02450: Introduction to Machine Learning and Data Mining

AUC and ensemble methods

Jes Frellsen

DTU Compute, Technical University of Denmark (DTU)

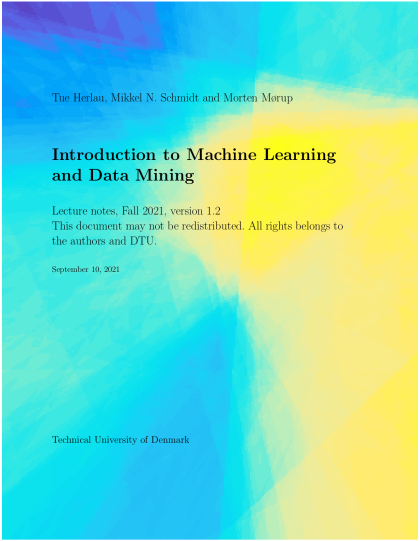
Today

Feedback Groups of the day:

Adrian Roed Schøning, Alaina Ann Martinez, Amanda Aagaard Uldal, Anna Venetsanou, Annette Lien, Antoni Wojciech Skrobisz, Asbjørn Ebenezer Magnussen, Asha Omar Abdirahman Haji, Asta Marie Nielsen, Camilla Lind Ommen, Caroline Ulstrup Larsen, Christian Adam Deding Nielsen, Christine Ibæk Topp Lindenhoff, Claes Jens Sjælborg Lindhardt, Daniel Pedrosa Martin, Danyu Shen, Dmitrij Mordasov, Elea Seidlmann, Emilie Østerdal Nilsson, Frey Emil Vestergaard, Grzegorz Wojciech Zaba, Hans Christian Godballe Lundberg, Harshit Shrivastava, Helene Scheel Wegener, Huanjun Liu, Jakob Malte Skou Lindstad, Jens Peter Sparresø, Jirì Tykva, Johan Kristian Petersen, Johannes Nørskov Toke, Josep Marín Llaó, Kenneth Paulsen, Kevin Thomas Mccabe, Line Egerod Lund, Mads Bundgaard Nørløv, Mads Cort Nielsen, Mads Dudzik Møller, Maria Maniati, Mario Cesar Rodriguez, Marion Motard, Mathilde Albrechtsen Mortensen, Mikkel Ditlev Sjøgren Olsen, Mikkel Thestrup, Niels Peter Lindegaard, Nils Rehtanz, Ole Martin Sørensen, PANAGIOTIS PAPADAMOS, Peter Gustav Rilenter Leunbach, Philip Tinggaard Thomsen, Rafael Parrado Gorga, Saud Abdulaziz A Shaheen, Sebastian Christian Harhoff Pieters, Signe Wulff-Andersen, Tanja Sølvsten, Thomas Spyrou, Torben Truong Nguyen, Txomin Perthuisot, Varun Shankar, Viktor Wilhelm Johannes Nordström, William Frederik Foldøy Steffens, Íris Björk Snorradóttir

Reading material:

Chapter 16, Chapter 17



Lecture Schedule

1. Introduction
   31 August: C1

Data: Feature extraction, and visualization

2. Data, feature extraction and PCA
   7 September: C2, C3
3. Measures of similarity, summary statistics and probabilities
   14 September: C4, C5
4. Probability densities and data visualization
   21 September: C6, C7

Supervised learning: Classification and regression

5. Decision trees and linear regression
   28 September: C8, C9
6. Overfitting, cross-validation and Nearest Neighbor
   5 October: C10, C12 **(Project 1 due before 13:00)**
7. Performance evaluation, Bayes, and Naive Bayes
   12 October: C11, C13
8. Artificial Neural Networks and Bias/Variance
   26 October: C14, C15
9. **AUC and ensemble methods**
   2 November: C16, C17

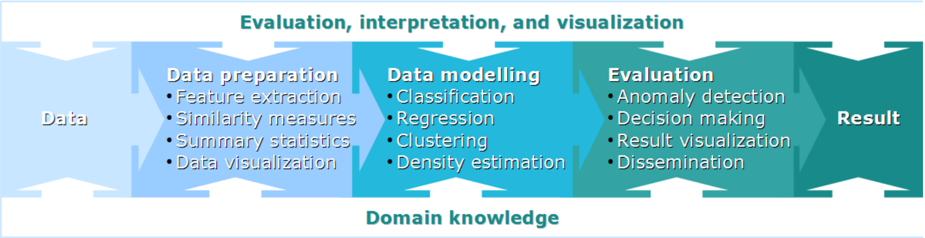
Unsupervised learning: Clustering and density estimation

10. K-means and hierarchical clustering
    9 November: C18
11. Mixture models and density estimation
    16 November: C19, C20 **(Project 2 due before 13:00)**
12. Association mining
    23 November: C21

Recap

13. Recap and discussion of the exam
    30 November: C1-C21

Online help: Forum on DTU Learn
Videos of lectures: `https://video.dtu.dk`
Streaming of lectures: Zoom (link on DTU Learn)

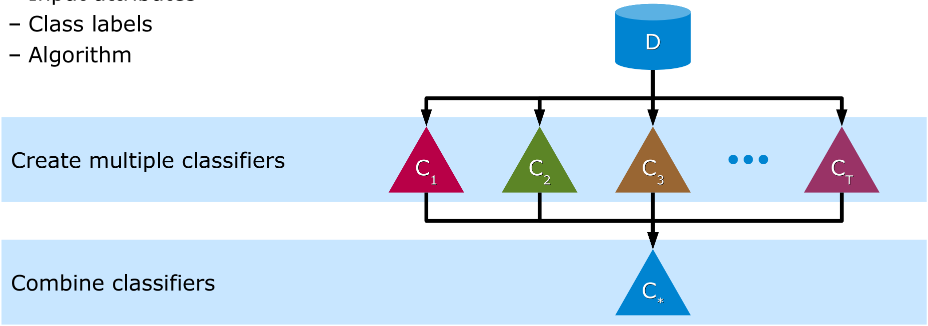


Learning Objectives

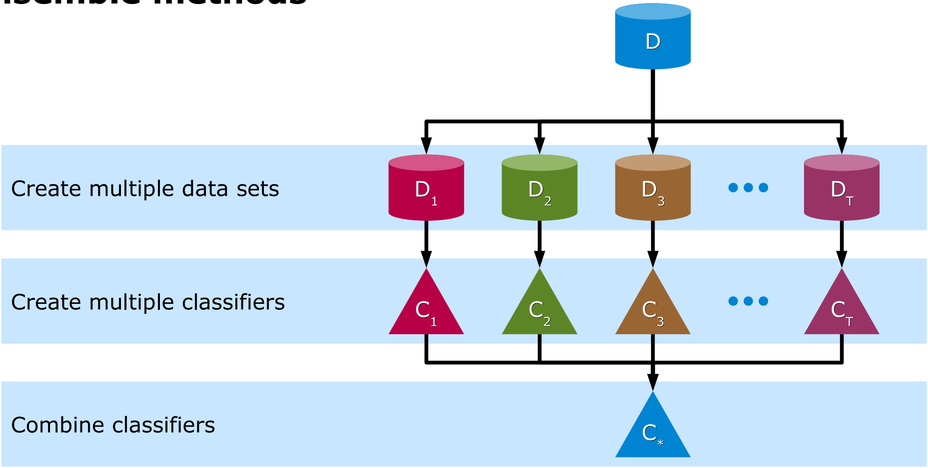
- Explain the principle behind boosting and bagging and apply it to improve classifiers
- Be able to address issues of class-imbalance and resampling
- Understand the definition of Precision, Recall, ROC, and AUC

Ensemble methods

- Combine multiple (weak) classifiers into one (strong) classifier
- Each classifier trained using different variations of
  - Data set
  - Input attributes
  - Class labels
  - Algorithm



Ensemble methods

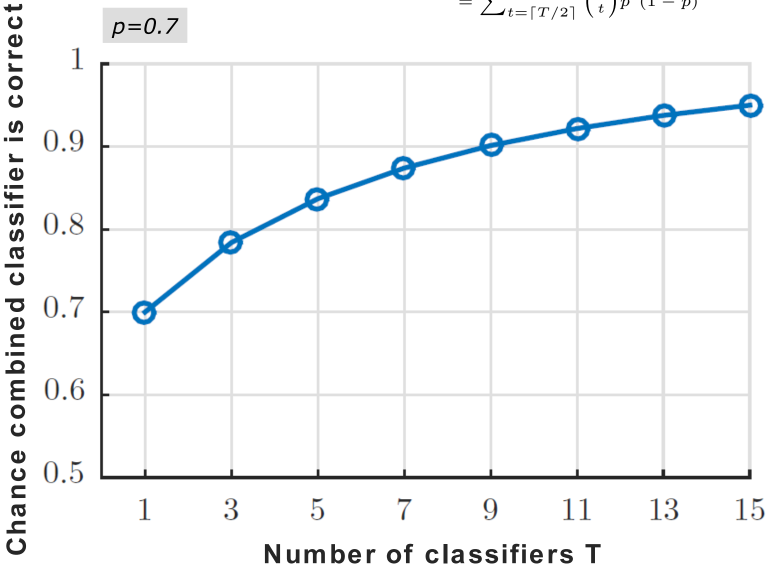


Why ensemble methods?

- Can improve classification algorithms in terms of
  - Better classification accuracy
  - Increased stability
  - Reduced variance
  - Less overfitting
- Consider T independent classifiers for binary classification, each with accuracy p.
- The probability a classifier which use majority voting is correct is then given by:

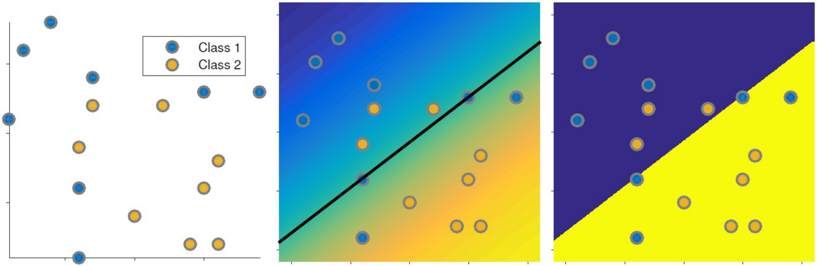
$$
\begin{aligned}
P(\text{Majority voting is correct}) &= \sum_{t=\lceil T/2 \rceil}^{T} P(\{t \text{ classifiers are correct}\}) \\
&= \sum_{t=\lceil T/2 \rceil}^{T} \binom{T}{t} p^t (1-p)^{T-t}
\end{aligned}
$$

$$P(\text{Majority voting is correct}) = \sum_{t=\lceil T/2 \rceil}^{T} P(\{t \text{ classifiers are correct}\})$$
$$= \sum_{t=\lceil T/2 \rceil}^{T} \binom{T}{t} p^t (1-p)^{T-t}$$



Data example

- Classification using logistic regression

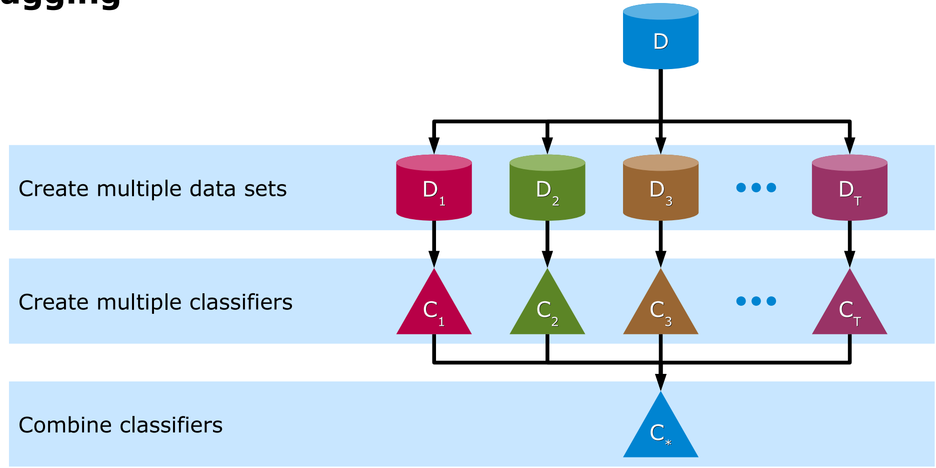


Bagging

- New training data sets drawn randomly from pool with replacement

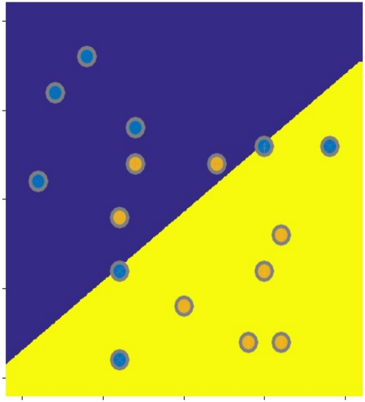
Pool of training data	1	2	3	4	5	6	7	8	9	10
New training data sets	3	5	4	3	9	7	9	5	1	1
	5	8	2	6	2	3	8	3	5	1
	1	7	4	1	10	6	10	8	8	7
					⋮					
	4	3	8	5	2	4	7	10	10	8

Bagging

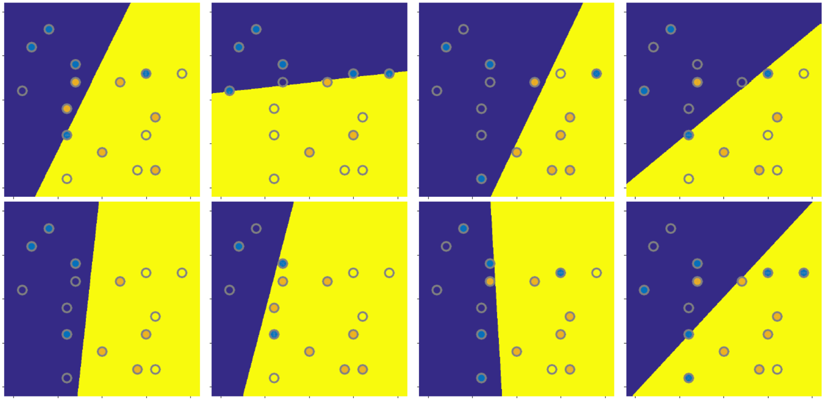

D
Create multiple data sets
D_1
D_2
D_3
D_T
Create multiple classifiers
C_1
C_2
C_3
C_T
Combine classifiers
C_*

Bagging

- **Single classifier**
  - Logistic regression
  - Two features, (x,y)



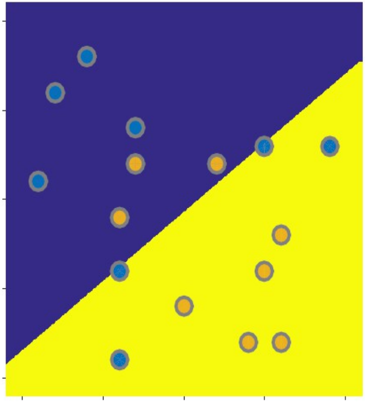
Bagging



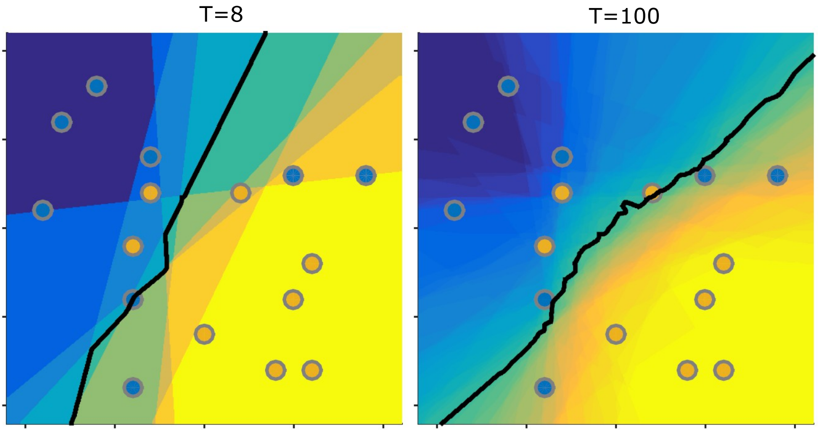
Notice, hollow dots are observations not included in bagging round

Bagging

- Single classifier



Bagging

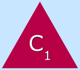


Boosting

Pool of training data	1	2	3	4	5	6	7	8	9	10
Weights	.1	.1	.1	.1	.1	.1	.1	.1	.1	.1

New training data set	3	5	4	3	9	7	9	5	1	1

Train classifier



Boosting

Pool of training data	1	2	3	4	5	6	7	8	9	10
Weights	.1	.1	.1	.1	.1	.1	.1	.1	.1	.1

New training data set	3	5	4	3	9	7	9	5	1	1

Train classifier C_1

Classify all data objects	1 ✓	2 ✗	3 ✓	4 ✗	5 ✓	6 ✗	7 ✓	8 ✓	9 ✓	10 ✓

Boosting

Pool of training data	1	2	3	4	5	6	7	8	9	10
Weights	.1	.1	.1	.1	.1	.1	.1	.1	.1	.1

New training data set	3	5	4	3	9	7	9	5	1	1

Train classifier

C_1

Classify all data objects	1 ✓	2 ✗	3 ✓	4 ✗	5 ✓	6 ✗	7 ✓	8 ✓	9 ✓	10 ✓
Update weights	.07	.17	.07	.17	.07	.17	.07	.07	.07	.07

Boosting

Pool of training data	1	2	3	4	5	6	7	8	9	10
Weights	.1	.1	.1	.1	.1	.1	.1	.1	.1	.1

New training data set	3	5	4	3	9	7	9	5	1	1

Train classifier

C_1

Classify all data objects	1 ✓	2 ✗	3 ✓	4 ✗	5 ✓	6 ✗	7 ✓	8 ✓	9 ✓	10 ✓
Update weights	.07	.17	.07	.17	.07	.17	.07	.07	.07	.07

New training data set	6	4	7	3	2	4	10	2	5	6

Train classifier

C_2

⋮

AdaBoost

Algorithm 6: AdaBoost algorithm

1: Initialize $w_i(1) = \frac{1}{N}$ for $i = 1, \ldots, N$
2: **for** $t = 1, \ldots, T$ **do**
3: Create $\mathcal{D}_t$ by sampling (with replacement) from $\mathcal{D}$ according to $\boldsymbol{w}(t)$
4: Let f_t be the classifier *trained* on $\mathcal{D}_t$
5: $\epsilon_t = \sum_{i=1}^{N} w_i(t) \left(1 - \delta_{f_t(\boldsymbol{x}_i), y_i}\right)$ *(weighted error of f_t on all data).*
6: $\alpha_t = \frac{1}{2} \log \frac{1-\epsilon_t}{\epsilon_t}$
7: For each i update weights using eq. (15.7):

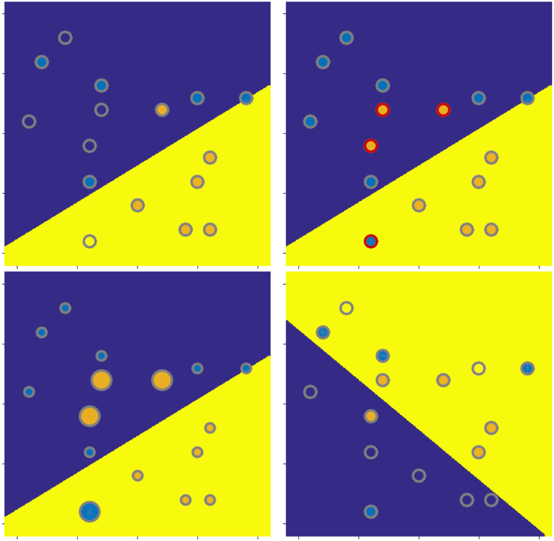
$$w_i(t+1) = \frac{\tilde{w}_i(t+1)}{\sum_{j=1}^{N} \tilde{w}_j(t+1)}, \quad \tilde{w}_i(t+1) = \begin{cases} w_i(t)e^{-\alpha_t} & \text{if } f_t(\boldsymbol{x}_i) = y_i \\ w_i(t)e^{\alpha_t} & \text{if } f_t(\boldsymbol{x}_i) \neq y_i. \end{cases}$$

8: **end for**
9: $f^*(\boldsymbol{x}) = \arg\max_{y=1,2} \sum_{t=1}^{T} \alpha_t \delta_{f_t(\boldsymbol{x}), y}$ *(Majority voting classifier)*

Boosting

A:
A dataset is sampled with replacement and a classifier trained.

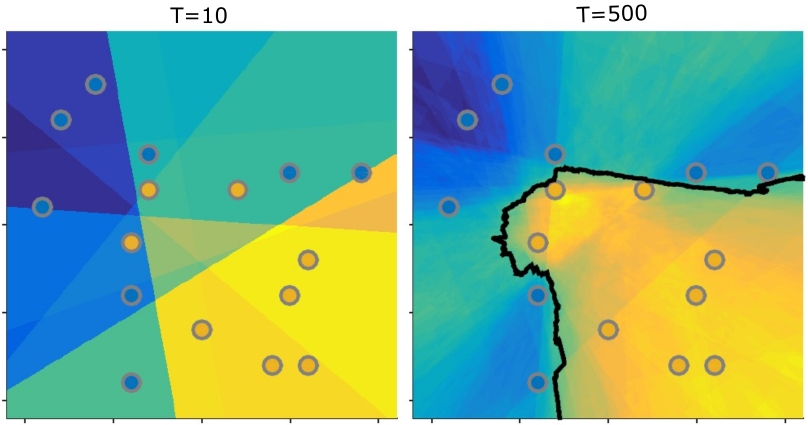
B:
Mis-classified observations are identified.



C:
Weighs are updated such that more emphasis is given to these mis-classified observations.

New round:
Based on the updated weights a new dataset is sampled and a classifier trained (shown), mis-classified observations identified and given more emphasis...

Boosting

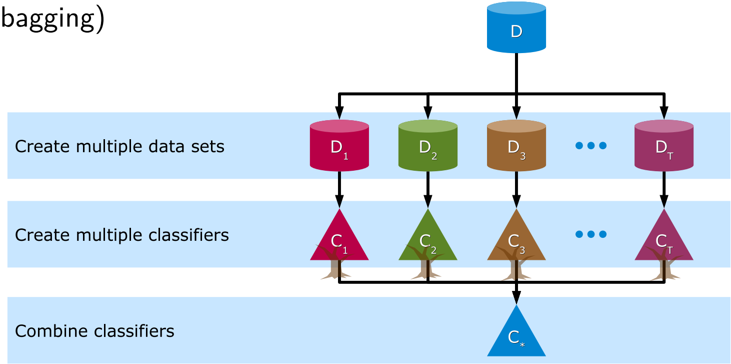


Bagging example: Random forest

Each tree is generated as follows:

- Sample dataset with replacement
- When generating each node in the tree, randomly select a subset of the features and only consider splits using these features

A large number of trees are generated and the trees are combined using majority voting (bagging)



Quiz 1 (please answer on Piazza): Adaboost (Spring 2016)

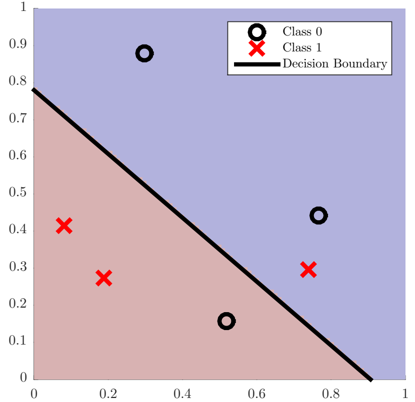


Figure 1: A binary classification problem and the decision boundary obtained by logistic regression. Observations left of the boundary are classified as belonging to the positive class 1 (red crosses) and observations right of the boundary to the negative class 0 (black circles)

We wish to apply a logistic regression model to the binary classification problem shown in Figure 1. We attempt to improve the performance by applying AdaBoost. AdaBoost works by first sampling a new dataset with replacement, then training a classifier on the dataset and then proceeding with the subsequent steps of the AdaBoost algorithm.

Suppose in the first iteration of the AdaBoost algorithm the classification boundary of the trained classifier is as indicated by the black line (i.e. observations left of the black line are classified as in the positive class). What is the resulting value of the weights $\boldsymbol{w}$?

A. $\boldsymbol{w} = \begin{bmatrix} 0.125 & 0.250 & 0.125 & 0.125 & 0.125 & 0.250 \end{bmatrix}$

B. $\boldsymbol{w} = \begin{bmatrix} 0.026 & 0.447 & 0.026 & 0.026 & 0.026 & 0.447 \end{bmatrix}$

C. $\boldsymbol{w} = \begin{bmatrix} 0.235 & 0.029 & 0.235 & 0.235 & 0.235 & 0.029 \end{bmatrix}$

D. $\boldsymbol{w} = \begin{bmatrix} 0.1 & 0.3 & 0.1 & 0.1 & 0.1 & 0.3 \end{bmatrix}$

E. Don't know.

(Hint: First compute ε_1, then α_1, then the weights)

Class imbalance problem

- Many data sets have **imbalanced class distributions**
  - Example: Detection of defects that only occur rarely (e.g. 1/1,000,000)
  - Danger: Algorithm that says nothing is defect will be 99.999% correct

- **Solution approaches**
  - Resample to balance data sets
  - Modify existing classification algorithms
  - Measure performance in a way that takes balance into account

Resampling balanced data

- New sample has equal number of data objects from each class

- **Approaches**
  - **Undersampling** majority class: Throws out potentially useful data
  - **Oversampling** minority class: Increase data size and computational burden
  - **Somewhere in between**…

Imbalanced training data	1	2	3	4	5	6	7	8	9	10
Oversampling	1	2	3	4	5	7	9	10	6	6
	6	6	8	8	8	8				
Undersampling	3	5	6	8						
Somewhere in between	3	5	4	3	9	6	6	8	8	8

Confusion matrix

		Predicted	
		positive	*negative*
Actual	*positive*	TP True Positive	FN False Negative
	negative	FP False Positive	TN True Negative

Precision and recall

- **Precision**
  - Fraction of true positive among objects predicted to be positive

$$p = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$$

- **Recall**
  - Fraction of objects predicted to be positive among all positive objects

$$r = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}$$

		Predicted	
		positive	*negative*
Actual	*positive*	TP True Positive	FN False Negative
	negative	FP False Positive	TN True Negative

Quiz 2 (please answer on Piazza): Precision/Recall

Consider two different classifiers, and suppose on a test set with 20 positive observations:

- Classifier 1 detects 54 positive of which 18 are actually positive
- Classifier 2 detects 16 positive of which 14 are actually positive

		Predicted: positive	Predicted: negative
Actual	positive	**TP** True Positive	**FN** False Negative
	negative	**FP** False Positive	**TN** True Negative

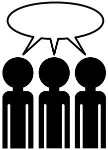
What is the precision and recall of the two classifiers?

A. Classifier 1: $p_1 = \frac{2}{3}, r_1 = \frac{7}{10}$
   Classifier 2: $p_2 = \frac{1}{3}, r_2 = \frac{1}{3}$

B. Classifier 1: $p_1 = \frac{1}{3}, r_1 = \frac{9}{10}$
   Classifier 2: $p_2 = \frac{2}{3}, r_2 = \frac{9}{10}$

C. Classifier 1: $p_1 = \frac{2}{3}, r_1 = \frac{7}{10}$
   Classifier 2: $p_2 = \frac{1}{3}, r_2 = \frac{9}{10}$

D. Classifier 1: $p_1 = \frac{1}{3}, r_1 = \frac{9}{10}$
   Classifier 2: $p_2 = \frac{7}{8}, r_2 = \frac{7}{10}$



Which classifier would you use if the objective was to detect credit-card fraud (the positive class corresponds to fraud)

- **Precision**
  - Fraction of true positive among objects predicted to be positive

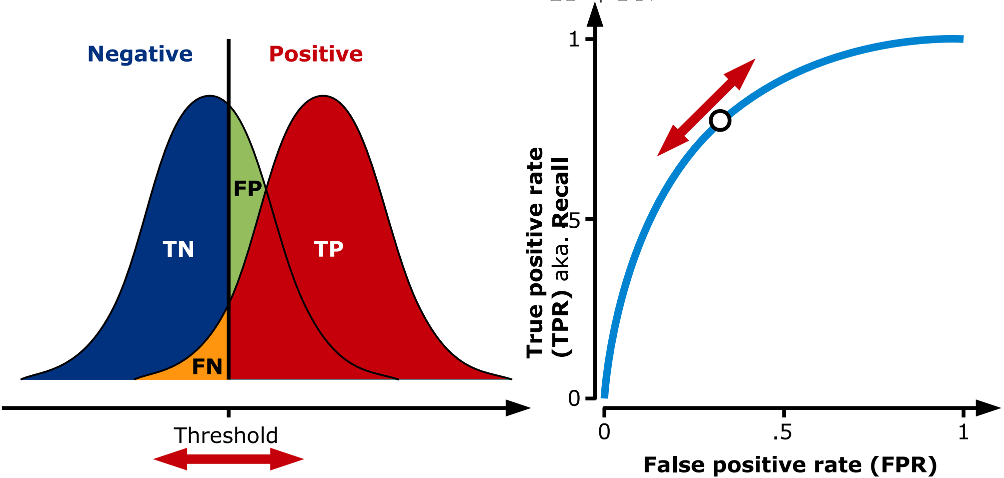
$$p = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$$

- **Recall**
  - Fraction of objects predicted to be positive among all positive objects

$$r = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}$$

Receiver operating characteristic

$$\mathrm{TPR} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}$$

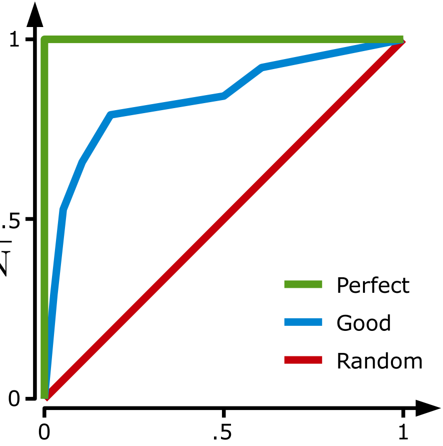


$$\mathrm{FPR} = \frac{\mathrm{FP}}{\mathrm{TN} + \mathrm{FP}}$$

Receiver operating characteristic

True positive rate
aka. **Recall**

$$\mathrm{TPR} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}$$



False positive rate

$$\mathrm{FPR} = \frac{\mathrm{FP}}{\mathrm{TN} + \mathrm{FP}}$$

Quiz 3 (please answer on Piazza): AUC (Spring 2017)

	3 gears ($x_5 = 3$)	4 gears ($x_5 = 4$)	5 gears ($x_5 = 5$)
Low mpg ($y = 0$)	13	2	2
High mpg ($y = 1$)	2	10	3

Table 1: Number of low mpg and high mpg cars (i.e. $y = 0$ and $y = 1$) according to the number of gears, i.e. $x_5 = 3$, $x_5 = 4$, or $x_5 = 5$.

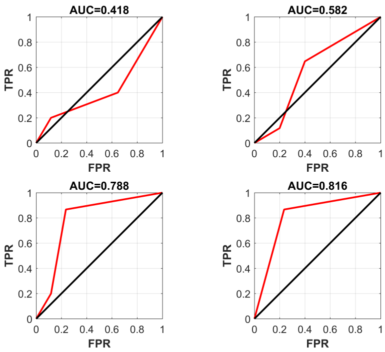


Figure 1: Four different receiver operator characteristic (ROC) curves and their area under curve (AUC) value.

A dataset representing cars contain an attribute x_5 corresponding to the number of gears. We wish to evaluate how well the number of gears predict low mpg, ($y = 0$, considered the negative class) from high mpg, ($y = 1$, considered the positive class) based on the data given in Table 1. For this purpose, we will evaluate the area under curve (AUC) of the receiver operator characteristic (ROC) using the feature x_5. Which one of the ROC curves given in Figure 1 corresponds to using x_5 to discriminate between low mpg ($y = 0$) and high mpg ($y = 1$)?

A. The curve having AUC=0.418

B. The curve having AUC=0.582

C. The curve having AUC=0.788

D. The curve having AUC=0.816

E. Don't know.

(Hint: Select a value e.g. $x_5 = 4$. We then predict cars with 4 or more gears as being in the positive class and otherwise negative. Compute the FPR and TPR using this prediction and use the (FPR, TPR) values to discriminate between the curves)

Resources

https://www.youtube.com Video tutorial on ROC curve and AUC (https://www.youtube.com/watch?v=OAl6eAyP-yo)

https://towardsdatascience.com More in-depth discussion of the Random Forrest algorithm and parameter choices (https://towardsdatascience.com/the-random-forest-algorithm-d457d499ffcd)

https://www.datacamp.com Practical use of the random forrest algorithm in python (https://www.datacamp.com/community/tutorials/random-forests-classifier-python)

https://citeseerx.ist.psu.edu Justification for the AdaBoost algorithm (technical) (https://citeseerx.ist.psu.edu/viewdoc/summary?doi=10.1.1.51.9525)