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ORIGINAL RESEARCH

Estimating the number of clusters using diversity

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Abstract

It is an important and challenging problem in unsupervised learning to estimate the number of clusters in a dataset. Knowing the number of clusters is a prerequisite for many commonly used clustering algorithms such as k-means. In this paper, we propose a novel diversity based approach to this problem. Specifically, we show that the difference between the global diversity of clusters and the sum of each cluster's local diversity of their members can be used as an effective indicator of the optimality of the number of clusters, where the diversity is measured by Rao's quadratic entropy. A notable advantage of our proposed method is that it encourages balanced clustering by taking into account both the sizes of clusters and the distances between clusters. In other words, it is less prone to very small "outlier" clusters than existing methods. Our extensive experiments on both synthetic and real-world datasets (with known ground-truth clustering) have demonstrated that our proposed method is robust for clusters of different sizes, variances, and shapes, and it is more accurate than existing methods (including elbow, Caliński-Harabasz, silhouette, and gap-statistic) in terms of finding out the optimal number of clusters.

Key Words: Clustering, Diversity

1. Introduction

Clustering is an important unsupervised learning task aiming to group a collection of items into subsets (clusters) such that those within the same cluster are more closely related (similar) to each other than to those in different clusters.[1] For many commonly used clustering algorithms (such as k-means,[1] k-medoids,[1] Gaussian mixtures,[2] and spectral clustering[3]), it is necessary to specify beforehand the number of clusters, a parameter often denoted by k as in k-means/k-medoids, to run the algorithm. However, we often do not have prior knowledge about the correct choice of k, and it is a very challenging problem to accurately estimate it by analysing the dataset itself only.[4–6] On one hand, increasing k will reduce the amount of error (in terms of data recovery[7]) in the resulting clustering, to the extreme case of full accuracy when $k = n$ the total number of items in the dataset. On the other hand, decreasing k will offer a higher compression ratio, to the extreme case of maximum compression when $k = 1$. The optimal choice of k probably lies somewhere in the middle ground, depending on the characteristics of the dataset such as its size, variance, and shape.

In this paper, we propose a novel diversity based approach to the problem of estimating the number of clusters in a dataset. A notable advantage of our proposed method is that it encourages balanced clustering by taking into account both the sizes of clusters and the distances between clusters. In other words, it is less prone to "outlier" clusters (that are much smaller than most other clusters in the dataset) than existing methods. Such a property of clustering is usually desirable in practice. For example, when using a clustering algorithm to perform image segmentation,[8] a very small cluster (segment) probably corresponds not to a complete meaningful object but only part of it, and therefore should

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be avoided. For another example, when using a clustering algorithm to perform market segmentation,[9] a very small cluster (segment) probably means that the market segment has too few customers to be profitable, and therefore should be discouraged. Obviously in some scenarios, small outlier clusters can be useful, e.g., for revealing exceptions or abnormalities in the data. However, there are many real-world applications where balanced clusters are preferred, which is the focus of this paper.

The rest of this paper is organised as follows. In Section 2, we review well-known existing methods for determining the number of clusters in a dataset. In Section 3, we describe our diversity based approach to this problem in detail. In Section 4, we present the experimental results on a number of datasets and empirically compare our proposed method with the existing methods. In Section 5, we make concluding remarks and discuss the future work.

2. Related work

The problem of estimating the number of clusters k in a dataset has been studied extensively, and many different methods have been proposed by researchers from various disciplines.[10] In this section, we review a few representative ones.

2.1 The elbow method

The elbow method[11] examines the percentage of variance explained by the clustering as a function of the number of clusters k. If we plot the percentage of variance explained against k, the first clusters will be able to explain a lot of variance, but at some point the marginal gain will drop, giving an "elbow" in the graph. The optimal k is chosen at this point, as introducing more clusters would not give a better explanation of variance in the dataset, though such an "elbow" cannot always be unambiguously identified.[12] In this paper, we use a slight variation of this method which plots the curve of the intra-cluster variance:[13]

$$E(k) = \sum_{r=1}^{k} W(C_r) \tag{1}$$

where $W(C_r)$ is the variance within the r-th cluster C_r.

2.2 The Caliński-Harabasz method

Milligan et al.[4] compared 30 different approaches to estimating the number of clusters in a dataset and found that the best performing method is given by Caliński and Harabasz:[14]

$$CH(k) = \frac{B(k)/(k-1)}{W(k)(n-k)} \tag{2}$$

where $B(k)$ is the inter-cluster variance (i.e. the sum of squared distances for the k clusters), and $W(k)$ is the intra-cluster variance. Maximising $CH(k)$ against different values of k gives the estimated number of clusters.

2.3 The silhouette method

Rousseeuw et al.[15] proposed the silhouette method, of which the main purpose is to examine whether an item i is classified well in the cluster or not. For every item or point i, its silhouette is calculated as:

$$S(i) = \frac{b(i) - a(i)}{\max(a(i), b(i))} \tag{3}$$

where $a(i)$ is the average distance of item i to all the items in the same cluster and $b(i)$ is its average distance to all the items in the nearest cluster. The i-th item is well clustered if the value of $S(i)$ approaches the maximum which is 1; and a $S(i)$ value 0 means that item i belongs to the other cluster. After plotting the silhouette score averaged over all the items against different values of k, the right number of clusters is estimated to be the k yielding the highest average silhouette score.

2.4 The gap-statistic method

Tibshirani et al.[16] proposed another method, gap-statistic, which compares intra-cluster variance with the expected values under the null reference distribution of the dataset. After clustering the dataset for different values of k, we get the intra-cluster variance for the observed dataset as well as the reference dataset, and then calculate the gap-statistic as:

$$Gap_n(k) = E_n^*\{\log(W(k))\} - \log(W(k)) \tag{4}$$

where $W(k)$ is the total intra-cluster variance and $E_n^*\{.\}$ denotes the expectation under a sample of size n from the reference distribution. The gap-statistic measures the deviation of the observed $W(k)$ value from its expected value under the null hypothesis.

3. Our approach

One drawback of the above mentioned methods for estimating the number of clusters is that they could lead to very imbalanced clustering, where some "outlier" clusters are much smaller than the other clusters. This is often undesirable for real-life clustering applications (see Section 1). Here we propose a novel *diversity* based approach to the problem of estimating the number of clusters, which is less tolerant to such "outlier" clusters and encourages balanced clustering by taking into account both the sizes of clusters and the distances between clusters.

3.1 Rao's quadratic entropy

The requirement of balance among clusters, in fact, implies that there should be no particular cluster dominating the dataset, i.e., there should be a certain level of diversity among clusters.

The concept of diversity, originated from ecology,[17] has been widely diffused into many other scientific disciplines[18,19] (such as linguistics and sociology). In recent years, a variety of quantitative measures of diversity have been successfully applied in computer science for web search,[20–24] text mining,[25] and recommender systems.[26]

Although there exist many different diversity measures (such as Simpson's and Shannon's) and it is debatable which diversity index is the best,[27,28] we choose to use Rao's quadratic entropy[29] to measure the diversity of data, because it takes into account both the sizes of species (groups) and the distances between species (groups). Rao's quadratic entropy is defined as:

$$Div = \sum_{i=1}^{s}\sum_{j=1}^{s} p_i p_j \delta(i,j) \tag{5}$$

where s is the number of species, p_i and p_j are the proportions of species i and j respectively, and $\delta(i,j)$ is the distance between them. Euclidean distance is used throughout this paper, but other distance metrics could be used as well.

3.2 The diversity method

To find out the optimal number of clusters in a dataset with n items, we use the output of the given clustering algorithm (such as k-means) and then measure the difference between the global diversity of clusters and the sum of each cluster's local diversity of their members, denoted by $Q(k)$ and given by

$$Q(k) = Div^G - \sum_{r=1}^{k} Div_r^L \tag{6}$$

where Div^G is the global diversity of k clusters (with each cluster as a species) while Div_r^L is the local diversity of the r-th cluster (with each member item of the cluster as a species) as measured by Rao's quadratic entropy given in Equation (5). We calculate the diversity based statistic $Q(k)$ for various values of k, i.e., for k from 1 to n, and the maximum value of $Q(k)$ should be able to tell us the optimal number of clusters in the dataset, i.e.,

$$\hat{k} = \arg\max_{1 \le k \le n} Q(k) \tag{7}$$

The underlying intuition of this diversity method is that in a good clustering, the items within each cluster should be as homogeneous as possible (i.e., less local diversity), while the clusters themselves should be as heterogeneous as possible (i.e., more global diversity). The balance of cluster sizes is actually implied by a high level of diversity among clusters.

The approaches to estimating the number of clusters can be divided into two categories, global methods and local methods, as pointed out by Gordon.[30] The former evaluate some measure over the entire dataset and optimise it as a function of the number of clusters; the latter consider individual pairs of clusters and decide whether they should be amalgamated.[16] Obviously the diversity method proposed by us is a global method. According to Gordon,[30] most global methods suffer from a serious disadvantage that they are undefined for one cluster (i.e., $k = 1$) and therefore cannot be used to determine whether the dataset should be clustered at all. It is worth mentioning that our diversity method does not have this shortcoming: $Q(k)$ is well defined for $k = 1$, as we show later in Section 4.2.

4. EXPERIMENTS

4.1 Balance

As can be seen in Equation (5), Rao's quadratic entropy takes into account the sizes of clusters and the distances between clusters, which is important to achieve *balanced* clustering desirable in many real-life clustering applications.

For the purpose of investigating the trade-off between the sizes of clusters and the distances between clusters, we first create two clusters from two 2-dimensional standard normal distributions which have 1,000 items each and are centred at (0,0) and (0,5) respectively, and then we create another cluster from one 2-dimensional standard normal distribution with varying number of items from 1 to 1,000 (i.e., we generate 1,000 different datasets). Following this, we move the third cluster's centre (x, y) as follows: we keep y at 2.5 (halfway from the first cluster's centre to the second cluster's centre), and gradually increase x from 0 to $+\infty$ until the third cluster is detected by our proposed diversity method as a separate, third, cluster.

The results of the simulation study are shown in Figure 1, which indicates that using the diversity method to estimate the number of clusters, a small cluster needs to be distant from the other clusters in the dataset to be regarded as a separate cluster, otherwise it will be assimilated into another nearby cluster: the smaller the cluster, the larger its distance to the other clusters should be. In other words, the diversity method tends to avoid suggesting very small clusters unless they are very far away from the rest of data.

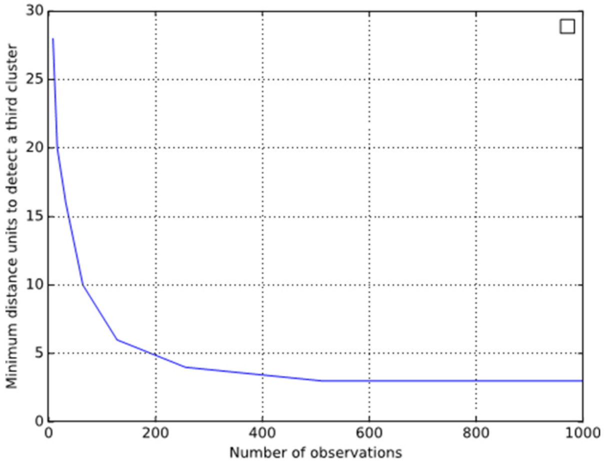
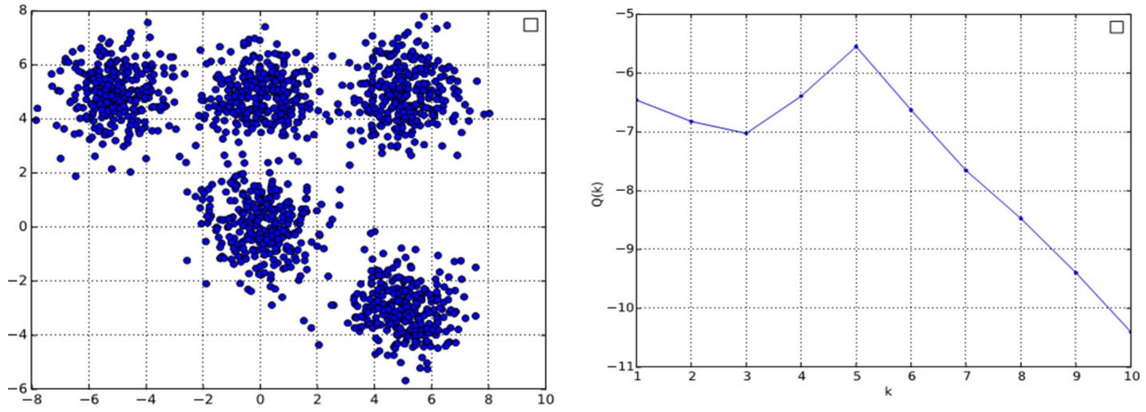


Figure 1. The trade-off between the sizes of clusters and the distances between clusters

4.2 Robustness

In this section, we investigate how robust our proposed diversity method is when it is applied to different types of datasets.

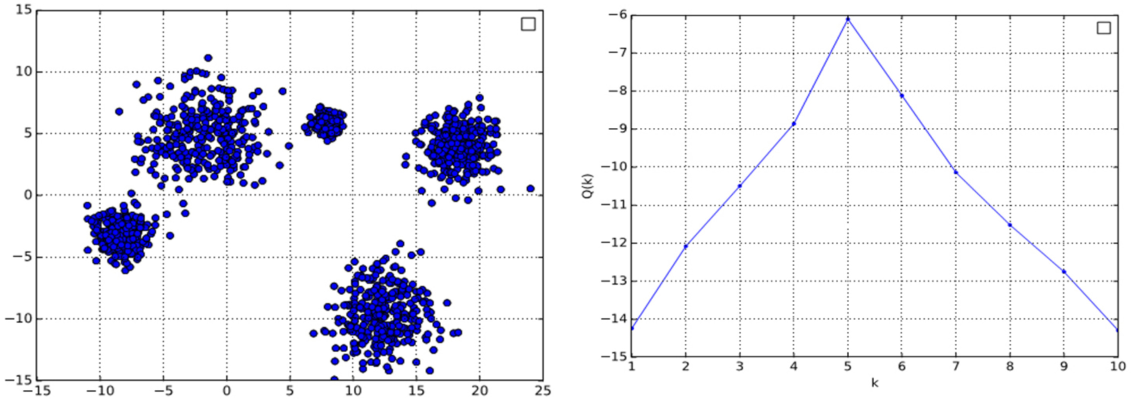
For this purpose, we create five synthetic datasets of different sizes, variances, and shapes. In addition, we also make use of three real-world datasets — Wine, Breast Cancer, and Thyroid Disease — from the UCI Machine Learning Repository.[31] On these synthetic and real-world datasets, we cluster the data points into k clusters with k from 1 to n (using k-means for the first three synthetic datasets and the first real-world dataset, but average-link hierarchical agglomerative clustering[32] for the remaining datasets), and calculate the value of $Q(k)$ for each k. The actual number of clusters in the dataset is estimated to be the k that maximises $Q(k)$ (see Section 3). It can be seen from the experimental results in Figures 2-7 that for both synthetic and real-world data, no matter what size, variance, or shape the dataset has, our proposed diversity method can successfully discover the correct number of clusters.



(a) Dataset

(b) Diversity based statistic $Q(k)$

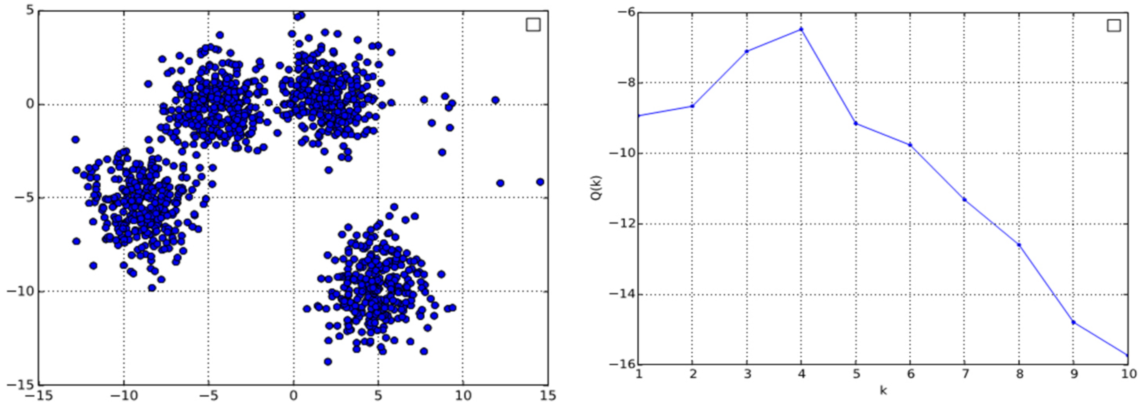
Figure 2. Experimental results on the synthetic dataset of five clusters with equal sizes and equal variances



(a) Dataset

(b) Diversity based statistic $Q(k)$

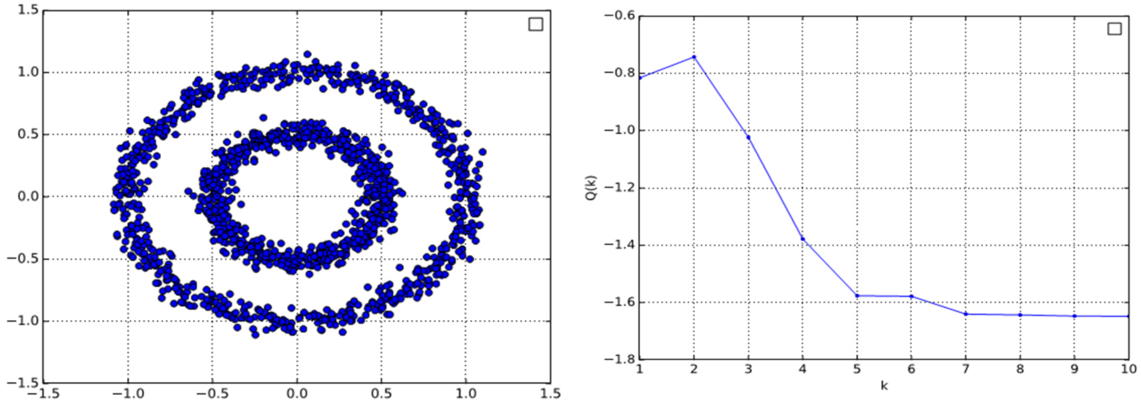
Figure 3. Experimental results on the synthetic dataset of five clusters with equal sizes but different variances



(a) Dataset

(b) Diversity based statistic $Q(k)$

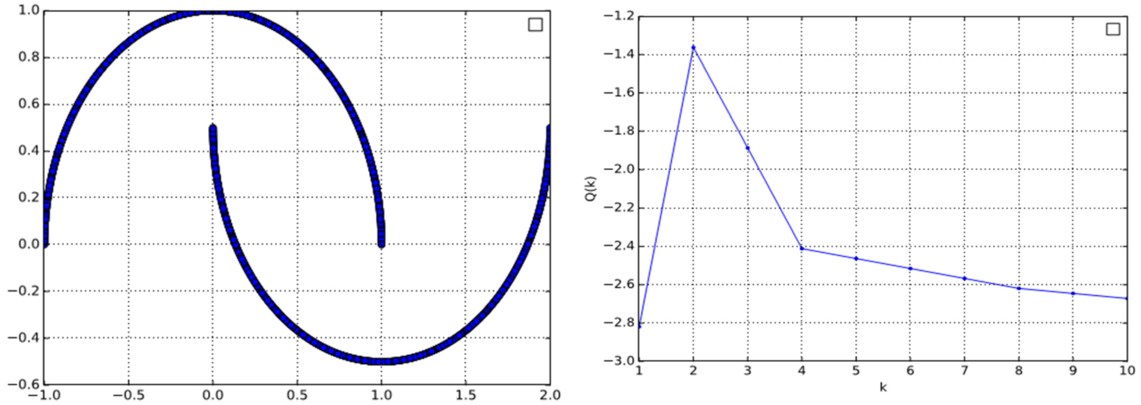
Figure 4. Experimental results on the synthetic dataset of four clusters with different sizes and some random noise



(a) Dataset

(b) Diversity based statistic $Q(k)$

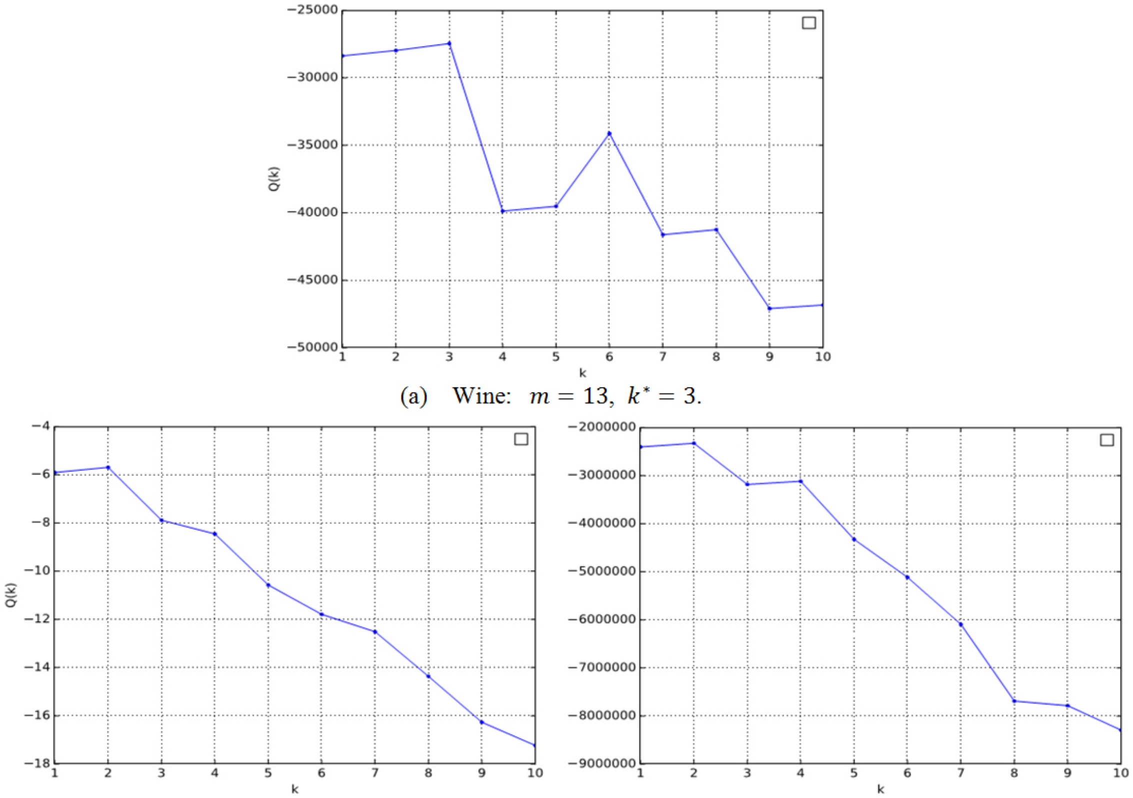
Figure 5. Experimental results on the synthetic dataset of two ring-shape clusters



(a) Dataset

(b) Diversity based statistic $Q(k)$

Figure 6. Experimental results on the synthetic dataset of two moon-shape clusters



(a) Wine: $m = 13,\ k^* = 3$.

(b) Breast Cancer: $m = 9,\ k^* = 2$.

(c) Thyroid Disease: $m = 5,\ k^* = 2$.

Figure 7. Experimental results on three real-world datasets from the UCI Machine Learning Repository, where m and k* are the number of features/dimensions and the actual number of clusters respectively in the corresponding dataset.

4.3 Comparison

We use four synthetic datasets to evaluate the proposed diversity method and compare it with the other methods reviewed in Section 2, i.e., elbow, Caliński-Harabasz, silhouette, and gap-statistic. Note that the same experimental methodology was used by the gap-statistic paper.[16]

Those datasets are intentionally made to differ in the number of clusters, the number of dimensions, and the number of items. They are defined as follows.

- Four clusters in 2 dimensions; their sizes are 250, 250, 250, and 500 respectively; their centres are (1,3), (0,8), (8,0) and (4,-2) respectively.
- Four “normal” clusters and one small “outlier” cluster in 2 dimensions; the sizes of those “normal” clusters are 1,000, 900, 900, and 850 respectively while the size of that “outlier” cluster is randomly set to a number between 50 and 100; their centres are chosen randomly.
- Five clusters in 10 dimensions; their number of items are randomly set to either 50 or 100; their centres are chosen randomly.
- Six clusters with the same settings as in the previous case of five clusters except that the number of dimensions is set to 4.

The items (data points) in each such cluster are all sampled from a particular standard multivariate normal distribution.

For each scenario defined above, we generated 50 concrete datasets so as to carry out 50 simulation trials. Then we used the chosen clustering algorithm to divide the generated dataset into k clusters with k varying from 1 to 9. On the basis of the clustering results, we apply the diversity method and the other methods in comparison to make estimations about the actual number of clusters.

The experimental results of the simulation study are summarised in Table 1. Each number in the table shows how many times a particular method detected the number of clusters mentioned in its column header. In the first case where there is little noise, all the methods performed almost equally well. In the second case where there is a lot of noise, it can be clearly seen that the diversity method outperformed all the other methods significantly. In the third and fourth cases, the diversity method worked best with near-perfect accuracy, closely followed by the gap-statistic method (which is widely regarded as the state-of-the-art).

Table 1. Experimental results on the synthetic datasets showing how many times out of 50 simulation trials a particular method estimated the number of clusters to be $\hat{k}$, where the column corresponding to the correct number of clusters is annotated with *.

Method	**Estimates of the following numbers of clusters $\widehat{k}$**								
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
a) Ground truth: 4 clusters (relatively clean)									
elbow	0	0	1	49^{*}	0	0	0	0	0
silhouette	0	0	0	50^{*}	0	0	0	0	0
Caliński-Harabasz	0	0	0	50^{*}	0	0	0	0	0
gap-statistic	0	0	0	50^{*}	0	0	0	0	0
diversity	0	0	0	50^{*}	0	0	0	0	0
b) Ground truth: 4 clusters (relatively noisy)									
elbow	0	0	5	29^{*}	16	0	0	0	0
Caliński-Harabasz	0	0	1	0^{*}	49	0	0	0	0
silhouette	0	0	0	39^{*}	11	0	0	0	0
gap-statistic	0	0	0	14^{*}	36	0	0	0	0
diversity	0	0	0	48^{*}	2	0	0	0	0
c) Ground truth: 5 clusters									
elbow	0	1	0	5	44^{*}	0	0	0	0
Caliński-Harabasz	0	7	0	6	37^{*}	0	0	0	0
silhouette	0	2	0	9	39^{*}	0	0	0	0
gap-statistic	0	0	0	0	48^{*}	2	0	0	0
diversity	0	0	0	1	49^{*}	0	0	0	0
d) Ground truth: 6 clusters									
elbow	0	0	0	0	8	42^{*}	0	0	0
Caliński-Harabasz	0	6	0	0	8	36^{*}	0	0	0
silhouette	0	0	0	0	12	38^{*}	0	0	0
gap-statistic	0	0	0	0	0	49^{*}	1	0	0
diversity	0	0	0	0	0	50^{*}	0	0	0

5. Conclusions

The main research contribution of this paper is a novel diversity based approach to the problem of estimating the number of clusters in a dataset. To the best of our knowledge, the underlying connection between diversity and clustering has not been revealed before in research literature.

Specifically, we show that the difference between the global diversity of clusters and the sum of each cluster's local diversity of their members can be used as an effective indicator of the optimality of the number of clusters, where the diversity is measured by Rao's quadratic entropy. A notable advantage of our proposed method is that it encourages balanced clustering by taking into account both the sizes of clusters and the distances between clusters. In other words, it is less prone to very small "outlier" clusters than existing methods.

Our extensive experiments on both synthetic and real-world datasets (with known ground-truth clustering) have demonstrated that our proposed method is robust to clusters of different sizes, variances, and shapes, and it is more accurate than existing methods (including elbow, Caliński-Harabasz, silhouette, and gap-statistic) in terms of finding out the optimal number of clusters.

It would be meaningful to explore the usage of diversity measures other than Rao's quadratic entropy, which is left for future work. It would also be interesting to compare our approach to estimating the number of clusters with those clustering algorithms that have built-in ability of detecting the number of clusters (such as DBSCAN,[33] OPTICS,[34] and affinity propagation[35]).

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