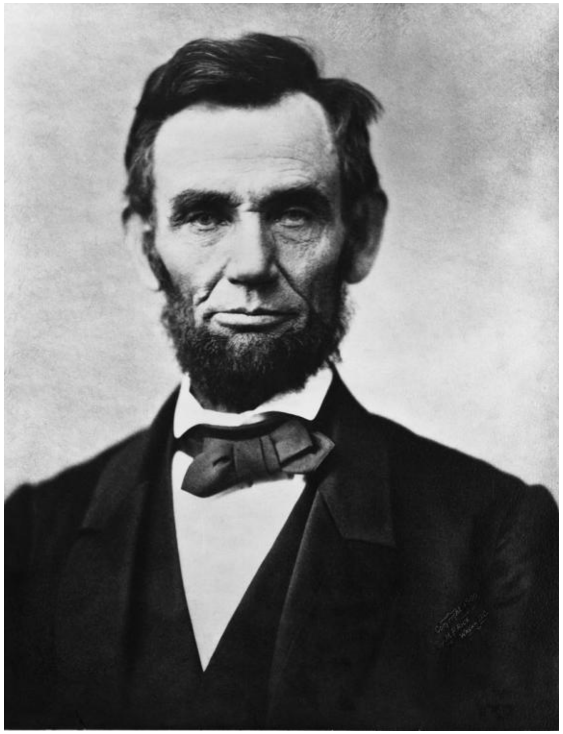
Preprocessing

IE500 Data Mining

UNIVERSITY OF MANNHEIM
Data and Web Science Group

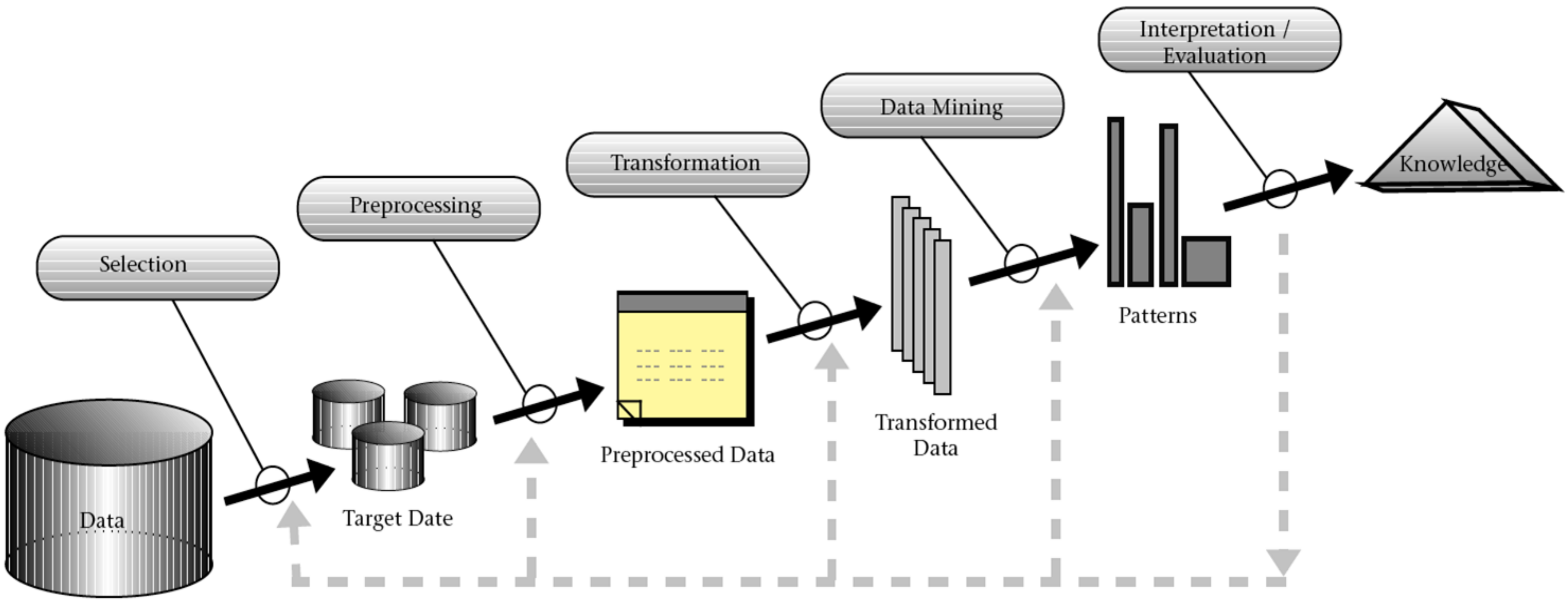
Introduction

- “Give me six hours to chop down a tree and I will spend the first four sharpening the axe.”



Abraham Lincoln, 1809-1865

Recap: The Data Mining Process



Source: Fayyad et al. (1996)

Data Preprocessing

- Your data may have some problems
  - i.e., it may be problematic for the subsequent mining steps
- Fix those problems before going on
- Which problems can you think of?

https://phdcomics.com/comics/archive.php?comicid=848

Data Preprocessing

- Problems that you may have with your data
  - Errors
  - Missing values
  - Unbalanced distribution
  - Different Scales
  - False predictors
  - Unsupported data types
    - Categorical data and Dates
    - Textual values
  - High dimensionality
    - Feature Subset Selection
    - PCA
    - Sampling

Errors in Data

- Sources
  - Malfunctioning sensors
  - Errors in manual data processing (e.g., twisted digits)
  - Storage/transmission errors
  - Encoding problems, misinterpreted file formats
  - Bugs in processing code
  - ...

Image: http://www.flickr.com/photos/16854395@N05/3032208925/

Errors in Data

- Simple remedy
  - Remove data points outside a given interval
    - This requires some domain knowledge
- Typical Examples
  - Remove temperature values outside -30 and +50 °C
  - Remove negative durations
  - Remove purchases above 1M Euro
- Advanced remedies
  - Automatically find suspicious data points (Anomaly Detection)

Missing Values

- Possible reasons
  - Failure of a sensor
  - Data loss
  - Information was not collected
  - Customers did not provide their age, sex, marital status, …
  - ...

Missing Values

- Treatments
  - Ignore records with missing values in training data
  - Replace missing value with...
    - Default or special value (e.g., 0, “missing”)
    - Average/median value for numerics
    - Most frequent value for nominals
    - `SimpleImputer(missing_values=np.nan, strategy='mean')`
  - Try to predict missing values:
    - Handle missing values as learning problem
    - Target: attribute which has missing values
    - Training data: instances where the attribute is present
    - Test data: instances where the attribute is missing
    - `KNNImputer(n_neighbors=2, weights="uniform")`

https://scikit-learn.org/1.5/modules/generated/sklearn.impute.SimpleImputer.html
https://scikit-learn.org/1.5/modules/generated/sklearn.impute.KNNImputer.html

Missing Values

- Note: values may be missing for various reasons
  - ...and, more importantly: **at random** vs. **not at random**
- Examples for not random
  - Non-mandatory questions in questionnaires
    - e.g., “how often do you drink alcohol?”
  - Values that are only collected under certain conditions
    - e.g., final grade of your university degree (if any)
  - Values only valid for certain data sub-populations
    - e.g., “are you currently pregnant”?
  - Sensors failing under certain conditions
    - e.g., at high temperatures
- In those cases, averaging and imputation causes information loss
  - In other words: “missing” can be information!

Handling Missing Values: Caveats

- Imagine a medical trial checking for side effects of a particular drug
- In the trial, there are 50 people who know their blood sugar value
  – Out of those, 4/5 have an increased blood sugar value

Overall, the side effects are moderate (~23%), but people with an increased blood sugar value have a 75% risk of side effects

		side effects	
		Yes (n=58)	No (n=192)
increased blood sugar	Yes (n=40)	**30**	**10**
	No (n=10)	**8**	**2**
	-- (n=200)	**20**	**180**

Handling Missing Values: Caveats (ctd.)

- Assume you handle the missing value for increased blood sugar
  - by filling in the majority value (“yes”)

Overall, the side effects are moderate (~23%), and even slightly lower (~21%) for people with an increased blood sugar value

		side effects	
		Yes (n=58)	No (n=192)
increased blood sugar	Yes (n=240)	**50**	**190**
	No (n=10)	**8**	**2**

Unbalanced Distribution

- Example:
  - learn a model that recognizes HIV
  - given a set of symptoms
- Data set:
  - records of patients who were tested for HIV
- Class distribution:
  - 99.9% negative
  - 0.01% positive
- Learn a decision tree
  - It will be hard to find any splitting that significantly improves the quality

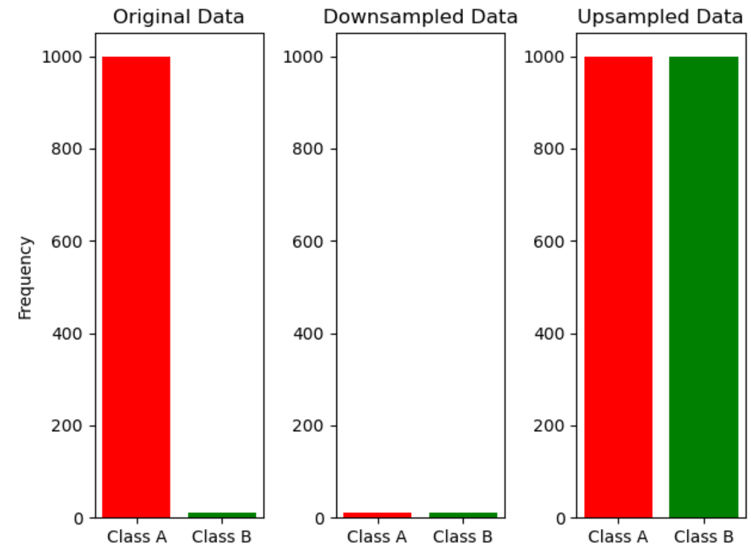
Decision tree learned:

false

Resampling Unbalanced Data

- Two conflicting goals
  - Use as *much* training data as possible
  - Use as *diverse* training data as possible
- Strategies
  - Downsampling larger class
    - Conflicts with goal 1
  - Upsampling smaller class
    - Conflicts with goal 2

Resampling Unbalanced Data



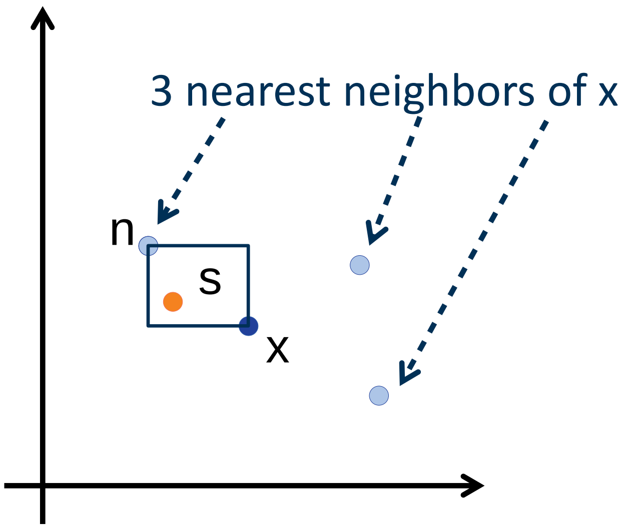
- Consider an extreme example
  - 1,000 examples of class A
  - 10 examples of class B
- Downsampling
  - does not use 990 examples
- Upsampling
  - creates 100 copies of each example of B
  - likely for the classifier to simply *memorize* the 10 B cases

- Python:
  - https://imbalanced-learn.org/

Imbalanced learn

Resampling

- SMOTE (Synthetic Minority Over Sampling Technique)
  - Creates synthetic examples of minority class
- Given an example x
  - Choose one neighbor *n* among the k nearest neighbors (w/in same class) of x
  - Create synthetic example s
    - For each attribute a
    - s.a ← x.a + rand(0,1) * (n.a – x.a)



N. V. Chawla, K. W. Bowyer, L. O.Hall, W. P. Kegelmeyer, “SMOTE: synthetic minority over-sampling technique,” Journal of artificial intelligence research, 321-357, 2002.

Different scales: Normalization

ID	Age	Income
371	25	70,000
433	30	85,000
864	40	90,000

- Recap:
  - k-NN: Sensitivity to scales
    - e.g. Euclidian distance between first and second entry:
    - $D = \sqrt{\sum_{i=1}^{n}(p_i - q_i)^2}$

      p_i: features of first example

      q_i: features of second example

      $= \sqrt{\underbrace{(25-30)^2}_{\text{age does not contribute much}} + (70000-85000)^2} = 15000$

  - Needs normalization
    - StandardScaler $z = \frac{x-\mu}{\sigma}$
      - Standardize features by removing the mean and scaling to unit variance
    - MinMaxScaler $X_{norm} = \frac{X-X_{min}}{X_{max}-X_{min}}$
      - Transform features by scaling each feature to a given range e.g. [0,1]

Preprocessors also Need to be Trained

- Many preprocessing methods also have an internal representation
  - E.g. Mean and variance, minimum and maximum values
  - Do NOT apply it on the whole dataset before splitting etc

```
import pandas as pd
from sklearn.preprocessing import MinMaxScaler
from sklearn.model_selection import train_test_split

golf = pd.read_csv('golf.csv')

scaler = MinMaxScaler()
golf_scaled = scaler.fit_transform(golf[['Temperature', 'Humidity']])

X_train, X_test, y_train, y_test = train_test_split(golf_scaled, golf['Play'], test_size=0.3, random_state=0)
```

https://scikit-learn.org/1.5/modules/compose.html

Preprocessors also Need to be Trained

- Many preprocessing methods also have an internal representation
  - Function **fit_transform** for training and **transform** for testing

```
golf = pd.read_csv('golf.csv')
X_train, X_test, y_train, y_test = train_test_split(golf, golf['Play'], test_size=0.3, random_state=0)

scaler = MinMaxScaler()
golf_scaled = scaler.fit_transform(X_train[['Temperature', 'Humidity']], y_train)

golf_test_scaled = scaler.transform(X_test[['Temperature', 'Humidity']])
```


https://scikit-learn.org/1.5/modules/compose.html

Preprocessors also Need to be Trained

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- How to compose multiple components
  - Pipeline

```
from sklearn.pipeline import Pipeline
from sklearn.svm import SVC
estimators = [
    ('scale', MinMaxScaler()),
    ('clf', SVC())
]
pipe = Pipeline(estimators)
pipe.fit(X_train, y_train)
pipe.score(X_test, y_test)
```

  - How to apply tranformations to only a few columns
    - ColumnTransformer

```
from sklearn.compose import ColumnTransformer
from sklearn.preprocessing import OneHotEncoder

column_trans = ColumnTransformer(
    [('categories', OneHotEncoder(dtype='int'), ['Outlook']),
     ('scale', MinMaxScaler(), ['Temperature'])],
    remainder='drop'
)

estimators = [
    ('preprocessing', column_trans),
    ('clf', SVC())
]
pipe = Pipeline(estimators)
pipe.fit(X_train, y_train)
pipe.score(X_test, y_test)
```

Name

Component

Columns

https://scikit-learn.org/1.5/modules/compose.html

False Predictors

- ~100% accuracy are a great result
  - ...and a result that should make you suspicious!

- A tale from the road
  - Working with our Linked Open Data extension
  - Trying to predict the world university rankings
  - With data from DBpedia

- Goal:
  - Understand what makes a top university

False Predictors

- The Linked Open Data extension
  - Extracts additional attributes from public knowledge graphs
    - e.g., DBpedia
  - Unsupervised (i.e., attributes are created fully automatically)

- Model learned: THE<20 → TOP=true
  - False predictor: target variable was included in attributes

- Other examples
  - Mark<5 → passed=true
  - Sales>1000000 → bestseller=true

Recognizing False Predictors

- By analyzing models
  - Rule sets consisting of only one rule
  - Decision trees with only one node
- Process: learn model, inspect model, remove suspect, repeat
  - until the accuracy drops
  - Tale from the road example: there were other indicators as well
- By analyzing attributes
  - Compute correlation of each attribute with label
  - Correlation near 1 (or -1) marks a suspect
- Caution: there are also strong (but not false) predictors
  - it's not always possible to decide automatically!

Unsupported Data Types

- Not every learning operator supports all data types
  - Some (e.g., SVM) cannot handle categorical data
  - Some (e.g., ID3) cannot handle numeric data
  - Dates are difficult for most learners
  - Textual values need to be transformed

- Solutions
  - Convert categorical to numeric data
  - Convert numeric to nominal data (discretization, binning)
  - Extract valuable information from dates
  - Transform textual attributes to vector representations

Conversion: Categorical to Numeric

- Two common ways to encode categorical attributes:
  - For **ordinal attributes (order is important)**
    - e.g. Grade=A, A-, B+, B, B-, C+, C, C-
    - Assign each distinct value a corresponding number preserving the order
      - A=8, A-=7, B+=6, B=5, B-=4, C+=3, C=2, C-=1

ID	Grade	…
371	A-	
433	B	

ID	Grade	…
371	7	
433	5	

    - Using such a coding schema allows learners to learn valuable rules, e.g.
      - grade>6 → excellent_student=true
    - Python: OrdinalEncoder

Conversion: Categorical to Numeric

- Two common ways to encode categorical attributes:
  - For **nominal attributes (no order)**
    - e.g. Color=Red, Orange,…, Violet
    - One Hot Encoding: For each value v, create a binary "flag" variable C_v , which is 1 if Color=v, 0 otherwise

ID	Color	…
371	red	
433	yellow	

→

ID	Color_red	Color_orange	Color_yellow	…
371	1	0	0	
433	0	0	1	

    - Python: [OneHotEncoder]
    - Special case: Binary attribute e.g. student=yes, no
      - Student = yes → student_binary = 0
      - Student = no → student_binary = 1

Conversion: Categorical to Numeric

- Many values:
  - US State Code (50 values)
  - Profession Code (7,000 values, but only few frequent)

- Approaches:
  - manual, with background knowledge
    - e.g., group US states
  - Use binary attributes
    - then apply dimensionality reduction (see later today)

Conversion: Numeric to Ordinal

- Remember: Discretization for decision tree
  - Values of the attribute, e.g., age of a person:
    - 0, 4, 12, 16, 16, 18, 24, 26, 28
  - **Equal-interval binning** – for bin width of e.g., 10:
    - Bin 1: 0, 4 [-∞,10) bin
    - Bin 2: 12, 16, 16, 18 [10,20) bin
    - Bin 3: 24, 26, 28 [20,+∞) bin
  - **Equal-frequency binning** – for bin density of e.g., 3:
    - Bin 1: 0, 4, 12 [-, 14) bin
    - Bin 2: 16, 16, 18 [14, 21) bin
    - Bin 3: 24, 26, 28 [21,+] bin

Dealing with Date Attributes

- Dates (and times) can be formatted in various ways
  - first step: normalize and parse

- Dates have lots of interesting information in them
- Example: analyzing shopping behavior
  - time of day
  - weekday vs. weekend
  - begin vs. end of month
  - month itself
  - quarter, season
- Python: use, e.g., `datetime`

Dealing with Textual Attributes

- Preprocessing
  - Text Cleanup (remove punctuation and HTML tags)
  - Tokenization (break text into single words or N-grams)
  - Stopword Removal (e.g. the, of, and, to, an, is, that, …)
  - Stemming (find the **stem of a word)**
    - User, users, used, using ➔ Stem: use

```
from nltk.stem.porter import PorterStemmer

# Stem tokens
stemmer = PorterStemmer()
tokens = ['Jupiter', 'is', 'the', 'largest', 'gas', 'planet']
stems = []
for item in tokens:
    stems.append(stemmer.stem(item))
```

Dealing with Textual Attributes

- Feature Generation: Bag-of-Words
  - Each word/term becomes a feature
  - Order of words/terms is ignored
- – Each document is represented by a vector

	Dokument																				
Term	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	Σ
oil	5	12	2	1	1	7	3	3	5	9	5	4	5	4	3	4	5	3	3	1	85
price	5	6	2	2	0	8	1	2	2	10	5	1	5	2	0	3	3	3	3	0	63
opec	0	15	0	0	0	8	1	2	2	6	5	2	2	4	0	0	0	0	0	0	47
mln	0	4	0	0	2	4	1	0	0	3	9	0	0	0	0	3	3	0	0	2	31
market	2	5	0	0	0	3	0	2	0	10	1	2	2	0	0	0	0	0	3	0	30
barrel	2	0	1	1	0	4	0	0	1	3	3	0	1	1	0	3	3	1	0	2	26
bpd	0	4	0	0	0	7	0	0	0	2	8	0	0	2	0	0	0	0	0	0	23
dlrs	2	0	1	2	2	2	1	0	0	4	2	0	0	0	0	1	1	5	0	0	23
crude	2	0	2	3	0	2	0	0	0	0	5	2	0	2	0	0	0	2	0	1	21
saudi	0	0	0	0	0	0	0	1	0	5	7	1	4	0	0	0	0	0	0	0	18
kuwait	0	0	0	0	0	10	0	1	0	3	0	1	0	2	0	0	0	0	0	0	17
offici	0	0	0	0	0	5	1	1	0	1	4	3	1	0	0	0	0	0	1	0	17
meet	0	6	0	0	0	3	0	1	0	1	0	1	0	2	0	0	0	0	0	0	14
pct	0	0	0	0	2	0	2	2	2	1	0	0	1	0	0	1	1	0	0	2	14
product	1	6	0	0	0	1	0	0	0	0	4	0	0	0	0	0	0	0	0	1	13
accord	0	0	0	0	0	0	0	0	0	5	1	0	2	0	0	0	0	0	4	0	12
futur	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	1	0	9	0	12
minist	0	0	0	0	0	3	0	0	1	3	1	2	1	1	0	0	0	0	0	0	12
govern	0	0	0	0	0	0	5	0	6	0	0	0	0	0	0	0	0	0	0	0	11
month	0	1	0	0	0	2	2	0	1	0	5	0	0	0	0	0	0	0	0	0	11
report	0	1	0	0	0	1	8	0	0	0	0	1	0	0	0	0	0	0	0	0	11
sheikh	0	0	0	0	0	3	0	0	5	2	0	0	0	1	0	0	0	0	0	0	11
industri	0	2	0	0	0	1	1	1	1	0	0	0	0	0	0	1	2	0	1	0	10
produc	0	0	0	0	0	4	1	1	0	3	0	0	0	0	0	0	0	0	0	1	10
quota	0	2	0	0	0	4	0	0	1	1	1	0	0	1	0	0	0	0	0	0	10
reserv	0	0	0	0	3	0	0	0	1	0	0	0	0	0	0	3	3	0	0	0	10
world	0	1	0	0	0	1	3	0	1	1	0	0	1	1	0	0	0	0	1	0	10
⋮																					
Σ	48	204	34	39	46	219	219	73	161	180	208	57	61	54	56	68	89	44	147	32	2039

Dealing with Textual Attributes

- Different techniques for vector creation:
  - **Binary Term Occurrence**: Boolean attributes describe whether or not a term appears in the document (one-hot encoding)
    - Python: CountVectorizer(binary=true)
  - **Term Occurrence**: Number of occurrences of a term in the document (problematic if documents have different length)
    - Python: CountVectorizer(binary=false)
  - **Terms Frequency**: Attributes represent the frequency in which a term appears in the document (number of occurrences / number of words in document)
    - Python: TfidfVectorizer(use_idf=False)
  - **TF-IDF**: see next slide
    - Python: TfidfVectorizer

Dealing with Textual Attributes

- The **TF-IDF weight** (term frequency–inverse document frequency) is used to evaluate how important a word is to a corpus of documents.
  - TF: Term Frequency (see last slide)
  - IDF: Inverse Document Frequency.

  N: total number of docs in corpus

  df_i: the number of docs in which t_i appears

$$w_{ij} = tf_{ij} * idf_i$$

$$idf_i = \log(\frac{N}{df_i})$$

- Gives more weight to rare words
- Give less weight to common words (domain-specific stopwords)

In scikit-learn:

$$idf_i = \log\left(\frac{1+N}{1+df_i}\right) + 1$$

Similarity of Documents

- **Jaccard Coefficient**
  - Similarity measure for vectors consisting of asymmetric binary attributes

$$Jaccard(A,B) = \frac{|A \cap B|}{|A \cup B|} = \frac{M_{11}}{M_{01}+M_{10}+M_{11}}$$

- Used together with binary term occurrence vectors (one-hot vectors)
  - 1 represents occurrence of specific word
  - 0 represents absence of specific word
  - most values are 0 as only small subset of the vocabulary is used in a document

Similarity of Documents

- **Jaccard Coefficient**
  - Similarity measure for vectors consisting of asymmetric binary attributes

$$Jaccard(A,B) = \frac{|A \cap B|}{|A \cup B|} = \frac{M_{11}}{M_{01}+M_{10}+M_{11}}$$

	Saturn	is	the	gas	planet	with	rings	Jupiter	largest	Roman	god	of	sowing
d1	1	1	1	1	1	1	1	0	0	0	0	0	0
d2	0	1	1	1	1	0	0	1	1	0	0	0	0
d3	1	1	1	0	0	0	0	0	0	1	1	1	1

- Jaccard similarities between the documents
  - $Jaccard(d_1, d_2) = \frac{4}{9} = 0.44$
  - $Jaccard(d_2, d_3) = \frac{2}{11} = 0.18$
  - $Jaccard(d_1, d_3) = \frac{3}{11} = 0.27$

Similarity of Documents

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- **Cosine similarity**
  - Similarity measure for comparing weighted document vectors such as term-frequency or TF-IDF vectors

$$\cos(d_1, d_2) = \frac{d_1 \bullet d_2}{\|d_1\|\|d_2\|}$$

where • indicates vector dot product

$$a \bullet b = \sum_{i=1}^{n} a_i b_i = a_1 b_1 + a_2 b_2 + \cdots + a_n b_n$$

and $\|d\|$ is the length of the vector

$$\|d\| = \sqrt{\sum_{i=1}^{n} d_i^2}$$

  - Example

d_1 = 3 2 0 5 0 0 0 2 0 0

d_2 = 1 0 0 0 0 0 0 1 0 2

$d_1 \bullet d_2$= 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5

$||d_1||$ = $(3*3+2*2+0*0+5*5+0*0+0*0+0*0+2*2+0*0+0*0)^{0.5}$ = $(42)^{0.5}$ = 6.481

$||d_2||$ = $(1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2)^{0.5}$ = $(6)^{0.5}$ = 2.245

$$\cos(d_1, d_2) = 0.3150$$

Dense and Sparse Representation

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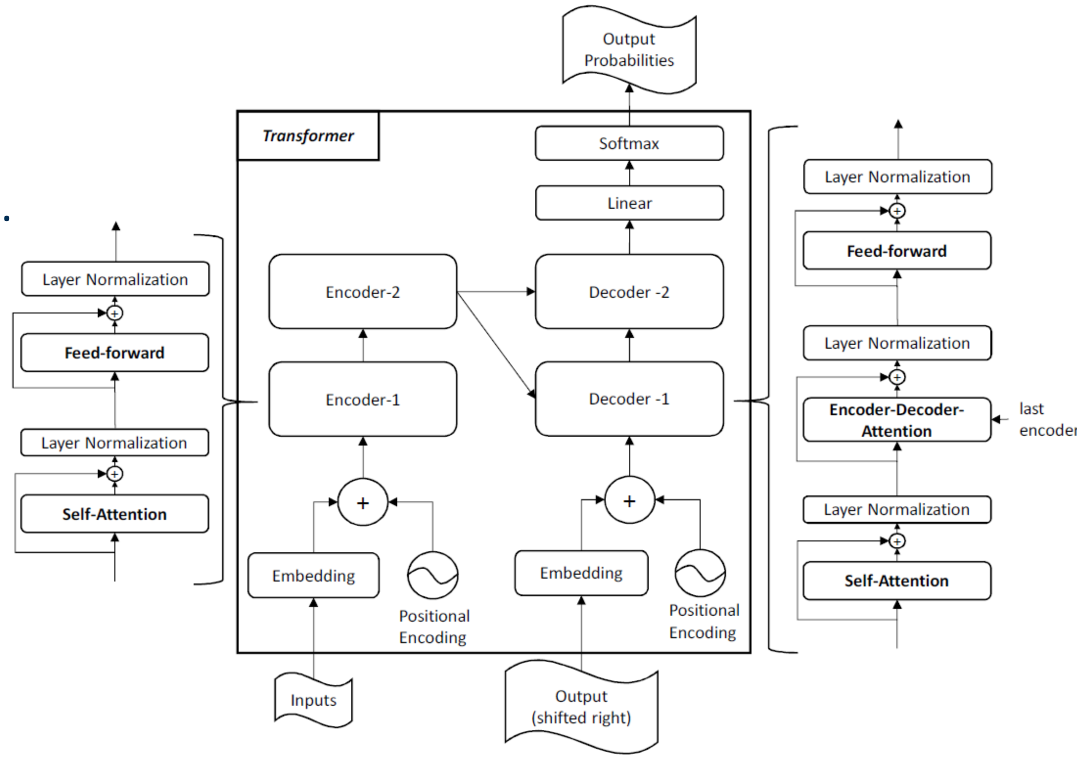
- Bag of Words is **sparse**
  - Vector dimension is tens of thousands
    - Most are zero

Term	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	Σ
	Dokument																				
oil	5	12	2	1	1	7	3	3	5	9	5	4	5	4	3	4	5	3	3	1	85
price	5	6	2	2	0	8	1	2	2	10	5	1	5	2	0	3	3	3	3	0	63
opec	0	15	0	0	0	8	1	2	2	6	5	2	2	4	0	0	0	0	0	0	47
mln	0	4	0	0	2	4	1	0	0	3	9	0	0	0	0	3	3	0	0	2	31
market	2	5	0	0	0	3	0	2	0	10	1	2	2	0	0	0	0	0	3	0	30
barrel	2	0	1	1	0	4	0	0	1	3	3	0	1	1	0	3	3	1	0	2	26
bpd	0	4	0	0	0	7	0	0	0	2	8	0	0	2	0	0	0	0	0	0	23
dlrs	2	0	1	2	2	2	1	0	0	4	2	0	0	0	0	1	1	5	0	0	23
crude	2	0	2	3	0	2	0	0	0	0	5	2	0	2	0	0	0	2	0	1	21
saudi	0	0	0	0	0	0	0	1	0	5	7	1	4	0	0	0	0	0	0	0	18
kuwait	0	0	0	0	0	10	0	1	0	3	0	1	0	2	0	0	0	0	0	0	17
offici	0	0	0	0	0	5	1	1	0	1	4	3	1	0	0	0	0	0	1	0	17
meet	0	6	0	0	0	3	0	1	0	1	0	1	0	2	0	0	0	0	0	0	14
pct	0	0	0	0	2	0	2	2	2	1	0	0	1	0	0	1	1	0	0	2	14
product	1	6	0	0	0	1	0	0	0	0	4	0	0	0	0	0	0	0	0	1	13
accord	0	0	0	0	0	0	0	0	0	5	1	0	2	0	0	0	0	0	4	0	12
futur	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	1	0	9	0	12
minist	0	0	0	0	0	3	0	0	1	3	1	2	1	1	0	0	0	0	0	0	12
govern	0	0	0	0	0	0	5	0	6	0	0	0	0	0	0	0	0	0	0	0	11
month	0	1	0	0	0	2	2	0	1	0	5	0	0	0	0	0	0	0	0	0	11
report	0	1	0	0	0	1	8	0	0	0	0	1	0	0	0	0	0	0	0	0	11
sheikh	0	0	0	0	0	3	0	0	5	2	0	0	0	1	0	0	0	0	0	0	11
industri	0	2	0	0	0	1	1	1	1	0	0	0	0	0	0	1	2	0	1	0	10
produc	0	0	0	0	0	4	1	1	0	3	0	0	0	0	0	0	0	0	0	1	10
quota	0	2	0	0	0	4	0	0	1	1	1	0	0	1	0	0	0	0	0	0	10
reserv	0	0	0	0	3	0	0	0	1	0	0	0	0	0	0	3	3	0	0	0	10
world	0	1	0	0	0	1	3	0	1	1	0	0	1	1	0	0	0	0	1	0	10
⋮																					
Σ	48	204	34	39	46	219	219	73	161	180	208	57	61	54	56	68	89	44	147	32	2039

- **Dense representation**
  - Word embeddings
    - Vector of a few hundred dimensions

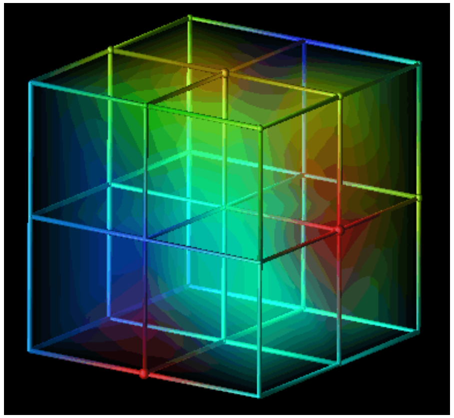
Transformer Architecture

- Encoder-only:
  - BERT, ALBERT (**a** **l**ite version of **BERT**),
    RoBERTa (A **Ro**bustly Optimized **BERT** Pretraining **A**pproach)
- Decoder-only:
  - LLMs like GPT, LLaMa, …
- Seq2Seq:
  - T-5 (**T**ext-**to**-**T**ext **T**ransfer **T**ransformer)
  - BART



High Dimensionality

- Datasets with large number of attributes
- Examples:
  - Text classification
  - Image classification
  - Genome classification
  - …
- (not only a) scalability problem
  - e.g., decision tree:
    search all attributes for determining one single split



Feature Subset Selection

- Preprocessing step
- Idea: only use valuable features
  - “feature”: machine learning terminology for “attribute”

- Basic heuristics: remove nominal attributes...
  - Which have more than p% identical values
    - Example: millionaire=false
  - Which have more than p% different values
    - Example: names, IDs
- Basic heuristics: remove numerical attributes
  - Which have little variation, i.e., standard deviation <s

Feature Subset Selection

- Basic Distinction: Filter vs. Wrapper Methods

- Filter methods
  - Use attribute weighting criterion, e.g., Chi², Information Gain, ...
  - Select attributes with highest weights
  - Fast (linear in no. of attributes), but not always optimal

- Example:
  - `X_f = SelectKBest(chi2,k=20).fit_transform(X, y)`

Feature Subset Selection

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- Remove redundant attributes
  - e.g., temperature in °C and °F
  - e.g., textual features “Barack” and “Obama”

- Method:
  - compute pairwise correlations between attributes
  - remove highly correlated attributes

- Recap:
  - Naive Bayes requires independent attributes
  - Will benefit from removing correlated attributes

Feature Subset Selection

- Wrapper methods
  - Use classifier internally
  - Run with different feature sets
  - Select best feature set

- Advantages
  - Good feature set for given classifier

- Disadvantages
  - Expensive (naively: at least quadratic in number of attributes)
  - Heuristics can reduce number of classifier runs

Feature Subset Selection

- Forward selection:

```
start with empty attribute set
do {
    for each attribute {
      add attribute to attribute set
      compute performance (e.g., accuracy)
    }
    use attribute set with best performance
} while performance increases
```

- An learning algorithm is used for computing the performance
  - Cross validation is advised

Feature Subset Selection

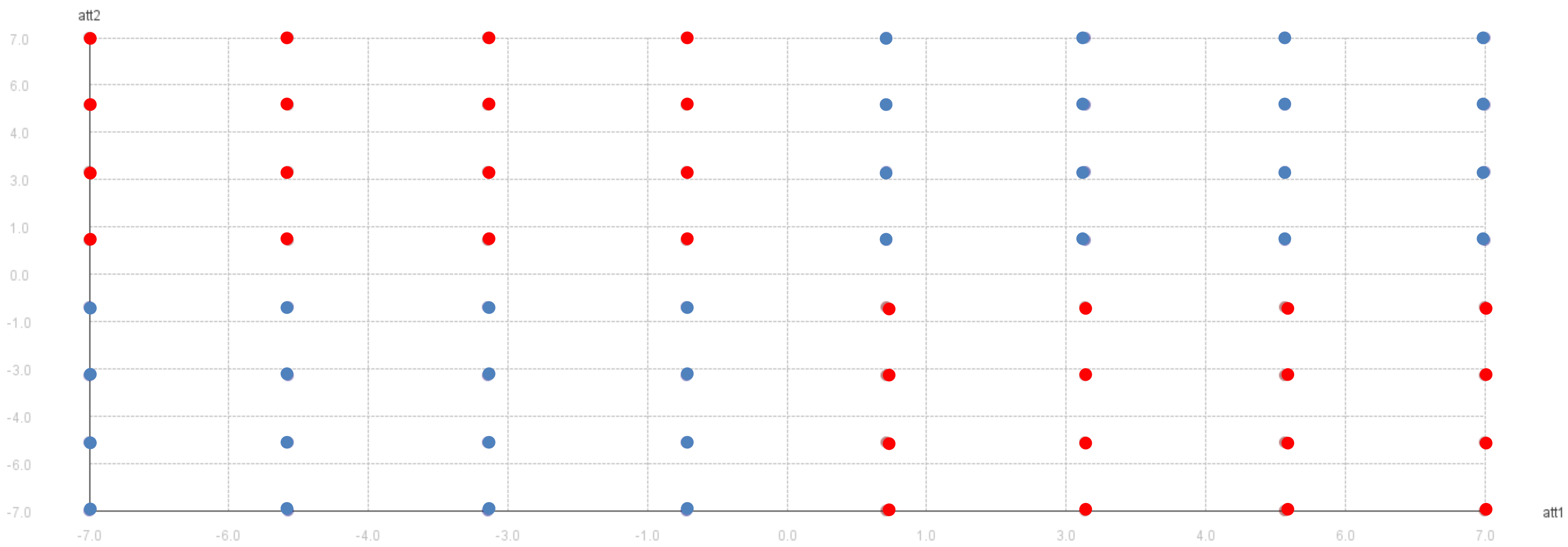
- Backward elimination:

```
start with full attribute set
do {
    for each attribute in attribute set {
      remove attribute to attribute set
      compute performance (e.g., accuracy)
    }
    use attribute set with best performance
} while performance increases
```

- An learning algorithm is used for computing the performance
  - Cross validation is advised

Feature Subset Selection

- The checkerboard dataset
  - Decision tree learners can perfectly learn this!
  - But what happens if we apply forward selection here?



Feature Subset Selection

- Python:
  - Forward selection:
    SequentialFeatureSelector(direction='forward’)
  - Backward elimination:
    SequentialFeatureSelector(direction=backward’)
    - If estimator has feature importances:
      - RFECV (**R**ecursive **f**eature **e**limination with **c**ross-**v**alidation)
  - Just one selection step based on feature importances
    - SelectFromModel

Feature Subset Selection

- Further approaches
  - Brute Force search
  - Evolutionary algorithms

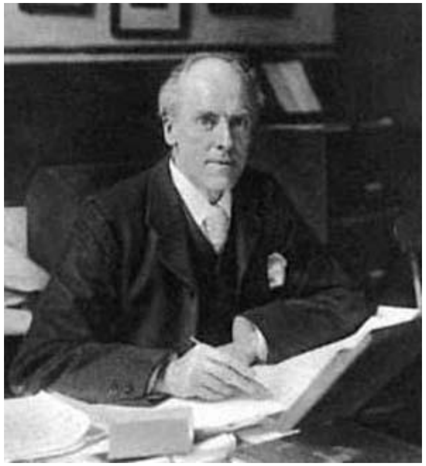
- Trade-off
  - Simple heuristics are fast
    - But may not be the most effective
  - Brute-force is most effective
    - But the slowest
  - Forward selection, backward elimination, and evolutionary algorithms
    - Are often a good compromise

Principal Component Analysis (PCA)

- So far, we have looked at feature selection methods
  - We select a subset of attributes
  - No new attributes are created

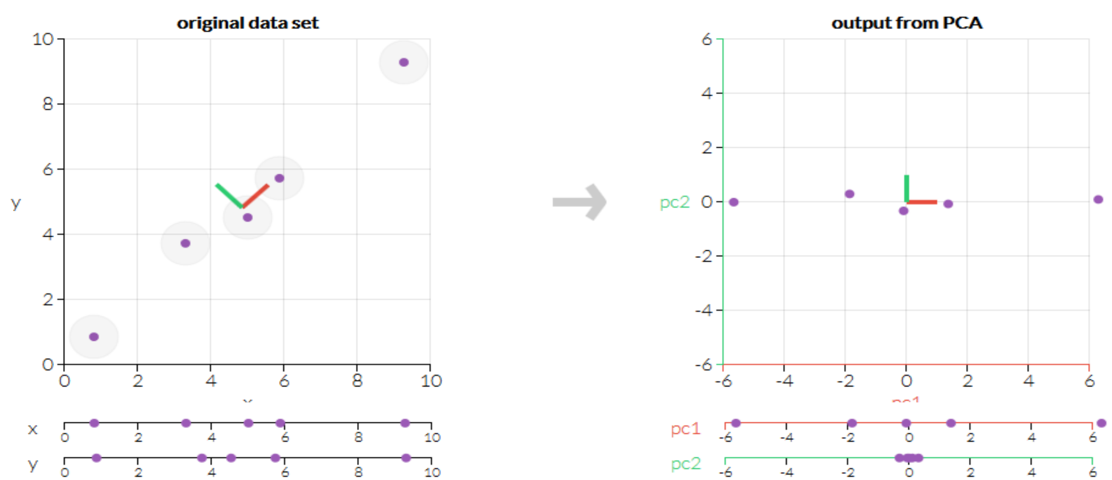
- PCA creates a (smaller set of) new attributes
  - Artificial linear combinations of existing attributes
  - As expressive as possible

- Dates back to the pre-computer age
  - Invented by Karl Pearson (1857-1936)
  - Also known for Pearson's correlation coefficient



Principal Component Analysis (PCA)

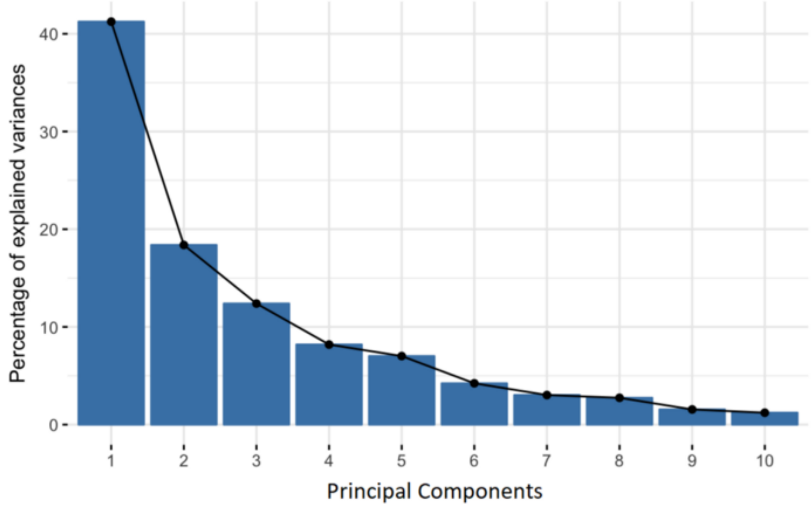
- Idea: transform coordinate system so that each new coordinate (principal component) is as expressive as possible
  – Expressivity: variance of the variable
  – The 1st, 2nd, 3rd... PC should account for as much variance as possible
    - further PCs can be neglected



http://setosa.io/ev/principal-component-analysis/

Principal Component Analysis (PCA)

- Principal components
  - Are *linear* combinations of the existing features
- General approach:
  - The first component should have as much variance as possible
  - The subsequent ones should also have as much variance as possible
    - And be perpendicular to the first one



https://builtin.com/data-science/step-step-explanation-principal-component-analysis

Sampling revisited

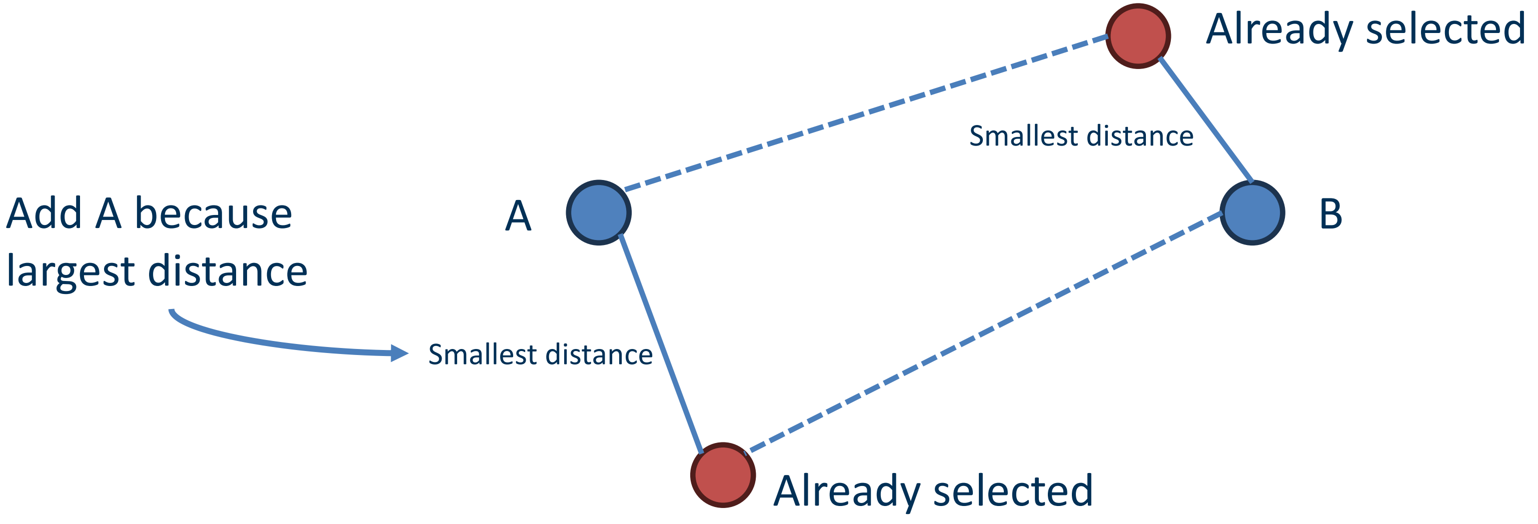
- Feature Subset Selection reduces the **width** of the dataset
- Sampling reduces the **height** of the dataset
  - i.e., the number of instances

- Trade-off
  - Maximum usage of information
  - Fast computation

- Notes
  - *Stratified* sampling respects class distribution
  - *Kennard-Stone* sampling tries to select heterogenous points

Kennard-Stone Sampling

1) Compute pairwise distances of points
2) Add points with largest distance from one another
3) While target sample size not reached
   1) For each candidate, find smallest distance to any point in the sample
   2) Add candidate with largest of those smallest distances



Kennard-Stone Sampling

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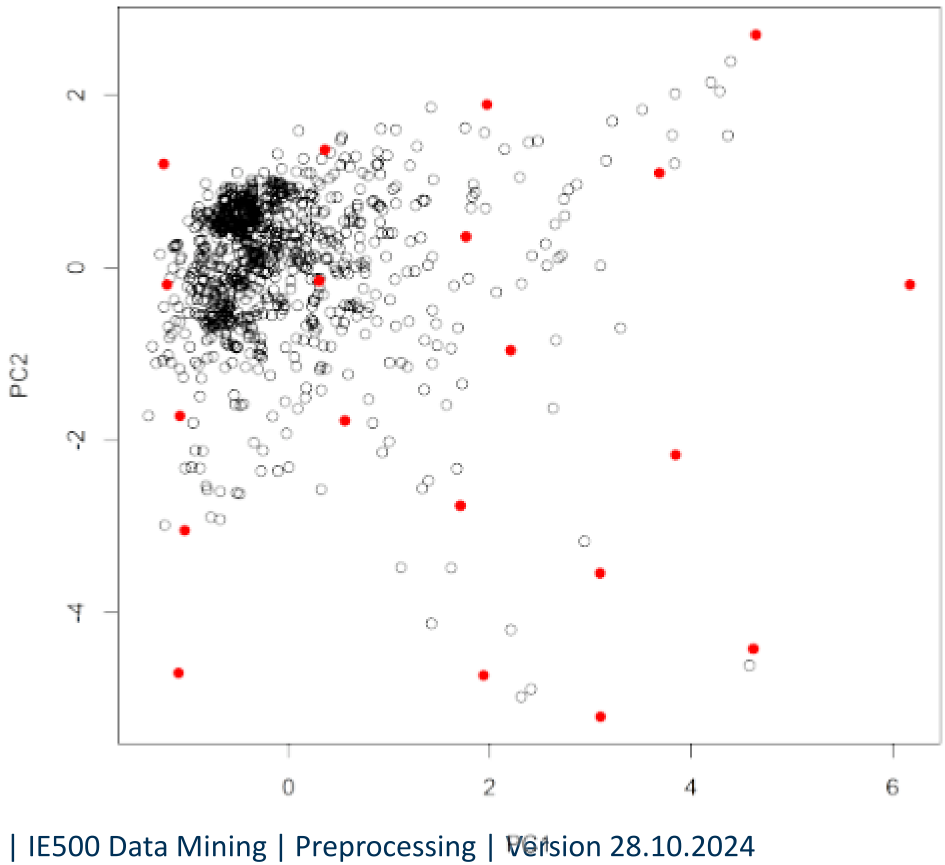
- This guarantees that heterogeneous data points are added
  - i.e., sample gets more diverse
  - Includes more corner cases
    - But potentially also more outliers
  - Distribution may be altered

- Python: Not included in scikit-learn by default
  - Need to install separate package "kennard-stone“
    - https://pypi.org/project/kennard-stone/

Kennard-Stone Sampling (Example)

- Pro: a lot of rare cases covered
- Con: original distribution gets lost



https://antoinestevens.github.io/prospectr/

Sampling Strategies and Learning Algorithms

- There are interaction effects
- Some learning algorithms rely on distributions
  - e.g., Naive Bayes
  - Usually, stratified sampling works better
- Some rely less on distributions
  - And may work better if they see more corner cases
  - e.g., Decision Trees

Titanic Dataset
Filter: 50 training examples

	Decision Tree	Naive Bayes
Stratified	.727	**.752**
Kennard Stone	**.742**	.721

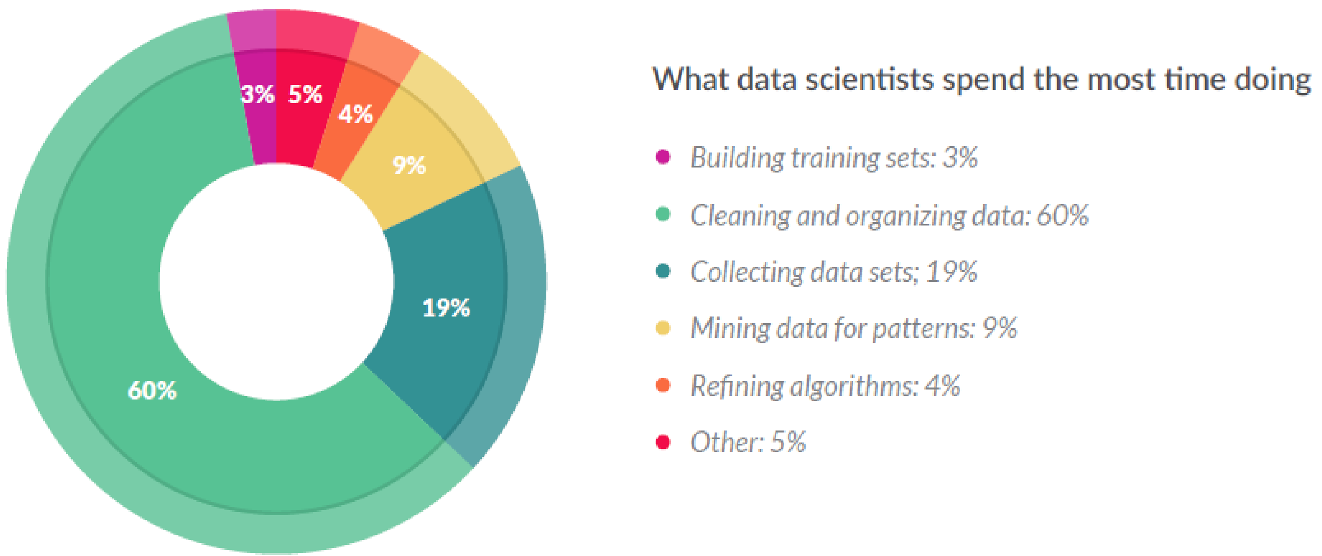
A Note on Sampling

- Often, the training data in a real-world project is already a sample
  - e.g., sales figures of last month
  - To predict the sales figures for the rest of the year
- How representative is that sample?
  - What if last month was December? Or February?
- Effect known as *selection bias*
  - Example: phone survey with 3,000 participants, carried out Monday, 9-17
  - Thought experiment: effect of selection bias for prediction, e.g., with a Naive Bayes classifier

Summary Data Preprocessing

- Raw data has many problems
  - Missing values
  - Errors
  - High dimensionality
  - …
- Good preprocessing is essential for good data mining
  - One of the first steps in the pipeline
  - Requires lots of experimentation and fine-tuning
    - often the most time consuming step of the pipeline

Prepare Your Data



Source: CrowdFlower Data Science Report 2016: http://visit.crowdflower.com/data-science-report.html

Reminder

- Content of online lectures are exercise and exam relevant

Week	Wednesday (Offline Lecture)	Online Lecture	Thursday (Exercise)
10.02.2025	no lecture		Introduction to Python (13:45–15:15)
17.02.2025	Introduction to Data Mining		Intro
24.02.2025	Preprocessing		Preprocessing
03.03.2025	Classification 1	Nearest Centroids	Classification 1
10.03.2025	Classification 2	Comparing Classifiers	Classification 2
17.03.2025	Regression	Ensembles	Regression
24.03.2025	Clustering and Anomalies	Hierarchical Clustering	Clustering
31.03.2025	Feedback on project outlines	Time Series	Time Series

Questions?

Literature for this Slideset

- Python:
  - Imputation
    - https://scikit-learn.org/1.5/modules/impute.html
  - Preprocessing
    - https://scikit-learn.org/1.5/modules/preprocessing.html
  - Text feature extraction
    - https://scikit-learn.org/1.5/modules/feature_extraction.html#text-feature-extraction
  - Feature Selection
    - https://scikit-learn.org/1.5/modules/feature_selection.html