Machine Learning
Data preparation

1

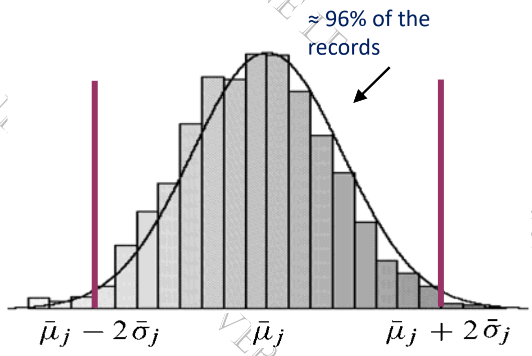
Incomplete data

- Elimination
- Inspection
- Identification
- Replacement
  - mean value of the attribute
  - mean value of the attribute for the same target class
  - value estimated using statistical inference

2

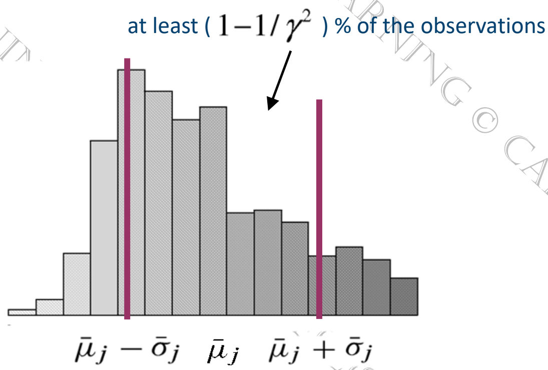
Noisy data

DISPERSION $\bar{\mu}_j \pm z_{\alpha/2}\bar{\sigma}_j$

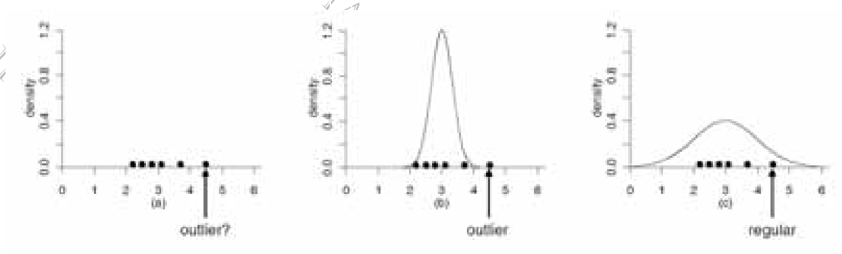


Noisy data

a percentage at least $1-1/\gamma^2$ of the observations, with $\gamma > 1$, falls in the interval $(\bar{\mu} \pm \gamma\bar{\sigma})$ (TCHEBYSHEFF theorem)



z-index method for outlier detection

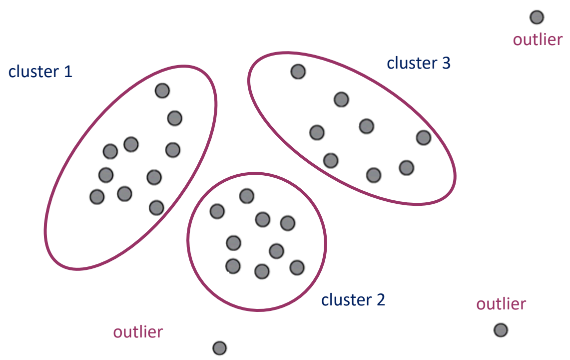


$$z_{ij}^{ind} = \frac{x_{ij} - \bar{\mu}_j}{\bar{\sigma}_j}$$

$$\left| z_i^{ind} \right| > 3$$

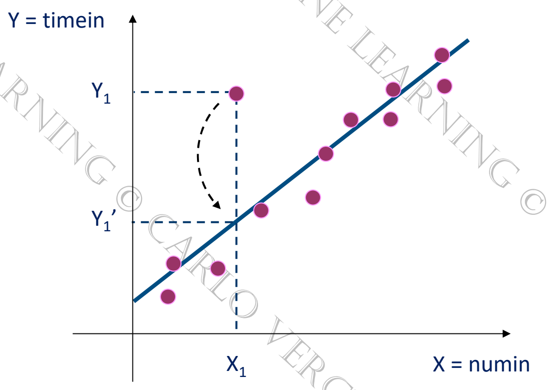
$$\left| z_i^{ind} \right| \gg 3$$

Noisy data



evaluate "density" in a neighborhood of a record: a record is an outlier if a percentage *p* of the records falls at a distance greater than *d*

Noisy data



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Data transformation

DECIMAL SCALING $$x'_{ij} = \frac{x_{ij}}{10^h}$$

MIN-MAX method

$$x'_{ij} = \frac{x_{ij} - x_{min,j}}{x_{max,j} - x_{min,j}}(x'_{max,j} - x'_{min,j}) + x'_{min,j}$$

Z-INDEX method $$x'_{ij} = \frac{x_{ij} - \bar{\mu}_j}{\bar{\sigma}_j}$$

8

Data standardization example

numout	decimal scaling	min-max method	z-index method
45	0.045	0.295	-0.006
20	0.02	0.078	-0.023
69	0.069	0.504	-0.01
66	0.066	0.478	0.008
11	0.011	0	-0.029
42	0.042	0.269	-0.008
126	0.126	1	0.049

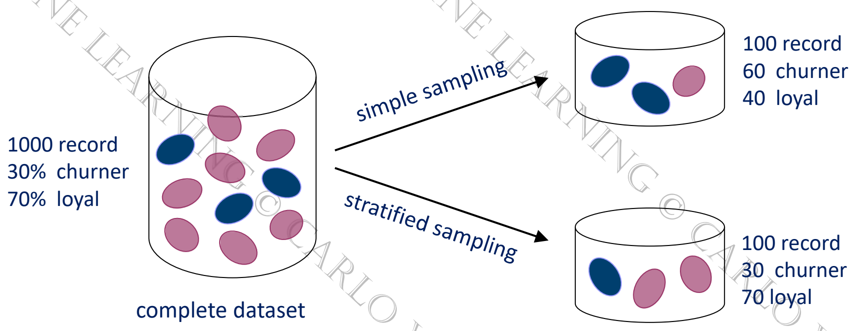
original values

Data reduction

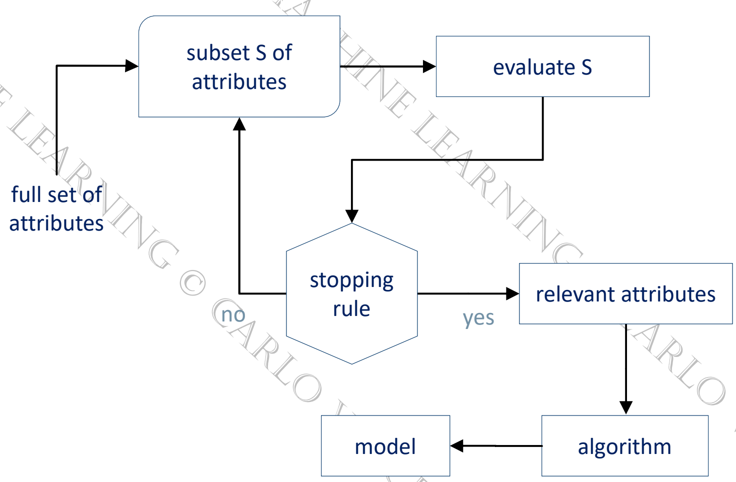
- improve efficiency in model identification
- preserve model accuracy
- achieve simpler models

- record reduction by SAMPLING
- attribute reduction by SELECTION or PROJECTION
- values reduction by DISCRETIZATION or AGGREGATION

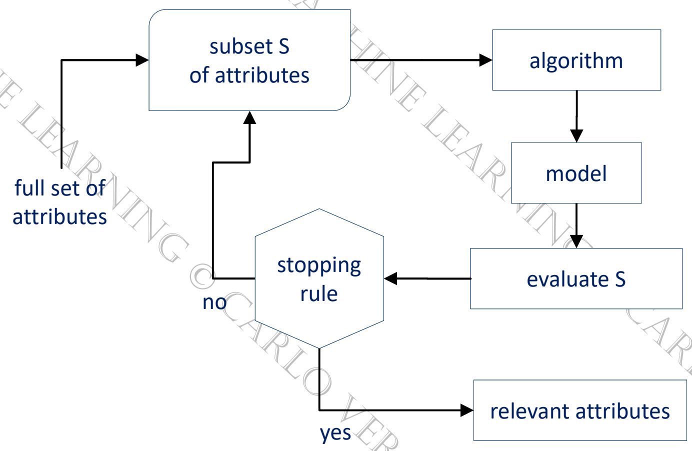
Dataset reduction



Attribute selection: filter methods

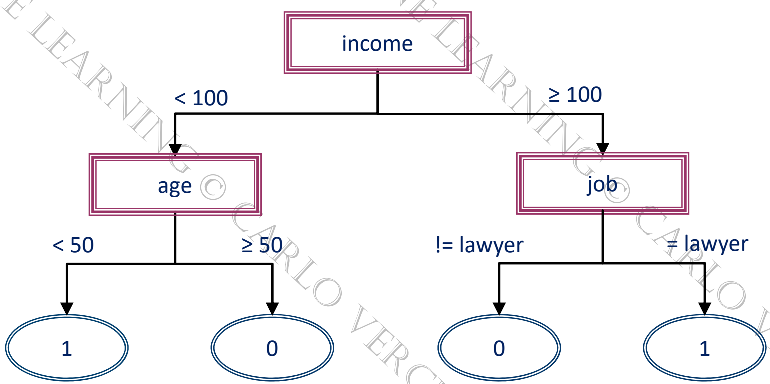


Attribute selection: wrapper methods



Attribute selection: embedded methods

Set of attributes: {age, sex, education, income, job}
Target: life insurance policy (class = 1)



Attribute selection

Given a dataset with n attributes, how many subsets to evaluate? ….2^n

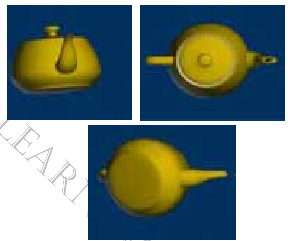
subset S
of attributes

full set of
attributes

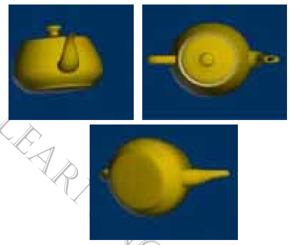
greedy search scheme:

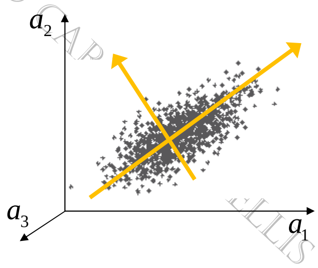
- FORWARD
- BACKWARD
- FORWARD-BACKWARD

Principal component analysis



Principal component analysis





Principal component analysis

- Principal component analysis (PCA) is the oldest and most popular technique of attribute reduction by means of projection.
- The n original attributes are replaced by n new attributes (principal components) obtained as a linear combination of the original ones.
- Principal components are generated in sequence by means of an iterative algorithm:
  - the first component is determined by solving an appropriate optimization problem, in order to explain the highest percentage of variation in the data.
  - at each iteration the next principal component is selected, among vectors orthogonal to components already determined, as the one which explains the maximum percentage of variance not yet explained by the previously generated components.
- In most cases, q principal components, with $q < n$, have information content almost equivalent to the original attributes.

Principal component analysis

$\mathbf{V} = \mathbf{X}'\mathbf{X}$ COVARIANCE matrix of data, after standardization: $\tilde{x}_{ij} = x_{ij} - \frac{1}{m}\sum_{i=1}^{m} x_{ij}.$

The principal components are obtained as linear combinations of the original variables:

$$\mathbf{p}_j = \mathbf{X}\mathbf{w}_j$$

where the coefficients $\mathbf{w}_j$ have to be determined.

The variance of the projection $\mathbf{w}_j'\mathbf{x}_i$ can be calculated as:

$$\begin{aligned} \mathrm{E}[\mathbf{w}_j'\mathbf{x}_i - \mathrm{E}[\mathbf{w}_j'\mathbf{x}_i]]^2 &= \mathrm{E}[(\mathbf{w}_j'(\mathbf{x}_i - \mathrm{E}[\mathbf{x}_i]))^2] \\ &= \mathbf{w}_j' \,\mathrm{E}[(\mathbf{x}_i - \mathrm{E}[\mathbf{x}_i])'(\mathbf{x}_i - \mathrm{E}[\mathbf{x}_i])]\mathbf{w}_j \\ &= \mathbf{w}_j'\mathbf{V}\mathbf{w}_j. \end{aligned}$$

Principal component analysis

The FIRST PRINCIPAL COMPONENT $\mathbf{p}_j = \mathbf{X}\mathbf{w}_j$ is obtained by solving an optimization problem

$$\max_{\mathbf{w}_1} \ \{ \mathbf{w}_1'\mathbf{V}\mathbf{w}_1 : \mathbf{w}_1'\mathbf{w}_1 = 1\}$$

It can be shown that:

the vector that solves the problem is the eigenvector $\mathbf{u}_1$ associated to the largest eigenvalue λ_1 of the covariance matrix $\mathbf{V}$

the eigenvalue λ_1 is equal to the amount of explained variance

The SECOND PRINCIPAL COMPONENT is obtained by solving a similar optimization problem with the additional condition

$$\mathbf{w}_2'\mathbf{w}_1 = 0$$

Principal component analysis

$$\max_{\mathbf{w}_1} \; \{ \mathbf{w}_1' \mathbf{V} \mathbf{w}_1 : \mathbf{w}_1' \mathbf{w}_1 = 1 \}$$

Lagrangean function

$$L(\mathbf{w}_1, \lambda_1) = \mathbf{w}_1' \mathbf{V} \mathbf{w}_1 - \lambda_1 (\mathbf{w}_1' \mathbf{w}_1 - 1)$$

KKT conditions

$$\frac{\partial L(\mathbf{w}_1, \lambda_1)}{\partial \mathbf{w}_1} = 2\mathbf{V}\mathbf{w}_1 - 2\lambda_1 \mathbf{w}_1 = \mathbf{0},$$
$$\frac{\partial L(\mathbf{w}_1, \lambda_1)}{\partial \lambda_1} = 1 - \mathbf{w}_1' \mathbf{w}_1 = 0.$$

$$\Rightarrow \quad (\mathbf{V} - \lambda_1 \mathbf{I}) \mathbf{w}_1 = \mathbf{0}.$$

This implies

$$\mathbf{w}_1' \mathbf{V} \mathbf{w}_1 = \lambda_1 \mathbf{w}_1' \mathbf{w}_1 = \lambda_1 \mathbf{u}_1' \mathbf{u}_1 = \lambda_1$$

$$\mathbf{p}_j = \mathbf{X} \mathbf{u}_j$$

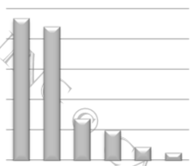
Principal component analysis

How many principal component to consider?

percentage of explained variance

$$I_q = \frac{\lambda_1 + \lambda_2 + \cdots + \lambda_q}{\lambda_1 + \lambda_2 + \cdots + \lambda_n}$$

scree-plot

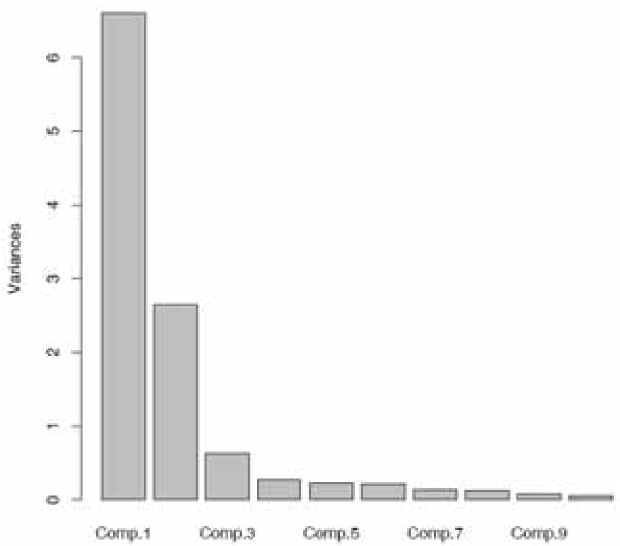


Principal component analysis

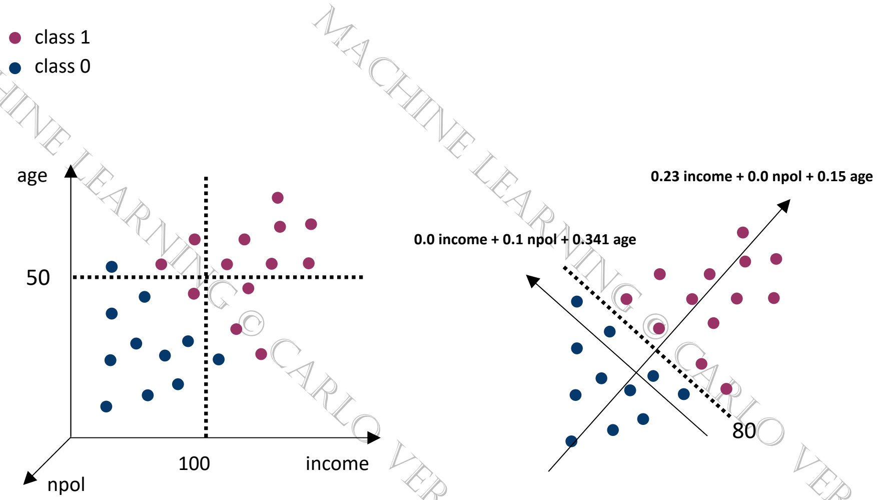
	Comp.1	Comp.2	Comp.3	Comp.4	Comp.5	Comp.6
mpg	0.363	-0.226	-0.103	-0.109	0.368	0.754
cyl	-0.374	-0.175	0.169	0.231	-0.846	
disp	-0.368	0.257	-0.394	-0.336	0.214	0.198
hp	-0.33	-0.249	0.14	-0.54	0.222	-0.576
drat	0.294	-0.275	0.161	0.855	0.244	-0.101
wt	-0.346	0.143	0.342	0.246	-0.465	0.359
qsec	0.2	0.463	0.403	0.165	-0.33	0.232
vs	0.307	0.232	0.429	-0.215	-0.6	0.194
am	0.235	-0.429	-0.206	-0.571	-0.587	-0.178
gear	0.207	-0.462	0.29	-0.265	-0.244	0.605
carb	-0.214	-0.414	0.529	-0.127	0.361	0.184

	Comp.7	Comp.8	Comp.9	Comp.10	Comp.11
mpg	0.236	0.139			0.125
cyl					0.141
disp					-0.661
hp	0.248				0.256
drat					
wt					0.567
qsec	-0.528	-0.271			-0.181
vs	-0.266	0.359	-0.159		
am					
gear	-0.336	-0.214			
carb	-0.175	0.396	0.171		-0.32

Principal component analysis



Principal component analysis



Customer Satisfaction Analysis

A survey in order to evaluate 20 different healthcare structures. 2000 customers have evaluated, with a 1-10 scale, each of six features of the service:

1. Courtesy
2. Clarity
3. Competence
4. Condition (of the structure)
5. Promptness (of the service)
6. Opening times

The following table shows the average results for each structure and each variable:

Structure	Courtesy	Clarity	Competence	Condition	Promptness	Opening times
A	7	5	9	8	6	7
B	5	6	8	4	4	6
C	5	5	8	7	7	7
D	6	6	9	7	6	7
E	7	5	10	4	3	6
F	6	4	8	4	5	6
G	5	6	9	4	3	5
H	5	5	8	5	4	6
I	4	4	7	7	5	6
L	5	5	8	7	6	7

Customer Satisfaction Analysis

	Courtesy	Clarity	Competence	Condition	Promptness	Opening.times
Courtesy	1.0000000	0.54586083	0.694808334	-0.115503469	0.00000000	0.1430140
Clarity	0.5458608	1.00000000	0.544426373	-0.081651741	0.04523081	0.1010995
Competence	0.6948083	0.54442637	1.000000000	0.003778134	-0.05860090	-0.1216282
Condition	-0.1155035	-0.08165174	0.003778134	1.000000000	0.71911387	0.4394498
Promptness	0.0000000	0.04523081	-0.058600904	0.719113873	1.00000000	0.7982825
Opening.times	0.1430140	0.10109950	-0.121628193	0.439449764	0.79828247	1.0000000

Relevant values of correlation among our variables

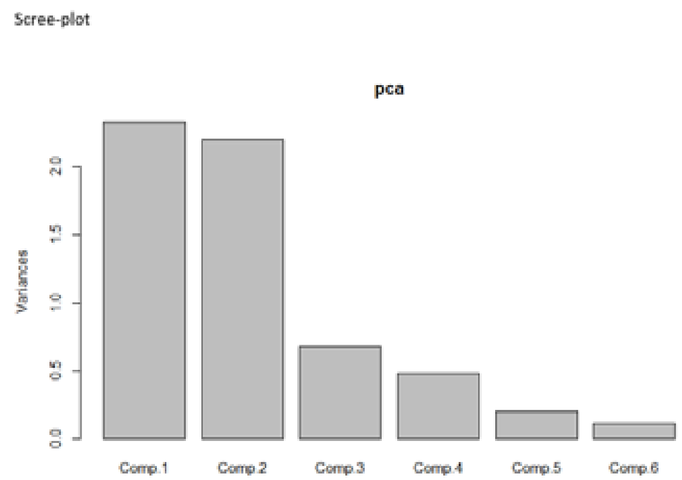
Customer Satisfaction Analysis

Importance of components:

	PC1	PC2	PC3	PC4	PC5	PC6
Standard deviation	1.5257	1.4824	0.8224	0.69466	0.45322	0.33260
Proportion of Variance	0.3879	0.3662	0.1127	0.08043	0.03423	0.01844
Cumulative Proportion	0.3879	0.7542	0.8669	0.94733	0.98156	1.00000

The first two components account for about 75% of the variance.

Customer Satisfaction Analysis



Customer Satisfaction Analysis

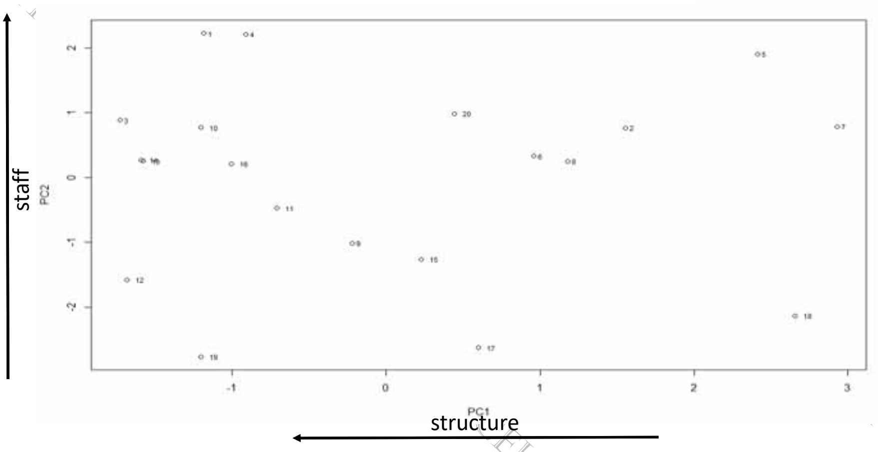
$$Y_1 = 0.1086X_1 + 0.0830X_2 + 0.1663X_3 - 0.5278X_4 - 0.6168X_5 - 0.5428X_6$$

$$Y_2 = 0.5869X_1 + 0.5389X_2 + 0.5621X_3 - 0.0515X_4 - 0.1356X_5 - 0.1678X_6$$

Customer Satisfaction Analysis

	PC1	PC2	PC3	PC4	PC5	PC6
[1,]	-1.1828628	2.2263798	-0.22186202	-0.91961937	-0.62306953	-0.028256138
[2,]	1.5546960	0.7654794	0.78344001	0.86684190	0.09347771	0.083846308
[3,]	-1.7240532	0.8856652	0.23333559	0.09592982	0.44168534	-0.549643694
[4,]	-0.9068263	2.2086511	0.27104063	0.28268453	-0.01769527	0.015156363
[5,]	2.4116996	1.9021137	0.13642506	-1.12399068	-0.19231098	0.556696687
[6,]	0.9589090	0.3290325	0.41935059	-1.18921989	0.09996898	-0.744915764
[7,]	2.9310884	0.7865377	-0.26154565	1.01955216	0.01685012	0.044668363
[8,]	1.1803912	0.2520779	0.17838250	0.15112222	-0.01811239	0.224943955
[9,]	-0.2186553	-1.0141899	-0.57707610	0.12265701	-0.04730614	-0.032665186
[10,]	-1.1967878	0.7697211	0.21721841	0.07567853	0.20680405	0.069612607
[11,]	-0.7035076	-0.4727002	1.47351814	0.28010514	-0.98973584	0.182605173
[12,]	-1.6784426	-1.5770088	0.22172883	-0.82491768	0.16201852	-0.005985052
[13,]	-1.5710926	0.2563197	-0.38783911	-0.64004115	0.09521395	0.210710254
[14,]	-1.5859659	0.2669501	-0.25381324	0.64140750	0.45630104	0.407718213
[15,]	0.2299627	-1.2612263	0.99588496	0.96178037	-0.49539272	-0.562470476
[16,]	-1.0041463	0.2102320	0.46394032	0.48311800	0.94487539	0.100527297
[17,]	0.6004681	-2.6257821	0.07073805	-0.26288977	0.43088624	0.333856443
[18,]	2.6569484	-2.1303118	-0.14433919	-0.75505323	0.34904884	-0.197022566
[19,]	-1.1987349	-2.7624412	-1.04413849	0.17521472	-0.71336311	0.211425882
[20,]	0.4469118	0.9845000	-2.57438929	0.55963983	-0.20014418	-0.320808668

Customer Satisfaction Analysis



Data discretization

For numerical attributes ⇒ DISCRETIZATION

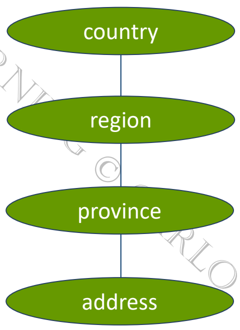
SUBJECTIVE SUBDIVISION

SUBDIVISION INTO CLASSES
of equal size or equal width

numin	
229	
235	low
237	
240	
245	medium
248	
253	
360	high
271	

Hierarchical discretization

For a categorical attribute



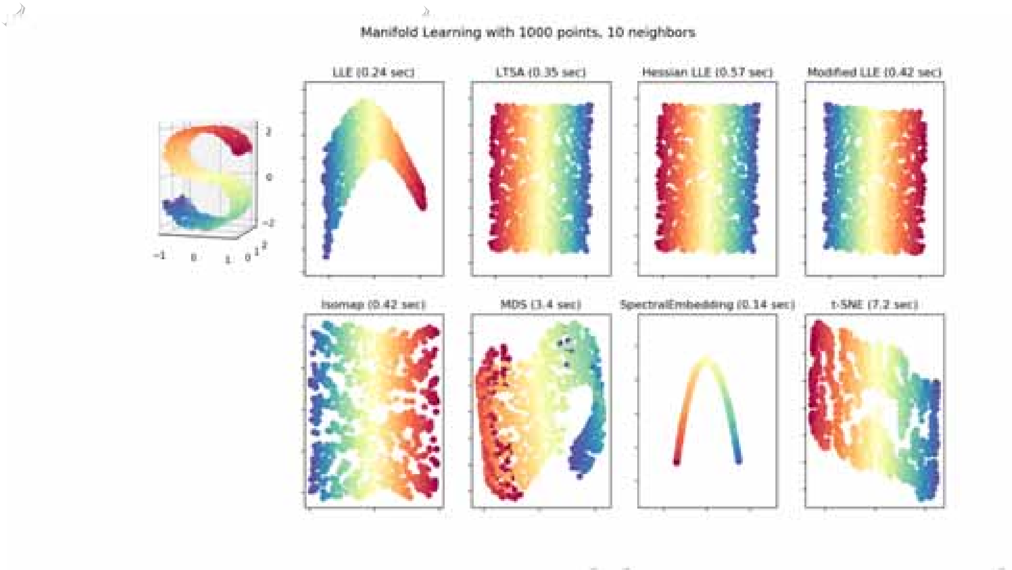
15 distinct values

65 distinct values

3567 distinct values

674.339 distinct values

Nonlinear dimensionality reduction - embedding



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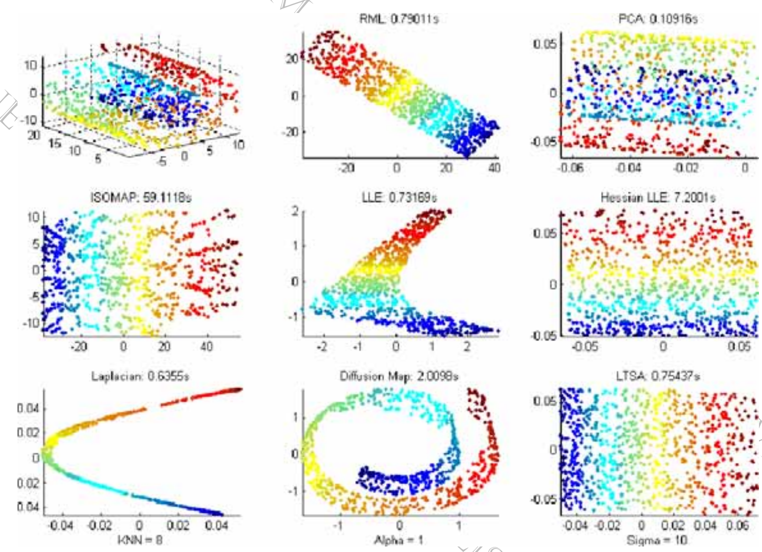
Nonlinear dimensionality reduction - embedding



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