PREDICTION OF LACTIC ACID CONCENTRATION USING ARTIFICIAL NEURAL NETWORK

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To my beloved mother and father
ACKNOWLEDGEMENT

“In the name of Allah (God) Most Gracious Most Merciful”

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ABSTRACT

This study investigates the application of artificial neural network in model development for lactic acid production. The current measurement of lactic acid concentrations is conducted offline, resulting in time delay in obtaining the results, not to mention that current analysis method is expensive and in need of specially trained personnel. In view of this, two model of artificial neural network; multilayer perceptron (MLP) and radial basis function (RBF) network, have been employed. For the development of MLP model, normalization method, the size of input layer, size of hidden layer and activation function have been varied. Effects of input combinations on the MLP performance have also been investigated. For RBF model development, effects of the tolerance (MSE), radius (σ) value, the number of input variables and input combinations on the RBF performance have been investigated. The results show that the optimum structure of MLP has four input variables (biomass concentration, glucose concentration, temperature and reaction time) and a transfer function of log sigmoid in the hidden layer and linear in the output layer. This model is capable of producing the error index (EI) test of 7.26% and R-value test of 0.9909 with seven nodes in the hidden layer. Also, the RBF model was able to obtain EI test of 6.48% and R-value of 0.9926 with a model of three input variables (biomass concentration, glucose concentration and reaction time) and a radius (σ) equal to 1.5. The optimum structure of the RBF model was 3-7-1. Both models exhibit comparable and good generalization ability. However, the RBF model out-performed the MLP model with regard to its generalization ability and reproducibility but overall both models have displayed satisfying ability in estimation of lactic acid concentration for the identified process.
ABSTRAK

Penyelidikan ini mengkaji aplikasi rangkaian neural buatan untuk digunakan dalam pembangunan model pengeluaran asid laktik. Ketika ini, proses analisis pengiraan untuk mendapatkan kepekatan asid laktik selalunya dilakukan di luar talian dan ini menyebabkan masa yang banyak terbuang, serta kaedah analisis yang mahal dan memerlukan kakitangan yang terlatih untuk mengendalikan alatan itu. Maka dengan itu, dua model neural buatan, rangkaian peseptron berbilang-lapis (MLP) dan fungsi asas jejian (RBF); telah digunakan dalam pembangunan ini. Dalam pembangunan MLP, kaedah normalisasi yang berbeza, saiz lapisan input, saiz lapisan tersembunyi dan fungsi pengaktifan telah dikaji. Kesan kombinasi input berlainan ke atas prestasi model MLP juga dikaji. Bagi pembangunan model RBF, kesan nilai MSE, nilai radius (σ), bilangan input dan kombinasi input juga turut dikaji. Keputusan kajian menunjukkan model MLP yang optimum ialah model dengan struktur empat input (kepekatan biojisim, kepekatan glukosa, suhu dan masa reaksi) dan penggunaan fungsi pengaktifan log sigmoid dan linear pada lapisan tersembunyi dan lapisan output. Model ini berkebolehan untuk mencapai nilai indek ralat (EI) sebanyak 7.26% dan nilai-R sebanyak 0.9909 dengan tujuh neuron dalam lapisan tersembunyi. Di samping itu, model RBF yang mempunyai struktur tiga input (kepekatan biojisim, kepekatan glukosa dan masa reaksi) dan nilai radius (σ) bersamaan dengan 1.5 memungkinkan model itu untuk mencapai nilai indek ralat sebanyak 6.48% dan nilai-R sebanyak 0.9926. Struktur yang optimum untuk model RBF ialah 3-7-1. Oleh sebab itu, kajian mendapati kedua-dua model mempunyai keupayaan penyeluruhan yang bagus. Walau bagaimanapun, kajian juga mendapati model RBF lebih sesuai digunakan kerana keupayaaannya yang lebih baik dari model MLP dan juga dari segi kadar keupayaaannya yang tinggi untuk mendapatkan nilai anggaran kepekatan asid laktik untuk proses yang dikenal pasti.
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<td>$N_p$</td>
<td>number of pattern</td>
</tr>
<tr>
<td>$\hat{y}$</td>
<td>estimated value of lactic acid concentration</td>
</tr>
<tr>
<td>$\Delta w$</td>
<td>weight and bias update vector</td>
</tr>
<tr>
<td>$a_{kl}$</td>
<td>actual (calculated output) at the output neuron $l$ for the input $k$</td>
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<tr>
<td>AI</td>
<td>alginate</td>
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<td>ANN</td>
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<tr>
<td>ATP</td>
<td>adenosine triphosphate</td>
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<tr>
<td>$b$</td>
<td>bias</td>
</tr>
<tr>
<td>$B$</td>
<td>normalized biomass concentration</td>
</tr>
<tr>
<td>BP</td>
<td>back-propagation training algorithm</td>
</tr>
<tr>
<td>$C$</td>
<td>carbon</td>
</tr>
<tr>
<td>Ca</td>
<td>calcium</td>
</tr>
<tr>
<td>cfu/L</td>
<td>colony forming unit per liter</td>
</tr>
<tr>
<td>$c_i$</td>
<td>center of RBF</td>
</tr>
<tr>
<td>$C_p$</td>
<td>specific heat ($J$/mole°C)</td>
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<tr>
<td>$d_{kl}$</td>
<td>desired (target) output neuron $l$ for the input $k$</td>
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<td>$e$</td>
<td>residual between the estimated and observed value</td>
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<td>$e$</td>
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<td>error index</td>
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<td>FFNN</td>
<td>feedforward neural network</td>
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<td>g/L</td>
<td>gram per liter</td>
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<td>Gl</td>
<td>normalized glucose concentration</td>
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<td>$H$</td>
<td>hydrogen</td>
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<tr>
<td>HPLC</td>
<td>high performance liquid chromatography</td>
</tr>
<tr>
<td>$I$</td>
<td>identity matrix</td>
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<td>$J$</td>
<td>Jacobian matrix</td>
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\( K \) - temperature
\( L \) - liter
\( Lai \) - normalized lactic acid concentration
\( LM \) - Levenberg-Marquardt training algorithm
\( mL \) - milliliter
\( MLP \) - Multilayer Perceptron
\( mm \) - millimeter
\( MSE \) - mean square error
\( n \) - total number of neurons in the output layer of network
\( Na \) - sodium / natrium
\( n_{h} \) - number of hidden nodes of RBF
\( Np \) - total number of training patterns
\( O \) - oxygen
\( OD \) - optical density
\( OLS \) - Orthogonal Least Square training algorithm
\( PCA \) - principle component analysis
\( pH \) - pH value
\( PLS \) - Partial least square
\( RBF \) - Radial Basis Function
\( rpm \) - rotation per minute
\( RSM \) - response surface methodology
\( R\)-value - coefficient of determination for regression analysis
\( t \) - reaction time
\( w \) - weights and biases of the network
\( x \) - variable \( x \)
\( x_{\text{max}} \) - maximum value of variable \( x \)
\( x_{\text{min}} \) - minimum value of variable \( x \)
\( x_{\text{norm}} \) - normalized value of variable \( x \)
\( y \) - observed value of lactic acid concentration
Greek letters

$\sigma$ - radius or width parameter of RBF
$\mu$ - adaptive learning rate
$\beta_j$ - bias parameter for the $j$th output node of RBF
$\|*\|$ - Euclidean norm
$\phi_i$ - output of the $i$th hidden node of RBF
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INTRODUCTION

1.1 Background of Study

Production of lactic acid is conducted either by a chemical synthesis process or by carbohydrate fermentation. The chemical process is done commercially based on lactonitrile (Marques et al., 2008, Narayanan et al., 2004). The chemical synthesis is performed by the hydrolysis of lactonitrile by strong acids. Base-catalyzed degradation of sugars, oxidation of propylene glycol, reaction of acetaldehyde, carbon monoxide and water at elevated temperature and pressure, nitric acid oxidation of propylene and hydrolysis of chloropropionic acid are also alternative routes to the chemical synthesis of the lactic acid (Mussatto et al., 2008). Unfortunately, this process depends on by-products from other industries and it produces a mixture of L (+) and D (-) lactic acid isomers (Nandasana and Kumar, 2008, Pal et al., 2009).

The other route to produce lactic acid is through fermentation. Fermentation of lactic acid is a carbohydrate fermentation whereby sugar is converted by the microorganism known as lactic acid bacteria (LAB). The typical sugar used in the fermentation is glucose. The most common LAB used for lactic acid fermentation is
from *Lactobacillus* strains such as *Lactobacillus amylophilus*, *Lactobacillus bulgaricus*, *Lactobacillus delbreuckii*, *Lactobacillus leichmanii* and *Lactobacillus plantarum* and others from fungal strains such as *Aspergillus niger* and from *Rhizopus* species (Pal *et al*., 2009). Production of lactic acid from the carbohydrate fermentation is preferred because it is less expensive compared to the chemical synthesis. This process has the advantage of selectively producing either of the single lactic acid enantiomers.

Fermentation of lactic acid can be carried out either by free cell fermentation or by immobilization. Immobilization involves entrapping the lactic acid bacteria (LAB) in beads under mildly confined conditions. These LABs are separated from their environment by a protective matrix, film or bead ensuring the extension of shelf life and also preventing exposure to the surround environment, in other words, the beads provide protection coats for these LABs.

In fermentation of lactic acid, the desired variable is the lactic acid concentration that shows how efficient the fermentation is. The key parameters of the fermentation are the substrate concentration, pH (Wee *et al*., 2004; Ye *et al*., 1996; Altaf *et al*., 2006; Huang *et al*., 2005; Marták *et al*., 2003), temperature (Huang *et al*., 2005; Idris and Suzana 2006) and the biomass concentration.

Instead of undergoing tedious analytical method in measuring of lactic acid and biomass concentrations, which results in delay of information, there is a need for a model to estimate and predict the concentration of lactic acid and biomass. Software sensors make use of easily available process knowledge, including a secondary process variables or a process model, to estimate primary variables of interest (Chatterjee and Saraf, 2004; Araúzo-Bravo *et al*., 2004; Facco *et al*., 2009). Software sensors are typically developed or designed from mathematical models based on growth kinetics or statistical analysis [such as multi-linear regression (MLR) or principal component analysis (PCA)], a ‘black box’ neural networks or combinations of all of these (Kiviharju *et al*., 2008).
Software sensors work by cause and effect; hence the inherent biologic relation between measured and unmeasured states can significantly affect the predictive accuracy (Chen, 2006). Software sensors are also known as virtual sensors (Dai et al., 2006); which is a software that processes several measurements together (Gonzaga et al., 2009) by using the history of the available data (Kadlec et al., 2009). In the process, each variable, also known as a signal, is interacting with each other, producing the desired responses by the end of the process. These kinds of interactions are used for calculating or to estimate new quantities that cannot otherwise be measured (Gonzaga et al., 2009). Some attributes of software sensors are as follows (Fortuna et al., 2005):

1. Software sensors recommend a low cost alternative to expensive hardware sensors.
2. Software sensors are able to work in parallel with hardware sensors giving useful information for fault detection tasks.
3. The sensors can easily be implemented on existing hardware (e.g. microcontrollers) and can easily be returned when system parameters change.
4. The sensors overcome the time delays introduced by slow hardware sensors (e.g. gas chromatography), allowing real time of data estimation thus improving the performance of the control algorithms.

Software sensors have been used in many different processes. Gonzaga et al. (2008) constructed a software sensor to provide a reliable real time of polyethylene terephthalate (PET) viscosity to be used in controlling polymerization process. Lee et al. (2008) used soft sensors in wastewater treatment plants (WWTPs) to control variables in order to monitor the plants’ status and to support the operation of local wastewater systems.

In wine stills, software sensors are applied to estimate the distillate ethanol concentration on-line, thus enabling predefined ethanol profiles to be tracked
throughout a distillation run (Osorio et al., 2008). Many studies have been conducted regarding the applications of software sensor to enhance, improve, optimize, monitor, predict, classify, and control (Kadlec et al., 2009) certain process. Therefore, the use of software sensors is a reasonable approach in order to make good estimations and predictions of product concentration in lactic acid production. Accordingly, it is practical to build a software sensor that is applicable to different conditions of the fermentation including the unseen data. Furthermore, software sensors that are well trained are capable of giving estimations for unseen data as long as the variables have been covered during training phase.

1.2 Problem Statement

Fermentation is a nonlinear, complex process. The complexity of the process includes the interrelation between each of variables. This process is also known as nonlinear process. Thus, supervision of the fermentation process must maintain certain variables within strict limits, since biological systems are highly sensitive to abnormal changes in operation conditions (Araúzo-Bravo et al., 2004). Meanwhile, the analysis of the lactic acid concentration in the fermentation is conducted by using high pressure liquid chromatography (HPLC) (Hábová et al., 2004; Marták et al., 2003; Resa et al., 2007; Shibata et al., 2007; Gao et al., 2009; Ding and Tan, 2006). These analysis methods are time consuming, tedious, and the apparatus is expensive (Rivier, 2000).

Traditionally, the optimizations of biology processes are based on mathematical models described by a set of differential equations derived from mass balances. There are models of lactic acid fermentation based on the mathematical models (Nandasana and Kumar, 2008; Schepers et al., 2000), yet due to the physiological complexity of the microorganisms, these models lack robustness and accuracy due to the physiological complexity of the microorganisms (Gueguim-Kana
Fermentation processes are difficult and complex, hence mathematical models find it difficult to represent the interrelations in the process itself. Moreover, the mathematical models are built with such complexes that they produce difficulties in estimation.

Most of the biology processes involve a nonlinear activity and this is the limitation to the classical modeling technique to describe the evolution of microorganisms (Esnoz et al., 2006). Considering these problems, using the artificial intelligence approach in estimating lactic acid concentration seems reasonable, since this approach requires less time for development and it has the capability of simulating nonlinear processes. Thus, artificial intelligence tools such as neural networks provide a new and better approach (Gueguim-Kana et al., 2007).

Experimental work for lactic acid production using cheap substrates can be found widely in literature. However, the modeling process using artificial intelligence (AI) has not been extensively explored. Nandasana and Kumar (2008) had developed mathematical modeling for lactic acid production from cheap substrate. The model was developed for the fermentation of cane sugar molasses for lactic acid production by Enterococcus faecalis RKY1. The model takes into account the substrate limitation and inhibition, growth- and non-growth associated lactic acid production and cell death rate and highly dependent on pH value.

Schepers et al. (2000) have developed a simple descriptive neural network model for Lactobacillus helveticus growth in pH controlled batch cultures, but the developed model was lacking in robustness and generalization. Acuña et al. (1998) have also performed work on the modeling of lactic acid production. They have developed two models, static modeling and dynamic modeling, which estimate the cell concentration of lactic acid fermentation. Though it was found out that, this model is able to give good estimates, but it was specifically modeled to estimate the cell number of fermentation.
1.3 Objective

Lactic acid is one of the foremost raw materials that have applications in many end-products, especially in foods. Therefore, an easy and rapid method of measurement should be employed as a way of maneuvering a productive fermentation. The general aim of this study can therefore be phrased as the desire to develop data based models to estimate the lactic acid concentration in lactic acid production as one of the analytical method in fermentation.

The objectives of this research are as follows:

1. To develop software sensor model to predict the lactic acid concentration from available process measurements (glucose concentration, biomass concentration, initial pH, temperature and reaction time) using Artificial Neural Network.
2. To evaluate a suitable scaling or normalization method for the data under consideration.
3. To design an optimum structure or model of the Multilayer Perceptron (MLP) and Radial Basis Function (RBF).
4. To compare both Multilayer Perceptron and Radial Basis Function neural network models in terms of their predictive performances on lactic acid concentrations.

Although this study’s approach is similar to Acuña et al. (1998), the system employed is different. Acuña et al. (1998) studied the growth of Lactobacillus bacteria, while in this study; the focus is on the formation product by Lactobacillus delbrueckii in an immobilization system. The developed models are of a great importance due to its capability to predict lactic acid concentration under varying operating conditions.
1.4 Scope of Study

In order to achieve those objectives, simulation work was conducted based on the following limitations.

i. This study is limited to the fermentation of lactic acid with pineapple waste as the substrate. In this work, data were obtained from work done by Idris and Suzana (2006).

ii. In the first stage of software sensor development, all raw data used underwent pre-processing. Three different normalization methods were used in order to scale the data to the same units and range.

iii. Multilayer Perceptron (MLP) models were developed under varying conditions. The learning algorithm used in this study was Levenberg Marquardt (LM) training algorithm. The MLP structures were optimized in regards to the performance goal, input number, input variables, the size of hidden nodes and the combinations of transfer function.

iv. Then, Radial Basis Function (RBF) based models were developed and optimized. RBF model was considered because of its performance, which is fast and has linear learning. The input layers were varied in terms of input numbers and the combination of variables used in input layer. Other features being varied were the radius and MSE value.

v. The predictive performances of each model were evaluated based on mean square error (MSE), error index (EI), regression analysis, graphical plot and residual plot.

vi. Finally, the performances of the best predictive ability between MLP and RBF structures were compared, and the one that had the better generalization and predictive ability was employed as the software sensor in the lactic acid production.
1.5 Thesis Outline

The outline of the thesis is arranged as follows. The literature review is presented in the Chapter 2 and it includes the review of lactic acid production and software sensors. This chapter also includes reviews on current applications of Multilayer Perceptron and Radial Basis Function, and the chapter ends by discussing the factors that affect the performances of a neural network models.

In Chapter 3, an explanation and overview of the fermentation process is presented extensively. This is followed by step-by-step development of the artificial neural network model covering both of MLP and RBF. The chapter gives a detailed, stage-by-stage description of each model development, including data normalization, input variables selection, training and testing.

The findings of the MLP and RBF model are discussed in Chapter 4. The effects of the normalization method, input number on MLP and RBF performances are presented. In this chapter, the effects of the normalization method, hidden nodes, model structure size and transfer function of MLP performances are discussed. Meanwhile for RBF, findings of the effects of tolerance goal (MSE), radius and goal value are also included in this chapter. These two models are compared at the end of the chapter. Lastly, in Chapter 5, general conclusions are drawn from this research and some recommendations for future work are suggested.
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