Mahalanobis-Distance 1.0
(MD)

NANOBRIDGES
-ACollaborative Project

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Background:

The multivariate chemometrical analysis involves the measurement of distances between objects and variables. The two widely and most commonly used distance measures are Euclidean distance (ED) and the Mahalanobis distance (MD). The ED is easy to compute and interpret but the calculation of MD takes into account the correlation in the data, since it is calculated using the inverse of the variance-covariance matrix of the dataset. When the data are measured over the large number of variables, due to the redundant or correlated information leads to singular or nearly singular variance-covariance matrix that cannot be inverted. Subsequently, for the calculation of variance-covariance matrix, the number of objects in dataset should be larger than the number of variables. So, feature reduction i.e selecting a small number of meaningful variables is required prior to the finalizing the input file for MD calculation [1].

The MD is useful for the many purposes such as detection of outliers, the selection of calibration samples from a larger set of measurement and for investing the representativity between the two datasets. In pattern recognition, the MD is applied in clustering techniques such as k-Nearest Neighbour method (kNN), in discrimination techniques such as linear, quadratic and regularised discriminating analysis (LDA, QDA and RDA) [2] and in class modelling techniques such as UNEQ (multivariate normal class model assuming an individual dispersion of each class) [3], EQ (multivariate normal class model assuming equal dispersion of each class) [4] and modifications of Soft Independent Modelling of Class Analogy (SIMCA).

About the algorithm: The algorithm involved in the calculation of MD is as follows:

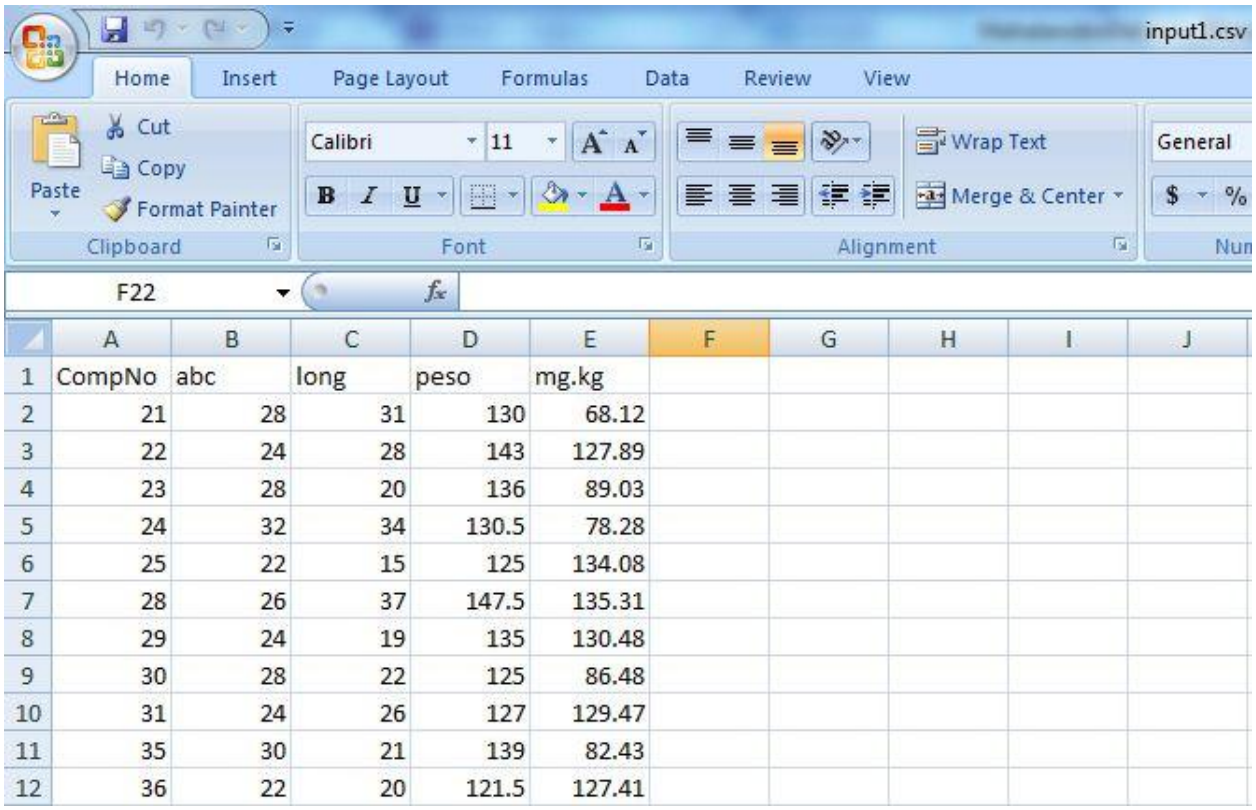
$$C_x = \frac{1}{(n-1)}(X_c)^T(X_c) \qquad \text{(i)}$$

$$MD_i = \sqrt{(x_i - x)C_x^{-1}(x_i - \bar{x})^T} \qquad \text{(ii)}$$

Where, C_x is the variance-covariance matrix; X is the data matrix containing n objects. X_c is the column-centered data matrix ($X - \overline{X}$)

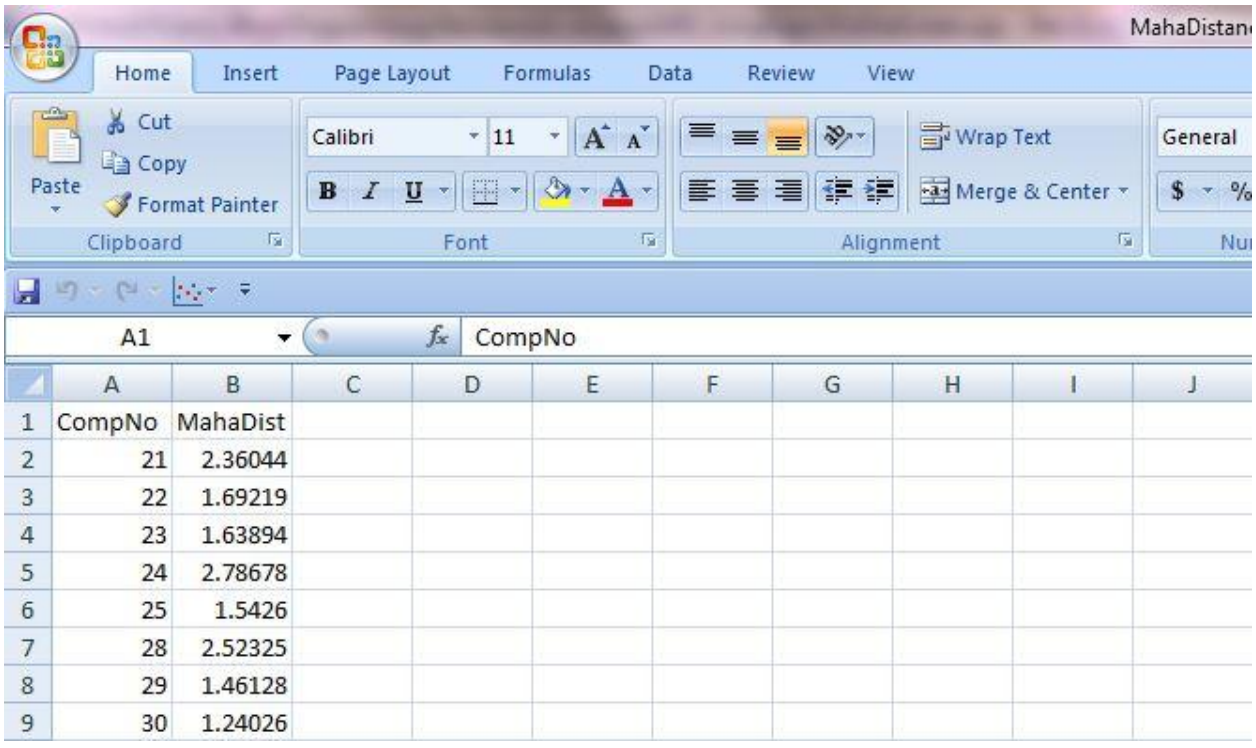
The eigen library was used for the calculation of matrix determinant and inverse calculation[5].

Input file format: This program takes a input file in CSV format.



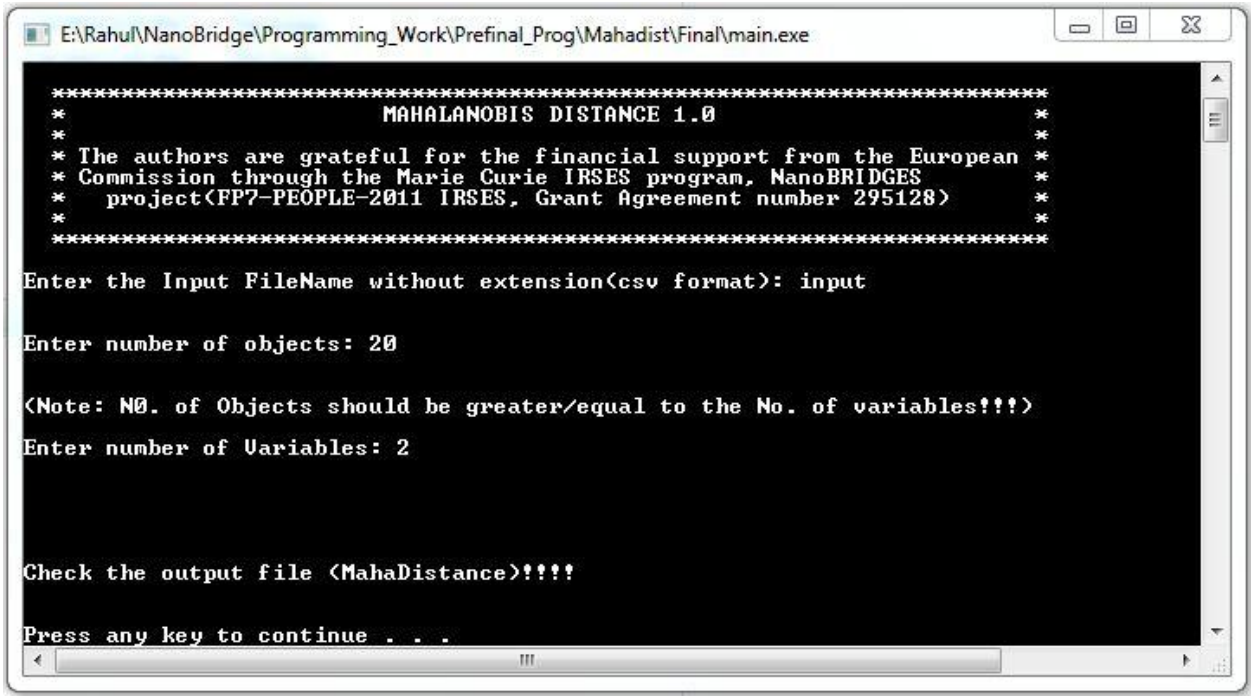
	A	B	C	D	E	F	G	H	I	J
1	CompNo	abc	long	peso	mg.kg					
2	21	28	31	130	68.12					
3	22	24	28	143	127.89					
4	23	28	20	136	89.03					
5	24	32	34	130.5	78.28					
6	25	22	15	125	134.08					
7	28	26	37	147.5	135.31					
8	29	24	19	135	130.48					
9	30	28	22	125	86.48					
10	31	24	26	127	129.47					
11	35	30	21	139	82.43					
12	36	22	20	121.5	127.41					

Output file format:



	A	B	C	D	E	F	G	H	I	J
1	CompNo	MahaDist								
2	21	2.36044								
3	22	1.69219								
4	23	1.63894								
5	24	2.78678								
6	25	1.5426								
7	28	2.52325								
8	29	1.46128								
9	30	1.24026								

How to run a program:



Disclaimer

For academic purpose only.

The program Mahalanobis-Distance 1.0 has been developed in C++ language and is validated on the known data sets. This program is compatible with both 32- and 64-bit Windows operating system. Please report for discrepancy of result for any other dataset. Contact us at any of the following addresses:

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References:

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