
# The Data - Pre–processing

## Data Mining

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# Why?

- Problems in data
  - Missing values
  - Skewed distributions
  - Outliers
  - Dimensionality
  - Errors and duplications
- Types not adequate for the processing required
- Necessary to point out particular aspects

# Data pre–processing

- Sampling
- Dimensionality Reduction
- Feature subset selection
- Feature creation
- Discretization and Binarization Attribute Transformation

# Aggregation

- Combining two or more attributes (or objects) into a single attribute (or object)
- Purpose
  - Data reduction
    - Reduce the number of attributes or objects
  - Change of scale
    - Cities aggregated into regions, states, countries, etc
  - *More stable* data
    - Aggregated data tends to have less variability

# Sampling I

- For both preliminary investigation and final data analysis
- Statistician perspective
  - obtaining the entire data set could be impossibile or too expensive
- Data processing perspective
  - processing the entire data set could be too expensive or time consuming

# Sampling II

1. using a sample will work almost as well as using the entire data sets, *if the sample is representative*
2. A sample is representative if it has approximately the same property (of interest) as the original set of data

# Types of sampling

1. Simple random
   - a single random choice of an object with given probability distribution
2. With replacement
   - repetition of independent extractions of type 1
3. Without replacement
   - repetition of extractions, extracted element is removed from the population
4. Stratified
   - used to split the data set into subsets with homogeneous characteristics
   - the representativity is guaranteed inside each subset
   - typically requested in cross–validation

# Sample size

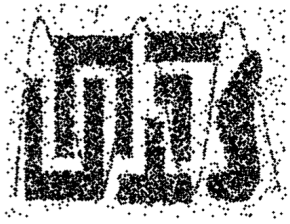
- Statistics provides techniques to assess
  - optimal sample size
  - sample significativity
- Tradeoff between data reduction and precision

# Sampling with/without replacement

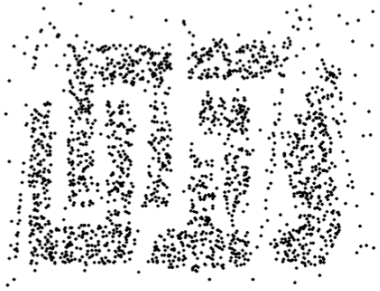
- they are nearly equivalent if sample size is a small fraction of the data set size
- with replacement, in a small population a small subset could be underestimated
- sampling with replacement is
  - much easier to implement
  - much easier to be interpreted from a statistical point of view
    - extractions are statistically independent

# Sample size – Example

Loss of information



8000 points



2000 points

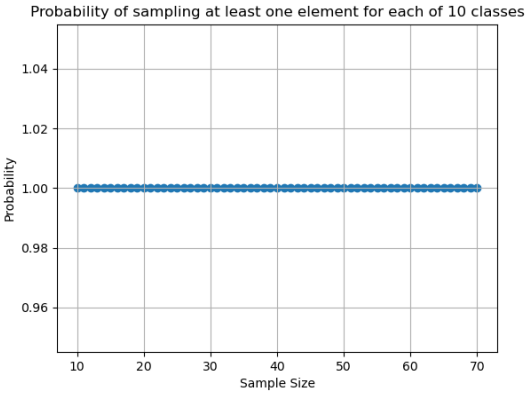
500 points

# Sample size – Missing class I[1]

- Probability of sampling at least one element for each class (with replacement)
  - it is independent from the size of the data set!

A B C D E
F G H I J

Ten classes



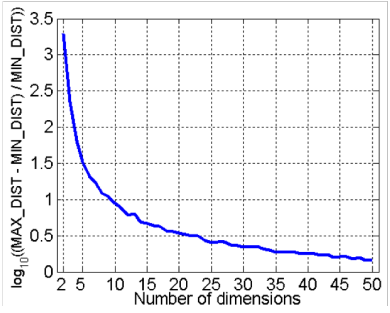

1 It is an instance of the Coupon Collector's Problem

# Sample size – Missing class - II

- This aspect becomes relevant, for example, in a supervised dataset with a high number of different values of the target
- If the number data elements is not big enough, it can be difficult to guarantee a stratified partitioning in train/test split or in cross–validation split
- Example:
  - $N = 1000$, $C = 10$, test–set–size $= 300$, cross–validation–folds $= 10$
  - the probability of folds without adequate representation of some classes becomes quite high
- When designing the training processes it is necessary to consider those aspects
  - in the example, one could use only 3 folds in cross–validation

# The curse of dimensionality

- When dimensionality is very high the occupation of the space becomes very sparse
- Discrimination on the basis of the distance becomes uneffective
- Experiment:
  - random generation of 500 points
  - plot the relative difference between the maximum and the minimum distance between pairs of points



# Dimensionality reduction

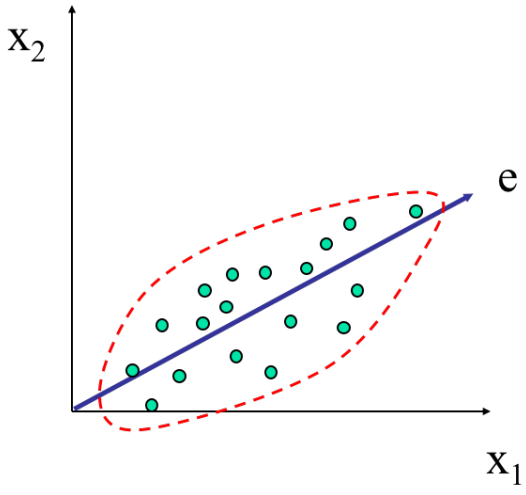
- Purposes:
  - avoid the *curse of dimensionality*
  - noise reduction
  - reduce time and memory complexity of the mining algorithms
  - visualization
- Techniques:
  - principal component analysis
  - singular values decomposition
  - supervised techniques
  - non–linear techniques

# PCA

Find projections that capture most of the data variation

- Find the eigenvector of the covariance matrix
- the eigenvectors define the new space

The new dataset will have *only the attributes* which capture most of the data variation



# Feature subset selection I

A *local* way to reduce dimensionality

- Redundant attributes
  - duplicate most of the information contained in other attributes
    - e.g. price and v.a.t. amount
- Irrelevant attributes
  - do not contain any information useful for analysis
    - e.g. SSN is not relevant to predict wealth

# Feature subset selection II

1. Brute force
   - try all possible feature subsets as input to data mining algorithm and measure the effectiveness of the algorithm with the reduced dataset
2. Embedded approach
   - Feature selection occurs naturally as part of the data mining algorithm
     - e.g. decision trees
3. Filter approach
   - Features are selected before data mining algorithm is run
4. Wrapper approaches
   - A data mining algorithm can choose the best set of attributes
     - try as in 1, but without exhaustive search

# Feature creation

New features can capture more efficiently data characteristics

- Feature extraction
  - pixel picture with a face $\Rightarrow$ eye distance, ...
- Mapping to a new space
  - e.g. signal to frequencies with Fourier transform
- New features
  - e.g. volume and weight to density

# Feature engineering, a.k.a. feature creation

- Feature creation is a crucial step in data mining
- It involves transforming raw data into meaningful features that can improve predictive models
- In the financial environment, feature creation plays a vital role in enhancing trading strategies, risk management, and fraud detection

# Examples of Feature Creation in Finance I

- **Moving Averages** Calculate the average closing price of a stock over a specific time window (e.g., 10 days, 50 days).
- **Volatility Measures** Compute metrics such as standard deviation or average true range to capture the level of price fluctuations.
- **Relative Strength Index (RSI)** Derive a momentum oscillator indicating overbought or oversold conditions in the market.

# Examples of Feature Creation in Finance II

- **Liquidity Ratios** Calculate ratios like bid-ask spread or trading volume to assess market liquidity.
- **Fundamental Analysis Indicators** Include financial metrics such as earnings per share (EPS), price-to-earnings (P/E) ratio, or debt-to-equity ratio.
- **Market Sentiment Analysis** Utilize sentiment scores from news articles, social media, or analyst reports to gauge market sentiment.
- **Technical Analysis Patterns** Identify chart patterns such as head and shoulders, double tops, or flags to predict future price movements.

# Feature Creation: closing prices of a stock

```
data = {'Date': ['2022-01-01', '2022-01-02', '2022-01-03', '2022-01-04', '2022-01-05'],
        'Close': [100, 102, 98, 105, 101]}
# Create a DataFrame
df = pd.DataFrame(data)

# Feature 1: Moving Average (10 days)
df['MA_10'] = df['Close'].rolling(window=10).mean()

# Feature 2: Daily Price Change
df['Price_Change'] = df['Close'].diff()

# Feature 3: Relative Strength Index (RSI)
# Calculation of RSI requires more data points and additional steps,
# so we'll simplify it here for demonstration purposes
df['RSI'] = 100 - (100 / (1 + (df['Close'].\
            pct_change()).rolling(window=14)\
            .apply(lambda x: x[x > 0].mean() / x[x < 0].mean())))
```

# Examples of Feature Creation in a Housing dataset I

- **Total Area**
  - Calculate the sum of sizes of all rooms in the house.
- **Price per Square Foot**
  - Divide the price of the house by its total area.
- **Age of the House**
  - Calculate the age of each house by subtracting the year it was built from the current year.
- **Neighborhood Median Income**
  - Include data on the median income of households in each neighborhood.

# Examples of Feature Creation in a Housing dataset II

- **Distance to City Center**
  - Measure the distance of each house from the city center.
- **Renovation Status**
  - Create a binary feature indicating whether the house has been recently renovated.
- **School District Rating**
  - Include data on the quality of school districts in which the houses are located.
- **Presence of Amenities**
  - Create a categorical feature indicating the presence of amenities such as a swimming pool, garden, garage, etc.

# Why do we need type conversion?

- Many algorithms require numeric features
  - categorical features must be transformed into numeric
  - ordinal features must be transformed into numeric, and the order must be preserved
- Classification requires a target with nominal values
  - a numerical target can be discretised
- Discovery of association rules require boolean features
  - a numerical feature can be discretised and transformed int a series of boolean features

# Binarization of discrete attributes

Attribute $d$ allowing $V$ values $\Rightarrow$ $V$ binary attributes.

| *Quality* | *Quality–Awful* | *Quality–Poor* | *Quality–OK* | *Quality–Good* | *Quality–Great* |
|---|---|---|---|---|---|
| Awful | 1 | 0 | 0 | 0 | 0 |
| Poor | 0 | 1 | 0 | 0 | 0 |
| Ok | 0 | 0 | 1 | 0 | 0 |
| Good | 0 | 0 | 0 | 1 | 0 |
| Great | 0 | 0 | 0 | 0 | 1 |

# Nominal to numeric

- One–Hot–Encoding
  - a feature with $V$ unique values is substituted by $V$ binary features each one corresponding to one of the unique values
  - if object $x$ has value $v$in feature $d$ then the binary feature corresponding to $v$ has `True` for $x$, all the other binary features have value `False`
  - `True` and `False` are represented as 1 and 0, therefore can be processed by also by procedures working only on numeric data, as is the case for the estimators available in `scikit-learn`
- `sklearn.preprocessing.OneHotEncoder`

link to manual page

# Ordinal to numeric

- The ordered sequence is transformed into consecutive integers
  - by default the lexicographic order is assumed
  - The user can specify the proper order of the sequence
- `sklearn.preprocessing.OrdinalEncoder`

link to manual page

# Numeric to binary with threshold

- Not greater than the threshold becomes zero
- Greater than the threshold becomes one
- `sklearn.preprocessing.Binarizer`

link to manual page

## Discretization/Reduction of the number of distinct values

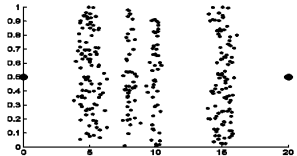
- Some algorithms work better with categorical data
- A small number of distinct values can let patterns emerge more clearly
- A small number of distinct values let the algorithms to be less influenced by noise and random effects

# Discretization

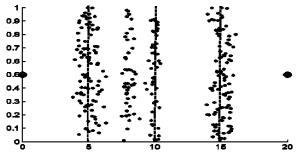
- Continuous ⇒ Discrete
  - thresholds
    - many options
  - binarization ⇒ single threshold
- Discrete with many values ⇒ Discrete with less values
  - guided by domain knowledge

# Continuous ⇒ Discrete

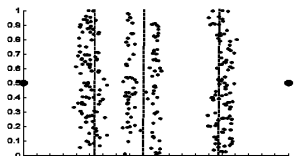
## Boundaries on x axis – Unsupervised



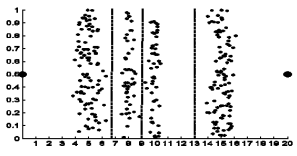
Data



Equal width



Equal frequency



K-means

# Numeric to $k$ values

- The numbers are discretised into a sequence of integers 0 to $k-1$
- Several strategies are available
  - {'uniform','quantile','means'}
- `sklearn.preprocessing.KBinsDiscretizer`

link to manual page

# Correlation of quantitative data (Pearson's) OPTIONAL

Measure of the linear relationship between a pair of attributes

- Standardize the values
- For two given attributes $p$ and $q$, consider as vectors the ordered lists of the values over all the data records
- Compute the dot product of the vectors

$$\mathbf{p} = [p_1, \ldots, p_N] \xrightarrow{standardize} \mathbf{p}'$$

$$\mathbf{q} = [q_1, \ldots, q_N] \xrightarrow{standardize} \mathbf{q}'$$

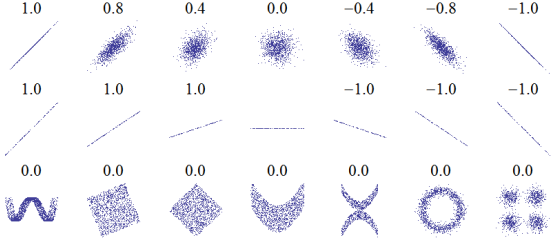
$$\mathrm{corr}(p, q) = \mathbf{p}' \bullet \mathbf{q}'$$

There is an alternative definition based on covariance and variances

# Correlation – Discussion

OPTIONAL

- Independent variables ⇒ correlation is zero
  - the inverse is not valid *in general*
- Correlation zero ⇒ absence of *linear relationship* between the variables
- Positive values imply positive linear relationship




From "Correlation and Dependence" on Wikipedia

# Correlation between nominal attributes OPTIONAL

Symmetric Uncertainty [Witten et al.(2011)Witten, Frank, and Hall]

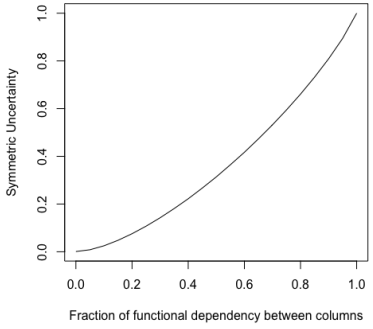
$$U(p,q) = 2\frac{H(p) + H(q) - H(p,q)}{H(p) + H(q)}$$

- where $H()$ is the entropy of a single attribute while $H(,)$ is the joint entropy, computed from the joint probabilities
- is always between 0 and 1

## Correlation between nominal attributes – Experiment

OPTIONAL

- Behavior of SU for two independent uniformly distributed discrete attributes, say $p$ and $q$
  - in a variable fraction of records the value of $p$ is copied to $q$
- from complete independence (left) to complete biunivocal correspondence (right)
- when there is independence, the joint entropy is the sum of the individual entropies, and SU is zero
- when there is complete correspondence, the individual entropies and the joint entropy are equal and SU is one



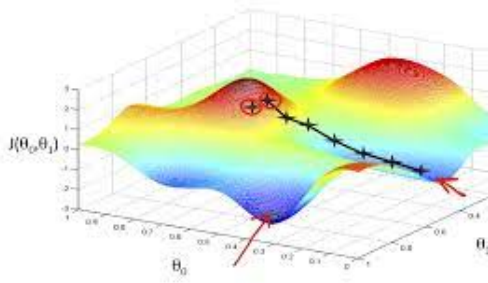
# Why Data Transformation

- the features may have different scales
  - this can alterate the results of many learning techniques
  - some machine learning algorithms are sensitive to feature scaling while others are virtually invariant to it
- there can be outliers

# Gradient descent

Machine learning algorithms that use *gradient descent* as an optimization technique require data to be scaled

- e.g. linear regression, logistic regression, neural network, etc.
- The presence of feature value X in the formula will affect the step size of the gradient descent
- The difference in ranges of features will cause different step sizes for each feature.
- Similar ranges of the various features ensure that the gradient descent moves smoothly towards the minima and that the steps for gradient descent are updated at the same rate for all the features



# Attribute transformation

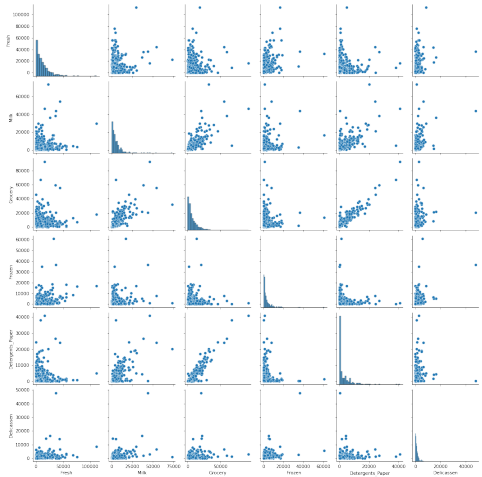
- Map the entire set of values to a new set according to a function
  - $x^k, \log(x), e^x, |x|$
  - in general they change the *distribution of values*
- Standardization: $x \rightarrow \frac{x-\mu}{\sigma}$
  - if the original values have a *gaussian* distribution, the transformed values will have a *standard* gaussian distribution ($\mu = 0, \sigma = 1$)
  - translation and shrinking/stretching, no change in distribution
- MinMax scaling (a.k.a. Rescaling): the domains are mapped to standard ranges

$$x \rightarrow \frac{x - x_{min}}{x_{max} - x_{min}} \quad \text{(0 to 1)} \qquad x \rightarrow \frac{x - \frac{x_{max}+x_{min}}{2}}{\frac{x_{max}-x_{min}}{2}} \quad \text{(-1 to 1)}$$

  - translation and shrinking/stretching, no change in distribution

# Attribute transformation – Example I

Data with skewed distribution

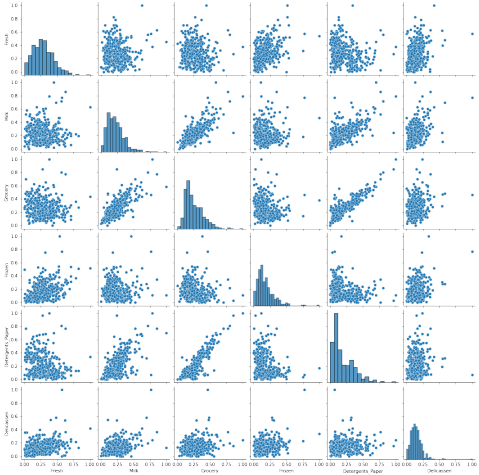


# Attribute transformation – Example II

Python code

```
from sklearn.preprocessing
      import PowerTransformer
pt = PowerTransformer(method='box-cox')
X = pd.DataFrame(pt.fit_transform(X0)
                 , columns = X0.columns)
```

After the transformation the data are
*less skewed*



# Distance–based algorithms

- KNN, K–Means, SVM, ...
- distances between points are used to determine their similarity

Example

| Original data | | |
|---|---|---|
| **Student** | **CGPA** | **Salary** |
| A | 3 | 60 |
| B | 3 | 40 |
| C | 4 | 40 |
| D | 4.5 | 50 |
| E | 4.2 | 52 |

| Scaled data | | |
|---|---|---|
| **Student** | **CGPA** | **Salary** |
| A | -1.18431 | 1.520013 |
| B | -1.18431 | -1.100699 |
| C | 0.41612 | -1.100699 |
| D | 1.21635 | 0.209657 |
| E | 0.736212 | 0.471728 |

# Distances before and after scaling

$$
\begin{aligned}
distance(A, B) &= \sqrt{(40-60)^2 + (3-3)^2} = 20 \\
distance(B, C) &= \sqrt{(40-40)^2 + (4-3)^2} = 1 \\
distance(A_s, B_s) &= \sqrt{(1.1+1.5)^2 + (1.18-1.18)^2} = 2.6 \\
distance(B_s, C_s) &= \sqrt{(1.1-1.1)^2 + (0.41+1.18)^2} = 1.59
\end{aligned}
$$

Before the scaling the two distances seemed to be very different, due to the a big numeric difference in the `Salary` attribute, now they are comparable

# Range–based scaling and standardization

operate on single features

- Range–based scaling stretches/shrinks and translates the range, according to the range of the feature (there are some variants)
  - good when we know that the data are not gaussian, or we do not make any assumption on the distribution
  - the base variant, the MinMax scaler, remaps to $0, 1$
- Standardization subtracts the mean and divides by the standard deviation
  - the resulting distribution has mean *zero* and *unitary* standard deviation
  - good when the distribution is gaussian
  - `StandardScaler`

# Range–based scalers in Scikit-Learn

affine transformations: linear transformation plus translation

- `MinMaxScaler` – remaps the feature to $[0, 1]$
- `RobustScaler` – centering and scaling statistics is based on percentiles
  - not influenced by a few number of very large marginal outliers
  - the resulting range of the transformed feature values is larger than the one given by `MinMaxScaler` and `StandardScaler`

# Normalization

- Normalization is mentioned sometimes with different meanings
  - frequently it refers to `MinMaxScaler`
- in `Scikit-learn` the `Normalizer` normalizes each data row to unit norm

# Workflow

1. transform the features as required both for the train and test data
2. fit and optimize the model(s)
3. test
4. possibly, use the original data to plot relevant views (e.g. to plot cluster assignments)

# Imbalanced data in classification

- The performance minority class (classes) has little impact on standard performance measures
- The optimised model could be less effective on minority class (classes)
- Some estimators allow to weight classes
- Some performance measures allow to take into account the contribution of minority class (classes)

# Cost Sensitive learning

Already introduced in *Machine-Learning-03-classification*

- several classifiers have the parameter `class_weight`
- it changes the cost function to take into account the imbalancing of classes
- in practice it is equivalent to oversampling the minority class, (repeating random examples) in order to produce a balanced training set

# Undersampling

- Obtains a balanced training set by randomly reducing the number of examples of the majority class
- Obviously part of the knowledge embedded in the training set is dropped out

# Oversampling with SMOTE

## Synthetic Minority Oversampling Technique – a type of data augmentation

let the minority class be $c_{min}$, synthesise new examples of class $c_{min}$

- choose from the *training set* random example $x_r$ of class $c_{min}$
- find in the training set the $k$ nearest neighbours of $x_r$ whose class is $c_{min}$
- choose randomly one of the neighbours, say $x_{rn}$ found above and *create* a new data element chosen randomly from the segment connecting $x_r$ $x_{rn}$ in the feature space $m = r * (x_r + x_{rn})/2$

Theory developed in SMOTE: Synthetic Minority Over-sampling Technique[Bowyer et al.(2011)Bowyer, Chawla, Hall, and Kegelmeyer]

# Workflow for *undersampling/oversampling*

- resample the training set
- fit and optimise the estimator
- test the fitted estimator on the test set (untouched)

# Bibliography I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