**Holy Bible**

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# Knowledge discovery in databases

# Frequent pattern mining

## Set theory

Powerset complexity: 2n where n is the length of the set

## Frequent itemsets

k-itemset: The length of an itemset

An itemset is a subset of a collection of items. They are ordered by a total ordering.

**Support:** The support is how often an itemset occurs in the database

**Frequency:** This is the support divided by the size of the database.

**Frequent itemset:** On itemset is frequent if its support or frequency is above a threshold.

## Association rules

A rules which states, that if one thing then something else. So if we buy milk, we also buy coffee:

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Automatisk genereret beskrivelse

IT describes co-occurences NOT causality. It does not have to hold for all cases.

**Support of the association rule**: The support is the union of how often the left hand side occurs and the right hand side occurs.

**The frequency:** is the support of the rule divided by the size of the database.

**Confidence:** How certain is the rule. This is the support of the full association rule divided by the support of the left hand side. (antecedent)

## Association rule mining

We try to find the associations rules, where the support is above a threshold and the confidence is above a threshold.

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**Brute force:** Take each possible itemset from the list of items and check the database if the count is frequent: The complexity is *2n \* length(database)* So the complexity is the 2 to the power of the number of items times the length (number of transactions) of the database.

## Monotonicity and anti-monotonicity

**Monotonicity:** If a set is frequent is subsets will be frequent as well

**Anti-monotinicity:** if a set is infrequent its subsets will be infrequent as well.

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The web above is called a lattice.

This is a positive border if the set cde is frequent.

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Automatisk genereret beskrivelse

This is a negative border:

Et billede, der indeholder diagram, kort, linje/række, cirkel

Automatisk genereret beskrivelse

### Max and closed frequent itemset

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**Closed frequent itemset:** An itemset is closed if none of its immediate superset has the same support and if it is frequent. So here is an example of a closed itemset with support = 3:

Et billede, der indeholder diagram, kort, Plan, tegning

Automatisk genereret beskrivelse

**Max frequent itemsets:** Is a set where, none if its immediate supersets are frequent. Here is an example with support = 3:

Et billede, der indeholder diagram, linje/række, Plan, kort

Automatisk genereret beskrivelse

These frequent itemsets do not have a frequent superset.

## Apriori algorithm

This algorithm utilizes the power of monotonicity and anti-monotinicity to only search the itemsets, that will be frequent by pruning itemsets, where its subsets are infrequent.

The algorithm is pretty simple:

1. Create all singleton itemsets
2. Count how often each singleton itemset occurs
3. C\_1 = Prune / remove those, that have a support lower than the threshold.
4. Create all 2-itemsets combinations of the remaining itemset
5. Return Set of items (set\_1)

K = 1

While set\_k is not empty

1. Join the itemsets where the first k-1 element is the same in set\_k.
2. C\_k = prune remove a set, if it contains a subset that is not part of set\_k
3. Count how often the c\_k occur in the database
4. Set\_k = Prune / remove those that have a lower support in the Db than the threshold
5. K = k + 1

**Complexity** O( 2n ) where n is the number of items

### Association rules in apriori

For each frequent itemset, that is left, we build association rules and delete rules with confidence below a given threshold.

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Support is useful for business, confidence measures how reliable a rule is. But there are other measrues called interestingness that can be used instead, since you can get a high confidence, let’s say 25% buy coffee and tea together, this might sound interesting, but if you then consider that 80% of all people buy coffee, then it is pretty uninteresting.

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# Feature spaces and distances

We can transform an object into a lower representation feature space. The goal is to only keep the relevant information.

3 types of features:

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Automatisk genereret beskrivelse

We can aggregate features, such as counting their frequency, relative frequency, their median or their average (slide 112)

## Centroids and medoids

A centroid is the mean of all our samples:

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Automatisk genereret beskrivelse



A medoid is the point which have the smallest distance to all other datapoints:

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Automatisk genereret beskrivelse

## Distance

A feature space have a distance function, it must be strict (that is one is higher than the other), it must be symmetric (if x > y then y < x) and reflexive (if distance from x to x must equal 0)

A metric space is a feature space, where the triangle inequality holds, most common is the euclidian space:

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Automatisk genereret beskrivelse

Z --> y --> x is greater than y 🡪x

We have this formula for calculating distances:

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We can also have euclidian weighted distance and quadratic matrix distance:

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Automatisk genereret beskrivelse

## Images

With a color histogram we can create a histogram where we count the frequencies of each color. Moreover, we can reduce the number of colors, which can be useful for reducing features.

# Clustering

Clustering is an unsupervised approach to categorize data points, since in the works case scenario (if we used a naïve method) we would end up having O(kn ) partitions.

## Partitional clustering

A data set is portioned into k cluster with the goal being minimizing a cost function.

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This strategy requires us to chose how many k we want. We then optimize iteratively, this is done by assigning the points to the same cluster as its closests representative. We can use a centroid, medoid or a gauissian distribution model.

The centroid of a cluster is the mean of all points in the cluster

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The measurement of its compactness is done by summing up the distance from each point to its centroid in the cluster. This is called the sum or squared error, and is a loss function we should minimize

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Automatisk genereret beskrivelse

We can see how the total clustering is by summing up the sum of squared error for all clusters:

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Automatisk genereret beskrivelse

## Clustering by minimization of Variance (Forgy, Lloyd)

We chose k random points, and assigns all points to its closest representative. Then we compute the centroid and assign each point to its closest centroid. We repeat this process until there are no new assignments

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## K-means clustering

This is ALMOST like the clustering by minimization of variance, but the centroid is recalculated as soon as a point is reassigned, rather than waiting for all points to be assigned.

Since the centroid is calculated immediately after a point is reassigned, the cluster will depend on the order the data is processed.

Runtime: O(k \* n) pr. Iteration (usually 10 iterations)

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## k-medoids

K-medoids is basically the same however it does not compute the centroid, but the medoid, this means that it can be used in more types of spaces, since it can work in non-euclidian spaces. It is also less sensitive to outliers.

## k-modes

This works with categorical data. This likewise minimizes distance. However, if two points are not the same category, their distance will just be one otherwise 0. If the categories are numerical, we can use a traditional centroid.

## Choosing k and evalutaing

There can max be n – 1 clusters

Chose the one with the best score. How to evaluate this is hard since TD2 becomes smaller with higher k, therefore we use silhouttes since it is independent of k

We are evaluating to things with silhouttes the cohesion (how tighly are members connection in a cluster) and separation, which evaluates how well clusters are separated.

There are the standard and the simplified version, the standard looks at the average distance between all members of a cluster and all members of the cluster that is closest. While The simplified only looks at the centroids.

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Automatisk genereret beskrivelse

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## Empty clusters

These cause problems since we cannot do the mean of an empty cluster.

We can remove one cluster (which I do), use a point that is farthest away from any centroid, or chose a random point as a new centroid.

# Classification

A supervised process where we have examples and information about the classes. The goal is to map an object o to a class c with a function, the goal of classification is to learn this function also known as the target function.

The function we learn will only be an approximation of the target function.

We train the model on training data.

A classifier has some assumptions on how the separation between classes can be achieved.

These assumptions define the hypothesis space or the set of hypotheses that are possible to create (example a decision tree will only separate verticaly and horizaontally). This hypothesis space is the bias, which means that certain algorithms tend to prefer certain hypotheses. However this is needed in order to avoid overfitting or learning the training data by heart.

## Evalutaion

We tend to get higher evaluation scores on training data than on test data, this is called overfitting. Moreover, it is hard to evaluate a classifier, since we do not know anything about the predictions on unseen data, we cannot verify them.

To avoid this problem we train the data on training data and evaluate on test data. The problem is that we are then reducing our training data.

## m-fold validation

This is a method to evaluate our performance. We basically split our data in m subsets. For each subset we leave one out for testing and use the rest for training. We then average the observed performances and get a more robust performance result. Et billede, der indeholder tekst, skærmbillede, Font/skrifttype, nummer/tal

Automatisk genereret beskrivelse

## Stratificaiton

With stratification we try to represent the class proportions in each fold. Each class must be present in the training set, and the distribution of each should reflect the distribution of classes in the whole training set.

## Bootstrap

With bootstrap we randomly draw objects with replacement (that is they can be reused) from the whole set and train on this.

## Leave-one-out or jack-knife

This is n-fold cross validation. For each sample we leave one out for testing and train on the rest of the dataset. We then average the results of all the test. This gives a pretty pessimistic performance.

## Confusion matrix

A confusion matrix shows the number of correctly predicted classes on the diagonal and how the classifier misclassified on the classes:

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Automatisk genereret beskrivelse

# Accuracy, true error and apparent error

Accuracy is the number of correctly classified predictions divided by the total number of predictions in the test set

True error is the number of misclassified predictions divided by the total number of predictions in the test set

The apparent error is the number of misclassified predictions in the training set divided by the length of the training set

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## True positives and false positives

We a binary classification problem we can split our observations into true positives and false positives in a matrix

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Automatisk genereret beskrivelse

This is useful if there for example is an intereset in minimizing false negatives (for example with medical tests, where we want to minize the number of sick people being classified as healthy).

## Precision, recall

Recall and precision are very similar, but they fundamentally try to answer the following questions for a class:

Precision: What proportion of a predicted class was actually correct? It is calculated by taking the number of correct predictions in a class and dividing it by the number of samples in that class

Recall: What proportion of a the class was correctly classified? It is calculated by taking the number correct predictions in a class and dividing it by the total number of samples that was predicted as belonging to this class.

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## KNN (K nearest neighbour)

K-nearest neighbour is a very simple algorithm. It takes a point and then depending on its k-nearest neighbours assigns the object to the majority class. If k = 1 it will assign it to the same class as the 1 closest neighbour, it is 3 it will look at the three nearest neighbours and assign it to the class, which contains the majority. It is a lazy learner, since it does not save a model, it only contains the data, and the learning process happens, when new data points are added to the training data.

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This will create a bunch of decision boundaries, which can be compared to a voronochi diagram

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K should not be too small, otherwiser it might be too sensitive to outliers. If it is to large, it might overreach and take unrelated classes into account. 1 < k < 10

It is possible to add a weight on classes. This can either be on distance or on on the class proportions, so smaller classes have a higher voting power.

Ties: If there is a tie, we can do one of the following:

* Chose a different k
* Randomly chose between one of the values
* Look at the distances between points and chose those, which have the shortest distance

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# Baysian learning

It is a way to calculate conditional probabilities, what is the probability of y given x. The best example is this, If I think I saw a donkey, but know it is most likely a horse, I will conclude that it is a mule.

**Sample space:** A set of all possible outcomes in a random process

**Event:** A subset of the sample space, which contains individual outcomes of this process is an event.

**Allowable events:** This is a set of events that are possible, where each subset each also a subset of the sample space.

**Probability function:** A function between 0 and 1, which returns the probability of an event, the probability of the whole sample space is always 1, and the sum of probabilities for k events is the same as the probability for the union of these events.

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Two events are independt if the probability of their co-occurrence is the same as the the events multiplied by each other. If events are independent, then knowledge about one event does not change the probability of the other events. So if I flip a coin and get heads, it wont influence the probability of my second coinflip.

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To get the conditional probability of (e and f) we take the probability of e and f together and divide it by the probability of f happening at all:

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Automatisk genereret beskrivelse

Quality measures of association rules can be seen as probabilities.

Support is the probability of a sample being in the databaseEt billede, der indeholder tekst, Font/skrifttype, hvid, design

Automatisk genereret beskrivelse

Confidence is the conditional probability of a association rule:

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The probability of an event is the same as the sum of all conditional probabilities for that event times the probability of the condition:

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## Bayes theorem

I sin simpleste form er bayes theorem for P(A | B) at vi tager den conditional probability for P(A | B) og ganger den med P(A) og dividerer den med P(B)

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Dette kan generaliseresEt billede, der indeholder tekst, skærmbillede, Font/skrifttype, nummer/tal

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This gives the following:

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With a baysian there is always different hypotheses, here we are hypothesizing wether the patient has flu, so there is a 1 – 0.13 = 87% percent chance that is it something else. To test the others we have to perform the same test but with other values in the top and bottom, they have to be swapped.

With a model we set a prior which in the formula below is Pr(B). If we don’t know it we can set it to ½, but if we then get some more knowledge about the prior, we can change it.

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## Baysian learning and probabilities

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With this we can observe the likelyhoof of an hypothesis given the observed data:

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Which can be used to get the most likely hypothesis

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Automatisk genereret beskrivelse

This gives that the likelihood of a hypothesis is just:

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So the amount of hypothesis d divided by the amount of hypotheses or said another way, the probability of each hypothesis is just the proportion of each hypothesis, so if P(h\_1 | D) = 0.7 and P(h\_2 | D ) = 0.3 then the MAP is h\_1

By letting P(D | h) take other values than 0 or 1 we can model noisy data.

## Bayes optimal classifier

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The bayes optimal classifier has a different hypothesis space since it can give a probability score

## Naïve bayes

The naïve bayes algorithm test the likelihood by combining the likelihood of each feature / attribute and which class is most likely is, it then choses the one based on this. Due to this is assumes that each feature is independent of each other.

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# Learning with distributions

We are often interested in some complex event, such as the sum of two dice rolls, here we are mapping the result of our sample space to a real number, this is a random variable.

The mean or average is the expected value of a random variable:

When we look at data we can either interpret it as a distribution, where the data set is a random sample, that can be used to make inferences about the population or we can view it as points in a space, where we can calculate distances.

Et billede, der indeholder diagram

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# EM clustering (parametric learning)

Each cluster follows a probability density function (normal distribution typically) points are assigned to a cluster depending on the probability of belonging to a cluster. For each point we check it probability with conditional probability:

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Each cluster is a hypothesis that tries to explain the data as k collections of distrivutions. We try to get the hypothesis that maximizes this expectation:

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Runtime:



The full model looks like this:

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Automatisk genereret beskrivelse

## Non-parametric learning

With parametric learning we assume that the data follows a specific distribution such as gaussian. We learn the mean vector and the covariance matrix of this distribution.

Non-parametric learning tries to infer probabilities directly from the sample without knowing the specific distribution or density function. K-nearest neighbours and naïve bayes are non-parametric, since they do not make any assumptions about the underlying probability density function for the whole data set.

## Density based clustering

With density based clustering we assume that a cluster if a area of high density separated from other clusters by a low density area

For am object in a cluster the local density must exceed a threshold:

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Automatisk genereret beskrivelse

Slide 438 gives a nice demonstration of how this threshold affect how many clusters we end up with. Moreover density based clusters often discard points outside clusters as noise instead of classifying them.

Density based structures makes an intuitive sense in natural data

The basic idea is that we have a core point, where the density is defined as having a threshold of points that must be reachable from this points, we then follow each reachable points until we hit a point without any reachable points, and then we have our cluster.

Et billede, der indeholder diagram

Automatisk genereret beskrivelse

It has two properties, which allow for efficient cluster searching:

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One problem is that sometimes different clusters have different density thresholds, this means that some clusters are more dense than others. A way to try and account for this is the shared neighbour similarity

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## Hierarchical clustering

The idea is that a cluster is made up of subclusters, which form hierarchies

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This is done using trees Et billede, der indeholder tekst, Font/skrifttype, skærmbillede, linje/række

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## OPTICS

Optics is almost like dbscan, but computes clusters for different density thresholds simultaneously. This gives a type of hierarchical clustering which is based on densityies.

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Here we have two parameters,

We have minpts or minimum number of points that must be reachable, and episolon, which is the area we are scanning for points in the cluster. Et billede, der indeholder tekst, diagram, linje/række, Kurve

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The OPTICS plots shows the reachability distances from one point to another and how the algorithm traverses the data points most effectively.

## Outlier detection

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### Statistical outlier detection

We calculate the mahalanobis distance for each data point to the center which is the mean vector

These distances should follow a chi-sqared distribution with d degrees of freedom (d is the number of dimensions).

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### Non-parametric outlier detection

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Density based outliers looks at the density and gets the outliers based on that.

Outliers can be local and global there can be outliers in a cluster, and there can be outliers globally. The ide is that that outliers have have lower local density than their neighbours.

### Outlier evaluation

Outlier detection is not a classification problem of outlier vs. inlier, since there are too few outliers to make any meaningful evaluations (if there is only three outliers it is hard to do any proper training and evaluation). Therefore they deliver a outlier score, and the detection of outliers if based on the scores ranking for each data point.

It can be done manually:

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And then create a two class confusion matrix:

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We then create a ROC curve, where the ROC AUC is between 0 and 1, the higher it is the better, if is 1 then it is perfect and there are no False positives.

# Entropy, purity, Separation

Entropy is a measurement of how much randomness there is in the data. A random variable with n outcomes is:

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For a binary variable the function is:

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If the variable has n outcomes of equal like probability the entropy is:

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The entropy of class distributions is given by:

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## Gini index

The gini-index measures the entropy / impurity of a dataset with k classes:

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## Decision trees

A decision tree works by partionioning the data until it eventually only contains one single classes. It does this by taking an attribute and measuring the information gain: Et billede, der indeholder tekst, skærmbillede, Font/skrifttype

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We can use the weighted gini index to compare partionionings:  
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