STATISTICAL METHODS IN ARTIFICIAL INTELLIGENCE COURSE PROJECT

Understanding of Internal Clustering Validation Measures

BY TEAM 62:
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INTRODUCTION:

Clustering is perhaps one of the most important tasks when it comes to machine-learning, it helps us in understanding the natural grouping in the dataset, finding which is a huge task in itself.
The reason for saying this is because there is no single criteria that can be said to reflect a good clustering.
However, it is necessary to validate how good our clustering actually is, in order to give some authority to our output.

In general, we can divide cluster validation into two classes, they are:
i) Internal clustering validation: This does not need any external information other than the data itself, which makes this a more generalised application in most of the cases.
ii) External clustering validation" In this, we make use of external data in order to validate our clustering . However, this kind of data might not always be available. To use this, one must know the true cluster number beforehand, which makes them applicable in only a few cases.

GOAL OF THE PAPER:

The main goal of the document is to present a detailed study of different clustering measures using some conventional aspects of clustering in general. We focus on 11 internal clustering validation measures and five aspects of clustering to be precise.

BASICS OF INTERNAL CLUSTER VALIDATION MEASURES:

In general, Internal cluster validation has two main components, they are:

i) Compactness: It tells us how tightly the cluster is packed. Different measures compute this in different ways. One can compute this using the variance of the points within the cluster or can be computed with the help of intra cluster distance.

ii) Separation: This tells us how well the clusters are separated from other clusters. This can also be realised as the inter cluster measure.

In general, we can determine the optimal cluster number by the general procedure of:

Step 1: Initialize a list of clustering algorithms which will be applied to the data set. Step 2: For each clustering algorithm, use different combinations of parameters to get different clustering results. Step 3: Compute the corresponding internal validation index of each partition obtained in step 2. Step 4: Choose the best partition and the optimal cluster number according to the criteria.
Most indices consider both of the evaluation criteria (compactness and separation) in the way of ratio or summation, such as DB, XB, and $S\ Dbw$. On the other hand, some indices only consider one aspect, such as $RMSSTD$, RS, and Γ

DIFFERENT INDICES USED FOR THE MEASURE:

Davies-Bouldin Index

In this metric, for a cluster maximum similarity with other clusters is computed. The average of similarity values of all clusters corresponds to Davies-Bouldin Index.

They capture this by estimating the cluster distribution and the distance between clusters. More nearer to the clusters and more similar the cluster distribution, more the similarity value.

Since, similarity is considered, minimum over all k's corresponds to optimal value.

Xie-Beni Index

The metric takes the from *compactness/separation.* Compactness is calculated as average intra cluster distance from centre. Separateness is calculated as maximum inter cluster distance.

Optimal value of Xie-Beni Index has to be low as compactness should be minimum and separation should be maximum.

SD Validity Index

Metric considers ratio of average standard deviation of all the clusters after training to standard deviation of total data. The ratio has to be minimum as good clustering should result in less average standard deviation. This captures compactness.

The separation value is captured using distance between the cluster centres.

Root-mean-Square std dev

Metric only measures compactness by calculating mean square of distances of sample points to their respective cluster centres.

R squared

Metric captures compactness by calculating sum of squares of distances of sample points to their respective centres. As k increases, sum of squares decreases and elbow point is taken as optimal value.

Modified Hubert T(Tow) Statistic

Metric captures separation by considering distance between cluster centres for each sample pair. As the number of clusters increases, inter cluster distance decreases so K corresponding to elbow point is optimal.

Calinski – Harabasz Index

Metric considers the form *separation/compactness.* Optimal K is given by maximum index value.

I Index

Metric is of the form *separation/compactness.* Separation captures minimum inter cluster distance and compactness captures sum of distances of sample points to respective clusters. Optimal K is given by maximum I index value.

Dunn's Index:

Metric is of form *separation/compactness.* Separation is given by minimum distance between two sample points belongs to different clusters. Compactness is given by maximum diameter among all the clusters.

Silhouette Index:

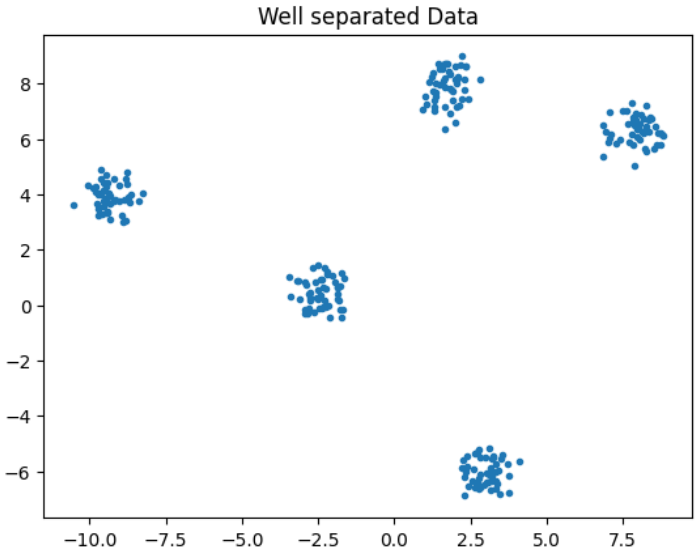
Index computes Silhouette Value for all the sample points in all the clusters. Silhouette value measures similarity of the sample point to its cluster and how distinct from the other clusters. Average value is considered as Silhouette Index.

S_Dbw validity Index:

Metric computes scattering value by computing ratio of variance of sample points belongs to a particular cluster to total data variance. The index considers density of clusters to calculate separation. K corresponding to Lowest S_Dbw value is optimal value.

WHAT WE IMPLEMENTED:

Our input data (synthetic):



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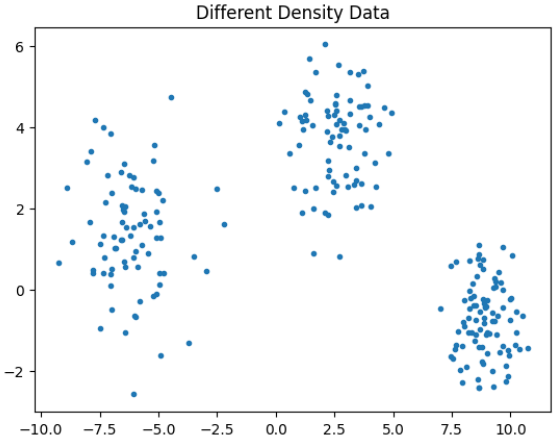
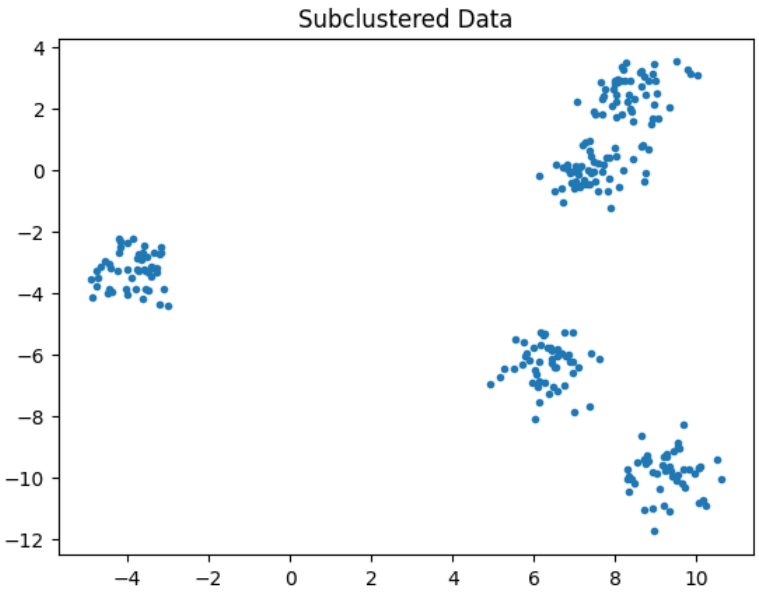
Number of clusters: 2 S_Dbw: 2.0418269705318 33
Number of clusters: 3 S_Dbw: 0.66133934489149 42
Number of clusters: 4 S_Dbw: 0.17127587255620919
Number of clusters: 5 S_Dbw: 0.089240978738393 98
Number of clusters: 6 S_Dbw: 0.1798547698635274
Number of clusters: 7 S_Dbw: 0.2753976763412074
Number of clusters: 8 S_Dbw: 0.260517316845619 96
Number of clusters: 9 S_Dbw: 0.268948157793118 87
```



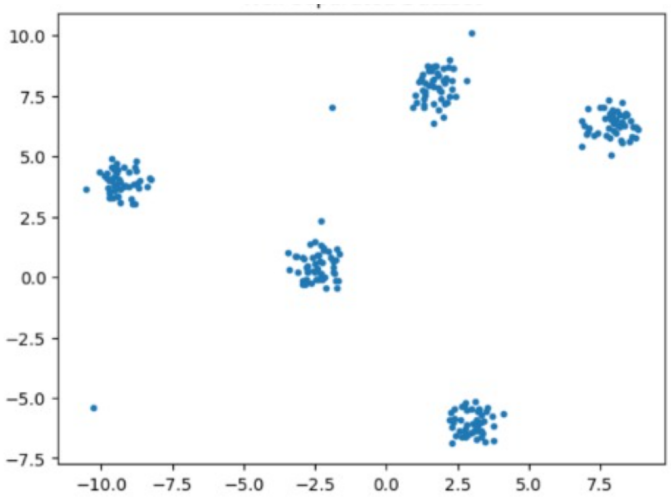

```
Number of clusters: 2 S_Dbw: 1.0403429671154 71
Number of clusters: 3 S_Dbw: 0.26014169275441 34
Number of clusters: 4 S_Dbw: 0.6090721180512298
Number of clusters: 5 S_Dbw: 0.639474699419227
Number of clusters: 6 S_Dbw: 0.7783660882230673
Number of clusters: 7 S_Dbw: 0.7997826490840996
Number of clusters: 8 S_Dbw: 0.7265993447356142
Number of clusters: 9 S_Dbw: 0.6420901651626552
```


```
Number of clusters: 2 S_Dbw: 0.9327312600163551
Number of clusters: 3 S_Dbw: 0.6822867993972872
Number of clusters: 4 S_Dbw: 0.8230960375216412
Number of clusters: 5 S_Dbw: 1.0879585647229113
Number of clusters: 6 S_Dbw: 0.8319852430748162
Number of clusters: 7 S_Dbw: 0.8680755085333061
Number of clusters: 8 S_Dbw: 0.7768138311332237
Number of clusters: 9 S_Dbw: 0.7513923900384873
```



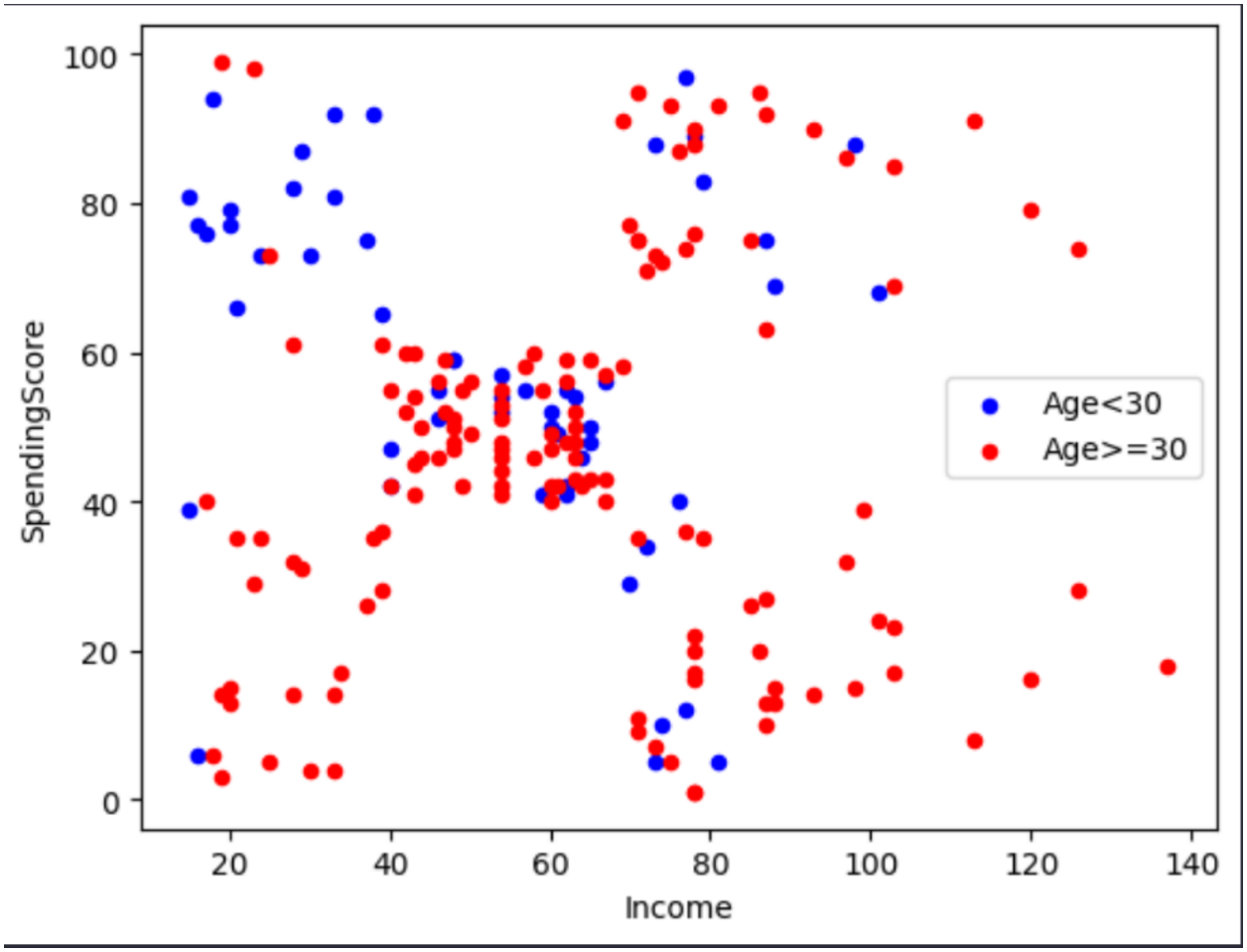

```
Number of clusters: 2 S_Dbw: 1.0643224147555246
Number of clusters: 3 S_Dbw: 0.8496724913507592
Number of clusters: 4 S_Dbw: 0.3788862164259825
Number of clusters: 5 S_Dbw: 0.3592774903104059
Number of clusters: 6 S_Dbw: 0.40883601811613
Number of clusters: 7 S_Dbw: 0.43804885090742407
Number of clusters: 8 S_Dbw: 0.39846676938302394
Number of clusters: 9 S_Dbw: 0.4218640101928597
```

On data with noise



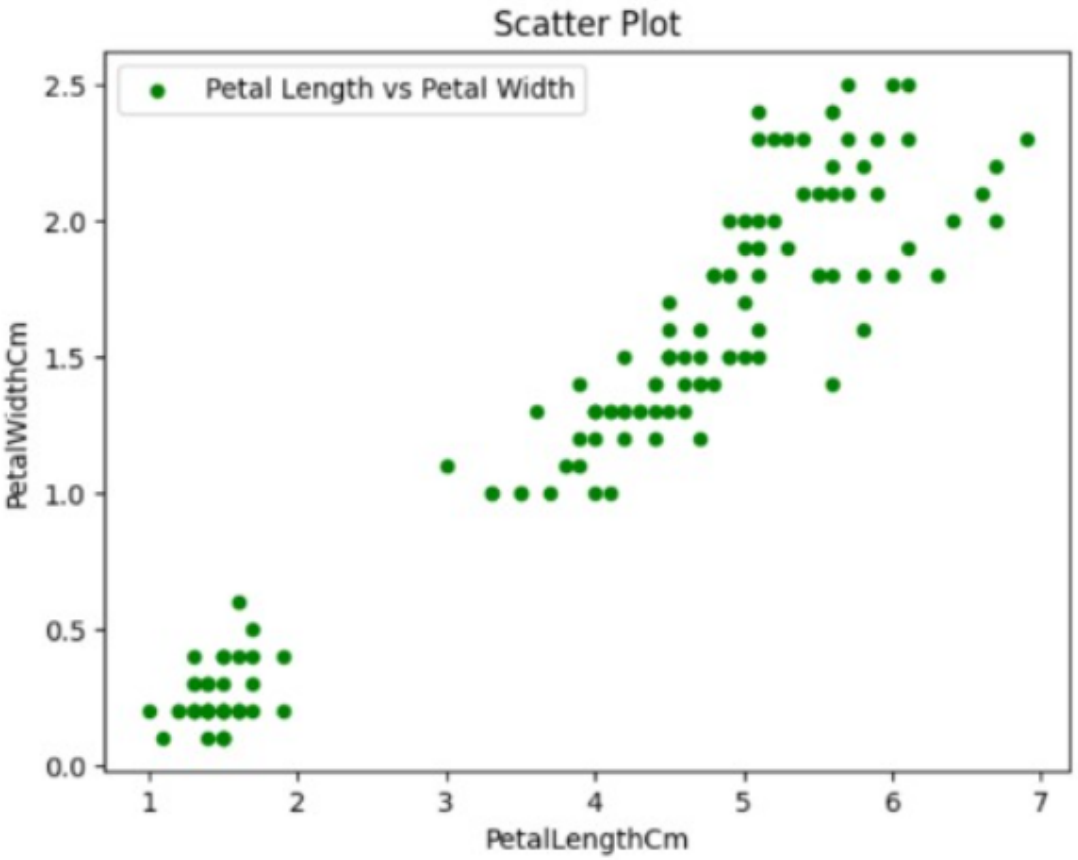
```
Number of clusters: 2 S_Dbw: 2.1296219701627104
Number of clusters: 3 S_Dbw: 0.6782522179304582
Number of clusters: 4 S_Dbw: 0.2122763755067506
Number of clusters: 5 S_Dbw: 0.11653256886266027
Number of clusters: 6 S_Dbw: 0.08003878497258043
Number of clusters: 7 S_Dbw: 0.15231010968191083
Number of clusters: 8 S_Dbw: 0.2185257781154865
Number of clusters: 9 S_Dbw: 0.223617645597107 48
```

The dataset of Mall_Customers.csv (Real life data)



```
Number of clusters: 2 S_Dbw: 1.06432241475552 46
Number of clusters: 3 S_Dbw: 0.8496724913507592
Number of clusters: 4 S_Dbw: 0.3788862164259825
Number of clusters: 5 S_Dbw: 0.3592774903104059
Number of clusters: 6 S_Dbw: 0.40883601811613
Number of clusters: 7 S_Dbw: 0.438048850907424 07
Number of clusters: 8 S_Dbw: 0.39846676938302394
Number of clusters: 9 S_Dbw: 0.4218640101928597
```

The dataset of iris.csv (Real life data)



```
Number of clusters: 2 S_Dbw: 0.6388164373972762
Number of clusters: 3 S_Dbw: 0.8156269894613086
Number of clusters: 4 S_Dbw: 0.7319831699184166
Number of clusters: 5 S_Dbw: 0.6734700533326072
Number of clusters: 6 S_Dbw: 0.5837203994935237
Number of clusters: 7 S_Dbw: 0.4019485234759874
Number of clusters: 8 S_Dbw: 0.44988288218073735
Number of clusters: 9 S_Dbw: 0.49811917692595203
```

CONCLUSION:

We concluded that out of all the measures, SDBW turned out to be the most optimal.
We also observed that when iris dataset (which has noise, is skewed and well separated) is applied, SDBW failed. Howener, we could observe that it worked well for all the synthetic data. Other than SDBW, others failed for atleast one of the variation is the data.

WHAT MORE CAN BE DONE?

Investigate further on why SDBW failed on the real world dataset.

CONTRIBUTIONS:

JAIN CHIRAG SHANTILAL(2021122004): Validation measures, data generation and Analysis on synthetic data set.
SHUBHAM PRIYADARSHAN(2020102027): Analysis of real life data.
K PAVAN KUMAR(2021122006): Validation measures and analysis of Synthetic data set.
YELLAPRAGADA SRI KRISHNA SARAT CHANDRA(2021122002): Analysed synthetically generated data.