Raport Badawczy
Research Report

RB/56/2001

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Pracę zgłosił: prof. dr hab.J.Kacprzyk

Warszawa 2001

IEEE Trans on SMC-B(to appear)

Granular Clustering: a Granular Signature of Data

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Abstract The study is devoted to a granular analysis of data. We develop a new clustering algorithm that organizes findings about data in the form of a collection of information granules – hyperboxes. The clustering carried out here is an example of a granulation mechanism. We discuss a compatibility measure guiding a construction (growth) of the clusters and explain a rationale behind their development. The clustering promotes a data mining way of problem solving by emphasizing the transparency of the results (hyperboxes). We discuss a number of indexes describing hyperboxes and expressing relationships between such information granules. It is also shown how the resulting family of the information granules is a concise descriptor of the structure of the data - a granular *signature* of the data. We examine the properties of features (variables) occurring of the problem as they manifest in the setting of the information granules. Numerical experiments are carried out based on two-dimensional synthetic data as well as multivariable Boston data available on the WWW.

Keywords information abstraction, information granules and granulation, principle of balanced information granularity, interval analysis, confidence limits analysis, complex systems, data mining, granular time series, feature analysis, hyperboxes

1. Introductory comments

Making sense of data has been a motto of data mining. Any in-depth analysis of data that leads to comprehensive and interpretable results has to address an issue of transparency of final findings. In one way or another, arises a need for casting the results in the language of information granules -- conceptual entities that capture the essence of the overall data set in a compact manner. It is worth stressing that information granules are a vehicle of abstraction that supports a conversion of clouds of numeric data into more tangible information granules [2][3][5]12][13][16][17][18].

The area of clustering with its long history has been an important endeavor of finding structures in data and representing the essence of such finding in terms of prototypes, dendrograms, self-organizing maps [8][9] and alike [1][4]. Commonly, if not exclusively, the direct aspect of granulation has not been tackled. The intent of this study is to address this important problem by introducing an idea of granular clustering. Being more descriptive, a simplest scenario looks like this: we start from collection of numeric data (points in $\mathbf{R}^n$) and form information granules whose distribution and size reflects the essence of the data. Forming the clusters (information granules) may be treated as a process of *growing* information granules – as the clustering progresses, we expand the clusters, enhance the descriptive facet of the granules while gradually reduce the amount of details being available to us. The information granules we are interested in this study are represented as hyperboxes positioned in a highly dimensional data space. The mathematical formalism of the interval analysis provides a robust framework for the analysis of information density of the granular structures that emerge in the process of clustering. The study reflects the intuitive objective of matching the granularity of data items used to describe the physical systems to the structure of these systems. In this sense the granulation process is attempting to achieve the highest possible generalization while maintaining the specificity of data structures.

The paper is organized into 7 sections. In Section 2, we start off with an introduction to information granules and spell out a rationale behind information granulation. As we are concerned with information granulation carried out in terms of sets (hyperboxes), this formalism is supported with all pertinent notation. The principle of granular clustering is covered in Section 3 that is followed by a complete algorithm (Section 4). Data analysis completed in the framework of information granules is studied in Section 5. Finally, experimental studies are included in Section 6.

2. Information granules and information granulation

Most experimental data available in a raw form are numeric. Granulation of information happens through a process of data organization and data comprehension. Interestingly; humans granulate information almost in a subconscious manner. This eventually makes the ensuing cognitive processes so effective and far superior over processes occurring under the auspices of machine intelligence. Two representative categories of problems in which information granulation emerges in a profound way involve processing of one and two-dimensional signals. The first case, we are concerned primarily with temporal signals. The latter case pertains to image processing and image analysis. In signal processing, analysis and interpretation the granules arise as a result of temporal sampling and aggregation. Several samples in the same time window can be represented as an information granule. In the simplest case, such interval can be formed by taking a minimal and maximal value of the signal occurring in this window of granulation, refer to Figure 1. Some other ways of forming information granules may rely on statistical analysis: one determines a mean or median as a representative of the numeric data points and then build a confidence interval around it (obviously, the use of this mechanism requires assumptions about the statistical properties of the population contained in the window as well as the numeric representative under discussion). Similarly, in image processing one combines pixels exhibiting some spatial neighborhood. Again, various features of an image can be granulated, say brightness, texture, RGB, etc.

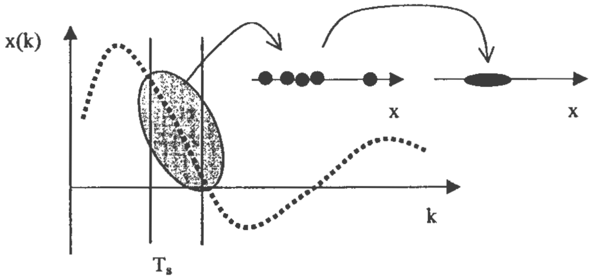


Figure 1. A fragment of a time series and its granulation trough sampling (T_s denotes a sampling interval)

Information granulation has been studied in [2][3][10][12] both in terms of the concept itself, computational aspects of it as well as resulting structures.

2.1. Set-based framework of information granules: the language of hyperboxes

In the overall presentation we adhere to a standard notation. A hyperbox defined in $\mathbf{R}^n$ is denoted by B and is fully described by its lower ($\mathbf{l}$) and upper corner ($\mathbf{u}$). To use explicit notation, we use $B(\mathbf{l}, \mathbf{u})$ where $\mathbf{l},\mathbf{u} \in \mathbf{R}^n$ and obviously a strict inclusion relationship holds true $\mathbf{l} \leq \mathbf{u}$. If $\mathbf{l} = \mathbf{u}$ the box reduces to a single point (numeric datum) $B(\mathbf{l}, \mathbf{l}) = \{\mathbf{l}\}$. Hyperboxes are elements of a family of relations defined in $\mathbf{R}^n$ More specifically we state that $B \in \mathcal{P}(\mathbf{R}^n)$ with $\mathcal{P}(.)$ being a class of sets. The volume of B, denoted by V(B), is viewed as a measure of specificity of the information granule. The point, $B(\mathbf{l},\mathbf{l})$ comes with the highest specificity that becomes reduced once the volume increases. Computationally, it is advantageous to consider the expression exp(-V) which captures the same aspect of granularity yet this measure is normalized as it attains 1 for the numeric datum and reduces to zero once the hyperbox starts growing.

3. The principle of granular clustering

Before we proceed with the details of the clustering technique for granular data, it is instructive to discuss the underlying principle, learn how the process proceeds and concentrate on the interpretation of some results generated by the proposed clustering mechanism.
As emphasized in the literature [1] [4], the essence of clustering (unsupervised learning) is to discover a structure in data. In essence, almost all existing clustering techniques operate on numeric objects (vectors in $\mathbf{R}^n$) and produce representatives (say, prototypes) that are again entirely numeric. In this sense, their form does not reflect how much data points they represent and how the distribution of these data points looks like (obviously, the nature of data is captured by a pertinent allocation of the prototypes). In the design of the clustering method, we add an extra dimension of granularity that helps sense the structure in the data as it becomes unveiled during the formation of the clusters.

3.1. The design

This approach introduced here is very much different in many ways from the others. The leitmotiv is the following

- abstraction (no matter whether dealing with numeric or granular elements) is achieved through *condensation* of original data elements into granules whose location and granularity reflects the essence of the structure of data. The more condensation, the larger the sizes of the information granules that realize this aggregation.

At the qualitative end, the granular clustering is carried out as the following iterative process

- find the two closest information granules (where the idea of compatibility guiding this search of information will be quantified later on) and on this basis build a new granule embracing them. In this way, one condenses the data while reducing the size of the data set
- repeat the first step until enough data condensation has been accomplished (here one has to come up with a certain termination criterion or introduce a sound validation mechanism)

Figure 2 illustrates how the clustering works. We start from a collection of small information granules (these are original data) and start growing larger information granules. Noticeably, through their growth they tend reflecting the essential characteristics of the original data. The size of the granules reflects quite evidently how much they incorporated the original data and convey an extra message about their dispersion (distribution).

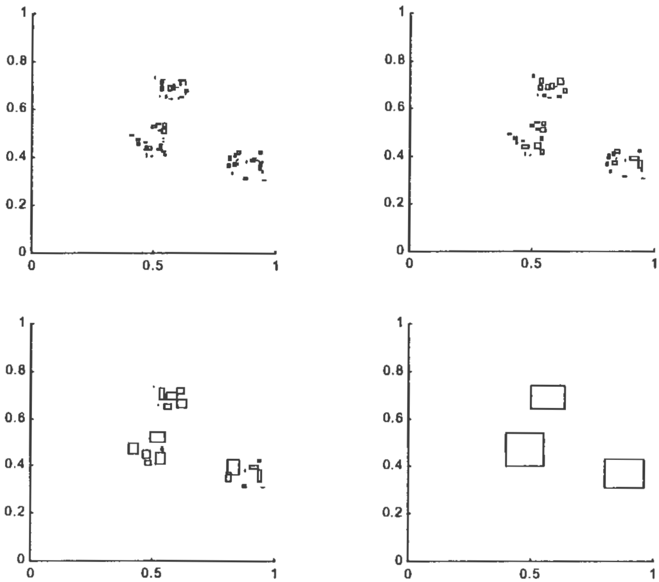


Figure 2. Several snapshots of cluster growing over the clustering process; observe that small information granules forming at the initial stage (first iteration) that are grouped in some well-confined regions and give rise to three apparent large information granules at the later stage of clustering

Considering a way in which the data points are merged together this approach resembles techniques of aggregative hierarchical clustering. There is a striking difference though: in hierarchical clustering we deal with numeric objects and the clusters are sets of the same objects. No conceptually new entities are formed. Here, we "grow" the clusters: from iteration to iteration they tend to form larger hyperboxes. Moreover the nature of these hyperboxes help monitor the clustering process more thoroughly and raise awareness about terminating the clustering. Essentially, once we have found that the evolved boxes become distant in the state space, the process of clustering (forming combined boxes) is terminated.

By the same token, this concept should be contrasted with the idea of min-max clustering discussed by Simpson [14] [15] as this technique seems to bear some resemblance with the method studied here. The similarity is superficial though. First, the Simpson's method deals with point-size data while we consider data that is represented by either points or hyperboxes in pattern space. Second, the fuzzy membership functions of the information granules (clusters) as proposed by Simpson promote formation of clusters that are having largely varying sizes in various dimensions which is exactly the opposite to what we are trying to promote through the "compatibility measure" (discussed in Section 4). To emphasise the latter point we present in Figure 3 a representative of a class of membership functions proposed by Simpson and refer the reader to Figure 9 for comparison with the functions that have been utilised in our clustering algorithm.

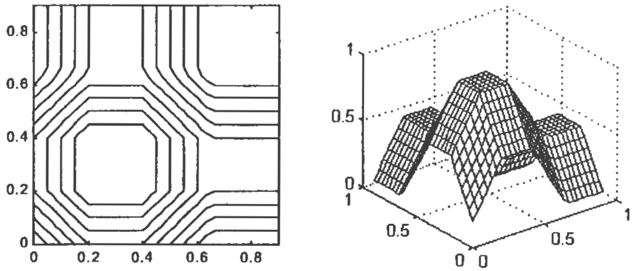


Figure 3. Simpson's membership function (as presented in [15]) for the hyperbox defined by the min point V=[0.2 0.2] and max point W=[0.4 0.4]. Sensitivity parameter γ is equal to 4.

3.2. Interpretation and validation of granular clustering

Clustering comes with a significant number of cluster validity indexes whose role is to identify the most "plausible" number of clusters. They help navigate the clustering process by stating what number of clusters should be. Commonly, their behavior does not lead to clear conclusions. What could be even worse, they may generate conflicting suggestions as to the termination condition (that is the number of clusters).
In granular clustering we take another position. As the clusters capture the core of the data (and obviously, this is regarded as an important benefit of the method), our conjecture is that such core should help establish a sound platform of assessment of the structure (granular clusters).

When progressing with an expansion of the information granules, a certain criterion worth investigating deals with measuring a volume of the smallest granule (V_{min}) that is constructed at this particular step (more specifically, we determine $e^{-V_{min}}$; the details will be covered in Section 4.1). The main point is that if such minimal volume grows quickly to cluster two granules, then it can be deduced that the compatibility of the component granules is low and the clustering process can be completed.

Again, it is worth emphasizing that the granularity of data adds an extra important dimension to any processing. Not only a location of the information granule is essential but also its size plays a crucial role in the process of clustering and afterwards during the validation of the clusters.

4. The computational aspects of granular computing

There are two essential functional elements of granular clustering that need to be constructed prior to moving to the detailed computing. These concern a way in which a distance between two information granules is determined and how we compute an inclusion relation between them. While the definitions generalize to a multidimensional case, we focus here on a two-dimensional case. Note also that these two concepts work for heterogeneous data that is granules and numeric entities.

4.1. Defining compatibility between information granules

In this section, we discuss details in which a compatibility and inclusion between two information granules are computed. The issue is more complicated than in a numeric case as these notions are granular and therefore the definitions of compatibility and inclusion should reflect this aspect as well.

Consider two information granules (hyperboxes) A and B. More explicitly, we follow a full notation $A(\mathbf{l}_a, \mathbf{u}_a)$ and $B(\mathbf{l}_b, \mathbf{u}_b)$ to point at their location in the space. The expression of compatibility, compat(A, B) involves two components that is a distance between A and B, d(A,B), and a size of a newly formed information granule that comes when merging A and B. The distance d(A,B) between A and B is defined on a basis of the distance between its extreme vertices, that is

$$d(A, B) = (\|\mathbf{l}_b-\mathbf{l}_a\| + \|\mathbf{u}_b-\mathbf{u}_a\|)/2 \tag{1}$$

that is an average of the two distances. Obviously $\|.\|$ is a distance defined between the two numeric vectors. To make the framework general enough, we treat $\|.\|$ as an L_p distance , p>1. By chaging the value of "p" we sweep across a spectrum of well known distances that depend upon a particular value of "p". For instance, p = 1 yields a Hamming distance, L_1. The value p = 2 produces a well – known Euclidean distance, L_2. For $p = \infty$ we refer to a Tchebyschev distance, L_∞.

Once A and B have been combined giving rise to a new information granule C, its granularity can be captured by a volume, $V(C)$ computed in a standard way

$$V(C) = \prod_{i=1}^{n} \text{length}_i(C) \tag{2}$$

where

$$\text{length}_i(C) = \max(u_b(i), u_a(i)) - \min(l_b(i), l_a(i)) \tag{3}$$

i=1, 2, …, n. For details, refer to Figure 4.

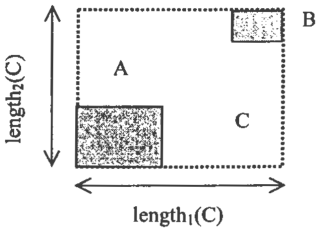


Figure 4. Information granule C as a result of combining A and B

The two expressions (1)-(2) are the contributing factors to the compatibility measure, compat(A, B) to be defined now in the form

$$\text{compat}(A, B) = 1 - d(A,B)e^{-\alpha V(C)} \quad (4)$$

The rationale behind the above form of the compatibility measure is as follows. In clustering we aggregate (cluster) two information granules that are the closest viz. their compatibility measure is the highest, compat(A, B) = 1. In light of the above criterion, the candidate granules to be clustered should not only be "close" enough (which is reflected by the distance component) but the resulting granule should be "compact" (meaning that the size of the granule in every dimension is approximately equal). The second requirement favors such A and B that give rise to a maximum volume for a given d(A, B), in other words it stipulates formation of hyperboxes that are as similar to hypercubes as possible. The particular exponential form of this expression has to do with the normalization criterion so that all values are kept in the unit interval. In particular, the volume of a point produces $e^{-0} = 1$ While the volume increases, its exponential function goes down to zero. The parameter α balances the two concerns in the compatibility measure and is chosen so as to control an extent to which the volume impacts the compatibility measure.
The compactness factor ($e^{-\alpha V(C)}$) introduced in the compatibility measure is critical to the overall processing (viz. clustering) of the information granules. By contrast, it is not essential and does not play any role when we proceed in a standard way and do not attempt to develop granules but retain a cluster of numeric data.
To retain the values of the compatibility measure to the unit interval, we consider the data to lie in the unit hypercube $[0,1]^n \subset \mathbf{R}^n$ (in other words we normalize the data before computing the value of (4)).
To gain a better insight of what really is accomplished when using the above compatibility measure, let us study two points (numeric values) A and B situated in $\mathbf{R}^2$. Furthermore let A be fixed and located at the origin of the coordinates while we allow B with some flexibility. d(A, B) is just a standard Euclidean distance. It becomes obvious that all elements (Bs) located on a circle of a fixed radius exhibit the same distance value. Restrict now a choice of Bs from this pool. If we connect A and any of such Bs, the resulting volume changes its value depending upon the location of B. Interestingly, out of all Bs, there are four of them (located on this circle) for which the volume of the resulting attains its maximum. This happens if such box(viz. the information

granule formed by clustering A and B) is a square, refer again to Figure 5. In other words, the compatibility measure attains a maximal value there.

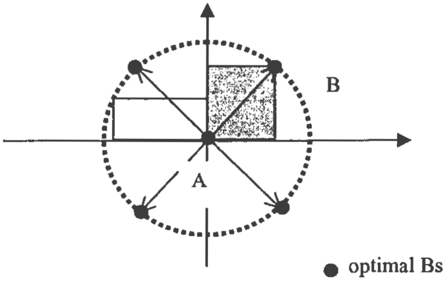


Figure 5. The calculations of the compatibility measure; note that there are four possible candidates (Bs) on the circle that maximize this measure

If we plot the compatibility measure as a function of τ (where τ is an angular position of B), we can easily see that the values of the compatibility measure is modulated by the angle (or equivalently the shape of the resulting information granule C), see Figure 6.

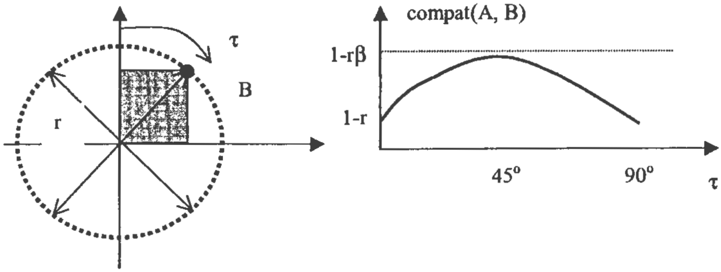


Figure 6. The compatibility measure expressed as a function of τ (the plot here plot is restricted to the first 90^0 degrees); $\beta = e^{-\alpha r . r/2}$

More importantly, the above graphical considerations shed light on the geometry of the information granules that are preferred by the introduced compatibility measure. Such preference reflects a principle that may be coined as a *principle of balanced information granularity*. In a nutshell, in building new information granules, we prefer to have entities whose granularity is balanced along all dimensions (variables) rather than constructing granules that are highly unbalanced. A number of selected examples of varying granularity are portrayed in Figure 7.

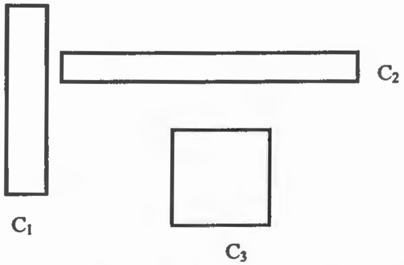


Figure 7. Examples of information granules characterized by various degrees of balance of information granularity; note that C_1 and C_2 are highly unbalanced as exhibiting different levels of information specificity along one of the variables (C_1 and C_2 with high specificity along x1 and x2, respectively) while C_3 is well-balanced.

When changing the distance function to the Hamming (p = 1) and Tchebyschev distance (p=∞), and carrying out the calculations of the compatibility measure, see Figure 5, now we have a number of Bs to choose from yet this selection can be made from different geometrical figures (that is a diamond and a square), Figure 8.

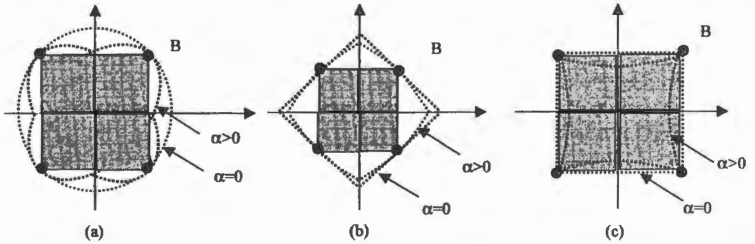
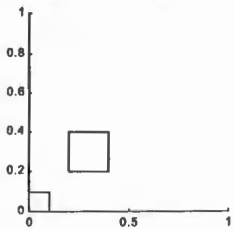
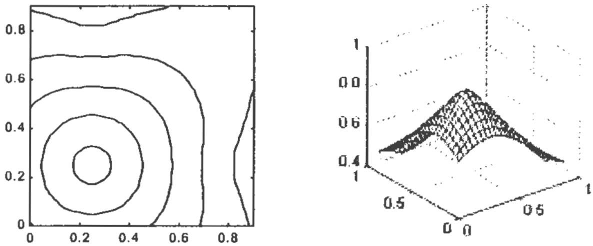


Figure 8. Identification of Bs leading to the highest value of the compatibility measure

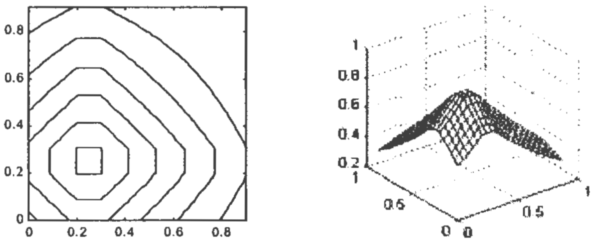
Moving on to the case where both A and B are two information granules, the resulting plots visualizing the compatibility measure are collected in Figure 9.



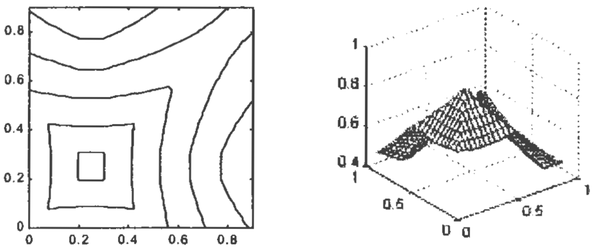
(a) Two hyperboxes representing information granules in a unit box in R^2



(b) Compatibility measure with L_2 distance measure



(c) Compatibility measure with L_1 distance measure



(d) Compatibility measure with L_∞ distance measure

Figure 9. Comparison of compatibility measures obtained with various distance measures. Note the preference that the compatibility measure gives to hyperboxes that are well balanced in all dimensions. This contrasts with the membership function proposed in [15] and illustrated in Figure 3.

As the clustering proceeds (refer to Figure 2) the process of merging the progressively less closely associated patterns finds its reflection in the gradual reduction of the compatibility measure (4). A typical plot of the evolution of the compatibility measure over the complete clustering cycle is shown in Figure 10.

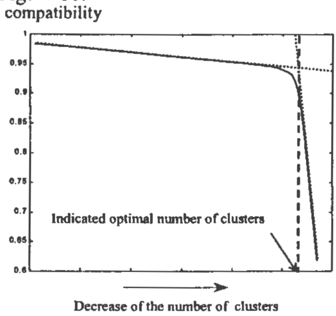


Figure 10. An example of the evolution of the compatibiliy measure over the full cycle of the clustering process.

It is self evident that the proximity of patterns that are being merged into granules at the early stages of the clustering process, is reflected in the relatively small gradient of the compatibility measure curve. By contrast, a large gradient of the curve, at the final stages of the clustering, indicates merging of incompatible clusters. The compatibility measure curve provides therefore a convenient reference for identifying which number of clusters captures the essential characteristics of the input data while providing the best generalization of them. The intersection of the two gradient lines (as indicated in Figure 10) can be used as an approximation to the optimal number of clusters. This number provides a good starting point in the subsequent optimization of the overlap of the identified clusters as discussed below.

4.2. Expressing inclusion of information granules

The inclusion relation expressing an extent to which A is included in B is defined as a ratio of two volumes

$$incl(A,B) = \frac{V(A \cap B)}{V(A)} \tag{5}$$

It is clear from the above that the inclusion measure is monotonic, non-commutative and satisfies the following boundary conditions: Incl(A,X)=1 and Incl(A,$\emptyset$)=0 where X and $\emptyset$ are the unit hyperbox and the empty set in $\mathbf{R}^n$, respectively. The calculations are straightforward; Figure 11 enumerates all cases for one-dimensional granules along with the pertinent values of this measure.

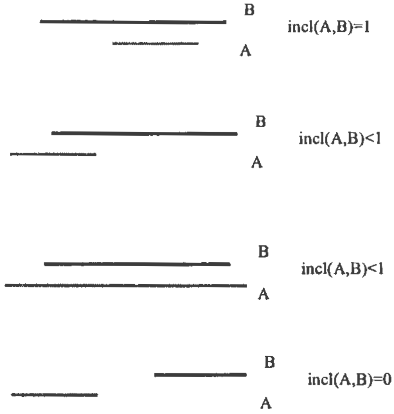


Figure 11. Computing the inclusion for two information granules A and B

It is worth mentioning that the value of the inclusion measure drop down quite substantially (at a rate of a^{-n} where $a \in (0, 1\}$ with the increasing dimension of the space in which the information granules are distributed. For example if there is an ½ overlap (a=2) in each variable in an n-dimensional space, the inclusion level expresses as 2^{-n}.

Clearly, the objective of effective information abstraction through clustering of information granules translates into identifying for which number of clusters there is a minimum overlap between the clusters. To encourage merging of clusters that have significant overlap we calculate an average of the maximum inclusion rates of each cluster in every other cluster, (6).

$$overlap(c) = \frac{1}{c-1}\sum_{i=1}^{c}\max_{\substack{j=1,..c \\ j\neq i}}(incl(A_i, A_j)) \tag{6}$$

where c is the current number of clusters and A_i and A_j are i-th and j-th cluster respectively.
It has to be pointed out however that, while the measure (5) is monotonic for any two pairs of clusters i.e. if $A \subset B$ and $C \subset D$, then $incl(A,C) \leq incl(B,D)$, the change of the number and the size of clusters during the clustering process results in the collective measure, (6), having various local optima. We illustrate this effect in Figure 12.

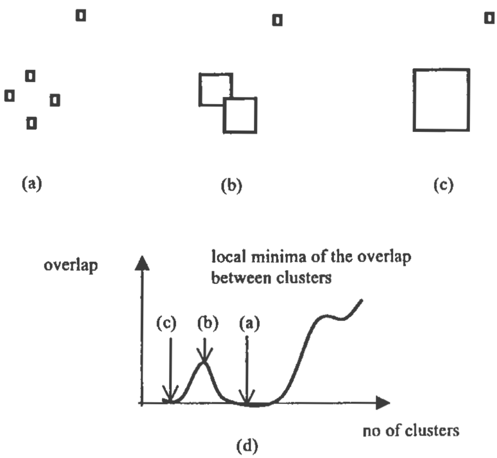


Figure 12. Progression from 5 to 2 clusters involves stage (b) during which clusters overlap. This is reflected in *overlap*(3) > 0 while *overlap*(5) = 0 and *overlap*(2) = 0

Because of the local minima of the *overlap*(.) function it is important to have a good initial estimate of the number of clusters as a starting point for the local minimization of the function. Such an estimate is provided by our earlier analysis of the compatibility measure as discussed in the previous section.

Having accomplished the clustering process the quality of data abstraction afforded by the given set of data clusters is measured using an independent validation data set. The generality of each of the identified clusters is well quantified by the sum of the inclusion rates of the validation data items in the respective cluster.

$$\mathrm{INCL}(i) = \sum_{j=1}^{M} \mathrm{incl}(V_j, A_i) \qquad i = 1,..c \tag{7}$$

where c is the number of clusters and M is the cardinality of the validation data set.
As well as indicating whether a given cluster is representative for a large proportion of data the INCL(.) measure can be used to assess how representative are the training and the validation data sets. If the sets are representative, then INCL(.) should correlate closely with the cardinality of the individual clusters.

5. The Granular Analysis

The hyperboxes constructed during the design phase are helpful in a thorough analysis. They shed light on the nature of data as they are perceived from the standpoint of information granularity established during the design of the hyperboxes. Two main aspects are distinguished. First, we characterize the hyperboxes themselves. Second, we analyze the properties of the variables (features) forming the data space. We should emphasize that the granular analysis follows the synthesis phase and does not impact it in any way. To maintain conciseness of the presentation, we consider that each out of "c" hyperboxes located in the n-dimensional space is fully described by vectors of its lower and upper corners (coordinates), that is $\mathbf{B}(k) = \{\mathbf{l}(k), \mathbf{u}(k)\}$, k=1, 2, …, c where $\mathbf{l}(k)$ and $\mathbf{u}(k)$ are vectors of the corresponding coordinates, that is $\mathbf{l}^T(k) = [l_1(k)\ l_2(k) \ldots l_n(k)]$ and $\mathbf{u}^T(k) = [u_1(k)\ u_2(k) \ldots u_n(k)]$

5.1. Characterization of hyperboxes

The most evident characterization of the hyperboxes can be provided in their volumes, V(B(k)). The computations are obvious. First, we determine a ratio (normalized length)

$$\text{norm\_length}_i(B(k)) = \frac{u_i(k) - l_i(k)}{\text{range}_i(B(k))}$$

where $\text{range}_i(B(k))$ is a range of the i-th feature (variable). Since the data is normalised to a unit hypercube the $\text{range}_i(B(k)) = 1$ for all i. Second, the volume is taken as a product

$$V(B(k)) = \prod_{i=1}^{n} \text{norm\_length}_i(B(k))$$

The volume quantifies the essence of granularity of the hyperboxes. Intuitively, it states how "large" (detailed) the hyperboxes are and how much details each of them captures. One can take an average of the volumes of the hyperboxes that gives a general summary of the hyperboxes

$$\bar{v} = \frac{1}{c}\sum_{k=1}^{c} V(B(k))$$

If one sides of the hyperbox is zero then the volume measure returns a zero value. This occurs because of the multiplicative nature of volume. To alleviate sch problem, we may also introduce a measure of an additive character. A plausible descriptor of a hyperbox could reflect a "circumference" of the hyperbox and read as follows

$$\sum_{i=1}^{n} \text{norm\_length}_i(B(k))$$

5.2. Granular feature analysis

The granulation of the data space (and each feature) provides an interesting insight into the nature of the variables occurring in the problem. In what follows, we provide their description in terms of sparsity and discrimination abilities. These two descriptors are exclusively implied by the granular nature of the hyperboxes.

Sparsity

When looking at a certain variable of the hyperboxes, we can visualize how much of the entire range of the variable is occupied by the hyperboxes (i.e., how *sparse* the boxes are in the given space). Take the i-th feature and calculate the sum of length of the corresponding sides of the hyperboxes that is

$$\text{tot\_length}_i = \sum_{k=1}^{c} \text{length}_i(B(k))$$

where $\text{length}_i(B(k)) = u_i(k) - l_i(k)$. The sparsity defined in the form

$$\text{sparsity}_i = \frac{\text{tot\_length}_i}{\text{range}_i}\frac{1}{c}$$

assumes values in the unit interval. If sparsity_i is less than 1 then this represents a situation when hyperboxes (more precisely its i-th coordinate) occupy a portion of the entire range of the feature. We may state that the variable is "underutilized". In other words, we witness a highly localized usage of this feature. The sparsity around 1 means a complete utilization of the variable. The effect of overutilization happens when sparsity achieves values higher than 1 (in this case we have some hyperboxes overlapping along this variable).
The sparsity does not capture the entire picture. A situation illustrated in Figure 13 shows two cases where the distribution of the hyperbox along the given feature is very different yet we end up having the same value of the sparsity. This leads us to another index (descriptor) that describes an overlap between the hyperboxes

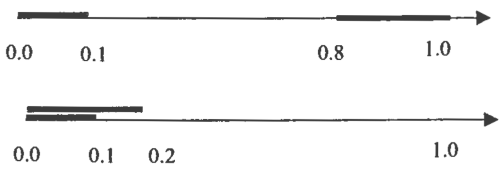


Figure 13. Two different distributions of hyperboxes (i-th feature) producing the same value of the sparsity index; in both cases the sparsity is equal to 0.3

Overlap index

We define the following index called coordinate overlap

$$c-overlap_i = \frac{2}{c(c-1)} \sum_{k=1}^{c-1} \sum_{l>k}^{c} \frac{length_i(I(k) \cap I(l))}{length_i(I(k) \cup I(l))}$$

i =1,2, …, n. In this definition, I(k) and I(l) are intervals (sides) of the hyperboxes for the i-th variable.The higher the value of this index, the more overlap between the hyperboxes expressed along the given variable. When I(k) and I(l) are pairwise disjoint then the overlap is equal to zero. This means that the feature is highly discriminative as it separated the hyperboxes. The higher the overlap measure, the lower the discriminatory aspects of the feature.

Each of the measures leads to a linear ordering of the variables. We can easily state which of the variables is highly "utilized" and which of them comes with the most significant discriminatory properties. To form a comprehensive picture, one can localize each feature in the sparsity – overlap space, Figure 14. By doing this, one can distinguish between the variables that are essential to the problem. More specifically, we prefer features that exhibit low overlap (as those come with strong discriminative properties) along with low values of sparsity that points at the issue of the localized usage of the variable.

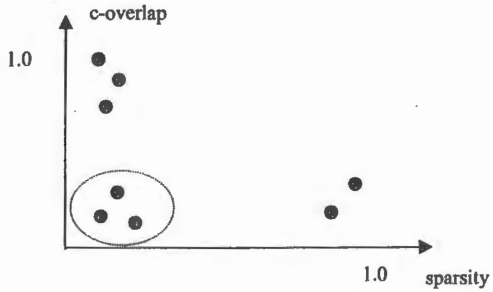


Figure 14. Sparsity – overlap space and feature arrangement; note a collection of highly discriminative features of low sparsity

It should be stressed that the above descriptors (sparsity and overlap) of the features emerge as important quantifiers because of the existence of information granules forming the hyperboxes.

6. Experimental studies

The series of experiments is aimed at visualizing the most essential features of granular clustering. We consider both synthetic data set and the one available on the WWW (Boston housing data).

6.1. Synthetic data

The synthetic data sets consist of 3 groups of information granules (hyperboxes), $A_i \in [0,1] \times [0,1]$, generated by a random number generator with a uniform distribution. Each group comprises 20 granules dispersed around pre-defined points: c_1=[0.4, 0.4]; c_2=[0.5, 0.6]; and c_3=[0.8, 0.3]. The dispersion factor σ is varied between 0.08 and 0.15 to establish the sensitivity of the clustering process to the dispersion of the data. The clustering process is governed by the compatibility measure, (4), with the distance defined according to L_2 norm and the "compactness" factor α=0.5.

An example of the evolution of the compatibility measure throughout the clustering process is shown in Figure 15. The intersection of the two asymptotes to the compatibility measure traced at the beginning and at the end of the clustering process indicates that 3 clusters (iteration 57) mark a natural 'change over' point in the behavior of the system. So, the clustering process should terminate with 3 clusters providing that the degree of overlap of clusters is also minimized for this number of clusters.

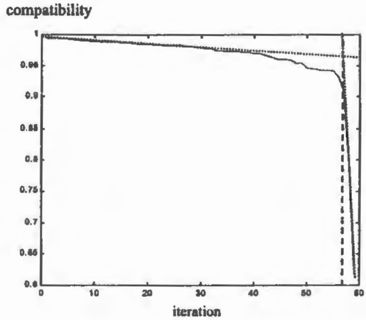


Figure 15. Compatibility measure for a single clustering process.

The degree of overlap of clusters was evaluated at each of the 59 iterative steps of the clustering process, according to (6), and is illustrated in Figure 16.

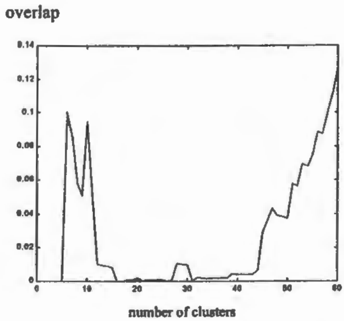


Figure 16. An average degree of overlap of clusters.

As expected, the results of the cluster overlap analysis clearly confirm that the test data naturally falls into 3 clusters.

The quality of data abstraction achieved through clustering is assessed by evaluating the inclusion rate, (7), of the independently generated data set (with the same statistical properties) in the constructed clusters. An example of the output of the validation process for 10, 3 and 1 cluster is illustrated in Figure 17.

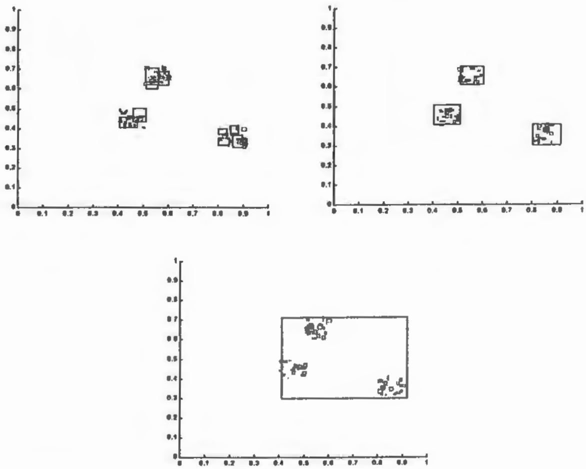


Figure 17. Inclusion of the validation data in 10, 3 and 1 cluster respectively.

The change of the overall inclusion rate of the validation data throughout the clustering process is illustrated in Figure 18. It is not surprising to see that the high value of the average inclusion rate for 3 or fewer clusters confirms that 3 clusters capture the essential features of the data while the high value of the compatibility measure confirms that the clusters retain high specificity. Should the number of clusters be reduced to 2 or 1, the inclusion rate of the validation data set would only be improved marginally while there would be a very significant reduction of specificity of the cluster(s).

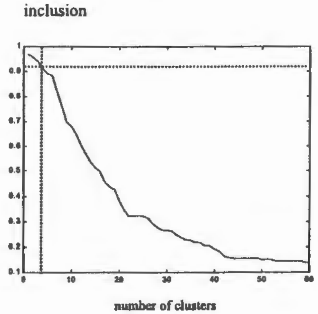


Figure 18. Average inclusion rate for the validation data set

In order to achieve a degree of independence from the statistical characteristics of the random number generator the evaluation of the inclusion of the validation data sets in the clusters was repeated 100 times for each value of $\sigma \in \{0.08, 0.09, 0.10, 0.11, 0.12, 0.13, 0.14, 0.15\}$ and the number of clusters varying from 1 to 10. A total of 8000 training sets and 8000 validation sets were processed.

Figure 19 illustrates how the inclusion measure, (5), depends on the dispersion parameter σ and the number of clusters. It is interesting to note that σ has little influence on the value of the inclusion measure. This is a very desirable characteristic of the clustering process since it suggests that the precise statistical properties of data sets do not need to be known for the clustering to be effective.

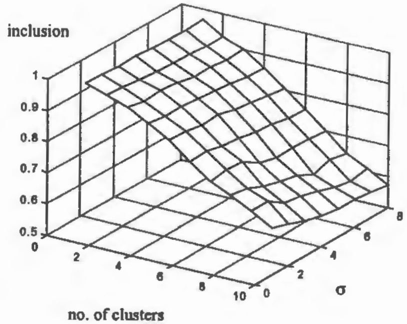


Figure 19. Average inclusion measure evaluated for 8000 training and validation sets.

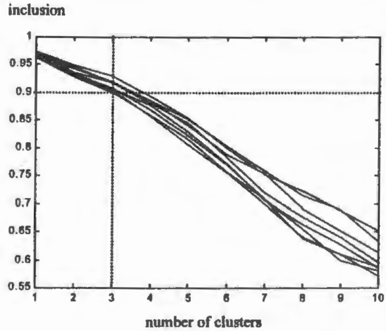


Figure 20. 2-D projection of the surface from Figure 15 resulting in a family of curves illustrating average inclusion rates of the validation data in clusters for the various values of σ.

It is easy to note, from Figures 19 and 20, that the inclusion rate of 0.9 or higher is attained consistently with 3 or fewer clusters.

6.2. Boston housing data

Although for 2-dimensional data sets B ∈ $\mathcal{F}(\mathbf{R}^2)$ the number of clusters can be easily established by visual inspection, the higher dimensional data presents a significant challenge. We have applied therefore the algorithm to a realistic 14-dimensional data set representing factors affecting house prices in Boston area (USA). The data set has been originally compiled by Harrison and Rubinfeld [6], and is available from the Machine Learning Database at University of California at Irvine (http://www.ics.uci.edu/~mlearn/MLSummary.html) The data set comprises of 506 records.

The 14 attributes of each data record are as follows:

1. CRIM	per capita crime rate by town
2. ZN	proportion of residential land zoned for lots over 25,000 sq.ft.
3. INDUS	proportion of non-retail business acres per town
4. CHAS	Charles River dummy variable (= 1 if tract bounds river; 0 otherwise)
5. NOX	nitric oxides concentration (parts per 10 million)
6. RM	average number of rooms per dwelling
7. AGE	proportion of owner-occupied units built prior to 1940
8. DIS	weighted distances to five Boston employment centres
9. RAD	index of accessibility to radial highways
10. TAX	full-value property-tax rate per $10,000
11. PTRATIO	pupil-teacher ratio by town
12. B	1000(Bk - 0.63)^2 where Bk is the proportion of blacks by town
13. LSTAT	% lower status of the population
14. MEDV	Median value of owner-occupied homes in $1000's

Study A

We divided the original set into two sets. The training set, comprising 253 odd-numbered records and the validation set comprising 253 even-numbered records. It should be noted that, as a pre-processing step, all data has been mapped into a 14-dimensional unit hyperbox. The compatibility measure provided direction for the clustering process and the evolution of this measure throughout the whole process is presented in Figure 21. The gradients of the compatibility measure at the beginning and the end of the process indicate that 7 clusters represent a good abstraction of the training data.

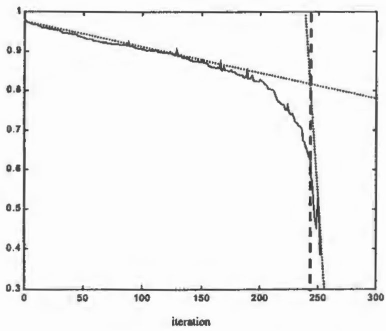


Figure 21. Compatibility measure of clusters formed from the odd-numbered records in the Boston housing data set.
Iteration step 245 corresponds to 7 clusters.

In the vicinity of 7 clusters the cluster overlap indicator is minimized for 7 and 8 clusters, as shown in Figure 22. Of these two possible numbers of clusters we select the smaller number so as to achieve greater granulation of the original data.

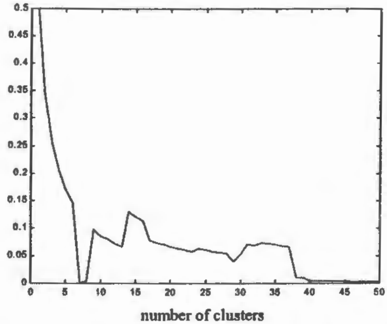


Figure 22. Degree of average overlap of clusters in the last 50 out of 252 iterations

The generality of the identified clusters was tested by evaluating average inclusion of the validation data set (even-numbered records from the original data set) in the sets of clusters identified in the last 50 steps of the clustering process. This is illustrated in Figure 23. The value of over 90%, achieved for 7 clusters, indicates a good abstraction of the detailed data that is achieved with this number of clusters.

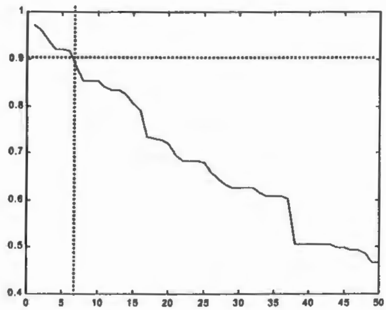


Figure 23. Average inclusion measure evaluated for 1 to 50 clusters.

To gain a more detailed insight into the makeup of the 7 clusters we evaluated an aggeregate inclusion measure (7), using the validation set, and compared the results with the cardinality of each cluster. It is clear, from Figure 24, that out of 7 clusters 3 have a significant support in the two data sets while the other 4 clusters represent data that could be described as significant exceptions. It is interesting to note however that the zero inclusion rates of the validation data in clusters 3, 4 and 7 indicate that the small data sample makes it difficult to do a proper evaluation of the clusters.

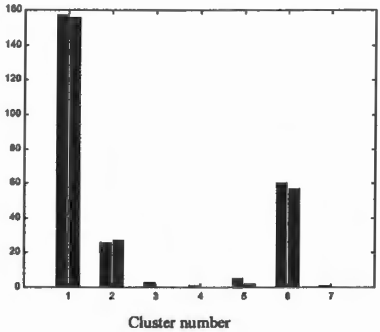


Figure 24. Cardinality (first bar) and the aggregate inclusion rate (second bar) for each of the 7 clusters

The full description of the identified clusters is given in Table 1.

TABLE 1. Description of the 7 clusters. (L_i represents minimum coordinates of the i-th hyperbox and U_i represents maximum coordinates)

Variables 1 through 7

L1	0.0063	0	0.7399	0	0.3850	4.9730	6.0004
U1	2.6354	95.0000	19.5800	1.0000	0.6470	8.3980	100.0000
L2	0.0686	0	8.1399	0	0.5200	4.9030	69.6999
U2	2.7795	0	27.7400	0	0.8710	6.4580	100.0000
L3	1.1265	0	19.5800	1.0000	0.8710	5.0120	88.0004
U3	3.3213	0	19.5800	1.0000	0.8710	6.1290	100.0000
L4	2.0099	0	19.5800	0	0.6050	7.9290	96.2005
U4	2.0099	0	19.5800	0	0.6050	7.9290	96.2005
L5	3.4744	0	18.1001	1.0000	0.6310	5.8750	82.8997
U5	8.9834	0	18.1001	1.0000	0.7700	8.7800	97.4997
L6	2.3783	0	18.1001	0	0.5320	4.1380	41.9002
U6	73.5337	0	18.1001	0	0.7700	7.0610	100.0000
L7	88.9762	0	18.1001	0	0.6710	6.9680	91.8999
U7	88.9762	0	18.1001	0	0.6710	6.9680	91.8999

Variables 8 through 14

L1	1.7984	1.0000	192.9998	12.6000	288.9906	1.9199	12.7000
U1	10.7103	8.0000	469.0011	22.0000	396.9000	30.8101	50.0000
L2	1.3459	2.0000	188.0008	14.7000	70.8002	6.4300	8.1000
U2	3.9900	4.9999	711.0000	21.2000	396.9000	29.6801	24.3000
L3	1.3216	4.9999	402.9980	14.7000	321.0184	12.1200	13.4002

U3	1.7494	4.9999	402.9980	14.7000	396.9000	26.8200	17.0002
L4	2.0459	4.9999	402.9980	14.7000	369.2980	3.7000	50.0000
U4	2.0459	4.9999	402.9980	14.7000	369.2980	3.7000	50.0000
L5	1.1296	24.0000	665.9989	20.2000	347.8787	2.9600	17.7998
U5	2.7227	24.0000	665.9989	20.2000	395.4287	17.5999	50.0000
L6	1.1370	24.0000	665.9989	20.2000	0.3200	3.2601	5.0000
U6	3.7240	24.0000	665.9989	20.2000	396.9000	37.9700	50.0000
L7	1.4165	24.0000	665.9989	20.2000	396.9000	17.2099	10.4000
U7	1.4165	24.0000	665.9989	20.2000	396.9000	17.2099	10.4000

The results of feature analysis is summarized in terms of their sparsity and overlap values. This analysis provides with an interesting insight into the discriminatory properties of the variables in the problem. The most dominant ones are: crime rate (1), nitric oxide concentration (5), index of accessibility to radial highways (9), and proportion of non-retail business acres (3). In other words, these are the variables that discriminate between hyperboxes (we stress that that the discriminatory aspects have been raised in the setting of the information granules).

Variable no.	sparsity	c-overlap
1	0.135	0.1826
2	0.136	0.7143
3	0.201	0.2194
4	0.143	0.3333
5	0.291	0.1933
6	0.326	0.3255
7	0.307	0.3759
8	0.210	0.3397
9	0.062	0.2109
10	0.218	0.2381
11	0.241	0.2234
12	0.344	0.4357
13	0.458	0.4399
14	0.426	0.3759

Study B

In order to ascertain whether the selection of records for the training and the validation data sets had influenced significantly conclusions regarding the number of clusters abstracting the original data set, we repeated the clustering process with the training and validation sets switched round. Again the compatibility measure directed the clustering process and the asymptotic evolution of the measure, at the initial and final stages of the process, indicated that 6 data clusters mark a 'change-over' point in the clustering process (Figure 25).

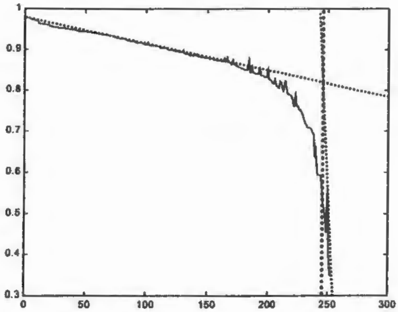


Figure 25. Compatibility measure of clusters formed from the even-numbered records in the Boston housing data set.
Iteration step 246 corresponds to 6 clusters.

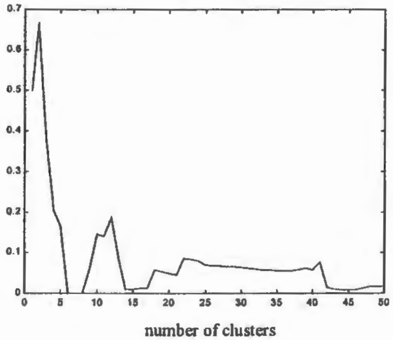


Figure 26. Degree of average overlap of clusters in the last 50 iterations

The curve showing the average degree of overlap between the clusters, illustrated in Figure 26, indicates that a minimum overlap is achieved with 6, 7 and 8 clusters. For the ease of comparison with the Study A case we select 7 clusters for the validation stage. The average inclusion rate of the validation data set (odd-numbered records from the original data set) in the 7 clusters is approx. 30% worse than in the previous case, averaging at 86%. This is illustrated in Figure 27. The reduction of the average inclusion rate in this case suggests that the training and validation sets contain a small number of unique patterns that do not have counterparts in the other set. The result is that although the distinctiveness of these patterns warrants their inclusion in separate clusters, the cross-comparison of these 'minority clusters' is very limited. This is further verified by the inspection of Figure 28, which shows that the clusters 3, 5 and 7 are representing by 1, 1 and 2 patterns respectively with no corresponding patterns in the validation set. It is also interesting to note that, compared to the Study A, there is a greater discrepancy between the cardinality of the clusters and the inclusion rate. We conclude therefore that the size of the data supports only firm conclusions about 2 clusters and the characterization of further clusters requires an order of magnitude greater data sample.

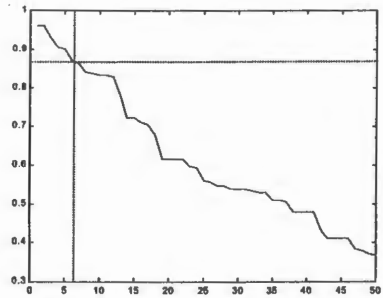


Figure 27. Inclusion measure evaluated for 1 to 50 clusters.

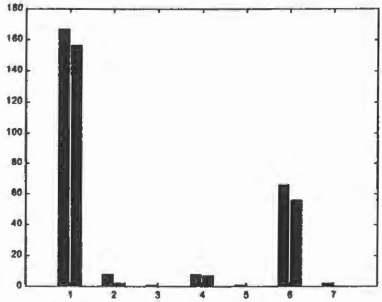


Figure 28. Cardinality (first bar) and the aggregate inclusion rate (second bar) for each of the 7 clusters

TABLE 2. Description of 7 clusters for the training and validation sets switched round (Li represents minimum and Ui represents maximum coordinates of the hyperbox)

Variables 1 through 7

L1	0.0108	0	0.4600	0	0.3890	5.0190	2.9000
U1	2.9236	100.0000	25.6501	0	0.6470	8.7250	100.0000
L2	0.7617	0	3.9701	0	0.6470	4.9260	62.8000
U2	4.0972	20.0000	19.5800	0	0.8710	6.5100	100.0000
L3	3.5349	0	19.5800	1.0000	0.8710	6.1520	82.5997
U3	3.5349	0	19.5800	1.0000	0.8710	6.1520	82.5997
L4	0.0615	0	6.2000	1.0000	0.4470	5.3440	27.6003

U4	1.5188	40.0000	19.5800	1.0000	0.6050	8.3750	100.0000
L5	0.0152	90.0000	1.2099	1.0000	0.4010	7.9230	24.7999
U5	0.0152	90.0000	1.2099	1.0000	0.4010	7.9230	24.7999
L6	2.8187	0	18.1001	0	0.5320	3.5610	40.3000
U6	67.9206	0	18.1001	1.0000	0.7700	7.3930	100.0000
L7	0.1060	0	27.7400	0	0.6090	5.4140	98.2998
U7	0.1834	0	27.7400	0	0.6090	5.9830	98.7998

Variables 8 through 14

L1	1.4394	1.0000	187.0000	12.6000	227.6119	1.7300	11.8999
U1	12.1265	8.0000	437.0004	22.0000	396.9000	34.4101	50.0000
L2	1.4118	4.9999	264.0018	13.0000	172.9116	7.3900	13.8002
U2	1.9865	4.9999	402.9980	14.7000	396.9000	29.5301	23.3001
L3	1.7455	4.9999	402.9980	14.7000	88.0118	15.0199	15.6002
U3	1.7455	4.9999	402.9980	14.7000	88.0118	15.0199	15.6002
L4	2.1620	3.0001	222.9988	14.7000	388.4489	3.3198	19.3001
U4	4.8628	8.0000	402.9980	18.6000	396.9000	23.9799	50.0000
L5	5.8850	1.0000	197.9988	13.6000	395.5199	3.1600	50.0000
U5	5.8850	1.0000	197.9988	13.6000	395.5199	3.1600	50.0000
L6	1.1691	24.0000	665.9989	20.2000	2.5210	3.7301	5.0000
U6	4.0983	24.0000	665.9989	20.2000	396.9000	34.7700	50.0000
L7	1.7554	3.9999	711.0000	20.1000	344.0517	18.0699	6.9998
U7	1.8682	3.9999	711.0000	20.1000	390.1106	23.9701	13.6000

The sparsity and c-overlap of the features (variables) are very similar as in Study A meaning that some global properties discovered in the data set have been retained.

Variable no.	sparsity	c-overlap
1	0.117	0.1414
2	0.229	0.2667
3	0.284	0.1432
4	0.143	0.5238
5	0.258	0.0985
6	0.348	0.3391
7	0.393	0.3144
8	0.221	0.1674
9	0.075	0.1769
10	0.155	0.1560
11	0.228	0.0760
12	0.303	0.3276
13	0.443	0.3762
14	0.412	0.3175

7. Conclusions

The study has articulated another look at data analysis by providing a constructive way of forming information granules that capture the essence of the large collections of numeric data. In this sense, the original data are compressed down to a few information granules whose location in the data space and granularity reflect the structure in the data. The approach promotes a data mining way of problem solving by emphasizing the transparency of the results (hyperboxes). The way in which information granules is guided by two aspects that is distance between information granules and a size (granularity) of the potential information granule formed through merging two other granules. These two aspects are encapsulated in the form of the compatibility measure. Moreover we discussed a number of indexes describing the hyperboxes and expressing relationships between such information granules. It has been shown how to validate the granular structure. The resulting family of the information granules is a concise descriptor of the structure of the data – we may call them a granular *signature* of the data.

Some further extensions of the hyperbox approach may deal with more detailed instruments of information granulation such as fuzzy sets [7][11].

It should be stressed that the proposed approach to data analysis is *noninvasive* meaning that we have not attempted to formulate specific assumptions about the distribution of the data but rather allow the data to "speak" freely. This is accomplished in two main ways

- first, the hyperboxes are easily understood by a user as each dimension (variable) comes as a part of the construct.
- second, the approach finds relationships that are direction-free meaning that we do not distinguish between input and output variables (which could be quite restrictive as we may not know in advance what implies what). Obviously, this feature is quite common to all clustering methods

Furthermore the granulation mechanism puts the variables (features) existing in the problem in a new perspective. The two indexes such as sparsity and overlap are useful in understanding the relevance of the variables, in particular their discriminatory abilities.

While the study was concerned with the development of information granules (hyperboxes), there are interesting inquires into their use in granular modeling. In particular, we are concerned with the fundamental inference problem

- given an input datum (information granule and numeric datum , in particular) X defined in a certain subspace of dimension n' of the original space $\mathbf{R}^{n'} \subset \mathbf{R}^{n}$ and a collection of information granules $\mathbf{B}$ = {B(1) B(2) ,..., B(c)} determine the corresponding information granule Y

The current paper provides a basis for this investigation.

Acknowledgment

Support from the Natural Sciences and Engineering Research Council of Canada (NSERC), Alberta Consortium of Software Engineering (ASERC) and from the Engineering and Physical Sciences Research Council (UK) is gratefully acknowledged.

8. References

1. M.R. Anderberg, *Cluster Analysis for Applications*, Academic Press, N. York, 1973.
2. A. Bargiela, Interval and ellipsoidal uncertainty models, In: W. Pedrycz (ed.) *Granular Computing*, Springer Verlag, to appear.

3. A. Bargiela, W. Pedrycz, Information granules: Aggregation and interpretation issues, submitted to *IEEE Trans. on Syst. Man and Cybernetics*.

4. J.C. Bezdek, *Pattern Recognition with Fuzzy Objective Function Algorithms*, Plenum Press, N. York, 1981.

5. B. Gabrys, A. Bargiela, General fuzzy Min-Max neural network for clustering and classification, *IEEE Trans. on Neural Networks*, Vol. 11, No. 3, pp. 769-783, 2000.

6. D. Harrison, D.L. Rubinfeld, Hedonic prices and the demand for clean air, *J. Environ. Economics & Management*, vol.5, 81-102, 1978.

7. A. Kandel, *Fuzzy Mathematical Techniques with Applications*, Addison-Wesley, Reading, MA, 1986.

8. T. Kohonen, Self-organized formation of topologically correct feature maps, *Biological Cybernetics*, 43, 59-69 (1982).

9. T. Kohonen, *Self-organizing Maps*, Springer Verlag, Berlin, 1995.

10. W. Pedrycz, *Computational Intelligence: An Introduction*, CRC Press, Boca Raton, FL, 1997.

11. W. Pedrycz, F. Gomide, *An Introduction to Fuzzy Sets*, Cambridge, MIT Press, Cambridge, MA, 1998.

12. W. Pedrycz, Fuzzy equalization in the construction of fuzzy sets, *Fuzzy Sets and Systems*, to appear.

13. W. Pedrycz, M. H. Smith, A. Bargiela, A granular signature of data, *Proc. 19th Int. (IEEE) Conf. NAFIPS'2000*, Atlanta, July 2000, pp. 69-73.

14. P. K. Simpson, Fuzzy Min-Max neural networks – Part1: Classification, *IEEE Trans. on Neural Networks*, Vol 3, No. 5, pp. 776-86, September 1992.

15. P. K. Simpson, Fuzzy Min-Max neural networks – Part2: Clustering, *IEEE Trans. on Neural Networks*, Vol 4, No. 1, pp. 32-45, February 1993.

16. L. A Zadeh, Fuzzy sets and information granularity, In: M.M. Gupta, R.K. Ragade, R.R. Yager, eds., *Advances in Fuzzy Set Theory and Applications*, North Holland, Amsterdam, 1979, 3-18.

17. L. A. Zadeh, Fuzzy logic = Computing with words, *IEEE Trans. on Fuzzy Systems*, vol. 4, 2, 1996, 103-111.

18. L. A. Zadeh, Toward a theory of fuzzy information granulation and its centrality in human reasoning and fuzzy logic, *Fuzzy Sets and Systems*, 90, 1997, pp. 111-117.