PHBS Course : Machine Learnings and Algorithms
Data Preprocessing

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Outlines

Data Types

- Tabular data : matrices, vectors, objects, relations, etc.
  - Data objects : also called samples, examples, instances, data points, objects, tuples, vectors
  - Attributes : each row of a table, also called dimensions, features, variables
- Graphical data : networks, graphs, etc.
- Multi-media data : texts, images, videos, audios, etc.

行星	周期（年）	平均距离	周期^2/距离^3
水星	0.241	0.39	0.98
金星	0.615	0.72	1.01
地球	1.00	1.00	1.00
火星	1.88	1.52	1.01
木星	11.8	5.20	0.99
土星	29.5	9.54	1.00
天王星	84.0	19.18	1.00
海王星	165	30.06	1.00

Types of Attributes

- Discrete : $\mathbf{x} \in$ some countable sets, e.g., $\mathbb{N}$
  - Nominal : Countries=$\{$China, US, UK, France, Germany$\}$, Universities=$\{$Peking U, Tsinghua U, SUSTech, Shenzhen U, HIT$\}$, not comparable
  - Boolean : 0 or 1, male or female, spam or non-spam, etc.
  - Ordinal : Heights=$\{$tall, short$\}$, Scores=$\{$A+, A, A-, B+, B, B-, C, C-, D, F$\}$, can be compared, but cannot operated arithmetically
- Continuous : $\mathbf{x} \in$ some subset in $\mathbb{R}^n$
  - Numerical : Income, exact marks, weights, etc., can be operated arithmetically

Basic Statistics

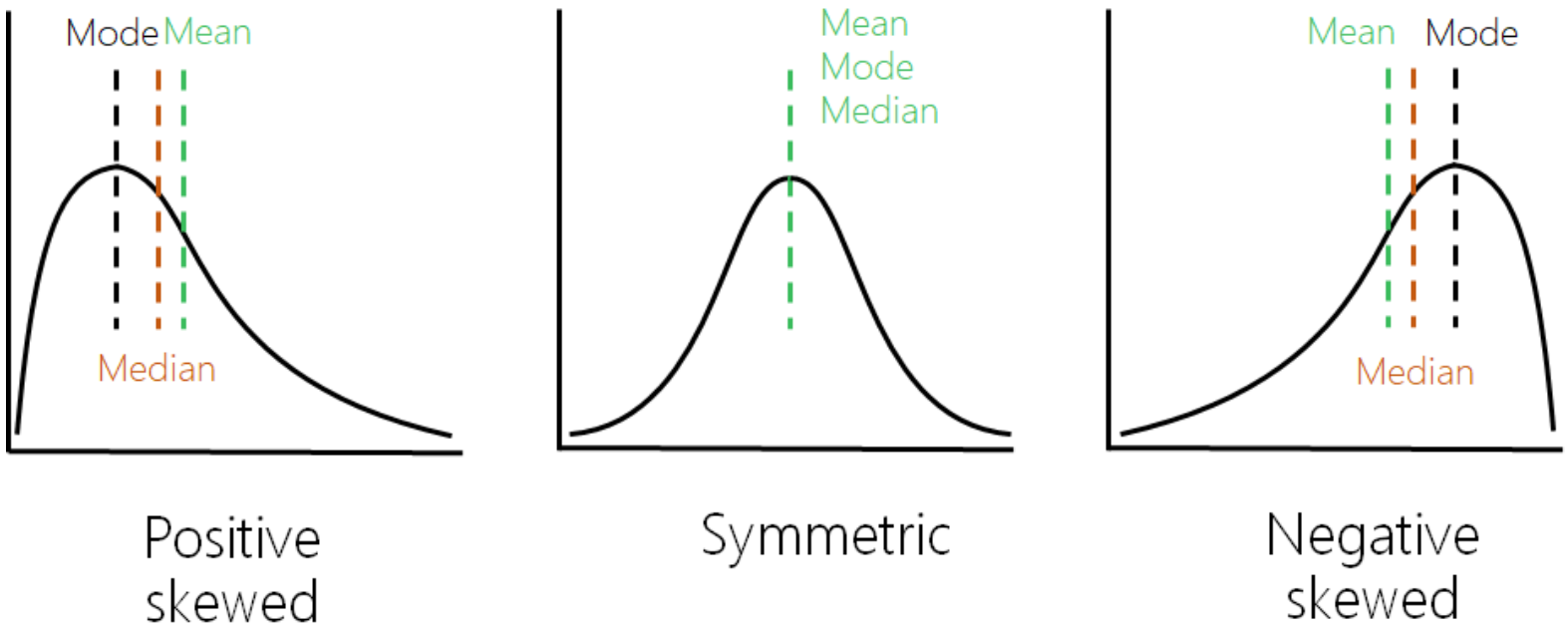
- Mean : $\mathrm{E}X = \min_c \mathrm{E}(X-c)^2 \approx \frac{1}{n}\sum_{i=1}^{n} x_i$
- Median :

$$\min_c \mathrm{E}|X-c| = \begin{cases} x_{(\frac{n+1}{2})} & \text{if } n \text{ is odd} \\ (x_{(\frac{n}{2})} + x_{(\frac{n}{2}+1)})/2 & \text{otherwise} \end{cases}$$

- Maximum : $\max_i x_i$; Minimum : $\min_i x_i$
- Quantile : a generalization of median, k-th q-quantile x_q : $P[X < x_q] \leqslant k/q$; interquartile range (IQR)$=Q_3(75\%) - Q_1(25\%)$
- Variance : $\mathrm{Var}(X) = \mathrm{E}[X - \mathrm{E}X]^2 \approx \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2$; Standard deviation : $\sqrt{\mathrm{Var}(X)}$
- Mode : $\min_c \mathrm{E}|X-c|^0 =$ the most frequently occurring value (define $0^0 = 0$)

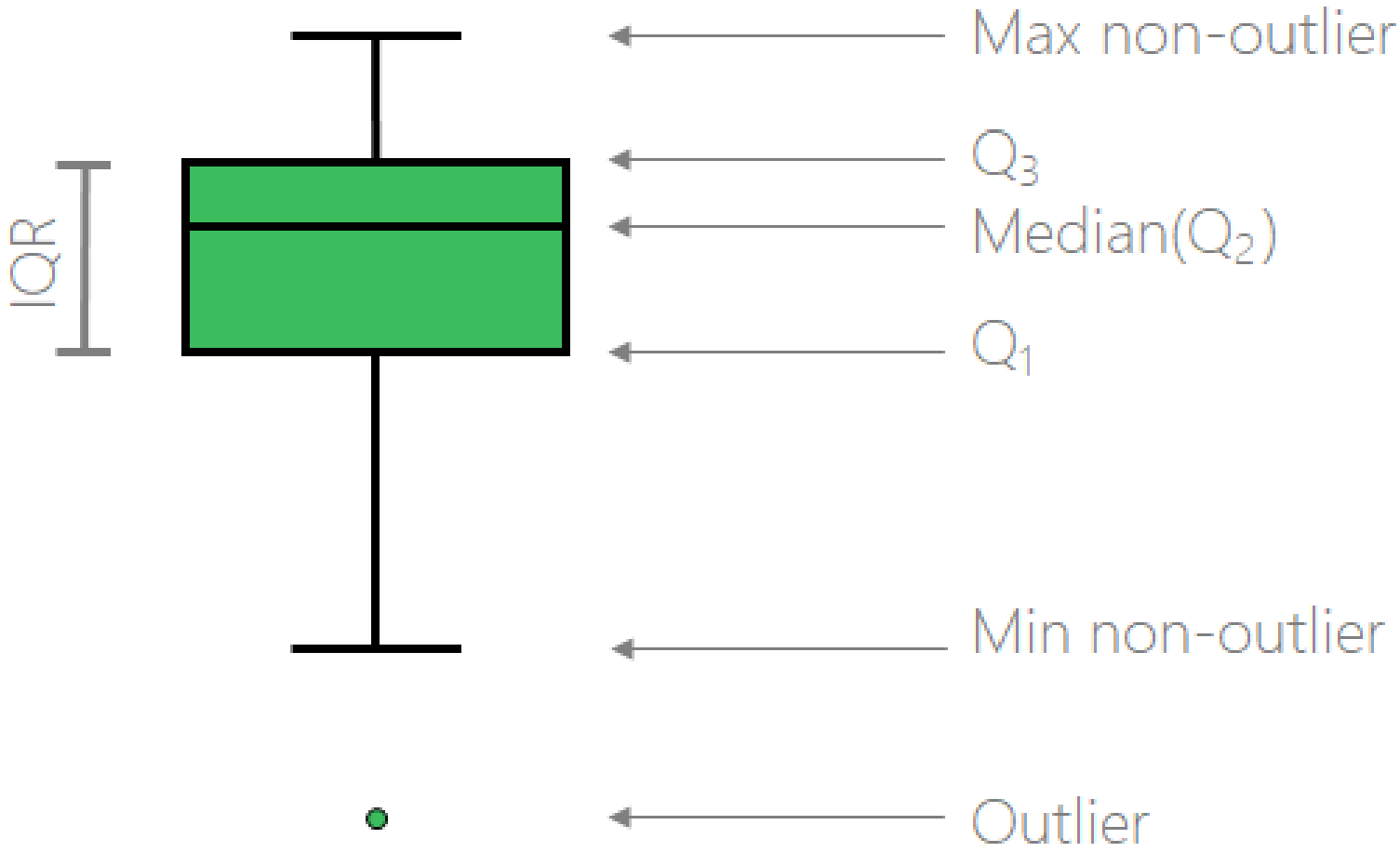
Central Tendency

For one-peak skewed density distribution, empirical formula :
$Mean - Mode = 3 \times (Mean - Median)$



Box Plot

Measure the dispersion of data



Metrics

- Proximity :
  - Similarity : range is $[0, 1]$
  - Dissimilarity : range is $[0, \infty]$, sometimes distance
- For nominal data, $d(\mathbf{x}_i, \mathbf{x}_j) = \frac{\sum_k I(x_{i,k} \neq x_{j,k})}{p}$; or one-hot encoding into Boolean data
- For Boolean data, symmetric distance $d(\mathbf{x}_i, \mathbf{x}_j) = \frac{r+s}{q+r+s+t}$ or Rand index $Sim_{Rand}(\mathbf{x}_i, \mathbf{x}_j) = \frac{q+t}{q+r+s+t}$; non-symmetric distance $d(\mathbf{x}_i, \mathbf{x}_j) = \frac{r+s}{q+r+s}$ or Jaccard index $Sim_{Jaccard}(\mathbf{x}_i, \mathbf{x}_j) = \frac{q}{q+r+s}$

		Sample j		
		1	0	sum
Sample i	1	q	r	$q+r$
	0	s	t	$s+t$
	sum	$q+s$	$r+t$	p

Metrics : Distance

- Example : Let $H = F = 1$ and $L = S = 0$, $d(LandRover, Jeep) = \frac{1+0}{4+1+0} = 0.20$, $d(LandRover, TOYOTA) = \frac{3+1}{1+3+1} = 0.80$, $d(Jeep, TOYOTA) = \frac{3+2}{1+3+2} = 0.83$
- Minkowski distance : $d(\mathbf{x}_i, \mathbf{x}_j) = \sqrt[h]{\sum_{k=1}^{p} |x_{ik} - x_{jk}|^h}$ is L_h-norm
  - Positive definiteness $d(\mathbf{x}_i, \mathbf{x}_j) \geqslant 0$ and "=" if and only if $i = j$;
  - Symmetry $d(\mathbf{x}_i, \mathbf{x}_j) = d(\mathbf{x}_j, \mathbf{x}_i)$;
  - Triangle inequality $d(\mathbf{x}_i, \mathbf{x}_j) \leqslant d(\mathbf{x}_i, \mathbf{x}_k) + d(\mathbf{x}_k, \mathbf{x}_j)$

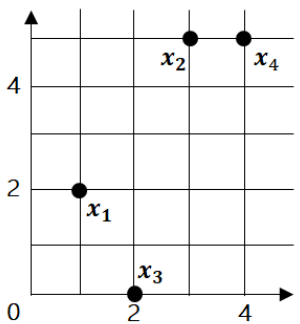
	Weight	Price	Acceleration	MPG	Quality	Sales Volume
Land Rover	H	H	F	H	H	L
Jeep	H	H	S	H	H	L
TOYOTA	L	L	F	L	H	H

		Jeep	
		1	0
Land Rover	1	$q = 4$	$r = 1$
	0	$s = 0$	$t = 1$

Metrics : Distance (Cont')

- Manhattan distance : $h = 1$, and $d(\mathbf{x}_i, \mathbf{x}_j) = \sum_{k=1}^{p} |x_{ik} - x_{jk}|$
- Euclidean distance : $h = 2$, and $d(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{\sum_{k=1}^{p} |x_{ik} - x_{jk}|^2}$
- Supremum distance : $h = \infty$, and $d(\mathbf{x}_i, \mathbf{x}_j) = \max_{k=1}^{p} |x_{ik} - x_{jk}|$

Point	Attr 1	Attr 2
x_1	1	2
x_2	3	5
x_3	2	0
x_4	4	5



L_1	x_1	x_2	x_3	x_4
x_1	0			
x_2	5	0		
x_3	3	6	0	
x_4	6	1	7	0

(a) Manhattan

L_2	x_1	x_2	x_3	x_4
x_1	0			
x_2	3.61	0		
x_3	2.24	5.1	0	
x_4	4.24	1	5.39	0

(b) Euclidean

L_∞	x_1	x_2	x_3	x_4
x_1	0			
x_2	3	0		
x_3	2	5	0	
x_4	3	1	5	0

(c) Supremum

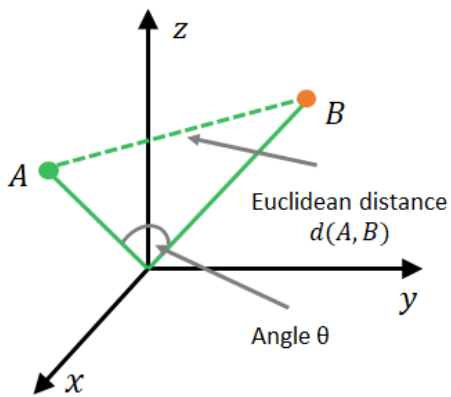
Metrics : Cosine Similarity

- Definition : $\cos(\mathbf{x}_i, \mathbf{x}_j) = \frac{\sum_{k=1}^{p} x_{ik} x_{jk}}{\sqrt{\sum_{k=1}^{p} x_{ik}^2} \sqrt{\sum_{k=1}^{p} x_{jk}^2}} = \frac{\mathbf{x}_i \cdot \mathbf{x}_j}{\|\mathbf{x}_i\| \|\mathbf{x}_j\|}$
- Example : $\cos(\mathbf{x}_1, \mathbf{x}_2) = 0.94$

Instance	Team	Coach	Hockey	Baseball	Soccer	penalty	Score	Win	Loss	Season
Instance 1	5	0	3	0	2	0	0	2	0	0
Instance 2	3	0	2	0	1	1	0	1	0	1

Euclidean vs. Cosine :

- Euclidean : measures the distance in absolute value, many applications
- Cosine : insensitive to absolute value, e.g., analyze users' interests based on movie ratings



Metrics : Other Distances

- For ordinal data, mapping the data to numerical data : $X = \{x_{(1)}, x_{(2)}, \ldots, x_{(n)}\}$, $x_{(i)} \mapsto \frac{i-1}{n-1} \in [0, 1]$
- For mixed type, use weighted distance with prescribed weights :

$$d(\mathbf{x}_i, \mathbf{x}_j) = \frac{\sum_{g=1}^{G} w_{ij}^{(g)} d_{ij}^{(g)}}{\sum_{g=1}^{G} w_{ij}^{(g)}}$$

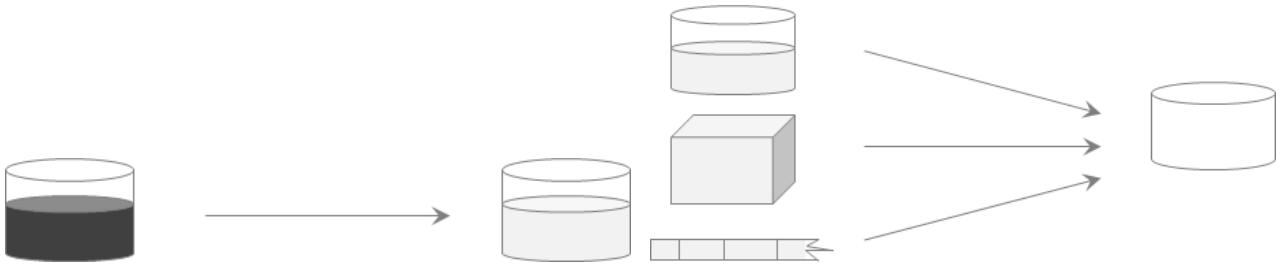
Put the attributes of the same type into groups, for each data type g, use the corresponding distance $d_{ij}^{(g)}$

Outlines

Why Data Preprocessing ?

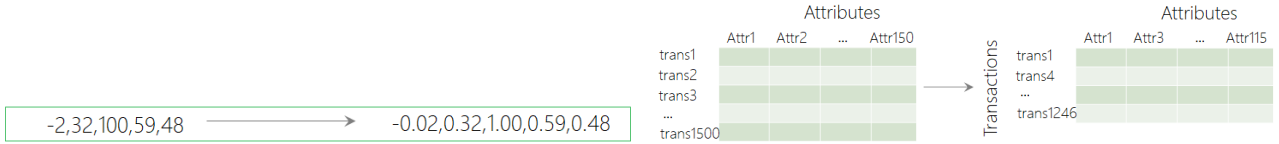
- Missing values
- Noisy with outliers
- Inconsistent representations
- Redundancy
- Errors may come during data input, data gathering, and data transferring
- Errors occur in about 5% of the data

Four Types of Data Preprocessing



(a) Data cleaning

(b) Data integration

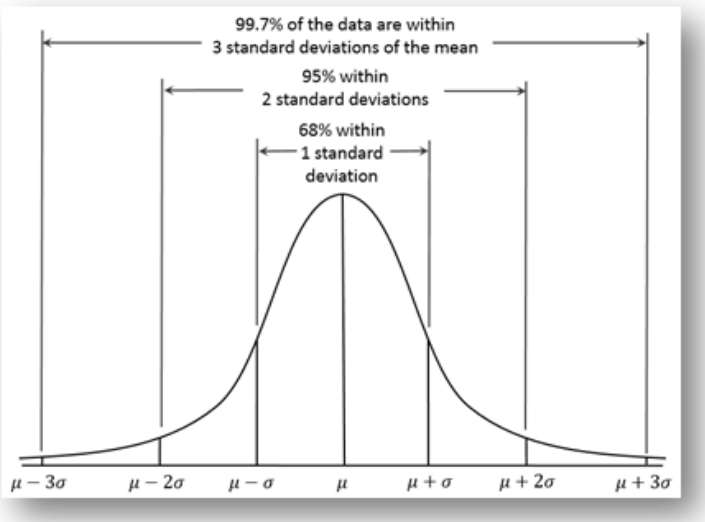


(c) Data conversion

(d) Data reduction

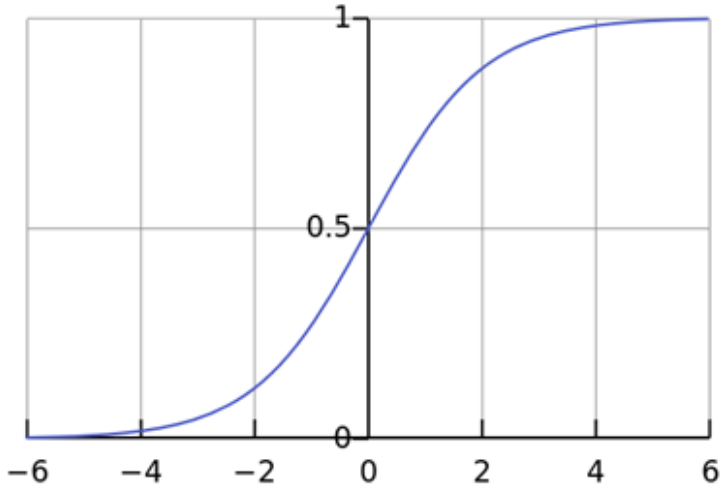
Data Scaling

- Why scaling :
  - For better performance : e.g., RBF in SVM and penalty in Lasso/ridge regression assume the zero mean and unit variance
  - Normalize different dimensions : many algorithms are sensitive to the variables with large variances, e.g., height (1.75m) and weight (70kg) in distance calculation
- Z-score scaling : $x_i^* = \frac{x_i - \hat{\mu}}{\hat{\sigma}}$, $\hat{\mu}$: sample mean, $\hat{\sigma}$: sample variance, applicable if max and min are unknown and the data distributes well



Data Scaling (Cont')

- 0-1 scaling : $x_i^* = \frac{x_i - \min_k x_k}{\max_k x_k - \min_k x_k} \in [0, 1]$, applicable for bounded data sets, need to recompute the max and min when new data arrive
- Decimal scaling : $x_i^* = \frac{x_i}{10^k}$, applicable for data varying across many magnitudes
- Logistic scaling : sigmoid transform $x_i^* = \frac{1}{1+e^{-x_i}}$, applicable for data concentrating nearby origin



Data Discretization

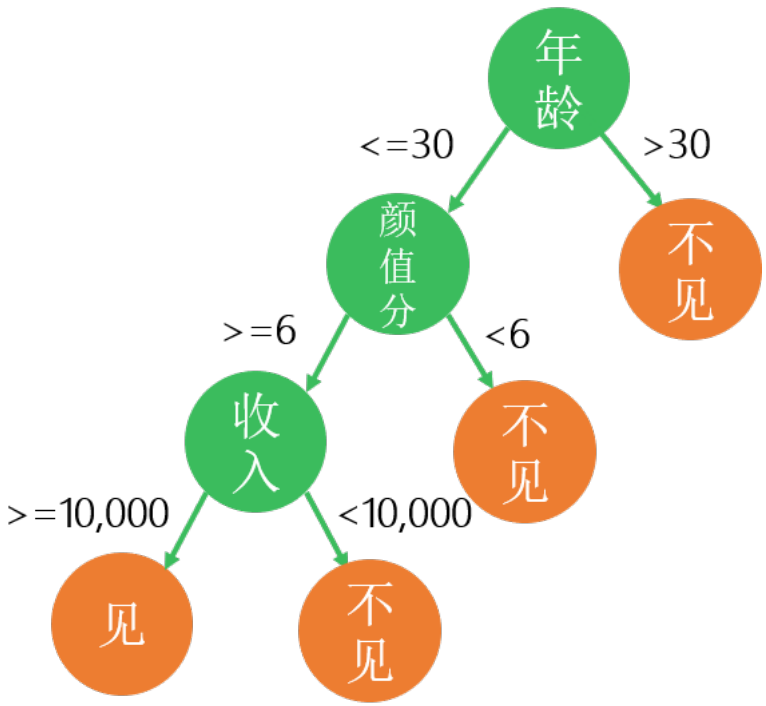
- Why discretization :
  - Improve the robustness : removing the outliers by putting them into certain intervals
  - For better interpretation
  - Reduce the storage and computational power
- Unsupervised discretization : equal-distance discretization, equal-frequency discretization, clustering-based discretization, 3σ-based discretization
- Supervised discretization : information gain based discretization, χ^2-based discretization

Unsupervised Discretization

- Equal-distance discretization : split the range to n intervals (bins) with the same length, group the data into each bin, sensitive to outliers
- Equal-frenquency discretization : group the data into n subset so that each subset has the same number of points, tend to separate samples with similar values and produce uniform distribution
- Clustering-based discretization : do hierarchical clustering and form a hierarchical structure (e.g., using K-Means), and put the samples in the same branch into the same interval (a natural example is family tree)
- 3σ-based discretization : put the samples into 8 intervals, need to take logarithm first

Supervised Discretization - Information Gain

- Top-down splitting, similar to create a decision tree
- Do a decision tree classification using information gain, find a proper splitting point for each continuous variable such that the information gain increases the most
- The final leaf nodes summarize the discrete intervals



Supervised Discretization - ChiMerge

- Bottom-up : similar to hierarchical clustering
- $\hat{\chi}^2$ statistics proposed by Karl Pearson, is used to test whether the observations dramatically deviate from theoretical distribution : $\hat{\chi}^2 = \sum_{i=1}^{k} \frac{(A_i - \mathbb{E}A_i)^2}{\mathbb{E}A_i} = \sum_{i=1}^{k} \frac{(A_i - np_i)^2}{np_i}$, where n_i is the number of samples in the i-th interval $A_i = [a_{i-1}, a_i]$ (frequency of observations), $\bigcup_{i=1}^{k} A_i$ covers the range of the variable, and $\mathbb{E}A_i = p_i$ is its expectation computed from the theoretical distribution ; it can be shown that $\hat{\chi}^2 \to \chi^2_{k-1}$
- ChiMerge : Given a threshold level t,
  1. Treat each value of the continuous variable as an interval and sort them in increasing order ;
  2. For each pair of adjacent intervals, compute its $\hat{\chi}^2$ statistics, if $\hat{\chi}^2 < t$, merge them into a new interval ;
  3. Repeat the above steps until no adjacent intervals can be merged.
- Two shortcomings : t is hard to set appropriately ; too long loop for large sample set, computationally intensive

ChiMerge : Iris Data Example

- $\hat{\chi}^2 = \sum_{i=1}^{m} \sum_{j=1}^{k} \frac{(A_{ij} - E_{ij})^2}{E_{ij}}$, where
  $m = 2$ (two adjacent intervals)
  k is the number of classes
  A_{ij} is the number of samples in i-th interval and in class k
  $R_i = \sum_{j=1}^{k} A_{ij}$ is the total number of samples in i-th interval
  $C_j = \sum_{i=1}^{m} A_{ij}$ is the total number of samples in class j
  $N = \sum_{i=1}^{m} \sum_{j=1}^{k} A_{ij}$ is the total number of samples
  $E_{ij} = R_i \cdot \frac{C_j}{N}$
- χ^2 of 4.3 and 4.4 : $C_1 = 4$, $C_2 = 0$, $C_3 = 0$, $N = 4$, $A_{11} = 1$, $A_{12} = A_{13} = 0$, $A_{21} = 3$, $A_{22} = A_{23} = 0$, $R_1 = 1$, $R_2 = 3$, $E_{11} = 1$, $E_{12} = E_{13} = 0$, $E_{21} = 3$, $E_{22} = E_{23} = 0$, $\hat{\chi}^2 = 0$.

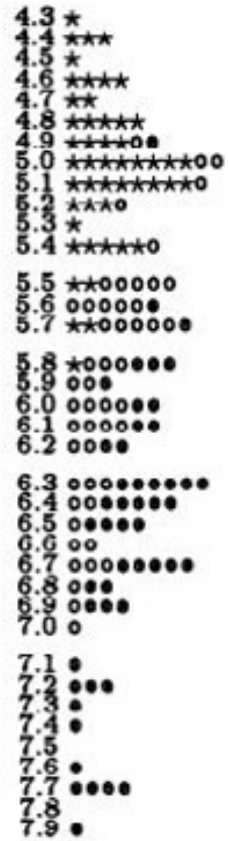


FIGURE: Sepal lengths of 3 types of iris

ChiMerge Results

Left : significance level is 0.5 and the threshold for χ^2 is 1.4 ;
Right : significance level is 0.9 and the threshold for χ^2 is 4.6 ;
The final results keep the intervals with χ^2 larger than the thresholds

Int	Class frequency			χ^2
4.3	16	0	0	4.1
4.9	4	1	1	2.4
5.0	25	5	0	8.6
5.5	2	5	0	2.9
5.6	0	5	1	1.7
5.7	2	5	1	1.8
5.8	1	3	3	2.2
5.9	0	12	7	4.8
6.3	0	6	15	4.1
6.6	0	2	0	3.2
6.7	0	5	10	1.5
7.0	0	1	0	3.6
7.1	0	0	12	

Int	Class frequency			χ^2
4.3	45	6	1	30.9
5.5	4	15	2	6.7
5.8	1	15	10	4.9
6.3	0	14	25	5.9
7.1	0	0	12	

Figure 2: ChiMerge discretizations for *sepal-length* at the .50 and .90 significance levels ($\chi^2 = 1.4$ and 4.6)

Data Redundancy

- When strong correlations exist among different attributes, then we say that the some attributes can be derived from the others (Recall linear dependency for vectors)
- E.g., two attributes "Age" and "Birthday", then "Age" can be calculated from "Birthday"
- Determine the data redundancy by correlation analysis
- For continuous variables A and B, compute the correlation coefficient $\rho_{A,B} = \frac{\sum_{i=1}^{k}(a_i-\bar{A})(b_i-\bar{B})}{k\hat{\sigma}_A\hat{\sigma}_B} \in [-1,1]$:
  1. If $r > 0$, A and B are positively correlated ;
  2. If $r < 0$, A and B are negatively correlated ;
  3. If $r = 0$, A and B are uncorrelated.

  Note that the correlation between A and B does not imply the causal inference.
- For discrete variables A and B, compute the χ^2 statistics : large $\hat{\chi}^2$ value implies small correlation

Missing Data

- Where missing data come from ?
  - Missing Completely At Random (MCAR) : the occurrence of missing data is a random event
  - Missing At Random (MAR) : depending on some control variables, e.g., the age > 20 is not acceptable in an investigation for teenager and thus is replaced by MAR
  - Missing Not At Random (MNAR) : missing data for bad performed employees after they are fired

Simple Methods

- Deleting samples : for small size of samples with missing values
- Deleting variables : for series missing values in variables

gradyear	gender	age	friends
2006	M	18.98	7
2006	F	18.801	0
2006	M	18.335	69
2006	F	18.875	0
2006	NA	18.995	10
2006	F		142
2006	F	18.93	72
2006	M	18.322	17
2006	F	19.055	52
2006	F	18.708	39
2006	F	18.543	8
2006	F	19.463	21
2006	F	18.097	87
2006	NA		0
2006	F	18.398	0
2006	NA		0
2006	NA		135
2006	F	18.987	26
2006	F	17.158	27
2006	F	18.497	123
2006	F	18.738	35

Filling Methods

- Filling with zero
- Filling with means for numerical type, and with modes for non-numerical type, applicable for MCAR ; drawback : concentrating in the mean and underestimating the variance ; solution : filling in different groups
- Filling with similar variables : auto-correlation is introduced
- Filling with past data
- Filling by K-Means : Compute the pairwise distances of the data using good variables (no missing values), then fill the missing values with the mean of the first K most similar good data, auto-correlation is introduced
- Filling with Expectation-Maximization (EM) : introduce hidden variables and use MLE to estimate the parameters (missing values)

Filling Methods (Cont')

- Random filling :
  - Bayesian Bootstrap : for discrete data with range $\{x_i\}_{i=1}^{k}$, randomly sample $k-1$ numbers from $U(0,1)$ as $\{a_{(i)}\}_{i=0}^{k}$ with $a_{(0)}=0$ and $a_{(k)}=1$; then randomly sample from $\{x_i\}_{i=1}^{k}$ with probability distribution $\{a_{(i)}-a_{(i-1)}\}_{i=1}^{k}$ accordingly to fill in the missing values
  - Approximate Bayesian Bootstrap: Sample with replacement from $\{x_i\}_{i=1}^{k}$ to form new data set $X^*=\{x_i^*\}_{i=1}^{k^*}$; then randomly sample n values from X^* to fill in the missing values, allowing for repeatedly filling missing values
- Model based methods : treat missing variable as y, other variables as $\mathbf{x}$; take the data without missing values as our training set to train a classification or regression model ; take the data with missing values as our test set to predict the miss values

Filling by Interpolation

- For the data of numeric type, each attribute (column vector) can be viewed as the function values $z_i = f(x_i)$ at the points x_i, where x_i is a reference attribute (the reference attribute usually has no missing values, it can be chosen as the index)
- We can interpolate a function f using the existing values (x_i, z_i), and then fill in the missing values z_k with $f(x_k)$
- Linear interpolation : treat $z = f(x)$ as linear function between the neighboring points x_{k-1} and x_{k+1} of x_k
- Lagrange interpolation : interpolate the $m+1$ existing values $\{(x_{l_i}, z_{l_i})\}_{i=1}^{m+1}$ by a degree m polynomial $L_m(x)$

```
gen_data.interpolate()
```

	feature1	feature2	feature3
1	1.728534	-0.371519	1.451700
2	0.795975	-1.067026	-1.861944
3	-0.030449	-0.050409	1.299994
4	-0.856872	0.966208	0.987861

Missing value

Missing value

Special Values and Dummy Variables

- In Python, "np.nan" means missing values (Not a Number, missing float value)
- "None" is a Python object, used to represent missing values of the object type
- Dummy variables : e.g., missing values in gender ("Male" or "Female"), then define a third value "unknown" for the missing values

```
import pandas as pd
import numpy as np

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

print teenager_sns['gender'].value_counts()

teenager_sns['gender'] = teenager_sns['gender'].replace(np.NaN, 'unknown')

print ""
print "哑变量方法处理后：\n"
print teenager_sns['gender'].value_counts()
```

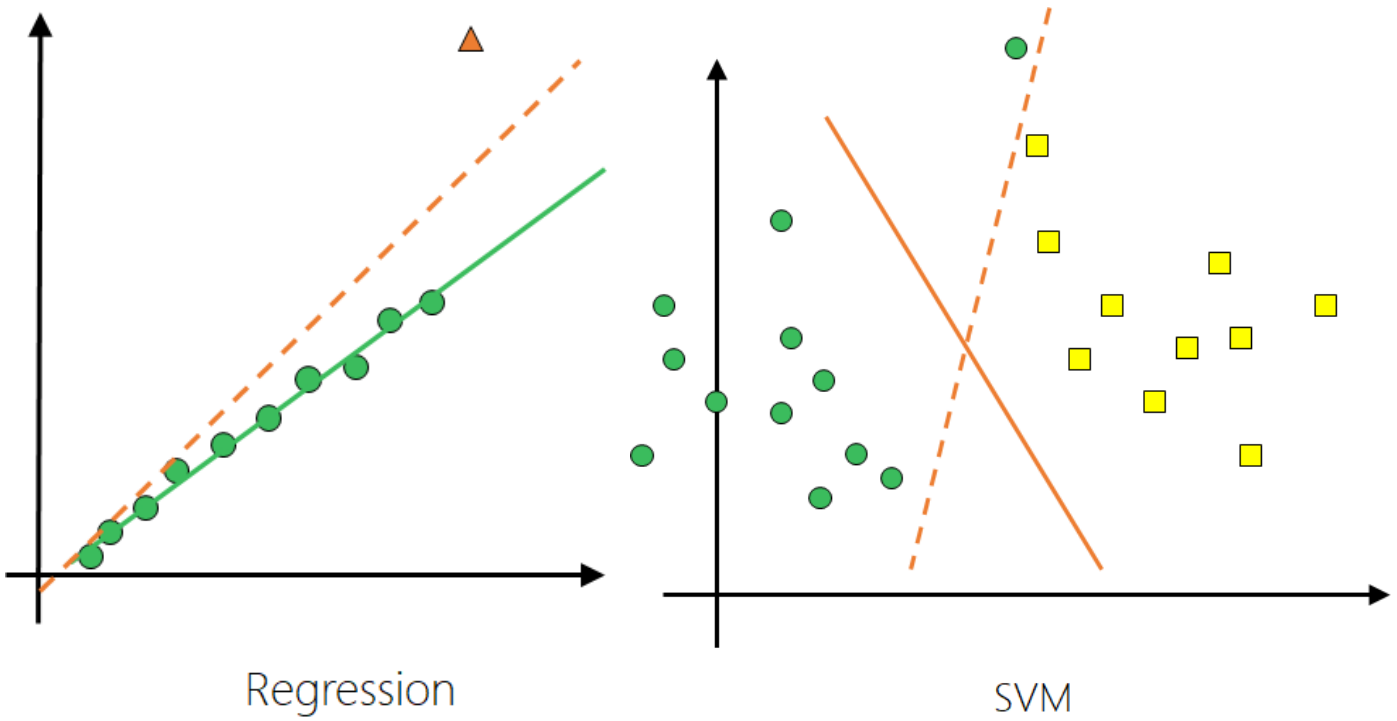
```
F    22054
M     5222
Name: gender, dtype: int64

哑变量方法处理后：

F          22054
M           5222
unknown     2724
Name: gender, dtype: int64
```

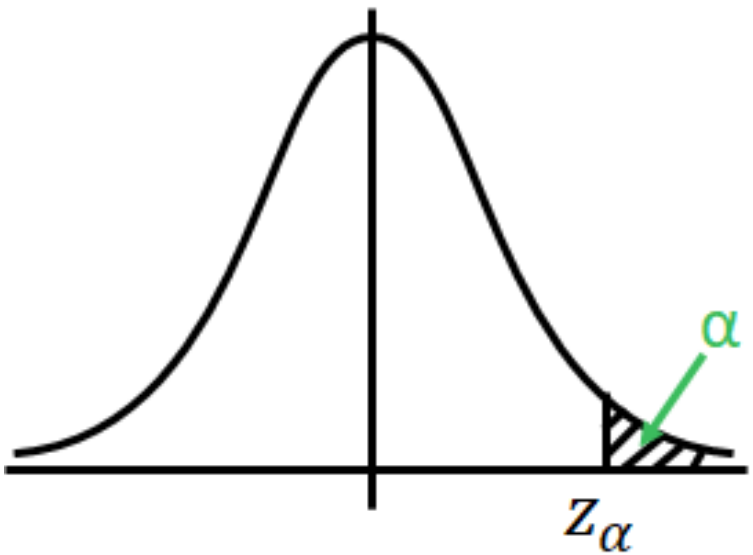
Outliers

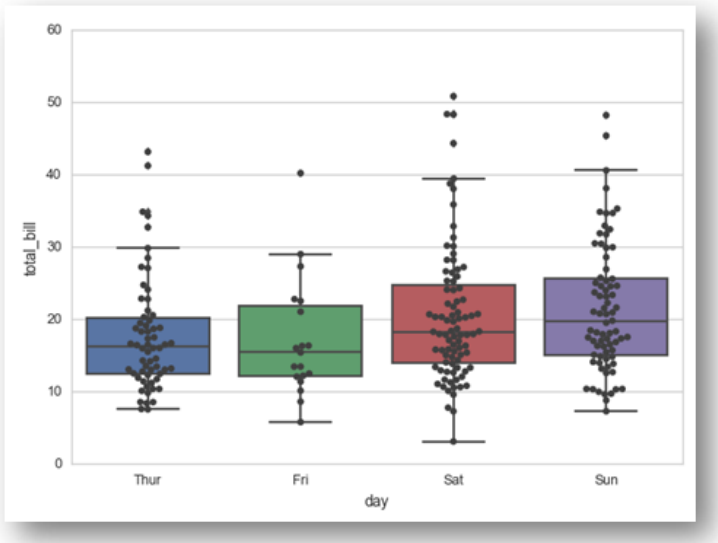
- Outliers : the data points seem to come from different distribution, or noisy data
- Outlier detection : unsupervised, e.g., Credit cheating detection, medical analysis, and information security, etc.



Outliers Detection - Statistics Based Methods

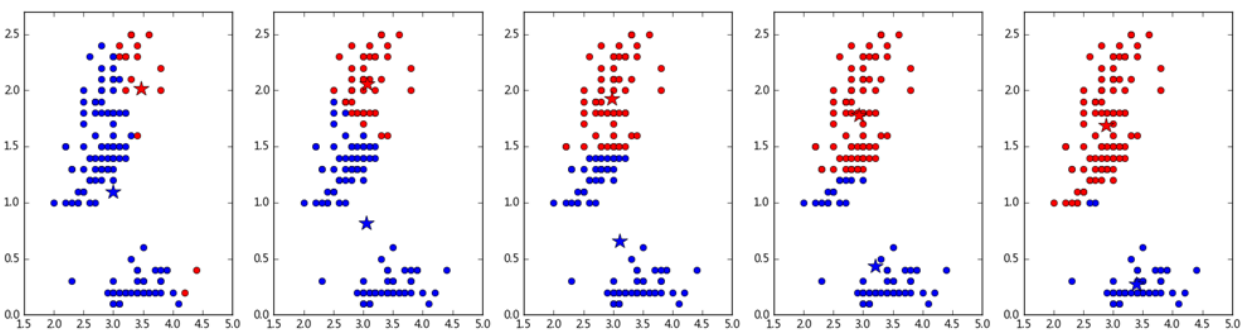
- The samples outside the upper and lower α-quantile for some small α (usually 1%)
- Observe from box plot
- 3σ-rule in 1D : the sample x with $x^*_{Z-score} > 3$ is an outlier

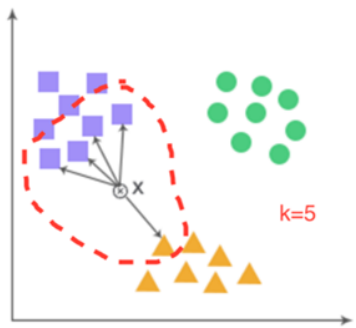




Outliers Detection - Distance Based Methods

- K-means : run K-means clustering first, and then select the farthest m points from their centers as outliers
- KNN : run KNN first, and then select the points that are far from their K nearest neighbors (distance $> C$) as outliers

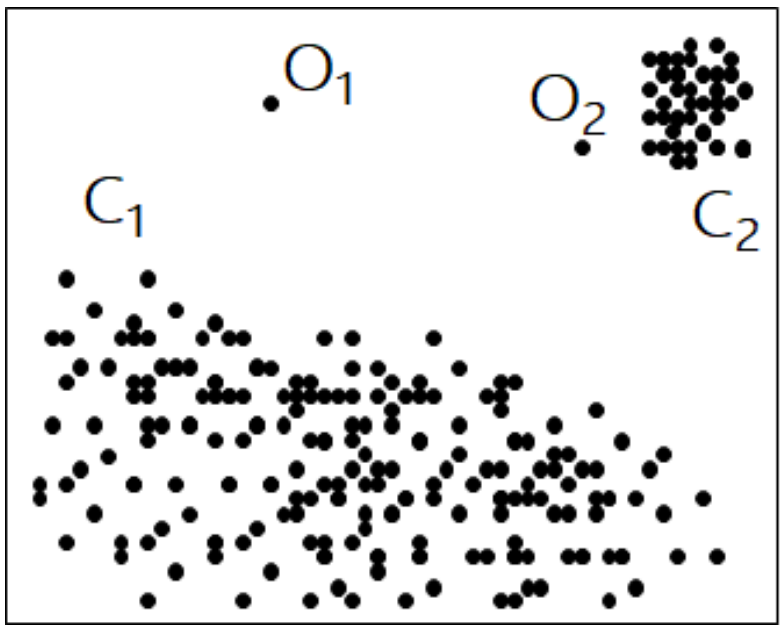




Outliers Detection - Local Outlier Factor

Local Outlier Factor (LOF) is a density based method :

1. We could compute the density at each position $\mathbf{x}$, e.g., $p(\mathbf{x})$ (how to define the density if we only have data samples) ;
2. We could compare the density of each point $\mathbf{x}$ with the density of its neighbors, i.e., compare $p(\mathbf{x})$ with $p(\mathbf{x}_k)$ where $\mathbf{x}_k$ is close to $\mathbf{x}$ (in a neighborhood of $\mathbf{x}$, but how to define the neighborhood)



Computing Density by Distance

Some definitions :

- $d(A, B)$: distance between A and B ;
- $d_k(A)$: k-distance of A, or the distance between A and the k-th nearest point from A
- $N_k(A)$: k-distance neighborhood of A, or the points within $d_k(A)$ from A ;
- $rd_k(B, A)$: k-reach-distance from A to B, the repulsive distance from A to B as if A has a hard-core with radius $d_k(A)$, $rd_k(B, A) = \max\{d_k(A), d(A, B)\}$; note that $rd_k(A, B) \neq rd_k(B, A)$, which implies that k-reach-distance is not symmetric.

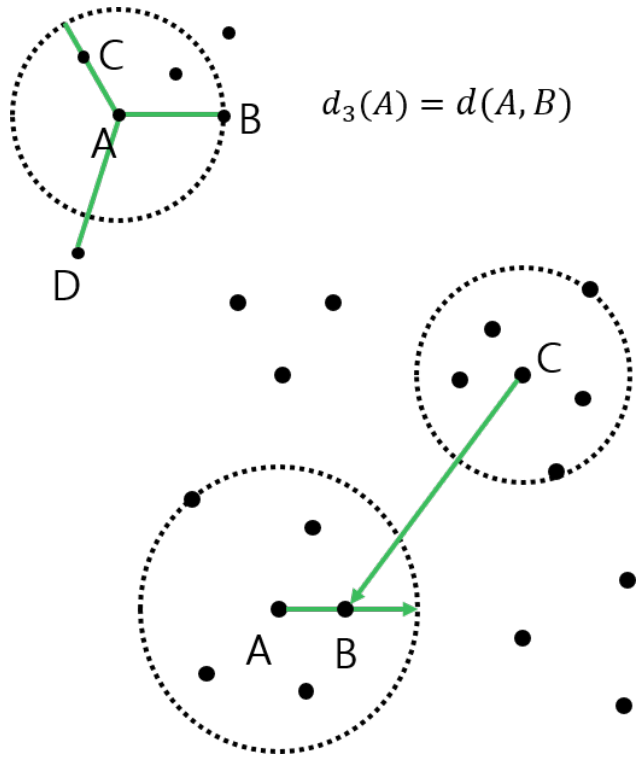
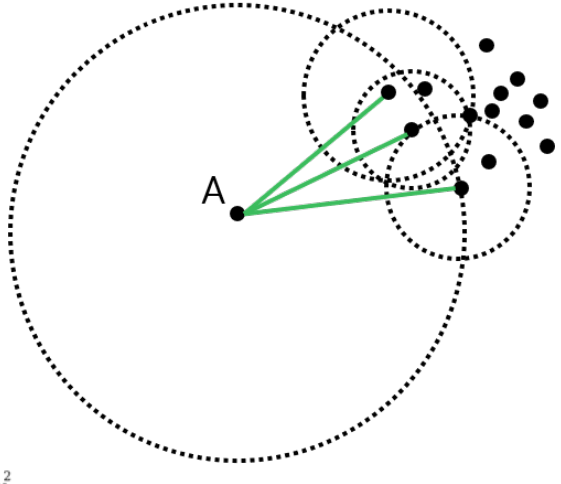


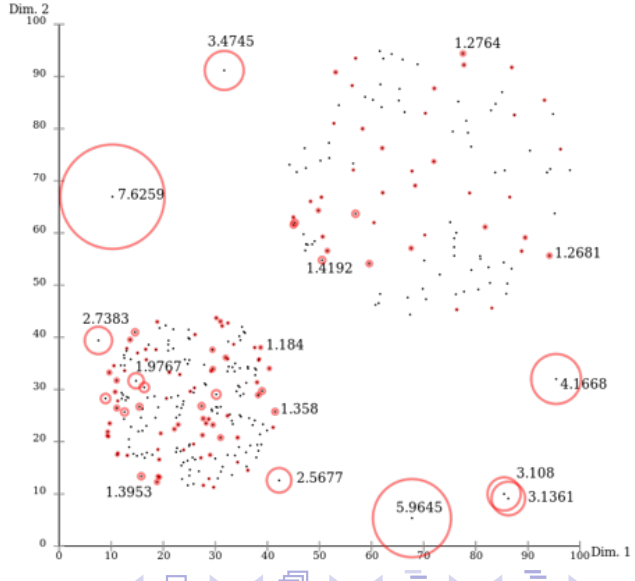
FIGURE: $rd_5(B, A) = d_5(A)$ and $rd_5(B, C) = d(B, C)$

Local Outlier Factor

Some definitions :

- $lrd_k(A)$: local reachability density is inversely proportional to the average distancep, $lrd_k(A) = 1/\left(\frac{\sum_{O \in N_k(A)} rd_k(A,O)}{|N_k(A)|}\right)$; intuitively, if for most $O \in N_k(A)$, more than k points are closer to O than A is, then the denominator is much larger than $d_k(A)$ and $lrd_k(A)$ is small ; e.g., $k = 3$ in the figure
- $LOF_k(A)$: local outlier factor, $LOF_k(A) = \frac{\sum_{O \in N_k(A)} \frac{lrd_k(O)}{lrd_k(A)}}{|N_k(A)|}$;
- $LOF_k(A) \ll 1$, the density of A is locally higher, dense point ; $LOF_k(A) \gg 1$, the density of A is locally lower, probably outlier





Further topics

- Other methods for outlier detection :
  - Isolation Forest : small path length (normally distributed) in a random forest (`sklearn.ensemble.Isolation`)
  - One-class support vector machine : classification as 1 (normal) vs. -1 (outlier) (`sklearn.svm.OneClassSVM`)
  - Robust covariance : based on Gaussian assumption, 3σ rule in high dimensions (`sklearn.covariance.EllipticEnvelope`)
- Outlier processing :
  - Delete outliers (treat them as missing values)
  - Robust regression : e.g., Theil-Sen regression, select the median of all possible slopes in two-point linear regression