MSc - Data Mining

Topic 06 : Classification

Part 01 : Introduction to Classification

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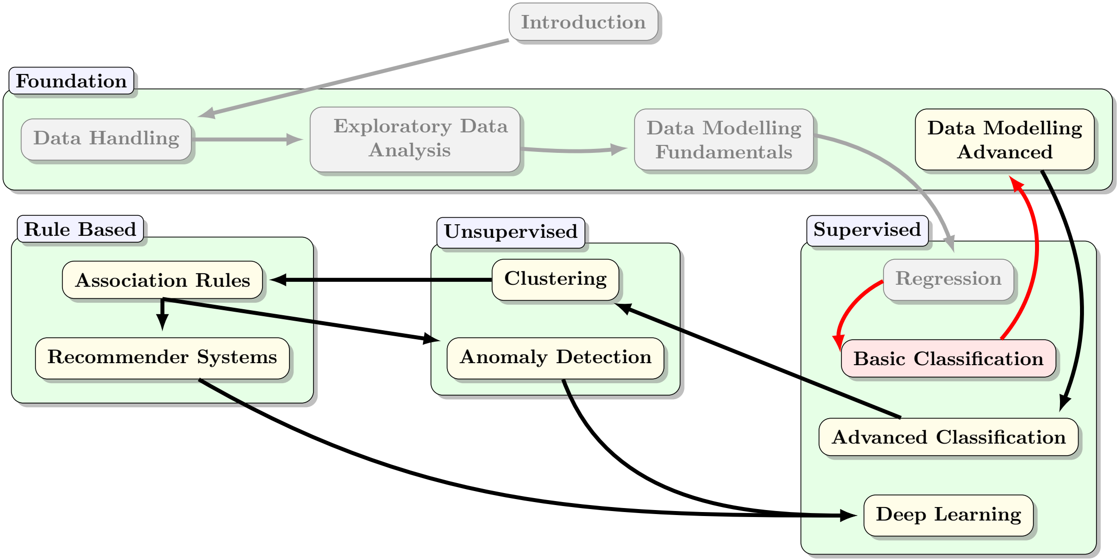
Outline

- How classification differs from regression
- Classification metrics
- Lazy vs Eager learners

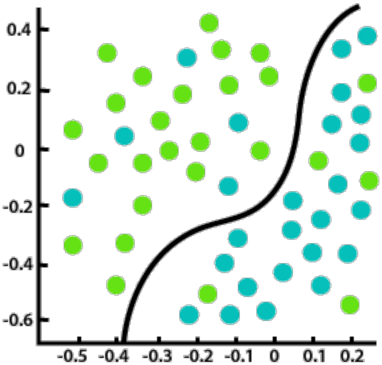
Data Mining (Week 6)

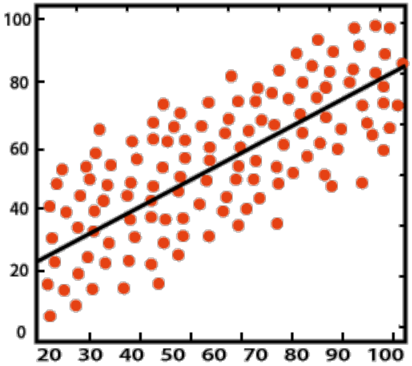


Outline

Classification vs Regression

Supervised data models have a target.
If target is quantitate (continuous) then have a regression model, if categorical then classification model.





Classification models aim to:
- predict class/label for each new observation,
- define a decision boundary between classes,
- and possibly the probability of being in each class.

Regression models aim to
- predict a continuous value for each new observation.

Classification vs Regression

- Unlike regression, statistical distributions play a limited role in evaluating a classifier:
  - Scope for hypothesis testing is limited (there is no equivalent of the `statsmodels` diagnostic output (covered by Bernard, in week 5).
  - Rely on empirical metrics — accuracy, precision, recall, f1-score, auc, …
- Classification metrics tend to be easier to use/understand than those in regression — classification metrics are based on counts of correct (or incorrect) cases divided by a subset of cases.
- Central concept in classification model is the confusion matrix:

		Predicted		
		Negative	Positive	
Actual	Negative	✔ True Negative (TN)	Type I error False Positive (FP)	N
	Positive	Type II error False Negative (FN)	✔ True Positive (TP)	P
		$\hat{N}$	$\hat{P}$	T

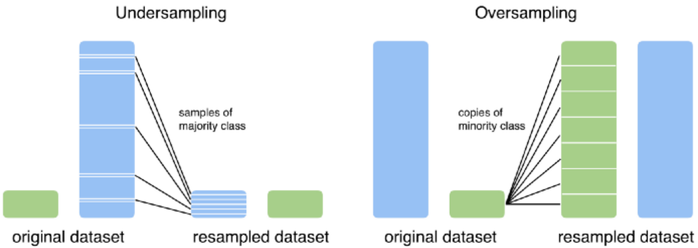
Unbalanced Classification Datasets

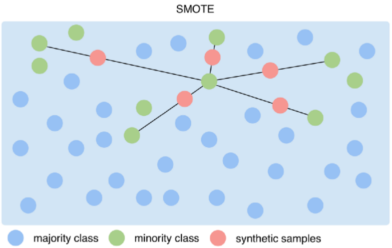
Practical classification datasets are often unbalanced — where the frequency of the classes in the target are very uneven:

- Telecommunication customer churn datasets. Churn rate of 2%–10%.
- Credit Card Fraud Detection 0.172% (492 frauds / 284,807 transactions).
- National Institutes of Health Chest X-Ray Dataset 14 cases, (size 13 to 3,044) in 5,606 cases

Solutions

Use suitable metrics and/or





Summary of Classification Models

Model	Data Pre-processing*		Impact from		Summary
	Normalisation	Scaling	Collinearity	Outliers	
Logistic Regression	✔	✘	✔	✔	• Descriptive with good accuracy • Reasonable computational requirements
Naïve Bayes	NA	NA	✔	✔	• Works with categorical features only • Suitable for small train datasets
KNN	✔	✔	✔	✔	• Local approximation, lazy learner • Heavy computational requirements
Random Forest (Week 8)	✘	✘	✘	✔	• High prediction accuracy • Limited explainability • Works with both continuous and categorical features
Support Vector Classifier (Week 8)	✘	✘	✘/✔	✔	• High prediction accuracy • Explainability depends on kernel • Computational effort depends on kernel
Neural Networks (Week 12)	✘	✔	✔	✔	• High prediction accuracy • Self-extract features • Heavy computational requirements

*Use `StandardScaler`, or `RobustScaler` if have outliers.

Lazy vs Eager Learners

Lazy learner

Stores training data (or only minor processing) and uses this to compute prediction when given test data.

- Does not generalise until after training
- Does not produce a standalone model
- Training data must be kept for prediction
- Local approximations
- Often based on *search*
- If new data is just added to the training data, it can respond more easily to changing conditions

Eager learner

Builds a model from the train set, before receiving new data for prediction

- Training has an extra goal: to generalise from the data
- Training has an extra output: standalone model
- Training data can be discarded after use
- Local and/or global approximations
- Based on *computation*
- Models *drift* with time, so not suited to highly dynamic contexts, as it needs retraining

Usually an (eager) model requires much less memory than a (lazy) training set.

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Outline

A Non-perfect Test — Type I and Type II Errors

Consider an imperfect test with two outcomes, there are four possible outcomes:

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		Predicted: Negative	Predicted: Positive	
Actual	Negative	✔ True Negative (TN)		N
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A Non-perfect Test — Type I and Type II Errors

Consider an imperfect test with two outcomes, there are four possible outcomes:

Confusion Matrix

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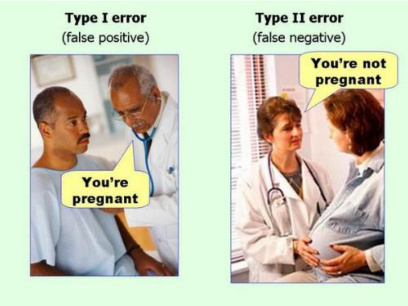
- If the test is applied to $T = P + N = \hat{P} + \hat{N}$ observations / subjects / instances then we have four independent quantities TP, TN, FP, and FN.
- How do we combines these quantities into a single metric ?
- The fraction of correct results seems like a good idea

$$\text{accuracy} = \frac{TP + TN}{P + N}$$

But what happens, if we are testing for an rare event? Maximising accuracy will result in the test always returning negative.



- Ideally we want the probability of either error to be zero but that may not be possible.
- Depending on the conditions we often modify the test to reduce probability of the type of error we don't want at the expense of increasing the probability of the other — think court case vs medical condition.

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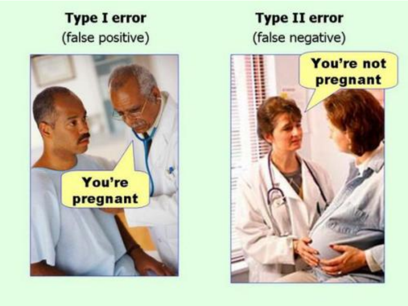

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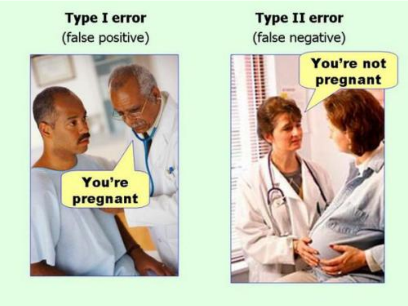

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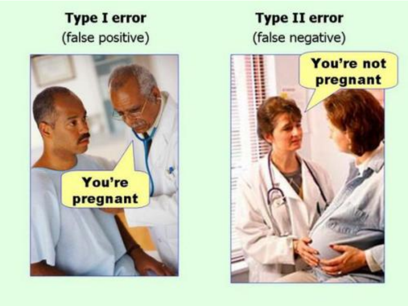

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Confusion matrix (Contingency table) Metrics I

$$\textbf{Accuracy} = \frac{\mathrm{TP}+\mathrm{TN}}{\mathrm{P}+\mathrm{N}}$$

(How often is the classifier correct?)

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- False negative rate (FNR) $= \frac{FN}{\mathrm{P}} = 1 - TPR$
- **Sensitivity** = **Recall** = True positive rate (TPR) $= \frac{TP}{\mathrm{P}} = 1 - FNR$
  (Of positive cases that exist how many did we mark positive?)
- **Specificity** $= \frac{\mathrm{TN}}{\mathrm{N}} = 1 - \mathrm{FPR}$
  (When it's actually no, how often does we predict no?)
  (Of cases that are negative, how many did we mark negative?)
- False positive rate (FPR) = false acceptance $= \frac{FP}{\mathrm{N}} = 1 - \mathrm{Specificity}$
- **Precision** = positive predictive value (PPV) $= \frac{TP}{\hat{\mathrm{P}}} = \frac{TP}{\mathrm{TP}+\mathrm{FP}}$
  (Of cases that we marked positive, how many were correct?)

Confusion matrix (Contingency table) Metrics I

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Confusion matrix (Contingency table) Metrics I

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Accuracy — how well model is trained and performs in general

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Recall — important when the costs of false negatives are high

Precision — important when the costs of false positives are high

Confusion matrix (Contingency table) Metrics II

F_1 Score

The F-measure or balanced F-score (F_1 score) is the harmonic mean of precision and recall:

$$F_1 = 2\left[\frac{1}{\frac{1}{\text{precision}} + \frac{1}{\text{recall}}}\right] = 2\left[\frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}}\right]$$

A word of Caution . . .

Consider the three binary classifiers A, B and C

	A		B		C	
	T	F	T	F	T	F
T	0.9	0.1	0.8	0	0.78	0
F	0	0	0.1	0.1	0.12	0.1

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Metric	**A**	**B**	**C**	(best)
Accuracy	0.9	0.9	0.88	**AB**
Precision	0.9	1.0	1.0	**BC**
Recall	1.0	0.888	0.8667	**A**
F-score	0.947	0.941	0.9286	**A**

Clearly classifier A is useless since it always predicts label T regardless of the input. Also, B is slightly better than C (lower off- diagonal total).

Yet look at the performance metrics – B is never the clear winner.

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A word of Caution ...

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Clearly classifier *A* is useless since it always predicts label T regardless of the input. Also, B is slightly better than C (lower off- diagonal total).
Yet look at the performance metrics – B is never the clear winner.

We use some metrics because they are easy to understand, and not because they always give the "correct" result.

Mutual Information is a Better Metric

The mutual information between predicted and actual label (case) is defined

$$I(\hat{y}, y) = \sum_{\hat{y}=\{0,1\}} \sum_{y=\{0,1\}} p(\hat{y}, y) \log \frac{p(\hat{y}, y)}{p(\hat{y})p(y)}$$

where $p(\hat{y}, y)$ is the joint probability distribution function.
This gives the intuitively correct rankings $B > C > A$

Metric	A	B	C
Accuracy	0.9	0.9	0.88
Precision	0.9	1.0	1.0
Recall	1.0	0.888	0.8667
F-score	0.947	0.941	0.9286
Mutual information	**0**	**0.1865**	**0.1735**

Micro Average vs Macro Average Performance

In a multi-class classifier we have more than two classes. To combine the metrics for individual classes to get an overall system metrics, we can apply either

Micro-Average Method
: Sum up the individual true positives, false positives, and false negatives of the system for different classes and then apply totals to get the statistics.

Macro-average Method
: Average the precision and recall of the system on different classes.

See `classification_report` from `sklearn.metrics` (Example: IRIS dataset)

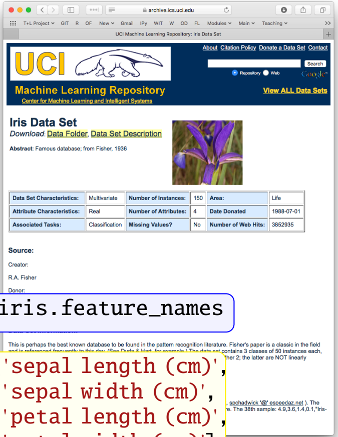
```
              precision    recall  f1-score   support

      setosa       1.00      0.95      0.97        19
  versicolor       0.81      0.74      0.77        23
   virginica       0.71      0.83      0.77        18

    accuracy                           0.83        60
   macro avg       0.84      0.84      0.84        60
weighted avg       0.84      0.83      0.84        60
```

Outline

Example: IRIS Dataset — Load




```
iris.feature_names
```

```
['sepal length (cm)',
 'sepal width (cm)',
 'petal length (cm)',
 'petal width (cm)']
```

```
from sklearn import datasets
iris = datasets.load_iris()

df = pd.DataFrame(iris.data)
df.columns = iris.feature_names
df['target'] = iris.target_names[iris.target]
df.sample(4)
```

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)	target
141	6.9	3.1	5.1	2.3	virginica
42	4.4	3.2	1.3	0.2	setosa
9	4.9	3.1	1.5	0.1	setosa
52	6.9	3.1	4.9	1.5	versicolor

The data set contains, four numeric features, 3 classes of 50 instances each, where each class refers to a type of iris plant. One class is linearly separable from the other 2; the latter are NOT linearly separable from each other.

Example: IRIS Dataset — Preprocess Data

We will cover some classifiers in a moment, but for now just treat the classifiers (`LogisticRegression`) as a black box and focus on the general process:

Extract the data (features and target)

The IRIS dataset has 4 features, but to simplify visualisation we are only going to use the first two ('sepal length' and 'sepal width'):

```
dataset_name = "IRIS"
X, y, target_names = iris.data[:,:2], iris.target, iris.target_names
```

Split dataset into `train` and `test`

We will keep 40% of the data for testing. Setting the parameter `random_state` to a value means that we will get a random — but sill reproducible — split.

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, train_size=0.6, random_state=666)
```

Example: IRIS Dataset — Fit Model and Predict

Select classifier

Scikit-learn supports a large set of classifiers, and aims to have a consistent interface to all. First import classifier and create instance …

```
from sklearn.linear_model import LogisticRegression
model = LogisticRegression(max_iter=500)
```

Train model

Then we train (fit) the classifier/model using only the features (`X_train`) and targets (`y_train`) from the train dataset …

```
model.fit(X_train, y_train)
```

```
LogisticRegression(max_iter=500)
```

Predict

Now that model is trained, we can use it to generate predictions, using the features (`X_test`) from the test dataset …

```
y_pred = model.predict(X_test)
```

Example: IRIS Dataset — Evaluate I

Scoring and confusion matrix

We could just compute the score using whatever metric we have picked ...

```
from sklearn.metrics import accuracy_score
accuracy_score(y_test, y_pred)
```

```
0.83333333333333
```

But this needs context, and even if good can hide critical flaws. Lets look at the confusion matrix ...

```
from sklearn.metrics import confusion_matrix
cm = confusion_matrix(y_test,y_pred)
cm
```

```
array([[18, 1, 0],
       [ 0, 17, 6],
       [ 0,  3, 15]])
```

or, to get a nicer output, convert to a DataFrame ...

```
df_cm = pd.crosstab(target_names[y_test],target_names[y_pred])
df_cm.index.name = 'Actual'
df_cm.columns.name = 'Predicted'
df_cm
```

Predicted	**setosa**	**versicolor**	**virginica**
Actual			
setosa	18	1	0
versicolor	0	17	6
virginica	0	3	15

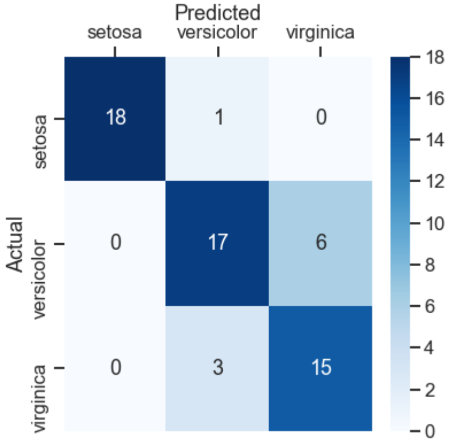
Example: IRIS Dataset — Evaluate II

The confusion matrix is fundamental in evaluating a classifier, so find a presentation/visualisation that you like and use it. Here I have a heat map representation that I tend to use.

Predicted	setosa	versicolor	virginica
Actual			
setosa	18	1	0
versicolor	0	17	6
virginica	0	3	15

The first class `setosa` was only misclassified once, while the classifier had more difficulty between the second two classes.

```python
plt.figure(figsize=(6,6))
g = sns.heatmap(df_cm, annot=True, cmap="Blues")
g.xaxis.set_ticks_position("top")
g.xaxis.set_label_position('top')
```



Example: IRIS Dataset — Evaluate III

The classification report, constructed from the confusion matrix, summaries the most common metrics per class and for overall averages …

```python
from sklearn.metrics import classification_report
print(classification_report(y_test, y_pred, target_names=target_names))
```

precision (setosa) = $11/(11+0) = 1$

recall (setosa) = $11/(11+1) = 0.92$

Predicted	setosa	versicolor	virginica
Actual			
setosa	18	1	0
versicolor	0	17	6
virginica	0	3	15

```
              precision    recall  f1-score   support

      setosa       1.00      0.95      0.97        19
  versicolor       0.81      0.74      0.77        23
   virginica       0.71      0.83      0.77        18

    accuracy                           0.83        60
   macro avg       0.84      0.84      0.84        60
weighted avg       0.84      0.83      0.84        60
```

accuracy = $(11+13+12)/45 = 0.8$

f1-score (virginica) = $2/(1/0.71+1/0.80) = 0.75$