# Feature Engineering

## Knowledge Discovery and Data Mining 1

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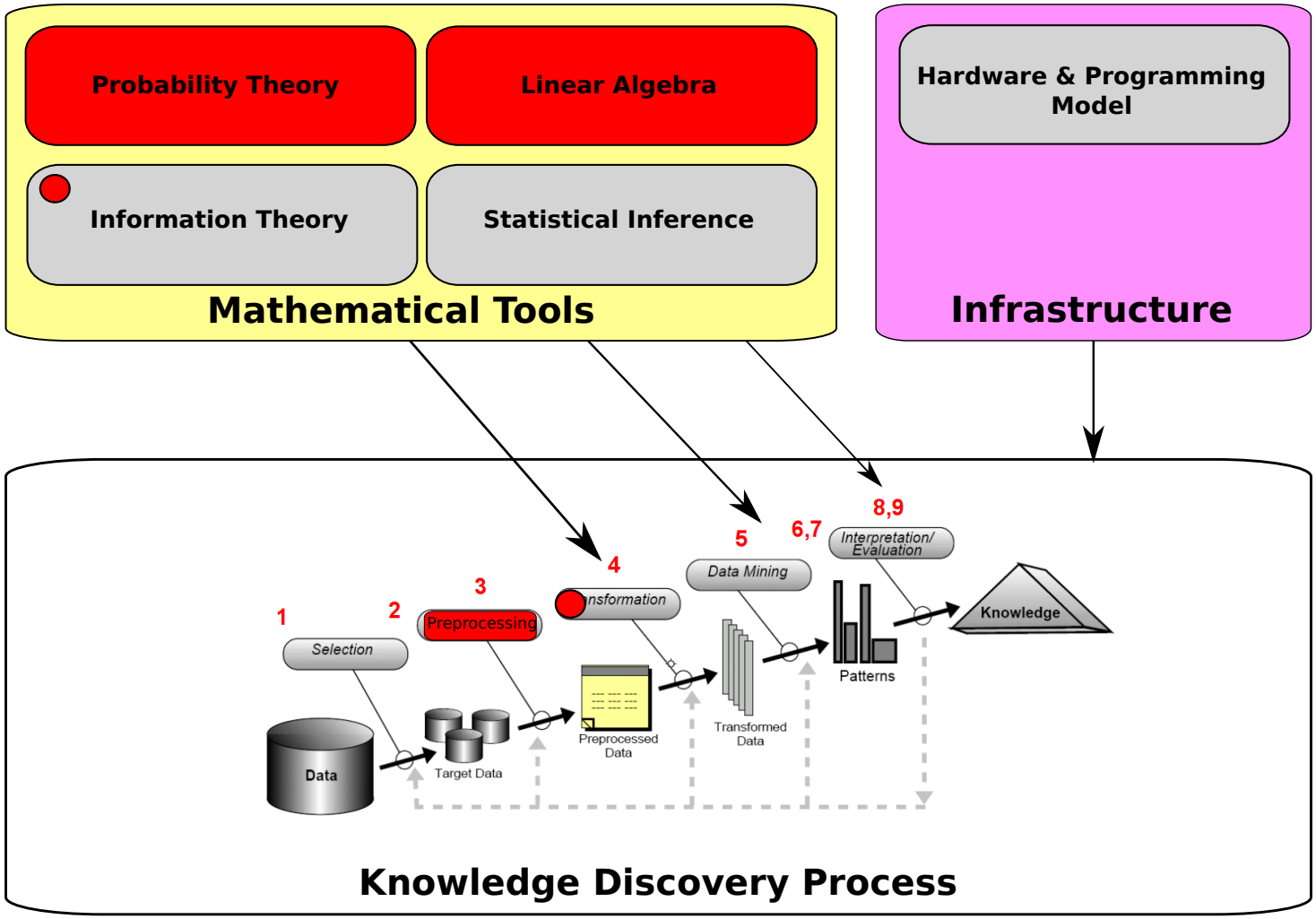
# Big picture: KDDM



# Outline


1. Information Theory
2. Introduction
3. Feature Value Processing
4. Feature Engineering for Text Mining
5. Feature Selection

# Recap

## Review of the preprocessing phase

# Recap - Feature Extraction

- Example of features:
- Images $\rightarrow$ colours, textures, contours, ...
- Signals $\rightarrow$ frequency, phase, samples, spectrum, ...
- Time series $\rightarrow$ ticks, trends, self-similarities, ...
- Biomed $\rightarrow$ dna sequence, genes, ...
- Text $\rightarrow$ words, POS tags, grammatical dependencies, ...

Features encode these properties in a way suitable for a chosen algorithm

# Recap - Feature Extraction

## What is Part-of-Speech?

- The process to apply word classes to words within a sentence
- For example
  - Car $\rightarrow$ *noun*
  - Writing $\rightarrow$ *noun* or *verb*
  - Grow $\rightarrow$ *verb*
  - From $\rightarrow$ *preposition*

## Open vs closed word classes

- Prepositions (closed, e.g. “of”, “to”, “in”)
- Verbs (open, e.g. to “google”)

# Recap - Feature Extraction

**Main approaches for POS tagging**

- Rule based
  - ENGTWOL tagger
- Transformation based
  - Brill tagger
- Stochastic
  - HMM tagger

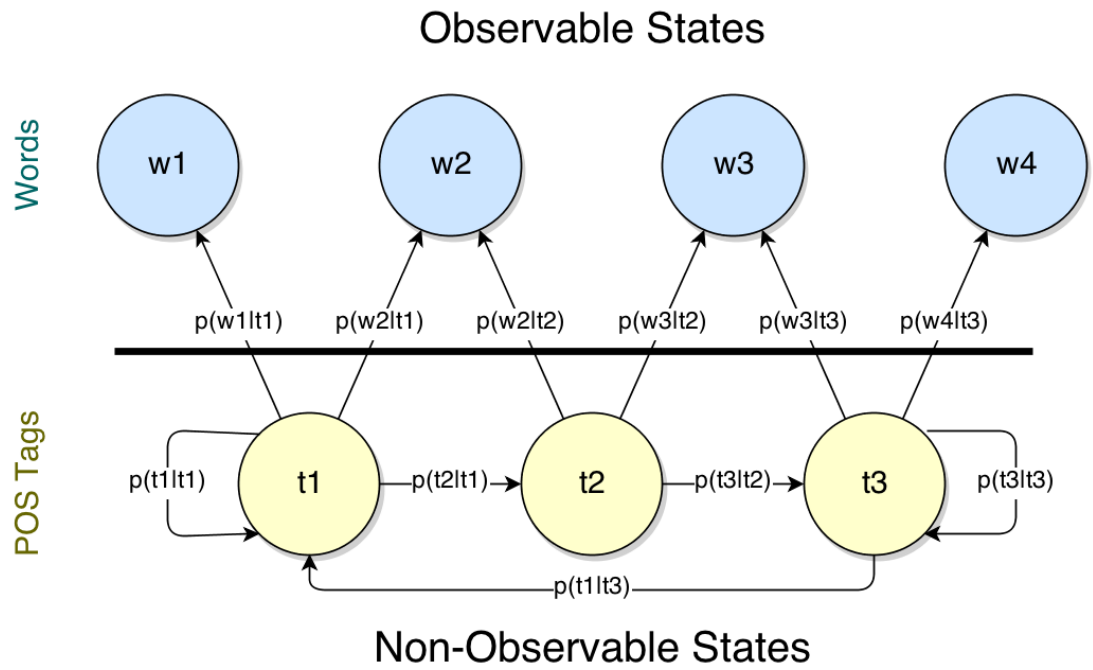
# Recap - Feature Extraction

**Sequence Tagging - Simplifications**

- $\text{argmax}_{t_{1,n}} P(t_{1,n}|w_{1,n}) = \text{argmax}_{t_{1,n}} P(w_{1,n}|t_{1,n})P(t_{1,n})$
  - $\rightarrow$ Not feasible in practice
- Limited horizon & independence assumption:
  $P(t_{1,n}) \approx P(t_n|t_{n-1})P(t_{n-1}|t_{n-2})...P(t_2|t_1) = \prod_{i=1}^{n} P(t_i|t_{i-1})$
- Words only depend on tags: $P(w_{1,n}|t_{1,n}) \approx \prod_{i=1}^{n} P(w_i|t_i)$
- The final equation is:
- $\text{argmax}_{\hat{t}_{1,n}} \prod_{i=1}^{n} P(w_i|t_i)P(t_i|t_{i-1})$

# Recap - Feature Extraction

## Hidden Markov Models




Needs three matrices as input: $A$ (transmission, POS $\mapsto$ POS), $B$ (emission, POS $\mapsto$ Word), $\pi$ (initial probabilities, POS)

# Recap - Feature Extraction

**Probability estimation for tagging**

- How do we get such probabilities?
- $\rightarrow$ With supervised tagging we can simply use **Maximum Likelihood Estimation (MLE)** and use counts (C) from a reference corpus
  - $P(t_i|t_{i-1}) = \frac{C(t_{i-1},t_i)}{C(t_{i-1})}$
  - $P(w_i|t_i) = \frac{C(w_i,t_i)}{C(t_i)}$

**Smoothing**

- To account for unseen words
- Lidstone smoothing: $\frac{C(t_{i-1},t_i)+\lambda}{C(t_{i-1})+\lambda V(t_{i-1},t)}$
- Need to estimate $\lambda$, e.g. by held-out data (development data set)

# Information Theory

Review of information theory

# Entropy

## What is Entropy?

- Let $X$ be a discrete random variable with alphabet $\mathcal{X}$ and probability mass function $p(x)$
- $p(x) = Pr\{X = x\}, x \in \mathcal{X}$
- The **entropy** of a variable X is defined as
- $H(X) = -\sum_{x \in \mathcal{X}} p(x) log_2 p(x)$
- ... entropy is a measure for information content of a variable (in bits)

Note 1: By convention $0 log_2 0 = 0$

Note 2: Entropy is the lower bound on the average number of yes/no questions to guess the state of a variable.

# Entropy

## Entropy Example 1/2

- For example, let $\mathcal{X} = \{A, B, C, D\}$
- ... each with the same probability of $\frac{1}{4}$
- One can encode each of the values with 2 bits
- e.g. $A = 00, B = 01, C = 10, D = 11$

# Entropy

## Entropy Example 2/2

- What if the probabilities are not evenly distributed?
- e.g. $A = \frac{1}{2}, B = \frac{1}{4}, C = \frac{1}{8}, D = \frac{1}{8}$
- One does only need 1.75 bits to encode
- e.g. $A = 0, B = 10, C = 110, D = 111$
- As one expects to see $A$ in 50% of all cases

# Entropy

## What is Entropy?

- Entropy is a measure for uncertainty
- High entropy $\rightarrow$ uniform distribution
  - Histogram of the frequencies would be even
  - Values are hard to predict
- Low entropy $\rightarrow$ peaks and valleys in the distribution
  - Histogram of the frequencies would have spikes
  - Values are easier to predict
- Entropy is always non-negative
- The entropy is always less (or equal) than the logarithm of the alphabet size

# Joint Entropy

## What is Joint Entropy?

- The joint entropy of a pair of discrete random variables $(X; Y)$ with joint probability mass function $p(x; y)$ is defined by
- $H(X, Y) = -\sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) log_2 p(x, y)$
- ... can be generalised to cover more than 2 variables
- $H(X, Y) = H(X) + H(Y)$, if $X$ and $Y$ are interdependent from each other

# Conditional Entropy

## What is Conditional Entropy?

- The conditional entropy of $Y$ given $X$ is defined as:
- $H(Y|X) = -\sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x,y) log_2 p(y|x)$
- ... how much uncertainty is left, once X is known
- Connection between joint entropy and conditional entropy:
- $H(Y|X) = H(X,Y) - H(X)$

# Conditional Entropy

## What is Specific Conditional Entropy?

- $H(Y|X = x)$ - the specific conditional entropy of $Y$ given a specific value $x$ of $X$
- e.g. if $H(Y|X = x) = 0$, then $x$ accounts for all the uncertainty of Y
- $H(Y|X) = \sum_{x \in \mathcal{X}} p(x) H(Y|X = x)$

# Information Gain

## What is Information Gain?

- $IG(Y|X) = H(Y) - H(Y|X)$
- ... how much is the uncertainty of $Y$ reduced, once $X$ is known
- or: One has to transmit $Y$; How many bits on average would it save if both ends of the line would know $X$?

# Information Gain

## What is Relative Information Gain?

- $RIG(Y|X) = \frac{H(Y) - H(Y|X)}{H(Y)}$
- One has to transmit $Y$; How many fraction of bits on average would it save if both ends of the line would know $X$?

# Mutual Information

## What is Mutual Information?

- The mutual information between random variables $X$ and $Y$ with joint probability mass function $p(x, y)$ and marginal probability mass functions $p(x)$ and $p(y)$ is defined as
- $I(X;Y) = -\sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x,y) log_2 \frac{p(x,y)}{p(x)p(y)}$
- The mutual information is a measure of the amount of information that one random variable contains about another random variable
- $I(X;Y) = 0$, if $X$ and $Y$ are independent from each other
- Conditional mutual information:
- $I(X;Y|Z) = H(X|Z) - H(X|Y,Z)$

# Pointwise Mutual Information

## What is Pointwise Mutual Information?

- The pointwise mutual information is defined as
- $pmi(X = x; Y = y) = i(x; y) = log_2 \frac{p(x,y)}{p(x)p(y)}$
- Can then be normalised to:
- $pmi_{norm}(X = x; Y = y) = \frac{pmi(X=x;Y=y)}{-log_2 p(x,y)}$

Example: For two binary variables:

| | y = false | y = true |
|---|---|---|
| x = false | $p(\neg x, \neg y)$ | $p(\neg x, y)$ |
| x = true | $p(x, \neg y)$ | $p(x, y)$ |

# Relative Entropy

## What is Relative Entropy?

- The relative entropy or between two probability mass functions $p(x)$ and $q(x)$ is defied by:
- $D(p||q) = \sum_{x \in X} p(x) log_2 \frac{p(x)}{q(x)}$
- ... also called Kullback-Leibler distance
- The relative entropy is always non-negative and zero if and only if $p = q$
- Connection between mutual information and relative entropy:
- $I(X;Y) = D(p(x,y)||p(x)p(y))$

Note: By convention $0 log_2 \frac{0}{0} = 0$, $0 log_2 \frac{0}{q} = 0$ and $p log_2 \frac{p}{0} = \infty$

# Entropy Overview

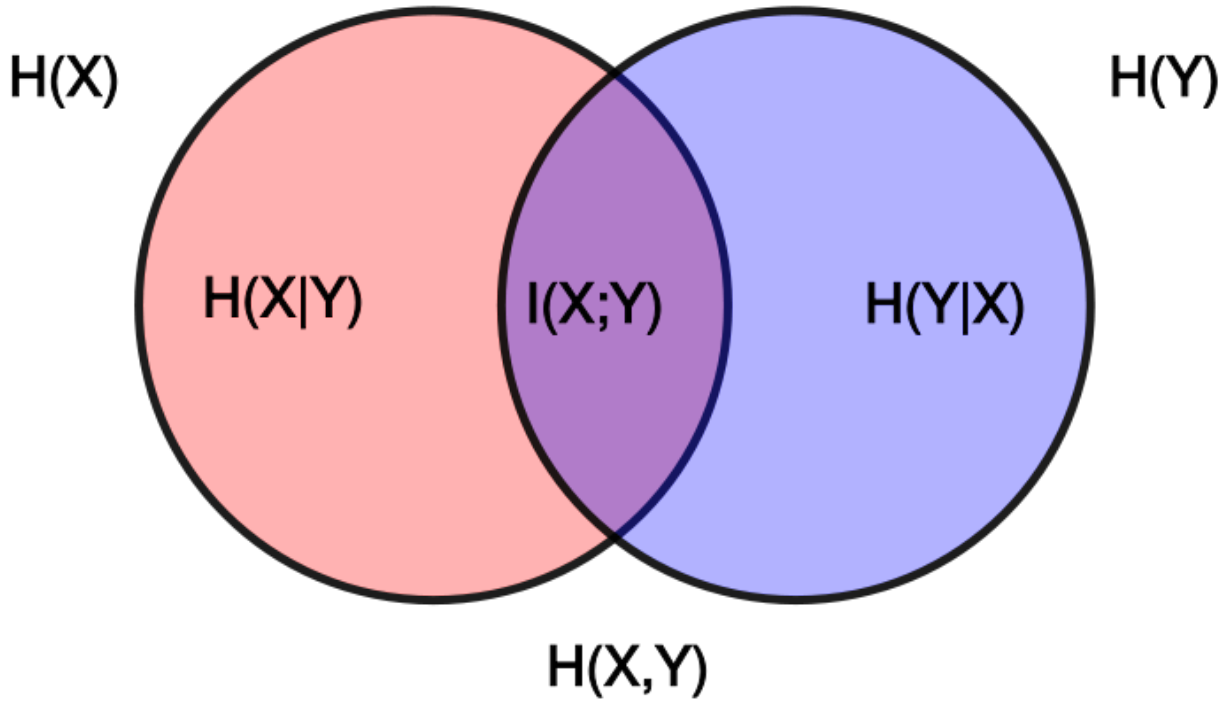



Figure: Overview of entropy, joint entropy, conditional entropy and mutual information (source: Wikipedia)

# Markov Chains

## Markov chains

Random variables $X, Y, Z$ are said to form a Markov chain in that order (denoted $X \to Y \to Z$) if the conditional distribution of Z depends only on Y and is conditionally independent of X, ie if the joint probability mass function can be written as:

$$p(x, y, z) = p(x)p(y|x)p(z|y)$$

$X \to Y \to Z$ if and only if $X$ and $Z$ are conditionally independent given $Y$.

## Markov chains and information theory

If $X \to Y \to Z$ then $I(X; Y) \geq I(X; Z)$

# Introduction

## What are features & feature engineering

# Introduction

## What is feature engineering?

The act to inject knowledge into a Machine Learning model.

## What are features?

The items, that represent this knowledge suitable for Machine Learning algorithms.

## What is a Machine Learning model?

The model represents the output of the learning process (knowledge representation)

Note: there is no formal definition of feature engineering

# Introduction

## Tasks of feature engineering

1. Understand the properties of the task - how they might interact with the strength and limitations of the model
2. Experimental work - test expectations and find out what actually works

# Introduction

## Process of feature engineering

- Remove unnecessary features
- Remove redundant features
- Create new features
  - Combine existing features
  - Transform features
  - Use features from the context
  - Integrate external sources
- Modify feature types
  - e.g. from binary to numeric
- Modify feature values

Note: depending on the task and the algorithms the results might differ

# Feature Engineering Goals

## Goals

The task also depends on the goal of feature engineering:

1. If the goal is to get the best prediction accuracy
2. ... or an explainable model

Note: Second use case is often only done by researchers, or as a first step, to get a better understanding of the problem/features

# Feature Engineering Terminology

## Important Terms

**Feature Set** Set of features used for a task

**Feature Space** High dimensional space spawned by the features (range of the feature values)

**Instance** Single assignment of features and values (an example)

# Introduction - Example

ARFF-Viewer - /home/rkern/apps/weka/weka-3-7-7/data/contact-lenses.arff

File Edit View

contact-lenses.arff

Relation: contact-lenses

| No. | 1: age Nominal | 2: spectacle-prescrip Nominal | 3: astigmatism Nominal | 4: tear-prod-rate Nominal | 5: **contact-lenses** Nominal |
|---|---|---|---|---|---|
| 1 | young | myope | no | reduced | none |
| 2 | young | myope | no | normal | soft |
| 3 | young | myope | yes | reduced | none |
| 4 | young | myope | yes | normal | hard |
| 5 | young | hypermetrope | no | reduced | none |
| 6 | young | hypermetrope | no | normal | soft |
| 7 | young | hypermetrope | yes | reduced | none |
| 8 | young | hypermetrope | yes | normal | hard |
| 9 | pre-presbyopic | myope | no | reduced | none |
| 10 | pre-presbyopic | myope | no | normal | soft |
| 11 | pre-presbyopic | myope | yes | reduced | none |
| 12 | pre-presbyopic | myope | yes | normal | hard |
| 13 | pre-presbyopic | hypermetrope | no | reduced | none |
| 14 | pre-presbyopic | hypermetrope | no | normal | soft |
| 15 | pre-presbyopic | hypermetrope | yes | reduced | none |
| 16 | pre-presbyopic | hypermetrope | yes | normal | none |
| 17 | presbyopic | myope | no | reduced | none |
| 18 | presbyopic | myope | no | normal | none |

Figure: Features to predict which type of contact lens is most appropriate (none, soft, hard)

# Introduction - Example

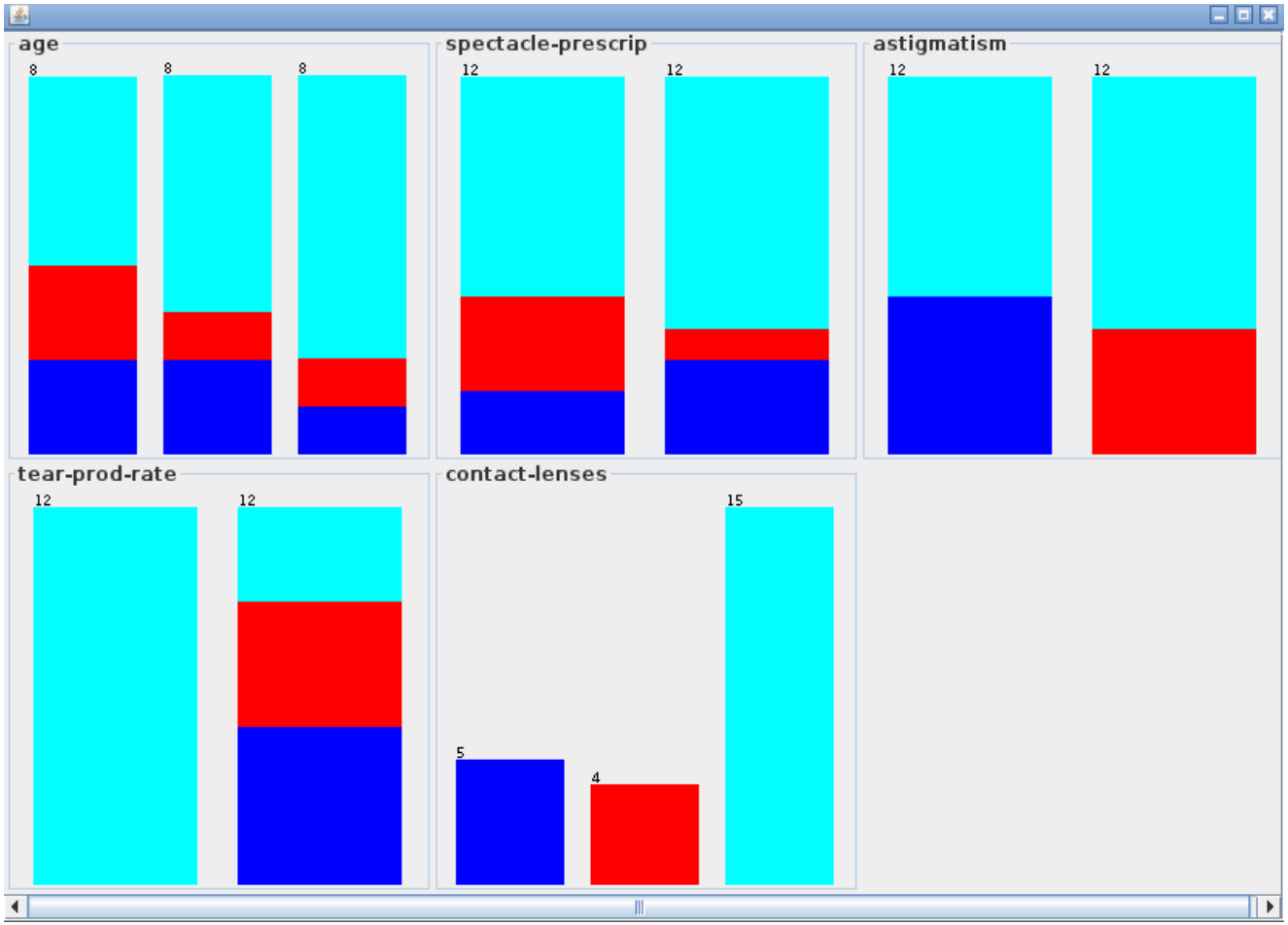



Figure: Relation between the features with the contact lens type

# Introduction - Example

ver - /home/rkern/apps/weka/weka-3-7-7/data/we

File Edit View

weather.arff

Relation: weather

| No. | 1: outlook Nominal | 2: temperature Numeric | 3: humidity Numeric | 4: windy Nominal | 5: **play** Nominal |
|---|---|---|---|---|---|
| 1 | sunny | 85.0 | 85.0 | FALSE | no |
| 2 | sunny | 80.0 | 90.0 | TRUE | no |
| 3 | overcast | 83.0 | 86.0 | FALSE | yes |
| 4 | rainy | 70.0 | 96.0 | FALSE | yes |
| 5 | rainy | 68.0 | 80.0 | FALSE | yes |
| 6 | rainy | 65.0 | 70.0 | TRUE | no |
| 7 | overcast | 64.0 | 65.0 | TRUE | yes |
| 8 | sunny | 72.0 | 95.0 | FALSE | no |
| 9 | sunny | 69.0 | 70.0 | FALSE | yes |
| 10 | rainy | 75.0 | 80.0 | FALSE | yes |
| 11 | sunny | 75.0 | 70.0 | TRUE | yes |
| 12 | overcast | 72.0 | 90.0 | TRUE | yes |
| 13 | overcast | 81.0 | 75.0 | FALSE | yes |
| 14 | rainy | 71.0 | 91.0 | TRUE | no |

Figure: Features to decide whether to play or not based on the weather

# Introduction

- Features are assigned to instances:
- No dependencies/relationships between instances (in practical applications)
- Thus relationships need to be flatted out (denormalisation)
- ... by modelling features
- Complex features need to be "simplified"
- ... by creating aggregate, compound features, e.g. by using averages
- Typically features have no fixed sequence (hence the term set)
- ... by creating features that express sequence information

# Feature Value Processing

Operations upon feature values...

# Feature Processing

**Feature binarisation**

- Threshold numerical values to get boolean values
- Needed as some algorithms just take boolean features as input

**Feature discretization**

- Convert continuous features to discrete features
- Equal sized partitions? Equal interval partitions?

**Feature value transformation**

- Scaling of values
- Move the centre

# Feature Normalisation

- Normalise the value of features
- For example, most of the features are in the range [0..1],
- ... but one ranges [-1000 .. +1000]
- Classifiers like SVM struggle with this (other algorithms do not need this step, e.g. decision trees)

# Feature Weighting

- Given numeric or binary features
- ... encode their impact into the feature value
- Can be seen as prior of a feature
- e.g. “term weighting” to separate potentially words with grammatical function from word with a semantic function

# Feature Engineering for Text Mining

## Tactics when dealing with text

# Contextual Features

**Bigram Features**

- When working with single words as features, often the sequence information is lost
- ... but, this could potentially a source of information
- $\rightarrow$ introduce new feature as a combination of two adjacent words

# Contextual Features

## Example Bigram Features

- Example: `The quick brown fox jumps over the lazy dog`
- Unigram features: `brown`, `dog`, `fox`, `lazy`, ...
- Bigram features: `brown_fox`, `fox_jumps`, `lazy_dog`, `over_the`, ...

# Contextual Features

**n-grams**

- Bigrams can be extended for more than two words
- $\rightarrow$ n-grams
- Can be extended to allow gap in between words (skip n-grams)

# Contextual Features

**Character n-grams**

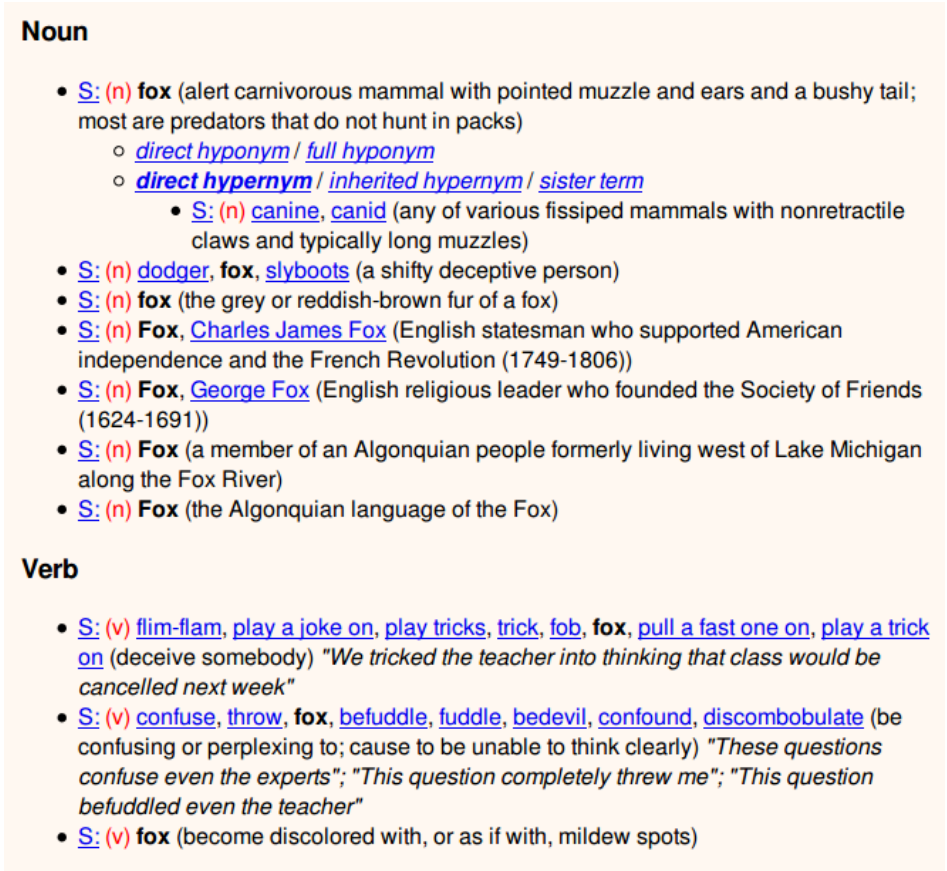
- n-gram can be created on words, but on characters as well
- e.g. `The quick brown fox jumps over the lazy dog`
- Character tri-grams: `the`, `qui`, `uic`, `ick`, `bro`, `row`, `own`, ...

# External Sources

**Integrate external sources**

- Integrate evidence from external sources
- e.g. WordNet for semantic relations
- Example: `The quick brown fox jumps over the lazy dog`
- Features: `the`, `quick`, `brown`, `fox`, `canine`, `canid`, `jumps`, ...
- Added *canine* and *canid* from the hypernyms found in WordNet

# External Sources



**Noun**

- S: (n) **fox** (alert carnivorous mammal with pointed muzzle and ears and a bushy tail; most are predators that do not hunt in packs)
  - *direct hyponym* / *full hyponym*
  - ***direct hypernym*** / *inherited hypernym* / *sister term*
    - S: (n) canine, canid (any of various fissiped mammals with nonretractile claws and typically long muzzles)
- S: (n) dodger, **fox**, slyboots (a shifty deceptive person)
- S: (n) **fox** (the grey or reddish-brown fur of a fox)
- S: (n) **Fox**, Charles James Fox (English statesman who supported American independence and the French Revolution (1749-1806))
- S: (n) **Fox**, George Fox (English religious leader who founded the Society of Friends (1624-1691))
- S: (n) **Fox** (a member of an Algonquian people formerly living west of Lake Michigan along the Fox River)
- S: (n) **Fox** (the Algonquian language of the Fox)

**Verb**

- S: (v) flim-flam, play a joke on, play tricks, trick, fob, **fox**, pull a fast one on, play a trick on (deceive somebody) *"We tricked the teacher into thinking that class would be cancelled next week"*
- S: (v) confuse, throw, **fox**, befuddle, fuddle, bedevil, confound, discombobulate (be confusing or perplexing to; cause to be unable to think clearly) *"These questions confuse even the experts"; "This question completely threw me"; "This question befuddled even the teacher"*
- S: (v) **fox** (become discolored with, or as if with, mildew spots)

Figure: Wordnet entry for the word fox, the first sense contains the hypernyms canine and canid.

# Feature Selection

Less is more - sometimes...

# Feature Selection

Feature engineering can be classified into two use cases

- Modelling for **prediction accuracy**
  - Default, if the goal is to have a productive system
  - ... with optimal performance
- Modelling for **explanations**
  - When the model should be easy to interpret
  - ... one can acquire better knowledge of the problem
  - ... and then to improve the feature engineering task

# Feature Selection

If a model uses fewer features

- ... it is easier to interpret
- ... it will generalise better (less risk of overfitting)
- ... it will be faster (more efficient)

# Feature Selection

**Curse of Dimensionality**

- The problem of having too many features
- More features make the model more expressive
- but not all of the features are relevant
- The higher the dimensionality, the higher the chances of spurious features

# Feature Selection

## Approaches towards reducing the complexity

- Feature selection
- Regularisation
- Kernels

# Feature Selection

**Feature selection**

- Approach: select the sub-set of all features without redundant or irrelevant features
- Set-of-all-subset problem $\rightarrow$ NP hard
- Need to find more practical approaches
  - Unsupervised, e.g. heuristics
  - Supervised, e.g. using a training data set
- Simple approach: each subset only consists of a single feature

# Feature Selection

- Simple approach $\rightarrow$ use heuristics
- Black & white lists
- ... list contains features, which either should not be used
- ... or an exclusive list of features

# Feature Selection

**Example for black list**

- Stop-word list for textual features
- ... list of frequent word, that carry little semantics
- e.g. the, you, again, can, ...
- Advantage: simple, yet effective
- Disadvantage: some may carry semantic, used in phrases or named entities ("The The"), homonyms (can.v vs. can.n)

# Feature Selection

## Unsupervised approach

- Unsupervised ranked feature selection
- Scoring function to rank the feature according to their importance
- ... then just use the top 5% (10%, 25%, ...)
- e.g. for textual data use the frequency of words within a reference corpus

| Feature | Count | Freq. |
|---|---|---|
| `the` | 3,032,573 | 0.879 |
| `in` | 2,919,623 | 0.846 |
| `a` | 2,903,352 | 0.841 |
| `of` | 2,888,379 | 0.837 |
| `is` | 2,639,282 | 0.765 |
| `and` | 2,634,096 | 0.763 |
| ⋮ | ⋮ | ⋮ |
| `with` | 1,703,251 | 0.494 |

Table: Top 50 word within the Wikipedia, the top ranked word (`the`) occurs in 88% of all instances.

# Feature Selection

## Supervised approaches

Filter approaches

- Compute some measure for estimating the ability to discriminate between classes
- Typically measure feature weight and select the best n features $\rightarrow$ supervised ranked feature selection
- Problems:
  - Redundant features (correlated features will all have similar weights)
  - Dependant features (some features may only be important in combination)

Wrapper approaches

- Search through the space of all possible feature subsets
- Each search subset is tried with the learning algorithm

# Feature Selection - Information Gain

**Information gain as ranking function**

- Recall: $IG(Y|X) = H(Y) - H(Y|X)$
- Select features by IG
  1. Compute the IG for each feature
  2. Rank the features based on IG
  3. Select the top-k features

## Example

Features on contact lenses

```
Ranked attributes:
 0.5488   4 tear-prod-rate
 0.377    3 astigmatism
 0.0395   2 spectacle-prescrip
 0.0394   1 age
```

# Feature Selection - Wrapper Approach

**Wrapper approach**

- General algorithm:
  1. Initial subset selection
  2. Try a subset with a learner
  3. Modify the feature subset
  4. Measure the difference
  5. GOTO 2
- Advantages: combination of features, ignore redundant/irrelevant features
- Disadvantage: computationally intensive
- 2 basic ways for i) initial subset selection, ii) modification of subset: forward selection and backward elimination

# Feature Selection - Wrapper Approach

## Forward Selection

- Start with empty set
- Add each feature not in set
- Pick the one with the highest increase
- Stop if there is no increase

## Backward Elimination

- Start with full feature set
- Try to remove features

# Feature Interactions

- From the field of statistics
- e.g. Principal Component Analysis (PCA)
- Non-trivial relationship between variables (features)
- Link to Information Theory - Interaction Information

# Regularisation

- Basic idea: Integrate penalty for complexity of a model
- The more features, the higher the complexity
- If the number of feature exceeds the number of observations
- Typically the regularizer is integrated into the cost function (or loss function)
- Example (negative log-likelihood): $cost(f) = -l(f) + regularizer(f)$
- e.g. $L_0$ ... taking the number of non-zero features, $L_1$ ... sum of the feature values, ...

# Feature Transformation

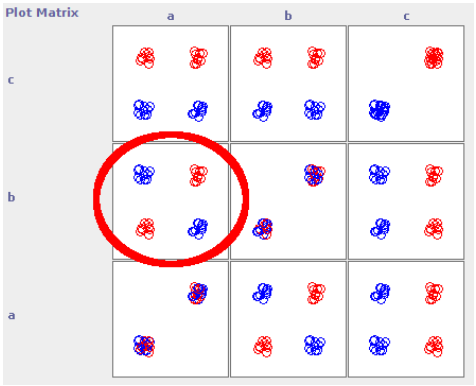
- Some algorithms can only solve certain problems
- e.g. Perceptrons apply only to linearly separable data
- XOR problem for single layer perceptrons
- $\rightarrow$ two main approaches: i) non-linear transformation of the features, ii) more sophisticated algorithms

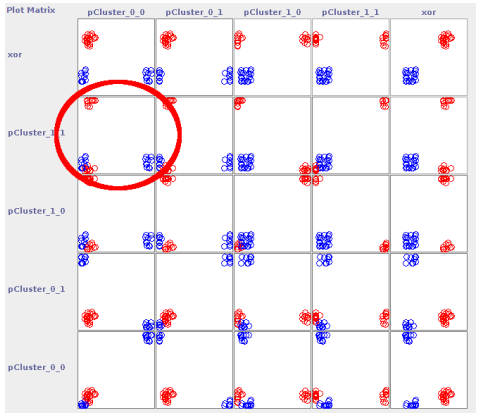
# Feature Transformation

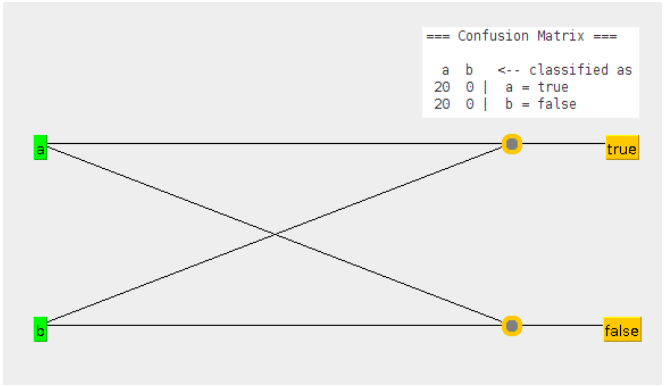
**Feature transformation**

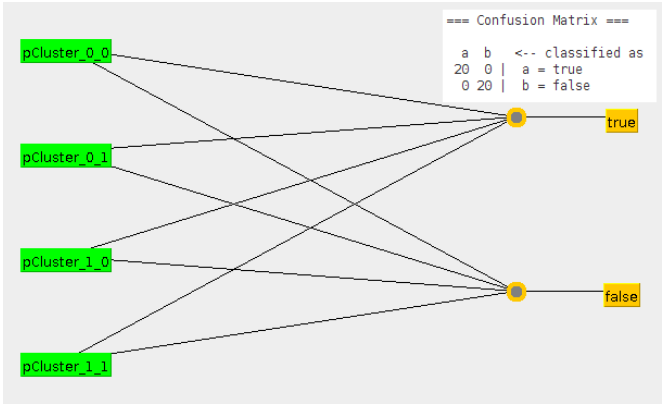
- Map features into high-dimensional space
- Create more features
- The more features, the higher the dimensionality
- The higher the dimensionality, the higher the chances that the problem is linearly separable

# Feature Transformation




Left: original features, which cannot be separated by a single layer perceptron;

Right: features transformed into a higher dimensional space, is linear separable

# Feature Transformation

**Kernel trick**

- Some algorithms employ a scalar product of the features (e.g. SVMs)
- Transform into higher dimensionality "on-the-fly"
- ... by introducing a function
- Original: $< x, y >$, with kernel function: $< \varphi(x), \varphi(y) >$
- Number of different well-known kernel functions (e.g. Gaussian kernel)
- ... which often require parameters (to tune)

# Thank You!

Next up: Data Matrices

## Further information

http://www.cs.cmu.edu/~awm/tutorials
http://www.icg.isy.liu.se/courses/infotheory/lect1.pdf
http://www.cs.princeton.edu/courses/archive/spring10/cos424/slides/18-feat.pdf
http://ufal.mff.cuni.cz/~zabokrtsky/courses/npfl104/html/feature_engineering.pdf
http://www.ke.tu-darmstadt.de/lehre/archiv/ss06/web-mining/wm-features.pdf