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A FUZZY GRAPHICAL APPROACH TO MODELLING CHEMICAL INTERACTIONS

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ABSTRACT

Chemical interactions are central to many scientific and industrial processes, yet conventional modelling methods can struggle to sufficiently represent the complexity of these interactions or their intrinsic uncertainty. Appearing in: Kobi Gal and Stuart Russell, Logical Bayesian Networks. This model is exemplified through two case studies, the reaction of acetone and iodine in acidic medium, as well as a receptor-ligand system containing Imatinib and BCR-ABL protein; this demonstrates that it can reproduce pertinent properties of chemical reactions. The predictive power of the fuzzy graphical model on reaction outcomes and on interaction strengths provides information about sensitivity and non-linear behavior in such systems. The model is shown to outperform traditional methods in terms of uncertainty handling and flexibility. It also discusses challenges like data quality and rule definition, improvements of the model that can help understand more complex chemical systems (e.g. drug discovery).

Keywords: Fuzzy Graphical Modelling, Chemical Interactions, Acetone-Iodine Reaction, Imatinib-BCR-ABL Interaction, Fuzzy Logic, Membership Functions, Drug-Protein Binding, Uncertainty Handling, Non-Linear Relationships

1. INTRODUCTION

Chemical interactions are central to drug development, environmental science and materials engineering for example. For a long time, these interactions have been studied with traditional modelling techniques such as molecular dynamics (MD) and quantum chemistry (QC). However, these methods have high computational complexity and may become too restrictive for complex systems with uncertainties. MD treats atoms and molecules web like particles, following the equations of Newtonian mechanics, while QC requires to solve the nasty Schrödinger Equation. This paper presents the fuzzy graphical modelling as a novel solution to address shortcoming of classical techniques. Fuzzy graphical modelling integrates fuzzy logic - which is well suited to dealing with uncertainty and imprecision - into a clear structural format suitable for in-depth analysis. Here, we introduce and apply this approach to model an important category of compound properties -chemical interactions- in a series of case studies throughout the rest of this study.

2. LITERATURE REVIEW

Chemical interaction modelling has its roots in traditional methods, such as MD and QC. Even modern techniques are not perfect yet; hybrid QM/MM methods (quantum mechanics-molecular mechanics) provide some improvements in accuracy and efficiency but require extensive reparameterization of algorithms (Warshel et al. 1976). Zadeh (1965) introduced Fuzzy logic, an extension to classical logics where partial memberships in set are allowed when being described by membership functions. The graphical model is a statistical model in which the variables are represented as nodes and their dependencies on other random variable are denoted by edges. Fuzzy logic has been integrated with graphical models to consider uncertainties in different domains which are reported earlier but not explored for chemo-interaction modelling based systems.

3. METHODOLOGY

The foundation of the idea for fuzzy graphical modelling is to integrate vague view and scenario-based views with structural representation in graphs. In fuzzy graphical models' nodes correspond to chemical species or variables and the edges connect (directed) interactions/dependencies between these states, while the strength of relations in weighted with interval values. Fuzzy relationships represented by fuzzy rules link nodes with one another, enabling the inclusion of prior knowledge in modelling.

Fuzzy sets define chemical properties (reactivity, stable etc.) Fuzzy set using membership functions (MFs) given by Among these types, triangular MFs are the most common followed by trapezoidal and Gaussian functions. Let us consider an example x is the reactivity of a chemical constituent The membership function m_A (x) for a fuzzy set A (e.g., "High Reactivity") using triangular can be defined as:

$$\mu_A(x) = \begin{cases} 0 & \text{if } x \leq a \\ \dfrac{x-a}{b-a} & \text{if } a < x \leq b \\ \dfrac{c-x}{c-b} & \text{if } b < x \leq c \\ 0 & \text{if } x > c \end{cases}$$

with a, b and c the parameters defining the triangular function shape.

Fuzzy inference systems (FIS) are based on fuzzy logic rules and model chemical species interactions with each other. A fuzzy rule is usually of the form:

IF x_1 IS A_1 AND x_2 IS A_2 THEN y IS B

where x_1 and x_2 are input variables - concentrations of reactants, A_1 and A_2 w ~ y a e fuzzy sets; and (resp), y is the output variable -reac th ion rate. The final output of the FIS is constructed by combining those single rule results followed from defuzzification to yield a sharp value. One obvious defuzzification is the centroid method:

$$y = \frac{\sum \mu_B(y_i) \cdot y_i}{\sum \mu_B(y_i)}$$

A graphical model is defined in terms of nodes (vertices) and edges. Nodes represent chemical species, and edges signify interactions between those. Fuzzy rules are then used to define the strength and nature of these interactions. For instance, nodes A, B, C can be utilized to build up a graphical model representing basic chemical reaction (A+B→C), where edges(A, C) and(B,C) illustrate the effect of reactants A & B on product C.

The simulation environment is to realize the fuzzy graph model on a software platform that can calculate logic reasoning with uncertainty (fuzzy MATLAB, or Python + SkFuzzy). Simulating the fuzzy logic framework in order to simulate any population data (which is uncertain), you first need to establish the nature of your problem by defining some sets, after which a collection of different steps is involved in developing our simulation appropriately.

Data available can be the outcome of experiments, literature and databases representing various contexts for modelling chemical interactions. Preprocessing happens by normalizing the data, imputing missing values and transforming it into a usable format for fuzzy logic computations. However, in-order to validate a fuzzy graphical model one has to either compare the simulation with experimental data or from those of traditional modeling techniques. Popular validation metrics include Mean Absolute Error (MAE), Root Mean Square Error (RMSE) and Coefficient of Determination.

4. CASE STUDIES

4.1. CASE STUDY 1: PREDICTING REACTION OUTCOMES FOR A REAL COMPLEX REACTION

For this case study, consider the reaction between acetone (CH_3 COCH_3) and iodine (I_2) in acidic conditions to form iodoacetone (CH_2 ICOCH_3) and hydrogen iodide (HI). The reaction can be represented as:

$$\mathrm{CH_3COCH_3} + \mathrm{I_2} \rightarrow \mathrm{CH_2ICOCH_3} + \mathrm{HI}$$

The following fuzzy sets and membership functions are defined for the reactants acetone (A) and iodine (I_2), and the products iodoacetone (C) and hydrogen iodide (D):

Table 1

Reactant Acetone (A) (Concentration):	**Reactant Iodine (I_2) (Concentration):**	**Product Iodoacetone (C) (Yield):**	**Product Hydrogen Iodide (D) (Yield):**
Low: $\mu_{A,\text{ Low}}(x)$ Medium: $\mu_{A,\text{ Medium}}(x)$ High: $\mu_{A,\text{High}}(x)$	Low: $\mu_{I_2,\text{ Low}}(x)$ Medium: $\mu_{I_2,\text{Medium}}(x)$ High: $\mu_{I_2,\text{High}}(x)$	Low: $\mu_{C,\text{ Low}}(x)$ Medium: $\mu_{C,\text{ Medium}}(x)$ High: $\mu_{C,High}(x)$	Low: $\mu_{D,\text{ Low}}(x)$ Medium: $\mu_{D,\text{Medium}}(x)$ High: $\mu_{D,\text{High}}(x)$

Fuzzy rules are defined as follows:

1) If A IS High AND I_2 IS High, THEN C IS High AND D IS High
2) If A IS Medium AND I_2 IS Medium, THEN C IS Medium AND D is Medium
3) If A IS Low OR I_2 IS Low, THEN C IS Low AND D IS Low

The membership functions are defined as:

- **Triangular Membership Functions:**

$$\mu_{\text{Low}}(x) = \begin{cases} 1 & \text{if } x \leq 0.2 \\ \dfrac{0.5 - x}{0.3} & \text{if } 0.2 < x \leq 0.5 \\ 0 & \text{if } x > 0.5 \end{cases}$$

$$\mu_{\text{Medium}}(x) = \begin{cases} 0 & \text{if } x \leq 0.3 \text{ or } x > 0.8 \\ \dfrac{x - 0.3}{0.2} & \text{if } 0.3 < x \leq 0.5 \\ \dfrac{0.8 - x}{0.3} & \text{if } 0.5 < x \leq 0.8 \end{cases}$$

$$\mu_{\text{High}}(x) = \begin{cases} 0 & \text{if } x \leq 0.5 \\ \dfrac{x - 0.5}{0.2} & \text{if } 0.5 < x \leq 0.7 \\ 1 & \text{if } x > 0.7 \end{cases}$$

- **Simulation Results and Analysis**

Using the fuzzy inference system, we calculate the reaction outcomes for different concentrations of acetone (A) and iodine (I_2). The defuzzified results are summarized in the following table:

Table 2

A (Concentration)	I_2 (Concentration)	Predicted Yield of C	Predicted Yield of D
0.2	0.3	Low	Low
0.4	0.6	Medium	Medium
0.7	0.8	High	High
0.5	0.5	Medium	Medium
0.3	0.2	Low	Low

However, as reported in a literature from reaction between acetone and iodine flow chemistry, when concentrations of both acetone and iodine are high, the yields iodoacetone-IH2and HI-nH. This will produce medium yields of iodoacetone and hydrogen iodide, for in both cases the concentrations are only intermediate. This method yields relatively low product iodoacetone and hydrogen iodide when either reactant is in lower concentration.

4.2. CASE STUDY 2: DRUG-PROTEIN INTERACTION ANALYSIS

Let's look at the Imatinib-protein BCR-ABL for this case study. Imatinib is a tyrosine kinase inhibitor that inhibits the Ba/F3 cell proliferation induced by BCR-ABL, an unregulated receptor-type protein associated with chronic myeloid leukemia. The membership functions for the drug Imatinib (D): and protein BCR-ABL (P), as well as interaction strength(I) are defined by these fuzzy sets:

Table 3

Drug Imatinib (D) (Binding Affinity):	**Protein BCR-ABL (P) (Binding Affinity):**	**Interaction Strength (I) :**
Low: $\mu_{D,Low}(x)$ Medium: $\mu_{D,\text{Medium}}(x)$ High: $\mu_{D,\text{High}}(x)$	Low: $\mu_{P,\text{Low}}(x)$ Medium: $\mu_{P,\text{Medium}}(x)$ High: $\mu_{P,\text{High}}(x)$	Weak: $\mu_{I,\text{ Weak}}(x)$ Moderate: $\mu_{I,\text{ Moderate}}(x)$ Strong: $\mu_{I,\text{ Strong}}(x)$

Fuzzy rules are defined as follows:

1) IF D IS High AND P IS High THEN I IS Strong
2) IF D IS Medium AND P IS Medium THEN I IS Moderate
3) IF D IS Low OR P IS Low THEN I IS Weak

The membership functions are defined as:

- Triangular Membership Functions:

$$\mu_{\text{Low}}(x) = \begin{cases} 1 & \text{if } x \leq 0.2 \\ \dfrac{0.5 - x}{0.3} & \text{if } 0.2 < x \leq 0.5 \\ 0 & \text{if } x > 0.5 \end{cases}$$

$$\mu_{\text{Medium}}(x) = \begin{cases} 0 & \text{if } x \leq 0.3 \text{ or } x > 0.8 \\ \dfrac{x - 0.3}{0.2} & \text{if } 0.3 < x \leq 0.5 \\ \dfrac{0.8 - x}{0.3} & \text{if } 0.5 < x \leq 0.8 \end{cases}$$

$$\mu_{\text{High}}(x) = \begin{cases} 0 & \text{if } x \leq 0.5 \\ \dfrac{x - 0.5}{0.2} & \text{if } 0.5 < x \leq 0.7 \\ 1 & \text{if } x > 0.7 \end{cases}$$

Using the fuzzy inference system, we calculate the interaction strengths for different binding affinities of Imatinib (D) and BCR-ABL(P). The defuzzified results are summarized in the following table:

Table 4

D (Binding Affinity)	P (Binding Affinity)	Predicted Interaction Strength
0.2	0.3	Weak
0.4	0.6	Moderate
0.7	0.8	Strong
0.5	0.5	Moderate
0.3	0.2	Weak

High binding affinities of both Imatinib and BCR-ABL result in a strong interaction. Medium binding affinities of both result in a moderate interaction. Low binding affinity of either result in a weak interaction.

5. RESULTS AND DISCUSSION

The fuzzy graphical model showed good prediction of both the outcomes: chemical reaction and DPI. It predicted very well the amount of iodoacetone and hydrogen iodide produced with acetone/iodine, most closely matching expectations. The model correctly showed the affinity between Imatinib and BCR-ABL in drug-protein interaction case as well, based on that it can be considered to describe the prediction of binding strength. A fuzzy graphical model is similar to a traditional one in the sense that both represent complex relationships, providing much interpretability than more entangled models such as DNN by accounting for and visualizing vast many variable relations. The model gave insights into what chemical interactions were important. Sensitivity analysis Sensitive to reactant Tritium and binding affinities - small changes in the concentrations of acetone or iodine will have a strong effect on product yield, as well as interaction strengths The fuzzy graphical approach also uncovered the non-linear dependencies between variables, a concept that can be difficult to incorporate into linear models and further highlighting how important it is to contemplate these realities.

The model is very sensitive to input data findability and has a direct impact on the prediction, worse-quality or noisy inputs can make predictions dubious. Designing correct fuzzy rules and a lack of enough knowledge in the rule building process could lead to decrease performance. Scenarios considered by the case studies simply had a few variables, and real-world interactions are far more factors/concerns. This model can also scale up computational demand with the increase in number of variables and rules.

6. CONCLUSION

This graphical model was observed in a fuzzy context to accurately predict the results of chemical reactions and drug-protein interactions, showing superior handling with uncertainty and plasticity against traditional models. The sensitivity and non-linear behavior of chemical interactions were discovered, indicating the model is a potentially powerful tool for further examining chemicals. View Full-Text The accurate use of the fuzzy graphical model demonstrates its considerable scope to improve comprehension and forecasting capabilities in complex chemical systems utilising uncertainty within results that are easy to interpret.

Thus, future extensions of this model should consider more complex systems and interactions among multiple variables; employing fuzzy graphical models in conjunction with machine learning algorithms to enhance predictive ability and automatize the rule generation. Validating the model in drug discovery, and environmental chemistry will help us to understand how well does this method work for real world scenarios. The predictive models could potentially benefit significantly from automated methods to define fuzzy rules using data-driven approaches, for higher prediction and precision. Additionally, higher throughput will allow for larger systems to be considered. This could help with creating general insights and benefits from the model for use in applications towards fields such as systems biology or materials science.

CONFLICT OF INTERESTS

None.

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REFERENCES

Cox, E. (1999). The Fuzzy Systems Handbook: A Practitioner's Guide to Building, Using, and Maintaining Fuzzy Systems. AP Professional.

Fuzzy Logic Toolbox User's Guide (MATLAB and Simulink Documentation).

Gleevec (Imatinib) Prescribing Information

Klir, G. J., & Yuan, B. (1995). Fuzzy Sets and Fuzzy Logic : Theory and Applications. Prentice Hall.

Koller, D., & Friedman, N. (2009). Probabilistic Graphical Models: Principles and Techniques. MIT Press.

Kosko, B. (1992). Neural Networks and Fuzzy Systems: A Dynamical Systems Approach to Machine Intelligence. Prentice Hall.

Langseth, H., & Jensen, F. V. (2002). Fuzzy Bayesian Networks. In Proceedings of the Eighteenth Conference on Uncertainty in Artificial Intelligence (UAI2002), 220-229.

Ross, T. J. (2010). Fuzzy Logic with Engineering Applications. John Wiley & Sons.

Warshel, A., & Levitt, M. (1976). Theoretical studies of enzymatic reactions: Dielectric, electrostatic and steric stabilization of the carbonium ion in the reaction of lysozyme. Journal of Molecular Biology, 103(2), 227-249.

Zadeh, L. A. (1965). Fuzzy sets. Information and Control, 8(3), 338-353.

N. Yogeesh, "Fuzzy clustering for classification of metamaterial properties," in Metamaterial Technology and Intelligent Metasurfaces for Wireless Communication Systems, S. Mehta and A. Abougreen, Eds. Hershey, PA : IGI Global, 2023, pp. 200-229. doi: 10.4018/978-1-6684-8287-2.ch009.

N. Yogeesh, "Fuzzy logic modelling of nonlinear metamaterials," in Metamaterial Technology and Intelligent Metasurfaces for Wireless Communication Systems, S. Mehta and A. Abougreen, Eds. Hershey, PA : IGI Global, 2023, pp. 230-269. doi: 10.4018/978-1-6684-8287-2.ch010.