Project 5 Report : Compare clustering methods

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Implementation details on parameters

My implementation uses all 4 methods : Kmeans clustering, Agglomerative clustering at Scipy, Agglomerative clustering at Sklearn and DBSCAN on their default setting except the following general parameters that could be changed:

- `random_state` : Random seed (set to 1 by default).
- `n_jobs` : Number of parallel threads allowed (set to 4 by default).
- `dist_metric` : To compute distance between two points (sample) (set to 'euclidean' by default).
- `n_cluster` : Number of clusters (set to 'auto' by default, estimated by the 'Elbow' method).

My implementation allows changes to the following clustering algorithm specific parameters:

- Agglomerative Clustering (at Scipy)
  - `method` denoted by `linkage_method` (set to 'ward' by default).
- Agglomerative Clustering (at Sklearn)
  - `linkage` denoted by `linkage_method` (set to 'ward' by default).
- DBSCAN
  - `eps` denoted by `eps_dbscan` (set to 'auto' by default, estimated by the nearest neighbor method).
  - `min_samples` denoted by `min_pts_dbscan` (set to 'auto' by default, estimated by the nearest neighbor method).

Apart from the above mentioned parameter some other clustering algorithm specific parameters were changed but were not provided to the user:

- Kmeans
  - `max_iter` was set to 100.
- DBSCAN
  - `algorithm` was set to 'kd_tree'.

The above represents the 'standard' setting for all regression methods when no parameter is changed.

The Elbow method for estimating n_cluster

The 'Elbow' method has been implemented in a separate class called `ClustUtility`. There were slight modifications made to the method in order to effectively pick a good `n_cluster` automatically.

A k_max was setup to avoid going over all n samples. It represents the maximum number of k the 'Elbow' method would check, it was computed as :

$$k\_max = round(\frac{n}{0.05 \cdot n}) \tag{1}$$

The idea was to push the requirement of min cluster size = 5% of data.

Next, the distortion (mse) was computed for each k $\in [1, k\_max]$:

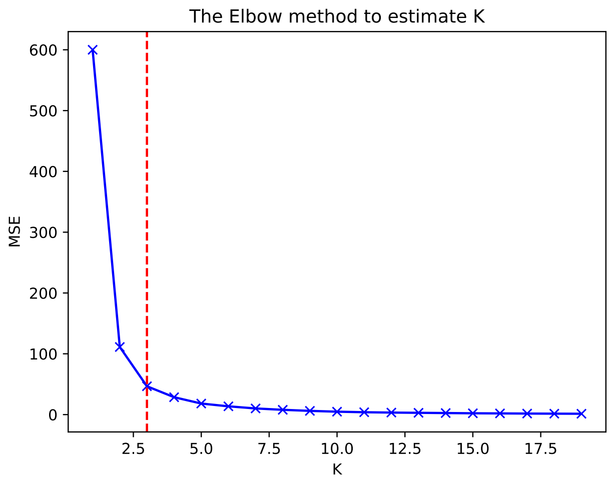
$$mse = \frac{1}{k} \sum_{i}^{n} \left(x^i - \mu_k\right)^2 \tag{2}$$

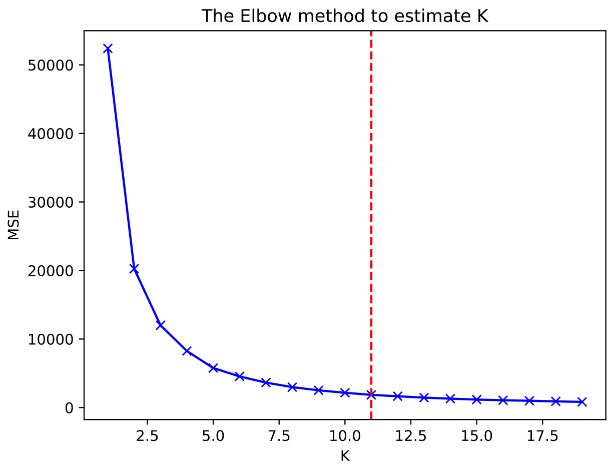
where μ^i represents the centroid of cluster k. In this case, mse is a better measure than sse as we want to compute the average pollution in each cluster as the k increases.

Next to determine a good k, the following cost function was computed :

$$cost = mse + k \cdot ||C||_1 \tag{3}$$

where $||C||_1$ is the l1 norm of C, that is, $range(1, k+1)$ or the unique labels in k clusters. This idea was borrowed from Lasso regression. It is known the the mse will decrease with increase in k, however, $k \cdot ||C||_1$ will heavily penalize larger k, causing an increase in the overall $cost$ after certain k. The last k that did not improve the $cost$, that is, the penalty term was heavier than mse (or the mse was not significant enough), was chosen as the appropriate k. It worked quite well in my humble opinion, atleast for Iris, it did pick 3 clusters which should be the optimal number. Figure 1 shows the k picked up for Iris and Faulty Steel Plates dataset.





The nearest neighbor method for estimating eps_dbscan and min_pts_dbscan

There were no major changes made for this method. I closely followed the steps mentioned in the notes, except that I choose the number of nearest neighbors K to be 5 instead of n - 1. This was done because the empirical evidence did not show any advantage of using a $K \geq 6$.

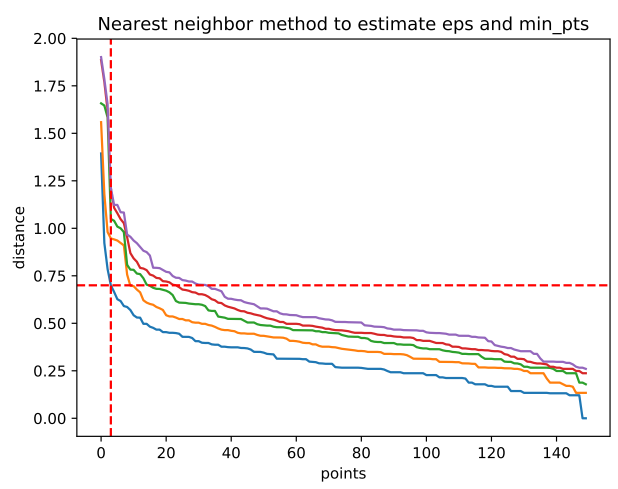
To choose the `eps_dbscan` and `min_pts_dbscan`, I again computed a $cost_k$ for each neighbor $k \in K$, given as :

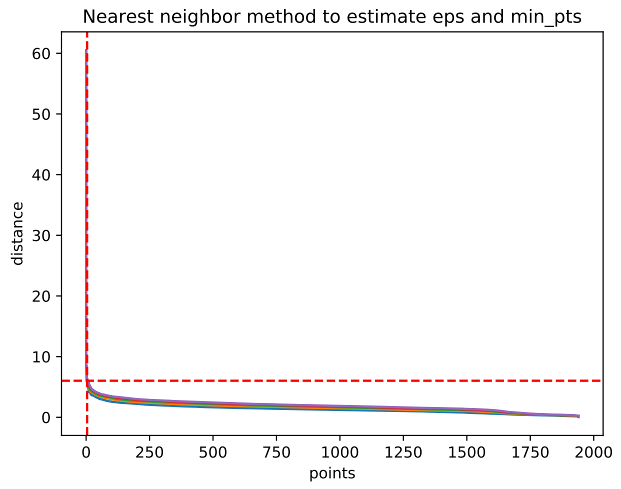
$$cost_k = argmin_{1 \leq j \leq n} dist[j] + 0.05 \cdot ||J||_2 \tag{4}$$

where $dist[j]$ was the distance jth entry of the k th column in the k-dist graph and $||J||_2$ represents the l2 norm of J, that is, $range(0, j)$. The idea here again was to penalize more number of points (j). However, this time I had to lower down the penalty by 5%, which seemed to work the best.

The smallest $cost_k$ was chosen to determine, `eps_dbscan` and `min_pts_dbscan`.

Figure 2 shows `eps_dbscan` and `min_pts_dbscan` picked up for Iris and Faulty Steel Plates dataset.





Performance evaluation

I computed the runtime, SSE and chi-square to judge the quality of the clustering methods. The chi-square method is an interesting way to utilize the class labels Y and see if the cluster labels were highly associative with Y. I used the p-value to determine the strength of association, a lower p-value better.

Performance on Iris Data-set

Info	**Kmeans**	**Agnes.scipy**	**Agnes.sklearn**	**DBSCAN**
runtime	0.029	0.003	0.0018	0.108
sse	139.8	148.8	148.8	225.2
chisq p-value	1.71E-39	5.03E-40	5.03E-40	9.95E-32

Table 1: Result on 'Iris' data-set with 'standard' configuration of 4 clustering methods.

Table 1 shows the runtime (in seconds), SSE and chisq-pvalue scores for 'Iris' data-set using the 'standard' configuration on 4 clustering algorithms : Kmeans, Agnes.scipy (Agglomerative clustering from scipy), Agnes.sklearn (Agglomerative clustering from sklearn) and DBSCAN. The data-set was scaled using the 'StandardScaler' method from sklearn. DBSCAN performs the worst on this data-set, however, I think it is expected as this dataset has more blobs than continuous patterns. Interestingly, even though Kmeans has a lower SSE, the association between the cluster labels and ground truth Y were better captured by the Agglomerative methods.

Performance on Faulty steel plates Data-set

I merged the 7 class label columns into one class label as the 'fault' always belonged to one class column for each sample.

Info	**Kmeans**	**Agnes.scipy**	**Agnes.sklearn**	**DBSCAN**
runtime	0.22	0.17	0.14	0.32
sse	20427.7	21564.9	21564.9	51401.9
chisq p-value	1	1	1	1

Table 2: Result on 'Faulty Steel Plates' data-set with 'standard' configuration of 4 clustering methods.

Table 2 shows the runtime (in seconds), SSE and chisq-pvalue scores for 'Faulty Steel Plates' data-set using the 'standard' configuration on 4 clustering algorithms : Kmeans, Agnes.scipy (Agglomerative clustering from scipy), Agnes.sklearn (Agglomerative clustering from sklearn) and DBSCAN. The data-set was scaled using the 'StandardScaler' method from sklearn. All methods do very poorly for this dataset (p-value is at its highest value of 1), however, DBSCAN was again the worst performer. Again, I think this dataset has more blobs than continuous patterns.

A more comprehensive evaluation

Since most of the parameters were automatically computed, the only parameters I could have changed were `linkage_method` and `dist_metric`, however, there were no major changes except when I changed `dist_metric` to 'cosine', all performances dropped. However, this was expected as 'cosine' distance does well for text clustering where the magnitude of the distance does not matter.