User Manual for KCC—a MATLAB package for K-means-based Consensus Clustering

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1. INTRODUCTION

This user manual systematically presents the usage of the MATLAB package[6] on K-means-based Consensus Clustering (KCC) accompanying the following paper:

> Hao Lin, Hongfu Liu, Junjie Wu, Hong Li, and Stephan Günnemann. 2023. Algorithm xxxx: KCC: A MATLAB Package for K-means-based Consensus Clustering. *ACM Trans. Math. Softw.*

For package installation, you need to first unpack the compressed archive into your current directory. It consists of a *source code* folder Matlab, a folder userManual with this comprehensive *user manual*, and a *license* file LICENSE indicating that the package is distributed under GNU GENERAL PUBLIC LICENSE (Version 3). Then under the Matlab folder, you need to add one of its subfolder, i.e., the Src folder, to the MATLAB path.

The directory structure of the Matlab folder is described as follows.

Src (core functions for conducting KCC)
- BasicCluster_RFS.m (function to generate BPs with RFS)
- BasicCluster_RPS.m (function to generate BPs with RPS)
- Preprocess.m (function to prepare for consensus clustering)
- KCC.m (consensus function)
- RunKCC.m (combined function for preprocessing and consensus clustering)
- exMeasure.m (function to compute external validity scores)
- inMeasure.m (function to compute internal validity scores)
- load_sparse.m (auxiliary function to load input text data as a sparse matrix)
- hungarian.m (auxiliary function for cluster label assignment)
- BasicCluster_RPS_missing.m (auxiliary function to generate IBPs with strategy-I)
- addmissing.m (auxiliary function to generate IBPs using strategy-II)
- distance_* (distance functions)
- gClusterDistribution.m (auxiliary function to calculate cluster distribution for BPs)
- Ucompute.m, Ucompute_miss.m (auxiliary function for utility calculation)
- gCentroid.m, gCentroid_miss.m (auxiliary function for centroid update)

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[6]The software package is publicly available at https://gitee.com/linhaobuaa/KCC.

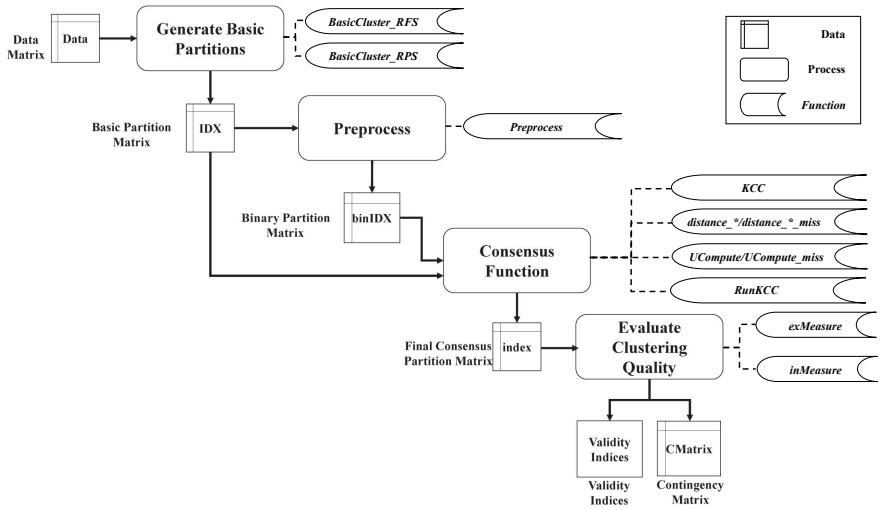


Fig. 1: Typical program flow of the KCC package.

sCentroid.m, sCentroid_miss.m (auxiliary function for centroid initialization)
CalinskiHarabasz.m (auxiliary function to calculate the Calinski and Harabasz index)
kmeans_octave.m (auxiliary function to conduct K-means clustering with Octave)
knee_pt.m (auxiliary function to find the elbow point of a curve)
majorityvote.m (auxiliary function to perform majority voting)

Drivers (illustrative examples)

data (input data for illustration)
demo.m (function for KCC with different utility functions)
demoIBPI.m (function for KCC with IBPs generated by strategy-I)
demoIBPII.m (function for KCC with IBPs generated by strategy-II)
demoNumberBP.m (function for KCC with varying number of BPs)
demoStrategyBP.m (function for KCC with RFS strategy for BP generation)
demoEvacluster.m (function for cluster evaluation and selection of K)
demoEvaTimeMem.m (function for recording execution time and memory usage)

The package was developed and tested in MATLAB R2022a under Linux. For those without access to MATLAB and those who prefer to use free open source software, we also investigate the usage of KCC with OCTAVE. Generally, the Octave supports drop-in compatibility with the MATLAB scripts in our KCC package. To use the KCC package with OCTAVE, the users need to firstly do an additional installation step, i.e., installing the statistics and io packages on the OCTAVE command line using "pkg install -forge statistics;" and "pkg install -forge io;", respectively. Then, the users should type the commands "pkg load statistics;" and/or "pkg load io;" on the OCTAVE command line before executing the functions/scripts of the KCC package if needed. All demonstration scripts with the prefix named "demo" under the Matlab/Drivers folder have passed the test on a personal computer with GNU OCTAVE 7.1.0 and macOS 12.4.

In Figure 1, we show the package's typical workflow, which provides a quick overview for using the package. The workflow starts by inputing a real-world data matrix Data into the basic partition generation functions in order to generate a basic partition matrix IDX.

The basic partition matrix is then input to a Preprocess function to produce a sparse representation of $\mathcal{X}^{(b)}$, i.e., the matrices, Ki, sumKi, and binIDX. They are then input to the final consensus clustering, i.e., the consensus function, which produces a consensus partition matrix index. Lastly, the clustering quality is evaluated with an inMeasure/exMeasure function, which outputs multiple internal/external validity indices.

Organization of this user manual. In Section 2, we give some typical examples with MATLAB code snippets, tables, and figures to help the readers to quickly understand how to work properly and effectively with the package. Next, we provide details for each of the package's available functions, such as syntax, input, and output, in Section 3.

2. ILLUSTRATIVE EXAMPLES

2.1 A quick introductory example for illustrating the typical workflow

Here we give illustrative examples with the UCI and TREC data sets to show how the KCC package works following the typical workflow as previously described.

Importing data. Firstly, we should import the data set into the MATLAB environment. For a UCI data set such as *iris*, the package KCC includes two files under the **Matlab/Drivers/data** folder, i.e., **iris.dat** and **iris_rclass.dat**, which correspond to the attribute information and ground truth cluster labels of data instances, respectively. As illustrated in Listing 1, the data attributes and ground truth cluster labels can be imported with the built-in MATLAB function **`load`**. For ease of understanding, we also illustrate the attribute information of the *iris* data set in Table Ia.

```
data = load('data/iris.dat');
true_label = load(strcat('data/', strcat('iris', '_rclass.dat')));
```

Listing 1: Using **`load`** to import data attributes and ground truth cluster labels.

For TREC data sets such as *mm*, as indicated in Listing 2, we use the function **`load_sparse`** implemented in the KCC package to import the data attributes as a sparse matrix `sp_mtx`, and use the built-in function **`load`** to import the ground truth cluster labels. The attribute matrix of the *mm* data set input to **`load_sparse`** is illustrated in Table Ib. We can see that the input attribute matrix is in a CLUTO sparse matrix format. The first line gives some meta information of the data set, which includes the number of instances n, the number of features d, and the total number of non-zero elements if recovering the data set as a $n \times d$ matrix. The file's remaining n lines preserve the non-zero values of the matrix in a sparse manner [Karypis 2002].

```
[sp_mtx, n, m, count] = load_sparse('data/mm.mat');
data = sp_mtx;
true_label = load(strcat('data/',strcat('mm', '_rclass.dat')));
```

Listing 2: Using **`load_sparse`**/**`load`** to import data attributes/ground truth cluster labels.

Generating basic partitions. As indicated in Figure 1, we should then generate basic partitions (BPs). Concretely, we can utilize the **`BasicCluster_RPS`** function to produce BPs with Random Parameter Selection (RPS) strategy. We set the number of BPs to 100 [Luo et al. 2011; Liu et al. 2016], because this setting can usually produce good consensus clustering results. For the data set *iris*, we use squared euclidean distance as the distance metric of clustering algorithm to generate BPs, while for the *mm* data

	$attr_1$	$attr_2$	$attr_3$	$attr_4$
$data_1$	5.1	3.5	1.4	0.2
$data_2$	4.9	3.0	1.4	0.2
$data_3$	4.7	3.2	1.3	0.2
⋮	⋮	⋮	⋮	⋮
$data_{150}$	5.9	3.0	5.1	1.8

(a) A $n \times d$ attribute matrix for *iris* data set, where $n = 150$ and $d = 4$.

	2521	126373	490062		
$data_1$	556	1	...	238	1
$data_2$	755	1	...	195	1
$data_3$	2202	2	...	7848	1
⋮	⋮	⋮	⋮	⋮	⋮
$data_{2521}$	595	1	...	20246	3

(b) A $n \times d$ attribute matrix for *mm* data set, where $n = 2521$ and $d = 126373$.

Table I: Illustration of the data attribute matrix for two data sets.

	BP_1	BP_2	BP_3	BP_4	BP_5	BP_6	BP_7	BP_8	BP_9	...	BP_{100}
$data_1$	1	1	1	4	7	4	6	1	10	...	7
$data_2$	1	8	4	3	1	2	4	1	1	...	7
$data_3$	1	8	10	3	1	2	4	1	6	...	7
$data_4$	1	8	10	3	1	2	4	1	6	...	7
$data_5$	1	1	1	4	7	4	6	1	10	...	7
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
$data_{150}$	2	3	3	1	8	1	5	2	11	...	8

Table II: A $n \times r$ basic partition matrix `IDX` for the *iris* data set, where $n = 150$ and $r = 100$.

set we use cosine distance. The code snippet is shown in Listing 3. We also illustrate the obtained basic partition matrix `IDX` for the *iris* data set in Table II. Each entry in `IDX` represents a cluster label that the corresponding data object is assigned to in a basic partition.

```
IDX = BasicCluster_RPS(data, 100, 3, 'sqEuclidean', 1); % for iris
IDX = BasicCluster_RPS(data, 100, 2, 'cosine', 1); % for mm
```

Listing 3: Using **`BasicCluster_RPS`** to generate BPs.

For further consideration of efficiency, we can also utilize the multicore-processor architecture to reduce the execution time of the KCC package. In fact, the parallel 'for-loop' function, i.e., **`parfor`**, in the MATLAB Parallel Computing Toolbox can be employed in the KCC package to accelerate the computation. Listing 4 demonstrates how the **`parfor`** function can be used to help accelerate the generation process of basic partitions with the **`kmeans`** function.

```
parfor i = 1:r
    IDX(:, i) = kmeans(Data, Ki(i), 'distance', dist, 'emptyaction', 'singleton', 'replicates', 1);
end
```

Listing 4: Using **`parfor`** to accelerate the process of generating BPs.

Preprocessing data and conducting consensus function. As a next step of the workflow in Figure 1, the function **`RunKCC`** is executed with the basic partition matrix `IDX` as the input. An illustrated code to conduct consensus clustering on the *iris* data set with U_h utility function and $K = 3$ is shown in Listing 5. The **`RunKCC`** function is composed of two key steps, which involves executing the **`Preprocess`** function to prepare input for consensus clustering and executing the core function **`KCC`** 10 times to find the best consensus partition `pi_index`, which has the best objective function value.

```
K = 3;
```

```
U = {'U_h', 'std', []};
r = size(IDX, 2);
w = ones(r, 1);
rep = 10;
maxIter = 40;
minThres = 1e−5;
utilFlag = 1;
[pi_sumbest, pi_index, ~, ~~, ~~~] = RunKCC(IDX, K, U, w, rep, maxIter, minThres, utilFlag);
```

Listing 5: Using **RunKCC** to conduct consensus clustering.

Evaluating clustering quality. As a last step of the workflow in Figure 1, users can utilize the external validity metrics to evaluate the clustering quality with the **exMeasure** function in the KCC package. The code to launch the **exMeasure** function is shown in Listing 6, which saves values of five external validity measurements to a result matrix file for further comparison.

```
[Acc, Rn, NMI, VIn, VDn, labelnum, ncluster, cmatrix] = exMeasure(pi_index, true_label);
filename = strcat('iris', strcat('_', lower(U{1, 1})));
filename = strcat(filename, strcat('_', lower(U{1, 2})));
if ~isempty(U{1, 3})
    filename = strcat(filename, strcat('_', num2str(lower(U{1, 3}))));
end
filename = strcat(filename, '.mat');
save(filename, 'Acc', 'VIn', 'VDn', 'Rn', 'NMI');
```

Listing 6: Using **exMeasure** to evaluate the clustering quality.

When the ground truth cluster labels are not available in real-world settings, we can utilize the internal validity metrics to evaluate a clustering with the **inMeasure** function in the KCC package. An illustrated code snippet is shown in Listing 7.

```
[Distortion, Silhouette, CH] = inMeasure(X, cluster, k);
```

Listing 7: Using **inMeasure** to evaluate the clustering quality.

2.2 An illustrative example of choosing an effective and efficient utility function

Choosing an effective and efficient utility function is a common need for the KCC package in practical clustering applications. In order to achieve this purpose, the KCC package provides demonstration scripts to compare the clustering quality and efficiency with different utility functions on 11 real-world data sets from the UCI and TREC repositories.

For effectiveness comparison, the KCC package provides the script **Matlab/Drivers/demo.m**. We briefly explain the main steps in this illustration. The first step utilizes an RPS strategy to generate basic partitions, which calls the **BasicCluster_RPS** function. The next step applies the **RunKCC** function to the obtained basic partition matrix to obtain the consensus partition. This step also involves executing consensus clustering with 10 different utility functions, namely U_c, U_H, U_{cos}, U_{L_5}, U_{L_8}, and their corresponding normalized versions NU_x. Then the script conducts clustering quality evaluation, and reports five external validity indices, including CA, NMI, R_n, VI_n, and VD_n. For robustness, the script conducts the **RunKCC** function 10 times to obtain the average validity values. In the following, we show the most important code snippet for this illustration.

```
U_array = {{'U_H','std',[]} {'U_H','norm',[]} {'U_c','std',[]} {'U_c','norm',[]} {'U_cos','std',[]}
{'U_cos','norm',[]} {'U_lp','std',[5]} {'U_lp','norm',[5]} {'U_lp','std',[8]} {'U_lp','norm',[8]}};
IDX = BasicCluster_RPS(data, r, K, dist_of_basic_cluster, randKi);
output_foldername='ResultDemo/';
mkdir ResultDemo;

for uidx = 1:length(U_array)
    avgAcc = 0;
    avgRn = 0;
    avgNMI = 0;
    avgVIn = 0;
    avgVDn = 0;
    U = U_array{1,uidx};
    for num = 1 : 10
        [pi_sumbest,pi_index,pi_converge,pi_utility,~] = RunKCC(IDX,K,U,w,rep,maxIter,minThres,utilFlag);
        [Acc, Rn, NMI, VIn, VDn, labelnum, ncluster, cmatrix] = exMeasure(pi_index, true_label);
        avgAcc = avgAcc + Acc;
        avgRn = avgRn + Rn;
        avgNMI = avgNMI + NMI;
        avgVIn = avgVIn + VIn;
        avgVDn = avgVDn + VDn;
    end
    avgAcc = avgAcc / num;
    avgRn = avgRn / num;
    avgNMI = avgNMI / num;
    avgVIn = avgVIn / num;
    avgVDn = avgVDn / num;
    filename = strcat([output_foldername '/' datafile],strcat('_',lower(U{1,1})));
    filename = strcat(filename,strcat('_',lower(U{1,2})));
    if ~isempty(U{1,3})
        filename = strcat(filename,strcat('_',num2str(lower(U{1,3}))));
    end
    filename1 = strcat(filename,'.mat');
    save(filename1,'avgAcc', 'avgVIn', 'avgVDn', 'avgRn', 'avgNMI');
end
```

Listing 8: Using **demo.m** to evaluate the clustering quality of the KCC package with different utility functions.

The clustering results in terms of the five external validity indices are presented in Tables III-VII. From these tables, we can see that 7 out of 10 utility functions achieve the best clustering performance over at least 1 data set. This suggests providing flexible utility functions can be crucial to accurate ensemble clustering in real-world applications. In practice, we can hardly know which utility function should be used in consensus clustering. We rate utility functions over a testbed, and select the utility function that achieves the best rating. More specifically, a final score is defined to assess the overall performance of an utility function on a set of data sets. The score is calculated as $score(U_i) = \frac{1}{11}\sum_j \frac{V(U_i,D_j)}{\max_i V(U_i,D_j)}$, where $V(U_i, D_j)$ denotes the clustering validity score obtained by applying an utility function U_i on a data set D_j. As can be seen, U_H obtains

	U_c	U_H	U_{cos}	U_{L5}	U_{L8}	NU_c	NU_H	NU_{cos}	NU_{L5}	NU_{L8}
breast_w	0.6403	0.9624	0.7172	0.6820	0.6896	0.6260	**0.9639**	0.6838	0.6820	0.6820
ecoli	0.5639	0.5789	0.5651	0.5756	0.5590	0.5831	0.5578	**0.5880**	0.5605	0.5657
iris	0.8940	0.8973	**0.9000**	**0.9000**	0.8940	0.8933	0.8907	**0.9000**	**0.9000**	0.8880
pendigits	0.6526	0.6584	**0.6837**	0.6422	0.6520	0.5947	0.6443	0.6833	0.6600	0.6533
satimage	0.5829	0.6571	0.6149	0.6060	0.6290	0.5229	0.6425	**0.6594**	0.6006	0.5597
dermatology	0.2913	**0.3128**	0.2729	0.2701	0.2723	0.3075	0.2975	0.2802	0.2760	0.2899
wine	0.5135	**0.5247**	0.5180	0.5112	0.5112	0.5208	0.5079	0.5219	0.5157	0.5152
mm	0.9337	0.9497	0.9532	0.9336	**0.9551**	0.7797	0.9495	0.9415	0.9439	0.9093
reviews	0.6153	0.6593	0.6313	0.6407	0.6569	0.6086	**0.6698**	0.6030	0.6353	0.6198
la12	0.4626	0.4912	**0.5064**	0.4755	0.4690	0.4349	0.4890	0.4853	0.4491	0.4476
sports	0.4497	**0.4858**	0.4715	0.4642	0.4502	0.4592	0.4584	0.4764	0.4693	0.4461
score	0.9182	**0.9898**	0.9462	0.9283	0.9314	0.8910	0.9707	0.9477	0.9265	0.9135

Table III: Clustering quality of KCC with different utility functions in terms of CA. The best results are highlighted with the bold font.

	U_c	U_H	U_{cos}	U_{L5}	U_{L8}	NU_c	NU_H	NU_{cos}	NU_{L5}	NU_{L8}
breast_w	0.2430	0.7558	0.2575	0.2024	0.1998	0.2326	**0.7690**	0.1850	0.2024	0.2024
ecoli	0.5809	0.5941	0.5861	0.5911	0.5855	0.5937	0.5922	**0.5952**	0.5839	0.5916
iris	0.7905	0.7937	**0.7981**	**0.7981**	0.7905	0.7908	0.7767	**0.7981**	**0.7981**	0.7829
pendigits	0.6978	0.6775	**0.7194**	0.6756	0.6663	0.6732	0.6749	0.7062	0.6816	0.6670
satimage	0.5388	0.5747	0.5695	0.5695	0.5839	0.4699	0.5790	**0.5840**	0.5469	0.5273
dermatology	0.1211	**0.1417**	0.1031	0.0990	0.0916	0.1395	0.1328	0.1238	0.0955	0.1083
wine	0.1675	0.1697	0.1689	0.1669	0.1519	0.1697	0.1511	**0.1701**	0.1682	0.1680
mm	0.6741	0.7249	0.7338	0.6501	**0.7487**	0.3531	0.7211	0.6924	0.7028	0.5949
reviews	0.4879	0.5347	0.5052	0.5375	**0.5575**	0.4538	0.5467	0.4765	0.5147	0.5091
la12	0.2646	**0.3371**	0.3095	0.2882	0.2764	0.2256	0.3234	0.2911	0.2515	0.2630
sports	0.4406	0.4641	0.4531	**0.4754**	0.4715	0.4319	0.4499	0.4693	0.4563	0.4472
score	0.8638	**0.9820**	0.8884	0.8671	0.8647	0.8070	0.9612	0.8842	0.8508	0.8408

Table IV: Clustering quality of KCC with different utility functions in terms of NMI. The best results are highlighted with the bold font.

	U_c	U_H	U_{cos}	U_{L5}	U_{L8}	NU_c	NU_H	NU_{cos}	NU_{L5}	NU_{L8}
breast_w	0.0687	0.8537	0.2104	0.1283	0.1391	0.0495	**0.8597**	0.1307	0.1283	0.1283
ecoli	0.3970	0.4230	0.4021	0.4128	0.4021	0.4213	0.4119	**0.4342**	0.4007	0.4110
iris	0.7352	0.7445	**0.7455**	**0.7455**	0.7352	0.7323	0.7287	**0.7455**	**0.7455**	0.7249
pendigits	0.4799	0.5236	**0.5662**	0.5073	0.5010	0.3996	0.5084	0.5551	0.5130	0.4961
satimage	0.3989	**0.5018**	0.4663	0.4650	0.4790	0.2704	0.4908	0.4958	0.4319	0.3955
dermatology	0.0428	**0.0553**	0.0305	0.0259	0.0275	0.0537	0.0442	0.0419	0.0285	0.0352
wine	0.1454	**0.1497**	0.1471	0.1447	0.1375	0.1480	0.1355	0.1484	0.1461	0.1459
mm	0.7564	0.8092	0.8215	0.7522	**0.8284**	0.3454	0.8081	0.7799	0.7893	0.6791
reviews	0.4231	0.5193	0.4797	0.4877	0.5305	0.3738	**0.5334**	0.4403	0.4821	0.4625
la12	0.2046	0.2671	**0.2770**	0.2344	0.2397	0.1574	0.2436	0.2449	0.2059	0.2063
sports	0.2639	0.3193	0.2989	0.3210	0.3229	0.2387	0.3002	**0.3283**	0.3081	0.3038
score	0.7834	**0.9798**	0.8578	0.8185	0.8339	0.6934	0.9342	0.8655	0.8062	0.7910

Table V: Clustering quality of KCC with different utility functions in terms of R_n. The best results are highlighted with the bold font.

	U_c	U_H	U_{cos}	U_{L5}	U_{L8}	NU_c	NU_H	NU_{cos}	NU_{L5}	NU_{L8}
breast_w	0.7572	0.2442	0.7425	0.7977	0.8003	0.7677	**0.2310**	0.8151	0.7977	0.7977
ecoli	0.4215	0.4079	0.4164	0.4113	0.4169	0.4083	0.4099	**0.4072**	0.4184	0.4109
iris	0.2096	0.2064	**0.2020**	**0.2020**	0.2096	0.2093	0.2234	**0.2020**	**0.2020**	0.2172
pendigits	0.3032	0.3227	**0.2808**	0.3247	0.3340	0.3289	0.3254	0.2940	0.3187	0.3333
satimage	0.4613	0.4253	0.4305	0.4306	**0.4161**	0.5311	0.4210	**0.4161**	0.4532	0.4727
dermatology	0.8790	**0.8584**	0.8970	0.9010	0.9084	0.8605	0.8672	0.8762	0.9045	0.8917
wine	0.8325	0.8303	0.8311	0.8331	0.8481	0.8303	0.8489	**0.8299**	0.8318	0.8320
mm	0.3259	0.2752	0.2662	0.3499	**0.2513**	0.6505	0.2789	0.3077	0.2972	0.4052
reviews	0.5125	0.4660	0.4956	0.4631	**0.4433**	0.5465	0.4539	0.5242	0.4857	0.4915
la12	0.7358	**0.6630**	0.6905	0.7119	0.7236	0.7754	0.6767	0.7090	0.7485	0.7370
sports	0.5612	0.5392	0.5497	**0.5278**	0.5315	0.5691	0.5534	0.5339	0.5467	0.5555
score	0.9060	**0.8145**	0.8721	0.8951	0.8869	0.9780	0.8256	0.8874	0.9027	0.9295

Table VI: Clustering quality of KCC with different utility functions in terms of VI_n. The best results are highlighted with the bold font.

the best score on all five validity metrics, and is closely followed by NU_H. As such, we take U_H as the default choice for the KCC package unless otherwise specified.

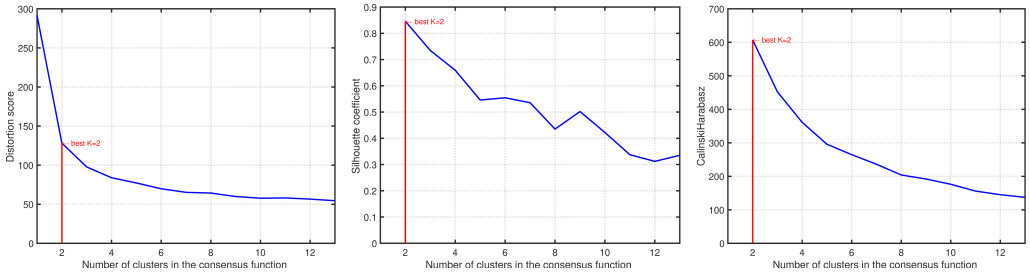
For efficiency comparison, the KCC package provides the script **Matlab/Drivers/de-**

	U_c	U_H	U_{cos}	U_{L5}	U_{L8}	NU_c	NU_H	NU_{cos}	NU_{L5}	NU_{L8}
breast_w	0.9511	0.1087	0.7664	0.8541	0.8378	0.9720	**0.1041**	0.8500	0.8541	0.8541
ecoli	0.4312	0.4323	0.4279	**0.4148**	0.4278	0.4161	0.4248	0.4173	0.4262	0.4270
iris	0.1729	0.1675	**0.1622**	**0.1622**	0.1729	0.1739	0.1779	**0.1622**	**0.1622**	0.1837
pendigits	0.3380	0.3386	**0.3006**	0.3418	0.3467	0.3859	0.3444	0.3133	0.3410	0.3582
satimage	0.4549	**0.3829**	0.4184	0.4198	0.4036	0.5686	0.3980	0.3859	0.4487	0.4805
dermatology	0.9170	**0.8877**	0.9342	0.9370	0.9328	0.9000	0.8977	0.9205	0.9293	0.9246
wine	0.7516	**0.7399**	0.7526	0.7512	0.7570	0.7531	0.7571	0.7534	0.7521	0.7520
mm	0.1546	0.1083	0.1016	0.1504	**0.0968**	0.5553	0.1091	0.1254	0.1244	0.2181
reviews	0.4749	0.4042	0.4089	0.4094	0.3866	0.4915	**0.3799**	0.4496	0.4315	0.4380
la12	0.7167	0.6286	**0.6270**	0.6695	0.6765	0.7898	0.6485	0.6725	0.7091	0.7066
sports	0.6014	0.5335	0.5512	0.5342	0.5372	0.6236	0.5555	**0.5295**	0.5360	0.5644
score	0.8801	**0.7425**	0.8054	0.8314	0.8250	0.9877	0.7536	0.8211	0.8423	0.8821

Table VII: Clustering quality of KCC with different utility functions in terms of VD_n. The best results are highlighted with the bold font.

	U_c	U_H	U_{cos}	U_{L5}	U_{L8}	NU_c	NU_H	NU_{cos}	NU_{L5}	NU_{L8}
breast_w	0.83	1.95	0.72	0.88	0.76	0.82	0.99	**0.64**	0.76	0.86
ecoli	1.61	3.50	1.24	1.67	1.51	**1.16**	2.06	1.23	1.50	1.40
iris	2.00	7.06	1.61	1.51	1.51	1.49	3.39	1.48	**1.46**	1.48
pendigits	**10.55**	12.87	11.45	13.84	11.87	11.39	13.00	11.19	14.01	13.12
satimage	1.25	1.80	**1.19**	1.42	1.73	1.22	1.62	1.22	1.58	1.96
dermatology	**1.11**	3.59	1.47	1.37	1.15	1.24	1.90	1.20	1.23	1.29
wine	1.86	6.55	2.30	1.84	1.61	1.80	3.28	1.78	1.56	**1.53**
mm	622.61	771.60	733.84	**571.96**	677.55	660.21	739.98	774.26	656.56	588.42
reviews	733.01	1209.34	769.65	693.93	647.68	977.17	1017.01	767.63	756.06	**629.17**
la12	255.44	302.76	283.09	258.23	252.70	266.36	**249.24**	256.89	267.51	252.64
sports	1043.65	1701.98	954.64	1008.88	929.79	989.38	1032.93	**899.55**	952.23	980.68
score	0.55	0.98	0.57	0.57	0.56	0.56	0.69	**0.54**	0.58	0.57

Table VIII: Full execution time of the KCC package with different utility functions. We collect the raw execution time in milliseconds, and normalize it by the number of data objects in the corresponding data set.



(a) Distortion Score (b) Silhouette Coefficient (c) Calinski and Harabasz index

Fig. 2: Impact of the number of clusters in the consensus partition on the *iris* data set.

moEvaTimeMem.m. We show the full execution time of the KCC with different utility functions in Table VIII. In the execution time computation, we consider the whole process of using the package, including loading data, generating basic partitions, conducting consensus function, and evaluating the clustering quality. As can be seen, NU_{cos} achieves the best score in terms of efficiency on the 11 data sets.

2.3 An illustrative example of determining the best number of clusters

Automatically determining the best number of clusters is another important need for the KCC package in practical clustering applications. The KCC package provides a demonstration script **Matlab/Drivers/demoEvacluster.m** for this purpose. The script is mainly composed of the following steps. The first step is to utilize three internal metrics, i.e., the

Distortion Score, Silhouette Coefficient, and Calinski and Harabasz index, to evaluate the quality of clustering results produced by KCC with varying number of clusters. Take the *iris* data set as an example, we show the results in Figure 2. As can be seen, on the iris data set, all three internal metrics generally decrease with the increase of K. The next step involves a selection process to find the best K based on the curve of each metric in Figure 2. For the Distortion Score, the Elbow method [Bholowalia and Kumar 2014] is used to pick the elbow point of the curve as the best K. For the Silhouette Coefficient, we choose the best K that produces a clustering solution with the maximum value of average silhouette coefficient. For the Calinski and Harabasz index, we choose the best K that produces a clustering solution with the maximum value of Calinski and Harabasz index. As indicated by the red line in Figure 2, all three methods consistently find the best number of clusters as $K = 2$ on the *iris* data set. The most important code snippet is shown below for this illustration.

```
MaxK = ceil(sqrt(size(data, 1))); % max number of clusters to choose from
distortions=zeros(MaxK, 1); % vectors storing the Distortion value for each K
silhouettes=zeros(MaxK, 1); % vectors storing the Silhouette value for each K
chs=zeros(MaxK, 1);
executiontimes=zeros(MaxK, 1); % vectors storing the execution time of running KCC
for K=1:MaxK % for each K
    tic; % record started computation time in seconds
    [pi_sumbest,pi_index,~,~~,~~~] = RunKCC(IDX,K,U,w,rep,maxIter,minThres,utilFlag);
    t = toc;
    [Distortion, Silhouette, CH] = inMeasure(data, pi_index, K);
    distortions(K,1) = Distortion;
    silhouettes(K,1) = Silhouette;
    chs(K,1) = CH;
    executiontimes(K,1)=t;
end
```

Listing 9: Using **demoEvacluster.m** to determine the best number of clusters for KCC.

3. MATLAB FUNCTIONS THAT ARE PROVIDED TO THE USER

In this section, we give the details of some important functions provided to the user. For each function, we give a brief description of the function, the syntax of invoking the function, the input parameters, the output parameters, and a discussion regarding the important details of the function.

3.1 BasicCluster_RFS

This function generates basic partition results by using K-means as a basic clustering algorithm with Random Feature Selection (RFS) strategy.

Syntax:

```
IDX = BasicCluster_RFS(Data, r, K, dist, nFeature)
```

Input parameters:

`Data` : the input data matrix

`r` : the predefined number of basic partitions in the cluster ensemble

`K` : the predefined number of clusters in the basic partitions
`dist` : the distance measure used in the K-means clustering
`nFeature` : the number of randomly selected partial features

Output parameters:

`IDX` : a matrix indicating the cluster labels of data points in the basic partitions

Discussion:

The parameter `Data` is an n × p matrix of data, whose rows correspond to n observations, and columns correspond to p features. The parameter `dist` is the distance measure used in the K-means clustering. The available options of the parameter `dist` can be found from the official documentation of the MATLAB kmeans function, and the most widely used distance metric is `'sqEuclidean'`, which denotes the squared Euclidean distance. For `'sqEuclidean'`, the centroid for each cluster is calculated as the mean of the data points in that cluster. To select features, we first sample nFeature values uniformly at random without replacement from the integers 1 to p, where p is the dimension of all features in the input data. Then the sampled values are used as the indices of the selected features. The output `IDX` is an n × r matrix indicating the cluster labels for n data points in r basic partitions. Note that this function is a non-deterministic function. Each call may yield a different output matrix IDX, due to the random feature sampling process, and the random initializations in the K-means algorithm.

3.2 BasicCluster_RPS

This function generates basic partition results using K-means as a basic clustering algorithm with Random Parameter Selection (RPS) strategy.

Syntax:

```
IDX = BasicCluster_RPS(Data, r, K, dist, randKi)
```

Input parameters:

`Data` : the input data matrix
`r` : the predefined number of basic partitions in the cluster ensemble
`K` : the groundtruth number of clusters for the input data
`dist` : the distance measure used in the K-means clustering
`randKi` : the parameter regarding the number of clusters in the basic partitions

Output parameters:

`IDX` : a matrix indicating the cluster labels of data points in the basic partitions

Discussion:

The parameter `K` indicates the groundtruth number of clusters for the input data, which is used as the lower bound of the randomized number of cluster for each basic partition when `randKi == 1`. The parameter randKi has the following options. If `randKi == 1`, this function generates a random number of cluster ranging from `K` to `sqrt(n)`, where n is the number of input data instances; if `randKi` is set to a r × 1 vector, this function produces

r basic partitions of which the i-th BP's number of clusters is RandKi(i); otherwise, this function produces r basic partitions with each partition having equal number (i.e., K) of clusters. Note that this function is a non-deterministic function. Each call may yield a different output matrix IDX, due to the random parameter selection process, and the random initializations in the K-means algorithm.

3.3 Preprocess

This function conduct some preprocessing on the input basic partition matrix `IDX` to produce the input for the final consensus clustering, as well as some auxiliary output variables that can help to save memory and accelerate computations.

Syntax:

```
 Ki, sumKi, binIDX, missFlag, missMatrix, distance, Pvector,
weight = Preprocess(IDX, U, n, r, w, utilFlag)
```

Input parameters:

`IDX` : the input basic partition matrix
`U` : the parameter regarding the chosen utility function
`n` : the number of data instances
`r` : the number of basic partitions in the cluster ensemble
`w` : the weight vector for all basic partitions
`utiFlag` : a flag indicating whether to calculate the utility value

Output parameters:

`Ki` : a row vector indicating the number of clusters in all basic partitions
`sumKi` : a matrix indicating the starting indexes for all basic partitions
`binIDX` : a sparse representation of the binary data set
`missFlag` : a flag indicating whether the input IDX matrix contains IBPs or not
`missMatrix` a matrix indicating the non-zero entries' positions in IDX for IBPs
`distance` : the distance function corresponding to a specific utility function
`Pvector` : a row vector calculated from the contingency matrix
`weight` : an adjusted weight vector adapted for convenient distance calculation

Discussion:

The parameter U is a 1×3 cell array. Its first cell U{1,1} defines the chosen type of the KCC utility function. It currently supports four different types of utility functions which correspond to four different K-means point-to-centroid distance functions, i.e., 'U_c' for Euclidean distance, 'U_H' for Kullback-Leibler Divergence, 'U_cos' for cosine similarity, and 'U_Lp' for Lp-norm. It is worth noting that 'U_Lp' corresponds the distance measure in L_p spaces, which are function spaces defined using a natural generalization of the p-norm for finite-dimensional vector spaces. The second cell U{1,2} is a parameter specifying the chosen form of the KCC utility function, i.e., 'std' for the Standard Form, and 'norm' for the Normalized Form. The third cell U{1,3} is only required to be set when 'U_Lp' is chosen as the utility function. The settings of $p = 1$, $p = 2$, and $p \rightarrow$

∞ correspond to the Manhattan distance, euclidean distance, and chebyshev distance, respectively. The parameter `w` is r $\times$ 1 weight vector, of which each entry indicates the weight value assigned to each basic partition in the optimization objective of consensus clustering. The parameter `utiFlag` is a variable indicating whether to calculate the utility value during the iterative process of the K-means clustering.

The output variable missFlag $\in \{0, 1\}$ indicates whether the input IDX matrix contains incomplete basic partitions (IBPs) or not. The output missMatrix is a mask matrix which represents the indices of the non-zero entries in IDX if there exists IBPs. The output variable distance determines the distance function to deal with the corresponding utility function defined by U{1,1}. The output vector Pvector is a 1 $\times$ r row vector calculated from the contingency matrix, i.e., $P_k^{(i)}$, which can later be used in calculating distance and utility functions. The output vector weight is a r $\times$ 1 adjusted weight vector adapted for convenient distance calculation in later K-means heuristic.

3.4 KCC

This function employs the K-means heuristic to generate a final consensus partition.

Syntax:

```
sumbest, index, converge, utility = KCC(IDX, K, U, w, weight,
distance, maxIter, minThres, utilFlag, missFlag, missMatrix, n,
r, Ki, sumKi, binIDX, Pvector)
```

Input parameters:

`IDX` : the input basic partition matrix
`K` : the number of clusters in the consensus partition
`U` : the parameter regarding the chosen utility function
`w` : the weight vector for all basic partitions
`weight` : an adjusted weight vector adapted for convenient distance calculation
`distance` : the distance function corresponding to a specific utility function
`maxIter` : the maximum number of iterations for the convergence
`minThres` : the minimum reduced threshold of objective function
`utiFlag` : a flag indicating whether to calculate the utility value
`missFlag` : a flag indicating whether there exist IBPs in IDX
`missMatrix` a matrix indicating the non-zero entries' positions in IDX for IBPs
`n` : the number of data points
`r` : the number of basic partitions in the cluster ensemble
`Ki` : a row vector indicating the number of clusters in all basic partitions
`sumKi` : a matrix indicating the starting indexes for all basic partitions
`binIDX` : a sparse representation of the binary data set
`Pvector` : a row vector calculated from the contingency matrix

Output parameters:

`sumbest` : the optimal value of the consensus clustering's objective function
`index` : the label vector for the final consensus partition

`converge` : the iterative values of objective function
`utility` : the final utility value

Discussion:

For convenience of computation, KCC function achieves the consensus clustering under four different conditions, e.g., (a) utility calculation is enabled and there are missing values (utilFlag==1 && missFlag==1); (b) utility calculation is enabled and there are no missing values (utilFlag==1 && missFlag==0); (c) utility calculation is disabled and there are missing values (utilFlag==0 && missFlag==1); (d) utility calculation is disabled and there are no missing values (utilFlag==0 && missFlag==0). Notably, we introduce a parameter called utilFlag in the KCC function to control whether the K-means heuristic computes the value of the KCC utility function, since the value of the KCC utility function might be of interest to some users in using the package. The users can choose to the enable or disable the computation of the value of the KCC utility function since it does not affect the process of K-means heuristic. Disabling the computation of the value of the KCC utility function does not affect the clustering performance and can accelerate the computation of KCC.

3.5 distance_euc

This function performs a point-to-centroid distance calculation with a euclidean distance measure.

Syntax:

```
D = distance_euc(U, C, weight, n, r, K, sumKi, binIDX)
```

Input parameters:

`U` : the 1×3 utility parameter cell array
`C` : the centroid matrix
`weight` : an $r \times 1$ adjusted weight vector
`n` : the number of data points
`r` : the predefined number of basic partitions in the cluster ensemble
`K` : the predefined number of clusters in the consensus partition
`sumKi` : a matrix indicating the starting indexes for all basic partitions
`binIDX` : a sparse representation of the binary data set

Output parameters:

`D` : an $n \times K$ point-to-centroid distance matrix

3.6 distance_cos

This function performs a point-to-centroid distance calculation with a cosine distance measure.

Syntax:

```
D = distance_cos(U, C, weight, n, r, K, sumKi, binIDX)
```

Input parameters:

`U` : the 1 × 3 utility parameter cell array
`C` : the centroid matrix
`weight` : an r × 1 adjusted weight vector
`n` : the number of data points
`r` : the predefined number of basic partitions in the cluster ensemble
`K` : the predefined number of clusters in the consensus partition
`sumKi` : a matrix indicating the starting indexes for all basic partitions
`binIDX` : a sparse representation of the binary data set

Output parameters:

`D` : an n × K point-to-centroid distance matrix

3.7 distance_kl

This function performs a point-to-centroid distance calculation with a KL-divergence measure.

Syntax:

```
D = distance_kl(U, C, weight, n, r, K, sumKi, binIDX)
```

Input parameters:

`U` : the 1 × 3 utility parameter cell array
`C` : the centroid matrix
`weight` : an r × 1 adjusted weight vector
`n` : the number of data points
`r` : the predefined number of basic partitions in the cluster ensemble
`K` : the predefined number of clusters in the consensus partition
`sumKi` : a matrix indicating the starting indexes for all basic partitions
`binIDX` : a sparse representation of the binary data set

Output parameters:

`D` : an n × K point-to-centroid distance matrix

3.8 distance_lp

This function performs a point-to-centroid distance calculation with a L_p norm measure.

Syntax:

```
D = distance_lp(U, C, weight, n, r, K, sumKi, binIDX)
```

Input parameters:

`U` : the 1 × 3 utility parameter cell array
`C` : the centroid matrix
`weight` : an r × 1 adjusted weight vector
`n` : the number of data points
`r` : the predefined number of basic partitions in the cluster ensemble

`K` : the predefined number of clusters in the consensus partition
`sumKi` : a matrix indicating the starting indexes for all basic partitions
`binIDX` : a sparse representation of the binary data set

Output parameters:

`D` : an n × K point-to-centroid distance matrix

3.9 distance_euc_miss

This function performs a point-to-centroid distance calculation over data of IBPs with a euclidean distance measure.

Syntax:

```
D = distance_euc_miss(U, C, weight, n, r, K, sumKi, binIDX,
missMatrix)
```

Input parameters:

`U` : the 1 × 3 utility parameter cell array
`C` : the centroid matrix
`weight` : an r × 1 adjusted weight vector
`n` : the number of data points
`r` : the predefined number of basic partitions in the cluster ensemble
`K` : the predefined number of clusters in the consensus partition
`sumKi` : a matrix indicating the starting indexes for all basic partitions
`binIDX` : a sparse representation of the binary data set
`missMatrix` a matrix indicating the non-zero entries' positions in IDX for IBPs

Output parameters:

`D` : an n × K point-to-centroid distance matrix

3.10 distance_cos_miss

This function performs a point-to-centroid distance calculation over data of IBPs with a cosine distance measure.

Syntax:

```
D = distance_cos_miss(U, C, weight, n, r, K, sumKi, binIDX,
missMatrix)
```

Input parameters:

`U` : the 1 × 3 utility parameter cell array
`C` : the centroid matrix
`weight` : an r × 1 adjusted weight vector
`n` : the number of data points
`r` : the predefined number of basic partitions in the cluster ensemble
`K` : the predefined number of clusters in the consensus partition

`sumKi` : a matrix indicating the starting indexes for all basic partitions
`binIDX` : a sparse representation of the binary data set
`missMatrix` a matrix indicating the non-zero entries' positions in IDX for IBPs

Output parameters:

`D` : an n × K point-to-centroid distance matrix

3.11 distance_kl_miss

This function performs a point-to-centroid distance calculation over data of IBPs with a KL-divergence measure.

Syntax:

```
D = distance_kl_miss(U, C, weight, n, r, K, sumKi, binIDX,
missMatrix)
```

Input parameters:

`U` : the 1 × 3 utility parameter cell array
`C` : the centroid matrix
`weight` : an r × 1 adjusted weight vector
`n` : the number of data points
`r` : the predefined number of basic partitions in the cluster ensemble
`K` : the predefined number of clusters in the consensus partition
`sumKi` : a matrix indicating the starting indexes for all basic partitions
`binIDX` : a sparse representation of the binary data set
`missMatrix` a matrix indicating the non-zero entries' positions in IDX for IBPs

Output parameters:

`D` : an n × K point-to-centroid distance matrix

3.12 distance_lp_miss

This function performs a point-to-centroid distance calculation over data of IBPs with a L_p norm measure.

Syntax:

```
D = distance_lp_miss(U, C, weight, n, r, K, sumKi, binIDX,
missMatrix)
```

Input parameters:

`U` : the 1 × 3 utility parameter cell array
`C` : the centroid matrix
`weight` : a r × 1 adjusted weight vector
`n` : the number of data points
`r` : the number of basic partitions in the cluster ensemble
`K` : the predefined number of clusters

`sumKi` : a matrix indicating the starting indexes for all basic partitions
`binIDX` : the sparse representation matrix
`missMatrix` a matrix indicating the non-zero entries' positions in IDX for IBPs

Output parameters:

`D` : an n × K point-to-centroid distance matrix

3.13 UCompute

This function performs a utility calculation on data sets without missing values.

Syntax:

```
util = UCompute(index, U, w, C, n, r, K, sumKi, Pvector)
```

Input parameters:

`index` : an n × 1 cluster assignment matrix
`U` : the 1 × 3 utility parameter cell array
`w` : the r × 1 adjusted weight parameter vector
`C` : the centroid matrix
`n` : the number of data points
`r` : the number of basic partitions in the cluster ensemble
`K` : the predefined number of clusters in the consensus partition
`sumKi` : a matrix indicating the starting indexes for all basic partitions
`Pvector` : a 1 × r row vector calculated from the contingency matrix

Output parameters:

`util` : the utility values calculated from the objective of consensus clustering

Discussion:

The output `util` is a 2 × 1 cell array including a utility gain and an adjusted utility value.

3.14 UCompute_miss

This function performs a utility calculation on data sets with missing values.

Syntax:

```
util = UCompute_miss(index, U, w, C, n, r, K, sumKi, Pvector, M)
```

Input parameters:

`index` : an n × 1 cluster assignment matrix
`U` : the 1 × 3 utility parameter cell array
`w` : the r × 1 adjusted weight parameter vector
`C` : the centroid matrix
`n` : the number of data points

`r` : the number of basic partitions in the cluster ensemble
`K` : the predefined number of clusters in the consensus partition
`sumKi` : a matrix indicating the starting indexes for all basic partitions
`Pvector` : a $1 \times r$ row vector calculated from the contingency matrix
`M` : a mask matrix indicating the indices of the non-zero entries in IDX

Output parameters:

`util` : the utility values calculated from the objective of consensus clustering

3.15 RunKCC

This function combines the two functions, i.e., Preprocess and KCC, for finding the consensus partition in one step.

Syntax:

```
[pi_sumbest, pi_index, pi_conv, pi_utility, t] = RunKCC(IDX,
K, U, w, rep, maxIter, minThres, utilFlag)
```

Input parameters:

`IDX` : the basic partition matrix
`K` : the predefined number of clusters in the consensus partition
`U` : the 1×3 utility parameter cell array
`w` : the $r \times 1$ adjusted weight parameter vector
`rep` : the number of repeated KCC experiments for selecting the best result
`maxIter` : the maximum number of iterations for the convergence
`minThres` : the minimum reduced threshold of objective function
`utiFlag` : a flag indicating whether to calculate the utility value

Output parameters:

`pi_sumbest`: the value of objective function in the best KCC experiment
`pi_index` : the cluster labels of the consensus partition in the best KCC experiment
`pi_conv` : the iterative values of objective function in the best KCC experiment
`pi_utility`: the utility values in the best KCC experiment
`t` : the execution time of the whole process for this function

3.16 exMeasure

This function assesses the clustering quality of the results obtained by a clustering algorithm with external validity indices.

Syntax:

```
[Acc, Rn, NMI, VIn, VDn, labelnum, ncluster, cmatrix] = exMeasure
(cluster, true_label)
```

Input parameters:

`cluster` : an $n \times 1$ cluster assignment matrix returned by a clustering algorithm

`true_label`: the true class labels for the data points

Output parameters:

`Acc` : the classification accuracy
`Rn` : the normalized Rand statistic
`NMI` : the normalized mutual information
`VIn` : the normalized Variation of Information
`VDn` : the normalized van Dongen criterion
`labelnum` : the number of unique labels in the groundtruth data
`ncluster` : the number of clusters returned by the algorithm
`cmatrix` : an ncluster × labelnum contingency matrix

Discussion:

This function implements five external validity indices, including the classification accuracy [Nguyen and Caruana 2007] (CA), normalized mutual information [Cover and Thomas 2012] (NMI), normalized Rand statistic [Rand 1971] (R_n), normalized van Dongen criterion [Dongen 2000] (VD_n), and normalized Variation of Information [Cover and Thomas 2012] (VI_n). In implementing the exMeasure function, we utilize a function called bestMap written by [Cai et al. 2005], in which a Hungarian method [Carpaneto and Toth 1980] is employed to resolve the label assignment issue in clustering.

3.17 inMeasure

This function assesses the clustering quality of the results obtained by a clustering algorithm with internal validity indices.

Syntax:

```
[Dist, Silh, CH] = inMeasure(X, cluster, k)
```

Input parameters:

`X` : the input data matrix
`cluster` : the clustering decision matrix returned by KCC
`k` : the number of clusters for KCC

Output parameters:

`Dist` : the distortion score
`Silh` : the average silhouette coefficient value of all data objects

Discussion:

This function implements two internal validity indices, including the Distortion Score [Bradley and Fayyad 1998] and Silhouette Coefficient [Kaufman and Rousseeuw 2009]. The Distortion Score corresponds to the sum of the squared distances between the data objects and the centroid of their assigned cluster.

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