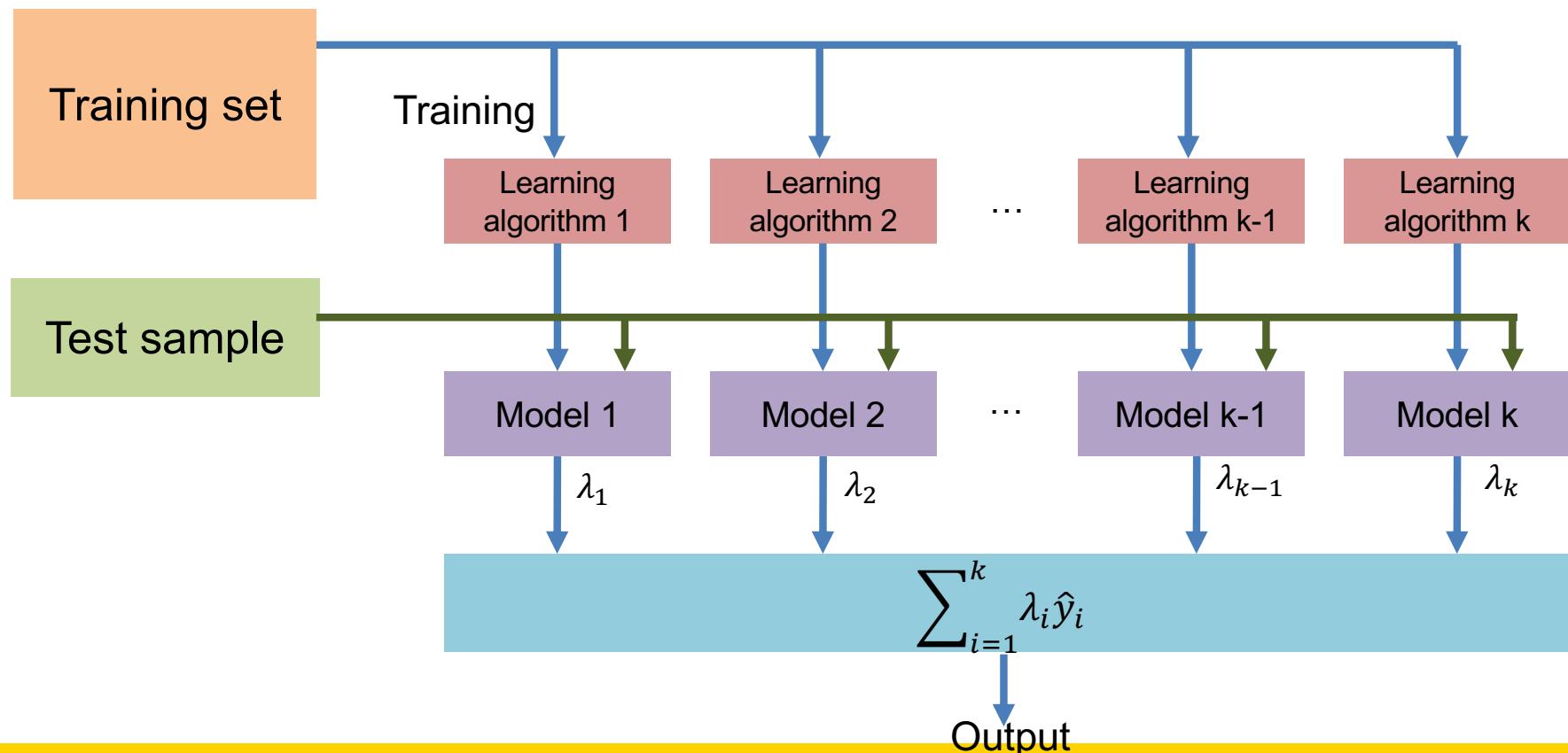
1. Simple ensembles like majority vote or unweighted average



Simple ensembles

2. weighted averages / weighted votes: Every model gets a weight (e.g. depending on its performance)

Type equation here.



Weighted average / weighted majority

In practice:

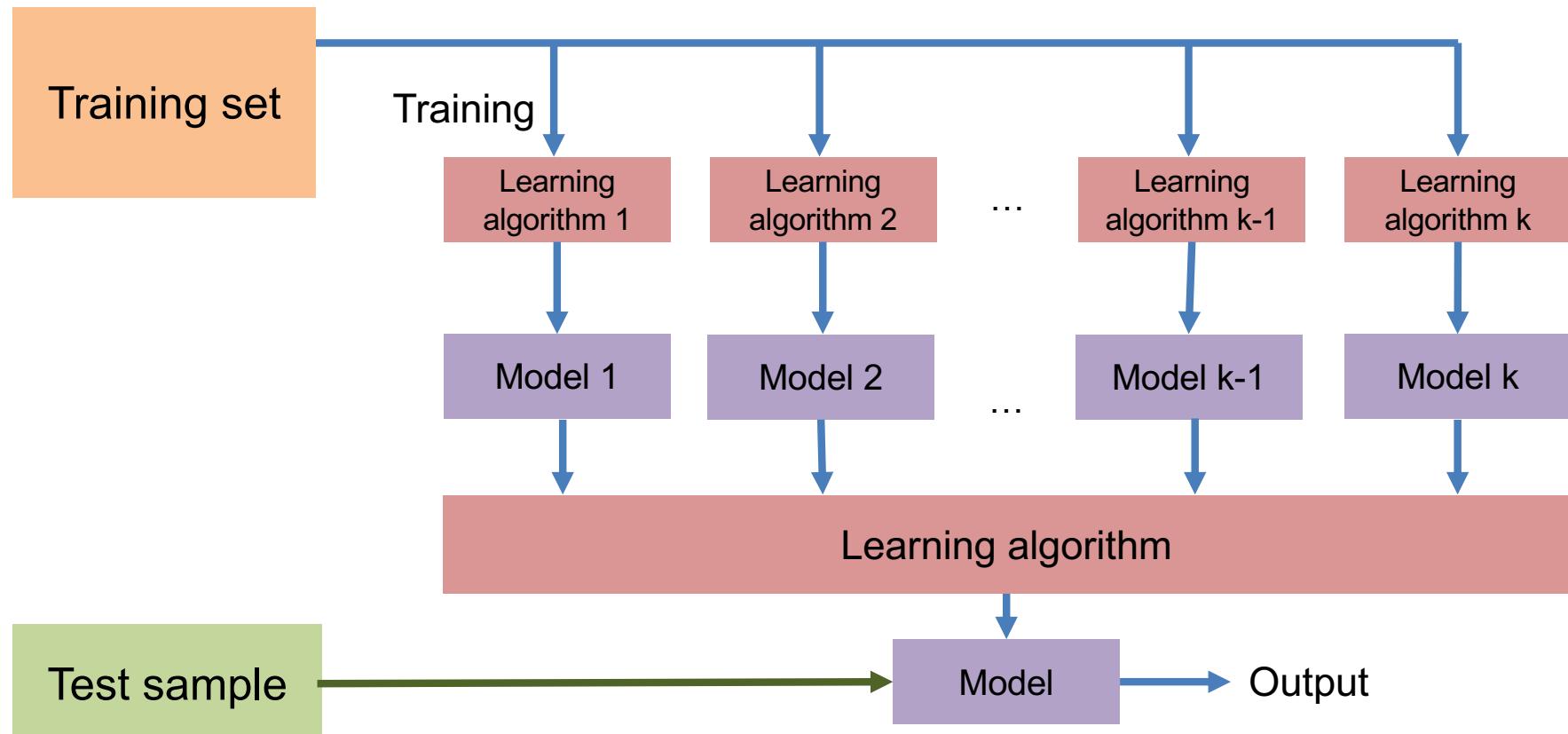
- Learning algorithms may not be independent
- Some better fit the data so make less error

We can define weights in different ways:

- Decrease weight of correlated learners
- Increase weight of good learners

Simple ensembles

3. Treat the output of each model as a feature and train a model on that



Simple ensembles

3. Treat the output of each model as a feature and train a model on that
 - If the task is a binary classification and we choose the fusion model to be a linear model then this will become a weighted vote
如果是二分，则相当于是linear model
 - We can train the fusion model on a validation set or a portion of training data that we have not used in training the initial models because otherwise it will always be biased towards the models that had a better performance on the training data

Simple ensembles

4. Mixture of experts:

- Weight $\alpha_i(x)$ indicates “expertise”
- It divides the feature space into homogeneous regions
- It may use a weighted average or just pick the model with the largest expertise
- It is a kind of local learning

Ensemble methods

5. “Bagging” method: (“Bootstrap **Aggregation**”) 选平均的，民主 不同的model 取部分data
- Training many classifiers, but each with only a portion of data
 - Then aggregate through model averaging / majority voting

We used data splitting in cross-validation (k-fold CV) to check overfitting and possibility avoid overfitting.

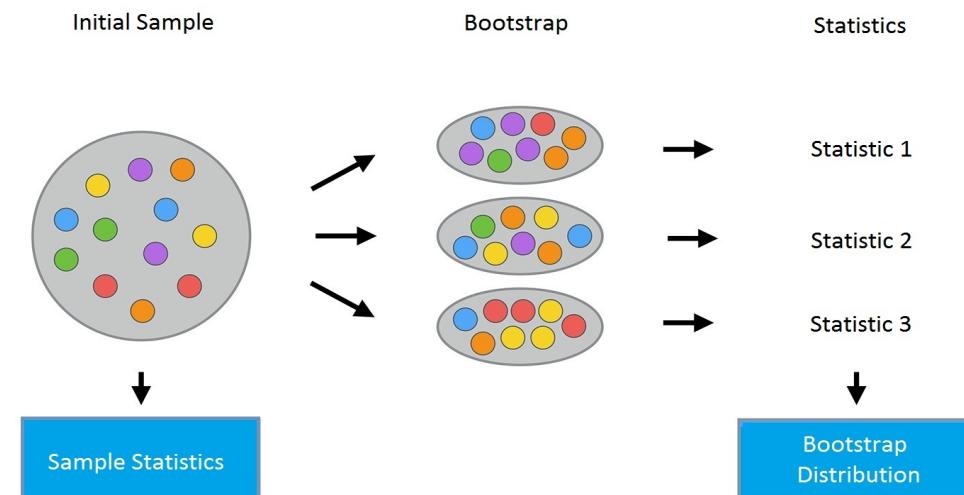
- But, maybe we can combine the models that we train on each split
- This will reduce the overfitting

Bagging

Bagging = Bootstrap + aggregation

Bootstrap: 使用样本数据的子集（刀切法）或从数据中有放回地随机抽样（自助法）

A standard “**resampling**” technique from statistics for estimating quantities about a population by averaging estimates from multiple small data samples. Importantly, samples are constructed by drawing observations from a large data sample one at a time and **returning them to the data sample after they have been chosen.**



<https://mlcourse.ai/articles/topic5-part1-bagging/>

Bagging

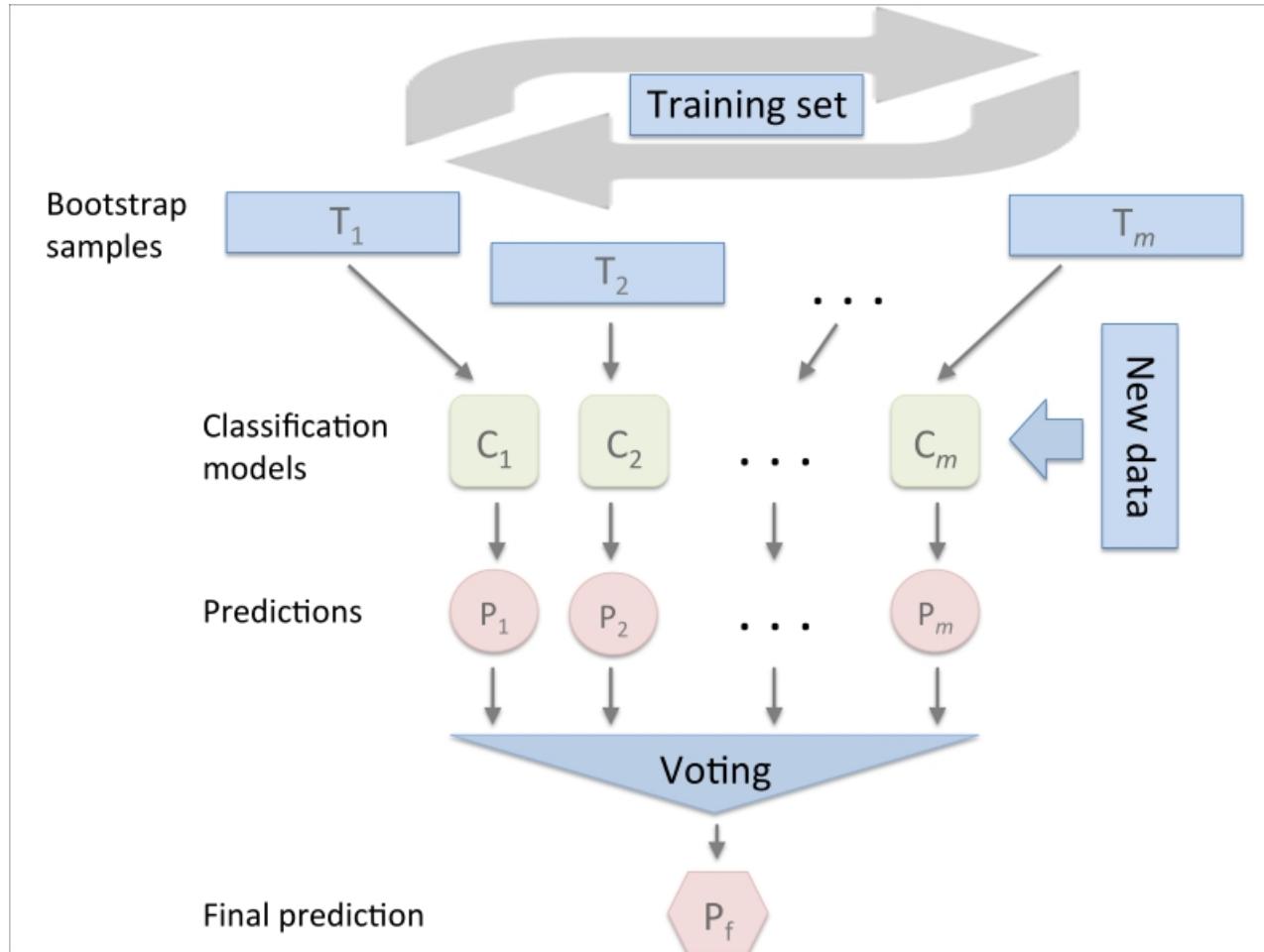
Bootstrap:

- Create a random subset of data by sampling with replacement
- Draw m' samples from m sample with replacement ($m' \leq m$)

Bagging:

- Repeat k times to generate k subsets
 - Some of the samples get repeated and some will not be left out
- Train one classifier on each subset
- To test, aggregate the output of k classifiers that you trained in the previous step using either majority vote / unweighted average

Bagging



https://subscription.packtpub.com/book/big_data_and_business_intelligence/9781783555130/7/ch07lvl1sec46/bagging-building-an-ensemble-of-classifiers-from-bootstrap-samples

Bias / Variance in Bagging

Error of any model has two components:

- Bias: due to model choice which
 - can be reduced by increasing complexity
- Variance: due to small sample size or high complexity of the model
 - Can be reduced by increasing the data or reducing the complexity

Bagging is applied on a collection of low-bias high-variance models and by averaging them the bias would not get affected, however the variance will be reduced

Bagging error

Assumption:

- If learners are independent
- If each learner makes an error with probability p (same error probability for all learners)

The probability that k' out of k learner make an error is:

$$\binom{k}{k'} p^{k'} (1 - p)^{k-k'}$$

If we use majority voting to decide about the output, then the error happens if more than $\frac{k}{2}$ of learners make an error, so the error for majority voting is:

$$\sum_{k' > \frac{k}{2}} \binom{k}{k'} p^{k'} (1 - p)^{k-k'}$$

If $k = 10$ and $p = 0.1$, then $\text{error}(\text{majority voting}) < 0.001$

Bagging

Advantage:

- Reduces overfitting (harder for the aggregated model to memorize full dataset, since some of the data will not be seen by the training models)
- This improves performance in almost all cases specially if learning scheme is unstable (i.e. decision trees are unstable because with slightly different sub-sample, the tree structure may change drastically)
- Can be applied to numeric prediction and classification
- Can help a lot if data is noisy

Bagging more precisely

Algorithm Bagging(D, T, \mathcal{A}) // train ensemble from bootstrap samples

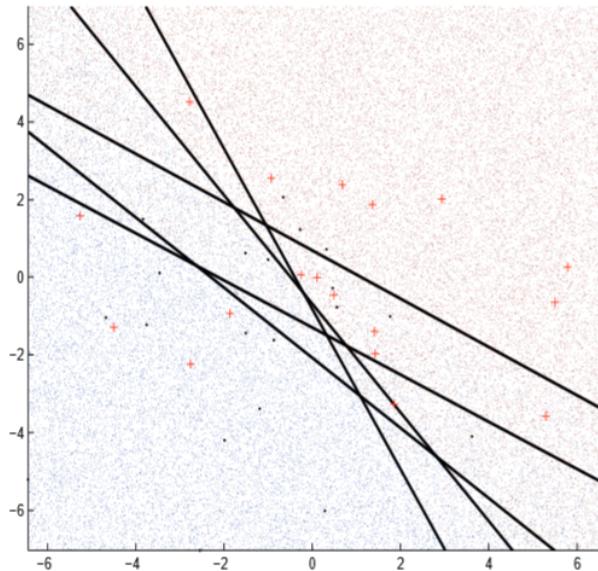
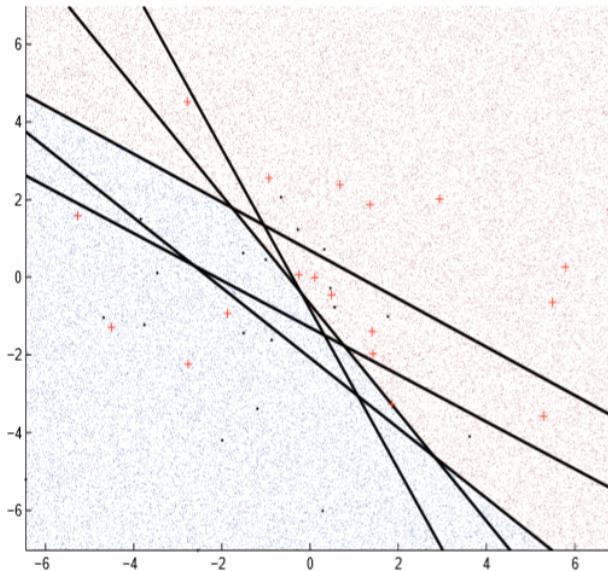
Input: dataset D ; ensemble size T ; learning algorithm \mathcal{A} .

Output: set of models; predictions to be combined by voting or averaging.

```
1 for  $t = 1$  to  $T$  do
2   | bootstrap sample  $D_t$  from  $D$  by sampling  $|D|$  examples with replacement
3   | run  $\mathcal{A}$  on  $D_t$  to produce a model  $M_t$ 
4 end
5 return  $\{M_t | 1 \leq t \leq T\}$ 
```

Bagging linear classifiers

based on training data



(left) An ensemble of five basic *linear classifiers* built from bootstrap samples with bagging. The decision rule is majority vote, leading to a piecewise linear decision boundary. (right) If we turn the **votes into probabilities**, we see the ensemble is effectively grouping instances in different ways, with each segment obtaining a slightly different probability.

Bagging trees

Example:

An experiment with simulated data:

- A sample set of size $m = 30$, two classes $\{0,1\}$ and 5 features
- Each feature has a standard Gaussian distribution with pairwise correlation 0.95
- The outputs are generated according to:

$$\Pr(Y = 1 | x_1 \leq 0.5) = 0.2 \text{ and } \Pr(Y = 1 | x_1 > 0.5) = 0.8$$

- A test set of size 2000 from same population
- The Bayesian error for this data is 0.2

Bagging trees

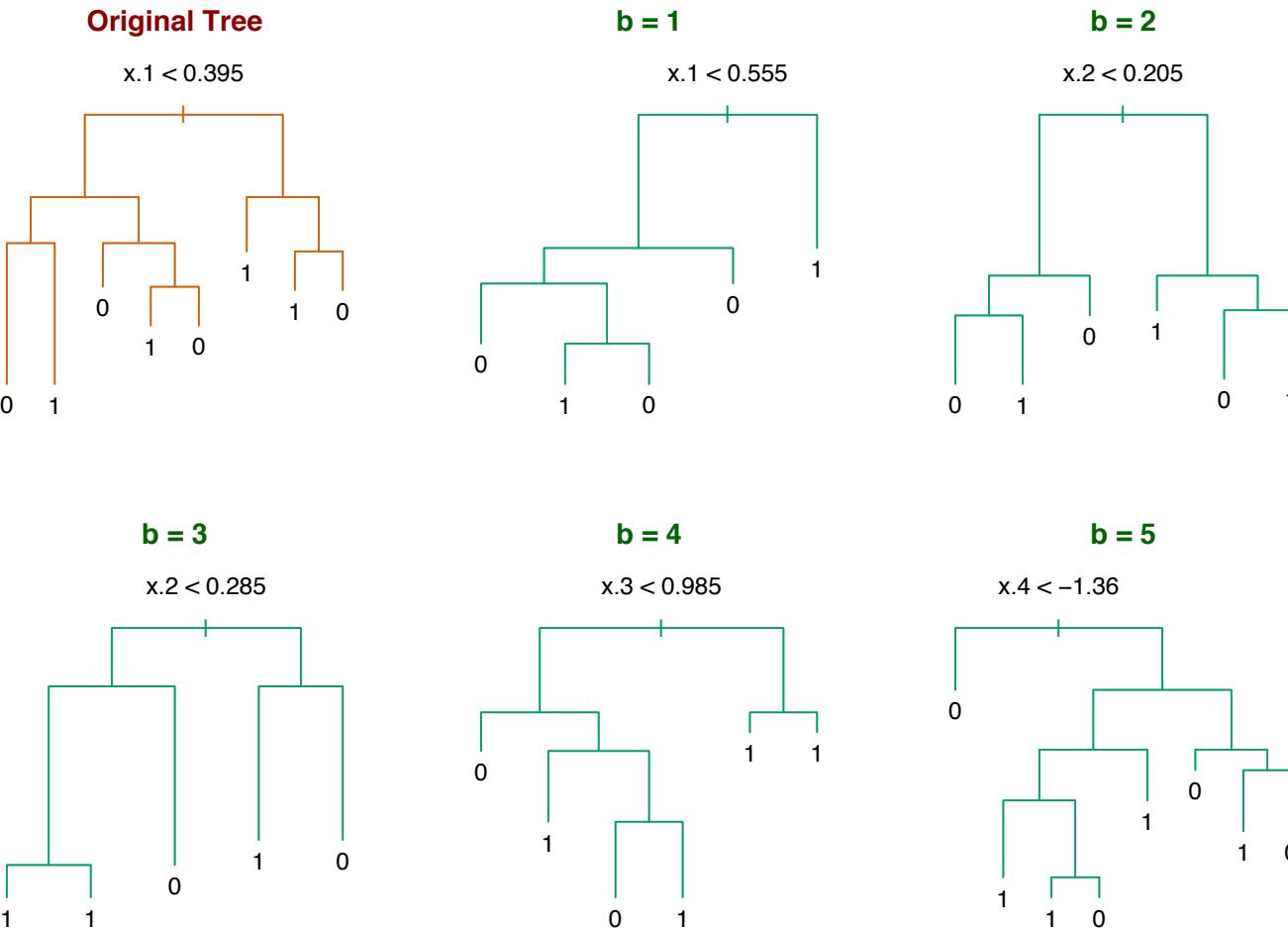
Approach:

- fit classification trees to training sample using 200 bootstrap samples
- No pruning was used
- trees are different (tree induction is *unstable*)
- therefore have high variance

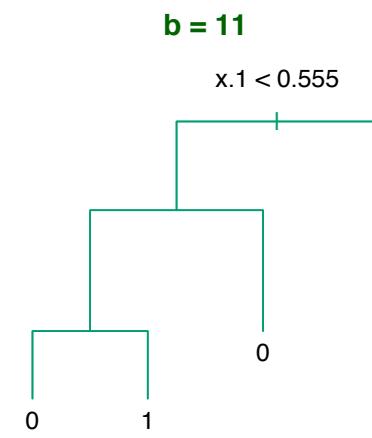
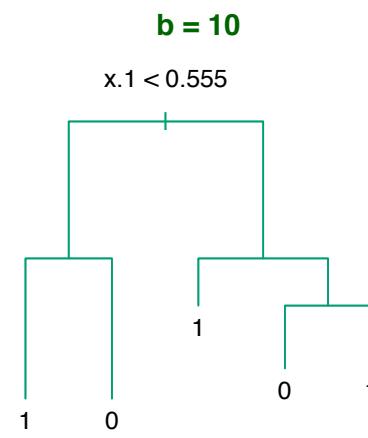
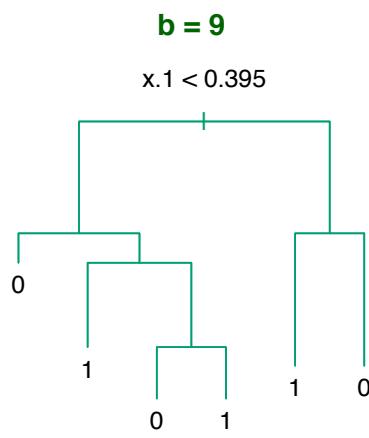
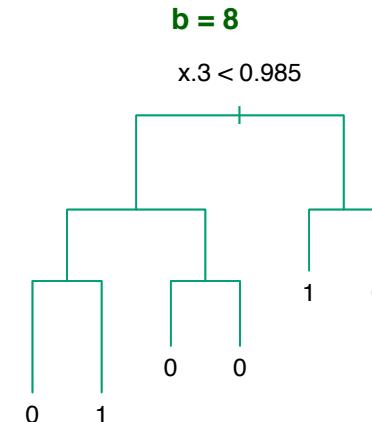
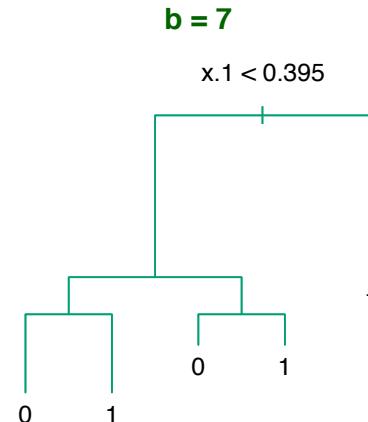
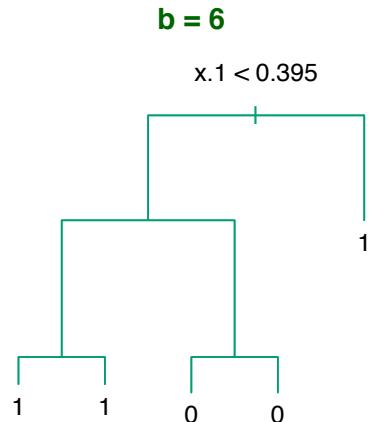
Results:

- averaging reduces variance and leaves bias unchanged

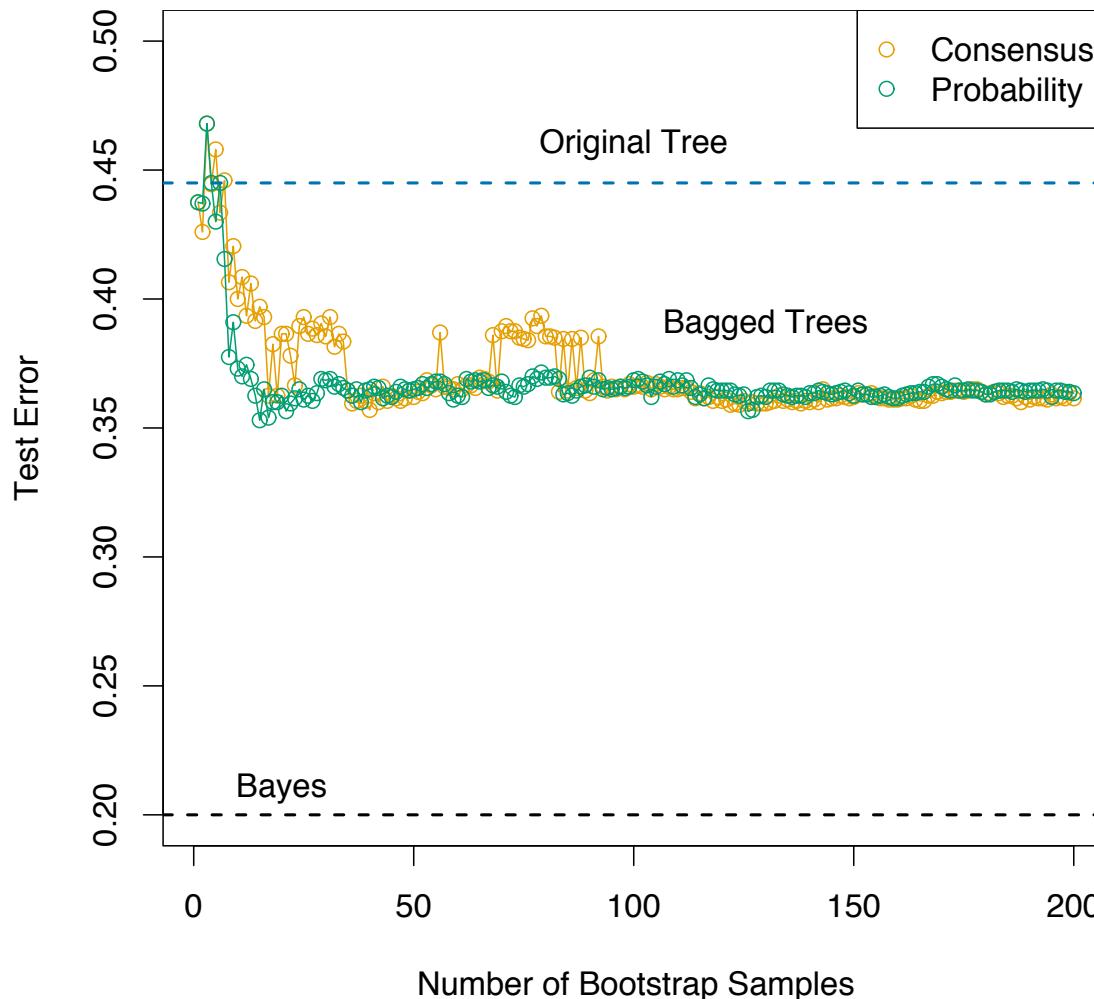
Bagging trees



Bagging trees



Bagging trees



Bagging trees

Pros:

- Reduces the overfitting
- Generalizes better

Cons:

如果数据很多， bagging产生的sample和original data差不多， 也会造成overfitting

- when we bag a model, any simple structure is lost
 - this is because a bagged tree is no longer a tree ... but a forest, so this reduces claim to interpretability
 - *stable* models like nearest neighbor not very affected by bagging but *unstable* models like trees most affected by bagging
- With lots of data, we usually learn the same classifier, so averaging them does not help

Random Forest

随机森林

What is the solution for ensemble decision trees with lots of data?

- Have extra variability in the learners and introduce more randomness to the procedure

How?

- For every model, use only a subset of features
 - This will create diversity in the trees
- Then, similar to before, take average/majority vote over trees (learners)

An ensemble tree with random subset of features is called Random Forest

Random Forests

Algorithm RandomForest(D, T, d) // train ensemble of randomized trees

Input: data set D ; ensemble size T ; subspace dimension d .

Output: set of models; predictions to be combined by voting or averaging.

```
1 for  $t = 1$  to  $T$  do
2     bootstrap sample  $D_t$  from  $D$  by sampling  $|D|$  examples with replacement
3     select  $d$  features at random and reduce dimensionality of  $D_t$  accordingly
4     train a tree model  $M_t$  on  $D_t$  without pruning
5 end
6 return  $\{M_t | 1 \leq t \leq T\}$ 
```

Random Forest (PlayTennis dataset)

Day	Outlook	Temp.	Humidity	Wind	Play
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Random Forest (PlayTennis dataset)

Example:

assign uniform number generator to make samples

Step 1: select 14 samples from the dataset with replacement

Day	Outlook	Temp.	Humidity	Wind	Play
D3	Overcast	Hot	High	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D3	Overcast	Hot	High	Weak	Yes
D8	Sunny	Mild	High	Weak	No
D14	Rain	Mild	High	Strong	No
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D12	Overcast	Mild	High	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D9	Sunny	Cool	Normal	Weak	Yes
D1	Sunny	Hot	High	Weak	No
D14	Rain	Mild	High	Strong	No

Random Forest (PlayTennis dataset)

Example:

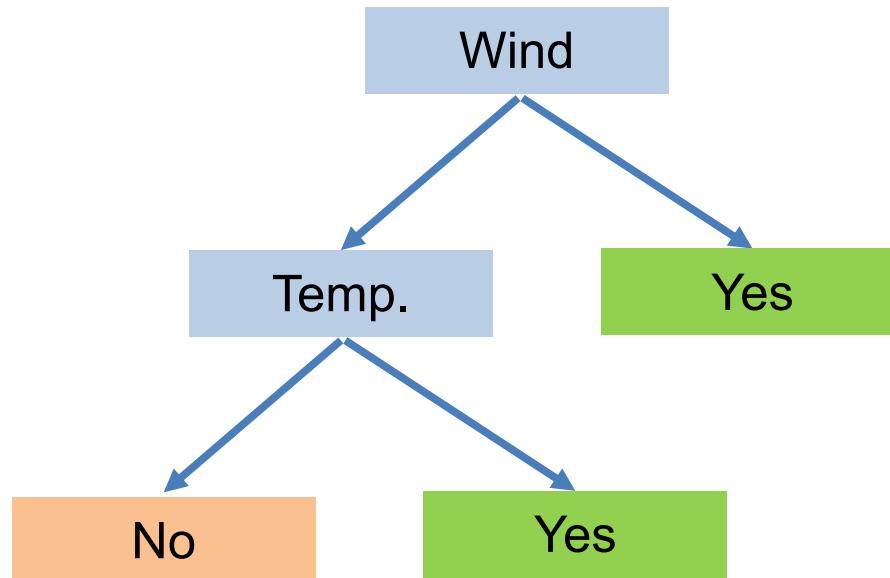
Step 2: select a subset of features randomly (for example 2 features out of 4)

Day	Temp.	Wind	Play
D3	Hot	Weak	Yes
D11	Mild	Strong	Yes
D3	Hot	Weak	Yes
D8	Mild	Weak	No
D14	Mild	Strong	No
D5	Cool	Weak	Yes
D6	Cool	Strong	No
D12	Mild	Strong	Yes
D8	Mild	Weak	No
D9	Cool	Weak	Yes
D10	Mild	Weak	Yes
D11	Mild	Strong	Yes
D9	Cool	Weak	Yes
D1	Hot	Weak	No
D14	Mild	Strong	No

Random Forest (PlayTennis dataset)

Example:

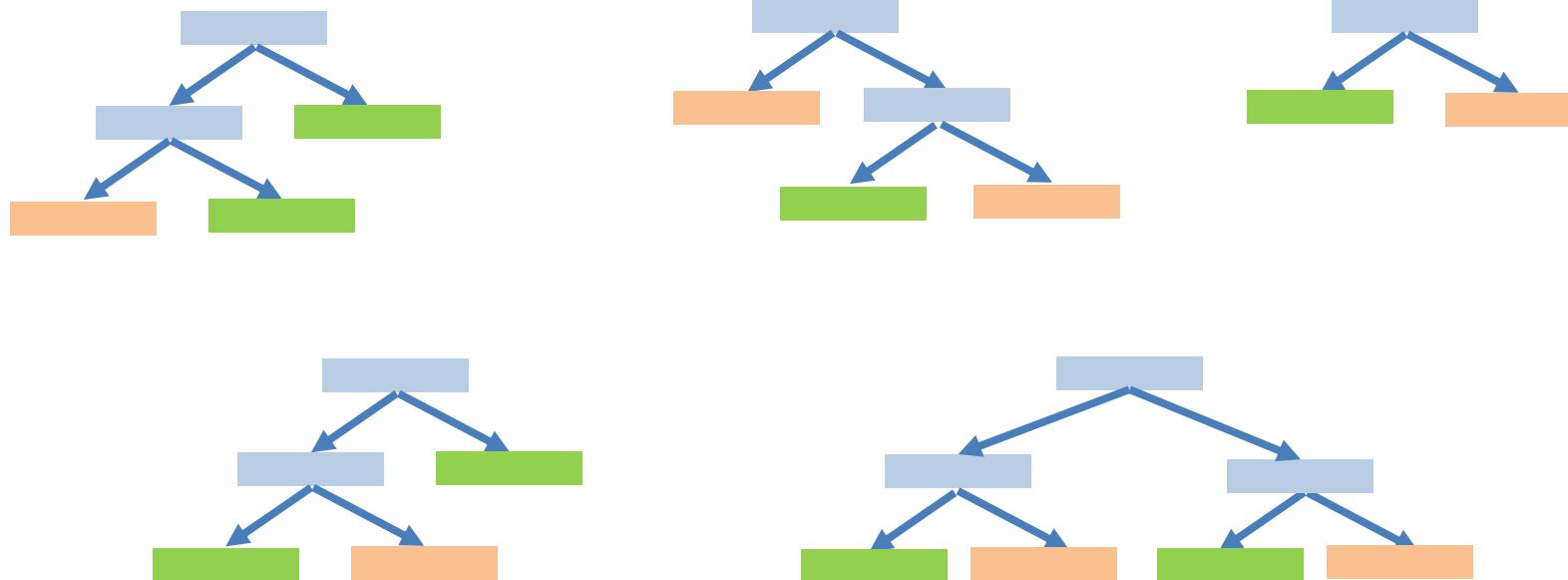
Step 3: build a full tree **without pruning** using the **selected features and samples**



Random Forest (PlayTennis dataset)

Example:

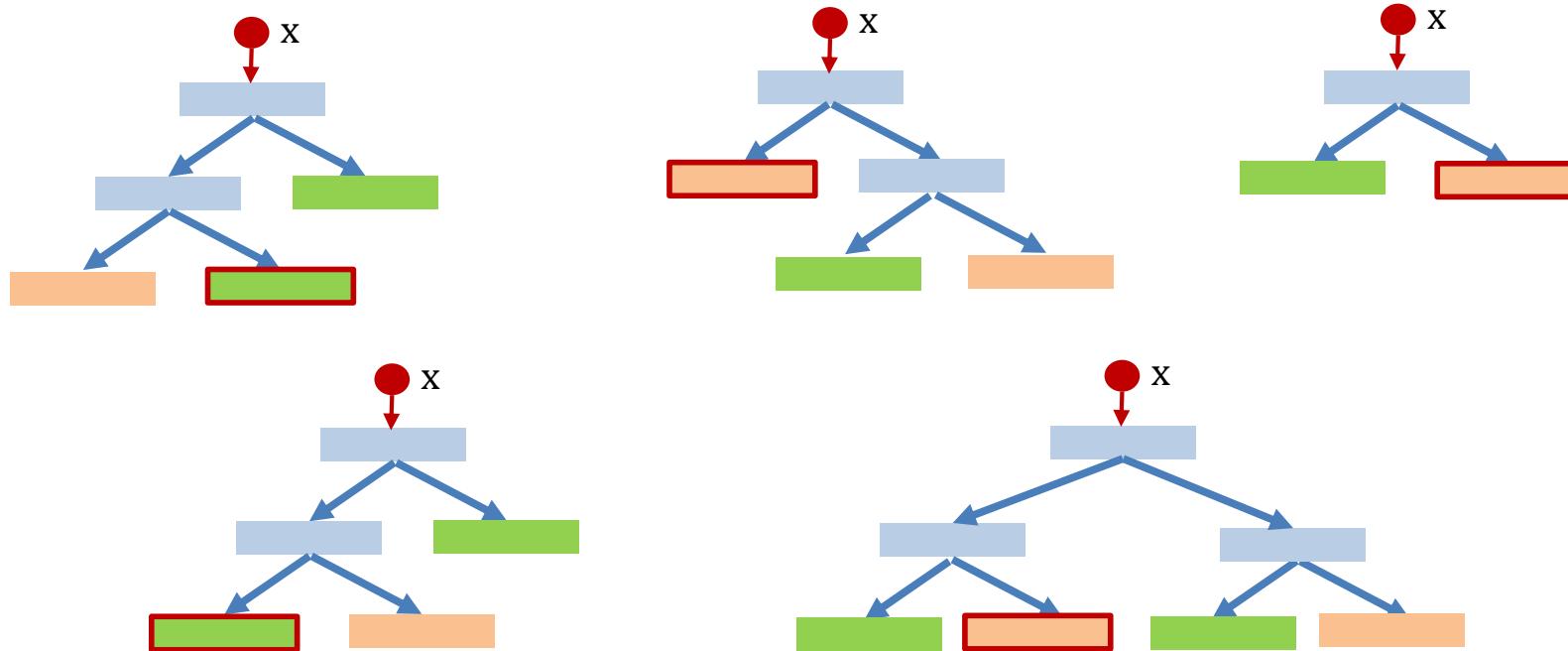
Step 4: Repeat previous steps $T = 5$ times (the value for T can be tuned by using cross validation)



Random Forest (PlayTennis dataset)

Example:

For every new sample, predict the output using all trees and then take the average/majority vote



Random Forests

Leo Breiman's Random Forests algorithm is essentially like Bagging for trees, except the ensemble of tree models is trained from bootstrap samples and random subspaces.

- each tree in the forest is learned from
 - a bootstrap sample, i.e., sample from the training set with **replacement** 有放回的取样
 - a subspace sample, i.e., randomly sample a subset of features
- advantage:
 - forces more diversity among trees in ensemble
 - less time to train since only consider a subset of features

Note: combining linear classifiers in an ensemble gives a piecewise **分段线性** linear (i.e., non-linear) model, whereas multiple trees can be combined into a single tree

Randomization

- Some algorithms already have a random component: e.g., initial weights in a neural net
- Most algorithms can be randomized, e.g., greedy algorithms:
 - Pick N options at random from the full set of options, then choose the best of those N choices
 - E.g.: attribute selection in decision trees
- More generally applicable than bagging: e.g., we can use random subsets of features in a nearest-neighbor classifier
 - Bagging does not work with stable classifiers such as nearest neighbor classifiers
- Can be combined with bagging
 - When learning decision trees, this yields the Random Forest method for building ensemble classifiers