Implementing Fuzzy Sets and Processing Fuzzy Logic Information by Molecules †

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Abstract: Fuzzy logic models human capacity to make decisions using natural language, and it is widely used in the field of Artificial Intelligence. This contribution supports the hypothesis that the effectiveness of fuzzy logic in mimicking human capability to compute with words is due to the structural and functional analogies between the human nervous system and fuzzy logic systems. Furthermore, this work demonstrates that fuzzy logic can be processed by molecules and chemical reactions in wetware beyond the traditional methods based on electronic circuits and software. This innovative way of processing fuzzy logic allows the development of Chemical Artificial Intelligence and the design of new computational machines, more similar to the brain rather than electronic computers, both in composition and performance.

Keywords: fuzzy logic; Artificial Intelligence; molecules; human nervous system; sensory system; brain; light; photochromism; photochemistry; conformations

1. Introduction

A universally accepted definition of intelligence does not exist yet [1]. However, human intelligence is undoubtedly valuable when facing complex scenarios for at least three reasons. First, human intelligence handles both numerical and vague information. Humans make rational decisions by speaking in natural language and compute by using numbers. Second, our intelligence allows us to make rational decisions in circumstances dominated by uncertainty, when the truth might be relative or partially understood. In other words, our intelligence allows us to face complex scenarios where the Incompatibility Principle holds: “As the complexity soars, our statements cannot be accurate and significant at the same time” [2]. Third, human intelligence supports us in recognizing variable patterns. Hence, it is evident that it is worth investigating the human nervous system that has human intelligence as its emergent property. Such an investigation should allow us to mimic human intelligence and develop Artificial Intelligence (AI) [3]. Currently, AI is a vast domain of research. Among the numerous successes of AI, it is worth highlighting fuzzy logic. Fuzzy logic reproduces the human capability to make rational decisions using natural language. Such power of fuzzy logic is based on a rigorous mathematical procedure [4].

This contribution supports the hypothesis that the effectiveness of fuzzy logic is due to some structural and functional analogies between the human nervous system and fuzzy logic systems [5]. Furthermore, this work demonstrates that fuzzy logic can be processed by molecules and chemical reactions in wetware beyond the traditional methods based on electronic circuits and software [6,7]. The innovative method of processing fuzzy logic through chemicals allows the development of Chemical Artificial Intelligence (CAI). A successful CAI will boost the implementation of new computational machines. The new generation’s computational devices will approach the human brain both in composition and performance [8].
2. Fuzzy Logic

Fuzzy logic is relevant in Artificial Intelligence because it models the human capability to compute with words. Fuzzy logic reproduces the human ability to make rational decisions using natural language. Such power of fuzzy logic is based on a rigorous mathematical procedure [9]. In 1965, the engineer Lotfi Zadeh proposed the core of fuzzy logic, i.e., the fuzzy set theory [10]. A fuzzy set differs from any traditional Boolean set. In Boolean algebra, any element either belongs or not to a Boolean set. Hence, any element cannot belong to a set and its complement simultaneously. This statement does not hold in the case of any fuzzy set. Actually, any item may belong to any fuzzy set, and the degree of membership (µ) of any element to a fuzzy set can be any real number included between 0 and 1. This degree of membership µ is the unit of fuzzy information, called “fit”. Since the range [0–1] contains an infinite amount of real numbers, fuzzy logic is an infinite-valued logic.

Fuzzy logic reproduces the human ability to make rational decisions by using the natural language through the construction of fuzzy logic systems (FLS). A FLS can be built by using the so-called method of Mamdani [11]. Three fundamental steps are required.

First, it is necessary to granulate both the input and the output variables in fuzzy sets. The operator must decide how many fuzzy sets to use for the granulation. Furthermore, the position and shape of the fuzzy sets must be defined. It is worth observing that the choices of the number, position and shape of the fuzzy sets must be performed by considering the context.

Secondly, the operator must graduate both the input and the output variables. The graduation requires the operator to label each fuzzy set by a word. The words that are used to mark the fuzzy sets are usually adjectives.

The third and final step requires the formulation of the fuzzy rules. The fuzzy rules are syllogistic sentences such as: “IF . . . , THEN . . . ”. The “IF . . . ” part includes the words chosen for labelling the fuzzy sets granulating the input variables. The “THEN . . . ” part of the fuzzy rules contains the words selected for marking the fuzzy sets that granulate the output variables. If the fuzzy rules include two or more input variables, the fuzzy sets granulating distinct variables are connected through the traditional logic operators: AND, OR, NOT. Formulating fuzzy rules requires preliminary data associated with the non-linear phenomenon that the FLS should describe. Any FLS consists of three components. The first component is the Fuzzifier. The Fuzzifier transforms the numerical inputs into degrees of membership to the fuzzy sets of the input variables. The second component is the Fuzzy Inference Engine. The Fuzzy Inference Engine has its roots in the collection of fuzzy rules. The fuzzy rules activate the output fuzzy sets. Finally, the third component is the Defuzzifier. The Defuzzifier transforms the activated output fuzzy sets into numerical output values. Such numerical values of the output variables are predictive values that can help make decisions in complex circumstances [12].

3. The “Similarity” Hypothesis

Fuzzy logic’s power of modelling the human capability to compute with words can be attributed to a similarity between fuzzy logic and the human nervous system (HNS). Many elements of the HNS are intrinsically fuzzy [5,6].

The HNS may be described as constituted by three systems. The first is the sensory system. The second is the central nervous system. Finally, the third is the system of effectors, which is made of glands and muscles [13]. The sensory system is sensitive to both physical and chemical stimuli. The chemical and physical stimuli are transduced into electrochemical signals. Such electrochemical signals are conveyed to the brain through the spinal cord. The brain collects the signals coming from the different sensors. It integrates and processes them. Finally, the brain transforms the data into information, making decisions. The final choices are electrochemical commands that the brain sends to the components of the effectors’ system.
Our sensory system comprises eight elements or subsystems. They are the visual, olfactory, gustatory, auditory, tactile, proprioceptive, thermo-receptive, and nociceptive subsystems. They work as Fuzzifiers. The information of any stimulus is polyhedral. It is related to its (a) modality \((M)\), (b) intensity \((I_M)\), (c) time-evolution \((I_M(t))\), and (d) spatial distribution \((I_M(x,y,z))\). Such multiple information is encoded hierarchically because any sensory subsystem is hierarchical from the structural point of view. At the molecular level, a collection of receptor proteins is present. At the cellular level, there is a group of receptor cells. Each receptor cell contains a vast number of molecular receptors. At the organ level, there are many replicas of the receptor cells. They are appropriately distributed in space, often covering a tissue.

The information regarding the modality of a stimulus is encoded at the molecular level. The intensity and time evolution information is encoded at the cellular level. Finally, its spatial distribution is encoded at the tissue level [5]. The sensory cells collect the multiple information of a stimulus and encode it in the values of graded membrane potentials. Then, the architecture of afferent neurons increases the acuity by highlighting the contrasts of the features of the stimuli in space and time. The receptive field of any afferent neuron is a fuzzy set granulating the receptor cells. Adjacent afferent neurons have receptive fields that are partially overlapped [6]. Afferent neurons encode information in trains of action potentials. Such action potentials constitute the ideal code for sending the information to the brain. The brain’s code is very abundant, and it is based on all the numerous spatiotemporal patterns of the activity of cortical neurons [14]. The network of cortical neurons gives rise to the neocortex. The neocortex can be described as being arranged horizontally in six laminae and vertically in a hive of cylinders, called cortical columns. Experimental evidence has demonstrated that cortical columns work as fuzzy and not Boolean sets [15–17].

4. Chemical Implementation of Fuzzy Logic

The similarities between the elements of any FLS and some components of the HNS spark new ideas for processing fuzzy logic through molecular, supramolecular, and systems chemistry [7].

Any molecule, which can assume many conformational structures or experience distinct micro-environments, is describable as a quantum mixed state:

\[
\rho = \sum_{i=1}^{N} w_i \left| \psi_i \right\rangle \left\langle \psi_i \right|
\]

In Equation (1), \(w_i\) is the weight (or probability) of the \(i\)-th wavefunction \(\left| \psi_i \right\rangle\). The molecular system represented by \(\rho\) can be used to encode Fuzzy information. The weight \(w_i\) represents the degree of membership of the state \(\left| \psi_i \right\rangle\) to the quantum fuzzy set \(\rho\). It is possible to determine the Fuzzy Entropy \(H\) for this molecular system through Equation (2):

\[
H = -\frac{1}{\log N} \sum_{i=1}^{N} w_i \log(w_i)
\]

\(H\) can assume any real value included between 0 and 1. When the molecule exists in only one state, \(N = 1, w_1 = 1\). It derives that \(H = 0\). When the compound exists in \(N\) distinct states, which are all equally probable, then \(w_i = 1/N\) and \(H = 1\). In any other case, the Fuzzy Entropy \(H\) assumes any value included in the \([0, 1]\) interval. The ensemble of the \(N\) states gives rise to a molecular fuzzy set [17]. Any physical or chemical input that modifies the distribution of the \(w_i\) values allows us to change the Fuzzy Entropy and hence to process fuzzy logic.

The weight \(w_i\) values appearing in Equation (2) defining \(H\) can be determined by recording any transient signal and fitting it through the Maximum Entropy Method (MEM).
MEM fits any transient spectroscopic signal (such as an absorbance $A(t)$ that changes over time) by using a poly-exponential function:

$$A(t) = \sum_{i=1}^{N} w_i e^{-\frac{t}{\tau_i}}$$

For example, the formation and depletion kinetics for a merocyanine photoproduced from a spiroporphyrin have been analyzed through MEM (see reference [18]). The kinetic constants’ distributions have been obtained. Such distributions are sensitive to temperature and the presence of a ducking compound, such as glycine. Glycine and temperature are two inputs that transform the molecular fuzzy set constituted by the conformers of the merocyanine.

The absence of transient signals does not prevent the possibility of processing fuzzy logic. The availability of smooth analog input–output relationships can be employed to build FLSs a posteriori. There are several examples in the literature. Those proposed in our group are described in references [19–22]. The software allows us to granulate physicochemical variables a posteriori. The granulation of the physicochemical variables can also be accomplished a priori. It is required to mix appropriately chosen compounds and imitate the structural principle that is at the basis of every human sensory subsystem.

For instance, the three retinals in the cones partition the visible spectral region in three fuzzy sets [5,6]. This molecular granulation of the visible region gives humans the capability of perceiving colours. This approach was applied to designing a system with three or more direct photochromic compounds [23,24]. The absorption bands of the uncoloured forms partition the UV region, whereas the bands of the coloured forms partition the visible region. By carefully selecting the composition of the photochromic mixture, it is possible to discriminate the UV frequencies based on the colour generated under UV irradiation. These photochromic systems extend human vision to the UV.

5. Conclusions

In conclusion, fuzzy logic mimics the human capability to make rational decisions based on natural language because structural and functional analogies exist between any Fuzzy Logic System and the human nervous system.

Fuzzy logic can be processed through molecules that exist in many micro-states or conformers. Alternatively, it can be encoded by mixing properly chosen chemical compounds that are responsive to the same kind of stimulus as it occurs in any sensory subsystem. If we want to approach the information processing power of the human nervous system, we need to design hierarchical structures similar to those we find in humans. Such hierarchical structures should also be autopoietic [25] and cognitive to approach the performances of living beings [26]. Implementing autopoietic and cognitive structures as well as processing fuzzy logic at the molecular level will boost the development of Chemical Artificial Intelligence [27]. Therefore, it will be reasonable to expect technology to approach some performances of human intelligence.

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