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 on K-means-based Consensus Clustering (KCC) accompanying the following paper:

Hao Lin, Hongfu Liu, Junjie Wu, Hong Li, and Stephan Günnemann. 2022. Algorithm xxxx: KCC: A MATLAB Package for K-means-based Consensus Clustering. *ACM Trans. Math. Softw.*

The package was developed and tested in Matlab R2022a under Linux. To those without access to Matlab and those who prefer to use free open source software, we also investigate the usage of KCC with Octave, and find it is also compatible with Octave without additional efforts. Octave version?

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)

exMeasure.m (function to compute validity scores for clustering results)

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)

sCentroid.m, sCentroid_miss.m (auxiliary function for centroid initialization)

Drivers (illustrative examples)

data (input data for illustration)

demo.m (function for KCC with different utility functions)

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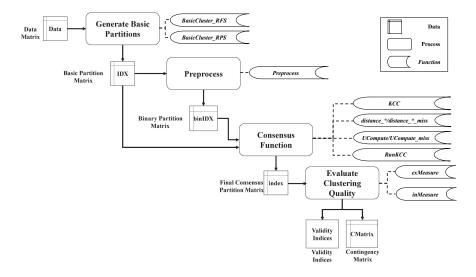


Fig. 1. Typical program flow of KCC package.

demolBPI.m (function for KCC with IBPs generated by strategy-I) demolBPII.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)

A typical workflow of the package as shown in Figure 1 is first to input a real-world data matrix Data into the basic partition generation functions for generating 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 binary matrix binIDX. The binary matrix binIDX is 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.

2. GUIDES

2.1 BasicCluster_RFS

This function generates basic partition results 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: 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 K-means clustering

nFeature : the number of randomly selected partial features

Output parameters:

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

Discussion:

The parameter Data is an $n \times p$ matrix of data, whose rows correspond to n observations, and columns correspond to p features. 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. For selecting features, we first sample n-Feature 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 a $n \times r$ cluster labels matrix 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.

2.2 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: input data matrix

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

K : the groundtruth number of clusters for the input data

 \mathtt{dist} : the distance measure used in K-means clustering

randKi : the parameter regarding the number of clusters in the basic partitions

Output parameters:

IDX : a $n \times r$ cluster labels matrix for n data points in r 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 $r \times 1$ 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.

2.3 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 partitionsutiFlag : whether to calculate utility function

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 binarization of IDX

missFlag : whether the input IDX matrix contains IBPs or not

missMatrix: indices matrix of the non-zero entries in IDX if there exists 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, $p \to \infty$ correspond to the Manhattan distance, the euclidean distance and the chebyshev distance, respectively. The parameter w is r × 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 utility function during the iterative process of K-means clustering.

The output variable $\mathsf{missFlag} \in \{0,1\}$ indicates whether the input IDX matrix contains incomplete basic partitions (IBPs) or not. The output $\mathsf{missMatrix}$ 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 corresponding distance function to deal with the specific 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.

2.4 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 partitionU : 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 : whether to calculate utility function missFlag : whether there exist IBPs in IDX

missMatrix: the indices matrix of the non-zero entries in IDX if there exists IBPs

n : the number of data points

r : the number of basic partitions in the cluster ensemble

 \mathtt{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 binarization of IDX

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 function 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. We have added more elaborations on the usage of the parameter utilFlag in the function KCC in the user manual.

2.5 distance_euc

This function performs point-to-centroid distance calculation using 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 ensembleK : 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 binarization of IDX

Output parameters:

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

2.6 distance_cos

This function performs point-to-centroid distance calculation using 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

 $\texttt{weight} \qquad : \text{an } r \times 1 \text{ adjusted weight vector}$

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 binarization of IDX

Output parameters:

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

2.7 distance_kl

This function performs point-to-centroid distance calculation using 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 $r \times 1$ adjusted weight vector

n : the number of data points

 ${\tt r}$: 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 binarization of IDX

Output parameters:

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

2.8 distance_lp

This function performs point-to-centroid distance calculation using 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 $r \times 1$ 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 binarization of IDX

Output parameters:

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

2.9 distance_euc_miss

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

Syntax:

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

Input parameters:

```
U: the 1 \times 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 binarization of IDX

missMatrix: the indices matrix of the non-zero entries in IDX if there exists IBPs

Output parameters:

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

2.10 distance_cos_miss

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

Syntax:

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

Input parameters:

```
U: the 1 \times 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 binarization of IDX

missMatrix : the indices matrix of the non-zero entries in IDX if there exists IBPs

Output parameters:

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

2.11 distance_kl_miss

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

Syntax:

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

Input parameters:

```
U: the 1 \times 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 binarization of IDX

missMatrix: the indices matrix of the non-zero entries in IDX if there exists IBPs

Output parameters:

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

2.12 distance_lp_miss

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

Syntax:

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

Input parameters:

```
U: the 1 \times 3 utility parameter cell array
```

C : the centroid matrix

weight : a $r \times 1$ 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: the indices matrix of the non-zero entries in IDX if there exists IBPs

Output parameters:

```
D \qquad : \text{an } n \times \mathsf{K} \text{ point-to-centroid distance matrix}
```

2.13 UCompute

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

Syntax:

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

Input parameters:

 $index : an n \times 1$ cluster assignment matrix : the 1×3 utility parameter cell array : the $r \times 1$ adjusted weight parameter vector

C : the centroid matrix

n : the number of data points

: the number of basic partitions in the cluster ensemble r

: the predefined number of clusters in the consensus partition sumKi: a matrix indicating the starting indexes for all basic partitions : a $1 \times r$ row vector calculated from the contingency matrix Pvector

Output parameters:

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

Discussion:

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

2.14 UCompute_miss

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

Syntax:

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

Input parameters:

 $index : an n \times 1$ cluster assignment matrix : the 1×3 utility parameter cell array

W : the $r \times 1$ adjusted weight parameter vector

С : the centroid matrix

: the number of data points

: the number of basic partitions in the cluster ensemble r

sumKi: a matrix indicating the starting indexes for all basic partitions

: a $1 \times r$ row vector calculated from the contingency matrix М : a mask matrix indicating the indices of the non-zero entries in IDX

: the predefined number of clusters in the consensus partition

Output parameters:

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

2.15 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_converge, 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

 \mathbf{w} : the $\mathbf{r} \times \mathbf{1}$ 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 : whether to calculate utility function

Output parameters:

```
pi_sumbest : the value of objective function for the best KCC experimentpi_index : the cluster assignment matrix in the consensus partition for the best KCC experiment
```

pi_converge: the iterative values of objective function for the best KCC experiment

pi_utility: the utility values for the best KCC experiment

t : the execution time cost of the whole process for this function

2.16 exMeasure

This function assesses the clustering quality of the results obtained by a clustering algorithm.

Syntax:

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

Input parameters:

```
cluster : a 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 : a ncluster × labelnum contingency matrix

Discussion:

This function implements five external validity indices, including classification accuracy [Nguyen and Caruana 2007] (CA), the normalized mutual information [Cover and Thomas 2012] (NMI), the normalized Rand statistic [Rand 1971] (R_n) , the normalized van Dongen criterion [Dongen 2000] (VD_n) , and the 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 the Hungarian method [Carpaneto and Toth 1980] is employed to resolve the label assignment issue in clustering.

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