A Hierarchical Clustering Method Based on the Computation of Gravity

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Abstract: In this paper a clustering algorithm based on the computation of gravity is described. The gravity supports the modeling of attractors in an artificial world. The classifier is decribed as an internal observer of the feature space.

Keywords: affinity, gravity, field, classifier, observer

1 Introduction

A lot of data must be computed on wide fields of information processing. Here algorithms are needed for the structuring of these data for further processing. The techniques of automatic classification are a possibility for information compression. Objects of data sets are assigned to classes by analysis of its features. Each class is an object set, whose elements have one or more similar characteristics of their features. Elements of such an object set can be distinguished from elements of other object sets, because these elements have other characteristics of the features.

1.1 An overview about Classification Methods

1.1.1 Supervised Learning

Methods of supervised learning are suitable for the assignment of objects or process situations to determined classes. The classifier is the algorithm, which makes a decision with aid of a priori knowledge. This knowledge is a learning sample, which contains characteristic objects of the observed classes and their class indexes. This learning sample makes the classifier able to valuate the object relations within the feature space and to classify new objects correctly.

The quality of the classifier is limited by the quality of the knowledge (the learning sample). The learning sample must reflect the working area of the process, whose states should be classified by the classifier. A faulty learning sample with incorrect class assignments for the objects can injure the quality of the classifier and can lead to incorrect classifications. Such incorrect classifications are possible by adaption of the observed systems. If the adaption will be not considered in the classifier then its decisions are based on invalid knowledge.

In general, the classifier is an observer of the feature space with trained knowledge.

1.1.2 Unsupervised Learning

In opposition to the supervised classification, no knowledge about the object set is necessary for the algorithms of unsupervised classification. In many cases, such a knowledge is not available, for instance, if a first glance about an object set should be given or it is necessary to make a first statement about the obejct set. In these cases, the algorithm must make the structuring of data by itself with the aid of given criteria. The goal of such algorithms is to create a partition which contains all objects of the unstructured object set as class members with its own *class identity*.

The revision of the classification are made with the aid of the given criterion. In many cases, the distance between two objects are used as criterion for similarity. Two objects are similar, if the distance between them has a small value. But the distance to objects of other classes should be significant larger – the dissimilarity to objects of other classes should be larger, too.

Hierarchical clustering methods introduce a hierarchy between the obtained classes. It can be visualized with the aid of a dendrogram. Starting from a start partition, it can be distinguished between ascend and descend clustering methods, which both result in the creation of a dendrogram. Starting from a descend method, at first all objects of the object set are assigned to the same class. With an increase of the differentiation, subclasses are visible in the main class. The objects of the subclasses can be distinguished from objects of other classes by a special feature. And so we can see more and more details in the observed subclasses, we can see subclasses in the subclasses and so on. The hierarchy ends, if each object respective identical objects build its own class. Such a hierarchy can be used as decision tree: if the main class of an object is known, only the contained subclasses must be considered for a more detailed classification. The classification problem can be simplified by this method.

2 Remarks to the Theory of Cognition

2.1 Two-worlds-model

Two basic worlds are face-to-face for the solution of the classification problem: the *reality*, in which the observed process is executed and a so-called *artificial world*, in which the analysis of signals and the classification takes place, see Figure 2.1.

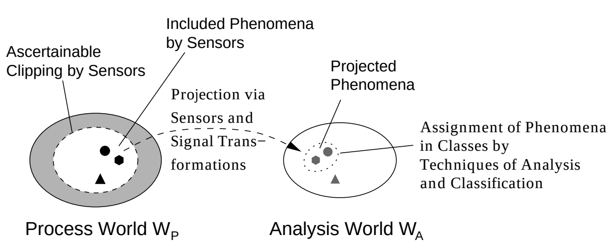

Figure 1: Structure of the Two-Worlds-Model

Similar to the sensual organs of humans, sensors are used for the projection of process situations in the artificial world. The system, which orients itself in the process world, needs not only knowledge about some process situations, it needs knowledge about a whole section of the process history. Similar to the sensual organs of humans, sensors deliver not a whole projection of the process world. Sensors have a limited working area and can registrate only a section of the observed world.

2.2 Noumena and Phenomena

2.2.1 Noumena

Things of the reality or things of the process world, which don't have an access to the artificial world, are called *noumena* [1]. Noumena are (possible) things of the reality, which cannot observed by the sensors, because its external characteristics are outside of the working range. It is also possible that the existence of noumena is not real, but noumena can felt only by its influence on other things.

2.2.2 Phenomena

In general, *phenomena* are appearances in a world. Phenomena have external features. By these featuers, phenomena can be observed by sensors and can be projected into the artificial world. But phenomena have internal features, too. In respect of the artificial world, phenomena are the result of a causal connection. A phenomenon, which appears in the artificial world, must have a corresponding phenomenon in the real world, which was observed by the sensors.

Phenomena can be described by a set of features. An observer resp. a self-oriented system cannot know the set of all possible features of a phenomenon and are not relevant for a significant description. Sensors can only observe a subset of features of real phenomena.

2.3 Belief and Knowledge

The theory of cognition discuss the question, in what kind it is possible to recognize this world. Starting from a realistic world view, the reality exists independently from the human consciousness. The access to this reality takes place by sensual organs, which map a part of the reality into the consciousness (here: the artificial world). Because the sensors can only observe a clipping area, we must proper call it as *belief*, that an object of the artificial world corresponds with the situation supposed in the reality. But this belief can be false. A false belief leads to false classifications and false conclusions.

The knowledge of an observer x about a situation p is defined in [2] as the follow:

x **knows,** that p, if

- p is true
- x believes, that p.

For the valuation, that the knowledge of x is really true, a further, higher observer is necessary, which have access to the knowledge of the observer x and the situation p believed from x. Such an observer must survey both worlds: the artificial world and the real process world. The "teacher" of a classifier can be such an observer.

2.4 Objects as Phenomena

The classifier has the part of the observer in the artificial world. "He" observes the objects of this artificial world and assigns them to determined object sets. The internal observer will be supplied with objects, which come from the external world. These objects are the *relation* between real process situations and the corresponding internal phenomena. Before the classifier can make a statement about the membership of an object, it must solve an elementary classification problem: the classifier must distuingish between an object and a non-object within the feature space. This basic knowledge must be rooted in the structure of the classifier resp. in the used laws.

Statistical and distance classifiers solve this problem by elimination of empty areas of the feature space. Each given position of space is valuated as an object implicitly, which corresponds with an external discrete event. However, it is impossible to valuate the external event by this way.

Fuzzy classifiers valuates given positions as objects, too. However, a membership value mu is allowed here. This membership value allows a statement about the membership of an object to a determined object set.

A phenomenological approach leads to a description of objects, which have *external* and *internal* features. The external features – especially the position in the feature space – correspond with the conditions of the external event resp. the characteristic features of the observed process situation. The internal features allow the detection of the object by an internal observer. In the simplest case, internal features can be *states*. Now it is possible to scan the whole feature space and look for objects. The case, that objects exist, can be detected by a change of states on these positions. A value for the state can be a degree for the *strength* of the believed external situation.

3 Structure of an Artificial World

3.1 Description of a generic field model

Altough a kind of intelligent behaviour is expected from a classifier, it must be able to model this intelligence with the aid of natural and physical laws respective this intelligence must *converge* against such physical laws. In the following, we want to describe some laws which are valid within the artifical world.

3.2 Affinity

Classical criteria for similarity use only the distance between two objects for the valuation of similarity. In opposition to this, we want to use a criterion for similarity for the clustering algorithm, which considers *external* features (like position in the feature space, distance) and *internal* features (the *state* in the simplest case). The state of an object can be interpreted as a kind of "loading" e of an object [3, 4]. The range of this state allows negative values for the modeling of *inverse* objects in the artificial world.

The valuation of external features of objects needs an inertial system in the feature space, with allows the orientation of an internal observer.

Now, a *force* between two objects can be assumed, which describes the tendency of two objects to build a cluster. This force is called *affinity*. The affinity can be computed by the equation

$$\vec{F}_{1,2} = \frac{e_1 \cdot e_2}{\left(d\left(\boldsymbol{m}_1, \boldsymbol{m}_2\right)\right)^3} \cdot \vec{d}\left(\boldsymbol{m}_1, \boldsymbol{m}_2\right) \qquad (1)$$

with d as the euclidean distance between this objects.

3.3 Field Strength

An *affinity field* spreads spherically around an affinity field with the field strength $\vec{A}$. It can be described by

$$\vec{A}_0 = \frac{e_1}{\left(d\left(\boldsymbol{m}_0, \boldsymbol{m}_1\right)\right)^3} \cdot \vec{d}\left(\boldsymbol{m}_0, \boldsymbol{m}_1\right) \qquad (2)$$

A scalar potential field exists in the artificial world, too. The affinity force has the direction that two objects with homonyous loadings are repelled from each other. This orientation leads to an increase of the entropy in the artifical world – if we discuss movable objects – and fulfills the second fundamental theorem of thermodynamics. It preserves the *stability* of objects in this world, because objects are anxious to save its own identity.

3.4 An Analysis-Space-System

3.4.1 The Cellular Space

The space of the artificial world is conform to the n-dimensional feature space, in which objects with n features exists. A discretized space is useful for numeric investigations of the feature space. Such a discretized space consists of a lot of orthogonal and disjoint subspaces, here called *hyxels* (hyperspace elements). You can find a detailed description of the cellular space in [4]. Each object projected into the feature space is located in a determined hyxel of the feature space.

Furthermore, each hyxel can be characterized by the state called *loading* e. If the loading of a hyxel is greater than zero than it can be reasoned, that this hyxel contains objects. The loading of a hyxel depends on the number of contained objects and is – if the loading of an object has a fix value – proportional to the object frequency within the hyxel.

The investigation of a discrete space has the advantage of a simplified numerical analysis, because the hyxels of the cellular space are analysed instead of the objects. For instance, such an algorithm can be realized by nested loops.

3.4.2 A Two-Space-System

If we try to compute the affinity at a position in the feature space, at which an object exists, we obtain $A \to \infty$. To avoid such singularities, we consider two n-dimensional spaces within a $n+1$-dimensional space. The object space $\mathcal{O}$ contains the objects of the object set only. In opposition to this, the analysis of the field behaviour is took place in the analysis space $\mathcal{A}$ which is displaced on the axis of the additional $n+1$st dimension by the value ζ in opposition to the object space. We only investigate the n-dimensional vector field in this space, because a n-dimensional observer cannot feel the $n+1$st field component. Now, the analysis space has no longer singularities in the field behaviour, so we can expect a smooth field behaviour in the analysis space [4].

3.5 Attractors

3.5.1 Attractors as Cause of Stable System Behaviour

A lot of systems of the reality have a stable system behaviour. For instance, controllers control a control variable of a system, the human organism has a stable blood heat, oscillators oscillate around an operating point, planets circulate around their fixed star, galaxies have a stable structure, etc. We can assume *attractors* behind all these cases as cause for the stable system behaviour. Attractors are hidden in most cases, so that only their influence on the system behaviour is ascertainable. Attractors are noumena.

The goal for unsupervised classification techniques is the reconstruction of these attractors with the aid of available observations of the system behaviour. This leads to a description of the cluster algorithm as an *inverse problem*: attractors cause a determined system behaviour in the reality or the process world. This system behaviour is observed by sensors and is projected into the feature space as objects. Now the internal observer has the task to reconstruct the original attractors from the object set.

An internal observer "has the feeling" that the objects are held together by a hidden attractor by a kind of *gravity*. It seems reasonable to investigate the field model of section 3.1 for the usage in a clustering method.

3.5.2 Attractors as Center of Gravity

Now we want to investigate how a field can be constructed from affinity which describes the coherence of objects of a cluster, and thereby, which has characteristics of *gravity*. In opposition of the affinity, the gravity must have an attracting behaviour for the objects. The gravity will be investigated in the analysis space – that is the reason for the consideration of ζ in the Euclidean distance – and can be computed in the point $\boldsymbol{m}_0$ as

$$\vec{G}_0 \quad \lhd\!\!\blacktriangleright \quad \frac{e_1}{\left(d_\zeta\left(\boldsymbol{m}_0, \boldsymbol{m}_1\right)\right)^3} \cdot \vec{d}\left(\boldsymbol{m}_0, \boldsymbol{m}_1\right) \qquad (3)$$

$$= \quad -\frac{e_1}{\left(d_\zeta\left(\boldsymbol{m}_0, \boldsymbol{m}_1\right)\right)^3} \cdot \vec{d}\left(\boldsymbol{m}_0, \boldsymbol{m}_1\right). \qquad (4)$$

You can see the behaviour of gravity in the analysis space for two object clusters and two features in Figure 2. The feature m_3 describes the displacement of the spaces only.

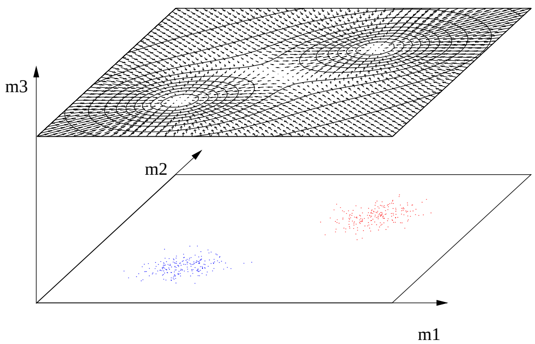

Figure 2: Behaviour of Gravity Using two Object Clusters

The vector field meets two points which are positioned exactly above the object clusters. The equipotential lines indicate two extremal points on these positions, too. An observer in the analysis point is in the curious situation that here the gravity goes to zero because he don't notice the maximum $n+1$st field component. Attractors are hided behind these extremum values which can be accounted as cause for these object clusters. An area exists between both attractors in which the gravity goes to zero, too. But this point is only the equilibrium between the attractors and appears as a saddle point in the field behaviour.

Now it is possible to give a geometrical explanation with the aid of a *mirroring plane*. Originally, this method is used for the solution of boundary value problems, see [3]. Each punctual n-dimensional object causes a spherical affinity field. A characteristic total field arises by the superposition of the partial fields. For the following remarks we assume a n-dimensional mirroring hyper plane in the origin of the $n+1$st feature which is parallel to the object space. The constellation of the spaces is shown in Figure 3.

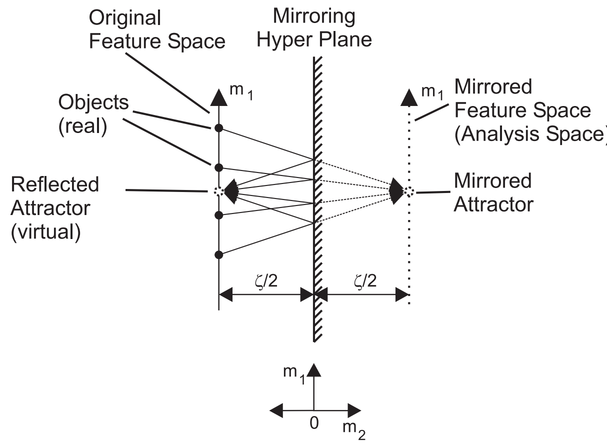

Figure 3: Emergence of Virtual Attractors in the Object Space

If the object space will be moved from the coordinate origin than the object space is mirroring in the hyperplane. The loadings of the objects can be added to a total loading which has – in opposition to the objects – a negative sign. Therefore, the total loading has the characteristic of an attractorand attracts the objects of the object clusters. The field vectors – here symbolized as *rays* – are reflected back into the object space. Now, a virtual atrtactor is come into being in the object space. This attractor cannot be noticed by an observer of the object space. However, it leads to an attraction of the objects and appears as center of gravity. The coherences are shown in Figure for the onedimensional feature space. In general, this method can be used in the n-dimensional space, too.

4 Description of the Classification Techniques

4.1 Unsupervised Classification

The circumstance that attractors have an attraction to objects can be used in a clustering algorithm. In this case, attractors have the function as *prototypes* for clusters. An increase of the distance of the object space to the hyperplane leads to an increase of the superposition of the affinity fields of the partiocular objects. The result is a merger of the attractors of the particular object clusters. A falling ζ leads to the decrease of the superposition and a division of attractors. The two emerging attractors migrate to the centres of the object sets, and a saddle point emerges at the position of the original common attractor. The division of an attractor can be shown as a bifurcation in a dendrogram. Saddle points in the field behaviour indicates a point of equilibrium of oppositional attractors.[1]

The search for attractors is equivalent to the search for local extrema in the potential behaviour. In a cellular space, the potential of the interesting hyxel must be compared with the potential of the neighbouring hyxels (von-Neumann-neighbourship). The scan of the whole cellular space with orthogonal hyxels is easy.

It is practical to start the algorithm with a high value for ζ. At first, the behaviour of the potential must be computed, and after this, the extremum must be searched. After each successful search, the value for ζ will be decreased. Then the search must be started again. We can abort the algorithm, if ζ has reached a minimum value. The algorithm has the following form:

1. Start with $\zeta = \zeta_{max}$
2. Compute the potential behaviour in the analysis space
3. Search for extrema in the potential $\rightarrow$ found extrema are positions of attractors
4. $\zeta = \zeta - \Delta\zeta$
5. $\zeta < \zeta_{min}$?
   (a) yes: abort
   (b) no: goto 2

4.2 Supervised Classification

Now, a assignment of new objects is easy with the aid of found atrtactors. We can simply compute the affinity of a new object to the attractors. The object will be assigned to the attractor with the highest affinity, and we can note

$$e = \operatorname{argmax}_{i=1}^{C} \vec{F}_i\left(\boldsymbol{m}_0\right). \tag{5}$$

[1]This is similar to a lever balance. The pivot in the middle can be compared with the saddle point.

5 Simulation and Applications

5.1 Similarity Between Two Signals

The fieldmodel can be used for the computation of the similarity of a measured signal to a given reference signal. An example for such signals is shown in Figure 4. You can see two test signals beside the reference signal. The signal comes from an automotive concern and show the simulated brake behaviour.

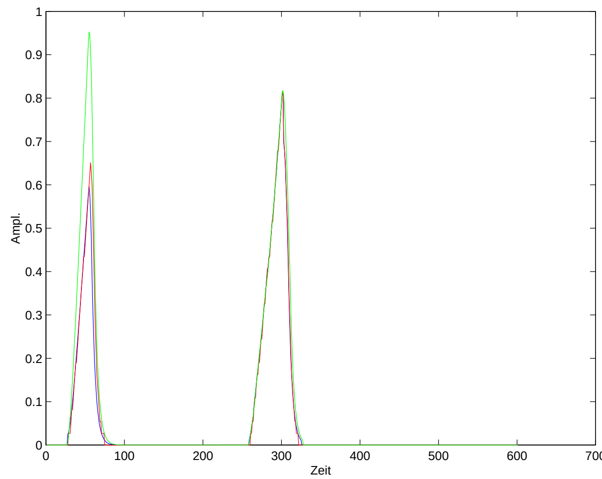

Figure 4: Behaviour of the Reference Signal and Three Test Signals

The signals include each 500 samples, so we can describe a brake event by 500 different features. Because the field model is also valid in higherdimensional spaces, we can project the reference signal as a point into the 500-dimensional analysis space. Here it has the function of an attractor. The test signal (also with 500 features) is an object in the obhect space. Now we can compute a determined affinity between the object and the attractor. This affinity depends on the distance between the highdimensional objects. The value of ζ controls the *sharpness* of the criterion of similarity. The affinity depends on ζ, too. Therefore we must normalize the affinity of the attractor to the test object with the affinity of the attractor to the attractor mirrored into the object space. We obtain for the similarity between two signals x_{ref} and x_{test} the criterion s

$$s_{ref,test} = \frac{\vec{F}_{ref,test}\left(\zeta\right)}{|\vec{F}_{ref,test}\left(\zeta\right)|}. \tag{6}$$

The geometric connection between attractor and test object is shown in Figure 5.

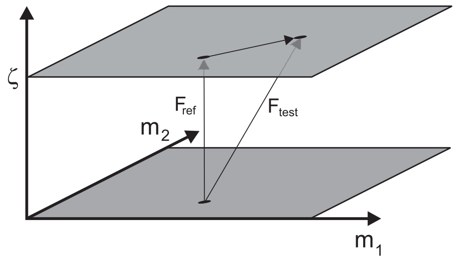

Figure 5: To Similarity of two Punctual Objects

For the three test signals and a distance $\zeta = 3$, we obtain the similarities $s_{1,1} = 1$ (the reference signal compared with itself), $s_{1,2} = 0.9743$ (the reference signal compared with test signal 1) and $s_{1,3} = 0.8$ (the reference signal compared with test signal 2).

5.2 The Clustering Algorithm

An unclassified data set consisting of five object clusters was used for the test of the clustering algorithm, see Figure 6.

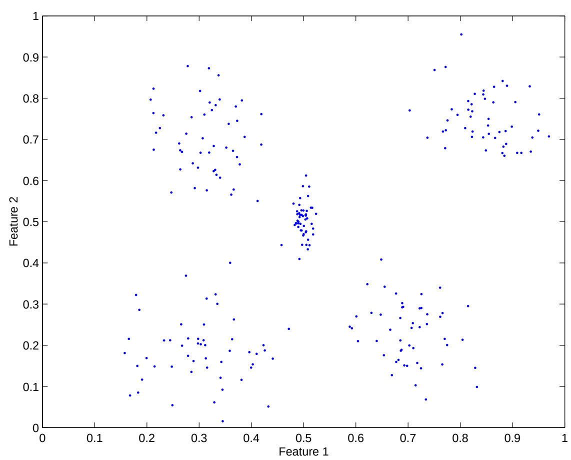

Figure 6: Unclassified Data Set

The potential maps were computed starting with high values for ζ, the parameter ζ was decreased successively after each computation. The extrema was searched for each potential map. The found extrema was used as attractors for a following supervised classification. The best potential map was the map with $\zeta = 100$. Their extrema correspond with the five given object clusters. The potential map for $\zeta = 100$ is shown in Figure 7. The following classification of objects affirms the assumed object clusters of Figure 6.

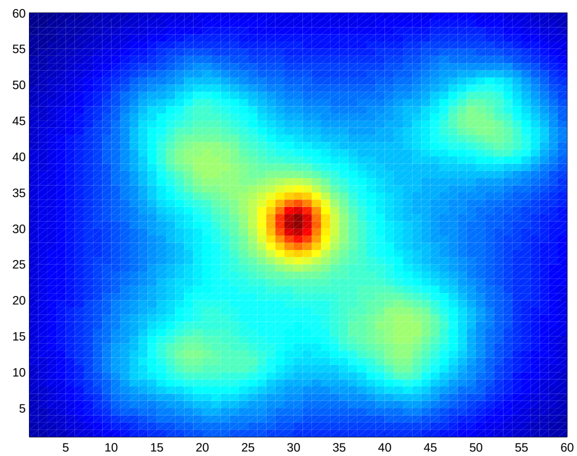

Figure 7: Potential Behaviour for $\zeta = 100$

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