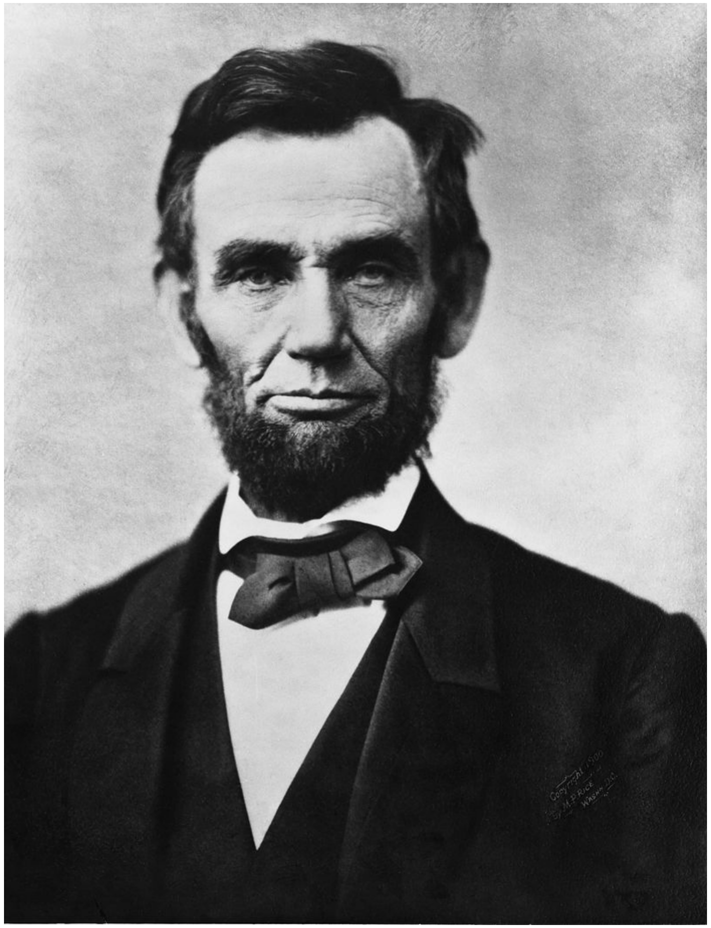
UNIVERSITÄT MANNHEIM

Data Mining II
Data Preprocessing

Heiko Paulheim

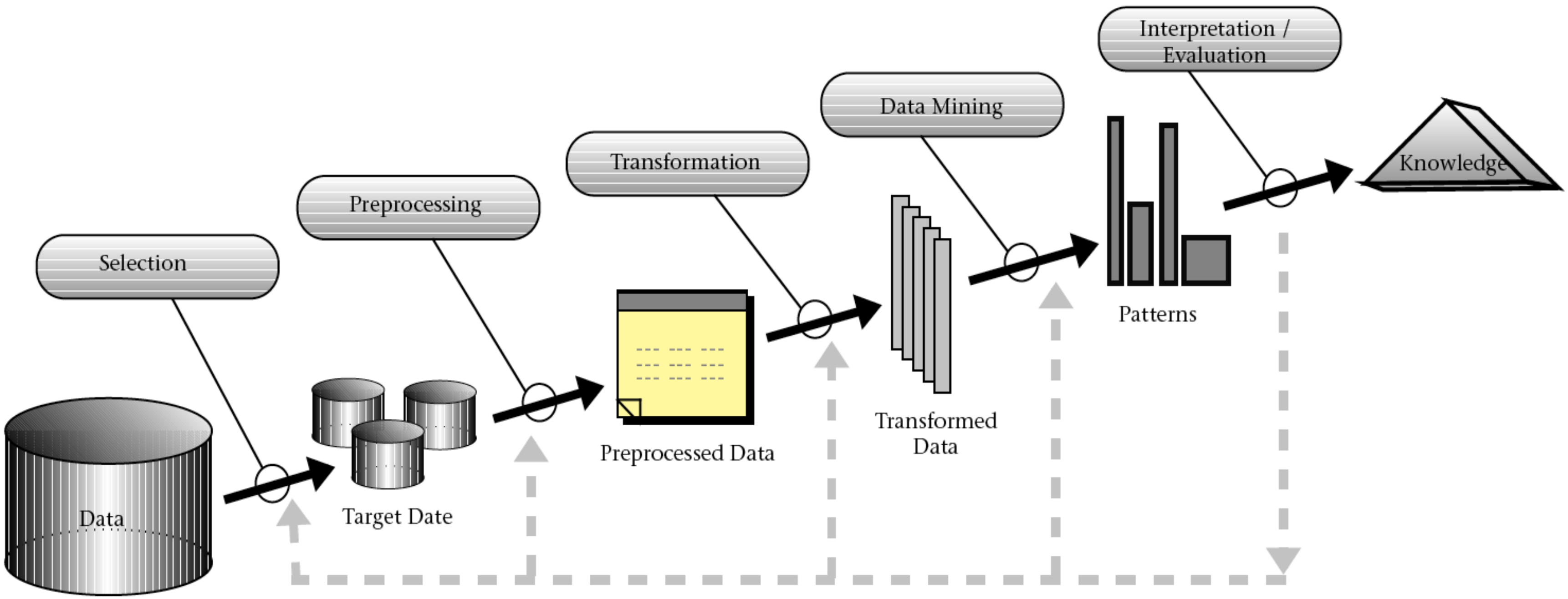
Introduction

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



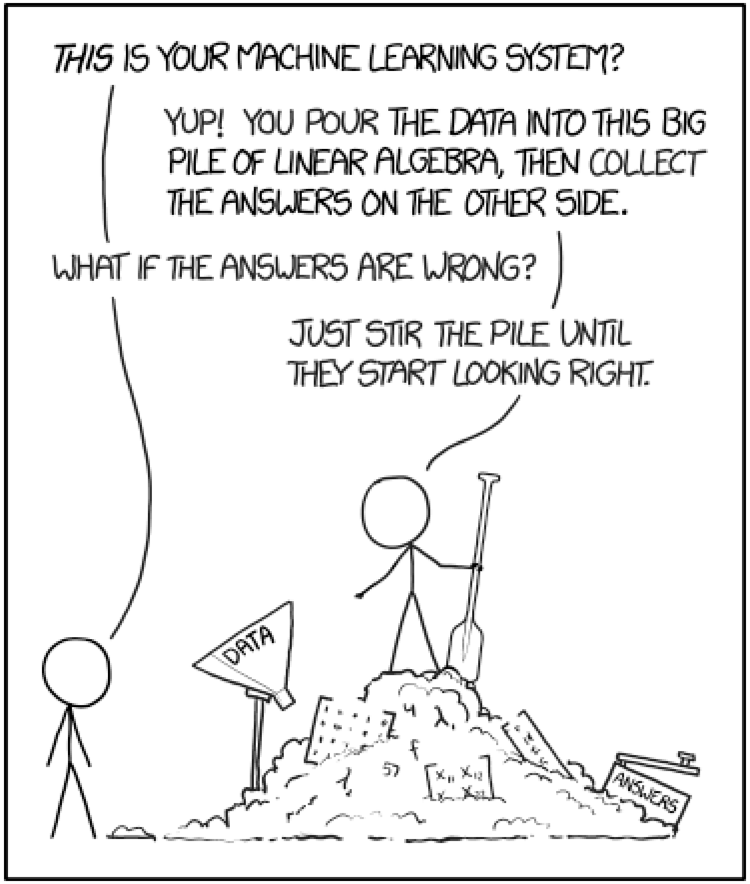
Abraham Lincoln, 1809-1865

Recap: The Data Mining Process



Source: Fayyad et al. (1996)

Recap: The Data Mining Process



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?

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
  - see lecture “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

```
imp = 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

```
imp = imputer = KNNImputer(n_neighbors=2, weights="uniform")
```

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

	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

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

Handling Missing Values: Caveats (ctd.)

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

	side effects	yes (n=58)	no (n=192)
increased blood sugar			
yes (n=240)		50	190
no (n=10)		8	2

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

Missing Values vs. Missing Observations

- Missing values:
  - Typically single fields in a record
  - Can be handled with imputation etc.
- Missing observations:
  - Entire records missing
  - Various forms:
    - Selection bias
    - Missing values in time series

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

Unbalanced Distribution

- Learn a decision tree
- Purity measure: Gini index
- Recap: Gini index for a given node t :

$$GINI(t) = 1 - \sum_j [p(j|t)]^2$$

  - (NOTE: p(j | t) is the relative frequency of class j at node t).

- Here, Gini index of the top node is

  $1 - 0.999^2 - 0.001^2 = 0.002$

Decision tree learned:

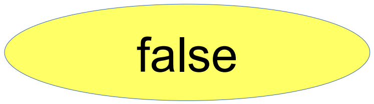
false

- It will be hard to find any splitting that significantly improves the purity

Unbalanced Distribution

- Model has very high accuracy
  - 99.9%
- ...but 0 recall/precision on positive class
  - which is what we were interested in

Decision tree learned:



- Remedy
  - re-balance dataset for training
  - but evaluate on unbalanced dataset!

- Balancing:

```
df_majority_downsampled = resample(df_majority,
                                   replace=False,
                                   n_samples=100)
```

Resampling Unbalanced Data

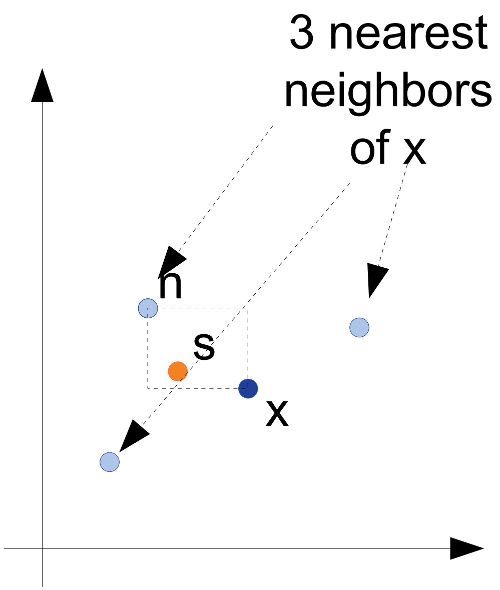
- Two conflicting goals
  1. use as *much* training data as possible
  2. use as *diverse* training data as possible
- Strategies
  – Downsampling larger class
    - conflicts with goal 1
  – Upsampling smaller class
    - conflicts with goal 2

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

Resampling

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



- Python has >80 variants of SMOTE

```
import smote_variants as sv
```

Sampling: the Story so Far

- Strategies seen
  - Upsampling (maximize data usage)
  - Downsampling (maximize performance)
  - Resampling w/ SMOTE

- Stratification vs. changing the distribution
  - *Stratified* sampling: keep class distribution
  - *Upsampling* and *downsampling*: balance class distribution
  - *Kennard-Stone* sampling tries to select heterogenous points

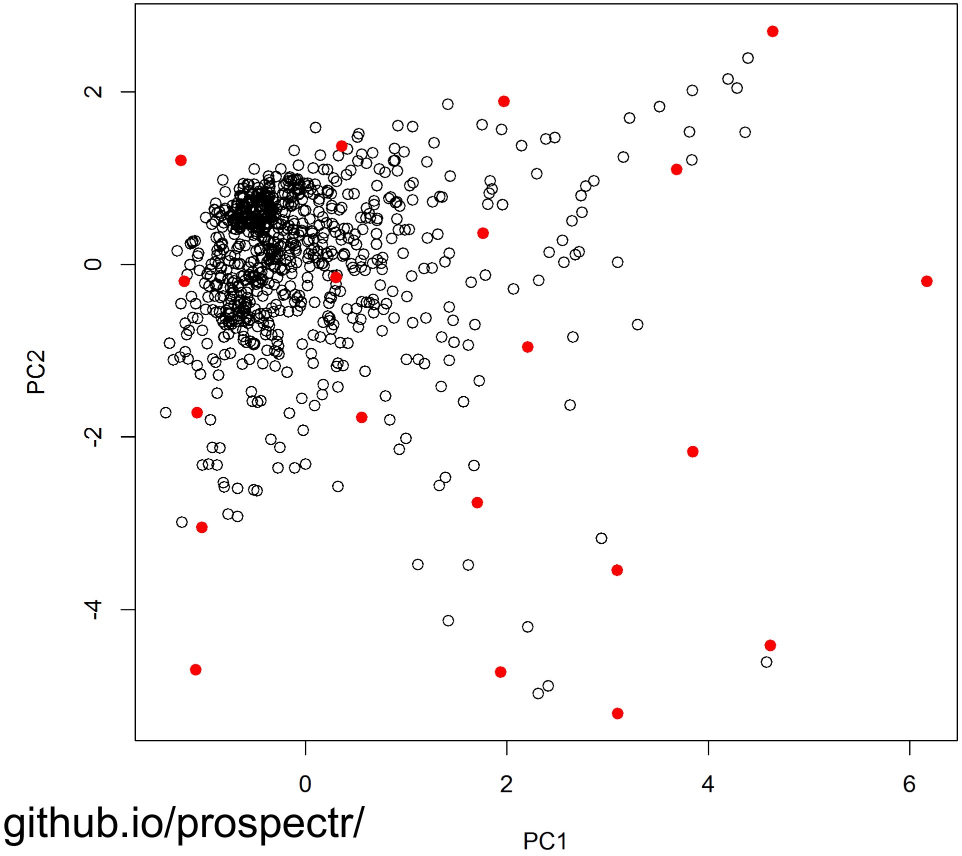
Kennard-Stone Sampling

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 smallest distance

- 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

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

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., ID3) cannot handle numeric data
  - others (e.g., SVM) cannot nominal data
  - dates are difficult for most learners

- Solutions
  - convert nominal to numeric data
  - convert numeric to nominal data (discretization, binning)
  - extract valuable information from dates

Conversion: Binary to Numeric

- Binary fields
  - E.g. student=yes,no
- Convert to Field_0_1 with 0, 1 values
  - student = yes → student_0_1 = 0
  - student = no → student_0_1 = 1

Conversion: Nominal to Numeric

- Multi-valued, unordered attributes with small no. of values
  - e.g. Color=Red, Orange, Yellow, …, Violet
  - for each value v, create a binary “flag” variable C_v , which is 1 if Color=v, 0 otherwise
- Aka “One hot encoding”
  - N binary or 0/1 variables, only one is “hot” (true or 1)

ID	Color	…
371	red	
433	yellow	

ID	C_red	C_orange	C_yellow	…
371	1	0	0	
433	0	0	1	

Conversion: Ordinal to Numeric

- Some nominal attributes incorporated an *order*
- Example: grades on scale A, A-, B+, B, ...
- Problem with one hot encoding:
  - d(Mary,John)=d(Mary,Jane)
  - Holds for almost all distance measures d

	A	A-	B+	B
John	0	1	0	0
Mary	1	0	0	0
Jane	0	0	0	1

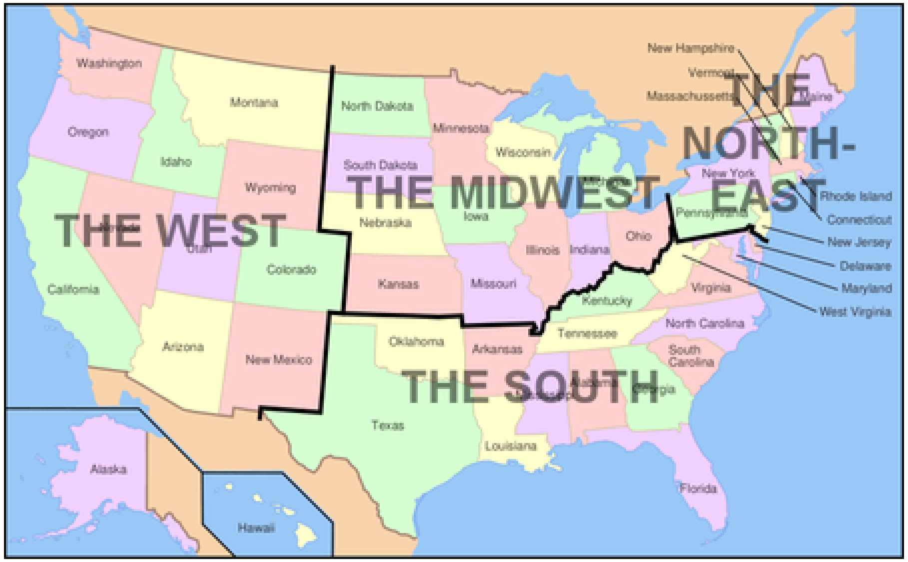
Conversion: Ordinal to Numeric

- Some nominal attributes incorporated an *order*
- Ordered attributes (e.g. grade) can be converted to numbers preserving natural order, e.g.
  - A → 4.0
  - A- → 3.7
  - B+ → 3.3
  - B → 3.0
- Now: d(Mary,John) < d(Mary,Jane)
- Using such a coding schema allows learners to learn valuable rules, e.g.
  - grade>3.5 → excellent_student=true

	grade
John	3.7
Mary	4.0
Jane	3.0

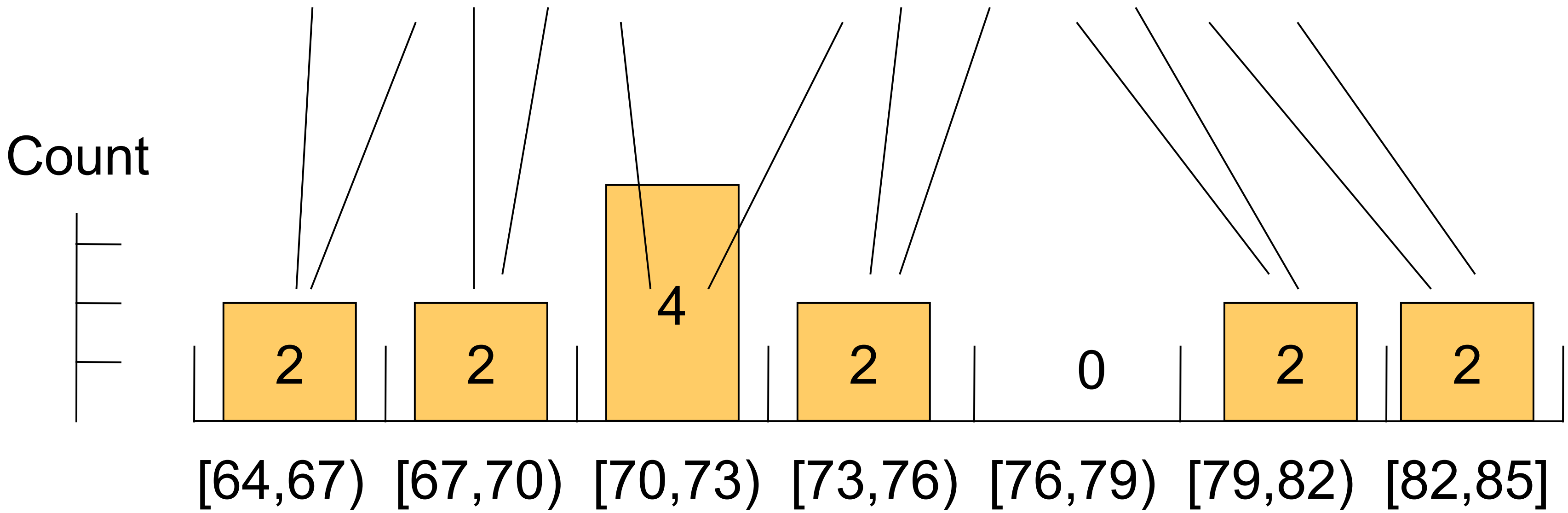
Conversion: Nominal to Numeric

- 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)



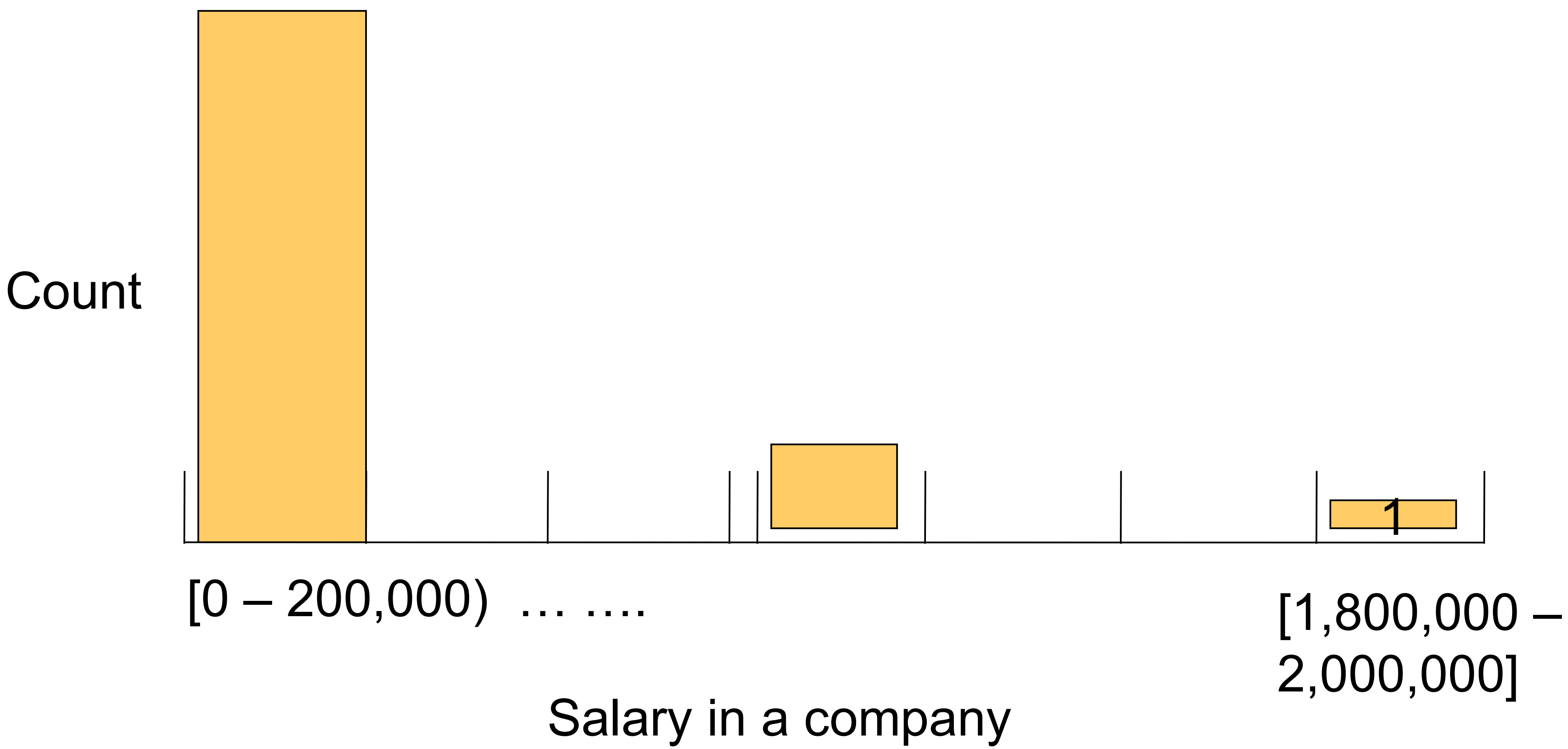
Discretization: Equal-width

Temperature values:
64 65 68 69 70 71 72 72 75 75 80 81 83 85



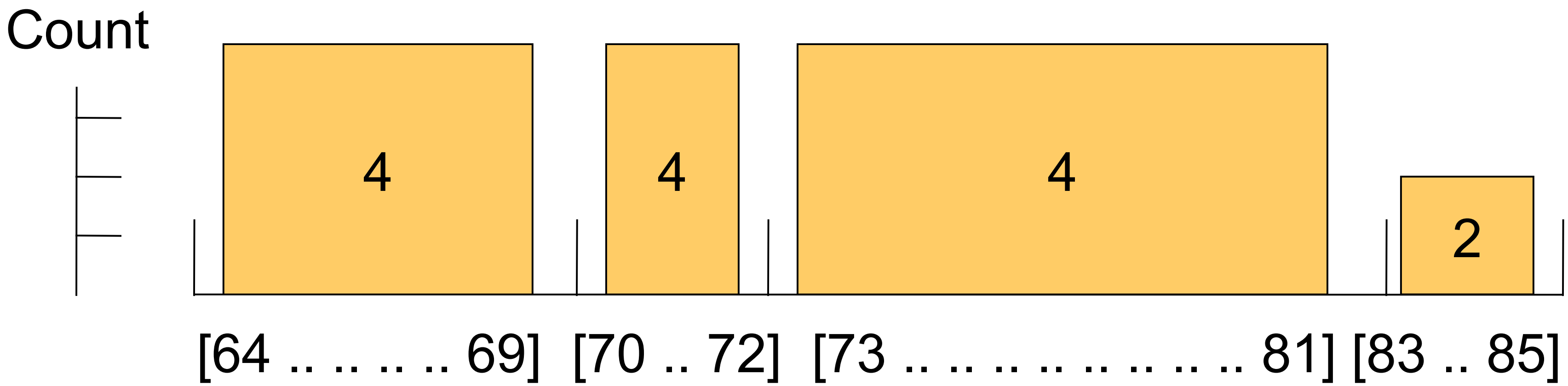
Equal Width, bins Low <= value < High

Discretization: Equal-width



Discretization: Equal-height

Temperature values:
64 65 68 69 70 71 72 72 75 75 80 81 83 85



Equal Height = 4, except for the last bin

Discretization by Entropy

- Top-down approach
- Tries to minimize the entropy in each bin
  - Entropy: $-\sum p(x)\log(p(x))$
  - where the x are all the attribute values

- Goal
  - make intra-bin similarity as high as possible
  - a bin with only equal values has entropy=0

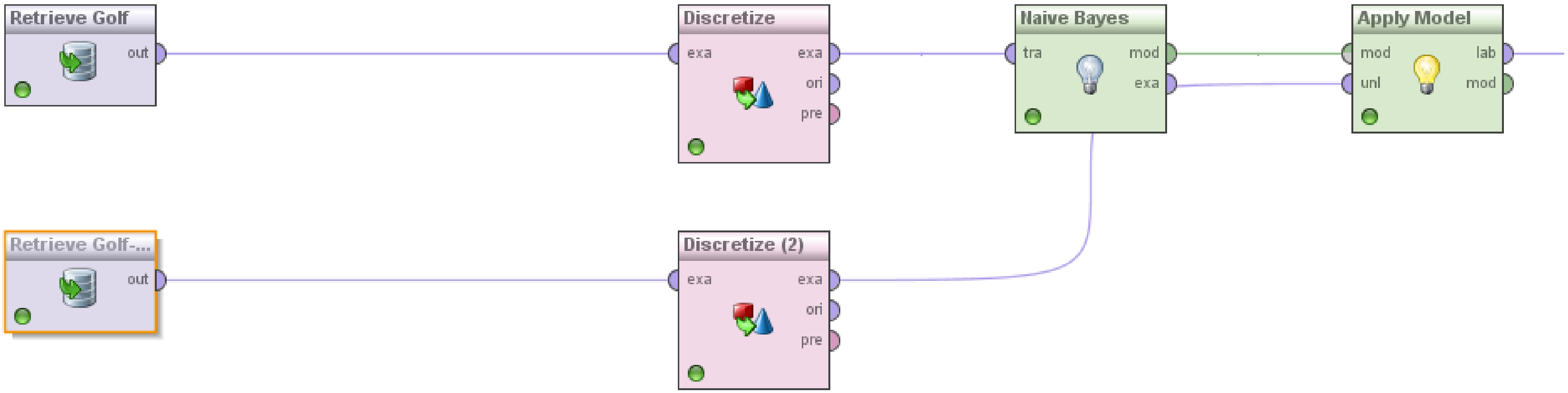
- Algorithm
  - Split into two bins so that overall entropy is minimized
  - Split each bin recursively as long as entropy decreases significantly

Discretization: Training and Test Data

- Training and test data have to be equally discretized!
- Learned model:
  - income=high → give_credit=true
  - income=low → give_credit=false
- Applying model:
  - income=low has to have the same semantics on training and test data!
  - Naively applying discretization will lead to different ranges!

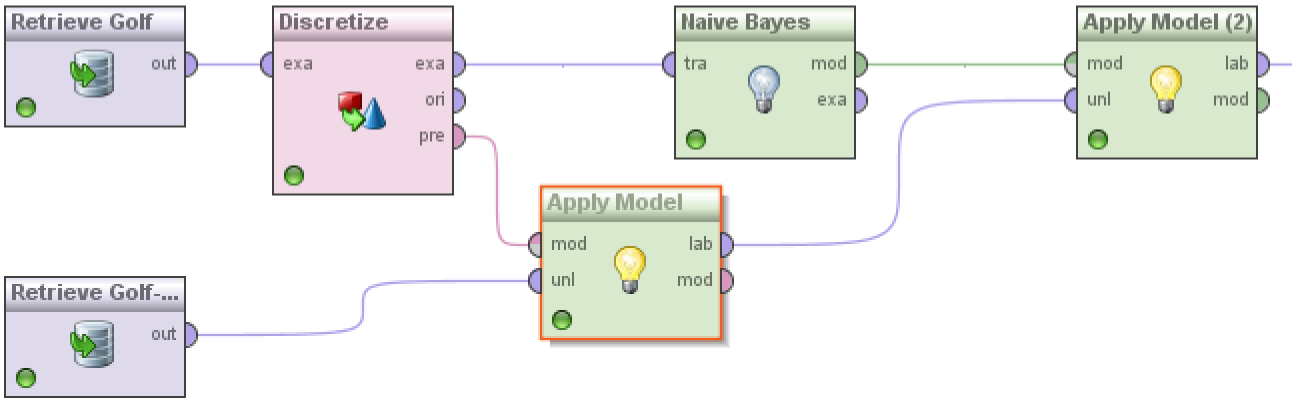
Discretization: Training and Test Data

- Wrong:



Discretization: Training and Test Data

- Right:



- Accuracy in this example, using equal frequency (three bins):
  - wrong: 42.7% accuracy
  - right: 50% accuracy
- Python: `fit` discretizer on training set, `transform` test set
  - fitting on the training+test set may lead to overfitting!

Discretization: Semi-supervised Learning

- Labeling data with ground truth can be expensive
- Example:
  - Medical images annotated with diagnoses by medical experts
- Typical case:
  - Smaller subset of labeled data (gold standard)
  - Larger subset of unlabeled data
- Semi-supervised learning
  - Tries to combine both types of data

- Semi-supervised learning can be applied to discretization
  - Learn distribution of an attribute on larger dataset

    → find better bins

Dealing with Date Attributes

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

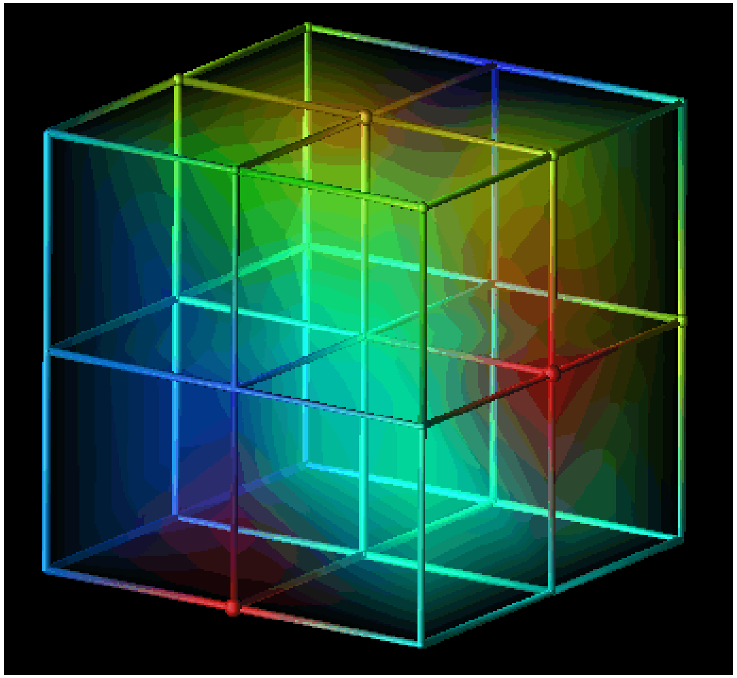
- Dates have lots of interesting information in them
- Example: analyzing shopping behavior
  - time of day
  - weekday vs. weekend
  - begin vs. end of month
  - month itself
  - quarter, season
- Python: use, e.g., `datetime`

Further Datatypes

- Text
  - We have come to know preprocessing techniques in Data Mining 1
- Multi-modal data, e.g.,
  - Images
  - Videos
  - Audio
- Typically, *encoders* are used to create (numeric) representations from such data
  - We will get back there when discussing neural networks

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



Curse of Dimensionality

- Learning models gets more complicated in high-dimensional spaces
- Higher number of observations are needed
  - For covering a meaningful number of combinations
  - "Combinatorial Explosion"
- Distance functions collapse
  - i.e., all distances converge in high dimensions
  - Nearest neighbor classifiers are no longer meaningful

$$euclidean\ distance = \sqrt{\sum_{k=1}^{n} (p_k - q_k)^2}$$

Why does Euclidean Distance Collapse?

- Imagine two randomly picked data points p and q, each with n attributes
- All attributes are equally distributed in [0;1]

  → the expected value of $|p_k-q_k|$ is 0.5,
  → i.e., it's 0.25 for $(p_k-q_k)^2$
- With n → ∞, the distance function will converge towards $\sqrt{n \times \frac{1}{4}}$
  – and the variance will converge to 0 for n → ∞!
- Now, remember that we picked p and q at random
  – i.e., the distance between each two points converges to a constant for high values n

$$euclidean\ distance = \sqrt{\sum_{k=1}^{n} (p_k - q_k)^2}$$

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

- 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

- Searching for optimal attribute sets

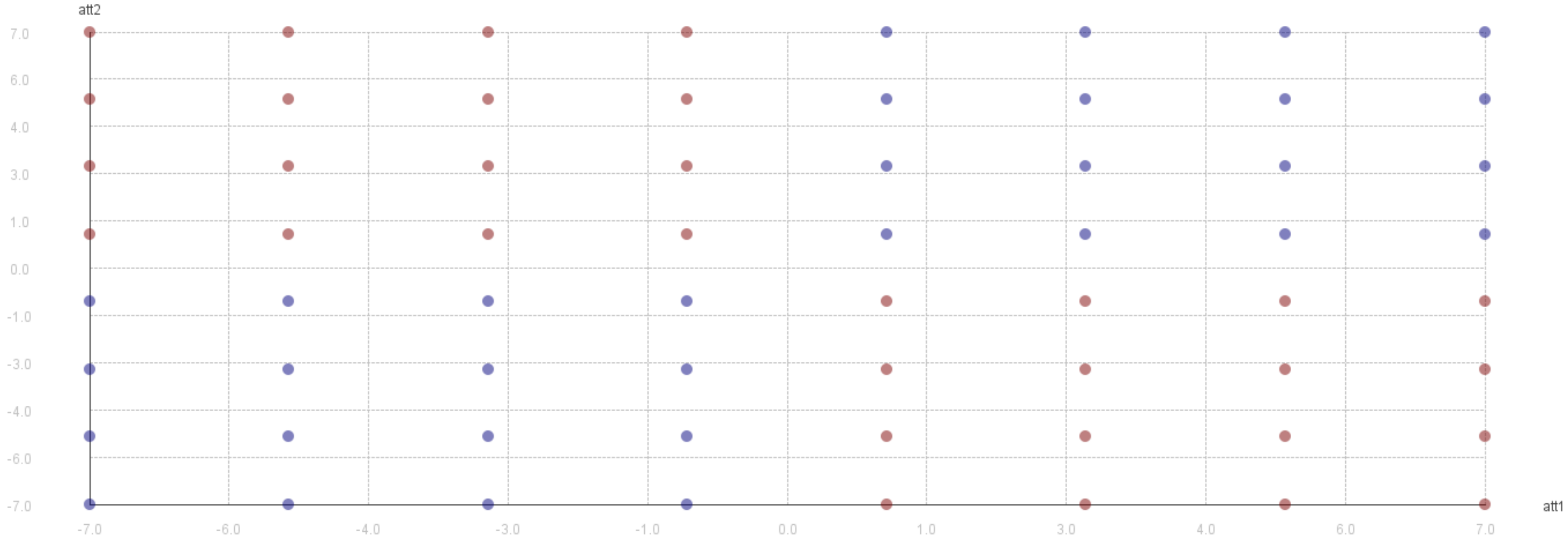
- Backward elimination:

```
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 example revisited
  - Recap: Rule learners can perfectly learn this!
  - But what happens if we apply forward selection here?



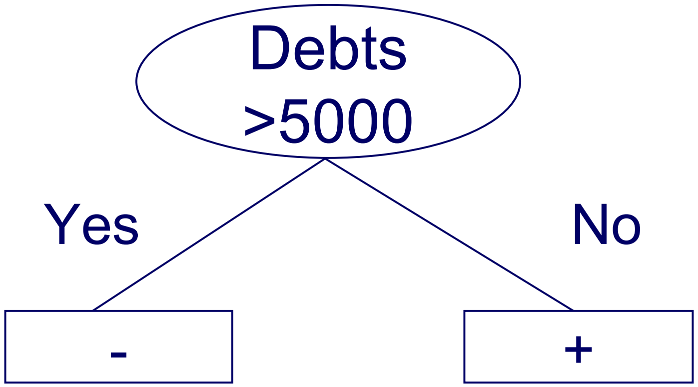
Feature Subset Selection

- Further approaches
  - Brute Force search
  - Evolutionary algorithms
    (will be covered in parameter optimization session)

- 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

Recap: Overfitting

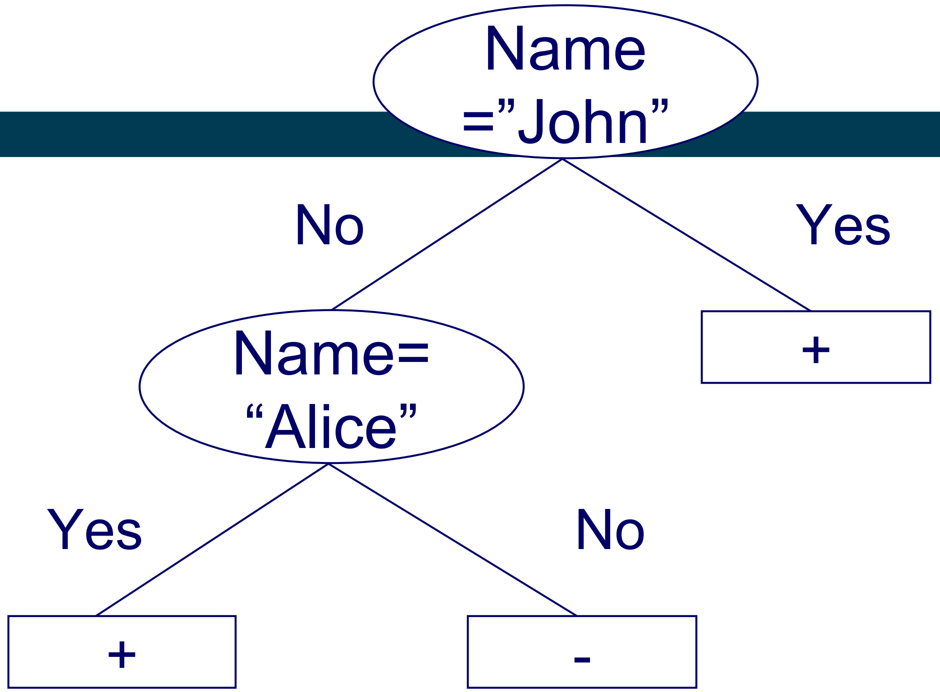
- Example: predict credit rating
  - possible decision tree:



Name	Net Income	Job status	Debts	Rating
John	40000	employed	0	+
Mary	38000	employed	10000	-
Stephen	21000	self-employed	20000	-
Eric	2000	student	10000	-
Alice	35000	employed	4000	+

Recap: Overfitting

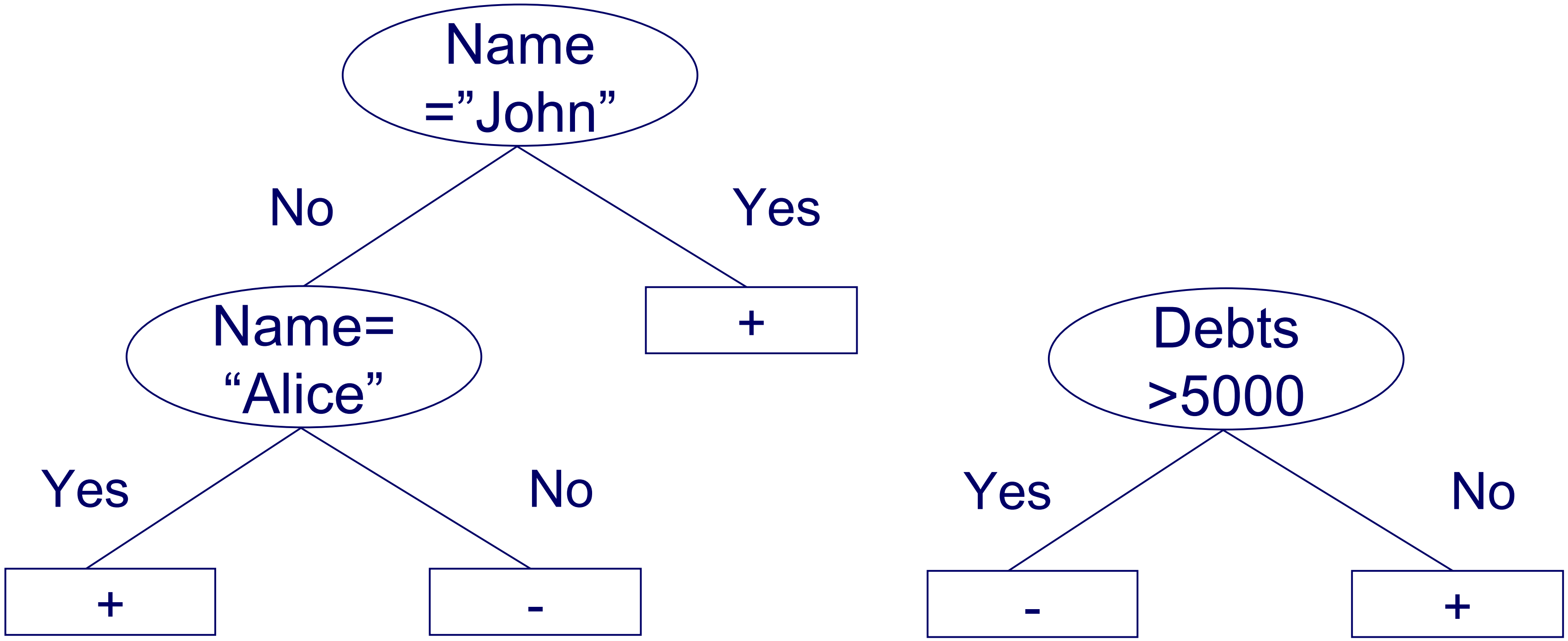
- Example: predict credit rating
  - alternative decision tree:



Name	Net Income	Job status	Debts	Rating
John	40000	employed	0	+
Mary	38000	employed	10000	-
Stephen	21000	self-employed	20000	-
Eric	2000	student	10000	-
Alice	35000	employed	4000	+

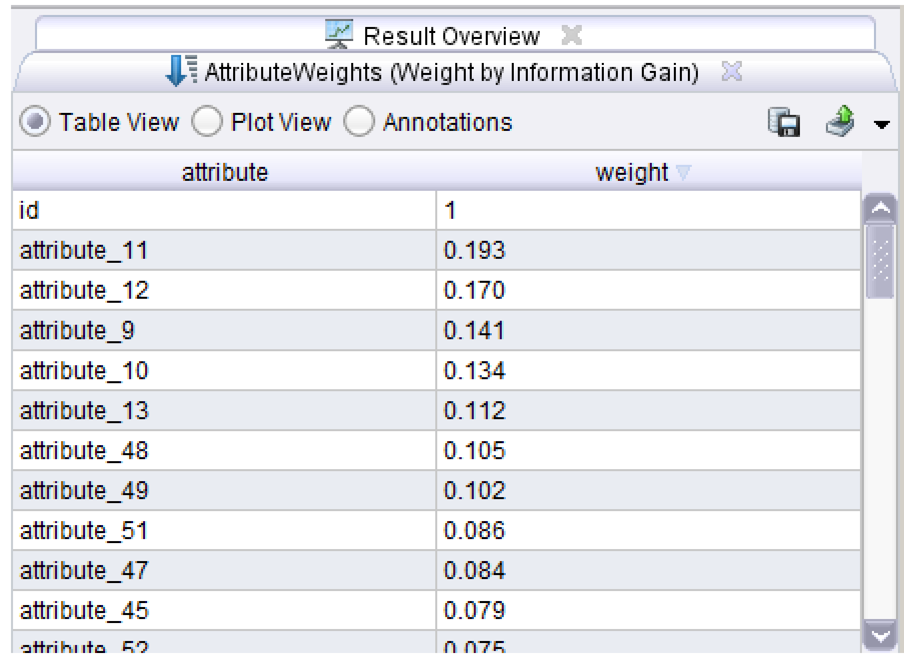
Recap: Overfitting

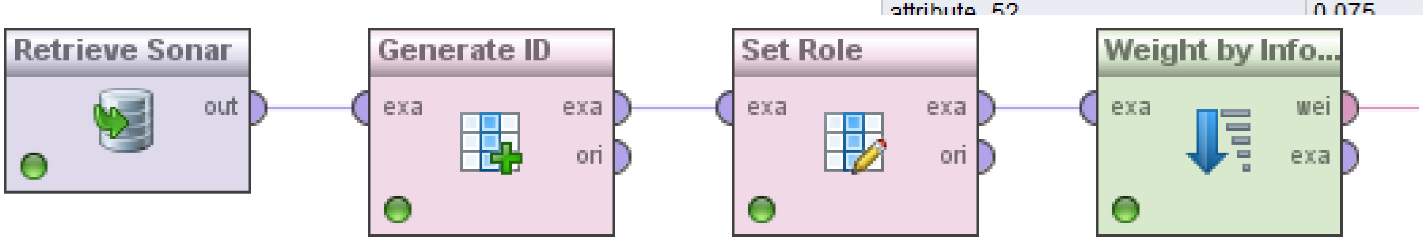
- Both trees seem equally good
  - Classify all instances in the training set correctly
  - Which one do you prefer?



Recap: Overfitting

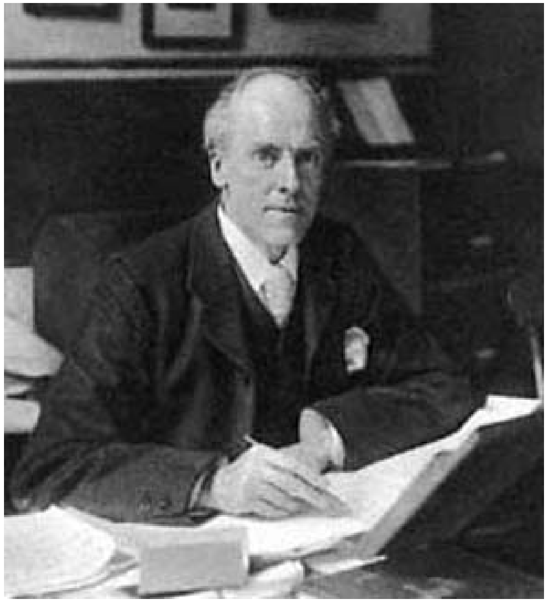
- Overfitting can happen with feature subset selection, too
  - Here, *name* seems to be a useful feature
  - ...but is it?
- Remedies
  - Hard for filtering methods
    - e.g., *name* has highest information gain!
  - Wrapper methods:
    - use cross validation inside!





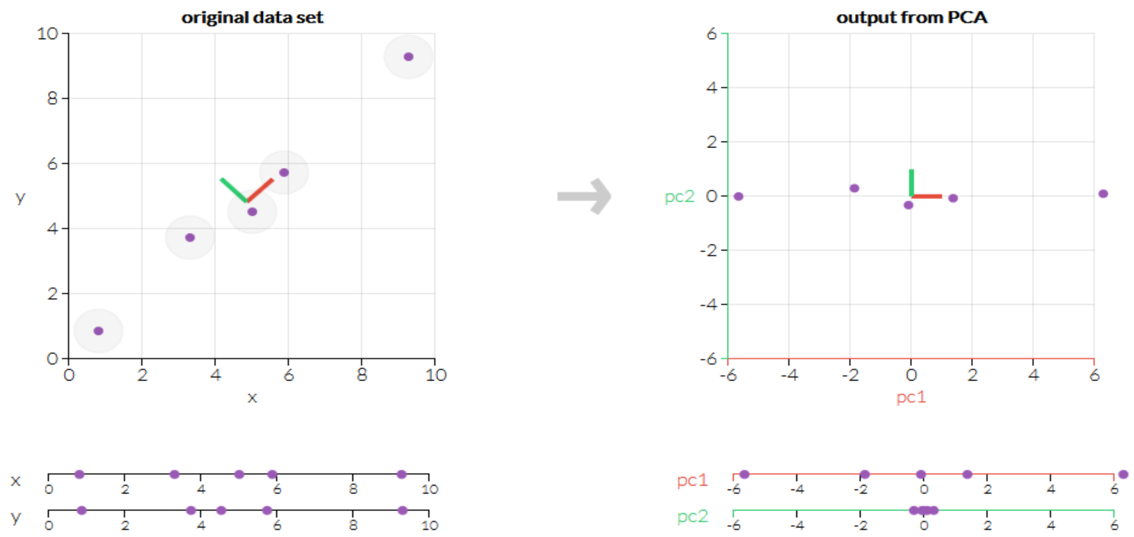
Principal Component Analysis (PCA)

- 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)

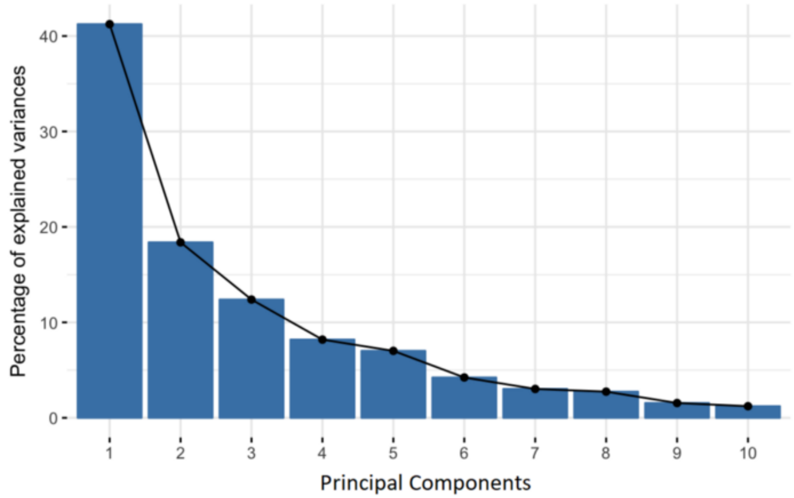
- Idea: transform coordinate system so that each new coordinate (principal component) is as expressive as possible
  - expressivity: variance of the variable
  - the 1st, 2nd, 3rd... PC should account for as much variance as possible
    - further PCs can be neglected



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

Principal Component Analysis (PCA)

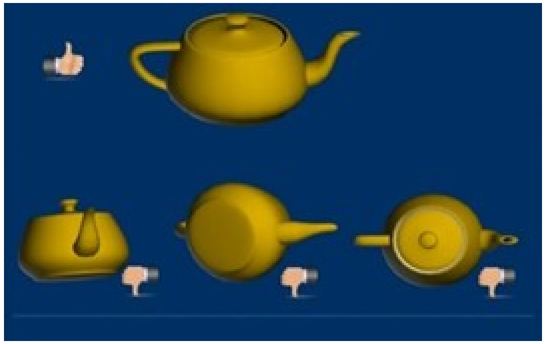
- Principal components
  - are *linear* combinations of the existing features
- General approach:
  - The first component should have as much variance as possible
  - The subsequent ones should also have as much variance as possible
    - and be perpendicular to the first one



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

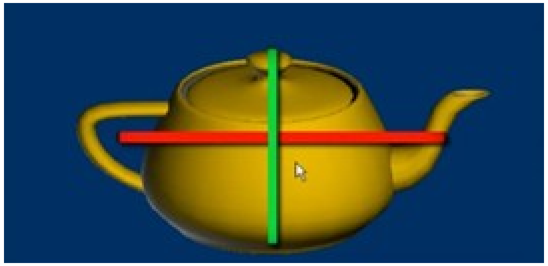
Principle Component Analysis illustrated

- Example by James X. Li, 2009
- Which 2D projection conveys most information about the teapot?



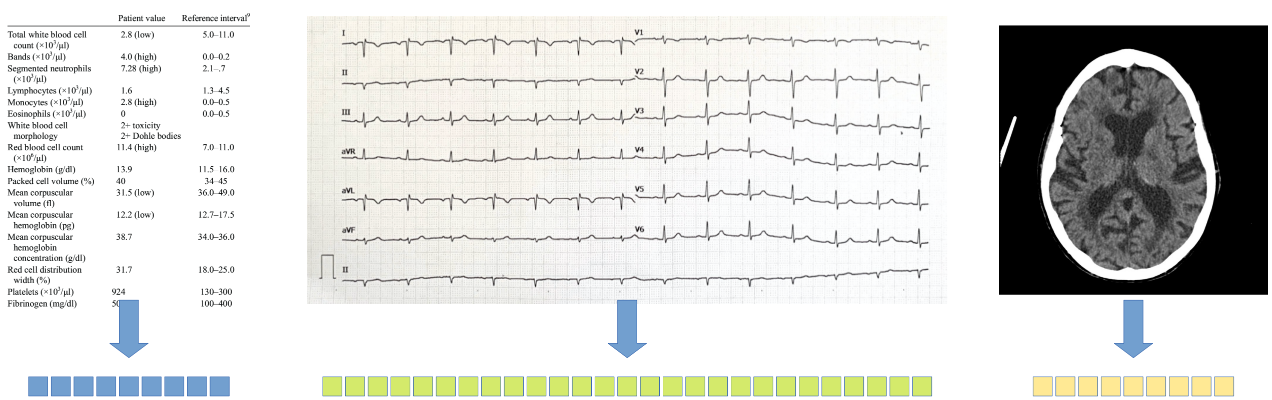
Approach:

- find longest axis first
  - in practice: use average/median diameter to limit effect of outliers
- fix that axis, find next longest



From PCA to Encoders

- PCA can be seen as an *encoder*
  - It computes a new representation (encoding) from an existing one
- Encoders have gained a lot of traction, e.g.,
  - for handling high-dimensional data
  - for handling multi-modal data
- Today, we mostly use neural encoders
  - We get back to that in the neural networks session

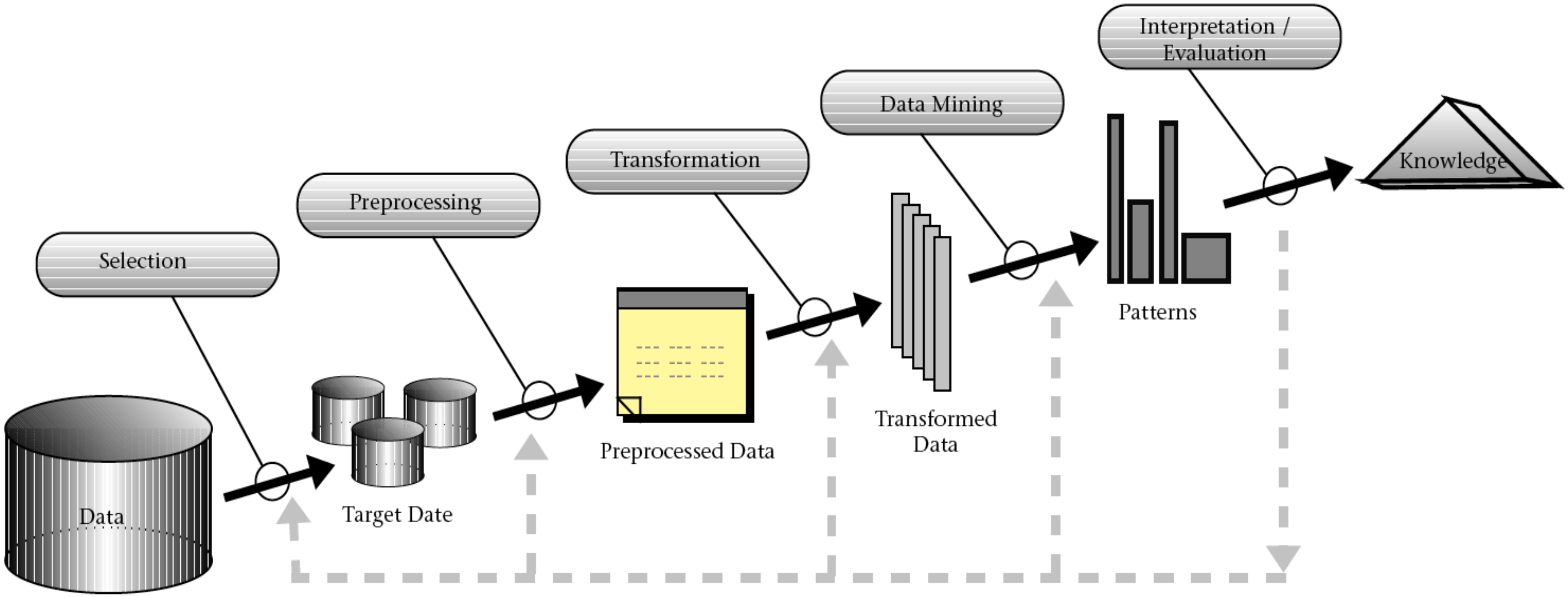


	Patient value	Reference interval[9]
Total white blood cell count ($\times 10^3/\mu l$)	2.8 (low)	5.0–11.0
Bands ($\times 10^3/\mu l$)	4.0 (high)	0.0–0.2
Segmented neutrophils ($\times 10^3/\mu l$)	7.28 (high)	2.1–.7
Lymphocytes ($\times 10^3/\mu l$)	1.6	1.3–4.5
Monocytes ($\times 10^3/\mu l$)	2.8 (high)	0.0–0.5
Eosinophils ($\times 10^3/\mu l$)	0	0.0–0.5
White blood cell morphology	2+ toxicity 2+ Dohle bodies	
Red blood cell count ($\times 10^6/\mu l$)	11.4 (high)	7.0–11.0
Hemoglobin (g/dl)	13.9	11.5–16.0
Packed cell volume (%)	40	34–45
Mean corpuscular volume (fl)	31.5 (low)	36.0–49.0
Mean corpuscular hemoglobin (pg)	12.2 (low)	12.7–17.5
Mean corpuscular hemoglobin concentration (g/dl)	38.7	34.0–36.0
Red cell distribution width (%)	31.7	18.0–25.0
Platelets ($\times 10^3/\mu l$)	924	130–300
Fibrinogen (mg/dl)	50	100–400

Summary Data Preprocessing

- Raw data has many problems
  - missing values
  - errors
  - high dimensionality
  - unfortunate distribution
  - …
- 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

Recap: The Data Mining Process



Source: Fayyad et al. (1996)

Questions?