Predictive Modelling Introduction

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Definition

Predictive modelling uses "statistics" to predict outcomes. (https://en.wikipedia.org/wiki/Predictive_modelling)

Terminologies of similar meaning: **Statistical learning**, **Machine learning**, https://en.wikipedia.org/wiki/Predictive_analytics

Things to be covered

- Supervised Learning Models / Predictive Models:
  - Classifiers: kNN, logistic regression, Naive Bayes, LDA, classification trees, ...
  - Regressors: kNN, linear regression and variations, regression trees, ...
- Validation Strategies
- Unsupervised Learning Models:
  - Dimensional Reduction: PCA, ...
  - Clustering: k-Means, HC, ...

May 2020 Final Assessment Q1(b)

Write an essay with no more than 3 pages to **summarise** the various **unsupervised learning models** and **predicative models** you learned by using **appropriate mathematical formulation**. Based on what you learned from your assignment and the Internet, suggest **improvements** on this course and propose a good online teaching learning environment. Be warned that non-constructive remarks and insults will receive ZERO mark. (7 marks)

Topics not cover

- Deep learning
- Self-supervised learning
- Reinforcement learning

Software and Data

Popular data analysis programming languages:

- R + misc libraries: `https://cran.r-project.org/`
- Python (+ Pandas + Sklearn + RPy2): Anaconda Python (`https://www.anaconda.com/products/individual`)
- Java (Weka)
- SQL, NoSQL, etc.

Popular data:

- https://archive.ics.uci.edu/ml/datasets.php
- Kaggle (need registration)

Online Learning Tools

- Microsoft Teams
- WBLE (based on Moodle)
- Lecturer Github Site: `https://liaohaohui.github.io/UECM3993`
- YouTube: E.g. Dr Kilian Weinberger's Machine Learning Lecture
- Internet Search

Reference Books

- Gareth James, Daniela Witten, Trevor Hastie and Robert Tibshirani, An Introduction to Statistical Learning: with Applications in R, Springer 2013
  https://statlearning.com/
- Trevor Hastie, Robert Tibshirani, Jerome Friedman, The Elements of Statistical Learning: Data Mining, Inference, and Prediction, Springer-Verlag, 2008
  https://web.stanford.edu/~hastie/ElemStatLearn/

Classes & Assessment

Week 4 Thursday: Day before CNY, class as usual.

Week 4 Friday: CNY Holiday. T1, join T2 or T3?; P3 cancel, recorded video?

Coursework (60%)

- Quiz: 12%
- Assignment: 48% (Report 24% + Programming Code 12% + Oral Presentation 12%). Starting: Week 4; Deadline: Wed Week 12
- Week 1: Start to find assignment group members, 4-7 in one group.

Final Assessment (40%)

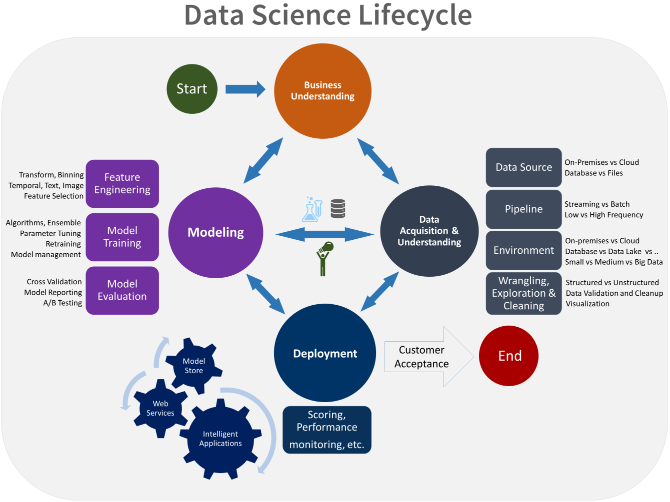
- 4 Compulsory Questions. Each 10%???

Data Science and CRISP-DM

Data Science / CRISP-DM (Cross Industry Standard Process for Data Mining)

- Business understanding
- Data understanding
- Data preparation / preprocessing
- Modelling
- Evaluation
- Deployment

Microsoft Data Science Lifecycle



https://docs.microsoft.com/en-us/azure/machine-learning/team-data-science-process/lifecycle-business-understanding

Business Understanding

- Define the business goals that the data science techniques can target.
- Find the relevant data that helps you answer the questions

Wrong Direction:

- Many of your seniors apply the predictive models on the data and choose the "best" model forgetting the "goal": How do the factors influence the target; OR How does the best model help business.

Data Understanding

Facts:

- Real-world data are noisy: missing values, wrong values, etc.

Exploratory Data Analysis (EDA):

- Data summary (mean, mode, median, etc.)
- Visualisation
- Data correlation?

Data Understanding (cont)

Unstructured Data (EDA cannot be used):

- Texts: Reports in Word, PDF; Twitters; etc.
- Images
- Biometric data
- Songs / Lyrics
- Time series: Stock price; Online game control sequence; Industrial robot control sequence; etc.

Observations:

- Most companies usually stored data in structured data format in SQL database using SQL.

Data Understanding (cont)

Structured data (EDA can be used):

- Tabular data containing:
  - Categorical (or nominal) data: Typical example: Gender. R's `factor`; Python's `astype("category")`
  - Ordinal data: Typical example: Student grade. R's `ordered`
  - Numerical data: Typical example: Temperature.
- With some assumptions, we can construct "structured" approximations to unstructured data.

EDA and Data Understanding (cont)

Exploratory data analysis tools for a single data:

- R's `summary`, Python's `describe`
- For (continuous) numerical data: R's `hist` (histogram), `stem` (stem-and-leaf plot)
- For integral data and categorical data, R's `table`.

EDA and Data Understanding (cont)

Exploratory data analysis tools for two data:

- categorical vs categorical: `barplot`, `table`
- categorical vs numerical: `boxplot`
- numerical vs numerical:
  - `cor(x, y, method="pearson")`,
  - (scatter) `plot`

Data Preparation / Preprocessing

https://scikit-learn.org/stable/modules/preprocessing.html)

- Standardisation of datasets — column scaling
- Normalisation — row scaling
- Non-linear and custom transformation
- Encoding categorical features
- Discretization
- Imputation of missing values
- Generating polynomial features

Modelling (Supervised Learning)

A "Predictive Model" as a "Blackbox"

$$\begin{aligned} output &= model(inputs), \\ Y &= f(X_1, \cdots, X_p) \end{aligned}$$

- Prediction: If we have inputs $x_1, \cdots, x_p$ and f, we can "know" a possible output y.
- Inference: Is the model correct? How Y is changing w.r.t X_i? E.g. What factors "improves" sales?

Modelling (cont)

The Bayesian approach allows us to classify "models" into

- Discriminative models:
$$\hat{Y} = \operatorname{argmax}_j \mathbb{P}(Y = j|X_1, \cdots, X_p)$$
E.g. kNN, logistic model
- Generative models:
$$\hat{Y} = \operatorname{argmax}_j \mathbb{P}(X_1, \cdots, X_p|Y = j)\mathbb{P}(Y = j)$$
E.g. Naive Bayes, LDA

Modelling (cont)

The “property” of the output allows us to classify “models” into

- Classifier:
  - Use to solve classification problems
  - Y is categorical / qualitative
- Regressor:
  - Use to solve regression problems
  - Y is numerical / quantitative

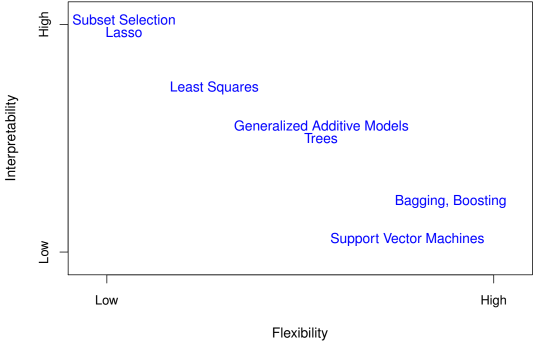
Modelling (cont)

The “fixed parameters” of the model allows us to classify “models” into

- Parametric models:
  - Models with fixed set of parameters
  - “Training” tries to find the most suitable parameter values to minimise “errors”
- Nonparametric models
  - Models without fixed set of parameters. Internal “representation” grows as data increases.
  - “Training” tries to “fit” the data!

Modelling: Flexibility vs Interpretability

Inflexible ⇒ Simpler math formula ⇒ Poorer Predictibility



Flexible ⇒ Complicated math formula ⇒ Good Predictibility

Predicting / Scoring

Suppose we have a "trained" model $\hat{f}$. It can be used for prediction / scoring in the following ways:

- Batch scoring: Classify documents / images / etc.
- Event-driven scoring: Detect atypical event (COVID-19 pandemic), spam filtering, detection of low fruits and vege by smart home / IoT system, ...
- Real-time scoring: Use in (credit card) fraud detection, ...

Predicting / Scoring (cont)

Examples

Training and batch scoring (predict) in R

```
lrmodel = lm(y ~ ., data=Xy)
predicted = predict(lrmodel, newdata=data.frame(x1=...,x2=...))
```

Training and batch scoring (.fit) in Python

```
from sklearn.linear_model import LinearRegression
lrobj = LinearRegression()
lrmodel = lrobj.fit(Xy.iloc[:,3:4],Xy.iloc[:,4])
newdata = pd.DataFrame({'x1':..., 'x2':...})
predicted = lrmodel.predict(newdata)
```

Predicting / Scoring (cont)

Examples of "Probabilistic" Scores

probability "cut-off" @ 0.5 (default)

$\mathbb{P}(Class = 1) = 0.4 \Rightarrow$ Predict = 0

$\mathbb{P}(Class = 1) = 0.7 \Rightarrow$ Predict = 1

$\mathbb{P}(Class = 1) = 0.9 \Rightarrow$ Predict = 1

probability "cut-off" @ 0.8

$\mathbb{P}(Class = 1) = 0.4 \Rightarrow$ Predict = 0

$\mathbb{P}(Class = 1) = 0.7 \Rightarrow$ Predict = 0

$\mathbb{P}(Class = 1) = 0.9 \Rightarrow$ Predict = 1

Model Validation / Evaluation

"Loss functions" — measuring "false prediction".

Regression:

- RSS = $\sum_{i=1}^{n}(y_i - f(x_1, \cdots, x_p))^2$
- $R^2 = 1 - \frac{\sum(Y_{actual} - Y_{predicted})^2}{\sum(Y_{actual} - Y_{mean})^2}$

Classification:

- Error rate: $\frac{1}{n}\sum_{i=1}^{n} I(y_i \neq \hat{y}_i)$
- Accuracy: $\frac{1}{n}\sum_{i=1}^{n} I(y_i = \hat{y}_i)$
- Kappa, ROC, etc.

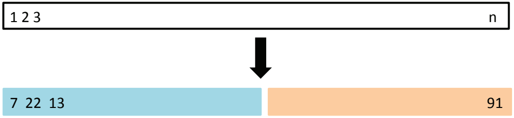
Model Validation (cont)

Holdout method, validation set approach:

Randomly dividing the available set of observations into two parts:

- Training set — to build/fit the model
- Validation/Test set — to test/evaluate the fitted model

Pictorially,



Model Validation (cont)

Holdout method, validation set approach in R:

```
library(datasets)
set.seed(0)
test.index = sample(1:nrow(iris), size=0.4*nrow(iris))
X_y.test  = iris[ test.index, ]
X_y.train = iris[-test.index, ]
library(e1071)
clf = svm(Species ~ ., data = X_y.train, kernel='linear')
predicted = predict(clf, newdata=X_y.test)
conftbl <- table(predicted, X_y.test$Species)
# Accuracy of prediction
sum(diag(conftbl))/sum(conftbl)
```

Model Validation (cont)

Holdout method, validation set approach in Python:

```
from sklearn.model_selection import train_test_split
from sklearn import datasets, svm
X, y = datasets.load_iris(return_X_y=True)
X_train, X_test, y_train, y_test = train_test_split(
         X, y, test_size=0.4, random_state=0)
clf_obj = svm.SVC(kernel='linear', C=1)
clf = clf_obj.fit(X_train, y_train)
# Accuracy of prediction (see Confusion matrix)
clf.score(X_test, y_test)
```

Model Validation (cont)

Example 1.7.1 (Final Exam Jan 2019, Q3)

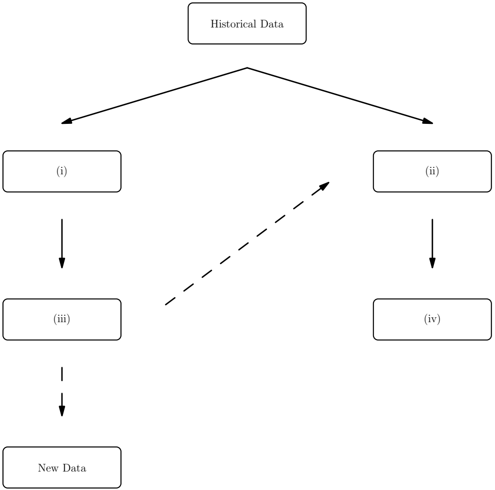
(a) A predictive model can be built when historical data with known response are presented. The predictive model is then used to predict the response of a new data set with predictors given. Figure Q3(a) shows the process to form a predictive model.

Fill in the blanks (i) to (iv) in Figure Q3(a). State the differences between regression and classification for each step in the process of forming a predictive model.

(b) Give three examples on how statistical learning can help in risk/fraud analytics.

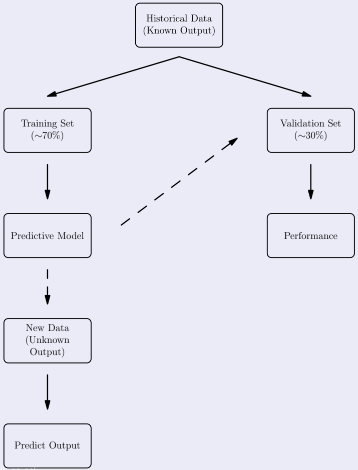
Model Validation (cont)

Figure Q3(a)



Model Validation (cont)

Example 1.7.1 (a) Answer



Regression vs. classification

	Regression	Classification
Response	Numerical	Categorical
Split	Linear sampling	Stratified sampling
Performance	RSS, R^2	Confusion matrix
Scoring	$\hat{y}(\boldsymbol{x}) \pm$ s.d.	$\mathbb{P}(Y = j \mid \boldsymbol{X} = \boldsymbol{x})$

(b) Answer

• Banking industry uses credit scores to decide if an applicant can get a loan.
• Insurance industry predicts changes of an event to calculate premium.
• Financial institutions predicts frauds in transactions

May 2020 Final Assessment Q1(a)

Describe the differences between regression and classification for each step in the process of forming a predictive model with appropriate justifications.

(3 marks)

Answer

	Regression	Classification
Response	Numerical	Categorical
Split	Linear sampling	Stratified sampling
Performance	RSS, R^2	Confusion matrix
Scoring	$\hat{y}(\boldsymbol{x}) \pm$ s.d.	$\mathbb{P}(Y = j \mid \boldsymbol{X} = \boldsymbol{x})$

. . . . [3 marks]

Confusion Matrix

For a classification problem with binary outcomes (only 2 classes), positive (+) and negative (-), the confusion matrix / contingency table can be presented as follows.

		Actual observations		
		Positive (+)	Negative (-)	**Precision**
Predicted	Positive (+)	True Positive Count (TP)	False Positive Count (FP)	Positive Predictive Value (PPV)
	Negative (-)	False Negative Count (FN)	True Negative Count (TN)	Negative Predictive Value (NPV)
	Recall	True Positive Rate (TPR) (Sensivity)	True Negative Rate (TNR) (Specificity)	Accuracy (ACR)

Confusion Matrix (cont)

Example 1.7.2: A predictive model has been built by using the training set. After predicting the outcome (fraud, not fraud) by implementing the model into validation set, the results are recorded as follow:

- Numbers of customer predicted to be fraud and the prediction is correct = 70
- Numbers of customer predicted to be fraud and the prediction is incorrect = 30
- Numbers of customer predicted not to be fraud and the prediction is correct = 80
- Numbers of customer predicted not to be fraud and the prediction is incorrect = 20

Confusion Matrix (cont)

		True Class	
		Fraud (+)	Not Fraud (-)
Predicted Class	Fraud (+)	70 (TP)	30 (FP)
	Not Fraud (-)	20 (FN)	80 (TN)

Calculate the accuracy measures sensitivity, specificity, PPV, NPV, ACR, FPR, FNR.

Confusion Matrix (cont)

```
lvs    <- c("not fraud", "fraud")  # -> class 1, 2
lvs.r <- c("fraud", "not fraud")  # Show fraud first
truth <- factor(rep(lvs, times=c(110, 90)),
                levels=lvs.r)
pred  <- factor(c(rep(lvs, times=c(80, 30)),
                  rep(lvs, times=c(20, 70))),
                levels=lvs.r)
xtab  <- table(pred, truth)
TPR = xtab[1,1]/sum(xtab[,1])  # Sensitivity
TNR = xtab[2,2]/sum(xtab[,2])  # Specificity
PPV = xtab[1,1]/sum(xtab[1,])
NPV = xtab[2,2]/sum(xtab[2,])
FPR = 1 - TNR
FNR = 1 - TPR
```

Decision Making Example

You have just landed a great analytic job with ACME Inc., one of the largest telecommunication firms in United States. They are having a major problem with customer retention in their wireless business. In the Mid-Atlantic region, 20% of cell phone customers leave when their contracts expire, and it is getting increasingly difficult to acquire new customers.

Since the cell phone market is now saturated, the huge growth in the wireless market has tapered off. Communications companies are now engaged in battles to attract each other's customers while retaining their own. Customers switching from one company to another is called churn.

Decision Making Example (cont)

You and your team have been called in to help understand the problem and to devise a solution. The data set given consists of 2,000,000 observations with 10 predictors. Your team decided to build several predictive models using different methods. The models are then tested with the validation data set. The results of testing are shown as below:

Model	TP	FP	TN	FN
3-Nearest Neighbour	281,609	31,291	263,077	24,023
500-Nearest Neighbour	181,301	51,014	243,354	124,331
LR (all predictors)	243,344	55,194	239,174	62,288
LR (significant predictors)	249,487	61,493	232,875	56,145

Based on the information given, make a decision on the model that is suitable for churn prediction to be proposed to the company. Discuss on your decision. . . . . **Online Class Discussion?**

Confusion Matrix (cont)

Multiclass Example 1.7.4: Use kNN with $k = 5$ (a kind of predictive model) to train on 75% of the iris data and then construct the confusion matrix on the remainder 25% iris data (as test data).

```
library(datasets)
data(iris)
N = nrow(iris)
set.seed(59) #set.seed(9)
train_idx = sample(N, size=0.75*N)
iris_train = iris[ train_idx,]
iris_test  = iris[-train_idx,]

library(class)  # for knn
M = ncol(iris)
iris_predict = knn(train=iris_train[,-M], test=iris_test[,-M],
                cl=iris_train[,M], k=5)
library(gmodels) # dependencies: gtools, gdata
CrossTable(x=iris_predict, y=iris_test[,M], prop.chisq=FALSE)
```

Confusion Matrix (cont)

```
             | iris_test[, M]
iris_predict |     setosa | versicolor |  virginica |  Row Total |
-------------|------------|------------|------------|------------|
      setosa |         14 |          0 |          0 |         14 |
             |      1.000 |      0.000 |      0.000 |      0.368 |
             |      1.000 |      0.000 |      0.000 |            |
             |      0.368 |      0.000 |      0.000 |            |
-------------|------------|------------|------------|------------|
  versicolor |          0 |         10 |          1 |         11 |
             |      0.000 |      0.909 |      0.091 |      0.289 |
             |      0.000 |      0.909 |      0.077 |            |
             |      0.000 |      0.263 |      0.026 |            |
-------------|------------|------------|------------|------------|
   virginica |          0 |          1 |         12 |         13 |
             |      0.000 |      0.077 |      0.923 |      0.342 |
             |      0.000 |      0.091 |      0.923 |            |
             |      0.000 |      0.026 |      0.316 |            |
-------------|------------|------------|------------|------------|
Column Total |         14 |         11 |         13 |         38 |
             |      0.368 |      0.289 |      0.342 |            |
-------------|------------|------------|------------|------------|
```

ROC Curve

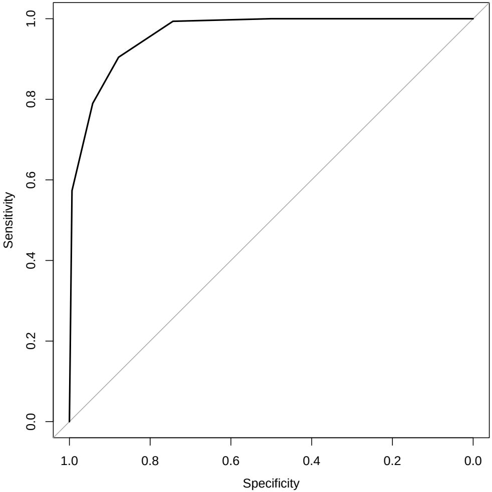
Receiver Operating Characteristic (ROC) curve = "sensitivity" vs "1−specificity" ("TPR vs FPR")
Only for **binary** classifiers.

```
library(ISLR)
Smarket = Smarket[,-1]  # Remove Year
N = nrow(Smarket)

set.seed(59) #set.seed(9)
train_idx = sample(seq(N), size=0.75*N)
Smarket_train = Smarket[ train_idx,]
Smarket_test  = Smarket[-train_idx,]

library(class)  # for knn
M = ncol(Smarket)
Smarket_predict = knn(train=Smarket_train[,-M], test=Smarket_test[,-M],
                cl=Smarket_train[,M], k=5, prob=TRUE)
suppressWarnings(library(pROC))
prob = attr(Smarket_predict,"prob")
prob = ifelse(Smarket_predict=="Up", prob, 1-prob)
proc.obj = roc(Smarket_test[,M], prob, plot=TRUE)
```

ROC Curve (cont)



Unsupervised Learning

- Descriptive Statistics / EDA
- Visualisation → Dashboard
- Clustering (for small dimension?) E.g. k-means, HC
- Dimensionality Reduction (for large dimension?). E.g. PCA
- `https://en.wikipedia.org/wiki/Association_rule_learning`
- `https://en.wikipedia.org/wiki/Anomaly_detection`

Use Cases

Classification:

- Email → spam / non-spam;
- Tumour → benign / malignant;
- Writing → characters / words;
- Image → label;
- Activity → fraud / non-fraud

Use Cases (cont)

Regression:

- Predicting insurance premiums
- Motor insurance pricing using GLM
- Econometrics
- Signal processing in sensors — industrial process tomography ?

Use Cases (cont)

Unsupervised learning:

- clustering COVID-19 viruses and other coronavirus
- market segmentation
- visualisation
- dimensionality reduction

Real-World Concern

Pros & Cons of AI.

E.g. AI in changing background

- Pro: Video production
- Con: Fake scene: A cooking background can be turned to a murder background.

E.g. AI in removing someone from the scene

- Pro: Video production, e.g. removing “tourists” from a documentary scene.
- Con: “Fake” CCTV.