Fermentation Process Modeling Using Takagi-Sugeno Fuzzy Model

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Abstract: Fermentation process is vital and important in many biotechnological applications. However modeling the fermentation process is considered a challenging and complex problem. The complexity of the problem is driven by the need of efficient, accurate, not expensive, and reliable predictive models. In this paper, we apply a Takagi-Sugeno Fuzzy Logic technique for modeling the lipase activity production based on nutritional and physico-chemical factors to estimate the lipase activities. The accuracy of the developed fuzzy model is measured, validated and compared with both the multiple regression and artificial neural network models. The fuzzy model successfully showed competitive and promising modeling results.

Key–Words: Fermentation process, Lipase activity production, Takagi-Sugeno Fuzzy Modele.

1 Introduction

Lipase production is getting more and more attention in the industry and business field recently due to their biotechnological applications [1]. Lipases have a wide range of uses in industry productions such as diary-based products, detergents, drugs, cosmetics and leather processes [2]. On the other side, Lipase production is a challenging, complex and not easy to model or monitor [2]. The complexity is due to the nature of lipase production which is highly dependent on its operating conditions that affect its growth. These operating conditions include nutritional and physico-chemical factors such as temperature, initial pH, incubation period, time, inoculum size and agitation rate [1–3]. Consequently, deciding upon an optimization method and choosing a modeling technique are vital issues in the process of producing reliable lipase products with high standards. Efficient optimization and modeling can dramatically improve the system performance and reduce the costs [3].

In biologyical research, response surface methodology (RSM) is one of the most applied methods in modeling the biological processes. RSM is a statistical and mathematical based system for modeling and optimizing complex processes. RSM explores the relationships between the response (output variable) and the independent variables (input variables). RSM has many advantages such as it reflects the significance of the input variables, alone or in combination, in a given model. Moreover, it reduces the cost of analysis by minimizing the number of experimental trials needed to evaluate input variables and their interactions [4].

Though, RSA is not applicable in all biological applications [3].

In many cases, output results are out of expectations when modeling and predicting systems based on mathematical equations are used for controlling the interactions between the input variables in the process for lipase fermentation. Therefore, a considerable number of previous studies employed empirical models based on artificial intelligence and machine learning approaches. By the following paragraphs we give an insight into some important studies in the field.

Among artificial intelligence and machine learning approaches, Artificial Neural Networks (ANNs) are the most applied in lipase modeling and prediction. In [3] authors used the best composition of production medium among the best previously published media, then they made a comparison by applying both RSM and ANN for optimizing the physical factors for extracellular thermostable lipase production. Although both techniques gave good predictions, the ANN showed better performance in data fitting and estimation capabilities. However ANN in general suffers some disadvantages; ANNs relatively need large amounts of data for training and they work as black input/output box, it is hard to interpret their results.

In [5] ANN model, based on feed forward architecture and back propagation as training algorithm was applied to predict the state of batch fermentations with grape juice extracted from grape waste. The Levenberg- Marquardt optimization technique has been used to upgrade the network by minimizing the sum square error (SSE). Authors found that the best performance of the model for predicting cell

mass and ethanol concentration is can be obtained using a neural network with two hidden layers of 15 and 16 neurons, respectively.

Other famous approaches are Genetic Programming (GP) and Genetic Algorithms (GA). Both approaches are evolutionary techniques inspired from biology concepts. GP and GA applied for modeling lipase production by researches but they are less common than ANN. For example, in [6] authors applied GP as evolutionary computation methodology for developing an efficient model for the fermentation process. Authors compared their results with others obtained from traditional experimental design approach (Box-Behnken). Their final results show the superiority of the GP in modeling the fermentation process.

In [7], a modified genetic algorithm is proposed for a parameter identification of an E. coli fedbatch fermentation model. Authors made some adjustments of the genetic parameters regarding the fermentation processes, to improve the conventional genetic algorithm. Authors claim that the modified GA for a parameter identification of the problem can be efficient and effective. Applying of the modified GA can decrease the running time but relatively still high.

In this paper we apply a Takagi-Sugeno fuzzy technique for modeling the lipase activity production based on Temperature, pH, Inoculum, Time and Agitation as input variables of 26 experiments. Then we measure the accuracy of the developed fuzzy model and compare it with a conventional polynomial model.

2 Multiple Regression (MR) Model

This approach uses the method of least squares estimation (LSE), to model a relationship between one dependent and many independent variables. Multiple regression models were used to solve variety of modeling problems. To show how the parameter estimation process work, we assume that a system with five input variables x_1, x_2, x_3, x_4, x_5 and single output y can be modeled with a single function f. the function f could have a different level of complexity.

For simplicity we will assume that f is a simple linear function as given in Equation 1. The level of complexity could be higher as we will discuss later in our case study which is given in Equation 9. The multiple regression model has the following mathematical

representation.

$$
\begin{aligned}
y &= f(x) \\
&= a_0 + \sum_{i=1}^{n=5} a_i x_i \\
&= a_0 + a_1 x_1 + a_2 x_2 + a_3 x_3 + a_4 x_4 + a_5 x_5
\end{aligned}
\tag{1}
$$

To find the values of the model parameters a's we need to build what is called the regression matrix Φ. This matrix is developed based on the experiment collected measurements. Thus, Φ can be presented as follows given there is a set of measurements m:

$$
\Phi = \begin{pmatrix}
x_1^1 & x_2^1 & x_3^1 & x_4^1 & x_5^1 \\
x_1^2 & x_2^2 & x_3^2 & x_4^2 & x_5^2 \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
x_1^m & x_2^m & x_3^m & x_4^m & x_5^m
\end{pmatrix}
$$

The parameter vector a and the output vector y can be presented as follows:

$$
\theta = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix}
\qquad
y = \begin{pmatrix} y^1 \\ y^2 \\ \vdots \\ y^m \end{pmatrix}
$$

The least squares solution of yields the normal equation:

$$
\begin{aligned}
\Phi a &= y \\
a &= \Phi^{-1} y
\end{aligned}
\tag{2}
$$

But since, the regression matrix Φ is not a symmetric matrix, we have to reformulate the equation such that the solution for the parameter vector a is as follows:

$$
a = (\Phi^T \Phi)^{-1} \Phi^T y
\tag{3}
$$

The second order regression model is given in Equation 4. This model can provide a better accuracy than the first order model since it provides more dynamics and nonlinearity.

$$
y = a_0 + \sum_{i=0}^{n} a_i x_i + \sum_{i=0}^{n} \sum_{j=0}^{n} a_{ij} x_i x_j
\tag{4}
$$

3 Fuzzy Modeling

Soft computing techniques were used to mimic the powerful parallel processing capabilities of the human brain. These techniques were capable of solving variety of modeling problems in computer science and engineering. These models can describe the non-linear

relationships between model parameters in an effective way. These techniques include artificial neural networks [5], fuzzy logic [8–10], swarm intelligence, agent based modeling [11], differential evolution, genetic algorithms [4, 12] and genetic programming [6]. A fuzzy model structure can be represented by a set of fuzzy If-Then rules [13]. A rule-based fuzzy model requires the identification of the following quantities:

- the antecedent,

- the consequent structure of the membership functions,

- the estimation of the consequent regression parameters and

- in this work, an additional parameters have to be selected which is the number of rules (clusters) σ. This parameter is specified by the user.

The above quantities have to be defined in various operating regions. The number of rules used to solve the nonlinear modeling problem can be determined automatically.

3.1 What is FIS?

In Figure 1, we show a flow diagram of the proposed fuzzy logic system used in this study. The system consists of number of stages.

1. **Fuzzification:** In this stage, the model inputs and outputs variables are defined.

2. **Inference:** Fuzzy inference is defined as the process of mapping from input state to an output state based fuzzy sets theory. The mapping constructs the system decision making. The process of fuzzy inference include: Membership functions, Fuzzy set operation, and If-Then rules. FIS may be summarized as two processes:

   - *Aggregation:* Compute the IF part (i.e. antecedent) of the rules. The antecedent variables reflect information about the process operating conditions.

   - *Composition:* Compute the THEN part (i.e. consequence) of the rules. The consequent of the rule is usually a linear regression model which is valid around the given operating condition [14–16].

3. **Defuzzification:** The output variable computed in the previous stage are then converted to real output value.

3.2 Takagi-Sugeno (TS) Fuzzy Model

This modified inference approach is a universal approximator of any smooth nonlinear system was proposed by Takagi and Sugeno [17, 18]. Takagi-Sugeno Fuzzy Model is represented by a small set of fuzzy IF-THEN rules that describe local input-output functions of a nonlinear system [19]. Each rule has the following form:

$$IF\ x_1\ is\ A_{r1}\ AND\ x_2\ is\ A_{r2}\ ..\ AND\ x_n\ is\ A_{rn}$$
$$THEN\ u = f_r(x_1, x_2, .., x_n)$$

where A_{ij} is a fuzzy set, X_k is input variable and u is a local output variable. Suppose that H_i is the validity of the logical expression $x_1\ is\ A_{r1}\ AND\ x_2\ is\ A_{r2}\ ..\ AND\ x_n\ is\ A_{rn}$ is R_i then the final output of the model can be computed as a weighted mean value over all rules according to 5.

$$u' = \frac{\sum_{i=1}^{N} H_i f_i(x_1, x_2, .., x_N)}{\sum_{i=1}^{N} H_i}$$

4 Problem Formulation

Our objective is to control the dynamics of the lipase production process during its growth and instead of representing it in a single nonlinear model by a set of local linear models. Each local model should be able to represents the relationship between the input variables x_1, x_2, x_3, x_4, x_5 which represent *Temperature, pH, Inoculum, Time and Agitation*, respectively, and the observed y in a certain range of operating conditions. Thus, we would like to find a function f for this relation as given in Equation 5 in a form of set of fuzzy rules as given in R_1. Such a proposed fuzzy model structure can be successfully represented by means of fuzzy If-Then rules.

$$\hat{y} = f(x_1, x_2, x_3, x_4, x_5) \tag{5}$$

R_1 : **If** x_1 is A_{11} **and** x_2 is A_{12} **and** x_3 is A_{13}
     and x_4 is A_{14} **and** x_5 is A_{15} **then**
     $y = a_0 + a_1 x_1 + a_2 x_2 + a_3 x_3 + a_4 x_4 + a_5 x_5$

Using membership functions and the antecedent of the rule we can define the fuzzy region in the product space. The $antecedent$ variables give the condition of the process status now. The consequent of the rule is typically a local linear regression model which relates y with x_1, x_2, x_3, x_4, x_5.
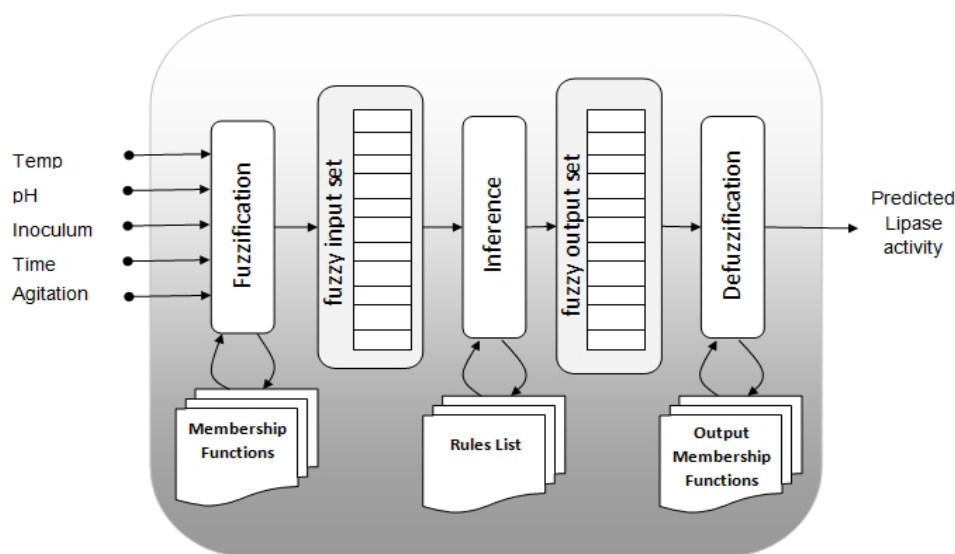
Figure 1: The proposed fuzzy logic system

A rule-based fuzzy model requires the identification of the *antecedent* and the *consequent* structure, the type of the membership functions for different operating regions and the estimation of the consequent parameters. The proposed presented technique does not require any *a prior* knowledge about the operating regimes. If a sufficiently number of measurements are collected which reflects the operating ranges of interest, the developed fuzzy model will be efficient one.

4.1 Evaluation Criteria

The performance of the developed two models; the regression and the fuzzy shall be evaluated using three evaluation criteria. They include:

- the Variance-Accounted-For (VAF):

$$VAF = [1 - \frac{var(y - \hat{y})}{var(y)}] \times 100\% \quad (6)$$

- The Euclidian distance (ED):

$$ED = \sqrt{(\sum_{i=1}^{n}(y_i - \hat{y}_i)^2)} \quad (7)$$

- The Manhattan distance (MD):

$$MD = (\sum_{i=1}^{n}|y_i - \hat{y}_i|) \quad (8)$$

where y and $\hat{y}$ are the actual lipase activates and the estimated activates based on proposed model and n is the number of measurements used in the experiments, respectively.

5 Lipase Data Set

The data set used in this study was presented in [20]. Author stated that the experimental data was collected for the included variables and their selected levels, after the preliminary study, for the lipase production optimization in SmF were: incubation temperature (27 - 45C); initial pH (6 - 9); inoculum size (1 - 5%); agitation rate (0 - 200 rpm) and incubation period (24 - 96 h). The variables and their levels in SSF were: incubation temperature $(27 - 45^{0}C)$; initial pH (6 - 9); moisture content (60 - 100%); olive oil (0 - 20%) and incubation period (72 - 168 h). In [20], authors used explored the use of Artificial Neural Networks to model the lipase activities. Their reported estimated lipase activities based ANN used five independent variables. They show the observed values of lipase activity in SmF. We report their results on Table 2.

6 Experimental Results

6.1 Developed MR Model

MR was used to find a relationship between several independent or predictor variables and a dependent variable. This relationship need to fit within acceptable level of error such that the relation is valid. MR particularly used since regression analysis helps the system designer to understand the status of a dependent variable changes while one or more of the independent variables also changed.

Many authors in the area of lipase production analysis and biocheisty used the first and second order MR model to solve this problem. For exam-

ple, in [21], author used the statistical software package Minitab version 15 (Minitab Ltd., Coventry CV3 2TE, UK) was used for analyzing the experimental data and developed a first order MR model. They checked the goodness of fit model by the determination of coefficient (R2) which indicated that the model could explain up to 98.67% variation of the data. In [22], the design of an optimum and cost-efficient medium for high-level production of hydrogen by Ethanoligenens harbinense B49 was attempted using the Plackett-Burman design model. The technique is based on the first-order polynomial model. They also used the multiple regression analysis on the experimental data and used the second-order polynomial model to explain the hydrogen production. The optimization of physical parameters for lipase production from Arthrobacter sp. BGCC No. 490 using MR second order model [23]. Many others used the second order MR model to solve diversity of problem in the area of Biochemistry [24, 25].

According to previous studies, it was found that the MR second order model is a promising choice to model the lipase activity. That is why in our study, we adopted it for the purpose of comparison. The adopted MR equation is given as:

$$
\begin{aligned}
\hat{y} \;=\; & a_0 + a_1 x_1 + a_2 x_2 + a_3 x_3 + a_3 x_4 + a_5 x_5 \\
& + \; a_6 x_1^2 + a_7 x_2^2 + a_8 x_3^2 + a_9 x_4^2 + a_{10} x_5^2 \\
& + \; a_{11} x_1 x_2 + a_{12} x_1 x_3 + a_{13} x_1 x_4 + a_{14} x_1 x_5 \\
& + \; a_{15} x_2 x_3 + a_{16} x_2 x_4 + a_{17} x_2 x_5 \\
& + \; a_{18} x_3 x_4 + a_{19} x_3 x_5 + a_{20} x_4 x_5 \qquad (9)
\end{aligned}
$$

where $\hat{y}$ is the predicted lipase activities, a_0 model constant; x_1, x_2, x_3, x_4 and x_5 are independent variables; a_1, a_2, a_3, a_4 and a_5 are linear coefficients; a_6, a_7, a_8, a_9 and a_{10} are the quadratic coefficients; a_{11}, a_{12}, a_{13}, . . . are the cross product coefficients. The values of the parameters a were obtained by solving this regression problem. We estimated the parameters of this model using Least Square Estimation (LSE). The model parameters are given in Table 1.

6.2 Developed Fuzzy Model

To develop our results, we used the Fuzzy Model Identification Toolbox (FMID), implemented in MATLAB [26]. The number of clusters σ need to be specified in advance. We have tested number of clusters and observed number of evaluation criterion. The developed fuzzy rules for lipase activities production are given in Table 3. In Figure 2, we show the error difference between the three techniques adopted in this study.

Table 1: Estmaited values of a's using LSE with a_0=155.6888

a_1	a_2	a_3	a_4	a_5
-1.6136	-22.8679	-20.4559	-0.7810	0.3274

a_6	a_7	a_8	a_9	a_{10}
0.0028	1.0607	-0.4272	-0.0010	-0.0003

a_{11}	a_{12}	a_{13}	a_{14}	a_{15}
0.0825	0.2319	0.0088	-0.0053	1.1630

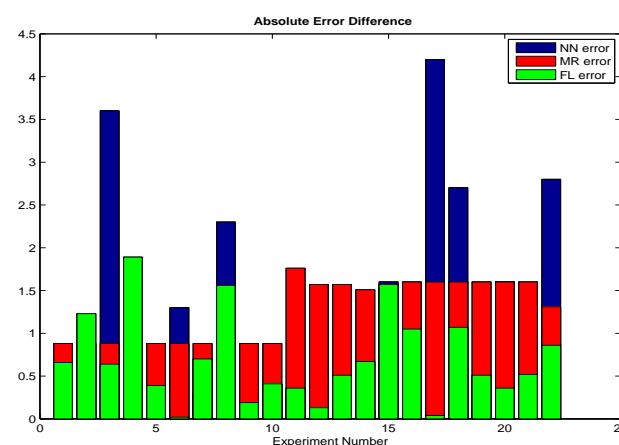| a_{16}	a_{17}	a_{18}	a_{19}	a_{20}
0.0570	-0.0119	0.0599	0.0195	-0.0003

Figure 2: Computed error in the NN, MR and FL cases

Table 2: Estimated Lipase Production Activity Using FL Model

Temp. C^o	pH	Inoculum (%)	Time (h)	Agitation (rpm)	Lipase Act. Measured	ANN model in [20]	MR model	Fuzzy model
40.9	8.3	1.9	79.8	45.1	8	7.9	8.8808	7.3466
40.9	6.7	4.1	79.8	45.1	3.6	3.7	4.4808	2.3755
31.1	8.3	4.1	40.2	154.9	10.6	7	11.4808	9.9609
40.9	8.3	4.1	40.2	45.1	5.5	7	6.3808	7.3989
40.9	8.3	1.9	40.2	154.9	4.8	4.1	5.6808	5.1985
40.9	6.7	1.9	79.8	154.9	2.4	1.1	3.2808	2.4247
31.1	6.7	4.1	79.8	154.9	7.2	7.5	8.0808	6.5098
31.1	8.3	1.9	79.8	154.9	8.5	6.2	9.3808	10.0611
40.9	6.7	4.1	40.2	154.9	5.6	6.3	6.4808	5.7953
31.1	8.3	4.1	79.8	45.1	5.2	5.6	6.0808	4.7972
31.1	6.7	1.9	40.2	45.1	8.3	8.6	10.0617	7.9416
27	7.5	3	60	100	11.2	10.2	9.6334	11.3319
45	7.5	3	60	100	9.4	10.4	7.8334	8.8956
36	6	3	60	100	9.8	9.9	8.2967	10.4795
36	9	3	60	100	15	13.4	13.4967	13.4307
36	7.5	1	60	100	9.2	9.5	7.6013	8.1593
36	7.5	5	60	100	7.6	3.4	6.0013	7.5686
36	7.5	3	24	100	9.2	11.9	7.6013	8.1315
36	7.5	3	96	100	8.4	8.3	6.8013	8.9156
36	7.5	3	60	0	4.2	5.8	2.6071	4.5621
36	7.5	3	60	200	10.6	9.8	9.0071	10.0889
36	7.5	3	60	100	7.2	10	8.5101	8.0652
36	7.5	3	60	100	7.6	X	8.5101	8.0652
36	7.5	3	60	100	5.9	X	8.5101	8.0652
36	7.5	3	60	100	8.1	X	8.5101	8.0652
36	7.5	3	60	100	8.6	X	8.5101	8.0652

Figure 3 shows the value of input variables of the fuzzy model in all experiments. While Figure 4, shows the five input variables in terms of fuzzy sets and their ranges. Finally, Figure 5 shows the actual and estimated lipase activities in real experiments and developed fuzzy model.
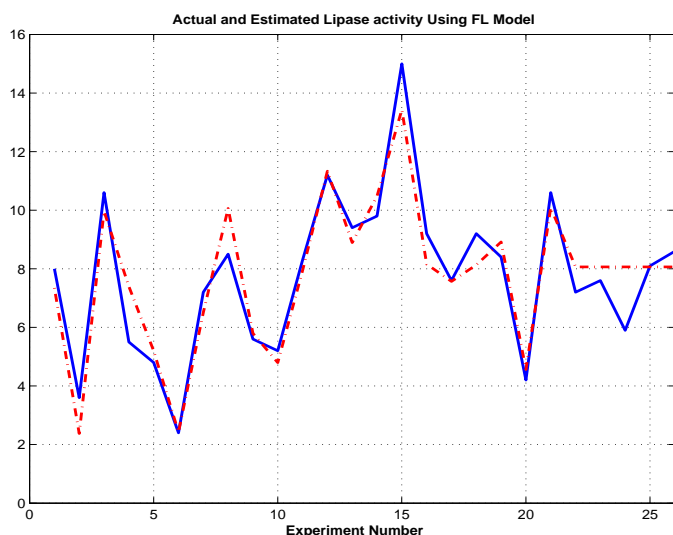

Figure 5: Actual and estimated response using Takagi-Sugeno fuzzy model

In order to compare the results of the fuzzy model with the polynomial one, the VAF was computed also for the polynomial model. The computed values are give in Table 4. It is clearly shown that the performance of the fuzzy model exceeds the polynomial model with more than 10% of increase and 25% increase over ANN models.

Table 4: VAF for the ANN, MR and FL models

No.	ANN Model in [20]	MR Model	Fuzzy Logic Model
VAF	64.15%	79.26%	90.98%
ED	3.90	3.89	2.18
MD	27.50	27.63	15.34

7   Conclusions and Future Work

In this paper, we used Takagi-Sugeno Fuzzy Logic technique for biotechnological process modeling of thermostable lipase production based on nutritional and physico-chemical factors. The proposed fuzzy model was able to estimate the lipase activities with high accuracy. In order to verify the approach applied, the results were compared with both the multiple regression and artificial neural network models.

The fuzzy model showed a superior performance in modeling the complex process.

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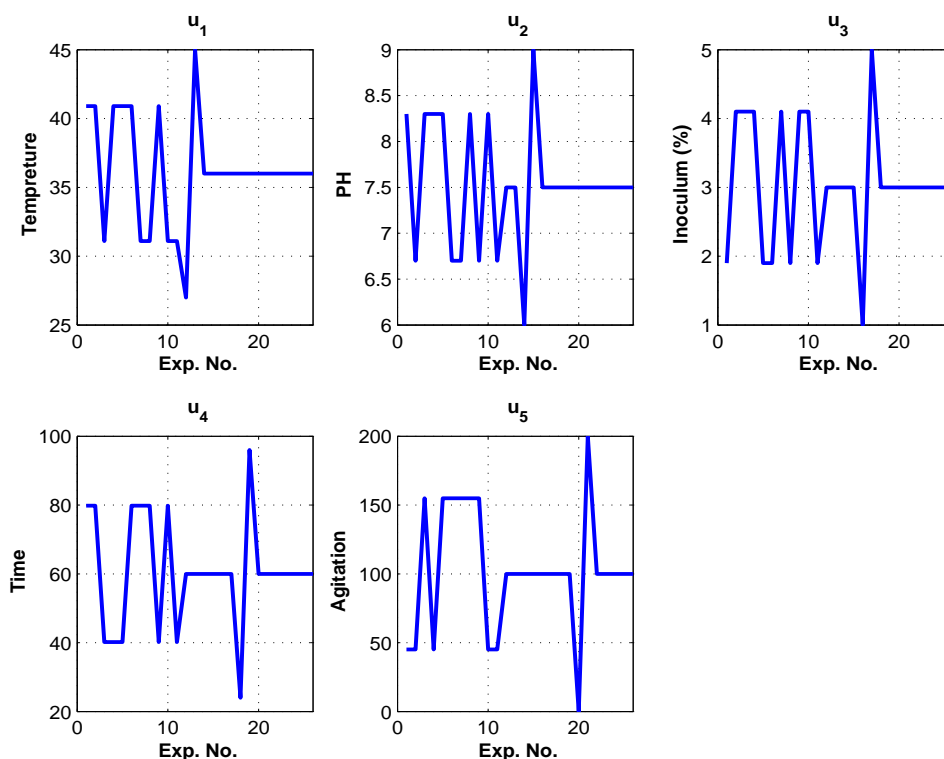[8] S. Vassileva. Advanced fuzzy modeling of integrated bio-systems. *WSEAS TRANSACTIONS on SYSTEM*, 11:234–243, 2012.

Figure 3: The input data for the Takagi-Sugeno fuzzy model

Table 3: Fuzzy Rules for lipase activities production

1. **If** x_1 is A_{11} **and** x_2 is A_{12} **and** x_3 is A_{13} **and** x_4 is A_{14} **and** x_5 is A_{15} **then**
   $y = 1.20 \cdot 10^0 x_1 + 7.12 \cdot 10^0 x_2 - 1.71 \cdot 10^0 x_3 - 2.31 \cdot 10^{-1} x_4 + 1.75 \cdot 10^{-1} x_5 - 7.18 \cdot 10^1$

2. **If** x_1 is A_{21} **and** x_2 is A_{22} **and** x_3 is A_{23} **and** x_4 is A_{24} **and** x_5 is A_{25} **then**
   $y = 9.73 \cdot 10^{-1} x_1 + 7.65 \cdot 10^0 x_2 - 1.95 \cdot 10^0 x_3 + 1.47 \cdot 10^{-2} x_4 + 8.00 \cdot 10^{-2} x_5 - 8.31 \cdot 10^1$

3. **If** x_1 is A_{31} **and** x_2 is A_{32} **and** x_3 is A_{33} **and** x_4 is A_{34} **and** x_5 is A_{35} **then**
   $y = 1.30 \cdot 10^0 x_1 + 1.07 \cdot 10^1 x_2 + 5.57 \cdot 10^0 x_3 + 1.36 \cdot 10^{-1} x_4 + 2.44 \cdot 10^{-1} x_5 - 2.07 \cdot 10^2$
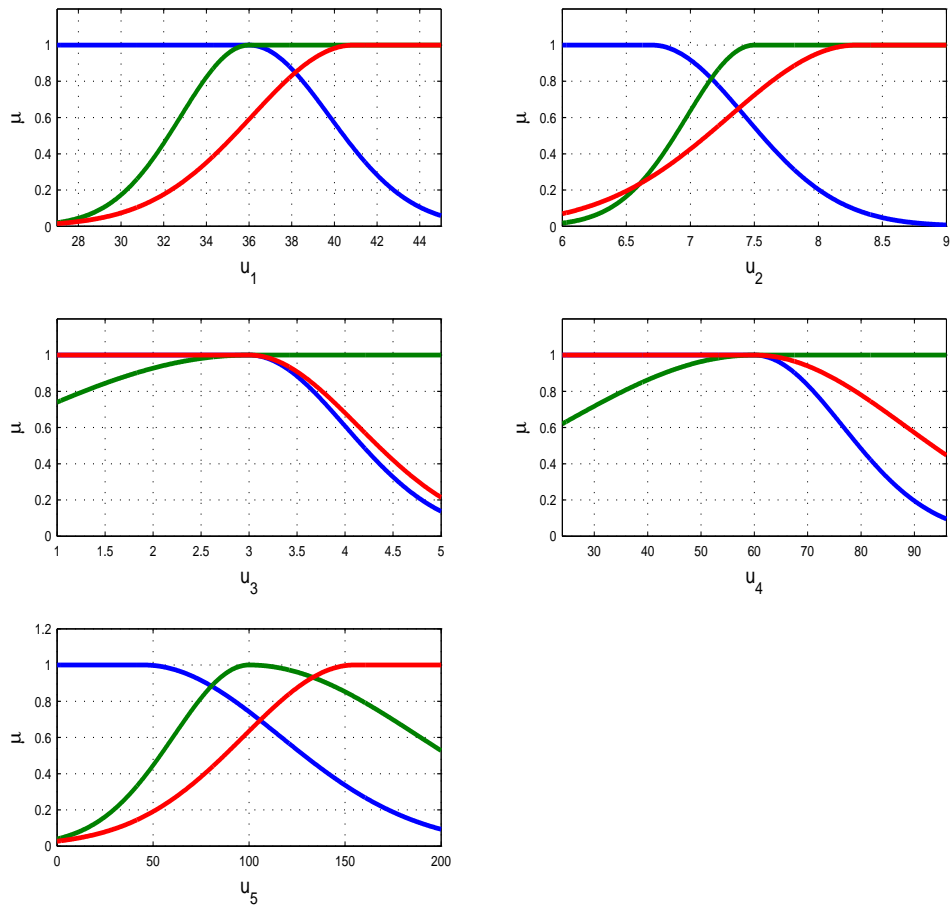
Figure 4: Fuzzy membership functions

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