Emergence in Self Organizing Feature Maps

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Abstract— This paper sheds some light on the claim that Emergent SOM (ESOM) are different from other SOM. The discussion in philosophy and epistemology about Emergence is summarized in the form of postulates. The properties of SOM are compared to these postulates. SOM fulfill most of the postulates. The most critical of the postulates are those concerned with "the whole is more than the sum of its parts". The epistemological postulates regarding this issue are hard, if not impossible, to prove. An alternative postulate relying on semiotic concepts, called "semiotic irreducibility" is proposed here. This concept is applied to U-Matrix on SOM with many neurons. This leads to the definition of ESOM as SOM producing a nontrivial U-Matrix on which the terms "watershed" and "catchment basin" are meaningful and which are cluster conform. It is demonstrated that a clustering algorithm (U*C) which exploits the emergent properties of such ESOM is superior to other popular clustering algorithms. Results on synthetic data in blind studies and a real world applications are convincing.

1 Introduction

When Emergence is discussed properties are meant, which appear unexpectedly in a system as holistic ("Gestalt-") phenomena. One part of the unexpectedness of emergent phenomena is that they can not be found when the constituents of the system are analyzed. An example of Emergence is the property of "wetness", which can be attributed to water, but not to H, O or H_2O molecules. Systems, which allow for Emergence, reward with properties that are "more than the sum of their parts" and "more than one could have expected". In this paper self organizing feature maps (SOM) [1] are discussed with respect to Emergence. It is shown that SOM possess many prerequisites for Emergence. To show this, the requirements for Emergence, as discussed in epistemology and philosophy, are reviewed (chapter 2). The practical application of these philosophical concepts to computer programs is addressed in chapter 3. Then the properties of SOM are compared to these requirements (chapter 4). In chapter 5 properties are defined which allow Emergence to happen in SOM. This approach has practical applications in the form of Emergent SOM (ESOM) clustering algorithms. The key differences of these algorithms in comparison to typical clustering algorithms are discussed in chapter 6. Chapter 7 and 8 present the results of a double blind study and real world application. In the last chapters, the results are discussed and summarized.

2 The Concept of Emergence

Emergence as an epistemological concept is not new. It seems, however, as Bentley puts it "that a clear definition of Emergence is very difficult to obtain"[3]. We follow here in most parts Stefan [2], who reviewed the evolution of the concept of Emergence from John Stuart Mill 1843 until today. For a complete philosophical discussion of different approaches to Emergence see [2]. Emergence is a central and essential concept of modern scientific disciplines like Artificial Life [4] and Connectionism [2]. The philosophical discussion is summarized here by the formulation of postulates attributed to Emergence. Postulates of Emergence:

(0) Postulate of materialism: Carriers of the emergent properties or structures consist exclusively of material parts

(I) Postulate of structural unpredictability: A novel property pn(S) of the structure of a system S is structural unpredictable if it is impossible to predict pn(S) before it is observed the first time.

(II) Postulate of temporal unpredictability: A novel property pn(S) of the structure of a system S is called temporal unpredictable if the time tn, when pn(S) can first be observed in S can not be predicted.

(III) Postulate of novelty: A property pn(S) of a system S is called novel if the system S did not have pn(S) at times t < tn and pn(S) is observable in times t >tn.

Sometimes this postulate is extended such that pn(S) is not observable anywhere in the universe in times < tn.

(IV)Postulate of systemic: A property p(S) of a system S is systemic, if no part S' of the system S possesses p.

(V) Postulate of dependence: If there are differences in the systemic properties of two systems S and T, then the systems S and T must differ in their parts or their arrangements or interactions. This postulate is also known as *"synchronistic determinism"* or *"supervenience"* [2].

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(VI) Postulate of irreducibility: A systemic property p(S) of a system S is irreducible, if there is no way to derive p(S) from any part, subset or partial structure of S.
Depending on what subset of the postulates above is used to define Emergence, several different flavors of Emergence may be defined. See [2], page 71 for an overview.
In epistemology the postulate of irreducibility is the most controversial postulate of the concepts of Emergence. This postulate is commonly referred to as "the whole is more than the sum of its parts". Sometimes it is interpreted such that the emergent properties can not even in principle be predicted by analyzing the parts of a system. In the next chapter we will analyze what properties programs must have in order to be able to produce Emergence.

3 Emergence in computer programs

In this chapter properties are given, that allow to differentiate between algorithms that can produce emergent phenomena and such that do not show Emergence. The epistemological postulates above can be grouped in three categories: first materialism (0), second unpredictability (I…III) and third "constructivistic" (IV…VI) postulates. Algorithms, defined as a finite list of well-defined instructions that can be translated into programs which run on a Turing Machine, certainly fulfill the postulate of materialism (0).
When an algorithm uses a source of (true) random numbers RND in the course of its calculation, the calculations of such an algorithm are nondeterministic. What the calculations of a nondeterministic algorithm are, can not be predicted. Therefore the postulates of structural unpredictability (II) and novelty (III) are fulfilled by such algorithms. If the time until a nondeterministic algorithm reaches a result depends on RND the algorithm can be termed temporal unpredictable (IV). So programs, which make use of RND fulfill the unpredictability postulates of Emergence (I…III).
What remains are the constructivistic postulates (IV…VI). To give a practical solution, we introduce the property "semiotic irreducibility" (SI): a systemic property p(S) of a system S consisting of parts e_i is *semiotic irreducible*, if the p(S) is described using a semiotic L = (G, Z, P) with syntax G, semantics Z and pragmatics P and L it is not meaningful to describe properties of the parts e_i in L.
A semiotic describes the signs, symbols and the interpretation of a language and its meaning [7]. For example, the pixels of a computer screen can be described within a semiotic. They can have a syntax, grammar and interpretation. "Color depth" or "contrast" might be properties formulated in pixel semiotics L_x. Another semiotics is the level of letters which may be formed by sets of pixels. In this semiotic L_{alpha} the properties "bold" or "italics" can be defined. With this examples the meaning of semiotic irreducibility can be exemplified: within the semiotics L_{alpha} the syntax, semantics and meaning (pragmatic) of "italics" is expressible. Although the letter is formed using pixels, "italics" make no sense when applied to pixels. The property "italics" of letters is semiotic irreducible to pixels. An analogical example from Physics is that the properties of "pressure" and "temperature" are irreducible to molecules.
When a property is semiotic irreducible (SI), it follows that the property is systemic. Since the language and concepts are not applicable for the parts of the system it is clear that these parts do not possess the semiotic irreducible property. Our approach using semiotics has another advantage: the property defined in a certain semiotic is useful, i.e. has a meaning, can be used for some purposes, can be used to formulate proofs or are even useful to make money etc. For programs or algorithm this concept has the consequence that a notion exists which can be constructed using elementary parts of the system. This Notion has a definite meaning when applied to the system as whole, but loses its meaning, when applied to single parts of the system. For example the notion "average" makes sense when applied to a reasonably large set of numbers, but is useless if applied one number. The notion of an average can therefore be considered to be semiotic irreducible (SI).
In summary a computer program has the prerequisites to show Emergence if

- the algorithm makes use of a source of random numbers for it's calculation (nondeterminism)
- semiotic irreducible properties can be defined on the results of the algorithm (SI)

4 Properties of SOM with respect to Emergence

From the viewpoint of systems theory SOM have the following properties: SOMs are

- complex
- multi agent
- dynamical
- adaptive
- nondeterministic
- bifurcating (history dependent)
- irreversible
- nonlinear

SOMs are complex, in the way that they are made up by multiple interconnected (communicating) elements: neurons, and neighborhoods. SOMs can be regarded as multi-agent system (MAS). MAS are composed of several agents which collaborate to reach a goal. The agents can be identified with the neurons, the collaboration is the modification of the neuron's weight within a neighborhood. The goal of MAS-SOM systems is the

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adaptation to the structure of the input data. SOMs can be regarded as a dynamical system. A dynamical system has a state determined by a collection of real numbers, or, more generally, by a set of points in an appropriate state space. The set of all weights of all neurons defines the state of a SOM. SOMs are nondeterministic. Systems are non-deterministic, if randomness is involved in the development of future states of the system. Typically there are two sources of randomness in SOMs: the choice of the initial configuration of the weights and the selection of the next input vector to be learned. A bifurcation occurs when a small smooth change made to the parameter values of a system causes a change in the system's long-term behavior. Finding the current best matching unit (BMU) depends on all the potentially small changes of the weight vectors. This also depends strongly on the sequence when the input vectors are processed. If a different BMU is found the future of the calculation is strongly altered. Irreversibility: the shrinking of the neighborhood and in consequence the inclusion or exclusion of neurons from a neighborhood produce an irreversible learning process. Irreversibility also follows from the bifurcations during the learning phase. Nonlinearity: the inclusion and exclusion of neurons in a neighborhood is the primary source of nonlinearity in SOM. With all this properties SOM fulfill many of the postulates of Emergence. *Materialism* is self understanding (O). The ordering of the neurons can be regarded as temporal and structural unpredictability and novelty of the results of a SOM. *Unpredictability* and *novelty* properties follow from the nondeterministic, bifurcating, irreversible and nonlinear leaning rule(I…III). *Supervenience* is also given. However, it is unclear, if there are systemic and irreducible properties of SOM. In particular, if properties can be found which can only be found for the whole SOM and not for its parts. In the next chapter a function on the U-Matrix of a SOM is defined, which is semiotic irreducible (SI).

5 Emergent SOM

For the lack of space, the basic notations of SOM are not defined here. For the definition of data space, input data, data distance, neurons, weight, neighborhood, best matching unit (BMU), cluster, output grid(=map space) and learning algorithm for SOM see, for example, [5] or Kohonen [1]. The *U-height* uh(N) of a neuron N is the average data distance from the weight vector of N to the weight vectors associated with neurons in its neighborhood. The display of the U-heights on top of the neurons of a map space is called U-Matrix [5]. A *step* on an U-Matrix is a movement from a neuron A to one of the neurons A's immediate neighborhood. A *path* is a connected sequence of steps. A step from a neuron A with U-height uh_A to a immediate neighboring neuron B with U-height uh_B is called *ascending* if $uh_B > uh_A$. Neuron A *drains to* neuron B if there is a path p from A to B and each step in p is not ascending and $uh_B < uh_A$. A *catchment basin* is a subset S of neurons of a SOM such that all neurons in S drain to the same local minimum. If such local minima are immediate neighbors, their catchment basins are merged. The *attractor* of all neurons within a catchment basin is a unique neuron chosen from the minima of the catchment basin. If there are more than one candidate for the role of an attractor, it can be chosen according to some data distribution criteria, like, for example, local density in data space. *Watersheds* are the frontier lines between catchment basins. There are efficient algorithms, for example [6], for the calculation of catchment basins and attractors for a U-Matrix.

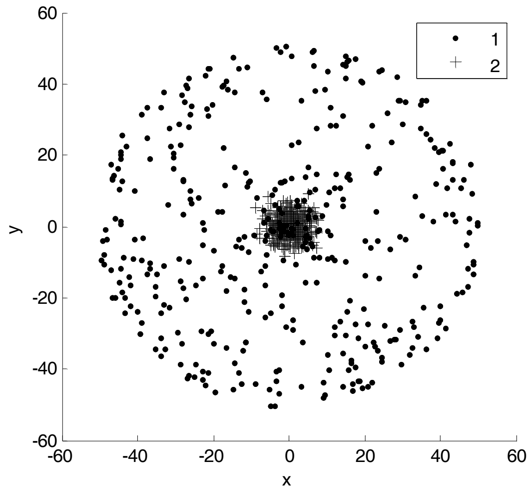

Figure 1: Atom data set

Consider, for example, the "Atom" data set shown above. This data set consists of two groups of data. One set is concentrated in a small sphere, the other group surrounds the first as the electrons in the hull of an atom. This data set is linear not separable. K-means and Ward clustering algorithms are not able to separate the two groups correctly. To be able to define catchment basins, a SOM of 50*82 = 4100 neurons on a planar grid was used. Figure 2 shows the catchment basins on the U-Matrix.

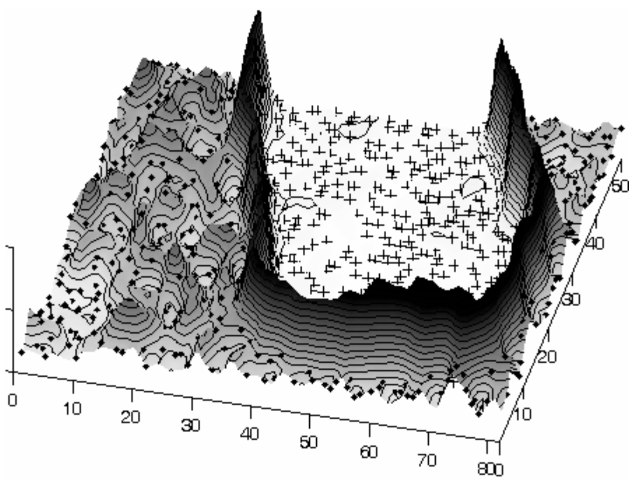

Figure 2: U-Matrix of Atom data with catchment basins

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Note that the basin for the data in the "hull" shows more internal structure due to the larger inter point distances in the "hull" cluster.

The watershed order of the U-Matrix U WO(U) is the number of distinctive catchment basins (= number of different attractors) on U. A U-Matrix is called *nontrivial*, if its watershed order WO(U) >1 and WO(U) is substantially smaller than the number of input data and the number of neurons on the SOM. A SOM is *locally ordered* if it produces a nontrivial U-Matrix U and U *conforms* with the cluster structure of the data. I.e. all the neurons within a catchment basin belong to the same cluster. In this case the catchment basin represents (a part of) the data's cluster. The watersheds on U represent (local) cluster borders. A U-Matrix is *cluster conform* if each cluster in the data is represented by either a single catchment basin or a set of directly adjacent catchment basins. Compare the catchment basins for the "hull" in figure 2.

We call a SOM Emergent (ESOM), if the definition of watersheds and catchment basins is meaningful on the SOM's U-Matrix and if the SOM learning algorithm produces a cluster conform, or at least a locally ordered, U-Matrix.

What needs to be shown is that this definition of ESOM fulfills the postulates of Emergence. Catchment basins and/or watersheds are not meaningful concepts for the U-heights of SOM with few neurons. These concepts emerge only when the whole structure of a large U-Matrix is regarded. Think of SOM with 2x2 or 3x3 neurons. No really meaningful catchment basin can be defined on those SOM. That a neuron belongs to a certain catchment basin is meaningless for such SOM. The property to be cluster conform is therefore semiotic irreducible (SI). The function which assigns to each neuron the attractor of the catchment basin to which it belongs, is a function which depends on the whole 'Gestalt" of the U-Matrix. The changing of the U-height of a single neuron, if it is on the watershed between two catchment basins may change the structure of the catchment basins completely. It follows that cluster conformity is systemic. A necessary condition for ESOM, is therefore to consist of enough neurons for a meaningful definition of watersheds and catchment basins. For practical applications, we found 4000 (for example 50x80) neurons to be a good lower limit to show Emergence. For the proper choice of the layout and dimensions of an ESOM the reader is referred to [14]. If the learning algorithm of an ESOM is topology preserving, it the corresponding U-Matrix is cluster conform. Such a SOM is therefore capable to produce Emergence.

6 Application

The SOM leaning algorithm can be interpreted as a variant of k-means clustering with additional topological constraints. This holds in particular for SOM with few neuron. Such SOM can be termed topological k-means SOM (TKM-SOM) With the canonical "Chainlink" example it could be demonstrated, however, that ESOM are different from TKM-SOM [12]. In TKM-SOM cluster are usually identified with neurons. So TKM-SOM can be directly used for clustering. ESOM, however, do not lead directly to a clustering. They can be considered as a visualization technique on top of the nonlinear and discontinuous projection of data onto the SOM's neuronal grid.

Clustering algorithms on top of ESOM have been published. Cluster algorithms on SOM are called emergent, if they use catchment basins on an ESOM's U-Matrix. U*F as defined in [8] and U*C as defined in [9] are examples of Emergent Clustering algorithms on SOM. U*C uses density information to merge elementary basins to cluster conform basins.

In this chapter we demonstrate that U*C working on ESOM is superior to other clustering algorithms. In 2005 a set of keystone clustering problems has been published [10]. The data is called Fundamental Clustering Problem Suite (FCPS). It can be obtained from www.mathematik.unimarburg.de/ ~databionics/en/.

From FCPS some data sets are in particular interesting to demonstrate the differences between Emergent and not Emergent cluster algorithms.One of these data sets in FCPS is called "WingNut" and is shown in figure 3. The clusters in WingNut have dense regions just at the borders between the clusters. There the other cluster is sparsely populated. This confuses many clustering algorithms. Single Linkage clustering did not distinguish between the two clusters. The result of a Ward clustering is shown in figure 4. K-means with its implicit requirement, that clusters are of spherical shape constructs a linear border between the two clusters. The global error function which is optimized by in K-means, however, is misled by the dense basins. Figure 5 shows the result

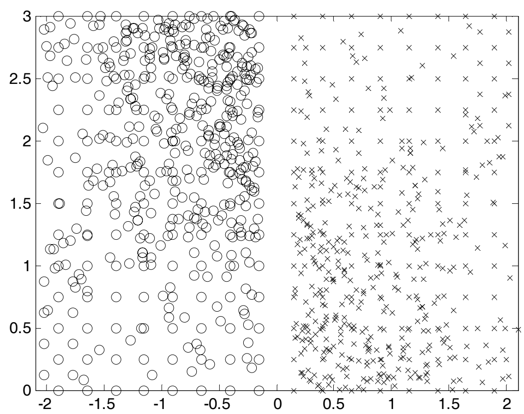

Figure 3: WingNut data set from FCPS

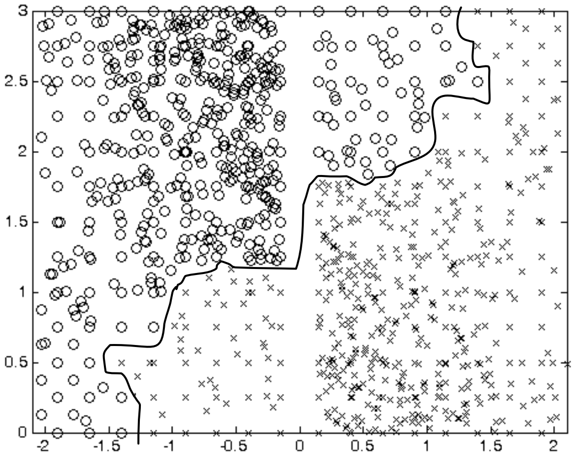

Figure 4 Ward clustering of WingNut

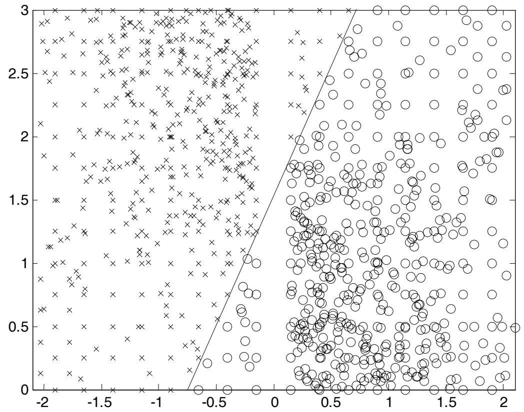

Figure 5 k-means clustering of WingNut

A ESOM consisting of a grid of 50x82 = 4100 neurons has been trained for 20 epochs using point-wise training. A U*-matrix (see [5]) has been constructed which had 62 elementary catchment basins. U*C combines these basins into two cluster conform basins.

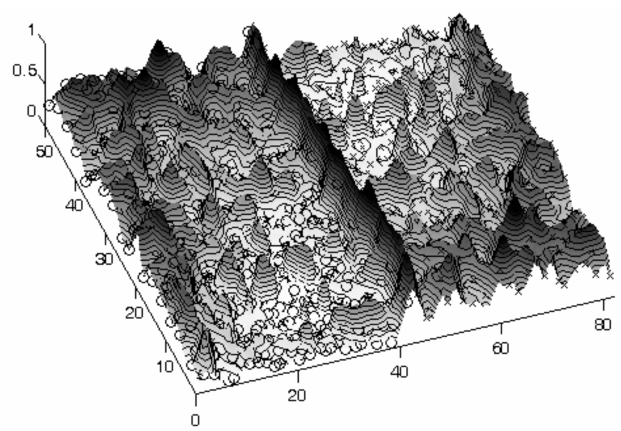

Figure 6: Catchment basins of ESOM for WingNut

For many clustering problems the borders of the clusters are defined as a combination of low density and large distances. In ESOM this can be accounted for by using the U*-matrix [10].

Table 1 summarizes the performance of U*C working on ESOM in comparison to other popular clustering algorithms. The correct number of clusters was used in Single-Linkage, Ward and K-means Clustering. U*C had to find the correct number of clusters by itself.

Table 1: Clustering of FCPS data

DataSet	Single	Ward	k-means	U*C
Hepta	100%	100%	100%	100%
Lsun	100%	50%	50%	100%
Tetra	0.01%	90%	100%	100%
Chainlink	100%	50%	50%	100%
Atom	100%	50%	50%	100%
EngyTime	0%	90%	90%	90%
Target	100%	25%	25%	100%
TwoDiamonds	0%	100%	100%	100%
WingNut	0%	80%	90%	100%
GolfBall	100%	0%	0%	100%

These results show that Emergent clustering is superior to non Emergent clustering algorithm even for very elementary clustering problems.

7 Blind experiment

In fall 2005, the working group of data analysis and numerical classification of the German classification society (GfKl/AG-DANK) performed a blind experiment (http://stoch.fmi.uni-passau.de/agdank/muenchen2005). A set of 11 synthetic data sets with known cluster structure were published without the a priori clustering. This suite was clustered using U*C, Single Linkage, Ward and k-means clustering.

Table 2 summarizes the results. All ESOM results were obtained using 80x50 neurons on a toroid grid in 20 learning epochs. Except U*C all other clustering algorithms needed an estimation of the number of clusters. The results shown are on the basis of the true number of clusters except for U*C which estimates this number by itself. For the data set “dankdata11” U*C identified only 4 instead of 5 clusters. In all other cases the correct numbers of clusters were found.

This shows that the superiority of Emergent clustering can be observed also in true double blind studies.

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Table2: Blind Clustering of AG-DANK data

DataSet	Single	Ward	k-means	U*C
dankdata1	83%	83%	83%	100%
dankdata2	27%	85%	85%	83%
dankdata3	56%	49%	71%	83%
dankdata4	81%	99%	99%	99%
dankdata5	26%	83%	82%	92%
dankdata6	100%	100%	99%	99%
dankdata7	78%	91%	64%	78%
dankdata8	63%	63%	63%	91%
dankdata9	65%	81%	81%	99%
dankdata10	100%	77%	67%	100%
dankdata11	28%	84%	91%	67%

8 Real world data: Protein Cavities

Many biochemical pathways are catalyzed and regulated via the complementary recognition properties of proteins and their substrates. The ligand accommodates the binding cavity of the protein according to the lock-and-key principle. If two binding cavities have common substructures, it can be assumed that the two active sites are capable to bind similar ligands and thus exhibit related function. Figure 7 shows a ligand inside a cavity.

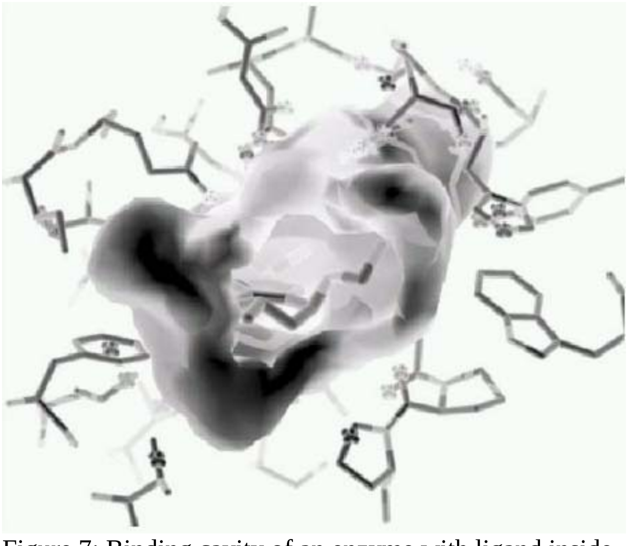

Figure 7: Binding cavity of an enzyme with ligand inside

Enzymes are a particular important class of biochemical agents. Enzymes can be classified with respect to their function. The bound ligand, each enzyme has a specific EC-number. Enzymes having the same EC-number are very similar. Enzymes with different EC-numbers have different cavities. The clustering task is to find common substructures within different cavities in order to identify a common functionality. This work was primarily undertaken by Katrin Kupas of our working group in collaboration of the Institute of Pharmaceutical Chemistry of the University of Marburg [11]. An U*C clustering of 774 binding pockets was performed. For these enzymes the EC class numbers were known. The enzymes belong to 13 different EC classes. The U*C clustering of these enzymes resulted in an accuracy of 98.3% compared to the true enzyme classes. Details of the clustering of enzymes are published in [11].

This demonstrates the applicability of Emergent clustering to large real world data sets with complicate high dimensional structures.

9 Discussion

In this paper an attempt is made to clarify the concept of Emergence in particular for SOM. Although Emergence is a central concept in many modern research areas, there is no precise definition has so far. This paper summarizes the discussion in philosophy and epistemology by giving a number of postulates for Emergence.

It is demonstrated, that SOM fulfill many of the requirements of Emergence. The most critical postulates for Emergent properties of a system are “systemic” and “irreducibility”. For short these postulates claim that emergent properties are “more than the sum of the parts of the system”. At the root of these postulate lies the idea that an Emergent property of a system is only produced by the system as whole (Gestalt-phenomenon). It should not, not even in principle, be possible to derive or even predict the emergent property when single parts of the Emergent system are analyzed. These requirements for Emergence are very hard, if not impossible, to prove. In this paper this postulate is replaced by an approach from semiotics. Semiotic irreducibile properties of a system are such, that the application of the properties, even the vocabulary, does not make sense, if applied to the parts of the system.

For the U-Matrix on SOM the concepts of “watersheds” and “catchment basins” can be defined. However, this makes only sense, if the SOM possesses enough neurons. The problem is the same as the definition of a forest, which is semiotic irreducible to one tree.

The concepts of watersheds and catchment basins are semiotic irreducibile to U-heights of single neurons. If a SOM produces an U-Matrix with watersheds that coincide with a clustering structure in the data, these watersheds are useful in the detection and definition of clusters in the data. Such SOM can be called Emergent SOM (ESOM). It is clear, that if the ESOM is topology preserving in consequence the U-Matrix is cluster conform, even for cluster structures which are not known beforehand.

The usage of these concepts are demonstrated with a clustering algorithm which exploits the Emergent properties (U*C of [9]). On data sets which are known to be simple, but hard to cluster, U*C outperforms clearly

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Single-Linkage, Ward and K-means (table 1). In a double blind experiment, where the true clustering became known only after the publication of the results U*C performed superior to the other clustering algorithms except in one case. In this case U*C estimated a wrong number of clusters. It has to be noted, however, that all other clustering algorithms had knowledge of the true number of clusters, while the ESOM clustering with U*C identified the number of clusters by itself.
On a real world problem, the clustering of three dimensional molecular structures, U*C made only 2% errors. As reason behind the excellent clustering results, the Emergent properties of catchment basins are identified. If a ESOM is formed during training, which is topology preserving, the attractors within watersheds of the corresponding U-Matrix are situated well within a cluster. Thus attractors alleviate the clustering problem at critical borders. A canonical demonstration of this is the WingNut data set of FCPS. In Figure 6 it can be seen, that the attractors are "immersed" in the clusters. The border between the two clusters is clearly marked by a large wall in the U-Matrix. This means that attractors are well within clusters and away from critical borders between clusters.

10 Conclusion

This paper sheds some light on the differences between non Emergent SOM and Emergent SOM (ESOM). The discussion in philosophy and epistemology is summarized here in the form of postulates. The properties of SOMs are compared to these postulates. All SOM fulfill the postulates except the constructivistic ones. The most critical of the postulate are those concerned with "the whole is more than the sum if its part". The original postulates regarding this issue in the epistemological Emergence discussion are hard, if not impossible, to prove. A postulate relying on semiotic concepts, called "semiotic irreducibility" is proposed here as a feasible alternative.
This concept is applied to U-Matrix on topology preserving SOM with many neurons. This leads to the definition of Emergent SOM (ESOM) as one on which the terms "catchment basins" and "watershed" are meaningful and furthermore useful for clustering.
The usefulness of the approach is demonstrated with an ESOM based clustering algorithm, which exploits the emergent properties of such SOM. Results on synthetic data even in a blind study are convincing. The application of ESOM clustering for a real world problem let to an almost 100% solution.

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