



Classical Machine Learning: Classification and Regression (IV)

Learning Objectives

- Learn how to choose the *best* machine learning model.
- Learn how to deal with class imbalance problems (with some useful performance metrics).

Compare and choose machine learning model

Choose the “best” machine learning model

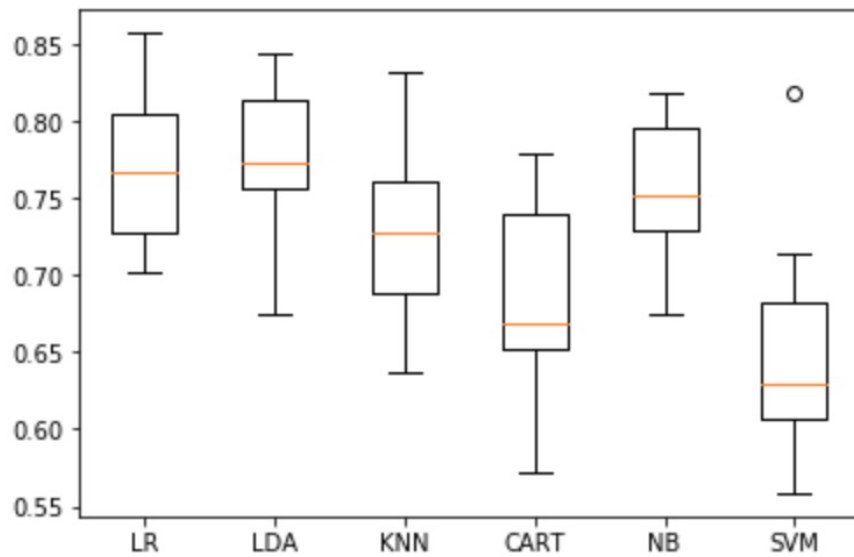


Model_compare.ipynb

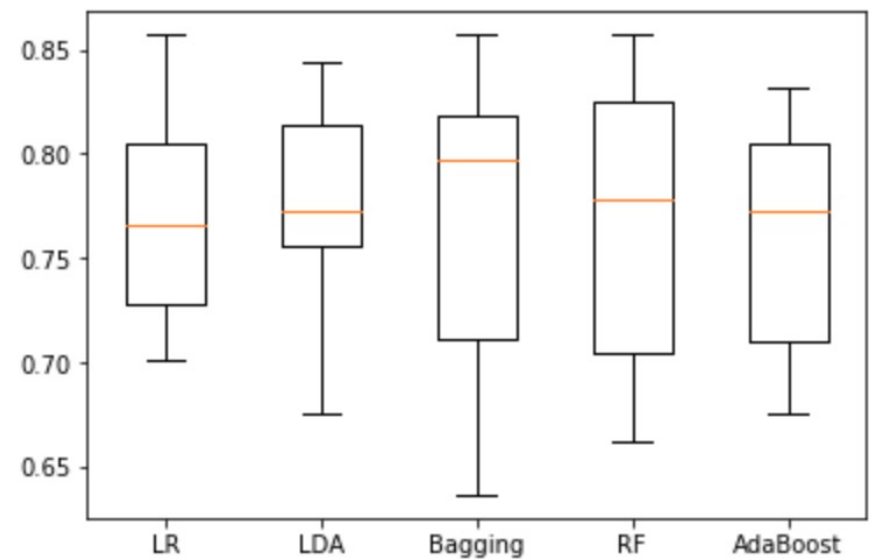
- Learning algorithm $\mathcal{A}$ depends on training examples $\mathcal{D}$ and hypothesis set $\mathcal{H}$ and there is no single learning algorithm dominated for every kind of data. (No free lunch!)
- You cannot know which algorithms are best suited to your problem beforehand.
- When comparing performance of different algorithms, make sure each algorithm is evaluated in the same way on the same data.



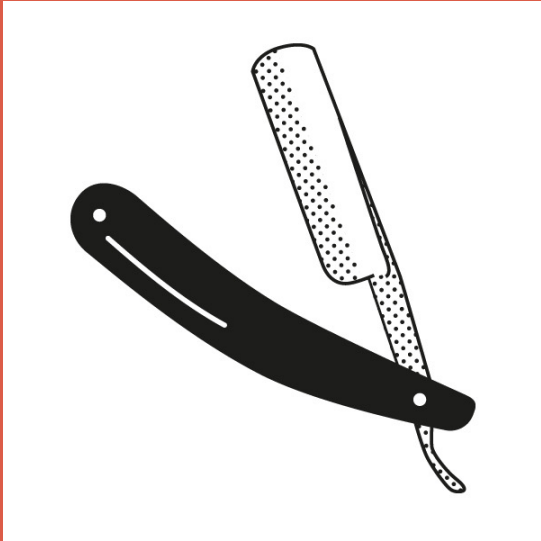
Algorithm Comparison



Algorithm Comparison



Learning Principle: Occam's Razor



Occam's Razor: The simplest model that fits the data is also the most plausible (合理).

- Occam's razor in machine learning means simpler model has a better chance of being right. However, if a complex explanation of the data performs better, we will take it.
- The argument that simpler has a better chance of being right goes as follows. With complex hypotheses, there would be enough of them to fit the data set regardless of what the labels are, even if these are completely random. Therefore, fitting the data does not mean much.
- If, instead, we have a simple model with few hypotheses and we still found one that perfectly fits. This is surprising, and therefore it means some thing.

Class imbalance problems and some alternative performance metrics

Class Imbalance Problem

- Lots of classification problems where the classes are skewed (more records from one class than another)
 - ✓ – Credit card fraud
 - ✓ – Intrusion detection
 - – Defective products in manufacturing assembly line
 - COVID-19 test results on a random sample
- Key Challenge:
 - Evaluation measures such as accuracy are not well-suited for imbalanced class

Class Imbalance Techniques

- **Choose better performance metrics**
- **Balance skewed classes**
- **Cost-sensitive learning**

Confusion Matrix

- Confusion Matrix:

ACTUAL CLASS	PREDICTED CLASS	
	Class=Yes	Class=No
	Class=Yes	Class=No
	Class=Yes	Class=No
	a	b
	c	d

a: TP (true positive)

b: FN (false negative)

c: FP (false positive)

d: TN (true negative)

Accuracy

ACTUAL CLASS	PREDICTED CLASS	
	Class=Yes	Class=No
	Class=Yes	Class=No
	a ✓ (TP)	b (FN)
	c (FP)	d ✓ (TN)

- Most widely-used metric:

$$\text{Accuracy} \equiv \frac{a + d}{a + b + c + d} \equiv \frac{TP + TN}{TP + TN + FP + FN}$$

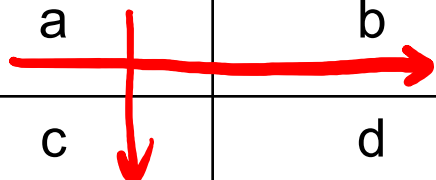
Problem with Accuracy

- Consider a 2-class problem
 - Number of Class NO examples = 990
 - Number of Class YES examples = 10
- If a model predicts everything to be class NO, accuracy is $990/1000 = 99\%$
 - This is misleading because this trivial model does not detect any class YES example
 - Detecting the rare class is usually more interesting (e.g., frauds, intrusions, defects, etc)

	PREDICTED CLASS		
		Class=Yes	Class=No
	Class=Yes	0	10
	Class=No	0	990

Alternative Measures

		PREDICTED CLASS	
ACTUAL CLASS		Class=Yes	Class=No
	Class=Yes	a	b
	Class=No	c	d



$$\text{Precision (p)} = \frac{a}{a + c}$$

$$\text{Recall (r)} = \frac{a}{a + b}$$

$$\text{F - measure (F)} = \frac{2rp}{r + p} = \frac{2a}{2a + b + c}$$

Alternative Measures

ACTUAL CLASS	PREDICTED CLASS		
		Class=Yes	Class=No
	Class=Yes	10	0
	Class=No	10	980

$$\text{Precision (p)} = \frac{10}{10+10} = 0.5$$

$$\text{Recall (r)} = \frac{10}{10+0} = 1$$

$$\text{F - measure (F)} = \frac{2 * 1 * 0.5}{1 + 0.5} = 0.62$$

$$\text{Accuracy} = \frac{990}{1000} = 0.99$$

ACTUAL CLASS	PREDICTED CLASS		
		Class=Yes	Class=No
	Class=Yes	1	9
	Class=No	0	990

$$\text{Precision (p)} = \frac{1}{1+0} = 1$$

$$\text{Recall (r)} = \frac{1}{1+9} = 0.1$$

$$\text{F - measure (F)} = \frac{2 * 0.1 * 1}{1 + 0.1} = 0.18$$

$$\text{Accuracy} = \frac{991}{1000} = 0.991$$

Recall (查全率) and Precision (精確率)

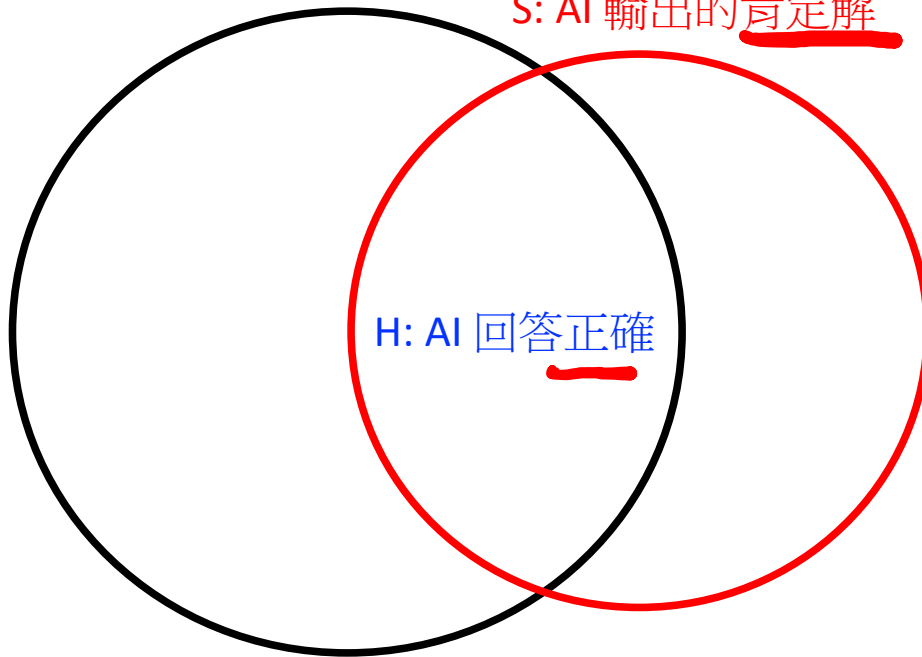
ACTUAL CLASS	PREDICTED CLASS	
	Class=Yes	Class=No
	Class=Yes	Class=No
	a	b
	c	d

$$\text{Recall} = \frac{a}{a+b}$$

$$\text{Precision} = \frac{a}{a+c}$$

A: 所有的肯定解

S: AI 輸出的肯定解



0 10
0 990

$$\text{Recall (查全率)} = \frac{H}{A}$$

$$\text{Precision (精確率)} = \frac{H}{S}$$

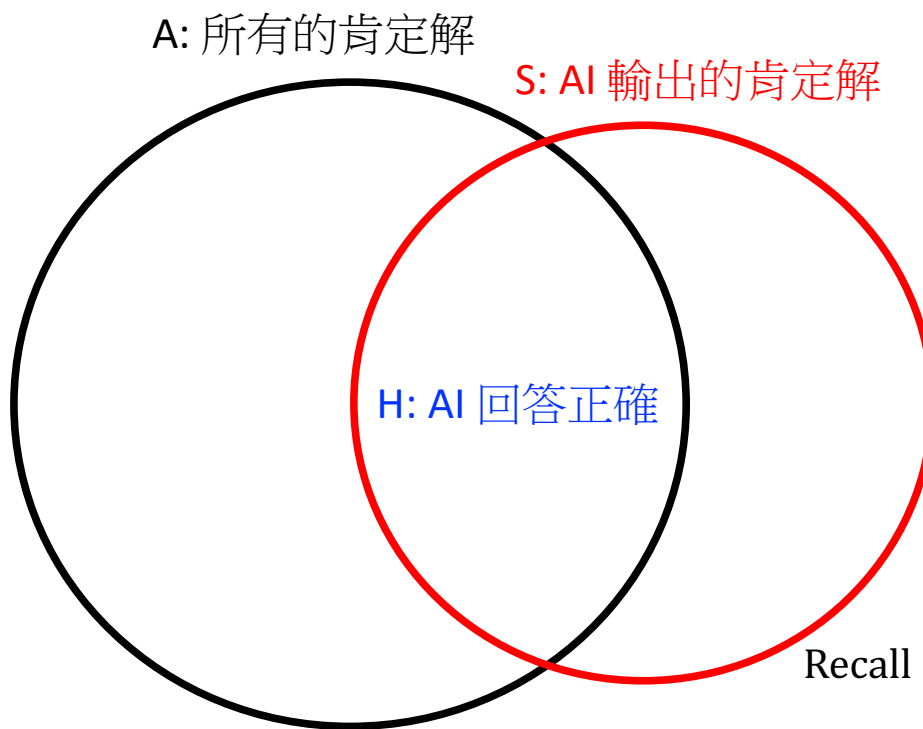
Learning from Movie: 要重視查全率還是精確率?



Fun Time:

要重視查全率
還是精確率?

「寧可錯殺，不可錯放」重視的是 (1) 查全率 Recall (2) 精確率 Precision



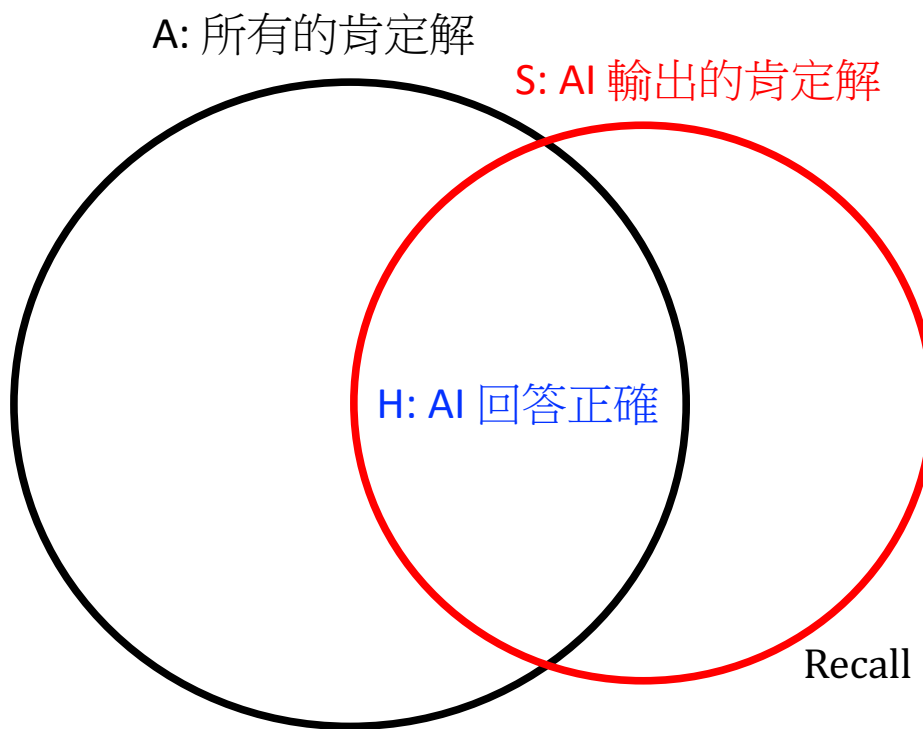
$$\text{Recall (查全率)} = \frac{H}{A}$$

$$\text{Precision (精確率)} = \frac{H}{S}$$

Fun Time:

要重視查全率
還是精確率?

開發人臉辨識系統我們應該要重視查全率
Recall 還是精確率 Precision? (1) 查全率
Recall (2) 精確率 Precision



$$\text{Recall (查全率)} = \frac{H}{A}$$

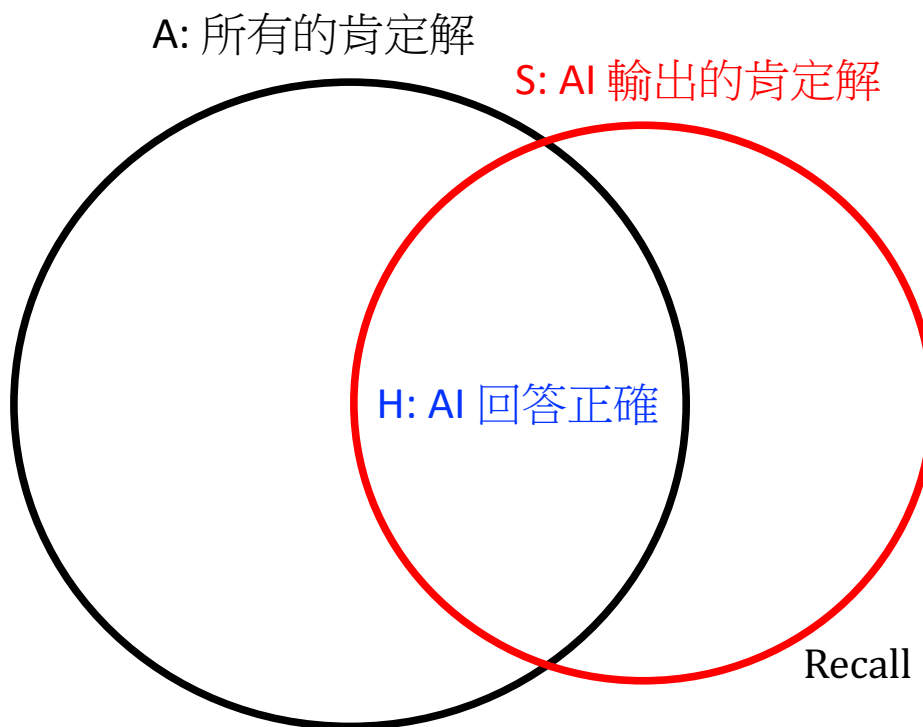
$$\text{Precision (精確率)} = \frac{H}{S}$$

Fun Time:

要重視查全率
還是精確率?

開發癌症檢測系統我們應該要重視查全率
Recall 還是精確率 Precision? (1) 查全率
Recall (2) 精確率 Precision

slide #872333
Polls



$$\text{Recall (查全率)} = \frac{H}{A}$$

$$\text{Precision (精確率)} = \frac{H}{S}$$

Measures of Classification Performance

ACTUAL CLASS	PREDICTED CLASS		
		Yes	No
	Yes	TP	FN
	No	FP	TN

α is a Type I error or a false positive (FP).

β is a Type II error or a false negative (FN).

$$\text{Accuracy} = \frac{TP + TN}{TP + FN + FP + TN}$$

$$\text{ErrorRate} = 1 - \text{accuracy}$$

F_α
 F_1 measure

$$\checkmark \text{Precision} = \text{Positive Predictive Value} = \frac{TP}{TP + FP}$$

$$\checkmark \text{Recall} = \text{Sensitivity} = \text{TP Rate} = \frac{TP}{TP + FN}$$

$$\rightarrow \text{Specificity} = \text{TN Rate} = \frac{TN}{TN + FP}$$

$$\text{FP Rate} = \alpha = \frac{FP}{TN + FP} = 1 - \text{specificity}$$

$$\text{FN Rate} = \beta = \frac{FN}{FN + TP} = 1 - \text{sensitivity}$$

$$\text{Power} = \text{sensitivity} = 1 - \beta$$

ROC (Receiver Operating Characteristic)

- A graphical approach for displaying trade-off between detection rate and false alarm rate
- Developed in 1950s for signal detection theory to analyze noisy signals
- ROC curve plots TPR against FPR
 - Performance of a model represented as a point in an ROC curve

ACTUAL CLASS	PREDICTED CLASS		
		Yes	No
	Yes	TP	FN
	No	FP	TN

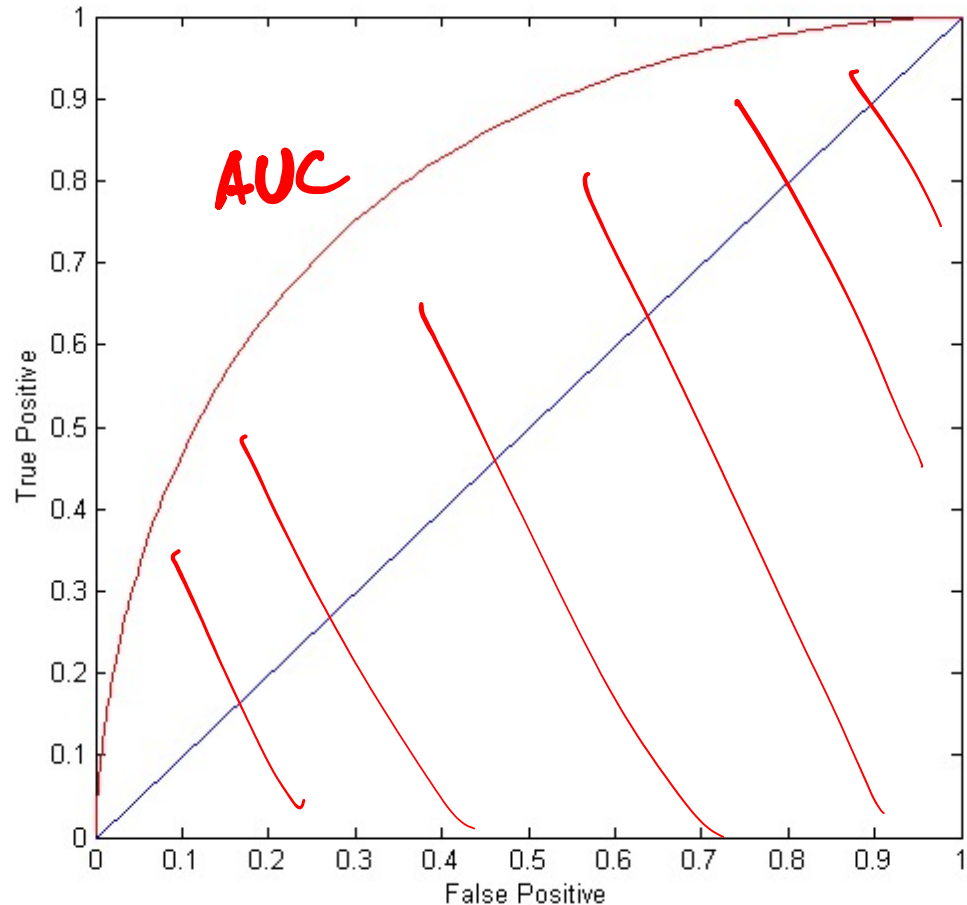
$$TPR = recall = \frac{TP}{TP + FN}$$

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

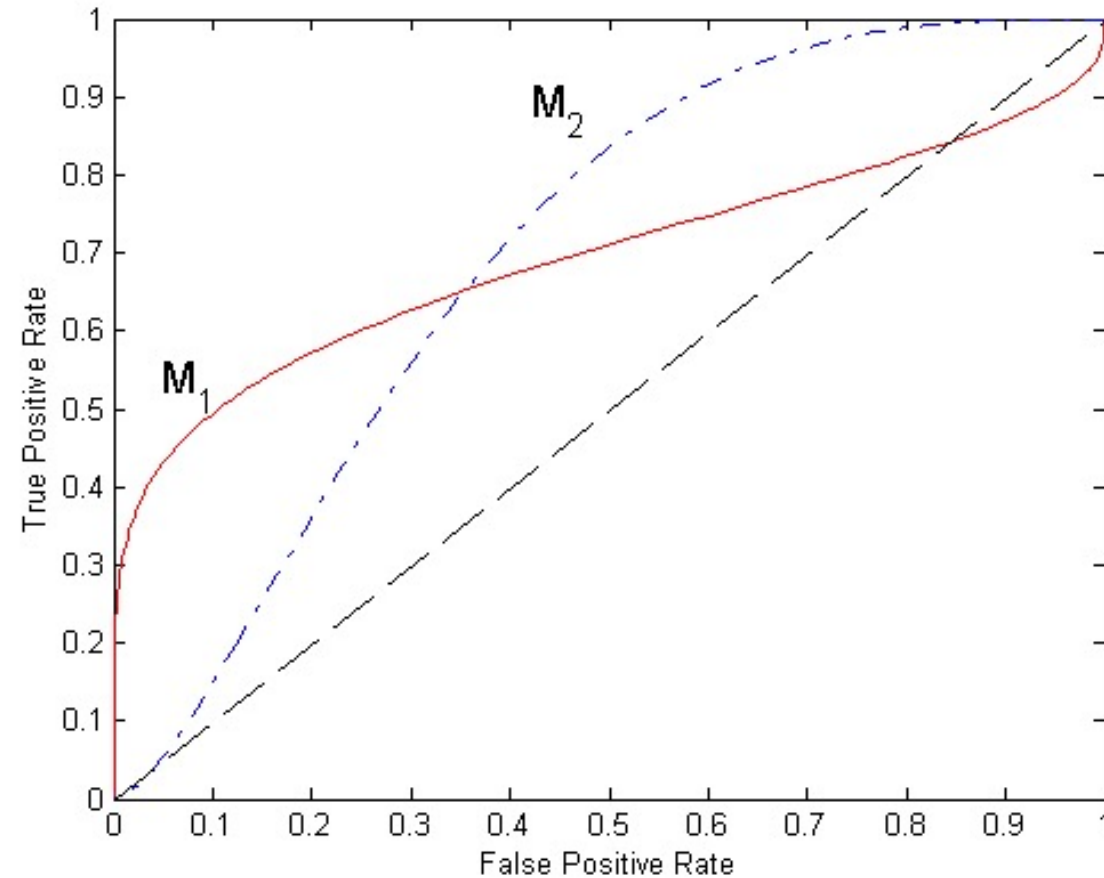
ROC Curve ^{Medium imbalance} PR Curve ^{Extreme imbalance}

(TPR, FPR):

- (0,0): declare everything to be negative class
- (1,1): declare everything to be positive class
- (1,0): ideal
- Diagonal line:
 - Random guessing
 - Below diagonal line:
 - ◆ prediction is opposite of the true class



Using ROC for Model Comparison



- No model consistently outperforms the other
 - M_1 is better for small FPR
 - M_2 is better for large FPR
- Area Under the ROC curve (AUC)
 - Ideal:
 - Area = 1
 - Random guess:
 - Area = 0.5

Common Performance Metrics for Classification and Regression

分類問題	迴歸問題
混淆矩陣 (<u>Confusion Matrix</u>)	均方誤差 (Mean Square Error)
✓ 正確率 (Accuracy)	決定係數 (Coefficient of Determination)
✓ 精確率 (Precision)	
✓ 召回率 (Recall)	
✓ F1 值 (F1-Score)	
✓ AUC (Area Under the Curve , 曲線下面積)	



Performance_metrics.ipynb

Class Imbalance

- **Choose better performance metrics**
 - Accuracy is often not a good metric for class imbalance problems.
 - Use precision, recall, ROC (AUC), F-score etc.
- ✓ • **Balance skewed classes**
 - Data oversampling and undersampling
- ✓ • **Cost-sensitive learning**

Class Imbalance: Balance Skewed Classes

- **Data Oversampling**
 - Random Oversampling
 - [– SMOTE
 - ...
- **Data Undersampling**
 - Random Undersampling
 - Tomek Links
 - Edited Nearest Neighbors
 - ...
- **Combined Oversampling and Undersampling**



IM_data_sampling.ipynb

Class Imbalance: Cost Sensitive Algorithms

- **Modified version of machine learning algorithms designed to take the differing costs of misclassification into account when fitting the model on training records.**
- **Many cost-sensitive algorithms to choose**
 - **Logistic regression**
 - **Support vector machines**
 - **Decision trees**
 - **Random forest**
 - **Gradient boosting**
 - **...**



IM_cost_sensitive_algo.ipynb

Summary: Class Imbalance Problems and Techniques

- Many practical classification problems are **class imbalance problems** where the classes are skewed (more records from one class than another)
- Sometimes you need to choose better performance metrics to train your model.
 - Accuracy is often not a good metric for class imbalance problems.
 - Use precision, recall, ROC (AUC), F-score etc.
- You can use techniques from data oversampling and undersampling (or combination) to balance the skewed class.
- Cost-sensitive learning algorithms are also very useful to attack class imbalance problems.