On the performance of ant-based clustering

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Abstract. Ant-based clustering and sorting is a nature-inspired heuristic for general clustering tasks. It has been applied variously, from problems arising in commerce, to circuit design, to text-mining, all with some promise. However, although early results were broadly encouraging, there has been very limited *analytical* evaluation of the algorithm. Toward this end, we first propose a scheme that enables unbiased interpretation of the clustering solutions obtained, and then use this to conduct a full evaluation of the algorithm. Our analysis uses three sets each of real and artificial data, and four distinct analytical measures. These results are compared with those obtained using established clustering techniques and we find evidence that ant-based clustering is a robust and viable alternative.

1 Introduction

Ant-based clustering and sorting [4] was inspired by the clustering of corpses and larval-sorting activities observed in real ant colonies [3]. The algorithm's basic principles are straightforward [16]: ants are modelled by simple agents that randomly move in their environment, a square grid with periodic boundary conditions. Data items that are scattered within this environment can be picked up, transported and dropped by the agents. The picking and dropping operations are biased by the similarity and density of data items within the ants' local neighbourhood: ants are likely to pick up data items that are either isolated or surrounded by dissimilar ones; they tend to drop them in the vicinity of similar ones. In this way, a clustering and sorting of the elements on the grid is obtained. Hence, like ant colony optimisation (ACO, [6]), ant-based clustering and sorting is a distributed process that employs positive feedback. However, in contrast to ACO, no artificial pheromones are used; instead, the environment itself serves as stigmergic variable [5].

One of the algorithm's particular features is that it generates a clustering of a given set of data through the embedding of the high-dimensional data items onto a two-dimensional grid; it has been said to perform both a vector quantisation and a topographic mapping at the same time, much as do self-organising feature maps (SOMs, [12]). While this would be an attractive property, (i) there has been little thorough analysis of the algorithm's actual performance in terms of *clustering* and (ii) it is unclear to what degree the *sorting* really is topology-preserving (cf. [10]).

In this paper, we address only the *first* of the above issues: *ant-based clustering*, that is, the algorithm's application to *pure cluster analysis*. Towards this goal we present:

- A technique to convert the spatial embedding generated by the ant algorithm, which *implicitly* contains clusters, to an *explicit* partitioning of the data set.

- Results on synthetic and real data sets. Evaluation is done using four different analytical evaluation measures. We compare the outcome to *k-means* and to *hierarchical agglomerative clustering* based on the linkage metric of *average link*.

The remainder of this paper is structured as follows. Section 2 briefly introduces the problem domain and Section 3 reviews previous work on ant-based clustering. Section 4 presents the algorithms used within our comparative study. The employed test data and evaluation measures are explained in Section 5. Results are presented and discussed in Section 6, and Section 7 concludes.

2 Clustering

Clustering is concerned with the division of data into homogenous subgroups. Informally, the objective of this division is twofold: data items within one cluster are required to be similar to each other, while those within different clusters should be dissimilar. Problems of this type arise in a variety of disciplines ranging from sociology and psychology, to commerce, biology and computer science, and algorithms for tackling them continue to be the subject of active research. Consequently, there exists a multitude of clustering methods, which differ not only in the principles of the algorithm used (which of course determine runtime behaviour and scalability), but also in many of their most basic properties, such as the data handled (numerical vs. categorical and proximity data), assumptions on the shape of the clusters (e.g., spherically shaped), the form of the final partitioning (hard vs. fuzzy assignments) or the parameters that have to be provided (e.g., the correct number of clusters).

The four main classes of clustering algorithms available in the literature are *partitioning methods*, *hierarchical methods*, *density-based clustering* and *grid-based clustering* (see [1] for an extensive survey). For the purpose of our comparative study we select two of the most popular and well-studied algorithms: k-means, a representative of the class of partitioning methods, and agglomerative average link clustering, which is a hierarchical approach. Both algorithms are described in more detail in Section 4.

3 Ant-based clustering in the literature

Ant-based clustering and sorting was originally introduced for tasks in robotics by Deneubourg et al. [4]. Lumer and Faieta [16] modified the algorithm to be applicable to numerical data analysis, and it has subsequently been used for data-mining [17], graph-partitioning [15, 14, 13] and text-mining [11, 20, 10].

While many of the obtained results 'look' promising, there is a lack of knowledge on the actual clustering performance of the algorithm. The evaluation of the results has, to a large extent, been based on visual observation. Analytical evaluation has mainly been used to track the *progress* of the clustering process, using evaluation functions (grid entropy and local dissimilarity) that provide only very limited information on the *overall quality* of the clustering and the sorting obtained [4, 16, 13, 20]. More enhanced analytical evaluation measures have been employed in [14] and [10] (non-metric stress and Pearson correlation), but their focus is on measuring the degree of *topology-preservation*, not the *clustering quality*. Classical evaluation measures for cluster analysis (cluster entropy and purity) have been used in a single paper, which, unfortunately, merely provides results for one single run on a small

document collection [11]. Only for the specialised application of graph-partitioning are analytical results (error rate and inter-vertex cuts) on a family of pseudo-random graphs and the corresponding values for the classical Fiduccia-Mattheyses heuristic, available [15]. Additionally, the range of benchmark data sets employed has been very limited. Apart from the pseudo-random graphs used by Kuntz et al. [15], one rather simple synthetical data set has been used in most of the work.

Note that Monmarché has introduced an interesting hybridisation of ant-based clustering and the k-means algorithm, and compared it to traditional k-means on various data sets, using the classification error for evaluation purposes [18]. However, the results obtained with this method are not applicable to ordinary ant-based clustering since it differs significantly from the latter.

Looking at the previous evaluations of ant-based clustering, one is inclined to ask why evaluation measures for cluster analysis have found so little application. Certainly, this is not for a lack of measures, as the data-mining literature provides a large pool of functions for the evaluation of partitionings both when the real cluster structure is known and when it is unknown (cf. [7] for a survey). The main problem is one related to the nature of the algorithm's outcome: it does not generate an *explicit partitioning* but a *spatial distribution* of the data elements. While this may contain clusters 'obvious' to the human observer, an evaluation of the clustering performance requires the retrieval of these clusters, and it is not trivial to do this without human interaction (e.g., 'marking' of the clusters) and without distorting the results (e.g., by assuming that the correct number of clusters has been identified, as done in [15]). A rigorous evaluation of the performance of ant-based clustering requires a solution to this problem.

4 Algorithms

We will now detail the three algorithms used in our comparative study, starting with a short description of the ant-based algorithm and the method developed to retrieve clusters from the grid.

Ant-based clustering: While the ant algorithm is mainly based on the version described in [10], a number of modifications have been introduced that improve the quality of the clustering, the time performance, and, in particular, the spatial separation between clusters on the grid, which is essential for the scheme of cluster retrieval introduced below. A detailed description can be found in an extended version of this paper [9], and results on the qualitative performance gains afforded by these extensions are provided in [8].

Cluster retrieval: In order to make the clusters identified by ant-based clustering explicit, we apply an agglomerative hierarchical clustering algorithm to the positions of the data items on the grid. The algorithm starts by assigning each data item on the grid to an individual cluster, and proceeds by merging the two least distant clusters (in terms of spatial distance on the grid) in each iteration, until a stopping criteria is met.

Given two clusters C_i and C_j on the grid and, without loss of generality, $|C_i| \leq |C_j|$, we define their spatial distance in grid-space as

$$weighted\_singlelink(C_i, C_j) = singlelink(C_i, C_j) \cdot weight(C_i, C_j).$$

Here, $singlelink(C_i, C_j)$ is the standard *single link* linkage metric, i.e. the minimal distance between all possible pairs of data elements i and j with $i \in C_i$ and $j \in C_j$. In our case, the

distance between two data elements is given by the Euclidean distance between their *grid positions*. The term $weight(C_i, C_j)$ is an additional scaling factor taking the relative sizes of the clusters into account:

$$weight(C_i, C_j) = 1.0 + \log_{10}(1.0 + 9.0 \cdot \frac{|C_i|}{|C_j|})$$

Clearly, $weight(C_i, C_j)$ is restricted to the range $(1, 2]$.

The spatial distribution generated by our version of the ant-based clustering algorithm has two interesting features, which are necessary for the robust performance of this retrieval scheme. These are, firstly, the high compactness of the clusters on the grid and, secondly, the clear spatial separation between the individual clusters. Given these properties, an agglomerative algorithm based on the single link criterion will clearly work very well and a stopping criteria for the clustering algorithm can easily be derived. However, as data items around the cluster borders are sometimes slightly isolated (so that they are prone to mislead the single link metric by establishing individual clusters or 'bridging' gaps between clusters), we have introduced the additional weighting term $weight(C_i, C_j)$ that encourages the merging of these elements with the 'core' clusters.

k-means: The first algorithm we compare against is the well-known k-means algorithm. Starting from a random partitioning, the algorithm repeatedly (i) computes the cluster centres (i.e., the average vector of each cluster in data space) and (ii) reassigns each data item to the cluster whose centre is closest to it. It terminates when no more reassignments take place. By this means, the intra-cluster variance, that is, the sum of squares of the differences between data items and their associated cluster centres, is locally minimised.

k-means' strength is its runtime, which is linear in the number of data elements, and its ease of implementation. However, the algorithm tends to get stuck in suboptimal solutions (dependent on the initial partitioning and the data ordering) and it works well only for spherically shaped clusters. It requires the number of clusters to be provided or to be determined (semi-) automatically.

In our experiments, we run k-means using the correct number of clusters k. Random initialisation is used, and the best result out of 20 runs (in terms of minimum variance) is selected in order to reduce the effects of local optima. If empty clusters arise during the clustering process, these are reinitialised using a randomly selected data item.

Average link: As a second method, an agglomerative hierarchical clustering algorithm based on the linkage metric *average link* is used. The algorithm starts with the finest partitioning possible (i.e., singletons) and, in each iteration, merges the two least distant clusters. The distance between two clusters C_i and C_j is computed as the average dissimilarity between all possible pairs of data elements i and j with $i \in C_i$ and $j \in C_j$.

Hierarchical clustering methods are thought to give higher quality solutions than partitioning methods. However, their runtime scales quadratically and results heavily depend on the linkage metric used. Also, the derivation of appropriate stopping criteria can be difficult, if the correct number of clusters is not known.

As for k-means, we provide the correct number of clusters, thus giving the same advantage to both algorithms. The Ward updating formula [19] is used to efficiently recompute cluster distances.

5 Evaluation

Comparative results are presented for three synthetic test sets and three real data collections taken from the Machine Learning Repository [2], which we describe below. In a preprocessing step, the data vectors are normalised in each dimension, and, for the ant-based algorithm and agglomerative clustering, all pairwise dissimilarities are precomputed. The employed distance function is the Euclidean distance[1] for the synthetic data sets, and the Cosine measure[2] for the real data sets.

Synthetic data: The *Square1* data set is the type of data most frequently used within previous work on ant-based clustering. It is two-dimensional and consists of four clusters arranged as a square. They are generated by the Normal Distributions $(N(-5,2),N(-5,2))$, $(N(5,2),N(5,2))$, $(N(-5,2),N(5,2))$ and $(N(5,2),N(-5,2))$, and are each of size 250. Hence, *Square1* contains four spherically shaped clusters with equal spread. In the experiments, a new sample is generated from these distributions in each run.

$2D$-$4C$ and $100D$-$10C$ are two examples of a range of benchmark test sets generated and used for our comparative study. Every set xD-yC (where x describes the dimensionality of the data and y gives the number of clusters) consists of 50 different instances, and we generate each individual instance as follows. We specify a set of y x-dimensional normal distributions $N(\vec{\mu},\vec{\sigma})$ from which we sample the data items for the y different clusters in the instance. The sample size s of each normal distribution, the mean vector $\vec{\mu}$ and the vector of the standard deviation $\vec{\sigma}$ are themselves randomly determined using uniform distributions over fixed ranges (with $s \in [50,450]$, $\mu_i \in [0,100]$ and $\sigma_i \in [0,5]$).

Consequently, the expected size of instances of $2D$-$4C$ and $100D$-$10C$ is 1000 and 2500 data items respectively. During the generation process, cluster centres are rejected if the resulting distributions would have more than 3% overlap. A different instance is used in each individual run of the experiments.

Real data: The *Iris* data contains 150 items described by 4 attributes. Its 3 clusters are each of size 50. Two of them are linearly non-separable. The *Breast Cancer Wisconsin* data contains 699 items described by 9 attributes. Its 2 clusters are of size 458 and 241 respectively. The *Yeast* data contains 1484 data elements described by 8 attributes. Its 10 clusters are of size 463, 429, 244, 163, 51, 44, 35, 30, 200 and 5. The real data sets are arbitrarily permuted in each run.

Evaluation functions: The clustering results of the different algorithms on the test sets are compared using four different evaluation measures. The first two of them make use of the correct classification, which is known for all six data sets.

- The *F-Measure* uses the ideas of precision and recall from information retrieval. Each *class* i (as given by the class labels of the used benchmark data set) is regarded as the set of n_i items desired for a query; each *cluster* j (generated by the algorithm) is regarded as the set of n_j items retrieved for a query; n_{ij} gives the number of elements of class i within cluster j. For each class i and cluster j precision and recall are then defined as

[1] The synthetic test sets are generated in Euclidean space and the Euclidean distance is therefore the appropriate measure to use.

[2] On the real data sets taken from the Machine Learning Repository the Cosine measure outperforms the Euclidean distance and is commonly used.

$p(i,j) = \frac{n_{ij}}{n_j}$ and $r(i,j) = \frac{n_{ij}}{n_i}$, and the corresponding value under the F-Measure is

$$F(i,j) = \frac{(b^2+1) \cdot p(i,j) \cdot r(i,j)}{b^2 \cdot p(i,j) + r(i,j)},$$

where we chose $b = 1$, to obtain equal weighting for $p(i,j)$ and $r(i,j)$. The overall F-value for the partitioning is computed as

$$F = \sum_i \frac{n_i}{n} \max_j \{F(i,j)\},$$

where n is the total size of the data set. F is limited to the interval $[0,1]$ and should be maximised.

- The *Rand Index* determines the degree of similarity (in terms of pairwise co-assignments) between the known correct classification U and the solution V generated by a clustering algorithm. It is defined as

$$R = \frac{a+d}{a+b+c+d},$$

where a, b, c and d are computed for all possible pairs of data points i and j and their respective cluster assignments $c_U(i), c_U(j), c_V(i)$ and $c_V(j)$:

$$a = |\{i,j | c_U(i) = c_U(j) \wedge c_V(i) = c_V(j)\}|, \quad b = |\{i,j | c_U(i) = c_U(j) \wedge c_V(i) \neq c_V(j)\}|,$$

$$c = |\{i,j | c_U(i) \neq c_U(j) \wedge c_V(i) = c_V(j)\}|, \quad d = |\{i,j | c_U(i) \neq c_U(j) \wedge c_V(i) \neq c_V(j)\}|.$$

R is limited to the interval $[0,1]$ and is to be maximised.

- The *Inner Cluster Variance* computes the sum of squared deviations between all data items and their associated cluster centre, which reflects the common agreement that data elements within individual clusters must be similar. It is given by

$$I = \sum_{c \in C} \sum_{i \in c} \delta(i, \mu_c)^2,$$

where C is the set of all clusters, μ_c is the centroid of cluster c and $\delta(i, \mu_c)$ is the distance function employed to compute the deviation between each data item i and its associated cluster centre. It is to be minimised.

- The *Dunn Index* determines the minimal ratio between cluster diameter and inter cluster distance for a given partitioning. Thus, it captures the notion that, in a good clustering solution, data elements within one cluster should be much closer than those within different clusters. It is defined as

$$D = \min_{c,d \in C} \left[\frac{\delta(\mu_c, \mu_d)}{\max_{e \in C} [diam(e)]} \right],$$

where the diameter $diam(c)$ of a cluster c is computed as the maximum inner cluster distance, and $\delta(\mu_c, \mu_d)$ is the distance between the centroids of clusters c and d. It is to be maximised.

Table 1: Results for k-means, hierarchical agglomerative average-link clustering and ant-based clustering on three synthetic and three real data sets. The quality of the partitioning is evaluated using the F-Measure, the Rand Index, the Inner Cluster Variance and the Dunn Index. Runtimes and the number of identified clusters (which is automatically determined only for the ant algorithm) are additionally provided. The table shows means and standard deviations (in brackets) for 50 independent runs. Bold face indicates the best and italic face the second best result out of the three algorithms.

Square1	k-means	average link	ant-based clustering
#Clusters	4 (0)	4 (0)	4 (0)
F-Measure	**0.987059** (0.00409363)	0.980654 (0.0076673)	*0.982561* (0.00518902)
Rand Index	**0.987212** (0.00398614)	0.981053 (0.00730242)	*0.982828* (0.00503838)
Variance	**0.461473** (0.0060167)	0.465201 (0.0086531)	*0.463618* (0.00883593)
Dunn Index	**3.78352** (0.105684)	3.22921 (0.298599)	*3.64224* (0.249045)
Runtime	**1.26** (0.795236)	*4.24* (0.427083)	10.14 (1.74367)
2D-4C	k-means	average link	ant-based clustering
#Clusters	4 (0)	4 (0)	4 (0.282843)
F-Measure	0.972734 (0.0740772)	**0.997365** (0.018445)	*0.990371* (0.0354898)
Rand Index	0.983066 (0.0464064)	**0.998241** (0.012311)	*0.99155* (0.031725)
Variance	0.177598 (0.16193)	**0.127346** (0.0372185)	*0.133784* (0.062165)
Dunn Index	4.45335 (2.09255)	**5.10569** (1.61428)	*5.02245* (1.78885)
Runtime	**0.74** (1.09197)	*6.8* (4.36807)	15.68 (6.60739)
10D-10C	k-means	average link	ant-based clustering
#Clusters	10 (0)	10 (0)	10 (0)
F-Measure	0.971745 (0.0410038)	**1.0** (0.0)	*0.999986* (0.0000960888)
Rand Index	0.993207 (0.0118778)	**1.0** (0.0)	*0.999995* (0.0000318648)
Variance	0.411021 (0.160722)	**0.331714** (0.0305796)	*0.331777* (0.0305041)
Dunn Index	8.22036 (6.67596)	**13.6787** 1.90435)	*13.445* (2.36789)
Runtime	*46.04* (13.1559)	83.26 (33.2955)	**19.2** (5.5715)
IRIS	k-means	average link	ant-based clustering
#Clusters	3 (0)	3 (0)	3.02 (0.14)
F-Measure	**0.824521** (0.0848664)	0.809857 (0.0)	*0.816812* (0.0148461)
Rand Index	0.816599 (0.101288)	*0.822311* (0.0)	**0.825422** (0.00804509)
Variance	0.922221 (0.221044)	*0.900175* (0.0)	**0.880333** (0.00405812)
Dunn Index	*2.65093* (0.4201)	2.5186 (0.0)	**2.9215** (0.298826)
Runtime	*0.16* (0.366606)	**0.02** (0.14)	3.36 (0.48)
WISCONSIN	k-means	average link	ant-based clustering
#Clusters	2 (0)	2 (0)	2 (0)
F-Measure	0.965825 (0.0)	*0.965966* (0.0)	**0.967604** (0.00144665)
Rand Index	*0.933688* (0.065321)	*0.933688* (0.0)	**0.93711** (0.00273506)
Variance	*1.61493* (0.0)	1.63441 (0.0)	**1.61257** (0.000838131)
Dunn Index	**5.47121**(0.000178411)	4.91649 (0.000000284355)	*5.4424* (0.0957218)
Runtime	**0.06** (0.237487)	*1.44* (0.496387)	10.54 (0.498397)
YEAST	k-means	average link	ant-based clustering
#Clusters	10 (0)	10 (0)	5.36 (1.17915)
F-Measure	0.431505 (0.00443954)	**0.448316** (0.0)	*0.435396* (0.0345797)
Rand Index	**0.750657** (0.00124985)	*0.742682* (0.0)	0.678131 (0.0752791)
Variance	**1.53798,** (0.001611)	*1.60028* (0.00000000652216)	1.89537 (0.115468)
Dunn Index	*1.69692* (0.109608)	1.55563 (0.000000120366)	**1.88049** (0.207959)
Runtime	**1.7** (1.0247)	14.04 (0.0)	*9.22* (0.54)

6 Results

Table 1 gives the means and standard deviations (over 50 runs) obtained for each of these measures. Additionally, it shows the average number of clusters (which is automatically determined only for the ant algorithm) and the algorithms' average runtimes. Note that the timings reported for the ant algorithm do *not* include the time required for cluster retrieval. This is justified as the cluster retrieval is a tool *only* necessary for the analysis process. In a typical application, the user would be presented with the visual representation and, in an interactive setting, clusters could then be identified with hardly any computational overhead.

Number of clusters: The results demonstrate that, if clear cluster structures exist within the data, the ant algorithm is quite reliable at identifying the correct number of clusters. This is the case both if the clusters are spatially well separated (as is the case in the test sets $2D$-$4C$, and $10D$-$4C$) and also if they touch but show clear density gradients (in *Square1*). Only on the *Yeast* data the detected number of clusters is far too low. However, the F-Measure reveals that all three algorithms perform very badly on this data, showing that both k-means and agglomerative clustering equally fail to correctly identify the clusters in spite of the fact that they have a priori knowledge of the correct number. This is an indication that the structure within the data is not very pronounced.

Solution quality: With the exception of the *Yeast* data set, ant-based clustering performs very well under all four measures. On the synthetic benchmarks, it always comes second best and is very close to the best solution. On the first two real data benchmarks it even shows the highest performance under three of the four measures.

It is interesting to note that on the $10D$-$10C$ test data, where both agglomerative clustering and ant-based clustering perform consistently well, k-means repeatedly generates very bad solutions. This happens in spite of the fact that k-means' solution is already the best selected out of 20 runs, and it is a trend that can (to a lesser degree) also be observed on the test set $2D$-$4C$. In the table this can be seen in the relatively high standard deviations in k-means' results.

Runtime: For the small data collections, the ant algorithm's runtimes are considerably higher than those of k-means and hierarchical clustering. However, it is worth observing that they scale linearly, such that ant-based clustering already outperforms the agglomerative scheme on the *Yeast* data set. As k-means is affected by the rise in dimensionality, ant-based clustering even becomes the fastest method on the $10D$-$2D$ data.

7 Conclusion

In contrast to previous studies on ant-based clustering and sorting, we have studied the algorithm's clustering solutions *in isolation*, in order to obtain an improved understanding of its performance relative to other methods for clustering. Nonetheless, it should not be forgotten that the mapping *simultaneously* provided by the algorithm is one of its most attractive features. To what extent this mapping really is (or can be improved to be) topology-preserving is investigated in [8].

Seen *purely* as a clustering algorithm, ant-based clustering performs well in our comparison to the popular methods of k-means and agglomerative hierarchical clustering. In addition to that, the algorithm has a number of features that make it an interesting candidate for clus-

ter analysis. Firstly, there is its linear scaling behaviour, which is attractive for use on large data sets as are frequently encountered today, e.g., in information retrieval. Also, the nature of the algorithm makes it fairly robust to the effects of outliers within the data. In addition, ant-based clustering has the capacity to work with any kind of data that can be described in terms of symmetric dissimilarities, and it imposes no assumption on the shape of the clusters it works with. Finally, an important strength of the algorithm is its ability to automatically determine the number of clusters within the data.

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