

Euclidean Based Kennard-Stone 1.0

NANOBRIDGES
-A Collaborative Project



Marie Curie
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Background:

The optimal division of dataset into training and independent test subset is an important and critical step in the QSAR modeling analysis. The test-set molecules will be predicted well, when they are structurally very similar to the training-set molecules. The reason is that the model would capture all features common to the training-set molecules. There are different techniques available for the rational division of the data-set into training and test sets such as statistical molecular design, self-organising map, clustering, Kennard–Stone (KS) selection, sphere exclusion, etc. [1]. The splitting of dataset by using rational way of division is a superior method as compared to the random splitting and activity sorting method.

About the algorithm: The KS algorithm was originally applied to generate a training set when no standard experimental design can be implemented. In this technique, all the objects are considered as candidates for the training set. The steps involved in the selection of training set based on Euclidean-based KS algorithm are as follows [2-3]:

1. The first two compounds of training set are selected by choosing two compounds that are quite farthest apart in terms of Euclidean distance. The normalized mean distance for all the compounds are calculated by following equations [4]:

$$d_{ij} = \|X_i - X_j\| = \sqrt{\sum_{k=1}^m (X_{ik} - X_{jk})^2} \quad (\text{i})$$

$$\bar{d}_i = \frac{\sum_{j=1}^n d_{ij}}{n-1} \quad (\text{ii})$$

$$\text{MeanDistance}_{(\text{Normalized})} = \frac{(\text{MeanDistance} - \text{Min_MeanDistance})}{(\text{Max_MeanDistance} - \text{Min_MeanDistance})} \quad (\text{iii})$$

Where,

d_{ij} : the distance score between two compounds

\bar{d}_i : Mean distance

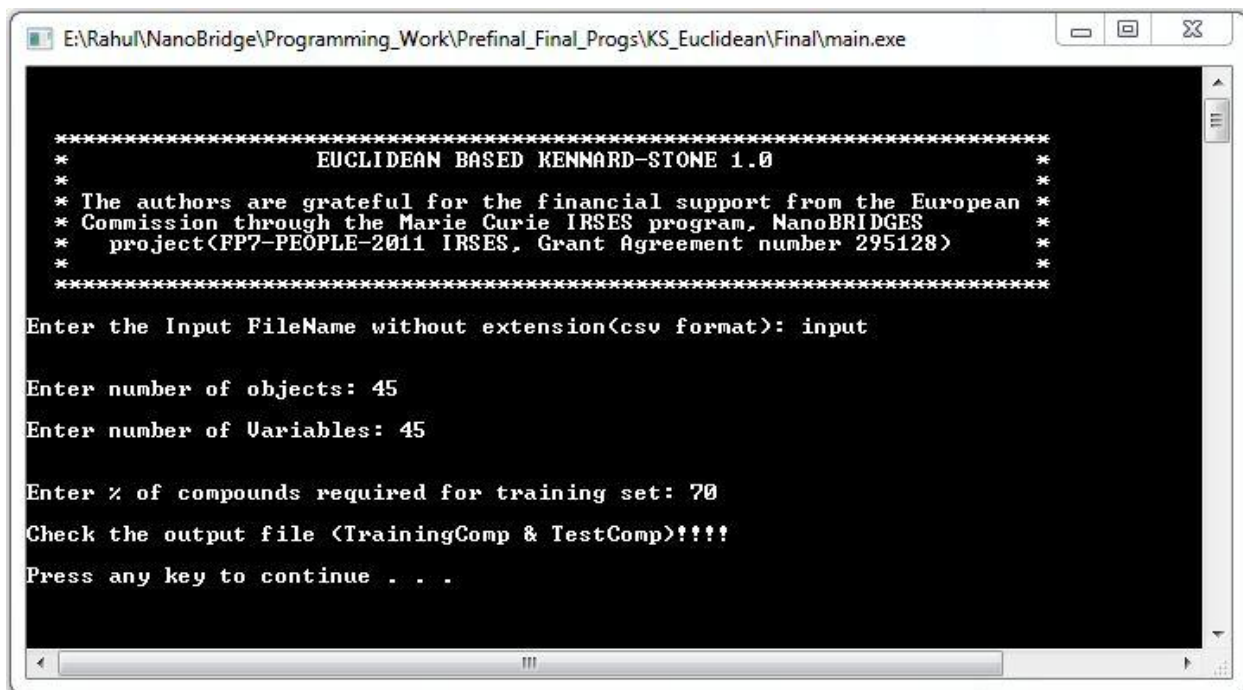
2. Find the compound which has the maximum dissimilarity (maximum minimum distance) from each of the previously selected chemicals and place this chemical in the training set.
3. Repeat step 2 until the desired number of chemicals have been added to the training set.

4. The remaining chemicals were placed in the test set.

Input file format: This program takes an input file in CSV format. Enter the standardized/scaled descriptors matrix.

	A	B	C	D	E	F	G	H	I	J
1	Comp	S_sCH3	S_ssCH2	S_dsCH	S_aaCH	S_dssC	S_aasC	S_aaaC	S_ssssC	S_sNH2
2	21	0.99786	-0.41755	1.05029	0.39528	0.68812	0.50956	-0.14907	0.17181	-0.28502
3	22	-0.50166	-0.41755	1.00002	0.35905	0.68812	0.47428	-0.14907	0.17181	-0.29834
4	23	2.11327	-0.41755	0.91396	-0.05687	0.10788	0.45357	-0.14907	0.17181	-0.27865
5	24	-0.50166	-0.41755	0.87386	0.082	0.68812	0.31016	-0.14907	0.17181	-0.31162
6	42	0.86771	-0.41755	0.93262	-0.34087	0.68812	0.48256	-0.14907	0.17181	-0.28599
7	29	-0.50166	-0.41755	1.0653	0.35235	0.68812	0.51415	-0.14907	0.17181	-0.29888
8	5	-0.50166	-0.41755	0.99624	0.22631	0.68812	0.3961	-0.14907	0.17181	-0.30674
9	3	-0.50166	0.1371	1.08978	0.30244	0.68812	0.47101	-0.14907	0.17181	-0.29181
10	2	-0.50166	-0.00186	0.88027	0.17143	0.68812	0.35283	-0.14907	0.17181	-0.2976
11	1	-0.50166	1.13381	0.9997	0.37329	0.68812	0.44626	-0.14907	0.17181	-0.28145
12	43	-0.50166	1.38075	1.28003	0.89713	0.68812	0.50564	-0.14907	0.17181	-0.27475

How to run a program:



```
E:\Rahul\NanoBridge\Programming_Work\Prefinal_Final_Progs\KS_Euclidean\Final\main.exe

*****
*                               *
*      EUCLIDEAN BASED KENNARD-STONE 1.0      *
*                               *
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* Commission through the Marie Curie IRSES program, NanoBRIDGES      *
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*                               *
*****

Enter the Input FileName without extension(csv format): input

Enter number of objects: 45
Enter number of Variables: 45

Enter % of compounds required for training set: 70
Check the output file <TrainingComp & TestComp>!?!?!
Press any key to continue . . .
```

Disclaimer

For academic purpose only.

The program Euclidean-based Kennard-Stone1.0 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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