International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor:6.887
Volume 5 Issue XI November 2017- Available at www.ijraset.com

Efficient Framework for Finding Optimal Data Partitions for Hierarchical Centroid Algorithm

Romana Riyaz[1], Irfan Rashid[2]
[1, 2] *Department of computer science University of Kashmir, Srinagar*

Abstract*: The most important task of clustering process is the validation of results obtained from clustering algorithms. There are many cluster validation criteria's but the most commonly used approaches are founded on internal validity indices. There are numerous indices that have been suggested from time to time but there are only some of them that have been popularly used. In this paper we have drawn a comparative analysis of external and internal validity measures using clustering results from hierarchical-centroid algorithm; we show the results of our experimental work which can be useful in selecting the most suitable index and providing an insight about the performance of different indices on different datasets. We have used four datasets: Iris, Gene dataset, liver disorder and Seeds datasets from UCI repository in our experiment.
Keywords: cohesion; separation; validity indices; clustering algorithms; dissimilarity; mediod.

I. INTRODUCTION

Clustering is a process of partitioning a set of data (or objects) into a set of meaningful subclasses called clusters. Data clustering is a method of creating groups of objects or clusters in such a way that objects which are in one cluster are very similar than the objects in different clusters. Clustering is an important tool for a variety of applications in data mining and has received attention in many areas including engineering, medicine, biology and data mining. Hierarchical clustering method works by grouping data objects into a tree of clusters. Hierarchical clustering methods can be further classified as either agglomerative or divisive depending on whether the hierarchical decomposition is formed in a bottom up (merging) or top down (splitting) fashion. The quality of pure hierarchical clustering method suffers from its inability to perform adjustment once a merge or split has done. If a particular merge or split decision is a poor choice the method cannot backtrack and correct it. As such, merge points need to be chosen carefully. For improving the quality of cluster integration of hierarchical agglomeration with iterative relocation method is emphasized. All agglomerative hierarchical clustering algorithms begin with each object as a separate group. These groups are successively combined based on similarity until there is only one group remaining or a specified termination condition is satisfied. For n objects, n-1 merging is done. In this paper we have presented an extensive comparison of cluster validity indexes on various real datasets in order to search for an optimal number of clusters for Hierarchical-centroid algorithm. The next section discusses work related to cluster validity indices comparison, section III provides a brief description of Proposed iterative merging framework which is used for clustering data in our experiment, section IV describes the variouscluster validity indices (CVI's) used in this paper and section V shows the experimental setup and section VI shows the main result work and finally we draw the conclusion and suggestion for further extensions.

II. RELATED WORK

Several methods have been proposed to solve the problem of cluster initialization. Some of the contributions have been discussed as under: Milligan and cooper[3] is the most citied and widely consulted paper as cluster validity indices comparison reference. They have compared 30 indices and authors have called them "stopping criteria" because they were used to stop agglomerative process of a hierarchical clustering algorithm. They used 108 synthetic datasets with a varying number of non-overlapped clusters, dimensionality and cluster size. They have presented their results in tabular format, showing the number of times that each CVI predicted the correct number of clusters. Tables also included the number of times each CVI overestimated or underestimated the real number of clusters. Dubes[14] compared two CVI's –Davies bouldin and modified Hubert statistics. The experiment is performed in 2 parallel works of 32 and 64 synthetic datasets,3 clustering algorithms(single-linkage, complete-linkage and CLUSTER) and 100 runs. Author has used statistics to test the effect of each factor on the behavior of the compared CVI's. Brunetal [15] made a comparison of 8 CVI's using several clustering's. They used 600 synthetic datasets based on 6 models with varying dimensionality(2 or 10),cluster shape and number of clusters(2 or 4).The author computed the error value for each partition by comparing it with correct partitions the correctness of CVI's is measured as its correlation with measured error values.

There are internal validity indices based on the compactness within a cluster and the separation between clusters. The sum-of-squares based indices are founded on sum-of-squares within cluster (SSW) and/or sum-of-squares between clusters (SSB) values, for example, Ball and Hall [4], Hartigan[5], Calinski-Harabasz (CH) [6] and Xu[7]. WB-index [8] is a sum-of-squares based index where a minimum value can be attained as the number of clusters. Other popular indices are given in [8–12].Dunn-type indices [9] are based on the inter-cluster distance and diameter of a cluster hyper sphere. A Dunn index is sensitive to outliers, whereas the Davies and Bouldin index is defined by the average of cluster evaluation measures for all the clusters. S_Dbw [11] replaces the total separation with the density of data objects in the middle of two clusters and omits the weighting factor. A model selection method called the Bayesian information criterion (BIC) [12] has been used in model-based clustering, it can be adapted to partition-based clustering[13], too.

III. ITERATIVE MERGING FOR CLUSTERING DATA

We propose an iterative merging approach for obtaining optimal clusters of the given data set. Two clusters are merged during each iterative step until stopping criteria (described in next section) is satisfied. The iterative merging process is described in detail below.

Iterative merging approach is based on the concept of agglomerative (bottom-up) clustering method. The idea is to build optimal clusters, where data elements are separated by natural boundaries. Merging of two clusters is based on the concept of closeness. During each iterative step, two closest clusters are merged to create a new cluster. This process is continued until optimal clusters are obtained.

The closeness of two clusters can be computed by using centroid-linkage distance. centroid linkage clustering, distance $D(c_1, c_2)$between two clustersc1 and c2 centers is used. The average distance$D(c_1, c_2)$ is the distance between the centers of two cluster C1 and C2. Mathematically it can be written as:

$$D = \|C_1 - C_2\|$$

Here, where C_1 and C_2 are the centroids of cluster C1 and C2.

IV. STOPPING CRITERIA FOR MERGING

We propose using Cluster Validity Indices(CVI)as a stopping criteria for obtaining the optimal number of clusters for the given dataset. CVI's determine how well each element is placed within its cluster. In general, clustering validity indices are defined by combining the measures of compactness and reparability. Compactness: This measure gives an indication of closeness of elements in a cluster. A common measure of compactness is given byintra cluster distance of elements in a cluster. Reparability: This measure gives an indication of how well a cluster is separated from other clusters. The intuitive way of expressing reparability is to compute inter cluster distances. On the type of the measure used (i.e. compactness measure reparability measure), we define three types of Cluster Validity Indices: i) Internal Cluster Validity Indices, this uses only compactness measure ii) External Cluster Validity Indices, this uses only reparability measure and iii) Hybrid Cluster Validity Indices, this uses both compactness and reparability measures.

A. Internal validity criteria

The internal validity indices quantify how good a particular partitioning is in terms of the compactness and separation between clusters and for this it utilizes the intrinsic structure of the data and does not require any supervised information. Some of internal validity indices are explained as under:

1) Silhouette index: Silhouete index refers to a method of interpretation and validation of clusters of data. The technique provides a succinct graphical representation of how well each object lies within its cluster by combining the measures of compactness and reparability. For each element ***i,*** leta (i) be the average distance of ***i*** with all other elements within the same cluster. a(i) canbe interpreted as how well ***i*** is assigned to its cluster(the smaller the value, the better the assignment).Let b(i) be the lowest average distance of ***i*** to any other cluster of which ***i*** is not a member. The cluster with this lowest average distance is said to be the "neighboring cluster" of ***i*** because it is the next best fit cluster for point ***i***. We now define:

$$Sil(i) = \frac{b\,(i) - a\,(i)}{max\,(a\,(i), b(i))}$$

Sil is the silhouette value for i , objectiis well fitted if Sil (i) is close to 1 and poorly fitted if Sil (i) is close to 0 or even negative. Negative values only occur when an object is not assigned to the best fitting cluster. Thus the average sil (i) over all data of the entire dataset is a measure of how appropriately the data has been clustered.

2) Calinski –Harabasz index: Calinski-Harabaszindexassess the quality of a clustering. It is given by the expression:

$$CH(k)=\frac{B(k)(k-1)}{W(k)(n-k)}$$

where *k* denotes the number of clusters and *B*(*k*) and *W*(*k*) denote the between (separation) and within (cohesion) cluster sums of squares of the partition, respectively. These are measured by the formula:

$$W=\sum_i \sum_{x\in Ci} (x-mi)2$$

$$B=\sum_i |Ci| (m-mi)^2$$

where |*Ci*| is the size of cluster *i*. An optimal number of clusters is then defined as a value of *k* that maximizes *CH*(*k*).

*3) Dunn index:*The Dunn index is based on the identification of clusters which are well separated and compact and therefore to maximize the inter-cluster distance while minimizing the intra-cluster distance. For any partition U ↔A :$A_1 \cup \cdots A_i \cup \cdots A_C$, where A_i represents the ith cluster of such partition, the Dunn's validation index, D, is given by equation:

DI (c) =$min_{i\varepsilon\, c}\left\{min_{j\varepsilon c, j\neq i}\left\{\frac{\delta(A_i,A_j)}{max_{k\varepsilon c}\{\Delta(A_k)\}}\right\}\right\}$

$$\delta(A_i,A_j) = min\{d(x_i,x_j)|x_i \varepsilon A_i\, , x_j \varepsilon A_j\}$$

$$\Delta(A_k) = max\{d(x_i,x_j)|x_i,x_j\, \varepsilon\, A_i\}$$

Where d is a distance function, $\delta(A_i,A_j)$is the inter-cluster distance and $\Delta(A_k)$ gives the maximum distance between the farthest two points within a cluster (diameter of cluster). Thus large values of D correspond to good clusters. Therefore, the number of clusters that maximizes D is taken as the optimal number of clusters.

4) Davies-bouldin index: Davies-Bouldin index was introduced by [10], it is an index which uses the measures of compactness and severability. Davies-Bouldin index (DB) is given by expression:

$$\text{DB(k)} = \frac{1}{k}\sum_{i=1}^{k} max_{j\neq i}\frac{(\Delta C_i+\Delta C_j)}{\delta(c_i,c_j)}$$

Where $\Delta(C_i)$ and $\Delta(C_j)$ denotes the intra-cluster distance, calculated as the average distance of all the cluster elements$C_i$and $C_j$to their respective cluster centers, whereas $\delta(C_i,C_j)$ denotes the distance between the clusters $C_i$and C_j(distance between the cluster centers).Therefore, the optimum number of clusters corresponds to the minimum value of DB (k).

B. External validity criteria

External validity indices measure the quality of a clustering result by bringing in some kind of external information such as known class labels or some supervised information. External validation measures know 'true' number of clusters in advance. These indices mainly quantify how good is the obtained partitioning with respect to prior class labeled information available.

1) Rand index: Rand index is an absolute criterion or referential standard that allows the use of classification datasets for performance assessment, not only of classifiers (which can produce different data partitions with the right number of classes), but of clustering results (in which different data partitions can be composed of different numbers of clusters) as well. This index handles two hard partition R=$\{R_1,\ldots.,R_k\}$ as the actual partition(reference partition)of the dataset D and Q= $\{Q_1,\ldots..,Q_s\}$ as the clustering structure of the dataset D The reference partition, R, encodes the class labels, i.e., it partitions the data into k known classes. Partition Q,in turn partitions the data into s categories(classes or clusters), and is the one to be evaluated. The categories encoded by Q will be, from now on, called clusters. This way one can easily distinguish between them and right classes encoded by R.

Thus, Rand index is given as:

$$W=\frac{a+d}{a+b+c+d}$$

Where:

a) Number of pairs of data objects belonging to the same class in R and to the same cluster in Q.

b) Number of pairs of data objects belonging to the same class in R and to different clusters in Q

c) Number of pairs of data objects belonging to different classes in R and to the same cluster in Q.
d) Number of pairs of data objects belonging to different classes in R and to different clusters in Q.

Rand index can have following values: (i) Wε [0, 1]; (ii) W = 0 iff Q is completely inconsistent, i.e., a = d = 0; and (iii) W= 1 iff the partition under evaluation matches exactly the reference partition, i.e., b = c = 0 (Q = R).

2) Adjusted Rand index: Rand index is defined as the number of pairs of objects that are either in the same group or in different groups in both partitions divided by the total number of pairs of objects. The Rand index lies between 0 and 1. When two partitions agree perfectly, the Rand index achieves the maximum value 1.Now if we adjust rand index for the chance grouping of elements then that forms adjusted rand index.

3) Jaccard index: The jaccard index is used to evaluate the stability of a clustering method. The rationale behind this index is essentially same as that of Rand index, except for the absence of term'd'. The term d is interpreted as a "neutral" term-counting pairs of objects that are not clearly indicative either of similarity or of inconsistency- in contrast to the others, viewed as counts of "good pairs"(term a) and "bad pairs"(terms b and c). From this viewpoint, the jaccard coefficient can be seen as a proportion of good pairs with respect to the sum of non-neutrals (good plus bad pairs).Given a pair of clustering solutions, R (reference partition) and Q (partition to be evaluated)for the same data set, the jaccard index between R and Q is then defined as:

$$J = \frac{a}{a+b+c}$$

Where

a) Number of pairs of data objects belonging to the same class in R and to the same cluster in Q.
b) Number of pairs of data objects belonging to the same class in R and to different clusters in Q.
c) Number of pairs of data objects belonging to different classes in R and to the same cluster in Q.

The jacquard index ranges from 0 to 1, where a higher value indicates a higher similarity between cluster solutions.

4) Fowlkes-Mallows (FM) index: Fowlkes-Mallows index measures the similarity of resulting clusters with real partition of a dataset. Consider Q=$\{Q_1,\ldots..,Q_s\}$ as a clustering structure of a dataset D, and R=$\{R_1,\ldots.,R_k\}$ as the actual partition of the dataset. The state of each pair of elements pertains to one of the following four states:

a) Number of pairs of data objects belonging to the same class in R and to the same cluster in Q.
b) Number of pairs of data objects belonging to the same class in R and to different clusters in Q.
c) Number of pairs of data objects belonging to different classes in R and to the same cluster in Q.

Thus, Fowlkes–Mallows index, is defined as

$$FM = \frac{a}{\sqrt{(a+b)(a+c)}}$$

A higher value for the Fowlkes–Mallows index indicates a greater similarity between the clusters and the benchmark classifications.

V. PROPOSED OPTIMAL CLUSTERING ALGORITHM

A. *Step 1*: Assign each data item to a cluster. N data items will result in N clusters where each cluster will have just one data item. Inter clusters distances between each pair of clusters is computed.
B. Step 2: Check for optimal number of clusters using indices. If optimal partition of data has been achieved then stop else proceed with step 3.
C. *Step 3*: Two closest clusters (determined using inter cluster distances) are merged into a single cluster.
D. *Step 4*: Inter cluster distances are updated.
E. *Step 5*: Steps 2 and 3 are repeated until all items are clustered until stopping criteria is satisfied.

VI. EXPERIMENTAL SETUP

In this section we describe the experiment performed to compare the CVI's listed in the previous section for finding optimal clusters for Hierarchical-centroid algorithm. The comparative methodology that we have used is to run Hierarchical-centroid algorithm over a dataset with different values for the 'k' parameter. Here we have used value of k =1 to 10.Then, the evaluated CVI is computed for all the partitions. The number of clusters obtaining the best results is considered as prediction of the index for that dataset. If this value matches the true number of clusters then the prediction is considered as successful. We have compared these CVI's using four real datasets from the UCI repository. Table 1-4 in the Results section shows the values of indices obtained for different values of 'k' and on different datasets respectively. Fig1-8 shows the optimal values obtained for each index for different datasets. The four datasets and their main characteristics are shown in table I.Plots1-4 in the Results section show the plots of indices obtained for

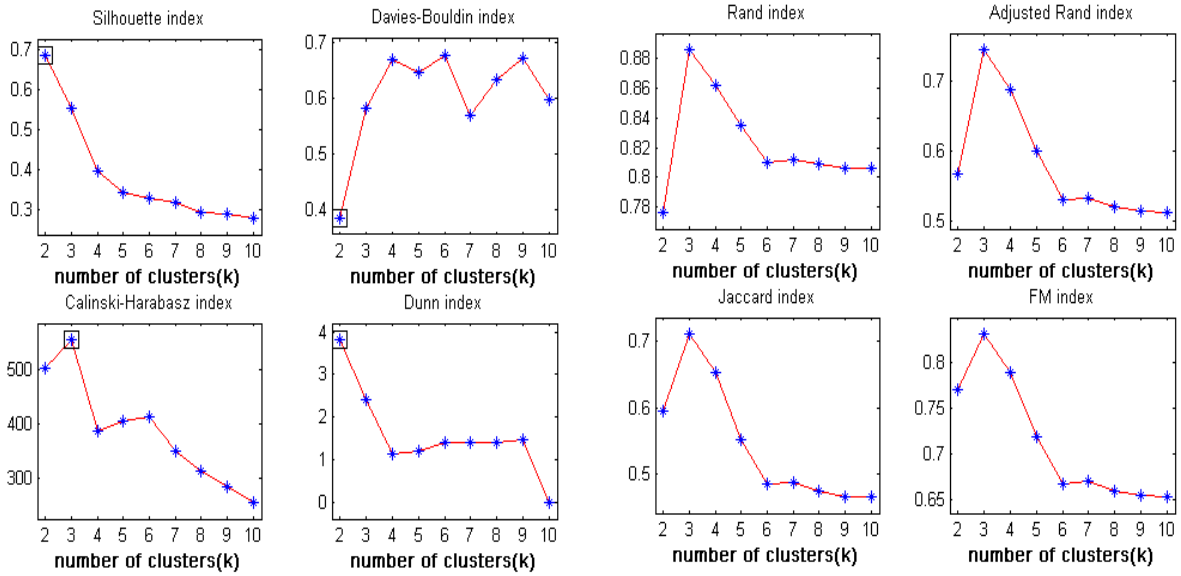
different values of 'k' and on different datasets respectively. Tables II-V shows the values obtained for each index for different datasets.

VII. RESULTS

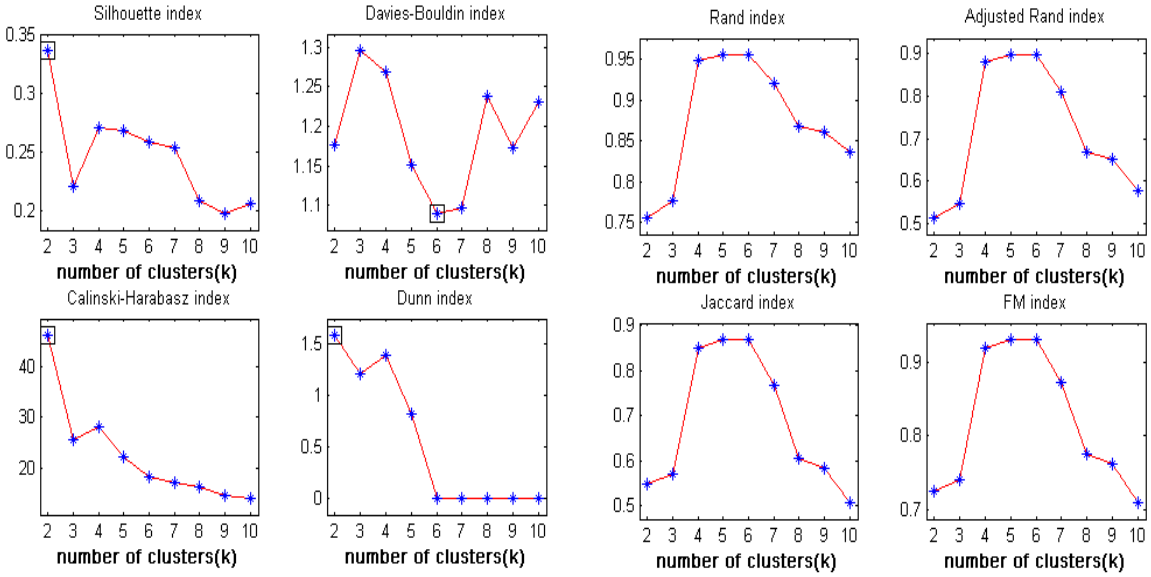
Table IThe characteristics of the real datasets.

Dataset	No. of Objects	Features	Classes
Iris	150	4	3
Gene	72	39	3
Seed	210	7	3
Liver	345	7	2

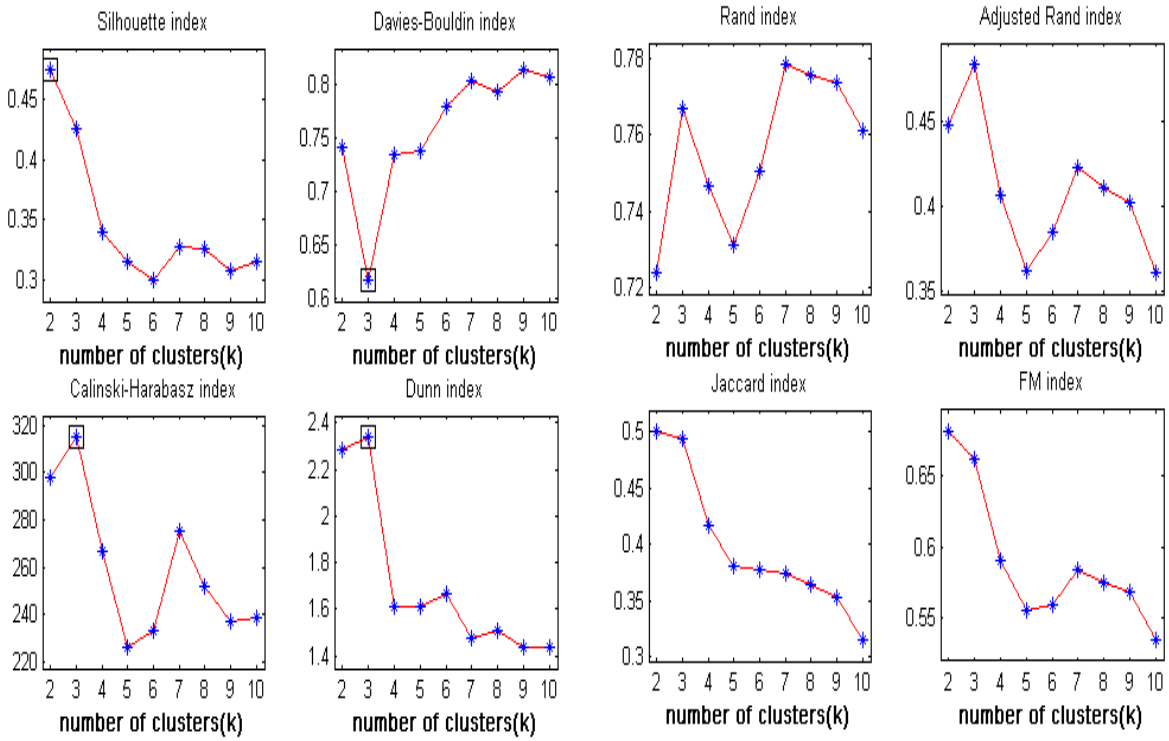
A. Plots For Iris Dataset



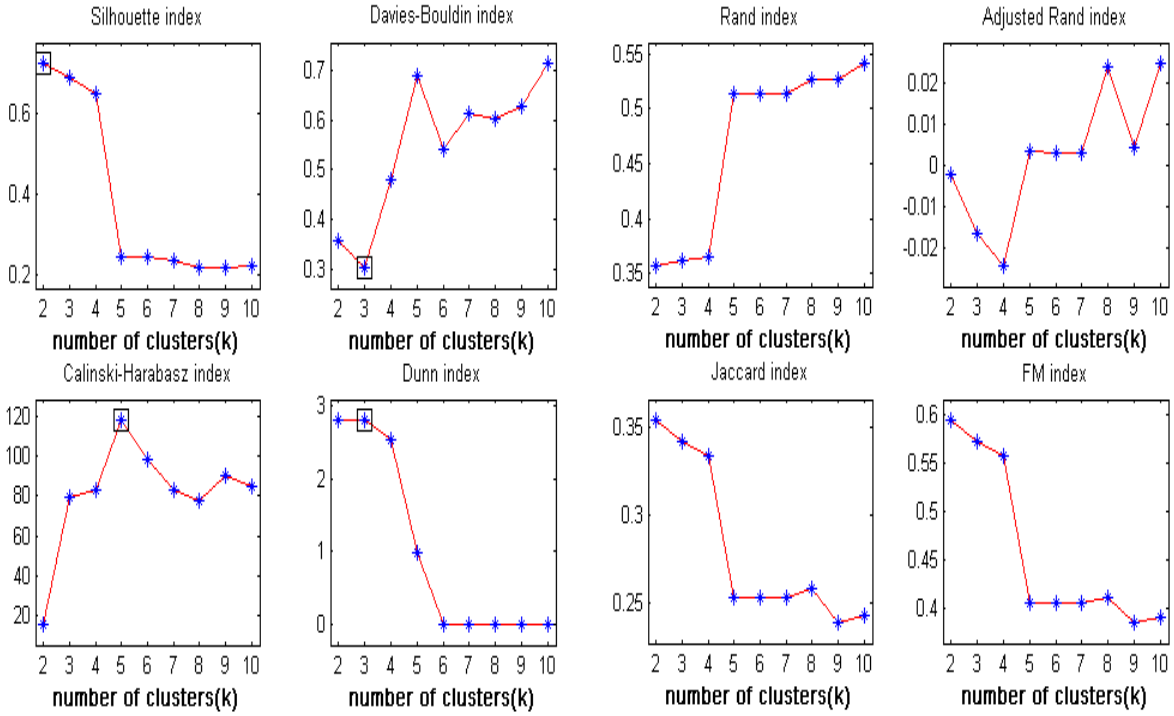
B. Plots For Gene Dataset



C. Plots For Seed Dataset



D. Plots For Liver Disorder Dataset



ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor:6.887
Volume 5 Issue XI November 2017- Available at www.ijraset.com

No. of clusters	Rand index	Adjusted Rand Index	Jaccard index	FM index	Silhouette index	Davies bouldin index	Dunn index	CH index
2	0.77629	0.56812	0.59514	0.77145	0.68639	0.3836	3.8212	501.9249
3	0.88591	0.7455	0.71186	0.83205	0.55508	0.5819	2.4132	554.9067
4	0.86228	0.68717	0.6522	0.78951	0.39645	0.67037	1.125	388.2909
5	0.83508	0.59963	0.55213	0.71967	0.34311	0.64608	1.2126	406.1216
6	0.81038	0.53003	0.48505	0.6671	0.32926	0.67791	1.4251	413.1072
7	0.81217	0.53376	0.48742	0.66986	0.31834	0.56939	1.4251	350.7682
8	0.80868	0.52061	0.47249	0.65969	0.29369	0.63393	1.4067	313.6823
9	0.80626	0.51355	0.46583	0.65425	0.28943	0.67366	1.4714	285.1101
10	0.80582	0.51224	0.46459	0.65324	0.27742	0.59895	0.0120	255.8146

TABLE I Values for k obtained for iris database

No. of clusters	Rand index	Adjusted Rand Index	Jaccard index	FM index	Silhouette index	Davies bouldin index	Dunn index	CH index
2	0.75587	0.51406	0.54848	0.72476	0.33686	1.1767	1.5819	46.0941
3	0.777	0.54944	0.57046	0.73997	0.22124	1.2957	1.2122	25.6523
4	0.94797	0.8809	0.85056	0.91953	0.27034	1.2678	1.3897	28.058
5	0.95501	0.89645	0.86812	0.93001	0.2682	1.1503	0.8137	22.2637
6	0.9554	0.89732	0.86912	0.93061	0.2584	1.0895	0	18.2421
7	0.92019	0.81105	0.76579	0.87152	0.25388	1.0966	0	17.2409
8	0.86815	0.67013	0.60446	0.77515	0.20896	1.2375	0	16.3212
9	0.8615	0.65152	0.58451	0.76205	0.19754	1.1723	0	14.6056
10	0.83568	0.57722	0.50704	0.7089	0.20638	1.2299	0	14.0701

TABLE II Values for k obtained for Gene database

No. of clusters	Rand index	Adjusted Rand Index	Jaccard index	FM index	Silhouette index	Davies bouldin index	Dunn index	CH index
2	0.72381	0.44782	0.50095	0.68201	0.47524	0.74269	2.2868	298.2568
3	0.76664	0.48391	0.49417	0.66205	0.42586	0.61777	2.3396	315.1461
4	0.7465	0.40696	0.4173	0.59035	0.3425	0.73483	1.608	266.5034
5	0.73092	0.3626	0.38148	0.55499	0.31504	0.73933	1.608	226.0421
6	0.75047	0.3847	0.37744	0.55887	0.29951	0.78018	1.6692	233.4473
7	0.77849	0.42253	0.37511	0.58349	0.32683	0.80426	1.4777	275.151
8	0.7753	0.4116	0.36448	0.57472	0.32578	0.79416	1.5102	252.0699
9	0.77366	0.4027	0.35342	0.56814	0.30785	0.81459	1.4369	237.026
10	0.76127	0.36112	0.31498	0.53372	0.31455	0.80761	1.4369	238.5425

TABLE III Values for k obtained for Seed database

No. of clusters	Rand index	Adjusted Rand Index	Jaccard index	FM index	Silhouette index	Davies bouldin index	Dunn index	CH index
2	0.35642	-0.0021772	0.35446	0.59388	0.72272	0.3576	2.7965	15.57962
3	0.36203	-0.016579	0.34146	0.57067	0.68498	0.30435	2.8087	79.77331
4	0.36517	-0.024645	0.33406	0.55767	0.64694	0.48046	2.5312	83.27218
5	0.51331	0.0032364	0.25243	0.40637	0.24537	0.68805	0.97659	118.0989
6	0.51325	0.0030192	0.25229	0.40618	0.24372	0.54097	0	98.18361
7	0.51325	0.0029597	0.25223	0.4061	0.23397	0.61346	0	83.3875
8	0.52747	0.023756	0.25771	0.41233	0.21864	0.60282	0	77.93691
9	0.52747	0.0043484	0.23808	0.38561	0.21784	0.62566	0	89.8495
10	0.54193	0.024893	0.24231	0.39062	0.22287	0.71338	0	84.59209

Table IV Values of K for Liver Disorder Dataset

VIII. CONCLUSIONS

The main conclusions that we drew by the comparison of CVI's is that external indicies outperformed internal indicies, however there are some of internal indices- Calinski-Harabasz index and duns index which gave good results on some of the datasets. However, the data does not show any conclusive observations to make any conclusion that some of the CVIs are significantly better than the rest. Although external indices performed better but the major limitation of these indices is that they need external information which for real datasets is rarely available. So, we suggest the use of multiple indices for more reliable results. This work however raises some question which suggest for further extension which will be done in future papers.

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