Supervised VS Unsupervised

- *Feature*: measurable property/characteristic of data instance
- *Concept*: output label/variable; what we are predicting
- *Supervised*: labelled
    - Classification, Regression
    - Learn relation between features and target
- *Unsupervised*: unlabelled data
    - Clustering, Dimensionality Reduction, Anomaly Detection
    - *Strongly*: no idea how many/what groups are
    - *Weakly*: know how many/what groups are
- *Semisupervised*: some labelled, majority unlabelled
- *Reinforcement Learning*: interaction and feedback
- *Hyperparameters*: parameters which <u>define and constrain</u> the learning process
- *Parameters*: <u>values learnt</u> and applied to particular training dataset

Feature Types

Numerical		**Categorical**	
Discrete	*Continuous*	*Nominal*	*Ordinal*
- whole number distinct categories/lvls	- range/interval - decimal	- no inherent order/ranking	- has natural order/ranking

Categorical → Numeric

Label/Ordinal Encoding
- assign unique number label to each category
- for ordinal: based on order/ranking
- eg. red, blue, green → 1, 2, 3
- CON: artificial order

One-Hot Encoding
- binary columns for each feature
- eg. "red" → [0, 0, 1]
- PRO: equal distance, CON: increases dimensionality

Target Encoding
- replace category with statistical aggregation (count, mean, median, etc.)
- eg. red, blue, green → 4, 10, 4
- CON: prone to overfitting

Hashing
- hash feature to fixed, unique numeric value
- PRO: reduces dimensionality of large-scale datasets

Categorical → Numeric

Equal-Width Discretisation
- partition into n bins of width $\frac{max-min}{n}$
- CON: sensitive to outliers; choosing n requires domain knowledge

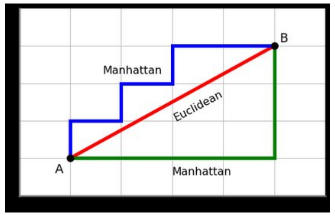
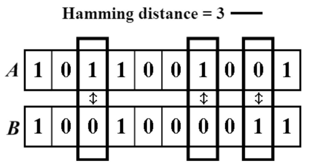
Equal Frequency
- sort values → find breakpoints to produce n bins with <u>equal frequency</u>

K-Means Clustering

Text
Bag of Words
- Vector of frequencies of each word
- CONS: curse of dimensionality, missing context, order, synonyms

Images
Bags of Pixels
- Can work for constrained tasks
- CONS: curse of dimensionality, no shapes/objects, just colours

Distance

Euclidean Distance	*Manhattan Distance*	*Hamming Distance*
		 Hamming distance = 3 A 1 0 1 1 0 0 1 0 0 1 B 1 0 0 1 0 0 0 0 1 1

0-R/1-Rule Classifier

0-R: Majority class classifier – predict majority class
1-R: Predict concept based on feature with least error
1. For each attribute/feature, create a frequency table and **calculate error**
    - assume we always pick majority class for that feature
    - Error = total all instances in minority classes
2. Pick feature with **least error**
3. Use feature to determine concept of test instances

Naive Bayes

- *Marginal Probability*: probability of event occurring for single random variable, without considering values of other variables
    - $P(X = A)$: probability of outcome X=A, considering all possible values of Y
- *Joint Probability*: probability of two or more events occurring together
    - P(X=A, Y=B)
- Bayes' Rule: $P(H|x) = \frac{P(H,x)}{P(x)} = \frac{P(x|H)P(H)}{P(x)}$
    - $P(A|B) = \frac{P(A\cap B)}{P(B)}$
- assumes that <u>all features are independent given the class</u>
- $\hat{c} = \arg\max_{c_j \in C} P(c_j) \prod_i P(x_i|c_j)$

- $\hat{c}$: Predicted Class
- $P(c_j)$: Prior Probability of class c_j
- $P(x_i|c_j) = \frac{\#feature=i}{\#class=j}$: Likelihood – probability of feature x_i given class c_j
- $\prod_i$: product – multiplying lots of numbers between (0, 1] can lead to underflow

Underflow

- Log Transformation: $\hat{c} = \arg\max_{c_j \in C} [\ \log(P(c_j)) + \sum_i \log(P(x_i|c_j))\ ]$
    - take log of each probability and sum instead of product

Zero Values

- If any $P(x_i|c_j) = 0 \Rightarrow$ Final value = 0
- *Simple Probabilistic Smoothing:* replace 0 with positive constant c
- *Laplace Smoothing*: increase counts by α (usually 1)
    -

Unsmoothed	Smoothed
$P_i = \frac{x_i}{N}$	$P_i = \frac{x_i + \alpha}{N + \alpha d}$

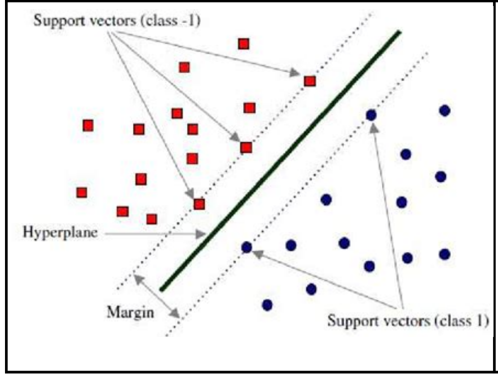
    - CONS: drastic change for small dataset; overestimates rare events
- *Other Options*: Add-k Smoothing, Regression

Decision Trees

Entropy: amount of uncertainty in dataset

ID3
Information Gain
Gain Ratio

Support Vector Machines (SVM)

 Support vectors (class -1) Hyperplane Margin Support vectors (class 1)	- GOAL: find optimal hyperplane to separate classes and maximises margin - PRO: good for high-dimensional spaces (captures feature relationships implicitly); strong generalisation; robust against overfitting (due to C) - CONS: sensitive to hyperparameter tuning (kernel, kernel params, C); computationally expensive; best for supervised binary classification (multi-class and regression is more expensive)

- *Confidence Measure*: distance between new instance and hyperplane
- *Soft Margins*: permits few points to be on the wrong side
- *Kernel Function*: transforms input data to higher-dimensional feature space

K Nearest Neighbours (KNN)

Hill Climbing

- finds best solution for search space (local optima)
- starts with initial solution and iteratively makes incremental improvements
- 1 initialise → 2 evaluate → 3 neighbourhood search (incremental change) → 4 selection (based on performance/evaluation) → repeat 3-4 until termination criterion

Logistic Regression

- binary classification

1. linear combination of input features: multiply each by weight and sum them tgt
2. logistic function (sigmoid function): maps value between 0 and 1
3. determine division boundary (threshold) to determine predicted class
4. trained using maximum likelihood estimation

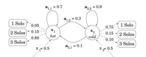
- O(num classes * num features)

Hidden Markov Model

- *Markov assumption*: the likelihood of transitioning into a given state depends only on the current state, and not the previous state(s) (or output(s)), i.e. P (qt|q1⋯qt−1) ≈ P (qt|qt−1)
- *Output independence assumption*: the likelihood of a state producing a certain observation (as output) does not depend on the preceding (or following) state(s) (or output(s)), i.e., P (ot|q1⋯qt, o1⋯ot−1) ≈ P (ot|qt)

Forward Algorithm

- P(3−Solos, 3−Solos, 1−Solo|μ)?



- Initialisation/induction: $\alpha_t(i) = P(o_1, o_2, \ldots, o_t, q_t = s_i|\mu)$

	$t = 1$	$t = 2$	$t = 3$
$\alpha_t(hot)$	$0.5 \times 0.8 = 0.4$	$[0.4 \times 0.7 + 0.05 \times 0.1] \times 0.8 = 0.228$	$[0.228 \times 0.7 + 0.0165 \times 0.1] \times 0.05 = 0.0080625$
$\alpha_t(cold)$	$0.5 \times 0.1 = 0.05$	$[0.4 \times 0.3 + 0.05 \times 0.9] \times 0.1 = 0.0165$	$[0.228 \times 0.3 + 0.0165 \times 0.9] \times 0.75 = 0.0624375$

- Termination:

P(3−Solos, 3−Solos, 1−Solo|μ) = 0.0080625 + 0.0624375 = 0.0705

- calculate the probability of observing a particular sequence of observations
-

Viterbi Algorithm

- find most likely sequence of hidden states given sequence of observations
-

K-Means Clustering

1. Select k points at random as initial cluster centroids
2. compute distance to each centroid for each instance & assign to nearest centroid
3. compute new centroid for each cluster (centroid = mean of all instances in cluster)
4. Repeat form 2. until no instances are reassigned

Gaussian Mixture Model (GMM) / Soft K-Means

- assigns probability associated with each cluster; allows instance to belong to multiple clusters simultaneously
- each cluster represented by Gaussian distribution
- algorithm iteratively updates means and covariance matrices of distribution and recalculates probabilities
- **Gaussian Mixture Model (GMM)**: distribution as composed of k Gaussian distributions
    - *Finite Mixture*: distribution composed of k component distributions

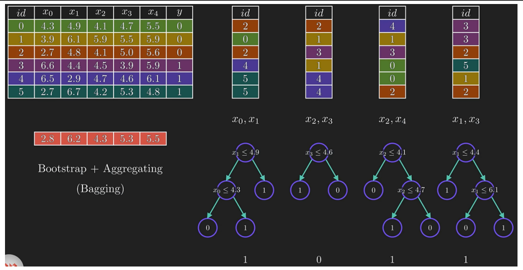
Expectation-Maximisation (EM) Algorithm

- iterative optimization algorithm; generalisation of (soft) k-means; guaranteed positive hill-climbing characteristics
- used to estimate parameters in statistical models with hidden variables

1. *(E)xpectation Step*: calculate posterior probability (expectation) of latent variables given observed data and current estimates of model parameters
2. *(M)aximisation Step*: maximises expected log-likelihood by updating model parameters
3. Repeated until algorithm converges (estimates of model parameters stabilise//reach convergence criterion)

Ensemble Learning

- Aggregate results from base classifiers ⇒ reduces variance
- *Bagging/Bootstrapping*: construct N new datasets with random sampling w/ replacement
    - Instance Absent Probability: $(1 - \frac{1}{N})^N$
    - PRO: simple (1 algo + simple vote); noisy datasets (outliers vanish); can parallelise; less overfitting
    - CON: unstable classifiers ⇒ high variance (and vv)
- *Stacking*: combining output of a number base classifiers as input to further supervised learning (meta) model; to smooth errors over range of algorithms with different biases
    - PRO: results usually better than best of base classifiers
    - CON: computationally expensive; many algorithms
- *Boosting*: focuses on hard-to-classify instances; iterative: sample → update weights → weighted voting
    - PRO: computationally cheap; guaranteed performance (error bounds over training data); minimise instance bias
    - CON: more expensive than bagging; overfitting
- *Random Forest*
    1. Create k new datasets using Bagging
    2. Use random subset of features for each tree



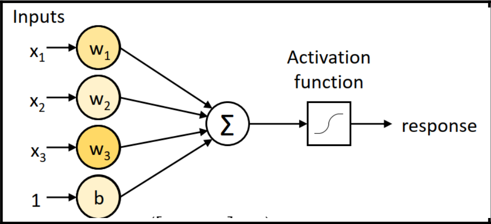
- ensemble of Random Trees
- *Random Tree*: decision tree with only some possible attributes

Neural Networks

Learns feature hierarchy

Embedding: low dimensionality representation of input; can be used for other tasks (not only original task)

Neuron



- Input: vector x_i, $< x_{i1}, x_{i2}, ... >$
- Output: scalar y_i
- Hyperparam: activation function f
- Parameters: weights w, $< w_1, w_2, ... >$

Perception

NN with single neuron

Binary linear classifier

Usually step function (if y_i > 0 then output 1, else 0)

Training Perceptrons

Find weights to minimise errors

1. Iterate over training set (1 iteration = 1 epoch); 2. compare prediction and true values; 3. Update weights

Lambda: learning rate

More penalty on larger inputs; less penalty on smaller inputs

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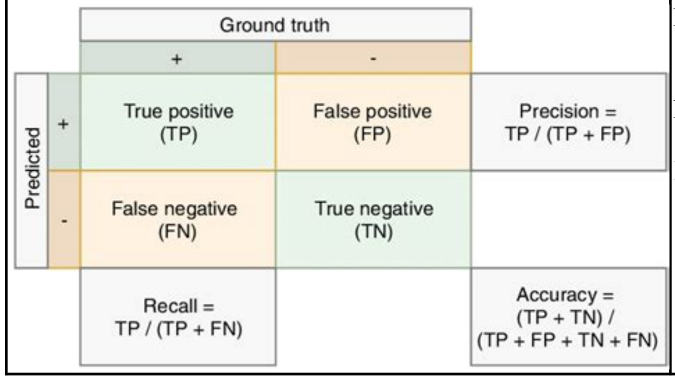
Evaluation

- *Generalisation*
- *Overfitting*
- *Learning Curve*
- *Bias*: tendency to produce same errors; □ Bias ⇒ predicted label distribution ≠ true labels//makes many mistakes; □ Bias ⇒ no mistakes//different kinds of errors on different instances; still similar distribution to true labels

- *Variance*: measure of model inconsistency; produce different classifications on different training sets (randomly sampled on same population)



		Ground truth +	Ground truth -	
Predicted	+	True positive (TP)	False positive (FP)	Precision = TP / (TP + FP)
Predicted	-	False negative (FN)	True negative (TN)	
		Recall = TP / (TP + FN)		Accuracy = (TP + TN) / (TP + FP + TN + FN)

Precision
- □ precision ⇒ □ FP

Recall
- □ recall ⇒ □ FN

Error Rate
- proportion of incorrect predictions
- = (FP + FN)/Total
- = 1 – Accuracy

- *Micro-average*: calculate metric for overall; kind of treat all data as from same class
- *Macro-average:* calculate metric for each class then average the resulting metric values (eg. $\frac{C1\ accuracy + C2\ accuracy + C3\ accuracy}{3}$)

MSE, RMSE and RRSE usually used for <u>regression</u>

Mean Squared Error (MSE)
1. for each prediction, subtract the corresponding true value
2. square the differences
3. calculate average of squared differences

Root Mean Squared Error (RMSE)
1. take square root of MSE
- same units as original data

Root Relative Squared Error (RRSE)
1. divide RMSE by range (max-min) of true values
2. multiply result by 100 (%)
- relative measure of error compared to range of true values

Baseline
Pearson's Correlation

<u>Feature Selection</u>

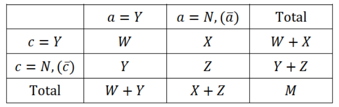
Dimensionality Reduction
- lossy: not possible to reproduce original data from reduced version

PCA
- Projects data to new coordinate system
- Identified Principal Components (linear combinations of original features that capture max variance in data)
- Arrange in descending order
- CONS: assumes <u>linear relationship</u> between features; hard to <u>interpret</u>; assumes □ variance components = informative features; influenced by <u>outliers</u>

Filtering
Pointwise Mutual Information (PMI)
Mutual Information (MI)
- amount of information shared between <u>two random variables</u>

Chi-Square, χ^2
- association between <u>two categorical variables</u> (usually feature and label)
- eval difference between observed and expected freq. → assess deviation
- □χ^2 ⇒ dependency between variables

1. Contingency Table



	$a = Y$	$a = N, (\bar{a})$	Total
$c = Y$	W	X	$W + X$
$c = N, (\bar{c})$	Y	Z	$Y + Z$
Total	$W + Y$	$X + Z$	M

2. Calculate <u>expected frequency</u> for each cell
   - $Expected = \frac{RowTotal \times ColTotal}{OverallTotal}$
3. Calculate Chi-Square Value for each cell and <u>sum</u> all up
   - $\chi^2 = \sum \frac{(Observed - Expected)^2}{Expected}$

set of patterns/principles of **assigning responsibilities** into an object; supports Responsibility-Driven Design (RDD)

Naive Bayes
B should create instances of A if: - B "contains" / compositely aggregates A - B records/closely uses A - B has initializing data for A
K Nearest Neighbours (KNN)
objects should communicate through **intermediary** rather than directly
reduces coupling; more flexible; easier maintain