J Mol Model (2004) 10:335–341
DOI 10.1007/s00894-004-0200-2

ORIGINAL PAPER

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Determination of fuzzy logic membership functions using genetic algorithms: application to structure–odor modeling

Received: 21 October 2003 / Accepted: 27 May 2004 / Published online: 31 July 2004

Abstract Fuzzy logic has been used as a tool in structure–camphoraceous odor relationships. The data base studied included 99 molecules. The rules used to discriminate between camphor and non camphor molecules lead to 77% correct discrimination. Such rules account for the shape and the size of the molecule. Their adjustment by means of genetic algorithms led to 84% correct discrimination between camphor and non-camphor molecules.

Keywords Fuzzy logic · Structure–activity relationship · Olfaction · Genetic algorithms

Introduction

Odor is a human sense for which no complete theory exists. This is due to the fact that the mechanisms of this activity are complex. Because of this lack of a final olfaction theory, many structure–odor relationships have been established, i.e. for musk, [1] sandalwood, [2] bitter almond [3] and camphor. [4] Efficient structure–odor relationships lead to models that can be used to predict the odor for new molecules. The variable descriptors identified to be pertinent in the models generally allow the formulation of efficient rules that can help understand olfaction mechanisms.

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The previous published papers on olfactory stimuli show that some odors depend closely on the stereochemistry of the chemical groups involved in the mechanisms, as for decalin structures with an amber odor, indan and tetralin series with a musk odor or campholenic structures with sandalwood character. In such examples, the stereochemistry is important around the groups involved in specific interactions such as hydrogen bonds. However, when hydrocarbon groups are involved in the interactions between receptor site and stimuli, the interaction energy depends on the size of the hydrocarbon group.

The previous studies [2, 4] of sandalwood and camphoraceous structure–odor relationships showed that the presence of odor depends on the presence of a hydrocarbon group, a hydroxyl group and a distance between them. The optimal value of the distance lies between 6.5 and 7.1 Å.

For a large set of odors, the activity is not well defined in relation to the chemical structure. This is the case, for example, with camphor and woody odors.

Therefore, the best approach to describe both the hydrocarbon group and a variable descriptor such as that above should be fuzzy. In addition we must consider a fuzzy description of odor. Such an approach was recently used by Chrétien et al. [5] for molecular-descriptor selection relative to three odors. However, their example was limited to 114 molecules.

Fuzzy concepts introduced by Zadeh [6] provide interesting alternative solutions to the classification problems within the context of imprecise categories, in which olfaction can be included. In fact, fuzzy classification represents the boundaries between neighboring classes as continuous, assigning to compounds a degree of membership of each class. It has been widely used in the field of process control, where the idea is to convert human expert knowledge into fuzzy rules, [7] and it should be able to extract relevant structure–activity relationships from a database without a priori knowledge. A fuzzy set is fully defined by its membership functions. For most applications, the sets to be defined are easily identifiable.

However, for other applications they have to be determined by knowledge acquisition from an expert or group of experts. Once the fuzzy sets have been established, one must consider their associated member functions. How best to determine the membership function is the first question to be tackled.

The approach adopted for acquiring the shape of any particular membership function often depends on the application. For most fuzzy logic control problems, the membership functions are assumed to be linear, triangular and usually trapezoidal in shape. So, typically the sets that describe various factors of importance in the application and the issues to be determined are the parameters that define the trapezoids. These parameters are elicited directly from the expert.

In addition to the use of the fuzzy approach, we used genetic algorithm (GA) methods, which are basically random-search techniques applied to many different problems such as function optimization, routing problems, design of neural networks, system identification, digital signal processing, computer vision, control and machine learning. [8] GAs have been used for the adjustment of membership function parameters, [9, 10, 11] as they offer a convenient way to model membership functions. However, there is no requirement for the membership function to be trapezoidal in shape.

In this paper we present a classification method using fuzzy rules of 99 camphoraceous molecules. GA was used to adjust the parameters that define the membership functions in the fuzzy rules, in order to minimize the error of classification.

Materials and methods

Data set and molecular description

The set of molecules chosen to illustrate our approach is taken from the work of Schnabel et al. [12] The molecules are described by means of physicochemical descriptors previously considered as pertinent for the determination of camphor odor. [13, 14] Some of these descriptors were obtained by the MMP molecular mechanics method. [15]

In order to take into account the shape of each molecule from its chemical structure, the molecular maximum length was oriented along the *x* axis and the molecular maximum width along the *y* axis. The following geometrical parameters were measured on the basis on the most stable conformation:

- *R*: molecular length, measured as the distance along the screen *x* axis between the extreme left and the extreme right atoms plus their van der Waals radii.
- *r*: molecular width is the distance along the screen *y* axis between the atoms at the top and the bottom plus their van der Waals radii.
- *R/r*: accounts for the shape of the molecule.
- *S*: accounts for the surface of the molecule.

Variables generated for 4-methyl-hexan-3-ol chosen as an example are given in Table 1. This molecule with camphoraceous character belongs to the class of camphor.

Table 1 Description and class of the 4-methyl-hexan-3-ol

R	*r*	*R/r*	*S*	*C*
10.42	1.63	6.4	11.64	Camph.

Fuzzy rules identification

The fuzzy rule (R_i) set characterizing the camphor odor is given below:

R_1: If the molecule is spherical and has a medium size then its odor is very camphorated.
R_2: If the molecule is spherical and has a small size then its odor is not camphorated.
R_3: If the molecule is spherical and has a large size then its odor is not camphorated.
R_4: If the molecule is not spherical then its odor is not camphorated.

For the sample studied, the shape of the molecule is defined by the variable *R/r*, if this ratio is close to 1, then the molecule has a shape close to spherical. The corresponding fuzzy variable of *R/r* is represented with membership functions denoted by: $f_{\text{spherical}}$ and $f_{\text{not spherical}}$.

The size of the molecule is expressed by the surface descriptor *S*. This descriptor has the fuzzy values: small, medium and large, with membership functions denoted by: f_{small}, f_{medium} and f_{large}. Limit values for such functions are identified on the basis of molecular descriptor calculated and discussions with experts (P_1=1.60, P_2=1.90, $P_{3=}$7.6, $P_{4=}$8.6, $P_{5=}$10.60, $P_{6=}$11.60) (Fig. 1).

The camphoraceous Schnabel's scores were transformed into two binary variables, respectively *TC* and *NC*. *TC* corresponds to molecules having 3, 4 and 5 Schnabel's scores and *NC* corresponds to molecules having 0, 1 and 2 Schnabel's scores. *TC* and *NC* are considered as fuzzy subsets with membership functions denoted by f_{TC} and f_{NC}, respectively (Fig. 2). As an example, the molecule number 6, with a Schnabel's score close to 2, is described by $f_{TC}(2)=0.33$ and $f_{NC}(2)=0.67$.

Classification method of the database examples using fuzzy rules

During the classification phase, a molecule can be classified directly using a fuzzy classification module (FCM), which uses fuzzy expert rules.

We have two fuzzy knowledge rules sets: $FR_{TC}=\{R_1\}$ which characterizes the odor *TC* and $FR_{NC}=\{R_2, R_3, R_4\}$ which characterizes the odor *NC*.

To illustrate this concept, consider the molecule m_x described by:

$$m_x = \langle A_1 = a_x^1 \rangle \text{and} \langle A_2 = a_x^2 \rangle \text{and} \langle C_x = \text{Schnabel's score} \rangle$$

$$\begin{aligned} A_i &\in \{\text{spherical, size}\} \\ a_x^1 &\in \{\text{spherical, not spherical}\} \\ a_x^2 &\in \{\text{small, medium, large}\} \\ \text{Schnabel's score} &\in \{0,\ 1,\ 2,\ 3,\ 4,\ 5\} \end{aligned}$$

We define the global degree of *TC* as:

$$\begin{aligned} A_i &\in \{\text{spherical, size}\} \\ a_x^1 &\in \{\text{spherical, not spherical}\} \\ a_x^2 &\in \{\text{small, medium, large}\} \\ \text{Schnabel's score} &\in \{0,\ 1,\ 2,\ 3,\ 4,\ 5\} \end{aligned}$$

with $R_k(m_x)$ the degree of *TC* inferred by using the rule $R_k \in FR_{TC}$, we use the Mamdani inference where the conjunction "and" is expressed with the min operator, and the disjunction "or" is expressed with the max operator. [16]

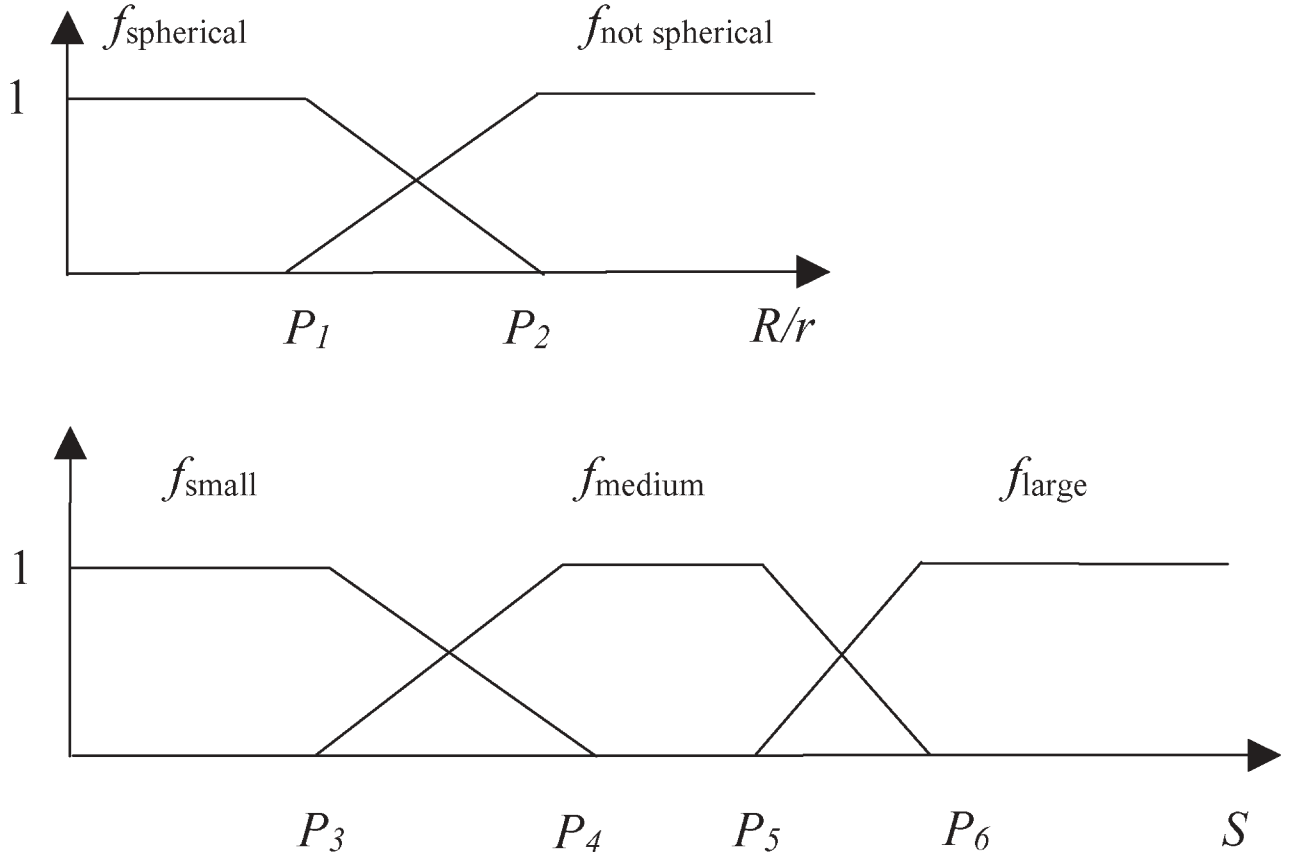

Fig. 1 Membership function for the chosen variables

For example (Fig. 3):

$$\text{If}: m_x = \langle R/r = 1.70\rangle \text{ and } \langle S = 8\rangle \text{and } \langle f_{TC}(Cx) = 0.67\rangle$$
$$FR_{TC} = \{R_1\}$$
$$R_1(m_x) = \min\left(f_{\text{spherical}}(0.70), f_{\text{medium}}(8)\right) = \min(0.75, 0.33) = 0.33$$
$$a_x = R_1(m_x) = 0.33$$

We define also the global degree *NC* as:

$$\beta_x = \underset{R_k \in FR_{NC}}{\text{Max}} (R_k(m_x))$$

with $R_k(m_x)$ the degree of *NC* inferred by using the rules $R_k \in FR_{NC}$.

For example (Fig. 4):

$$\text{If}: m_x = \langle R/r = 1.70\rangle \text{ and } \langle S = 8\rangle \text{ and } \langle f_{NC}(C_x) = 0.33\rangle$$
$$FR_{NC} = \{R_2, R_3, R_4\}$$
$$R_2(m_x) = \min\left(f_{\text{spherical}}(0.70), f_{\text{small}}(8)\right) = \min(0.75, 0.45) = 0.45$$
$$R_3(m_x) = \min\left(f_{\text{spherical}}(0.70), f_{\text{large}}(8)\right) = \min(0.75, 0) = 0$$
$$R_4(m_x) = f_{\text{not spherical}}(0.55) = 0.55$$
$$\beta_x = \max(R_2(m_x), R_3(m_x), R_4(m_x)) = \max(0.45, 0, 0.55) = 0.55$$

The aggregation of the global degrees and the membership degree gives a degree of strong odor presence *DegTC* and a degree of odor absence *DegNC* defined by:

$$DegTC = T(\alpha_x, f_{TC}(C_x))$$
$$DegNC = T(\alpha_x, f_{NC}(C_x))$$

T: aggregation operator that combines several information sources [17]C_x: the m_x molecule class (Schnabel's score)

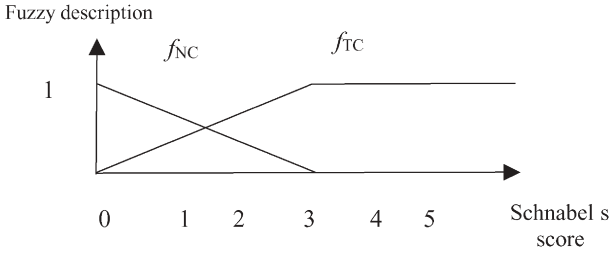

Fig. 2 Membership functions for odor activity

Example: The degrees *DegTC* and *DegNC* of m_x molecule with *T* as the max operator:

$$DegTC(m_x) = \max(\alpha_x, f_{TC}(m_x)) = \max(0.33, 0.67) = 0.67$$
$$DegNC(m_x) = \max(\beta_x, f_{NC}(C_x)) = \max(0.55, 0.33) = 0.55$$

In this study we used the following three aggregation operators: Zadeh, Lukasiewicz and Ordered Weighted Averaging (OWA), $w \in [0,1]$ [18] (Table 2).

Adjustment of parameters of membership functions using genetic algorithms

A genetic algorithm was used to adjust the variable descriptors using database examples in order to have a minimal error for the classification. The GA used has the following specificities:

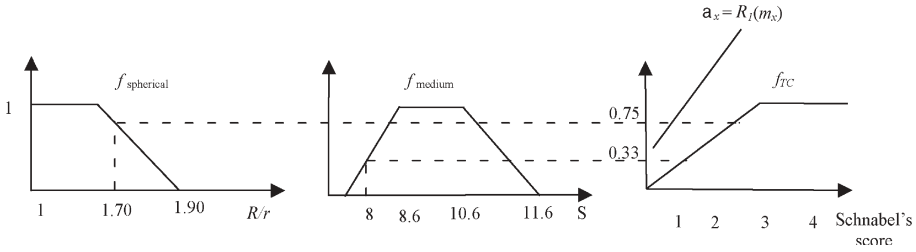

Fig. 3 Calculation of $R_1(mx)$ for m_x molecule

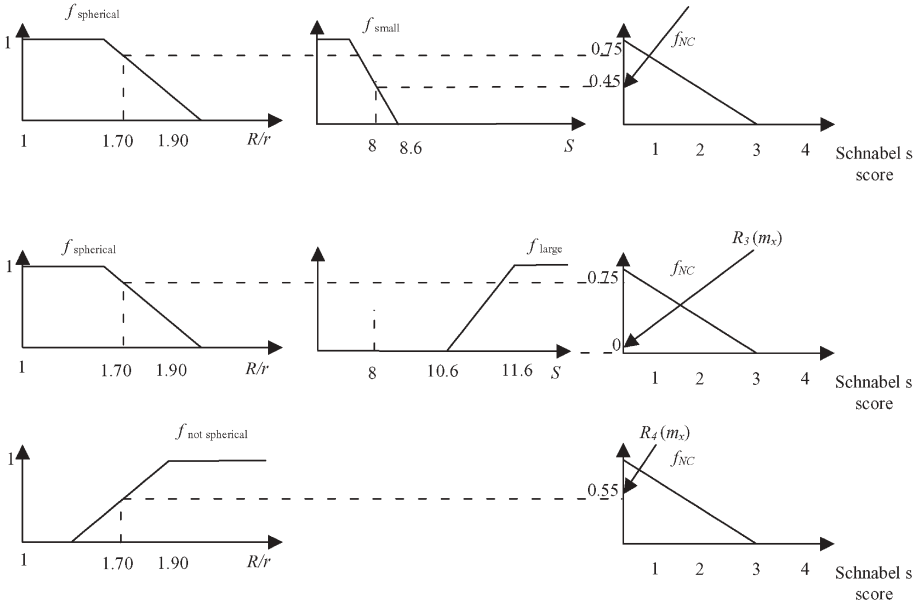

Fig. 4 Calculation of R_2 (m_x), R_3 (m_x) and R_4 (m_x) for m_x molecule

Table 2 Aggregation operators to calculate *DegTC* and *DegNC*

T	*DegTC*	*DegNC*
Zadeh	$\max(\alpha_x, f_{TC}(C_x))$	$\max(\beta_x, f_{NC}(C_x))$
Lukasiewicz	$\max(\alpha_x+f_{TC}(C_x)-1, 0)$	$\max(\beta_x+f_{NC}(C_x)-1, 0)$
OWA	$\min(\alpha_x, f_{TC}(C_x))w+\max(\alpha_x, f_{TC}(C_x)(1-w)$	$\min(\beta_x, f_{NC}(C_x))w+\max(\beta_x, f_{NC}(C_x)(1-w)$

1. $(p_l)_{l=1..6}$ the membership function parameters of the various variables used in fuzzy expert rules.
2. For each parameter family and each molecule m_i belonging to database, the FCM generates two degrees *DegTCi* and *DegNCi*.
3. The purpose is to find an adequacy between a given *DegTCi* and $f_{TC}(C_i)$ and on another *DegNCi* and f_{NC} (C_i) for all molecules in the database, C_i is the class of m_i. This is evaluated by:

$$Er_{mi} = \max\left(|DegTC, -f_{TC}(C_i)|, |DegNC, -f_{NC}(C_i)|\right)$$

Thus, the problem consists in finding the parameters $(p_{\hat{i}})_{\hat{i}=1..6}$ which minimize:

$$Er_{mi} = \max\left(|DegTC, -f_{TC}(C_i)|, |DegNC, -f_{NC}(C_i)|\right)$$

The GA procedure developed unfolds in the following steps:

- Step 1: generation of the initial population (limits P_1 to *P6*)
- Step 2: generation of database set (set of studied camphoraceous molecules)
- Step 3: evaluation of the error (objective function) using initial set of P_1 to P_6
- Step 4: generation of a new set of P_1 to P_6 values and calculation of the error
- Step 5: stop if the error becomes constant, else go to step 3

Results and discussion

We use the FCM method to predict the class of all 99 molecules using the Zadeh operator. For each molecule, the method generates two degrees of odor response to be determined within 0 to 1. The comparison between predicted and experimental values for all molecules tested is reported in Table 3. The classification method leads to satisfactory results (77%), as seen in this table, with a prediction error:

$$\text{Error} = 23.23\left(\text{Error} = \sum_i (Er_{mi})\right)$$

The classification score obtained using the FCM method only may be improved. That is, a GA was used to adjust membership functions in the fuzzy expert rules used initially. For the shape variable (input 1), it was assumed that there are two different membership functions "spherical" and "not spherical", and it is assumed that one of them is triangular. For the size variable (input

Table 3 Classification results using FCM method

Compound	Schnabel's score	Fuzzy description		Predicted score		Er_{mi}
		TC	*NC*	*DegTC*	*DegNC*	
1	0	0.00	1.00	0.00	1.00	0.00
2	0	0.00	1.00	0.00	1.00	0.00
3	0	0.00	1.00	0.00	1.00	0.00
4	0	0.00	1.00	0.00	0.99	0.02
5	3	1.00	0.00	0.50	0.48	0.50
6	1	0.33	0.67	0.29	0.71	0.04
7	1	0.33	0.67	0.47	0.53	0.14
8	1	0.33	0.67	0.47	0.53	0.14
9	4	1.00	0.00	0.94	0.06	0.06
10	1	0.33	0.67	0.17	0.83	0.17
11	0	0.00	1.00	0.25	0.75	0.25
12	0	0.00	1.00	0.23	0.77	0.23
13	1	0.33	0.67	0.40	0.60	0.06
14	4	1.00	0.00	0.91	0.09	0.09
15	4	1.00	0.00	0.86	0.14	0.14
16	0	0.00	1.00	0.32	0.68	0.32
17	3	1.00	0.00	0.86	0.14	0.14
18	0	0.00	1.00	0.00	1.00	0.00
19	0	0.00	1.00	0.00	1.00	0.00
20	1	0.33	0.67	0.17	0.83	0.17
21	4	1.00	0.00	0.50	0.50	0.50
22	0	0.00	1.00	0.00	1.00	0.00
23	0	0.00	1.00	0.00	1.00	0.00
24	4	1.00	0.00	0.50	0.50	0.50
25	0	0.00	1.00	0.00	0.75	0.25
26	0	0.00	1.00	0.00	1.00	0.00
27	0	0.00	1.00	0.00	0.50	0.50
28	0	0.00	1.00	0.00	0.50	0.50
29	0	0.00	1.00	0.00	0.50	0.50
30	0	0.00	1.00	0.00	1.00	0.00
31	2	0.67	0.33	0.33	0.65	0.33
32	4	1.00	0.00	0.55	0.43	0.45
33	1	0.33	0.67	0.44	0.56	0.11
34	5	1.00	0.00	0.89	0.11	0.11
35	4	1.00	0.00	0.89	0.11	0.11
36	2	0.67	0.33	0.52	0.48	0.14
37	4	1.00	0.00	0.80	0.20	0.20
38	4	1.00	0.00	0.81	0.19	0.19
39	4	1.00	0.00	1.00	0.00	0.00
40	5	1.00	0.00	0.94	0.06	0.06
41	5	1.00	0.00	0.94	0.06	0.06
42	0	0.00	1.00	0.00	1.00	0.00
43	0	0.00	1.00	0.00	1.00	0.00
44	5	1.00	0.00	0.50	0.50	0.50
45	0	0.00	1.00	0.00	1.00	0.00
46	3	1.00	0.00	0.50	0.50	0.50
47	4	1.00	0.00	0.50	0.50	0.50
48	3	1.00	0.00	0.50	0.50	0.50
49	3	1.00	0.00	0.50	0.50	0.50
50	0	0.00	1.00	0.00	1.00	0.00
51	0	0.00	1.00	0.00	0.87	0.13
52	0	0.00	1.00	0.00	1.00	0.00
53	4	1.00	0.00	0.50	0.19	0.50
54	0	0.00	1.00	0.00	0.74	0.26
55	4	1.00	0.00	0.50	0.50	0.50
56	0	0.00	1.00	0.00	1.00	0.00
57	0	0.00	1.00	0.00	1.00	0.00
58	0	0.00	1.00	0.00	1.00	0.00
59	0	0.00	1.00	0.00	0.50	0.50
60	4	1.00	0.00	0.78	0.22	0.22
61	4	1.00	0.00	0.72	0.28	0.28
62	4	1.00	0.00	0.80	0.20	0.20
63	5	1.00	0.00	0.80	0.20	0.20
64	0	0.00	1.00	0.00	1.00	0.00
65	4	1.00	0.00	0.50	0.50	0.50
66	4	1.00	0.00	0.50	0.50	0.50
67	4	1.00	0.00	0.50	0.50	0.50

Table 3 (continued)

Compound	Schnabel's score	Fuzzy description		Predicted score		Er_{mi}
		TC	*NC*	*DegTC*	*DegNC*	
68	4	1.00	0.00	0.50	0.50	0.50
69	4	1.00	0.00	0.50	0.50	0.50
70	4	1.00	0.00	0.50	0.50	0.50
71	4	1.00	0.00	0.50	0.50	0.50
72	4	1.00	0.00	0.50	0.50	0.50
73	2	0.67	0.33	0.33	0.67	0.33
74	3	1.00	0.00	0.50	0.50	0.50
75	0	0.00	1.00	0.00	0.88	0.12
76	4	1.00	0.00	0.50	0.50	0.50
77	1	0.33	0.67	0.17	0.83	0.17
78	1	0.33	0.67	0.17	0.83	0.17
79	4	1.00	0.00	0.50	0.50	0.50
80	4	1.00	0.00	0.50	0.21	0.50
81	4	1.00	0.00	0.50	0.21	0.50
82	4	1.00	0.00	0.50	0.50	0.50
83	4	1.00	0.00	0.50	0.50	0.50
84	4	1.00	0.00	0.50	0.23	0.50
85	4	1.00	0.00	0.50	0.13	0.50
86	0	0.00	1.00	0.00	1.00	0.00
87	0	0.00	1.00	0.00	1.00	0.00
88	0	0.00	1.00	0.00	1.00	0.00
89	0	0.00	1.00	0.00	0.50	0.50
90	0	0.00	1.00	0.00	1.00	0.00
91	0	0.00	1.00	0.00	1.00	0.00
92	4	1.00	0.00	0.50	0.50	0.50
93	4	1.00	0.00	0.50	0.50	0.50
94	1	0.33	0.67	0.17	0.71	0.17
95	0	0.00	1.00	0.00	1.00	0.00
96	0	0.00	1.00	0.00	1.00	0.00
97	0	0.00	1.00	0.00	1.00	0.00
98	0	0.00	1.00	0.00	1.00	0.00
99	0	0.00	1.00	0.00	1.00	0.00

Table 4 Error and parameters for each operator

Operator	Error	P_1	P_2	P_3	P_4	P_5	P_6	w
Zadeh	21.13	1.22	1.78	6.36	8.17	10.15	12.35	–
Lukas	25.75	1.17	1.85	6.53	8.15	10.96	12.05	–
OWA	14.64	1.09	2.25	6.12	9.18	9.86	11.30	0.48

2), it was adopted that there are three different membership functions "small", "medium" and "large", and it is assumed that one of them is trapezoidal. The ranges of input 1 variables P_1 and P_2 are 0–1.75 and 1.75–4 respectively, and the ranges of input 2 variables P_3, P_4, P_5 and P_6 are 0–8.1, 8.1–9.6, 9.6–11.1 and 11.1–13 respectively. The sum of errors to be optimized by the GA is done using various aggregation operators to compute $DegTC_i$ and $DegNC_i$.

In addition, the results depend on the choice of the GA parameters (crossover probability, mutation probability, population size, and number of generations). We tested several parameter values. The best values are: 20 for population size, 0.8 for crossover probability, 0.01 for mutation probability and 30 for the number of generations. The results of the computation are given in Table 4. In this table, we give the minimal error and optimal parameters P_1,..,P_6 of the membership functions using Zadeh, Lukasiewicz and OWA operators. The application of the OWA operator leads the minimal error, with the good parameters, with the weight w=0.48.

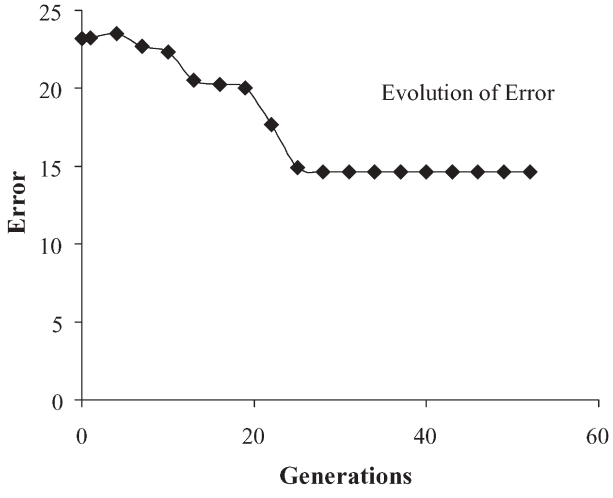

Fig. 5 Evolution error using GA

Table 5 Statistical values defining the robustness of the FCM optimized model

Test set	Validation ratio (%)
S_1	79.8
S_2	85.6
S_3	82.5
S_4	87.3
Mean	83.8

The evolution of the error is shown in Fig. 5 with the OWA operator in order to calculate this error. GA was trained on all 99 molecules of the data set. The optimized parameters using the GA method were used to classify the 99 molecules of the data set, using the cross-validation method. As a cross-validation procedure, we choose randomly four subsets with 24 or 25 molecules for each and we tested it using the optimized parameters. The classification ability of each is given in Table 5. The statistical criteria concerning the test set reported in Table 5 show that the average value of prediction efficiency is close to 84%. This demonstrates that the model is relatively robust.

As a conclusion, this paper presents a prediction method, combining fuzzy logic and GA, of the camphor odor. In addition to its classification efficiency, this method allows the chemist to localize the eventual optimal parameters responsible for a given odor, as shown in this paper, or an activity in general. Our goal in the paper is to find and to test this new tool for olfaction modeling.

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