1 Introduction

Artificial Intelligence

- different interpretations
- we do not have a definition of inteligence

Statistical machine learning

• Algorithms and applications where computer learn from data AGI

- Artificial General Intelligence
- Hypothetical computer program that can perform intellectual tasks as well as, or better than a human.

Turing Test • Also called imitation game

- Tests of a machine's ability to exhibit intelligent behaviour equivalent to, or indistinguishable from that of a human

 • Has some philosophical problems (Complex problems, humans

cant solve / AI must learn to lie) Examples of application (today)

- Personalization of news feeds
 Product searching and recommendation s on eCommerce plat-
- Voice-to-text
- Predictive maintenance

Rias

- · Results that are systematically prejudiced due to faulty assump-
- The inability for a machine learning method (like linear regression) to capture the true relationship, eg. Straight Line can't be curved like the true relationship
- Difference of fits between data sets
- The difference in fits between training and testing set (different data sets in general)
- Low variance Sum of Squares are very similar for different data-

The ideal ML algorithm has low bias and can accurately model the true relationship and it has low variability by producing consistent predictions across different datasets.

1.1 Tasks and Algorithms of Machine Learning



1.2 Dialogflow

Intents An intent categorizes an end-user's intention for one con-

- Recognizes the need of a user
- Require training to match to user inputs
- Follow up Intents (on Success) Fallback Intents (on Failure)

Entities Each intent parameter has a type, called the entity type, which dictates exactly how data from an end-user expression is extracted.

- Extract information from user inputs
- Help to identify required intent
 System Entities Date and time / Numbers / Amounts / Units /
- Developer Entities defined by list of words (@pizza-type / @drink / etc.)

 • User Entities transient, temporary Information based on Con-
- versation (@previous-orders)

Dialog

Linear Gather a list of information
Non Linear Using Contexts

Context

Each Intent can have Input & Output Context
 Intents are active based on active Context

- Expire automatically Fulfillment
- Action triggered on fullfilled Intents

e g Webbook

Predictive modeling Train model for predictions

Feature Engineering

• The process of identifying useful, additional input from the data

· A typical preprocessing step before the actual learning process Deep neural network ANNs with multiple hidden layers

Feature e.g. Years of working experience, school grades

1.3 7 Steps of Machine Learning

- 1. Gathering data Collect quantity/quality data for training/tes-
- 2. Preparing that data Cleanup data (remove duplicates, correct errors, deal with missing values, normalize data, convert data
- types) 3. Choosing a model Select the right algorithm(s)

- 4. Training Train the model, each iteration of process is a training
- 5. Evaluation Use metrics to measure objective performance of the model, test model against previously unseen data, good train/e-val split is 80/29, 70/30
- 6. Hyperparameter tuning Try to improve upon the positive results achieved during the evaluation through gamble with stepNumber of training steps, learning rate, initialization values and distri-
- 7. Prediction Model should be ready for practical applications

2 Natural Language Processing (NLP)

- Automated processing of human language (written & spoken)
 Aims to understand and generate human (natural) language
 Understanding spoken text is still difficult
- Understanding written text became BIG business (searchengines)
 • Generating human-like conversations is still very hard

2.1 4 Ingredients of Machine Learning

1. Data

- Dataset
 Pre-Processing Pipeline including cleansing, feature-engineering, data augmentation etc.

2. Cost-Function (Loss)

- Formal mathematical expression for good / bad Commonly Mean Squared Error (MSE)

3. Model

- From linear model: $\hat{y_i} = ax_i + b$ To complicated million parameter neural networks
- Different tasks require different models (regression / decision

4. Optimization Procedure

- Algorithm that changes the parameters of the model that the
- cost-function is minimized.

 E.g. Stochastic Gradient Descent (SGD), ADAM, RMSProp...

For successful ML, there are many more ingredients ...

- 5. Performance optimization • Building of efficient pipelines
- Folowwing tool specific recommendations
- 6. Visualization and evaluation of the learning Process
- · Learning curves
- Performance measures
- Tensorboard
- 7. Cross-Validation & Regularization
- · Train models that generalize well to unseen data
- Estimate the generalization error

2.2 Representation of Words

Vectors can be used to represent words based on their meaning

2.2.1 One-hot representation

- Vector with a single 1-Value
- All other Values are set to 0
- Count the Number of different Words, Define one unique vector per word

Dini Mom isch fett

l	10]	$\begin{bmatrix} 0 \\ 1 \end{bmatrix}$		0				0	
l	Dini: 0	Mom:	0	isch:		fett:	Ŏ	·. ·:	Õ	
ı	0		l N		0		히		1	

Disadvantages

- Very high dimensional vector space (1 Dimension / unique Word)
 Sparse Representation: Each vector has a single 1 and N Zeroes. (Memory Inefficient)

 No Generalization: All words are unrelated to each other.
- Does not capture any aspect of the meaning of a word

Make a list of words (optionally alphabetically). Use the index to represent each word

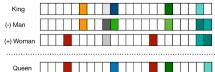
Example: Dini Mom isch fett.

Dini: 0, Mom: 1, isch: 2, fett: 3, '.': 4

- Dense Equivalent of one-hot encoding
 Indexes are not more useful that one-hot vectors
- Often used as preprocessing step
 Indices / One-Hot Vectors are fed into a network which learns more useful representations

2.2.3 Distributed Representation

- vectors that capture (at least partially) the semantics of a word
 Words that occur in similar contexts (neighboring words) tend
- to have similar meanings Similar words share similar representations
- Distributed representations can be learned



Words to Vectors

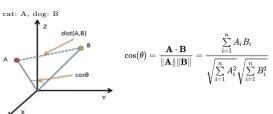
- Mathematical function maps word to high dimensional Vector
 In neural networks, this function is implemented in the Embedding Laver

Advantage (of vectors)

- Good embedding maps similar/related words to similar regions of the vector space (nearby words have a semantic similarity)
 Dot-Product (Skalarprodukt) is a measure of similarity
 Possible to add/subtract vectors
- Calculate Similarities between words Dot-Product (Skalarprodukt) of 2 Vectors is • maximal when parallel (0°), both vectors with norm 1 results in
- max value 1
- zero when orthogonal (90°)
 minimal (negative) when opposite directions (180°) both vectors with norm 1 results in max value -1

Cosine Distance

• Way to calculate how similar two words (vectors) are



 $||A||||B|| = \sqrt{(9+36+4+1)} * \sqrt{(4+49+4+0)} = 53.38539$

A*B/(||A||||B||) = 0.9740high value equals high similarity (to be an animal)

Example

A: (3, 6, 2, 1), B: (2, 7, 2, 0) $A \cdot B = 6 + 42 + 4 + 0 = 52$

3.1 Random Variables

- · Values depend on outcomes of a random phenomenon Random variable X is a variable that takes a numerical value x,
- which depends on a random experiment
- Discrete X takes any of a finite set of values 1.5, 2.123, 6.2, 10 Continous X takes any value of an uncountable range e.g. real numbers from an interval

Best we can know

- All possible values
- Probability of each value

E.g. The discrete random variable X is the number observed when rolling a fair dice. P(X = x) / P(x): 1/6 for each possible value

Joint Probability

- Joint Properties of two random variables
- Defined by the Joint Probability Mass Function

E.g. Dice1 = 5 AND Dice2 = 4
$$P_{XY}(5,4) = P_X(5) * P_Y(4) = 1/6 * 1/6 = 1/36$$

X=1 X=2 X=3 X=4 X=5 X=6

Y=1 1/36 1/36 1/36 1/36 1/36 1/36 1/36

	X=1	X=2	X=3	X=4	X=5	Х=6
Y=1	1/36	1/36	1/36	1/36	1/36	1/36
Y=2	1/36	1/36	1/36	1/36	1/36	1/36
Y=3	1/36	1/36	1/36	1/36	1/36	1/36
Y=4	1/36	1/36	1/36	1/36	1/36	1/36
Y=5	1/36	1/36	1/36	1/36	1/36	1/36
Y=6	1/36	1/36	1/36	1/36	1/36	1/36

Independant random Variables

• Joint Probability is the product of the individual probabilities

P(X,Y)=P(X)*P(Y) (only if independant) P(X,Y,Z)=P(X)*P(Y)*P(Z) (only if independant) Correlated random Variables

- · There are events that are not independant
- Such random variables are correlated
 X: observe clouds (0=no, 1=small, 2=big)
- Y: observe rain (0=no, 1=light, 2=moderate, 3=heavy)

Conditional Probability

- One variable is no longer random
- X is observed, its value is fixed
- Calculate the probabilities of Y given X: P(Y|X)

$$\begin{split} P(X,Y) &= P(X|Y) * P(Y) \\ P(X,Y) &= P(Y|X) * P(X) \\ P(Y|X) &= \frac{P(X,Y)}{P(X)} \end{split}$$
 Bayes Rule

Bayes Rule
$$P(X|Y) * P(Y) = P(Y|X) * P(X)$$

Therefore

$$P(Y|X) = \frac{P(X|Y)*P(Y)}{P(X)}$$

3.2 Probability mass function (PMF)

Wahrscheinlichkeitsfunktion, a function f(x) that provides the probability for each value x of a discrete random variable X

Graph of a PMF



4 Data Visualization

- See trends, clusters and local patterns in data
- Difficult to see in raw data
- Detect outliers and unusual groups
 Validate Hypothesis/Conjecture/Theory

Important in a Plot

- X-Axis labels which data is represented and its units
 Y-Axis labels which data is represented and its labels
- Scale linear, logarithmic
- Dimensionality of the data 2D / 3D

Dataframe a two-dimensional labelled data structure with columns

4.0.1 Data Analysis Libraries

NumPv

- Package for scientific computing in Python
 Multidimensional array object
- Routines for fast array operations (sorting, selecting, FFT, line-

pandas

- Built on top of NumPy
 Routines for accessing tabular data from files (.csv, xls, etc.)
 Supports 2-dimensional data (dataframe and series)
- Dataframes are something like database tables

MatPlotLib

Library for visualizing data
Provides bargraphs, histograms, piecharts, scatter plots, lines, boxplots, heatmaps, ...

Seaborn

- · Extension of MatPlotLib, NumPy and pandas
- More user friendly
 Plots are aesthetically better

4.0.2 Line Plots

• Bivariate, Continuous Recognizes trend (pattern of change) (over time)

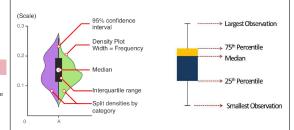
4.0.3 Bar Chart

- Used for categorical data
 Counting based on each category

4.0.4 Histogram

- $\bullet\,$ Represents the empirical distribution of a variable
- Automatically creates bins (interval) along the range of values
 Shows vertical bars to indicate the number of observations per

4.0.5 Descriptive Statisics: Box Plots and Violin Plots



4.0.6 Scatter Plot

Relationship between (two) continuous variables
Helps to get an idea of the degree of correlation between varia-

5 Linear Regression

a simple method to analyse data

- Only consideres a linear relationship between input and output In the simplest case, x and y are scalars and the linear model therefore has only two free parameters The goal is to identify a (slope) and b (intercept) for which the linear model best explains the data

$$\hat{y_i} = ax_i + b$$

Applications

- Interpretation has some input an effect on the output, eg. Is there a relationship between smoking cigaretts and the risk of lung
- Prediction Given some sensor data like oil pressure, temperature
 ..., eg. a model could predict (and thereby hopefully prevent) an

5.1 Model

In ML, we use the term model for any mathematical function that explains the data

$$y_i \approx f(x_i) \\ y_i = f(x_i) + \epsilon_i$$

where ϵ_i is unexplained noise. It is often assumed that ϵ_i follows a normal distribution. Instead of approximating y_i , we calculate an estimate $\hat{y_i}$ (y hat) of the usually unknown y_i :

$$\hat{y_i} = f(x)$$

5.2 Mean Squared Error (MSE)

Loss we want to minimize
Usually divided by 2

$$\begin{split} \hat{y_i} &= ax_i + b \\ e_i &= y_i - \hat{y_i} \\ \text{The difference } e_i, \text{ called residual} \\ E &= \frac{1}{2N} * \sum_{i=1}^N e_i^2 \\ E &= \frac{1}{2N} * \sum_{i=1}^N \left(y_i - (a * x_i + b) \right)^2 \end{split}$$

5.3 Correlation and Causality

- · Correlation is not causality
- Correlation refers to the degree to which a pair of variables are • Linear regression is a tool to detect correlations between two or
- more variables

 Correlation can be quantified using the Pearson correlation coefficient

6 Optimization

- Training or learning in AI often suggests an algorithm performing some sort of optimization
- It is the problem of finding a set of inputs to an objective function that results in a maximum or minimum function evaluation
- In our examples the objective is to minimize the loss function

6.1 Gradient Descent

At any location [a,b] we look at the error-gradient in the neighbourhood of [a,b] and move a (small) step in the direction where the error shrinks the most. By repeating this procedure, we will eventually arrive at the location where the error is smallest.

- Iterative Method/Procedure
 Each iteration, the model parameters are updated such as that the Loss (MSE) is reduced
- Move along a trajectory which includes fewer points
 At each point of the trajectory we evaluate the gradient of the
- error function • At each iteration, we would have to iterate over all N = 1'000
- points to calculate the gradient of the loss function.

Calculate Gradient

Gradient of E =
$$\begin{bmatrix} \frac{\partial E}{\partial a} \\ \frac{\partial E}{\partial b} \end{bmatrix}$$

Calculate these two partial derivatives

$$\frac{\partial E}{\partial a} = \frac{1}{N} \sum_{i=1}^{N} (y_i - (a \cdot x_i + b)) \cdot - x_i$$

$$\frac{\partial E}{\partial b} = \frac{1}{N} \sum_{i=1}^{N} (y_i - (a \cdot x_i + b)) \cdot -1$$

$$\text{Gradient of E} = \begin{bmatrix} \frac{\partial E}{\partial p} \\ \frac{\partial E}{\partial b} \end{bmatrix} = \begin{bmatrix} \frac{1}{N} \sum_{i=1}^{N} (y_i - (a \cdot x_i + b))(-x_i) \\ \frac{1}{N} \sum_{i=1}^{N} (y_i - (a \cdot x_i + b))(-1) \end{bmatrix}$$

6.2 Stochastic Gradient Descent (SGD)

we do not need the exact gradient to find a trajectory toward the minimum. Instead, at each iteration we can randomly pick a few datapoints and use them to calculate an approximation of the gradient.

- At each iteration, the gradient is calculated on a (randomly selected) subset of the data
- For a fixed learning rate, SGD does not converge

Mini-batches

- 1 < n < N• Increasing the batch-size will reduce the variance of the gradient estimation
- batch-size n = 1 yields a very noisy gradient
 batch-size n = N is expensive to calculate
- often mini-batches of size n = 32 or n = 64 are used

Annealed SGD

- The learning rate alpha is reduced over time
 This is called (simulated) annealing
 There are different options (called schedules) how to reduce alpha over time
 • A fixed learning rate α does not converge. The algorithm keeps
- fluctuating around the minimum. Annealed SGD solves this appearent contradiction by adapting the learning rate. It starts with a large α and reduces it over time

6.2.1 General remarks on SGD

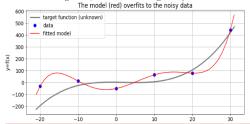
- Gradient-based methods only work if we can express a Loss function as a differentiable function
- SGD is dealing with only a single datum at each iteration. This
 is very inefficient and rarely used.
- · Batch- or mini-batch gradient-descent is usually used

7 Generalization and Regularization

- Out-of-sample Error Generalization Error (Test Error) is the MSE of new Data
- A good model has a low Generalization Error

7.1 Overfitting

- A model that perfectly fits the data does not have to be perfect
 In-Sample Error (Training error) was minimized (MSE = 0)
 Overfitting happens if the MSE of Training Error is small thanks to a complex model but the Generalization Error is large (Good with training data, bad with testing data)



7.2 Underfitting

- Using a too simple model
 In-Sample Error is large
- Generalization Error is large



7.3 Training-Set, Test-Set, Model Evaluation

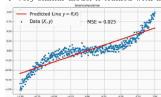
- The Generalization Error can't be calculated, but estimated
- Split the data into 2 sets
 Training-Set (80% of data)
 Test-Set (20% of data)

- Training
 Fit the model to the training set
- · This minimizes the in-sample error
- Evaluating
- Using the Test-Set
 Produces the Test-Error
 This is an estimate of the Generalization Error

7.4 Bias-Variance Trade-off

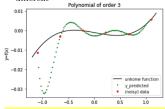
High Bias

- A too simple model for the given data
 Low Variance
 The model is relatively stable
 Very similar model if trained with new data



Low Bias

- A more complex model can better explain the data High Variance
- Given a new datapoint, the MSE can be very large
 For a different set with more datapoints, the model may be very different



- Higher bias implies lower variance
 Lower bias implies higher variance
- In practice, all we want is low variance
 The model can only be as complex as the data permits
- You have to find an optimal balance between bias and variance

← Underfitting Overfitting >

model complexity

Training Error

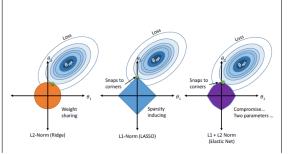
7.5 Regularization

Technique to measure the model complexity

Technique to control the model complexity

- Add a penalty term to the Loss (optimization problem)
- More complex models get a higher penalty
 Add a constrain to the optimization process
- ullet Modified optimization error target regularized loss = MSE + λ model-complexity

$$\sum_{i=1}^{n} (y_i - \sum_{j=1}^{p} x_{ij} \beta_j)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$



8 Cross-Validation (CV)

- a technique to compare (and select from) different models (=different parameter values)

 • Use case 1: Obtain a better estimate of the generalization error
- Use case 2: Selection of hyper parameters, split/train pattern of cross validation can be used to find optimal hyper parameters

Problem with (80/20) Data Separation

- Test Error depends on random set
 For different sets, the test error would be different

without cross-validation



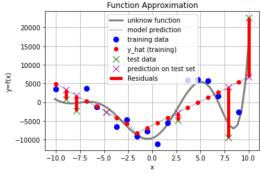
8.1 k-fold Cross-Validation

With k-Fold Cross-Validation

- The data is split once into k folds Repeats the split-train-test procedure k times, using a systematic resampling procedure
- Then train/test is repeated k-times.
 Each fold participates in k-1 training phases and is used once for testing



- Typical Values for k are 5,10 or N
 The data of a fold does not change during procedure
- Do not preprocess the whole dataset
- Apply the preprocessing pipeline (standardization) to each split
 Each split generates a different model
- With regularization, each split may yield a different model and a different optimal λ



9 Artificial Neural Networks (ANN)

An ANN is a data-structure to define arbitrarily complex mathe-

9.1 Artificial Neurons

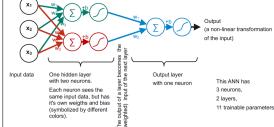
- Receives an input vector $[x_1, x_2, ...]$
- Each neuron has its own input weights $[w_1, w_2, ...]$ and bias b
- (=intercept)
 Calculates the sum of the weighted input (dot product $\vec{x} * \vec{w}$). adds a bias b, and passes it through a nonlinear activation function



example of a popular non-linear activation

The Rectified Linear Unit (Rel II) cuts-off negative values (y=0). Positive-values are passed through (y=x)

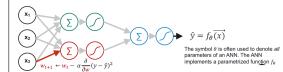
9.2 Simple Artificial Neural Network (ANN)



9.3 Training an ANN

Supervised learning

- Data with label
- For each input \vec{x} we are given the output \vec{y} ANN is initialized with random weights
- An optimizer reduces a cost-function (e.g. MSE)
 At every iteration, and for every single weight w and bias b.
- the partial derivative needs to be calculated. (Backpropagation algorithm)



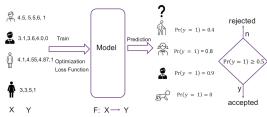


Classification method

10.1 Binary Classification

- Decision with 2 possible outcomes
 Hail in Lausanne (yes/no)
 Master admission (admission / no admission)
 Based on different data / entity

y=1 implies yes/accepted/admission, y=0 implies no/rejected $P(y=1,x_1=4.5,x_2=5,x_3=5.5)$



10.2 Predicting Probabilities: Logistic Regression

Decision using Linear Regression

- Train the model with gradient descent

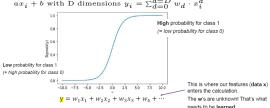
Models the response (y) and post process the response (e.g. by thresholding) to compute the probability

The model: sigmoid function

- Values between 0 and 1. y is interpreted as probability
- Function is not parametrized
 Has a single input value

$$sigmoid(y) = \frac{1}{1+e^{-y}}$$

- calculated from the input data
 a linear combination of the input features, with one feature $ax_i + b$ with D dimensions $y_i = \sum_{d=0}^{d=D} w_d \cdot x_i^d$



Probabilities

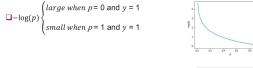
- We can write the estimated probabilityFor a prediction we can write

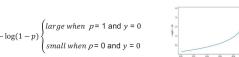
$$P(x) = \frac{1}{1 + e^{-(W^T x)}}$$

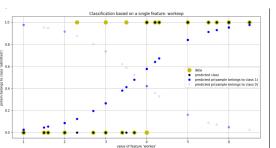
$$\text{e.g. } Pr(y_i = 1 | x_i; w) = \frac{1}{1 + e^{-\left(w_0 + w_1 \cdot x_{i,1} + w_2 \cdot x_{i,2} + w_3 \cdot x_{i,3}\right)}}$$

10.3 Optimization: Maximum Likelihood Estimation

- Given all the data points (X,Y) we want to maximize the probability that all the predictions are correct.
- For each of the training data, we want to maximize the likelihood
- of correct prediction \bullet We can use Gradient Descent to find optimal W

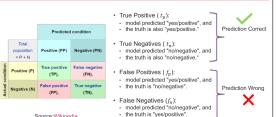






11 Classifier Evaluation

11.1 Confusion Matrix



Source:Wikipedia Mean Accuracy

• How often is the classifier correct? • $A = (t_p + t_n)/n$

Mean Error

- How often is the classifier wrong? $E = (f_p + f_n)/n$

Precision

Sensitivity, Recall, True Positive Rate (TPR)

• How often the prediction is 1 when it's actually 1 $\bullet \ R = t_p/(t_p + \dot{f}_n)$

Miss Rate, False Negative Rate (FNR)

• MR = 1 - TPR

11.2 Why Accuracy is not enough?

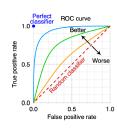
- If the prediction is constant the accuracy may still look decent
- E.g. always predict false 90% of the data is false
- Accuracy = 90% (decent)
 Precision = 0
 Recall = 0

11.3 Precision vs. Recall

- Increasing precision reduces Recall and vice versa
 Threshold is a business decision (depending on goals)

11.4 Receiver Operating Characteristics (ROC)

- Defined by FPR and TPR as x and y axes
 Visualizes tradeoff between TP (benefits) and FP (cost)



Area under the curve

- Area under the ROC curve
 Shows how well the TPR and FPR is looking in the aggregate
- The greater the area under the curve, the higher the quality of the model
- The greater the area, the higher the ratio of TP to FP

12 K-Nearest Neighbour (KNN)

Classification method

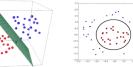
12.1 Linear Separability

linearly separable in 2D









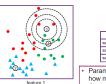
- Based on logistic regression model, you can draw a line
 This is the Linear decision boundary
 If a simple line perfectly seperates the classes, then the classes are said to be linear separable

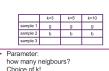
12.2 Non-Linear decision boundary

- When classes are not linearly separableResort to polynomial terms

12.3 k-Neares Neighbors (KNN)

- A datapoint is know by the company it keeps
- Computes k nearest neighbours
- Returns the most frequent class of the k neighbours





Process

- 1. Load the training and test data 2. Choose value of k (number of nearest neighbours to consider for classification)
- 3. For each test data points x_{test}

For all training data x_{train} calculate $d(x_{test}, x_{train})$ with distance metric

Sort training data in ascending order of distance Choose first k data points from sorted training data Choose most frequently occurring class from k data points as classification result

Distance Metric

- Cosine Distance $cost\theta = \frac{x_1 \cdot x_2}{||x_1|||||x_2||}$ Manhattan Distance $d_M = \sum_{i=1}^n |x_{1,n} x_2, n|$
- Euclidean Distance (most used) $d_E = \sqrt{\sum_{i=1}^n (x_{1,n} x_{2,n})^2}$
- Minkowski Distance

Advantages

- Easy and simple ML model
 Few hyperparameters to tune

Disadvantages

- k should be wisely selected
 Large computation cost during runtime if sample size is large
- Not efficient for high dimensional datasets
 Proper scaling should be provided for fair treatment among fea-

- K Value how many neighbours to participate in the KNN algo-
 - Distance Function Euclidean distance is most used

13 Clustering

13.1 Unsupervised Learning

- We are given Data (features, x) without labels (y)
 It learns something through the structure of the data
 The goal of unsupervised learning is to self-discover patterns from the data

Clusters

- Data points which have shared properties
 Fall into one cluster or one alike group
 Similar Data Points are close together
- Group n data points into k_c number of clusters

Applications

- Social Network Analysis
 Astronomical Data
- Marked segmentation
 Recommendation systems

13.2 Naive K-means

- Let us assume we know the number of clusters k.
- 2. Initialize the value of k cluster centres (aka, means, centroids) $(C_1, C_2, \dots, C_{k_c})$

- 1. Find the squared Euclidean distance between the centres and all the data points.
- 2. Assign each data point to the cluster of the nearest centre
- 4. Update: Each cluster now potentially has a new centre (mean). Update the centre for each
- 1. New Centres $((C'_1, C'_2, \dots, C'_{k_c}))$ = Average of all the data points in the cluster $(1, 2, \dots, k_c)$
- 5. If some stopping criterion met, Done

6. Else, go to Assignment step 3

- Initialization: choose (C_1,C_2,\ldots,C_{k_c}) . $(C_1\ldots$ are vectors in the same space as the features. They can be randomly initialized)
- · Assignment Step:

$$\forall_{k=1}^{k_{c}} \ \forall_{l=1}^{N} \ \mathrm{d}_{i,k} = (x_{l} - C_{k})^{2}$$
 (squared euclidean distance)

$$\begin{array}{ll} d_{i,k}^{min} = \ \textit{Minimum} \big(\mathbf{d_{i,1}}, \mathbf{d_{i,2}}, \ldots, \mathbf{d_{i,k_c}} \big) \\ x_i \in \textit{Cluster } k \end{array}$$

Update Step: (centre_k = mean of all data in cluster_k)

$$\forall_{k=1}^{k_c} C_k = \frac{1}{size(C_k)} \sum_{\mathbf{x}_i \in state(\mathbf{x}_i)} \mathbf{x}_i$$

- Stopping Criterion
 When centres don't change (time consuming)
- The datapoints assigned to specific cluster remains the same (takes too much time)
- The distance of datapoints from their centres >= treshold we have set
- Fixed number of iterations have reached (choose wisely)

Initialization

- Performance depends on the random initialization
- Some seeds can result in a poor convergence rate
 Some seeds can converge to suboptimal clustering
 If centres are very close, it takes a lot of iterations to converge
 Initialize randomly, run multiple times
 Standardization of data
- Features with large values may dominate the distance value
 Features over small values will have no impact
- Normalize values! 13.3 Sklean k-means

Initialization

- Init = K-means++
- Only initialization of the centroids will change
- Chosen centroids should be far from each other
- max iter
- Number of iterations before stopping
- n init
- Number of time the k-means algorithm will be run with different centroid seeds

13.4 Evaluate Cluster Quality

• Make clusters so that for each cluster the distance of each cluster member from its center is minimizes

Inertia or within-cluster sum-of-squares (WCSS)

- Sum of squared distances of samples (each point) to their closest
- As small as possible

Y-Values									
3.5									
2.5									
2	• • •)								
1.5									
1									
0.5									

	Squared Euclidean distance from red centre	Squared Euclidean distance from red centre			
	1.25,2	2.5, 1			
1,3	$(1.25 - 1)^2 + (3 - 2)^2 = 1.0625$	-			
1,2	0.0625	-			
1,1	1.0625	-			
2,1	-	0.25			
2,2	0.5625	-			
3,1	-	0.25			
wcss	2.75	0.5			

Silhouette Score

- How far the datapoints in one cluster are from the datapoints in another cluster
- Silhouette Score of a point: $\frac{b-a}{max(a,b)}$
- a: average intra-cluster distance (distance between each point

• b: average inter-cluster distance (distance between a cluster and

Silhouette Score

- Silhouette(1,3) = $\frac{(3.65 1.47)}{3.65}$ = 1 $\frac{1.47}{3.65}$ = 0.59
- Silhouette(2,2) = $\frac{(1.2-1.27)}{1.27}$ = $\frac{1.2}{1.27}$ 1 = -0.05
- · The range of silhouette score is from -1 to 1
- · Score should be closer to 1 than -1

	Distance from points in the GREEN cluster					Distance from other points in the cluster				П
						1,3	1,2	1,1	2,2	a
	2,1	3,1	b	1.	-	_	4	2	$\sqrt{2} = 1.41$	1.4
1,3	√5	√8	3.65	1 25			'	2	V2 = 1.41	1.7
1.2	√2	√5	1.8	1,	2	1	-	1	1	1
	V2	- 43	_	1,	1	2	1	-	√2	1.4
1,1	1	2	1.5	l 📙						1
2,2	1	√2	1.2	2,	2	$\sqrt{2}$	1	√2		1.2

14 Ensemble Methods

- Suppose we have many different weak models (better than ran-
- Get prediction from all of them and take a vote
- Class with most votes is the predicted class
 Commonly used towards the end of a project
 Requirement enough models / diverse models
 Wisdom of Crowd
- Suppose you have a difficult question
- Ask many people and aggregate the answer
 This might work very well instead of finding the best suited per-

- Wisdom of Crowd can be applied to ML
 Instead of finding the best model, aggregate the results of weak models
- Aggregate predictions of regressors or classifiers
 Might get better accuracy than the best predictor
 Ensemble: group of predictors

- Aggregate predictions

 Hard voting Predict class with most votes • Soft voting Predict class with the highest class probability

14.1 Bagging and Pasting

Bagging (Bootstrap Aggregating)

- Sampling with replacement
 Allows data points to be used several times



Pasting • Sampling without replacement

14.2 No free lunch theorem

No single machine learning algorithm is universally the best-performing algorithm for all problems

14.2.1 Out of Bag (oob) Evaluation

- Using Bagging
- Some Data Points may not be used at all
 Use them for evaluation