Clustering with Swarm Algorithms Compared to Emergent SOM

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Abstract. Swarm-based methods are promising nature-inspired techniques. A swarm of stochastic agents performs the task of clustering high-dimensional data on a low-dimensional output space. Most swarm methods are derivatives of the Ant Colony Clustering (ACC) approach proposed by Lumer and Faieta. Compared to clustering on Emergent Self-Organizing Maps (ESOM) these methods usually perform poorly in terms of topographic mapping and cluster formation. A unifying representation for ACC methods and Emergent Self-Organizing Maps is presented in this paper. ACC terms are related to corresponding mechanisms of the SOM. This leads to insights on both algorithms. ACC can be considered to be first-degree relatives of the ESOM. This explains benefits and shortcomings of ACC and ESOM. Furthermore, the proposed unification allows to judge whether modifications improve an algorithm's clustering abilities or not. This is demonstrated using a set of critical clustering problems.

1 Introduction

Flocking behaviour of social insects has inspired various algorithms in numerous research papers over the last decade due to the ability of simple interacting entities to exhibit sophisticated self-organization abilities. A particularly interesting field of application is cluster analysis, i.e. the retrieval of groups of similar objects in high-dimensional spaces. The idea behind Ant Colony Clustering (ACC) is that autonomous stochastic agents, called ants, move data objects on a low-dimensional regular grid such that similar objects are more likely to be placed on nearby grid nodes than dissimilar ones. This task is referred to as *topographic mapping*.

In the following sections, the basic ACC algorithm by Lumer/Faieta is introduced in a notation consistent with SOM for non-vectorial data, i.e. Dissimilarity-SOM. A unifying representation for both methods is therefore derived in Section 3. Sections 4 and 5 describe how to improve topographic mapping and cluster analysis of ACC methods on basis of SOM. Finally, in Section 6 the effect of altered objective functions is empirically verified.

J.C. Príncipe and R. Miikkulainen (Eds.): WSOM 2009, LNCS 5629, pp. 80–88, 2009.

2 Ant Colony Clustering

The ACC method proposed by Lumer and Faieta [9] operates on a fixed regular low-dimensional grid $\mathbb{G} \subset \mathbb{N}^2$. A finite set of input samples X from a vector space with norm $\|.\|$ is projected onto the grid by $m : X \rightarrow \mathbb{G}$. The mapping m is altered by autonomous stochastic agents, called ants, that move input samples $x \in X$ from $m(x)$ to new location $m'(x)$. Ants move randomly on neighbouring grid nodes. Ants might pick input samples when facing occupied nodes and drop input samples when facing empty nodes. Probabilities for picking and dropping actions, respectively, are determined using objective function $\phi : \mathbb{G} \times X \rightarrow \mathbb{R}_0^+$, at which $\phi(x, i)$ denotes the average similarity between $x \in X$ and input samples located on the so-called perceptive neighbourhood around node $i \in \mathcal{G}$. Usually, the perceptive neighbourhood consists of $\sigma^2 \in \{9, 25\}$ quadratically arranged nodes at which the ant is located in the center. The set of input samples mapped onto the perceptive neighbourhood around $i \in \mathbb{G}$ is denoted with $N_x(i) = \{y \in X : y \neq x,\ m(y)$ neighbouring $i\}$.

$$\phi_x(i) = \frac{1}{\sigma^2} \sum_{y \in N_x(i)} \left(1 - \frac{\|x - y\|}{\alpha}\right) \tag{1}$$

ACC methods lead to a local sorting of input samples on the grid in terms of similarities. Ants gather scattered input samples into dense piles. In literature, it has been noticed that ACC derivatives are prone to produce too many and too small clusters [1] [5]. For illustration see Figure 1.

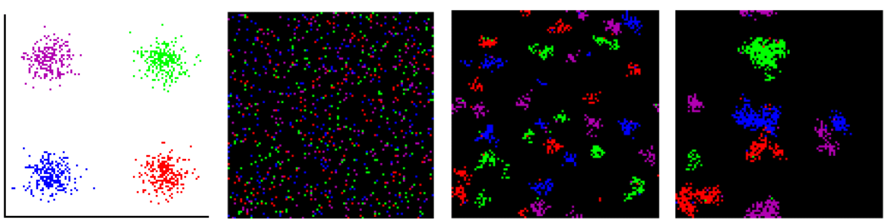


Fig. 1. Typical result of ACC methods. From left to right: gaussian data with 4 clusters, initial mapping of data objects, dense clusters appear, too many clusters with topological defects have finally emerged [1].

3 Analysis of Ant Colony Clustering by Means of Dissimilarity-SOM

The Self-Organizing Batch Maps (Batch-SOM) and its derivatives are particularly interesting for analyiss of Ant Colony Clustering (ACC) methods. Batch-SOM consist of grid $\mathbb{G}$, codebook vectors $w_i \in \mathbb{R}^n, i \in \mathbb{G}$ and a mapping function $m : X \rightarrow \mathbb{G}$ with $m(x) = \arg\min_{i \in \mathbb{G}} \|x - w_i\|$. It was shown in [5] how the objective ϕ of each ant is related to $m : X \rightarrow \mathbb{G}$ of Batch-SOM.

The so-called Dissimiliarity-SOM [8], often referred to as Median SOM, is a generalization of the Batch-SOM for nonvectorial input data. For the sake of simplicity, let $\|x-y\| \in \mathbb{R}_0^+$ denote the dissimiliarity of each $x, y \in X$. Codebook vectors are updated according to the generalized median, i.e. $w_i = \arg\min_{x \in X} \Phi_x(i)$. Here, $h : \mathcal{G} \times \mathcal{G} \to [0,1]$ denotes the neighbourhood function of SOM.

$$\Phi_x(i) = \sum_{y \in X} h(m(y),i) \cdot \|x-y\| \quad \text{with} \quad \sum_{y \in X} h(m(y),i) = 1 \tag{2}$$

In the following, the mechanism of picking and dropping ants is no longer subject of consideration. In [10] it was shown that collective intelligence can be discarded in ACC systems, i.e. same results were achieved without ants but using objective function ϕ directly for probabilistic cluster assignments. This simplification is evident: over a sufficient period of time, randomly moving ants may select any arbitrary subset of input samples, but re-allocation through picking and dropping depends on ϕ only. Probability of selection is the same on all input samples such that ants might be omitted in favor of any other subset sampling technique.

A meaningful symmetrical neighbourhood function $h : \mathbb{G} \times \mathbb{G} \to [0,1]$ for ACC methods is defined according to the perceptive neighbourhood of ants, i.e. $h(i,j)$ is 1 if $j \in \mathbb{G}$ is located in the perceptive neighbourhood of node $i \in \mathbb{G}$ and 0 elsewhere. Equation 3 reformulates the ants' objective ϕ by incorporating Φ (see Equation 2).

$$\phi_x(i) = \frac{|N_x(i)|}{\sigma^2} \cdot \left(1 - \frac{\Phi_x(i)}{\alpha}\right) \quad \text{with} \quad \Phi_x(i) = \frac{\sum_{y \in X} h(m(y),i) \cdot \|x-y\|}{\sum_{y \in X} h(m(y),i)} \tag{3}$$

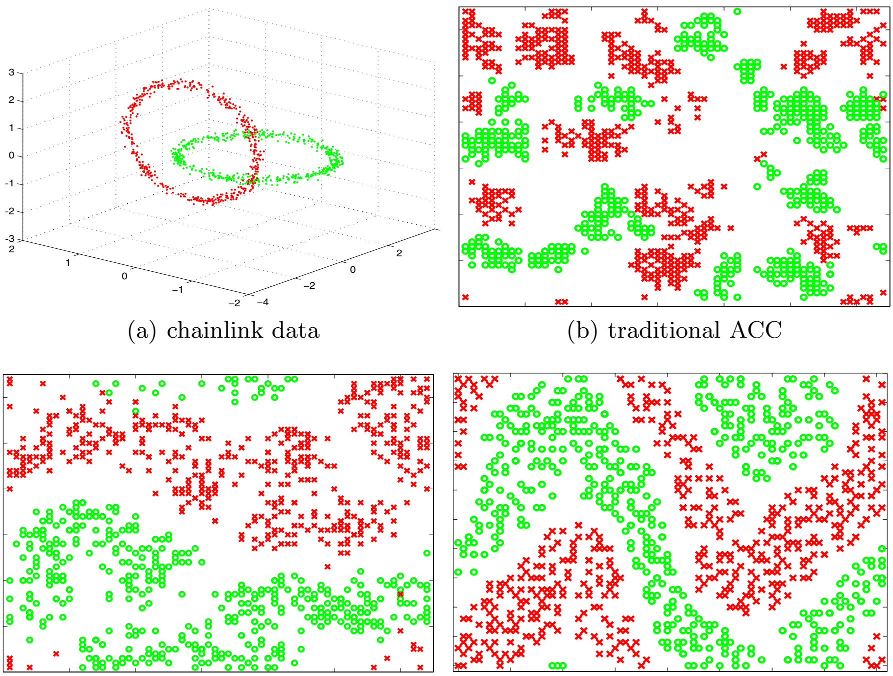
The ACC method uses a fixed neighbourhood function with small radius, whereas Dissimilarity-SOM uses shrinking neighbourhood functions with large radiuses. ACC has a probabilistic update of mapping $m : X \to \mathbb{G}$, whereas Dissimilarity-SOM is deterministic. The objective function of ACC algorithms decomposes into an output density term $\frac{|N|}{\sigma^2}$ and a term $1 - \frac{\Phi}{\alpha}$ related to topographic quality. Therefore, the ACC algorithm is easily convertible into a special case of Dissimilarity-SOM, and vice versa. For a brief overview of differences see Table 1.

Table 1. varieties of Dissimilarity-SOM and Ant Colony Clustering

	Dissimilarity-SOM	ACC
neighbourhood $h : \mathbb{G} \times \mathbb{G} \to [0,1]$	large shrinking	small, fixed
update of $m : X \to \mathbb{G}$	deterministic	probabilistic
searching for update of $m : X \to \mathbb{G}$	global $\mathbb{G}$	local $\subset \mathbb{G}$
objective function	Φ	$\frac{\lvert N \rvert}{\sigma^2}(1 - \frac{\Phi}{\alpha})$
termination	cooling scheme	never

4 Improvement of Ant Colony Clustering

From Dissimilarity-SOM, minimization of Φ is known to produce sufficiently topography preserving mappings $m : X \rightarrow \mathbb{G}$, e.g. when using Dissimilarity-SOM. In contrast to that, the *output density term* $\frac{|N|}{\sigma^2}$ has some major flaws. First, the output density term leads to maximization of output space densities, instead of preservation. Obtained mappings are, therefore, not related to the configuration of available clusters in the input space. Traditional ACC algorithms are not allowed to assign two or more objects to a single grid node (see Section 2) in order to prevent the mapped clusters from collapsing into a single grid node. Due to that, densities of input data can hardly be preserved on grid $\mathbb{G}$. In comparison with the topographic term, the output density term is much easier to maximize and, therefore, will distort the objective function ϕ. Accounting of output densities is prone to distort the formation of correct topographic mappings because it is responsible for additional local optima of ϕ.



(a) chainlink data

(b) traditional ACC

(c) emergent ACC

(d) emergent SOM

Fig. 2. ACC projects looped cluster structures on a *toroid* grid. (a) Chainlink data from FCPS [11]. (b) Traditional ACC with small σ produces too many small clusters. (c) Emergent ACC enables the formation of looped clusters. (d) Emergent SOM enables the formation of looped clusters.

The topographic term $1 - \frac{\Phi'}{\alpha}$ of the ACC objective function depends on the shape of the neighbourhood function $h : \mathbb{G} \times \mathbb{G} \to \{0, 1\}$. Usually, neighbourhoods' sizes are chosen as $\sigma^2 \in \{9, 25\}$, i.e. the immediate neighbours. From SOM it is known that the cooling scheme of the neighborhood radius vitally influences the obtained topographic mapping quality. (see [6] for details). A bigger radius enables a more continuous mapping in the sense that proximities existing in the original data are visible on the grid. This is evident because smaller neighbourhoods are more likely to exclude parts of a cluster.

In order to cope with the shortcomings mentioned above, we introduce the *Emergent Ant Colony Clustering* method. An ACC method is said be be emergent if it fulfills the following conditions:

- Ants' modifications of mapping $m : X \to \mathbb{G}$ is directed by minimization of Φ
- Ants do not account for output densities.
- The perceptive neighbourhood of ants is not limited to immediate neighbours on grid $\mathbb{G}$. Instead, bigger neighbourhood radiuses are to be chosen in order to obtain SOM-like mappings.

Figure 2 illustrates the ability of emergent ACC method to preserve even looped input space clusters, which is hardly possible for traditional ACC.

5 Data Analysis with Emergent Ant Colony Clustering

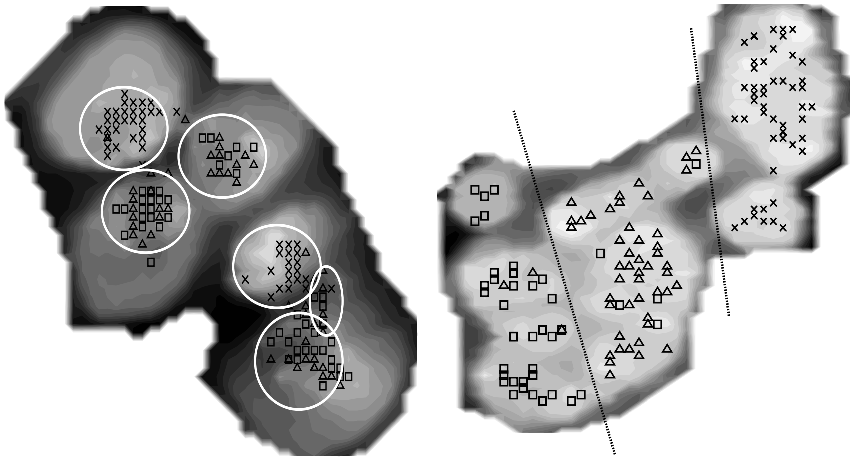
Emergent ACC usually will provide an ESOM-like projection, i.e. input samples are uniformly mapped onto the grid. See Figure 2 for illustration. In this case, cluster retrieval cannot be achieved according to sparse regions dividing dense clusters on the grid.

A promising technique for cluster retrieval is based on so-called U-Maps [12]. Arbitrary projections from normed vector spaces onto grid $\mathbb{G} \subset \mathbb{N}^2$ are transformed into landscapes, so-called U-Maps. The U-Map technique assigns each grid node a height value that represents the averaged input space distance to its' neighbouring nodes and codebook vectors, respectively. Clusters lead to valleys on U-Maps whereas empty input space regions lead to mountains dividing the cluster valleys. This is illustrated in Figure 3 using Fisher's well-known iris data [3]. Traditional ACC produces too many valleys, whereas Emergent ACC preserves cluster structures.

The U*C cluster algorithm uses the so-called watershed transformation to retrieve cluster valleys on U-Maps. See [13] for details.

6 Experimental Settings and Results

In order to measure the distortion of a topographic mapping method in question, a collection of fundamental clustering problems (FCPS) is used [11]. Each data set represents a certain problem that arbitrary algorithms shall be able to handle



(a) Traditional ACC (b) Emergent ACC

Fig. 3. Well known iris data [3]: setosa (×), versicolor (△), virginica (□). U-Maps shown as islands generated from toroid grids. Dark shades of gray indicate high inter-cluster distances. (a) Too many small clusters emerge from traditional ACC. (b) Emergent ACC preserves three clusters after the same number of learning epochs.

when facing unknown real-world data. Here, traditional and emergent ACC are tested on which one delivers the best topographic mapping.

A comprehensive overview on topographic distortion measurements can be found in [4]. Here, the so-called *minimal path length* (MPL) measurement is used.

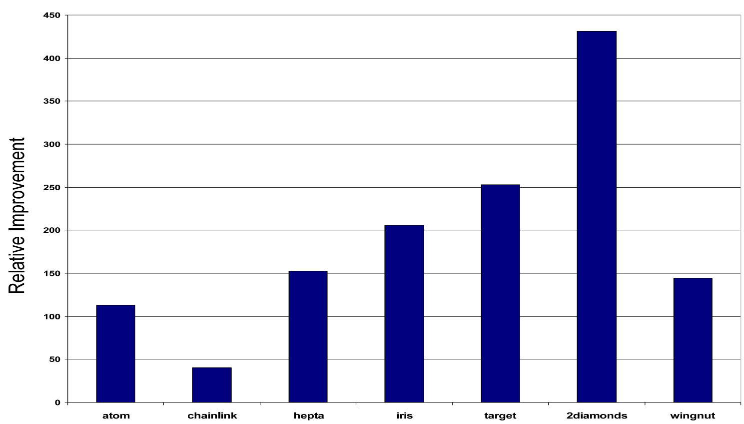


Fig. 4. Improvement of topographic quality measured by *minimal path length* method: percental z-scores of traditional over emergent ACC. Emergent ACC leads to improvements between 50% to 400% when compared to traditional ACC on different FCPS data sets.

It is an easy-to-compute measurement that sums up input space distances of grid-neighbouring data objects and codebook vectors, respectively.

$$mpl = \sum_{x \in X} \frac{1}{|N_x|} \sum_{y \in N_x} \|x - y\| \tag{4}$$

Lower MPL values indicate less topographic distortion when moving on the grid and, therefore, a more trustworthy topographic mapping. Each algorithm is run several times with the same parametrization. MLP values indicate if accounting for output densities assists the formation of good topographic mappings, or not. All data sets from the FCPS collection were processed with the same parameters established in literature, i.e. $\alpha = 0.5$, $\sigma^2 = 25$, $k_1 = 0.3$ and $k_2 = 0.1$ on a 64×64 grid with 100 ants during 100000 iterations. The results are illustrated in Figure 4. Accounting for output densities leads to increasing MPL values on an average, i.e. worsenings of topographic mappings. Significance has been confirmed using a Kolmogorov-Smirnov test on a $\alpha = 5\%$ level. All obtained p-values are below 10^{-5}.

7 Discussion

This work shows a previously unknown relation of two topographic mapping techniques, namely Dissimilarity-SOM and Ant Colony Clustering (ACC). It is based on the assumption [10] that stochastic agents, e.g. ants, are nothing more than an arbitrary sampling technique that is to be omitted for further analysis of formulae. This simplification is evident but may be invalid for stochastic agents guided by more than just randomness and topographic distortion, e.g. ants following pheromone trails. Our analysis of formulae does not cover algorithms that are not ACC derivatives following the Lumer/Faieta scheme. In contrast to hybrid approaches, like KohonAnts [2], our work creates a unifying basis for comprehension and creation of techniques from the fields of artificial neural networks and swarm-intelligence.

Minimal path lengths (MPL), as proposed in Section 6, are well-known topographic distortion measures. The length of input space *paths* is normalized by the cardinality $|N_x|$ of the corresponding grid neighbourhood, i.e. the number of objects mapped onto the grid neighbourhood. This is supposed to decrease error values of locally dense mappings, as produced by traditional ACC, because small radial neighbourhoods usually do not cover objects of another cluster, since locally dense mappings imply sparse dividing grid regions around clusters. Nevertheless, traditional ACC produces bigger MPL errors than emergent ACC that is not accounting for densities. We conclude that the topographic mapping quality is improved beyond our empirical evaluation.

Traditional and emergent ACC methods do not converge due to the architecture of stochastic agents. Instead, they enable perpetual machine learning. ACC methods are, therefore, to be favored over traditional methods, like Self-Organizing Maps and hierarchical clustering, when dealing with incremental learning tasks.

8 Summary

This work continues our last publication [5] at which the Ant Colony Clustering (ACC) method by Lumer and Faieta [9] was related to Self-Organizing Batch Maps [7]. The mechanism of picking and dropping ants was omitted in favor of a formal analysis of the underlying formulae and comparison with Kohonen's Dissimilarity-SOM. It could be shown that a unifying framwork for both methods does exist in terms of a common topographic error function. The ACC method is to be considered a probabilistic, first-class relative of Batch-SOM and, especially, Dissimilarity-SOM. The behaviour of ACC methods becomes explainable on that unifying basis.

ACC methods exhibit poor clustering abilities because of distorted topographic mappings. Improvements of topographic mapping were derived by means of SOM architecture. Perceptive areas are to be increased, and accounting for density of mapped data is futile. The novel method *Emergent ACC* does not produce dense clusters any more but uniformly distributed, SOM-like projections. Due to that, clusters are to be retrieved using U-Map technology. As predicted by our theory, an empirical evaluation showed on critical clustering problems that disregarding the density of mapped data improves the quality of topographic mapping despite of unfavorable settings.

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