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FUZZY LOGIC FOR CHEMOINFORMATICS – A REVIEW

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ABSTRACT

Fuzzy logic and fuzzy systems are gaining widespread acceptance in a large variety of fields, including but not limited to engineering, commercial, forecasting, artificial intelligence, etc. This paper is for beginners who try to use fuzzy logic in Chemoinformatics. Since, there are lot of uncertainties, vagueness and ambiguity during drug design and other simulations carried out in Chemoinformatics, there is a high need of understanding the ability of fuzzy logic in representing and modeling these parameters in much effective and efficient way. This paper presents an introductory review of fuzzy logic and its applications to Chemoinformatics.

Keywords: *Fuzzy Logic (FL), Membership Functions (MF), Semi-Circular Membership Function (SCMF), Fuzzy Rules (FR), Fuzzy Control (FC), Fuzzy Inference Systems (FIS), Chemoinformatics*

1. INTRODUCTION

Fuzzy logic (one of the components of softcomputing) and fuzzy systems are gaining widespread acceptance in almost all fields [2]-[4], [9], [21], [40]-[53], [57], [59]. Figure 1 shows first author along with Prof. L.A. Zadeh (Father of fuzzy logic) in World Congress on Computational Intelligence held in Hong Kong during 2008.

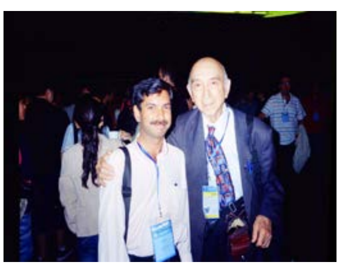

Figure 1: Dr. R. Rajesh Along With Prof. L.A. Zadeh

It should be noted that significance and precision cannot be achieved together. Whenever you are having high significance, precision will be very low and vice-versa. So in real life applications when you compromise between precision and significance, certain level of uncertainty comes in. There are three types of uncertainties, namely, stochastic uncertainty (for eg. throwing a die/coin), linguistic uncertainty (for eg. low price, tall tree, huge stone) and informational uncertainty (for eg. honesty, creditworthiness, brilliant). Another two types of problem that we see in real life are vagueness and ambiguity. Whenever, we have these types of uncertainties, ambiguity and vagueness in systems, fuzzy logic based systems will work better than conventional systems.

Recently it is seen that fuzzy logic (FL) has widely applied to the brain child of Frank Brown [7] [8], namely, the Chemoinformatics [1] [54]. Since, there are lot of uncertainties, vagueness and ambiguity during drug design and other simulations carried out in Chemoinformatics, there is a high need of understanding the ability of fuzzy logic in representing and modeling these parameters in much effective and efficient way. This paper deals with the review of Chemoinformatics applications which makes use of techniques / methods / algorithms related with fuzzy logic. This paper is organized as follows. Section 2 deals with an introduction to fuzzy systems. Section 3 deals with fuzzy logic applications in Chemoinformatics. Section 4 concludes the paper.

2. FUZZY LOGIC – A REVIEW

2.1 Fuzzy Set and Classical Set

In classical set, for example tallness can be represented as given below

$$Tall = \{x / x>160 \text{ cm}).$$

You can visualize it as a set containing sharp boundary at 160. If a person is having 159.999, he has to be considered as not tall as it does not belong to the above set. But in fuzzy you will get an

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inclined boundary based on membership functions. So that you can say the person belongs to the tall group with certain degree of membership. A fuzzy set can be described as follows using an ordered pair with the value along with its membership grade.

$$A = \{(x, \mu_A(x)) : x \in X, \mu_A(x) \in [0,1]\}$$

2.2 Membership Functions

Various types of membership functions used in fuzzy logic are triangular function, trapezoidal function, Gaussian membership function, sigmoid function, semi-circular membership function, etc. Mathematical expressions of few of them are shown here.

2.2.1 Zadeh's Z-shaped function (ZMF) [59]

$$z = \begin{cases} 1-2\left(\frac{x-a}{c-a}\right)^2 & if \quad a < x \le (a+c)/2 \\ 2\left(\frac{x-c}{c-a}\right)^2 & if \quad (a+c)/2 < x \le c \\ 1 & if \quad x \le a \\ 0 & otherwise \end{cases}$$

2.2.2 Triangular Membership Function (Trimf)[59]

$$F(x) = \begin{cases} \frac{x-a}{b-a} & if \quad a \le x \le b \\ \frac{c-x}{c-b} & if \quad b \le x \le c \\ 0 & otherwise \end{cases}$$

2.2.3 Rajesh's Asymmetric Semi-Circular Membership Function [48], [49]

$$F(x) = \begin{cases} abs\left(\sqrt{1-\frac{(c-x)^2}{r^2}}\right) & if \quad 0 \le x-c < r \\ abs\left(\sqrt{1-\frac{(c-x)^2}{R^2}}\right) & if \quad -R < x-c < 0 \\ 0 & otherwise \end{cases}$$

2.2.4 Rajesh's Drum Shaped Semi-Circular Membership Function [48], [49]

$$F(x) = \begin{cases} abs\left(\sqrt{1-\frac{(c_1-x)^2}{r^2}}\right) & if \quad c_1 - r < x < c_1 \\ abs\left(\sqrt{1-\frac{(c_2-x)^2}{r^2}}\right) & if \quad c_2 < x < c_2 + r \\ 1 & if \quad c_1 \le x \le c_2 \\ 0 & otherwise \end{cases}$$

2.2.5 Rajesh's Generalized Semi-Circular Membership Function [48], [49]

$$F(x) = \begin{cases} abs\left(\sqrt{1-\frac{(c_1-x)^2}{R^2}}\right) & if \quad c_1 - R < x < c_1 \\ abs\left(\sqrt{1-\frac{(c_2-x)^2}{r^2}}\right) & if \quad c_2 < x < c_2 + r \\ 1 & if \quad c_1 \le x \le c_2 \\ 0 & otherwise \end{cases}$$

2.3 Fuzzy Inference Systems

The essential parts of fuzzy inference system are the fuzzification module, rule base, inference engine and defuzzification (see Fig. 2). Fuzzification module converts a crisp value of a variable into a fuzzy value. Rule base consists of a set of fuzzy rules. Inference engine computes the overall firing value of all rules based on the current fuzzy values of all variables. Defuzzification module calculates the defuzzified value of the overall fuzzy output of the inference engine.

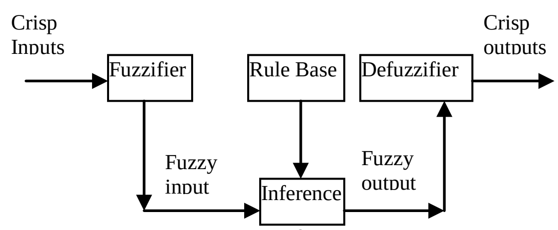

Figure 2: Fuzzy inference system

2.4 Fuzzy Rules

There are three different types of fuzzy rules, namely, Mamdani-type fuzzy rules [35], Takagi-Sugeno [57] and Tsukamoto types. Extensions of the above fuzzy rules are Takagi-Sugeno fuzzy models with nonlinear consequence and T-S fuzzy models with variable coefficient.

2.4.1 Takagi-Sugeno fuzzy models with nonlinear consequence [44]

Suppose that the nonlinear function $f(x):R^n \rightarrow R$ is defined over a compact region $D \subset R^n$ with the following assumptions:

A_1: $f(0) = 0$

A_2: $f \in C_1^2$. Therefore, f, $\partial f/dx$ and $\partial^2 f/\partial x^2$ are continuous and therefore bounded over D.

A_3: f(x) is expressible in the form of $f(x)=a(x)\psi(x)$ and can be approximated as $f_0(x) = a_0\psi(x)$ in the region $D_0 = \{x \ / \ |x_i| < \varepsilon_0\}$ and $f_{j_1 j_2 \ldots j_n}(x) = a_{j_1 j_2 \ldots j_n}\psi(x)$ in the region $D_{j_1 j_2 \ldots j_n} = \{x / x \in D, j_1\varepsilon \le x_i \le (j_i+1)\varepsilon \quad \forall i\}$

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where j_i are integers, ε_0 and ε are small positive numbers. $x = [x_1,x_2, \ldots, x_n]^T$. a(x) is continuous and $a_0=a(x_{00\ldots0})$, $a_{j_1j_2\cdots j_n} = a(x_{j_1j_2\cdots j_n}) \in R^{1xn}$. $\psi(x):R^n \rightarrow R$ is defined over a compact region $D \subset R^n$. $\psi(x)=[\psi_1(x_1), \psi_2(x_2), \ldots, \psi_n(x_n)]^T$ and $\psi_i(x_i)$ is either equal to $\sin(x_i)$ or equal to x_i.

Then f(x) can be approximated by TSFMNC. The rules of TSFMNC are of the following form:

Rule 0: If x_1 is about 0 … and x_n is about 0

Then $\hat{f}(x) = a_0\psi(x)$

Rule $j_1,j_2, \ldots, j_n$: If x_1 is about $j_1\varepsilon$ … and x_n is about $j_n\varepsilon$

Then $\hat{f}(x) = a_{j_1j_2\cdots j_n}\psi(x)$

For Rule 0, choose the possibility of firing $h_0(x)$ as, 1 inside D_0 and, 0 outside. The possibility of firing for the $j_1,j_2, \ldots, j_n$ th rule is given by the product of all membership functions associated with $j_1,j_2, \ldots, j_n$ th rule and is $h_{j_1j_2\cdots j_n}(x(t)) = \prod_{i=1}^{n} M_{j_i}(x_i(t))$ where the membership function for x_i is given below. It is assumed that $h_{j_1j_2\cdots j_n}(x)$ has already been normalized, i.e. $h_{j_1j_2\cdots j_n}(x) \geq 0$ and $\sum h_{j_1j_2\cdots j_n}(x) = 1$

$$M_{j_i}(x_i) = \begin{cases} 1 - \dfrac{|x_i - j_i\varepsilon|}{\varepsilon}, & |x_i - j_i\varepsilon| < \varepsilon \\ 0 & else \quad where \end{cases}$$

Then by using center of gravity method for defuzzification, the TSFMNC can be represented as:

$$y = \hat{f}(x) = h_0(x)a_0\psi(x) + \sum h_{j_1j_2\cdots j_n}(x)a_{j_1j_2\cdots j_n}\psi(x)$$

2.4.2 Takagi-Sugeno fuzzy models with variable coefficient (TSFMVC) [47]

A general representation of TSFMVC is as described below. Suppose that the nonlinear function $f(x):R^n \rightarrow R$ is defined over a compact region $D \subset R^n$ with the following assumptions:

A_1: $f(0) = 0$

A_2: $f \in C_1^2$. Therefore, f, $\partial f/dx$ and $\partial^2 f/\partial x^2$ are continuous and therefore bounded over D.

A_3: f(x) can be approximated as $f_{j_1j_2\cdots j_n}(x) = a_{j_1j_2\cdots j_n}(x)x$ in the region $D_{j_1j_2\cdots j_n} = \{x / x \in D, j_1\varepsilon \leq x_i \leq (j_i+1)\varepsilon \quad \forall i\}$ where j_i are integers, ε is a small positive numbers. $x = [x_1,x_2, \ldots, x_n]^T$. a(x), $a_{j_1j_2\cdots j_n}(x)$ are continuous.

Then f(x) can be approximated by TSFMVC. The rules of TSFMVC are of the following form:

Rule $j_1,j_2, \ldots, j_n$: If x_1 is about $j_1\varepsilon$ … and x_n is about $j_n\varepsilon$

Then $\hat{f}(x) = a_{j_1j_2\cdots j_n}(x)x$

The possibility of firing for the $j_1,j_2, \ldots, j_n$ th rule is given by the product of all membership functions associated with $j_1,j_2, \ldots, j_n$ th rule and is $h_{j_1j_2\cdots j_n}(x(t)) = \prod_{i=1}^{n} M_{j_i}(x_i(t))$ where the membership function for x_i is given below. It is assumed that $h_{j_1j_2\cdots j_n}(x)$ has already been normalized, i.e. $h_{j_1j_2\cdots j_n}(x) \geq 0$ and $\sum h_{j_1j_2\cdots j_n}(x) = 1$

$$M_{j_i}(x_i) = \begin{cases} 1 - \dfrac{|x_i - j_i\varepsilon|}{\varepsilon}, & |x_i - j_i\varepsilon| < \varepsilon \\ 0 & else \quad where \end{cases}$$

Then by using center of gravity method for defuzzification, the TSFMVC can be represented as:

$$y = \hat{f}(x) = \sum h_{j_1j_2\cdots j_n}(x)a_{j_1j_2\cdots j_n}(x)x$$

3. FUZZY IN CHEMOINFORMATICS

Fuzzy clustering has wide applications in Chemoinformatics. Feher et. al. used fuzzy clustering as means of selecting representative conformers and molecular alignments [22]. Friederichs et. al. has done fuzzy clustering of existing chemicals according to their ecotoxicological properties [23]. Holliday et. al. used fuzzy k-means clustering for chemical structures [24]. Misra et. al. have proposed a novel feature extraction technique for fuzzy relational clustering of flexible dopamine reuptake inhibitor [37]. Other fuzzy clustering applications include, but not limited to, fuzzy clustering of alcohols [31], analysis of spectroscopic imaging data by Fuzzy C-Means Clustering [36], fuzzy hierarchical cross-clustering algorithm [38], FCM and G-K clustering of chemical dataset using topological indices [55], etc.

Fuzzy clustering has also been used for classification, for example, Lin et. al has done classification of some active HIV-1 protease inhibitors and their inactive analogues using fuzzy c-means alogirthm [30].

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Fuzzy logic has also been widely used for similarity measures. Bonachera et. al. have developed topological fuzzy pharmacophore triplets and adapted molecular similarity scoring schemes [5]. Horvath et. al. have proposed fuzzy similarity measures [25], [26] and fuzzy molecular descriptors [26], [27] for similarity searching and drug design.

Monitoring and control utilization in medicine is another area where fuzzy logic can be applied [33].

Most interesting applications of fuzzy logic include, but limited to, fuzzy restrictions and inherent uncertainties in chirality studies, fuzzy classical structures in genuine quantum systems, fuzzy measures of molecular shape and size, fuzzy logic strategies for molecular recognition, segmentation/ matching of molecular surfaces with fuzzy logic strategies, fuzzy graphs in chemical structure research, fuzzy graph theory applications in computer assisted biopolymer NMR assignment, fuzzy rules for structure elucidation research based upon multiple spectra, fuzzy logic in computer aided structure elucidation, fuzzy hierarchical classification methods in analytical chemistry. Table I shows some of the applications of fuzzy logic in chemoinformatics. More details about these can be had from [10], [15], [17], [19], [20], [28], [29], [54].

Table 1: Fuzzy Logic In Chemoinformatics

No	Applications of FL in Chemoinformatics
1	Fuzzy Logic Molecular recognition [6], [12], [13], [16], [18]
2	Docking algorithm [11]
3	Identification of complementarity of molecular surfaces [14], [15]
4	Fuzzy virtual ligands for virtual screeing by Lower et. al. [32]
5	Fuzzy differentials in atmospheric and medical cybernetics [34]
6	Fuzzy Expert System for Fluid management in general anaesthesia [39]
7	Fuzzy fragment selection strategies in applications of the ADMA method of Macromolecular quantum chemistry [56]
8	Fuzzy pharmocophores and its application to RNA targets [58]

4. CONCLUSION

Since the introduction of fuzzy logic in 1965 by Prof. L.A. Zadeh, it has seen its fruits in various applications. More over fuzzy logic will act as an intelligent layer above any conventional systems. The most important fact is that, fuzzy logic is able to handle uncertainties, vagueness, and ambiguity in a much better way than any other conventional techniques.

This paper has made review of fuzzy logic and its applications in Chemoinformatics. This review will surely help any beginner in the field of Chemoinformatics.

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