Genetic algorithms for symbolic clustering

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Abstract. This paper introduces a novel methodology for clustering of symbolic objects by making use of Genetic Algorithms (GAs). GAs are a family of computational models inspired by evolution. These algorithms encode potential solutions to specific problems on simple chromosome-like data structures and apply recombination operators to these structures so as to preserve critical information. A new type of representation for chromosome structure is presented here along with a new method for mutation. The efficacy of the proposed method is examined by application to numeric data of known number of classes and also to assertion type of symbolic objects drawn from the domain of fat oil, microcomputers, microprocessors and botany. The validity of the clusters obtained is examined.

Keywords. Symbolic clustering; symbolic similarity; symbolic dissimilarity; genetic algorithms; path length; spanning length; best spanning length.

1. Introduction

In conventional data analysis, objects are taken as numerical vectors. The clustering of such objects is achieved by minimizing intra cluster dissimilarity and maximizing inter cluster dissimilarity. A good survey of cluster analysis can be found in the literature (Duda & Hart 1973; Diday & Simon 1976; Bock 1987; Diday *et al* 1987; Jain & Dubes 1988; Diday 1989).

Symbolic objects are extensions of classical data types. In conventional data sets, the objects are *individualized*, whereas in symbolic data sets, they are more *unified* by means of relationships. Based on the complexity, the symbolic objects can be of *assertion*, *hoard* or *synthetic* type. Some references to clustering of symbolic objects can be found in Diday (1990), Gowda & Diday (1991a, 1992).

A symbolic clustering methodology is proposed in this paper, which makes use of GAs. An implementation of a genetic algorithm begins with a population of (typically random) chromosomes. One then evaluates these structures and allocates reproductive opportunities in such a way that chromosomes which represent a better solution to the target problem

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BEGIN /* genetic algorithm */
Generate initial population
Compute Fitness of each individual
WHILE NOT FINISHED Do
BEGIN /* Produce new generation */
For Population Size Do
BEGIN /* Reproductive Cycle */
Select two individuals from old generation
for mating /* biased in favour of fitter ones */
Recombine the two individuals to give two offspring
Compute Fitness of the two offspring
Insert offspring in new generation
END
If population has converged THEN
finished = TRUE
END
END.

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Figure 1. A traditional genetic algorithm.

are given more chances to *reproduce* than those which are poorer solutions. The goodness of a solution is typically defined with respect to the current population. In a broader usage of the term, a genetic algorithm is any population-based model that uses selection and recombination operators to generate new sample points in a search space. The standard GA can be represented as shown in figure 1.

2. Proposed modified similarity and dissimilarity measures

Similarity between A and B is written as,

$$S(A, B) = S(A_1, B_1) + \cdots + S(A_k, B_k). \quad (1a)$$

For the k th feature, $S(A_k, B_k)$ is defined using the following three components:

- (1) $S_p(A_k, B_k)$ due to position p ,
- (2) $S_s(A_k, B_k)$ due to span s ,
- (3) $S_c(A_k, B_k)$ due to content c .

Dissimilarity between A and B is written as,

$$D(A, B) = D(A_1, B_1) + \cdots + D(A_k, B_k). \quad (1b)$$

For the k th feature, $D(A_k, B_k)$ is defined using the following three components:

- (1) $D_p(A_k, B_k)$ due to position p ,
- (2) $D_s(A_k, B_k)$ due to span s ,
- (3) $D_c(A_k, B_k)$ due to content c .

2.1 Quantitative interval type of A_k and B_k

Let

$$\begin{aligned} al & \text{ and } au \text{ represent lower and upper limit of interval } A_k, \\ bl & \text{ and } bu \text{ represent lower and upper limit of interval } B_k, \\ inters & = \text{length of intersection of } A_k \text{ and } B_k, \\ ls & = \text{span length of } A_k \text{ and } B_k, \\ & = |\max(au, bu) - \min(al, bl)|, \end{aligned}$$

where $\max()$ and $\min()$ represent maximum and minimum values respectively. The similarity and dissimilarity between two samples A_k and B_k is defined on position and span. Similarity due to position is defined as

$$S_p(A_k, B_k) = \sin[(1 - ((al - bl)/u_k)) \times 90]. \quad (2)$$

Similarity due to span is defined as

$$S_s(A_k, B_k) = \sin[((la + lb)/(2 \times ls)) \times 90], \quad (3)$$

where u_k denotes the length of the maximum interval of the k th feature and

$$\begin{aligned} la & = |au - al|, \\ lb & = |bu - bl|. \end{aligned}$$

Net similarity between A_k and B_k is

$$S(A_k, B_k) = S_p(A_k, B_k) + S_s(A_k, B_k). \quad (4)$$

Dissimilarity due to position is defined as

$$D_p(A_k, B_k) = \cos[(1 - ((al - bl)/u_k)) \times 90]. \quad (5)$$

Dissimilarity due to span is defined as

$$D_s(A_k, B_k) = \cos[((la + lb)/(2 \times ls)) \times 90]. \quad (6)$$

Net dissimilarity between A_k and B_k is

$$D(A_k, B_k) = D_p(A_k, B_k) + D_s(A_k, B_k). \quad (7)$$

2.2 Qualitative type of A_k and B_k

For qualitative type of features the similarity component and dissimilarity component due to position are absent. The two components that contribute to similarity and dissimilarity are

- (1) span,
- (2) content.

Let la = length of A_k or number of elements in A_k ,
 lb = length of B_k or number of elements in B_k ,
 $inters$ = number of elements common to A_k and B_k ,
 ls = span length of A_k and B_k combined,
 $= la + lb - inters$.

The similarity component due to span is defined as

$$S_s(A_k, B_k) = \sin[(la + lb)/(2 \times ls) \times 90]. \quad (8)$$

The similarity component due to content is defined as

$$S_c(A_k, B_k) = \sin[(inters/ls) \times 90]. \quad (9)$$

Net similarity between A_k and B_k is

$$S(A_k, B_k) = S_s(A_k, B_k) + S_c(A_k, B_k). \quad (10)$$

The dissimilarity component due to span is defined as

$$D_s(A_k, B_k) = \cos[((la + lb)/(2 \times ls)) \times 90]. \quad (11)$$

The dissimilarity component due to content is defined as,

$$D_c(A_k, B_k) = \cos[(inters/ls) \times 90]. \quad (12)$$

Net dissimilarity between A_k and B_k is

$$D(A_k, B_k) = D_s(A_k, B_k) + D_c(A_k, B_k). \quad (13)$$

In conventional data analysis, whenever two samples that are merged are to be represented by a single sample, one of the frequently used methods is the mean of the two as a single representative. In symbolic data analysis, the concept of composite symbolic object (Gowda & Diday 1991a, 1992) is used. A new method of forming a composite symbolic object is proposed in which

$$\begin{aligned} a^1m &= am \times (n_1/n), \\ b^1m &= bm \times (n_2/n), \end{aligned}$$

where a, b are the lowest and highest values considering n samples, n_1 represents the number of samples between a and m , n_2 represents the number of samples between b and m .

3. Methodology

The problem here is to find the number of classes and class memberships in a data set of N samples. In order to obtain the natural groups, the following method is proposed. The methodology makes use of the principle of mutation to obtain better solutions. Another important feature of the proposed method is that it makes use of a new type of representation for chromosome structure.

Figure 2. Formation of mutated offspring

Stage 1: Generate C number of random solutions. The solution would contain the samples connected in some order. If there are N samples, randomly generate a number between 0 and N . Let it be A_0 . Now generate one more number other than A_0 . Let it be B_0 . Connect A_0 and B_0 . Next generate some number between 0 and N other than A_0 and B_0 . Let it be C_0 . Connect B_0 and C_0 . Repeat this until all the N numbers are included. The solution would be in the form of a string (chromosome).

Compute the dissimilarities between A_0 and B_0 and hence find the path length. In the same way find the path length between B_0 and C_0 and so on. The sum of all the path lengths in the string would represent the spanning length.

Repeat the above procedure for C solutions and hence find the strings and corresponding spanning lengths of each solution.

This would form the initial population.

Stage 2: Having C random spanning lengths, our aim would be to obtain the best spanning length which has the least value. In order to obtain the best spanning length, we select an individual from the initial population and mutate it. The mutation is done in two phases.

Phase 1: The mutation is done by generating two crossover points and rearranging the samples in order to obtain a different string structure (chromosome). This is depicted in figure 2.

Phase 2: The mutated offspring is further subjected to mutation as follows: Each sample in the string has two links connected to two different samples. Among the two links, the one that has the highest dissimilarity value is selected and replaced by a shorter link. This process is repeated for all the samples in the string.

Stage 3: The process of mutation, i.e. stage 2, is repeated till 90% of the initial population selected has the same spanning lengths.

Stage 4: Among the C populations, the one that has the least spanning length is selected which would represent the best spanning length. This string structure would represent

Table 1. Experimental results of randomly generated classes.

No. of Gaussian clusters generated	No. of samples generated	Mean values used for generating samples	Classes obtained by proposed method
2	80	1,3	2
3	120	1,3,5	3
4	160	1,3,5,7	4
5	200	1,3,5,7,9	5
6	240	1,3,5,7,9,11	6
7	280	1,3,5,7,9,11,13	7
8	320	1,3,5,7,9,11,13,15	8

the best solution to the given data. In order to obtain the classes, we adopt the following procedure.

- (1) Compute the dissimilarities between each sample in the string, i.e. path lengths.
- (2) Identify the inconsistent length, which is the path length having the highest value between two samples. Remove the inconsistent length to form two groups.
- (3) Merge all the samples of each group and form two composite symbolic objects.
- (4) Compute the similarity S and dissimilarity D between the two groups. If dissimilarity D is greater than similarity S then the inconsistent length is removed so as to result in two clusters or else the inconsistent length is placed back.
- (5) Repeat steps 1 to 4 until no sample has dissimilarity greater than similarity.

4. Results of simulation

In order to corroborate the efficacy of the algorithm, several simulation studies were made, the results of which are given below. The clusterings obtained using the proposed method are examined for their validity using Hubert's T statistics (Jain & Dubes 1988) approach. In order to compare the results, the validity of the clustering structures obtained by other methods is presented in table 11 below.

Table 2. Description of 2 classes of Iris data.

Cluster no.	Feature 1	Feature 2	Feature 3	Feature 4
1	5.47–5.92	2.55–2.73	3.62–4.19	1.13–1.31
2	4.83–4.86	3.07–3.09	1.38–1.43	0.28–0.35

Figure 3. Plot of iris data; x -axis – feature SW; y -axis – feature PL.

Example 1. The first example is such that the input data are of numeric type and the output data are symbolic. The objects of numeric type were drawn from a mixture of normal distributions with a known number of classes and classification so that the results show the efficacy of the algorithm. The test set was drawn from a mixture of C normal distributions with mean m_i and covariance matrix C_i having individual variances of 0.15 and zero covariances. The different values of the number of classes and the means chosen are shown in table 1 and the test samples were independently generated using a Gaussian vector generator. The proposed method was used on this test data set. As indicated in table 1, there is perfect agreement between the number of classes used for generating Gaussian clusters and the number of classes obtained by the proposed method. In all the seven cases, the classification results were in full agreement with the test samples generated.

Table 3. Fat oil data.

Sample	Sp. gravity (g/cm ³)	m.p. (°C)	Io. value	Sa. value	Fatty acids
Linseed oil	0.930–0.935	–27 to –8	170–204	118–196	L,Ln,O,P,M
Perilla oil	0.930–0.937	–5 to –4	192–208	188–197	L,Ln,O,P,S
Cotton seed	0.916–0.918	–6 to –1	94–113	189–198	L,O,P,M,S
Sesame oil	0.920–0.926	–6 to –4	104–116	187–193	L,O,P,S,A
Camellia	0.916–0.917	–21 to –15	80–82	189–193	L,O
Olive oil	0.914–0.919	0 to 6	79–90	187–196	L,O,P,S
Beef tallow	0.860–0.870	30 to 38	40–48	190–199	O,P,M,S,C
Lard	0.858–0.864	22 to 32	53–77	190–202	L,O,P,M,S,Lu

Abbreviations: Io – ionisation; sa – saponification; L – linoleic acid; Ln – linolenic acid; O – oleic acid; P – palmitic acid; M – myristic acid; S – stearic acid; A – arachic acid; C – capric acid; Lu – lauric acid

Table 4. Description of classes in fat oil data.

Cluster no.	Samples	Sp. gravity (g/cm ³)	(0°C) m.p.	Io. value	Sa. value	Fatty acids
1	0,1,2,3, 4,5	0.917–0.933	–7.75 to +3	191.25–196.75	165.87–183.25	L,Ln, O,P, M,S,A
2	6,7	0.862–0.864	28.75–34.62	49.75–60.25	194.87–195.62	L,O,P, M,S, Lu,C

Abbreviations: Io – ionisation; sa – saponification; L – linoleic acid; Ln – linolenic acid; O – oleic acid; P – palmitic acid; M – myristic acid; S – stearic acid; A – arachic acid; C – capric acid; Lu – lauric acid

Example 2. The example is so chosen so as to demonstrate the efficacy of the algorithm in clustering data belonging to two classes with many overlaps. The data set used is the well-known iris data set. This data set contains measurement of two species of iris. There are 50 patterns for each species and four features, namely petal length, petal width, sepal length and sepal width. The proposed method was applied to the two classes of iris data having 100 samples. The method resulted in two classes in perfect agreement with the data set considered. Two symbolic objects representing the two classes are shown in table 2, which also gives the descriptive information about the classes. The plot of the two classes obtained is as shown in figure 3.

Table 5. Microcomputer data.

Microcomputer	Display	RAM (k)	ROM (k)	MP	Keys
Apple II	Colour TV	48	10	6502	52
Atari 800	Colour TV	48	10	6502	57–63
Commodore VIC 20	Colour TV	32	11–16	6502A	64–73
Exidi Sorcerer	B&W TV	48	4	Z80	57–63
Zenith H8	Built-in	64	1	8080A	64–73
Zenith H89	Built-in	64	8	Z80	64–73
HP-85	Built-in	32	80	HP	92
Horizon	Terminal	64	8	Z80	57–63
Ohio Sc Challenger	B&W TV	32	10	6502	53–56
Ohio Sc II Series	B&W TV	48	10	6502C	53–56
TRS-80 I	B&W TV	48	12	Z80	53–56
TRS-80 III	Built-in	48	14	Z80	64–73

Table 6. Description of classes in microcomputer data.

Cluster no.	Samples	Display	RAM (k)	ROM (k)	MP	Keys
1	0,1,2,3,4,5, 7,8,9,10,11	Colour TV, B & W TV Terminal Built-in	32,64	6-10	6502X	55-73
2	6	Built-in	32	80	HP	92

Table 7. Botanical data of 9 trees of 3 classes.

Class 1 (Annonaceae)	Class 2 (Clasiaceae)	Class 3 (Mimosaceae)
0 degjknpcFR	3 aehilmoswxzDFR	6 begikmpBJKPR
1 dfhjknpcFR	4 cfgilmoswxzDFR	7 begiknpBJKPR
2 dehjknpcFR	5 cegjmoswxzDFR	8 begjkmpBJKPR

Example 3. The data set for this example (table 3) is chosen from the domain of fats and oils (Ichino & Yaguchi 1989) having four quantitative features of interval type and one nominal qualitative feature. The proposed method resulted in two classes. The samples of the classes were {0, 1, 2, 3, 4, 5} and {6, 7}. Table 4 shows the two symbolic objects representing the two classes.

Example 4. The data set of microcomputers (table 5) (Ichino & Yaguchi 1989) is considered for this experiment. The proposed method resulted in two classes. The samples of the classes were {0, 1, 2, 3, 4, 5, 7, 8, 9, 10, 11} and 6. Table 6 shows the description of the two classes.

Example 5. The data for this experiment (table 7) is considered from botany (Gowda & Diday 1992). It consists of 9 trees belonging to 3 classes. The proposed method resulted in 3 classes. The samples of the classes were {0, 1, 2}, {3, 4, 5} and {6, 7, 8}. Table 8 shows the three symbolic objects representing the three classes.

Table 8. Description of classes in botanical data.

Cluster no.	Description	Samples in cluster
1	degjknphcFR	0,1,2
2	cfgilmoswxzejahDFR	3,4,5
3	begjkmppinBJKPR	6,7,8

Table 9. Microprocessor data.

MPU	Clock (MHz)	Gen. reg*	Inst. (byte)	Cache size	Cache type
i386DX	16–33	8	123	—	Null
i386SX	12–20	8	123	—	Null
i486DX	25–50	8	214	8192	Common
i486SX	20	8	129	8192	Common
68020	12–33	8	99	256	Instruction
68030	16–50	8	105	512	Independent
68040	25	8	140	8192	Independent
MB86901	20–25	120	64	—	Null
MB86930	20–40	136	68	4096	Independent

*General registers

Example 6. The data set of microprocessors (table 9) (Ichino & Yaguchi 1989) is considered for this experiment. The proposed method resulted in two classes. The samples of the classes were {0, 1, 2, 3, 4, 5, 6, 8} and {7}. The description of the 2 classes is shown in table 10.

As mentioned earlier, for purpose of comparison, results obtained by other methods are given in table 11.

5. Conclusion

A new method for clustering symbolic objects is developed using GAs. A new type of representation for chromosome structure is presented along with two ways of mutating the chromosome structure. Several artificial and real-life data with known number of classes and classification assignments were used to establish the efficacy of the proposed methodology. Subsequently, the proposed methodology was applied to assertion type of symbolic data sets drawn from the domain of fat oil, microcomputers, botany, and microprocessors.

Table 10. Description of classes in microprocessor data.

Cluster no.	Samples	Clock (MHz)	Gen. reg.	Instructions (byte)	Cache size	Cache type
1	0,1,2,3,4,5,6,8	22–28	8	123,99,140,214,129,105,68	8192,256,4096,512	Common, instruction, Null, independent
2	7	20–25	120	64	—	Null

Table 11. Level of significance values for validating the clusters using Hubert's T statistics.

Data	Proposed method	Gowda & Diday (Using similarity)	Gowda & Diday (Using dissimilarity)	Ichino
Fat oil	0.98	0.98	0.96	0.98
Microcomputer	0.90	0.67	0.67	0.90
Microprocessor	0.79	—	—	0.66
Botanical	1.00	1.00	1.00	—

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