

# Data Mining 2

## Topic 05 : Ensemble Learning

### Lecture 01 : Introduction to Ensemble Learning

Dr Kieran Murphy

Department of Computing and Mathematics, WIT.  
([kmurphy@wit.ie](mailto:kmurphy@wit.ie))

Spring Semester, 2021

#### Outline

- Ensemble learners
- Bootstrapping and Bagging
- Boosting, AdBoost

# Outline

---

1. Introduction	2
1.1. Ensemble Methods	6
1.2. Bias/Variance Tradeoff	8
1.3. Bootstrapping	10
2. Bagging	13
3. Boosting	17

# Motivation

Condorcet's jury theorem is a political science theorem about the relative probability of a given group of individuals arriving at a correct decision:

## Theorem 1 (Condorcet's jury theorem)

*Assume a group of  $n$  independent voters wishes to reach a decision by majority vote. One of the two outcomes of the vote is correct, and each voter has an independent probability,  $p$ , of voting for the correct decision.*

- If  $p > 0.5$ , then adding more voters increases the probability that the majority decision is correct. In the limit, the probability that the majority votes correctly approaches 1 as the number of voters,  $n$ , increases.*
- If  $p < 0.5$  then adding more voters makes things worse: the optimal jury consists of a single voter.*

### Take Home Message

- Even weak decision makers have benefit as long as they individually perform better than chance ( $p > 0.5$ ).
- “Wisdom of Crowds” needs independence!
- What happens if  $p < 0.5$ ?

# Condorcet's Jury Theorem

```
from scipy.stats import binom
nValues = np.array(range(1,41,2))

prob_correct = lambda n,p: 1-binom.cdf(n//2, n, p)

for p in [0.9, 0.8, 0.7, 0.6, 0.55, 0.51]:
    muValues = prob_correct(nValues,p)
    plt.plot(nValues,muValues,label="$p=%s$" % p)

plt.title("Probability of overall correct decision")
plt.xticks(nValues)
plt.legend(loc="center right")
plt.savefig("jury_decision.pdf",bbox_inches="tight")
plt.show()
```

... just calculating cumulative binomial distribution probabilities.

# Condorcet's Jury Theorem

```

from scipy.stats import binom
nValues = np.array(range(1,41,2))

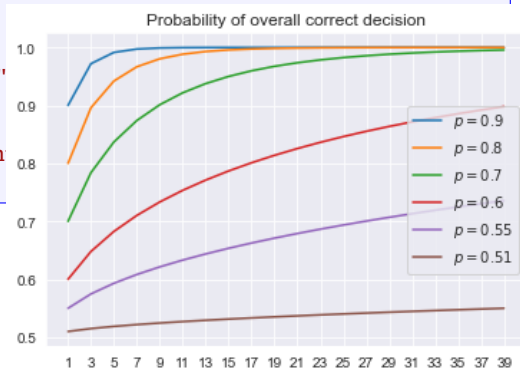
prob_correct = lambda n,p: 1-binom.cdf(n//2, n, p)

for p in [0.9, 0.8, 0.7, 0.6, 0.55, 0.51]:
    muValues = prob_correct(nValues,p)
    plt.plot(nValues,muValues,label="$p=%s$" % p)

plt.title("Probability of overall correct decision")
plt.xticks(nValues)
plt.legend(loc="center right")
plt.savefig("jury_decision.pdf",bbox_inches="tight")
plt.show()

```

... just calculating cumulative binomial distribution probabilities.  
 With enough voters the probability of correct decision approaches one.  
 'enough' gets large for  $p \approx 0.5$ .



# Practical Motivation — Netflix Prize\*

- Open competition to predict user ratings for films, based only on previous ratings.
- Prize was awarded on 2009 to BellKor's Pragmatic Chaos team which bested Netflix's own algorithm for predicting ratings by 10.06%. was an ensemble of 107 modules.

## Leaderboard

Display top  leaders.

Rank	Team Name	Best Score	% Improvement	Last Submit Time
1	<a href="#">The Ensemble</a>	0.8553	10.10	2009-07-26 18:38:22
2	<a href="#">BellKor's Pragmatic Chaos</a>	0.8554	10.09	2009-07-26 18:18:28
<b>Grand Prize - RMSE &lt;= 0.8563</b>				
3	<a href="#">Grand Prize Team</a>	0.8571	9.91	2009-07-24 13:07:49
4	<a href="#">Opera Solutions and Vandelav United</a>	0.8573	9.89	2009-07-25 20:05:52
5	<a href="#">Vandelav Industries I</a>	0.8579	9.83	2009-07-26 02:49:53
6	<a href="#">PragmaticTheory</a>	0.8582	9.80	2009-07-12 15:09:53
7	<a href="#">BellKor in BigChaos</a>	0.8590	9.71	2009-07-26 12:57:25
8	<a href="#">Dace</a>	0.8603	9.58	2009-07-24 17:18:43
9	<a href="#">Opera Solutions</a>	0.8611	9.49	2009-07-26 18:02:08
10	<a href="#">BellKor</a>	0.8612	9.48	2009-07-26 17:19:11
11	<a href="#">BigChaos</a>	0.8613	9.47	2009-06-23 23:06:52
12	<a href="#">Feeds2</a>	0.8613	9.47	2009-07-24 20:06:46
<b>Progress Prize 2008 - RMSE = 0.8616 - Winning Team: BellKor in BigChaos</b>				
13	<a href="#">xiangliang</a>	0.8633	9.26	2009-07-21 02:04:40
14	<a href="#">Gravity</a>	0.8634	9.25	2009-07-26 15:58:34
15	<a href="#">Ces</a>	0.8642	9.17	2009-07-25 17:42:38
16	<a href="#">Invisible Ideas</a>	0.8644	9.14	2009-07-20 03:26:12
17	<a href="#">Just a guy in a garage</a>	0.8650	9.08	2009-07-22 14:10:42
18	<a href="#">Craig Carmichael</a>	0.8656	9.02	2009-07-25 16:00:54
19	<a href="#">J Dennis Su</a>	0.8658	9.00	2009-03-11 09:41:54
20	<a href="#">acmehill</a>	0.8659	8.99	2009-04-16 06:29:35
<b>Progress Prize 2007 - RMSE = 0.8712 - Winning Team: KorBell</b>				
<b>Cinematch score on quiz subset - RMSE = 0.9514</b>				



# Ensemble Methods

## Definition 2 (Ensemble Learner)

An **ensemble learner** is a set of models whose individual decisions are combined in some way to classify new examples.

- Simplest approach:
  - Generate multiple classifiers
  - Each votes on test instance
  - Take majority as classification
- Classifiers are different due to different sampling of training data, or randomised parameters within the classification algorithm.
- Aim: take simple mediocre algorithm and transform it into a super classifier without requiring any fancy new algorithm.
- Differ in training strategy, and combination method:
  - Parallel training with different training sets: **Bagging** or **Cross-validated committees**
  - Sequential training, iteratively re-weighting training examples so current classifier focuses on hard examples: **boosting**
  - Parallel training with objective encouraging division of labor: **mixture of experts**

# Why do Ensemble Methods Work?

## Variance reduction

If the training sets are completely independent, it will always help to average an ensemble because this will reduce variance without affecting bias (e.g., bagging)

- Reduce sensitivity to individual data points.

## Bias reduction

For simple models, average of models has much greater capacity than single model (e.g., hyperplane classifiers, Gaussian densities).

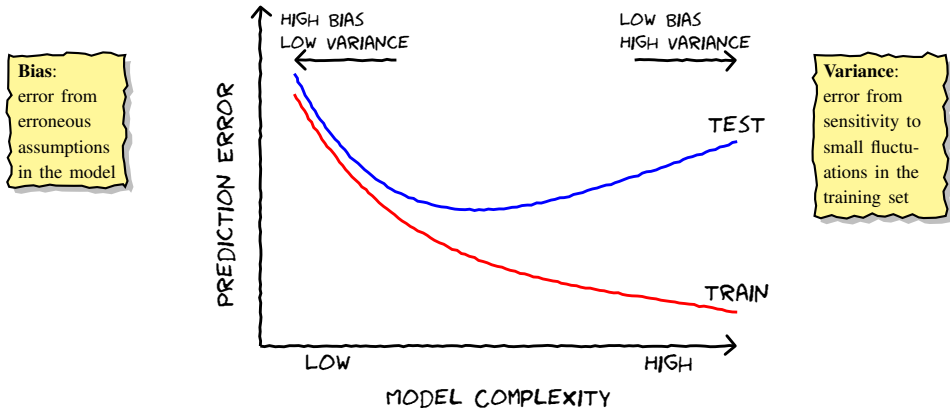
- Averaging models can reduce bias substantially by increasing capacity, and control variance by fitting one component at a time (e.g., boosting)

## Classification vs Regression

- Regression models can be averaged.
- Classification models can be averaged if output is probability of being in a class, otherwise can use majority vote if classifier only outputs class.



# Bias/Variance Tradeoff



- Model too simple then has large bias (as model is too simple to learn signal) but small variance (as model is too simple to learn/be affected by noise).
- Model too complicated then has small bias (as model can learn signal) but has large variance (as model also can learn noise).

# Reduce Variance Without Increasing Bias

It seems that all we can do to is select how complicated our model is to minimise the generalisation error ( $\text{bias}^2 + \text{Var} + \text{noise}$ ). But this is not the case:

- It is possible to reduce variance without affecting bias by averaging.

Averaging reduces variance

- Given  $N$  independent estimates for  $X$ , each with variance of  $\text{Var}(X)$ , we have

$$\text{Var}(\bar{X}) = \frac{\text{Var}(X)}{N}$$

But only if independent!

## One Problem

We have only one training set, so where do multiple models (independent estimates) come from? — apply Bootstrap sampling

### Bootstrap sampling

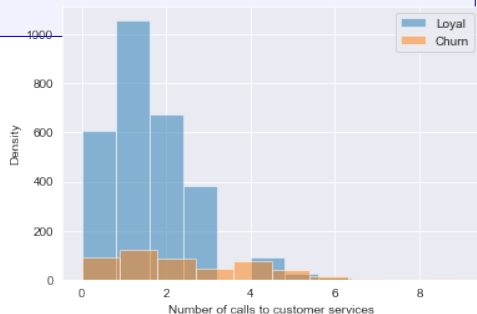
Given set  $D$  containing  $N$  training examples, create  $D'$  by drawing  $N$  examples at random with replacement from  $D$ .

## Example — Bootstrapping for Small Samples

Consider our Churn dataset with only 3333 rows. Lets look at the distribution of Cust\_Serv\_Calls for both the loyal customers and the churning customers ...

```
df.loc[df['Churn']==0,'Cust_Serv_Calls'].hist(label='Loyal',alpha=0.5)
df.loc[df['Churn']==1,'Cust_Serv_Calls'].hist(label='Churn',alpha=0.5)
plt.xlabel('Number of calls to customer services')
plt.ylabel('Density')
plt.legend()
plt.savefig("churn__Cust_Serv_Calls__hist.pdf",bbox="tight")
plt.show()
```

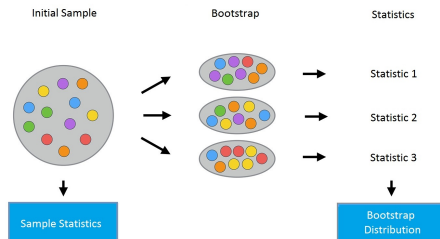
- Looks like loyal customers make fewer calls to customer service than those who eventually leave.
- So we should estimate the average number of customer service calls in each group.
- As dataset is small, we would not get a good estimate by simply calculating the mean of the original samples.
- We would be better off applying the bootstrap method
- ...



# Example — Bootstrapping for Small Samples

Create two utility functions to generate the bootstrap samples and to compute statistic estimates:

- We could have used `np.random.choice` with option `replace=True` to get the same effect.
- $\alpha\%$ -confidence intervals are computed as done back in semester 2.



```
def get_bootstrap_samples(data, n_samples):
    """Generate bootstrap samples using the bootstrap method."""
    indices = np.random.randint(0, len(data), (n_samples, len(data)))
    samples = data[indices]
    return samples

def stat_intervals(stat, alpha):
    """Produce an interval estimate."""
    boundaries = np.percentile(stat, [100*alpha/2, 100*(1-alpha/2)])
    return boundaries
```

# Example — Bootstrapping for Small Samples

Next we split the data set, generate bootstrap samples and resulting confidence intervals ...

```
np.random.seed(42)

loyal_calls = df.loc[df['Churn']==0, 'Cust_Serv_Calls'].values
churn_calls = df.loc[df['Churn']==1, 'Cust_Serv_Calls'].values

# Generate the samples using bootstrapping and calculate the mean
loyal_mean_scores = [np.mean(sample)
    for sample in get_bootstrap_samples(loyal_calls, 1000)]
churn_mean_scores = [np.mean(sample)
    for sample in get_bootstrap_samples(churn_calls, 1000)]

print("Service calls from loyal: mean interval",
      stat_intervals(loyal_mean_scores, 0.05))
print("Service calls from churn: mean interval",
      stat_intervals(churn_mean_scores, 0.05))
```

```
Service calls from loyal: mean interval [1.40700877 1.4922807 ]
Service calls from churn: mean interval [2.06625259 2.38307453]
```

# Outline

---

1. Introduction	2
1.1. Ensemble Methods	6
1.2. Bias/Variance Tradeoff	8
1.3. Bootstrapping	10
2. Bagging	13
3. Boosting	17

# Bagging

aka **B**ootstrap **A**Ggregation

## Method

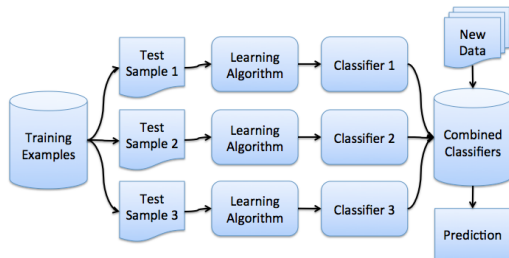
- Create  $M$  bootstrap samples,  $D_1, D_2, \dots, D_M$  of size  $N$ .
  - When picking each element of sample  $D_i$ , each element in  $D$  has probability of  $1/N$  of being selected.
  - The probability of an element of  $D$  not being selected for  $D_i$  is

$$(1 - 1/N)^N \xrightarrow{N \rightarrow \infty} 1/e$$

- Hence the probability of an element of  $D$  being selected for  $D_i$  is  $1 - 1/e = 0.632$ .

A bootstrap sample contains 63% of the original data.

- Separately train classifier on each  $D_i$ .
- Classify new instance by majority vote / average.



\*Leo Breiman (1994)

# Bagging

aka **B**ootstrap **A**Ggregation

## Method

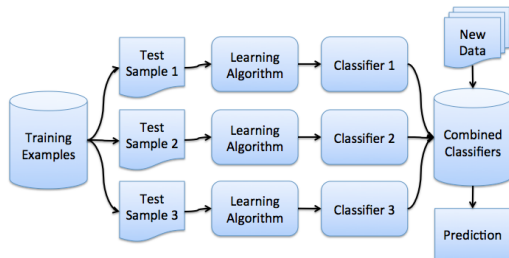
- Create  $M$  bootstrap samples,  $D_1, D_2, \dots, D_M$  of size  $N$ .
  - When picking each element of sample  $D_i$ , each element in  $D$  has probability of  $1/N$  of being selected.
  - The probability of an element of  $D$  not being selected for  $D_i$  is

$$(1 - 1/N)^N \xrightarrow{N \rightarrow \infty} 1/e$$

- Hence the probability of an element of  $D$  being selected for  $D_i$  is  $1 - 1/e = 0.632$ .

A bootstrap sample contains 63% of the original data.

- Separately train classifier on each  $D_i$ .
- Classify new instance by majority vote / average.



\*Leo Breiman (1994)



# Bagging — Performance

## Definition 3 (Unstable learner)

A learner is **unstable** if its output classifier undergoes major changes in response to small changes in training data

- Unstable: decision-tree, neural network, rule learning algorithms, ...
- Stable: linear regression, nearest neighbour, linear threshold algorithms, ...

Bagging tends to

- works well for unstable learners
- can have a mild negative effect on the performance of stable methods

Best Case

$$\text{Var}\left(\text{Bagging}(L(x, D))\right) = \frac{\text{Var}(L(x, D))}{M}$$

However, in practice the models are correlated, so reduction is smaller than  $1/M$ . Also variance of models trained on fewer training cases can be somewhat larger.

# Bagging — Performance

- Bagging reduces the variance of a classifier by decreasing the difference in error when we train the model on different datasets.
- In other words, bagging prevents overfitting.
- The efficiency of bagging comes from the fact that the individual models are quite different due to the different training data and their errors cancel each other out during voting.
- Additionally, outliers are likely omitted in some of the training bootstrap samples.
- Bagging is effective on small datasets.
  - Dropping even a small part of training data leads to constructing substantially different base classifiers.
  - If you have a large dataset, you would generate bootstrap samples of a much smaller size.

## Example

The `skikit-learn` [documentation](#) has a simulation showing the effect of bagging.

# Outline

---

1. Introduction	2
1.1. Ensemble Methods	6
1.2. Bias/Variance Tradeoff	8
1.3. Bootstrapping	10
2. Bagging	13
3. Boosting	17

# Motivation — ‘How May I Help You?’

## Problem

Automatically categorise type of call requested by phone customer (Collect, CallingCard, PersonToPerson, etc.)

- ‘Yes I’d like to place a collect call long distance please’ (Collect)
- ‘Operator I need to make a call but I need to bill it to my office’ (ThirdNumber)
- ‘Yes I’d like to place a call on my master card please’ (CallingCard)
- ‘I just called a number in sioux city and I musta rang the wrong number because I got the wrong party and I would like to have that taken off of my bill’ (BillingCredit)

## Observations

- Easy to find ‘rules of thumb’ that are ‘often’ correct  
e.g. ‘IF "card" occurs in utterance THEN predict ‘CallingCard’
- Hard to find single highly accurate prediction rule.

---

\*Gorin et al

# Boosting Approach

## Outline

- Devise procedure for deriving rough rules of thumb
- Apply procedure to subset of examples
- Obtain rule of thumb
- Apply to 2nd subset of examples
- Obtain 2nd rule of thumb
- Repeat T times

## Key Steps

- How do we choose examples on each round?
  - Concentrate on hardest examples (those most often miss-classified by previous rules of thumb) — focus by sampling or weighing the whole data set.
- How do we combine rules of thumb into a single prediction rule?
  - Take (weighted) majority vote of rules of thumb.

## If Boosting is possible, then

- can use (fairly) wild guesses to produce highly accurate predictions.
- for any learning problem:
  - either can always learn with nearly perfect accuracy
  - or there exist cases where cannot learn even slightly better than random guessing

# Boosting

## Boosting

General method of converting rough rules of thumb into highly accurate prediction rule.

- Assume given ‘weak’ learning algorithm that can consistently find classifiers (‘rules of thumb’) at least slightly better than random, say, accuracy  $\geq 55\%$  (in two-class setting).  
‘weak learning assumption’
- Then given sufficient data, a boosting algorithm can provably construct single classifier with very high accuracy, say, 99%.
- In contrast to bagging which has little effect on Bias, boosting reduces both bias and variance.

### History

Schapire '89 — first provable boosting algorithm

Freund '90 — ‘optimal’ algorithm that ‘boosts by majority’

Freund & Schapire '95 — introduced ‘AdaBoost’ algorithm, strong practical advantages over previous boosting algorithms

# AdaBoost Algorithm

## Outline

- First train the base classifier on all the training data with equal importance weights on each case.

Given weights and data how do we train a classifier?

- Then re-weight the training data to emphasise the hard cases and train a second model.

How do we re-weight the data?

- Repeat above steps.
- Finally, use a weighted committee of all the models for the test data.

How do we weight the models in the committee?

## Notation

- Input: feature matrix,  $X$ ; target vector,  $\mathbf{y} \in \{-1, 1\}$ 
  - Recall:  $X_m$  is  $m$ (th) feature/column and  $X^n$  is  $n$ (th) row/example — superscript represent rows/examples/cases.
- Output:  $m$ (th) classifier predicted output  $f_m(X) = \{-1, 1\}$

# AdaBoost Algorithm — How do we train a classifier?

## Weights

Let  $w_m^n$  represent the weights of example  $n$  for classifier  $m$ . With

$$w_1^n = 1/N$$

Whenever, we change these weights, we will rescale so that they sum to one.

## Training

Given feature matrix,  $X$ , target vector,  $y$  and weights  $w_m^n$ , we train a (weak) classifier using **cost function** for classifier  $m$ :

$$J_m = \sum_{n=1}^N w_m^n \underbrace{[f_m(X^n) \neq y^n]}_{\substack{1 \text{ if error, else } 0}} = \sum \text{weighted errors}$$



# AdaBoost Algorithm — How do we update weights?

- Define the **unnormalized error rate** of a classifier as

$$\epsilon_m = J_m$$

and the **quality of the classifier** as

$$\alpha_m = \frac{1}{2} \ln \left( \frac{1 - \epsilon_m}{\epsilon_m} \right)$$

This is zero if the classifier has weighted error rate of 0.5 and infinity if the classifier is perfect.

- The weights for the next round are then

$$w_{m+1}^n = w_m^n \cdot \frac{\exp\{-\alpha_m y^n f_m(X^n)\}}{\sum_{n=1}^N w_m^n \exp\{-\alpha_m y^n f_m(X^n)\}}$$

Notice the product  $y^n f_m(X^n)$ .

- This is +1 when prediction matches actual and -1 otherwise.
- So  $\exp\{-\alpha_m y^n f_m(X^n)\}$  will be small when prediction matches actual and big otherwise  $\implies$  increases weight for harder cases to focus on them.

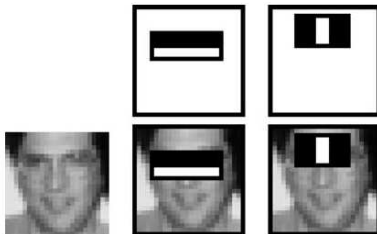
# AdaBoost Algorithm — How do we make predictions?

After  $M$  boosting iterations, we have  $m$  classifiers. To use in prediction of new cases we weight the binary prediction of each classifier by the quality of that classifier:

$$f(X_{\text{test}}) = \text{sign} \left( \sum_{m=1}^M \alpha_m f_m(X_{\text{test}}) \right)$$

## Example Application of boosting

- Viola and Jones created a very fast face detector that can be scanned across a large image to find the faces.



- Two twists on standard algorithm:
  - Pre-define weak classifiers, so optimisation=selection
    - The base classifier/weak learner just compares the total intensity in two rectangular pieces of the image — very fast operation.
  - Change loss function for weak learners: false positives less costly than misses