MODELING OF BIOPOLYMERIZATION PROCESS USING FIRST PRINCIPLE MODEL AND BOOTSTRAP RE-SAMPLING NEURAL NETWORK

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“In the name of Allah, The Most Gracious, The Most Merciful”

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LIST OF ABBREVIATIONS

ε-CL	Epsilon Caprolactone
ACS	American Chemical Society
ANN	Arficial neural network
ANN-SS	Artificial neural network-soft sensor
ANOVA	Analysis of variance
ART	Adaptive resonance theory
BAGNET	Bootstrap aggregated network
BP	Backpropagation
CAL-B	Candida antarctica Lipase B
CSTR	Continuous stirred tank reactor
EKF	Extended Kalman filter
FDA	Foods and Drugs Administration
FFN	Feed forward network
FID	Free inductive detector
GC	Gas chromatograph
GPC	Gel permeation chromatograph
HNN	Hybrid neural network
HNNRF	Hybrid neural network rate function
HPLC	High performance liquid chromatograph
IRN	Internal recurrent network
LM	Levenberg-Marquardt
MISO	Multiple input single ouput
MLP	Multi-layer perceptron
MLR	Multiple linear regression

MLRN	Multi-layer recurrent network
MMA	Methyl methacrylate
MPC	Model predictive control
MW	Monomer molecular weight
NMAX	Nonlinear moving average with exogenous inputs
NMAX-MLRN	Nonlinear moving average with exogenous inputs multi-layer recurrent network
NMAX-RTRL	Nonlinear moving average with exogenous inputs real time real learning
NNMPC	Neural network model predictive control
NNRF	Neural network rate function
PCL	Polycaprolactone
PCR	Principal component regression
PDF	Probability density function
PI	Proportional-Integral
PID	Proportional-Integral-Derivative
PRMS	Pseudo random multi-state signal
R	Correlation coefficient
RMSE	Root mean squared error
RNN	Recurrent neural network
ROP	Ring-opening polymerization
RTRL	Real time real learning
SISO	Single input single output
SPUD	Sequential pseudo-uniform design
SSE	Sum squared error

THF	Tetrahydrofuran
USEPA	United States Environmental Protection Agency
VA	Vinyl acetate
VLE	Vapor-liquid equilibrium
VLSI	Very large scale integration

LIST OF SYMBOLS

		Unit
σ	Transfer function	-
α	Significance level	-
E	Energy function	-
N	Total number of nodes	-
ΔG	Free energy	Joule
[S]	Substrate concentration	mol/cm^3
[P]	Product/biopolymer concentration	mol/cm^3
[E]	Enzyme concentration	mol/cm^3
[ES]	Enzyme-substrate complex	-
[M]	Monomer concentration	mol/cm^3
[EM]	Enzyme-monomer complex	-
[HA]	ω-hydroxy carboxylic acid	mol/cm^3
$[E]_T$	Total enzyme concentration	mol/cm^3
$[P]_{eq}$	Equilibrium product concentration	mol/cm^3
$[S]_{eq}$	Equilibrium substrate concentration	mol/cm^3
$[M]_o$	Initial monomer concentration	mol/cm^3
h_j	Hidden layer output	-
H_{0A}	Null hypothesis for all samples from factor A	-
H_{0B}	Null hypothesis for all samples from factor B	-
k_i	Rate constant of particular pathway	mol/s, s^{-1}
$k_1,\ldots, k_3$	Forward rate constant	mol/s, s^{-1}
$k_{-1},\ldots, k_{-3}$	Reverse rate constant	mol/s,s^{-1}

K_{eq}	Equilibrium rate constant	-
K_m	Michaelis-Menten constant	mol/cm^3
K_{mM}	Monomer Michealis-Menten constant	mol/cm^3
K_{mP}	Polymer Michaelis-Menten constant	mol/cm^3
k_p	Rate constant for the breakdown of ES to E + P	mol/s, s^{-1}
M_n	Number-average molecular weight	g/mol
M_w	Weight-average molecular weight	g/mol
u_j	Hidden layer weighted sum	-
v	Velocity	min^{-1}
v_j	Output layer weighted sum	-
V_r	Reverse velocity	min^{-1}
V_f	Forward velocity	min^{-1}
V_{max}	Maximum velocity	min^{-1}
V_{maxf}	Maximum forward velocity	min^{-1}
w_{ji}	Hidden layer weight	-
w_{kj}	Output layer weight	-
y_k	Output layer output	-
$(x_1,\ldots,x_p)$	Vector of predictor variable value	-
$\frac{d[S]}{dt}\Big/\frac{d[M]}{dt}$	Rate of substrate/monomer concentration over time	-
$\frac{d[ES]}{dt}\Big/\frac{d[EM]}{dt}$	Rate of enzyme-substrate concentration over time	-
$\frac{d[HA]}{dt}$	Rate of concentration over time	-
$\frac{d[P]}{dt}$	Rate of polymer/product concentration over time	-

LIST OF SCHEMES

PERMODELAN PROSES BIOPOLIMERISASI MENGGUNAKAN MODEL PRINSIP PERTAMA DAN JARINGAN NEURAL PERSAMPELAN SEMULA IKAT BUT

ABSTRAK

Kemunculan isu alam sekitar seperti kesan rumah hijau dan pemanasan global telah mencetuskan idea bagi para pengkaji dan saintis untuk mencipta bahan baru yang mampu menangani isu alam sekitar dan sekaligus memenuhi kehendak manusia iaitu biopolimer. Kualiti biopolimer adalah dinilai melalui berat molekulnya. Sehingga kini tiada pengukuran atas talian bagi berat molekul polimer. Oleh itu, kajian ini membangunkan model untuk menyerupai proses sebenar dengan menggunakan kaedah permodelan seperti jaringan neural. Model prinsip pertama juga telah menjadi antara kaedah paling digunakan untuk membangunkan model selain dari menggunakan kaedah permodelan seperti jaringan neural. Jadi, jaringan neural dan model prinsip pertama telah digunakan dalam untuk membangunkan model process biopolimerirasi dan keputusan bagi kedua-dua model ini dibandingkan. Bagi membangunkan model-model ini, eksperimen dijalankan untuk mendapatkan data untuk kedua-dua model. Data bagi model jaringan neural adalah berat molekul biopolimer manakala data bagi model prinsip pertama adalah data kinetik. Kedua-dua model menggunakan pendekatan berlainan iaitu pendekatan secara teori dan empirikal. Kedua-dua model juga memberikan keputusan yang baik dari segi nombor berat molekul mahupun trendnya. Berdasarkan keputusan dari kedua-dua model, model jaringan neural memberikan keputusan terbaik dengan ralat jumlah kuasa dua sebanyak 0.9996 dan pekali kolerasi sebanyak 0.9999. Model prinsip pertama pula dinilai berdasarkan analisis varian (ANOVA). Dalam kajian ini, ANOVA mengambil aras kepentingan, α sebagai 0.01. Oleh itu, keputusan yang memberi nilai kurang dari 0.01 menunjukkan bahawa ianya berbeza dari satu sama lain. Ini adalah situasi yang tidak dikehendaki kerana keputusan yang baik adalah yang memberi keputusan yang hampir kepada berat molekul sebenar dari eksperimen. Berdasarkan keputusan ANOVA, semua keputusan adalah lebih dari 0.01. Ini bermakna keputusan dari model prinsip pertama adalah hampir sama dengan keputusan dari eksperimen. Berdasarkan keputusan yang diberi oleh kedua-dua model telah membuktikan bahawa kedua-dua model adalah kaedah yang tepat dalam membangunkan model bagi meramal berat molekul biopolimer. Kaedah jaringan neural bagaimanapun telah memberi keputusan yang lebih baik berbanding model prinsip pertama.

MODELING OF BIOPOLYMERIZATION PROCESS USING FIRST PRINCIPLE MODEL AND BOOTSTRAP RE-SAMPLING NEURAL NETWORK

ABSTRACT

The emergence of the environmental issues such as green house and global warming have triggered scientists and researchers to create new materials that can cope both environmental and humanity needs i.e. biopolymer. Biopolymer quality assesses by its molecular weight. Apparently, there is no online measurement for molecular weight measurement. Therefore, in this study models are developed to mimic the real process using a reliable modeling tool such as neural networks. First principle model also become one of the most applied methods to model a process other than using a modeling tool such as neural network. Therefore in this research, neural network and first principle model have been chosen to model the biopolymerization process and followed by the comparison between the aforementioned models. In order to develop the models, experimental work is conducted to obtain data for first principle model and neural network model. The data for the neural network model are the molecular weight of the biopolymer whereas the data for the first principle model are the kinetics data. Both models delivered predicted molecular weight of biopolymer using different approaches i.e. fundamental and empirical model. Both models delivered convincing results in terms of molecular weight number as well as molecular weight trend. Based on the results from both models, neural network model gives closest prediction with sum squared error (SSE) is 0.9996 and correlation coefficient, *R* value is 0.9999. First principle model results on the hand assessed based on Analysis

of Variance (ANOVA). In this work, ANOVA takes the significant level, α as 0.01. Hence, the results that give the value that is less that 0.01, is showing that the compared data are significantly different from each other which is undesirable as the actual and predicted data should be projected similar trend and number. According to the ANOVA for first principle model, all the results are more than 0.01 which mean that the actual and predicted molecular weights are similar. These results have proved that both neural network and first principle model are reliable tools in prediction of molecular weight of biopolymer which neural network model appeared to be the more precise model in terms of biopolymer molecular weight prediction.

CHAPTER ONE

INTRODUCTION

1.0 Research Background

The world now has loudly spoken about ‘going green’. One of the ways to support this manifesto is to utilize biodegradable materials such as biopolymer. One of the methods to achieve this is by ring opening polymerization process of lactones to polyester (polycaprolactone) catalyzed by enzyme (lipase) (Kumar and Gross, 2000). Despite of this ambitious goal, the intricacy of polymerization and the difficult-to-measure variable such as molecular weight have become obstacle us to achieve an optimum condition of the process and also to produce the desired product without much waste to be thrown away. Beside the difficulties in measuring and analyzing the molecular weight of the biopolymer, the biopolymerization process itself exhibits a very non-linear behavior. Modeling and control of non-linear process is an uneasy task and requires a powerful and reliable tool to tackle the process. Thus, artificial intelligent application using neural network model can be said as the solution of this puzzle (Zhang, 1999; Zhang et al., 2006).

Through a lab-scale reactor with adequate instrumentation, the desired biopolymerization process can be done and the data retrieved from the experiment is then used to model the process using neural network. The developed model can be used to predict the output (molecular weight) of biopolymerization process of lactones to polyester using lipase as catalyst which can possibly heal our biggest ‘headache’ for analyzing the polymer in order to obtain its molecular weight. The good news is that there are many researchers have employed polymerization processes in their researches and many of them have somehow tried to model the process in order to mimic chemically catalyzed polymerization process using either first principle model or empirical model. Even though this work is focusing on biopolymerization process, it seems that the success of previous works on modeling chemically catalyzed polymerization process have become proofs that a nonlinear polymerization process can be modeled using the aforementioned approaches and have also exhibited convincing results. Such circumstances have shed some light on this particular process and became a sign that biopolymerization process also can be modeled using either first principle model or empirical model. All the succeeded works can be discovered in Chapter 2.

Since half a century ago, researchers have discovered the ultimate tool and the so-called artificial intelligence to render a new method in order to cope with processes that require precision and accuracy especially when dealing with a nonlinear process that unfortunately cannot properly be interpreted mechanistically. Since the discovery of the tool, researchers have realized that the 'control targets' should be able to achieve by using this tool. Neural network has been shown to be able to approximate any continuous non-linear functions and it has been used to build data base empirical models for non-linear processes (Hertz, 1991).

Neural network or artificial neural network is said to mimic the human brain in solving problems. According to Haykin (Haykin, 1994), a neural network is a massive parallel-distributed processor that has a natural capability for storing experiential knowledge and making it available for use in the future system. It resembles the brain in two respects; firstly, the knowledge is acquired by the networks through a learning process and secondly, the interneuron connection strengths known as synaptic weights are used to store the acquired knowledge.

Based on the above observation, neural networks can be said as a remedy to cope with intricate processes. One of the main advantages of neural network- based process models is that they are easy to build (Zhang et al., 2006; Zhang, 2008). This feature is particularly useful when modeling complicated processes where detailed mechanistic models are difficult to develop. Nonetheless, many researches on neural networks are mainly focus on feed forward neural networks. This is due the fact that it is the simplest neural network architecture yet reliable to be applied in various applications and processes (Zhang et. al, 1999). Therefore, this work has set to focus more on feed forward neural network. It is just a matter of modification of the neural network architecture such as single, multiple networks, hybrid, etc. that determine the performance of the network in each applications. Other neural network architectures such as recurrent network has received quite a tremendous consent amongst researchers, however, feed forward neural network is still the most implemented neural network architecture to date (Gonzaga et al., 2009; Zhang, 2008; Gomm et al., 1993).

However, a critical shortcoming of all neural networks is that they often lack robustness, unless a proper network training and validation procedure is used (Zhang et al., 1999, Zhang, 2009). Robustness of the model can be defined as one of the baselines to judge the performance of neural network models and it is really related to the learning or training classes as what Bishop (Bishop, 1995) described in his work. The importance of neural networks in this context is that they offer very powerful and general framework to represent non-linear mappings from several input variables to several output variables, where the form of the mapping is governed by a number of adjustable parameters (Gomm et al., 1993).

Many factors can contribute to the success of the neural network implementations (Hinton, 1992; Haykin, 1994). In particular, neural network is non-linear models, which are very useful in modeling nonlinear systems that cannot be successfully modeled by linear models. The second factor is that neural network is easy to use and develop and they basically learn by examples (Zhang et al., 2006; Zhang et al., 2008). The neural network users gather representative data, and then invoke a training algorithm to automatically learn the structure of the data (English, 1996; Chen et al., 1999).

Because of the tremendous capability of neural networks, currently there are a lot of applications of neural network in industry and business and they are applied in pattern recognition such as automated recognition of hand-written text, finger print identification and moving target on a static background (Seong-Wan, 1999; Chen et al., 1997). Neural networks have also been used in speech production where a neural network model is connected to a speech synthesizer (Baig et al., 1999; Furlanello et al., 1999).

Real time control is also a major application of neural networks with neural network models having been applied in the monitoring and control of complex plants such as chemical plants (Zhang et al., 1998a; Jazayeri-Rad, 2004). Neural network has been employed in business where neural network model have played a role in predicting the stock market trend in certain period of time (Fletcher and Goss, 1993; Desai and Bharati; 1998). Another area of applications of neural network models is in signal processing and other typical applications such as noise suppression, filtering and digital signal processing technology (Larsson et al., 1996). These broad applications of neural networks can be a substantiation of the superiority of neural network. Despite of their advantages, researchers have continuously attempted to improve neural network to better suit many complex processes.

In order to improve the robustness of neural networks a number of techniques have been developed lately like regularization (Girosi et al., 1995) and the early stopping method (Morgan and Bourlard, 1990). Ohbayashi and co-workers (Ohbayashi et al., 1998) implemented the universal learning rule and second order derivatives to increase the robustness in neural network models. Robustness is enhanced by minimizing the change in the values of criterion function caused by the small changes around the nominal values of system parameters. Lack of the robustness in individual neural networks is basically due to the overfitting of the models (Caruana et al., 2000).

Overfitting basically refers to the poor generalization of the networks due to fitting the noise in the data (Mc Loone and Irwin, 2001). Furthermore, the trained network might not minimize the error on the training data set because it has uncontrolled excess dynamics capability or because the training data itself is corrupted with noise. The representation capability of a neural network is determined by its size (number of neurons). If networks are too large, they can find many solutions which exactly fit the training set data but without the presence of the frequency dynamics in the underlying function. When the data is corrupted with noise, a second form of overfitting occurs and will result in the networks fitting the noise (McLoone and Irwin, 2001).

In order to inhibit all the drawbacks that are mentioned earlier, a modified neural network that offers better presentation of a model can be developed based on available method such as bootstrap re-sampling method. Sometimes, a complicated process may experience problem such as insufficient data. Therefore, bootstrap re-sampling has been identified to as a method to overcome this problem by re-sample original data to produce additional data without interfere with the integrity of the data. Basically, data re-sampling is the act of rearranging the original data to form new sets of data. It is better known as the bootstrap re-sampling method. Further discussion about neural networks can be found in Chapter 2.

Figure 1.1 is a pictograph in the form of flowchart can be a simplified way to convey the whole idea behind this work.

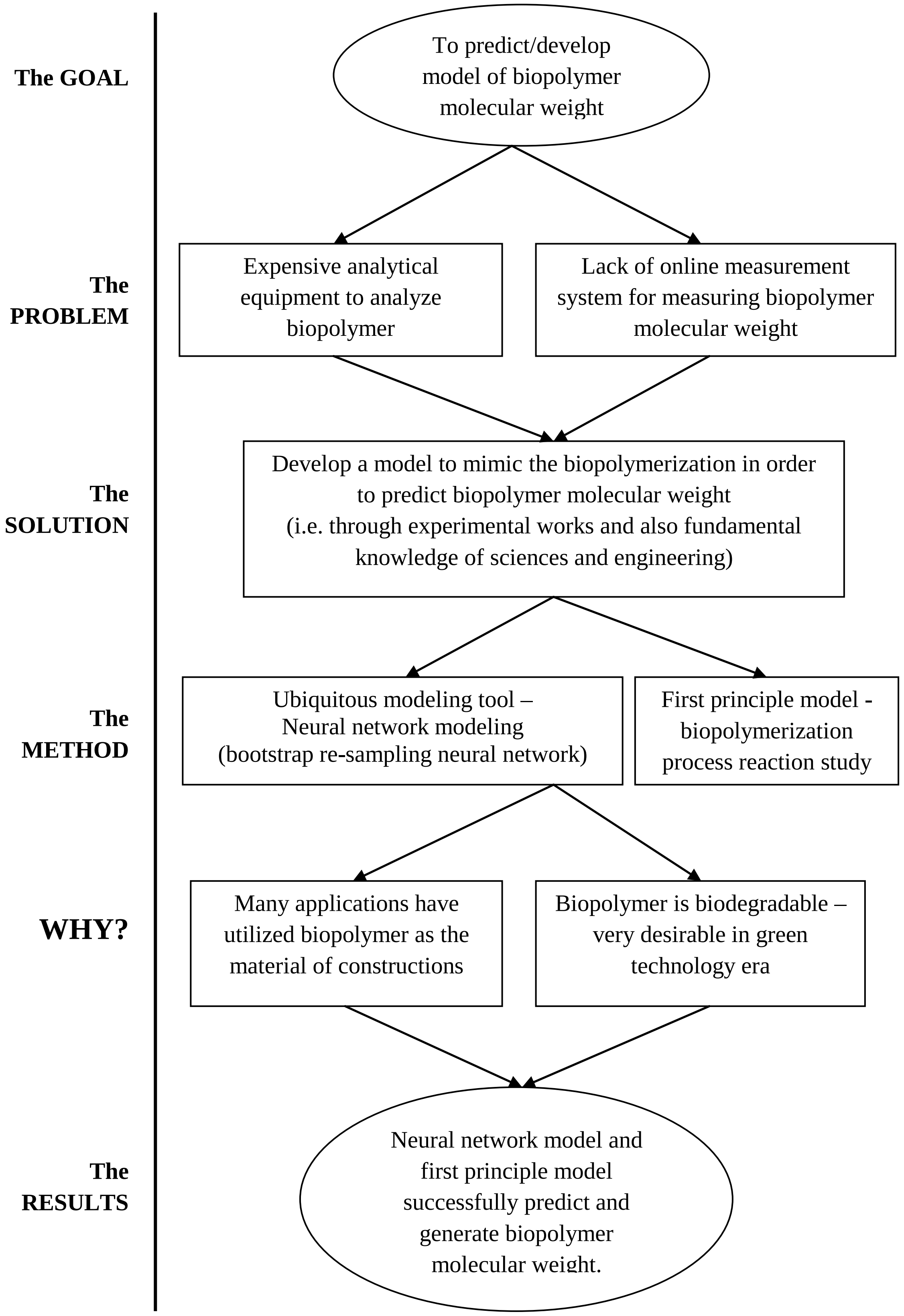

The GOAL
To predict/develop model of biopolymer molecular weight
The PROBLEM
Expensive analytical equipment to analyze biopolymer
Lack of online measurement system for measuring biopolymer molecular weight
The SOLUTION
Develop a model to mimic the biopolymerization in order to predict biopolymer molecular weight (i.e. through experimental works and also fundamental knowledge of sciences and engineering)
The METHOD
Ubiquitous modeling tool – Neural network modeling (bootstrap re-sampling neural network)
First principle model - biopolymerization process reaction study
WHY?
Many applications have utilized biopolymer as the material of constructions
Biopolymer is biodegradable – very desirable in green technology era
The RESULTS
Neural network model and first principle model successfully predict and generate biopolymer molecular weight.

Figure 1.1: A Simplified Flowchart of the Whole Research Work

1.1 Problem Statement

Polymerization process which always classified as a complex process and also lack of instrumentation which can deliver a fast and accurate measurement of polymer molecular weight have become the motivation to start this research. Demanding and fast-growing polymer industries have sent this conventional measurement scheme over the edge. A truly reliable and trustworthy system for coping with the intricacy of the polymerization process meanwhile still can guarantee the highest process safety, the ultimate product quality and also maximum profit is indeed being a highlight in recent research phenomena. When putting reliability, simplicity and intricacy as the desirable criteria of the model, neural networks have emerged as primary choice to bring such criteria into reality.

Moreover, complicated process such as biopolymerization that requires a long reaction time has resulted to the problem such as insufficient data from the real process. Such a problem can lead to undesired conditions in neural network modeling such as underfitting. Besides, measurement for polymer molecular weight also has caused such a problem where online measurement for polymer molecular weight is impossible. Most biopolymers are assessed by offline analyzer such as Gel Permeation Chromatograph (GPC) for their molecular weight. Thus, a tool that can solve both problems in a model has to be created in order to be able to mimic the real biopolymerization process. Neural network model has been found to be the most eligible tool to tackle these problems. With latest computer technology, the model can be implemented easily. Moreover, neural network also comes with several improved methods such as bootstrap re-sampling method that can be applied to generate additional data for training and testing processes.

Therefore, artificial intelligence (i.e. neural network) has been identified to be able to tackle both problems with the ability to mimic real process as well as the ability to generalize model even with insufficient data for training and testing processes. Apart from merely applied neural network in modeling biopolymerization process, another method that can be utilized is by using knowledge-based model or first principle model. The method is developed purely based on the biopolymerization process reaction and its kinetics. Both models – neural network model (empirical model) and first principle model are applied in this work and comparison is made to evaluate the performance of both models.

1.2 Research Objectives

The primary objective of this research is to develop a model for the nonlinear biopolymerization process of lactones to polyester using bootstrap neural network model and also mechanistic model of the process. Nevertheless, the elaborated objectives are as follows:

1) To fabricate a batch/fed-batch biopolymerization reactor with a necessary instrumentations.

2) To develop the process model of the proposed biopolymerization process using bootstrap re-sampling neural network model in MATLAB™ environment (empirical model).

3) To develop the process model of the proposed biopolymerization using first principle model .

4) To validate the bootstrap re-sampling neural network model and first principle model with the experimental output and to analyze the results from experiment, bootstrap re-sampling neural network model and also first principle model.

1.3 Organization of Thesis

In general, this thesis comprises of five main chapters. Each chapter is detail out by the following paragraphs.

Chapter 1 gives an introduction of the research, the current problems regarding biopolymerization process and the possible solution to these predicaments. This chapter also briefly explains what is neural network, some applications of neural network, what is the role of neural network in solving and unweaving the nonlinearity of biopolymerization process through neural network modeling.

Chapter 2 discusses and reviews extensively about neural network and its applications in polymerization processes. Biopolymerization of lactones to polyester is also scrutinized in a matter of ring-opening polymerization process and its reaction elements, such as monomer and enzyme. Application of biopolymer is also listed as one of the sections in this chapter.

Chapter 3 presents the methods of experiments and analysis. This chapter consists of two main parts. The first part would present the method of experiments which is the biopolymerization reaction process from ε-caprolactone to polycaprolactone for both reactor and flask level. The second part covers the methods of analysis which include the biopolymer molecular weight analysis using Gel Permeation

Chromatograph (GPC) and residual monomer analysis using Gas Chromatograph (GC).

Chapter 4 discusses the methods of developing bootstrap re-sampling neural network model and first principle model. The bootstrap re-sampling neural network model employs feedforward neural network with re-sampled data using bootstrap method. First principle model is developed based on biopolymerization reaction mechanism. These models are used to predict the biopolymer molecular weight which is compared to the actual biopolymer molecular weight.

Chapter 5 covers the results and discussion obtained from bootstrap re-sampling neural network model and first principle model as well as experimental works. Comparison of these results between neural network model and first principle model can also be found in this chapter. Analysis of the results for both models are also presented in this chapter based on SSE, *R* and ANOVA.

Chapter 6 states the conclusions from this work and also future hopes and expectations.

CHAPTER TWO

LITERATURE REVIEW

2.0 Introduction

Interest in artificial neural networks began in the early 1940s when pioneers, such as McCulloch et al. (1943), investigated neural networks based on the neuron and attempted to formulate the adaptation laws which applied to such systems. During 1950s and 1960s, several basic architectures were developed and a background body of knowledge was built up from many diverse disciplines: biology, psychology, physiology, mathematics and engineering. General interest in the subject waned after the analysis of the perceptron by Minsky and Papert in the early 1970s highlighted the limitations of several of the models. However, several groups did continue and by the mid 1980s the work of Hopfield and of Rumerhalt gave a renewed impetus to the area (Gomm et al., 1993).

The study of neural networks is an attempt to understand the functionality of the brain. In particular, it is of interest to define an alternative artificial computational form to mimic the brain's operation in one or a number of ways. Essentially, artificial neural networks is a 'bottom up' approach to artificial intelligence in that a network of processing elements is designed, these elements being based on the physiology and individual processing elements of the human brains. Neural networks have several important characteristics which are of interest to control engineers:

1) Modeling: Because of their ability to get trained using data records for the particular system of interest, the major problem of developing a realistic system model is obviated.

2) Nonlinear systems: The networks possess the ability to learn nonlinear relationships with limited prior knowledge about the process structure. This is possibly the area in which they show the greatest promise.

3) Multivariable systems: Neural networks, by their very nature have many inputs and many outputs and so can be readily applied to multivariable systems.

4) Parallel structure: The structure of neural networks is highly parallel in nature. This is likely to give rise to three benefits, very fast parallel processing, fault tolerance and robustness.

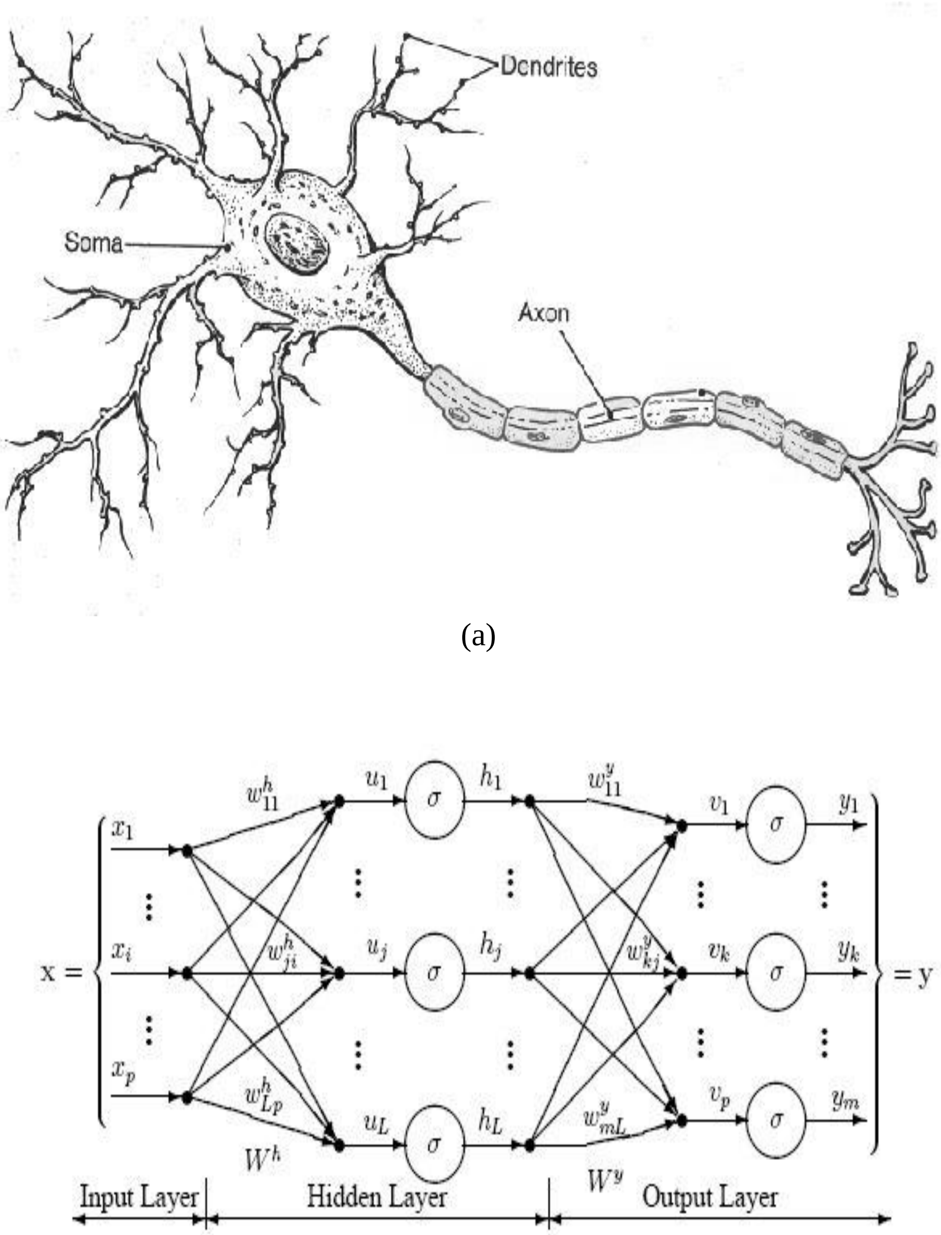
The great promise held out by these unique features is the main reasons for the enormous interest which is currently being shown in this field. The next paragraph is intended to provide a general knowledge about neural networks. Concepts of neural networks are introduced with background of biological aspects and their attributes are described. Artificial neural networks have emerged from studies of how human and animal brains perform operations. The human brain is made up of millions of individual processing elements, called neurons that are interconnect (Gomm et al., 1993).

Information from the outputs of other neurons in the form of electrical pulses is received by cells at connections called synapses. The synapses connect to the cell inputs, known as dendrites and the single output of the neuron appears at the axon. An electrical pulse is sent down to the axon when the total input stimuli from all of the dendrites exceed a certain threshold. Artificial neural network (ANN) on the other hand are made up of individual models of the artificial neurons that are connected together to form a network. Information is stored in the network often in the form of different connection strengths or weights associated with the synapses in ANN.

In other words, ANN is a simplified version of biological neuron. Biological-artificial neuron analogy can be shown as in Table 2.1 below. Figure 2.1 gives a pictorial representation of this biological-artificial terminology.

Table 2.1: Biological-Artificial Neuron Analogy (Statsoft Electronics Statistical Textbook, 2010)

Biological Neurons	**Artificial Neural Networks**
Soma	Neuron
Dendrite	Input
Axon	Output
Synapse	Weight



(a)

(b)

Figure 2.1: (a) Biological Neuron; (b) Artificial Neural Network Representation (Statsoft Electronics Statistical Textbook, 2010)

Therefore, neural network becomes one of the artificial intelligence techniques. It is very similar to biological neurons in so many levels. Besides similarities with biological neurons, neural network comprises of three common layers:

1) Input layer: A vector of predictor variable values ($x_1 ... x_p$) is presented to the input layer. The input layer (or processing before the input layer) standardizes these values so that the range of each variable is -1 to 1. The input layer distributes the values to each of the neurons in the hidden layer. In addition to the predictor variables, there is a constant input of 1.0, called the *bias* that is fed to each of the hidden layers; the bias is multiplied by a weight and added to the sum going into the neuron.

2) Hidden layer: Arriving at a neuron in the hidden layer, the value from each input neuron is multiplied by a weight (w_{ji}), and the resulting weighted values are added together producing a combined value u_j. The weighted sum (u_j) is fed into a transfer function, σ, which outputs a value h_j. The outputs from the hidden layer are distributed to the output layer.

3) Output layer: Arriving at a neuron in the output layer, the value from each hidden layer neuron is multiplied by a weight (w_{kj}), and the resulting weighted values are added together producing a combined value v_j. The weighted sum (v_j) is fed into a transfer function, σ, which outputs a value y_k. The *y* values are the outputs of the network.

To simplify the previous section, the next paragraph should be a decent explanation to conclude the aforementioned neural network components. The most commonly used neuron model is depicted in Figure 2.2 and is based on the model proposed by McCulloch and Pitts in 1943 (McCulloch and Pitts, 1943). Each neuron input, $x_1 – x_N$, is weighted by the values $w_1 – w_N$. A bias, or offset in the node is characterized by an additional constant input of 1 weighted by the value w_o. The output, *y*, is obtained by summing the weighted inputs to the neuron and passing the results through a nonlinear activation function, *f ( )*. Various types of nonlinearity are possible and some of these are hard limiter, threshold logic, tanh and sigmoidal functions. The general equation can be seen as the following:

$$y = f\left(\sum_{i=1}^{N} w_i x_i + w_o\right) \tag{2.1}$$

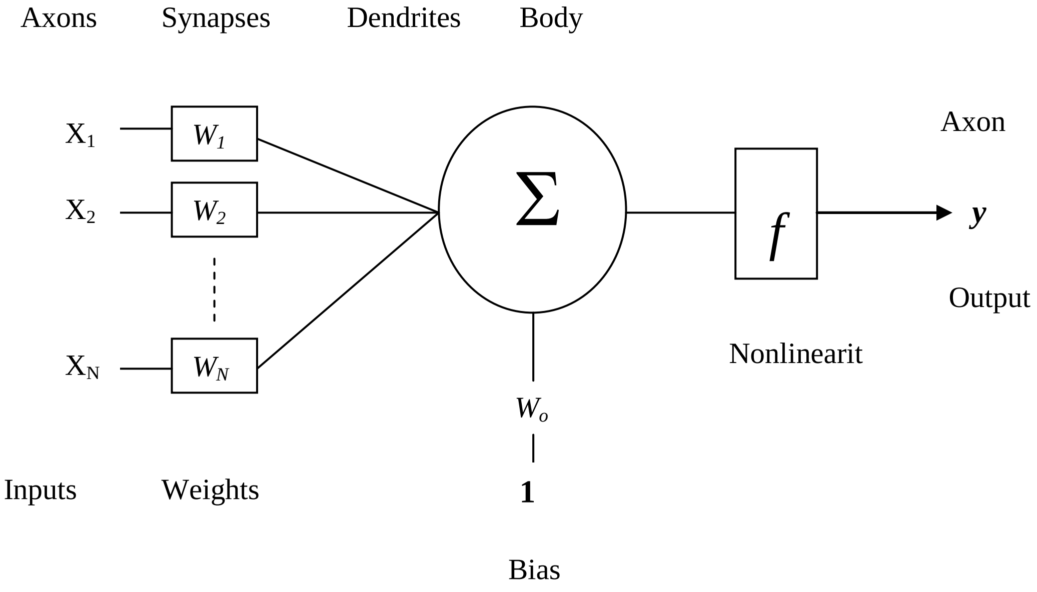


Figure 2.2: Biological Neuron Elements-Artificial Neural Network Elements (Warwick, 1995)

Among the numerous attributes of neural networks that have been found in many application areas are (Warwick, 1995):

1) Inherent parallelism in the network architecture due to the repeated use of simple neuron processing elements. This leads to the possibility of very fast hardware implementations of neural networks.

2) Capability of learning information by example. The learning mechanism is often achieved by appropriate adjustment of the weights in the synapses of neural networks.

3) Ability to generalize to new inputs (i.e. trained ANN is capable of providing ‘sensible’ outputs when presented with input data that has not been used before).

4) Robustness to noisy data that occurs in real world applications.

5) Fault tolerance. In general, ANN performance does not significantly degenerate if some of the network connections become faulty.

The above attributes of neural networks indicate their potential in solving many problems. Hence, the considerable interest in neural networks that has occurred in recent years is not only due to significant advances in computer processing power that has enabled their implementation but because of the diverse possibility of application areas. Many different types of neural network architectures are available for modeling and also control purposes. The next section is over viewing on types of neural networks.

2.1 Types Of Neural Network

Nowadays, many types of neural network architectures are available to be implemented. Amongst them are Hopfield, Kohonen, Radial Basis Function and the most common network is Feedforward artificial neural network (FANN). A Hopfield network is a type of recurrent network which was invented by John Hopfield. The Hopfield network comprises of two layers, an input layer and a Hopfield layer. Each node in the input layer is directly connected to only one node in the Hopfield layer. The nodes in the latter layer are neuron models previously described with either hard limiter or sigmoidal activation functions. Binary input signals are introduced such that each of the network node elements has an output which acquires one or two possible states, either +1 or -1.

Operation of the Hopfield network is as follows. During training, the network output is often required to be the same as the input. Connection strengths are weakened by reducing the corresponding weight values if the output of a neuron is different from the input, and strengthened when the converse is true. The trained network is used by applying an input pattern to the network. The network outputs are then continually fed back through the weights until a convergence criterion is met, typically when there are no changes at the network output nodes on successive iterations.

The weights are adjusted to arrive at a local minimum of a defined global energy function. The energy function is given by,

$$E = -\frac{1}{2}\sum_{ij=1}^{N} b_{ij} S_i S_j \tag{2.2}$$

where E is the energy function, N is the total number of nodes, S_i and S_j are the output values either +1 or -1, of the ith and jth node elements and b_{ij} is the weighting applied to the link from the jth node output to the ith node input. The applications of Hopfiled networks include modeling and control of dynamical systems (Warwick, 1995).

A Kohonen network is constructed of a fully interconnected array of neurons that is the output of each neuron is an input to all neurons including itself and each neuron receives the input pattern. The distinguishing feature of this network from other networks is that no output data is required for training. It has been developed by Teuvo Kohonen (1989, 1995). There are two sets of weights; 1) an adaptable set, to compute the weighted sum of the external inputs, 2) fixed set between neurons that controls neuron interactions in the network.

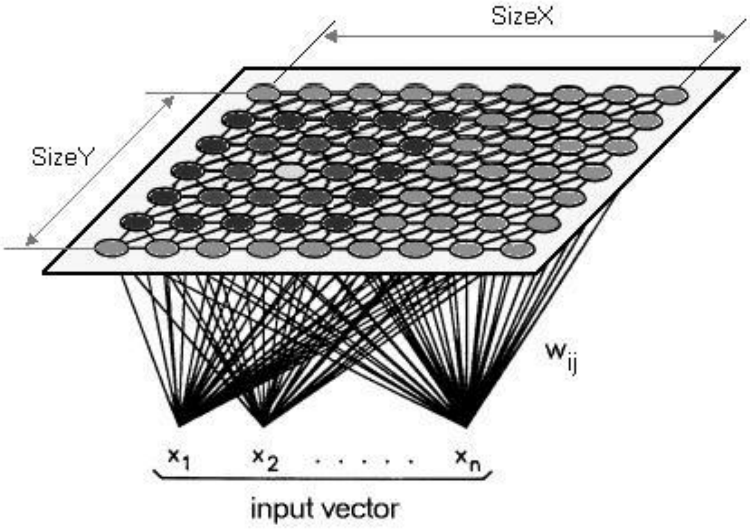


Figure 2.3: A Simplified Kohonen Network (Heaton Research, 2010)

Kohonen network defines a mapping from the input data space spanned by $x_1..x_n$ onto a one- or two-dimensional array of nodes. The mapping is performed in a way that the topological relationships in the n-dimensional input space are maintained when mapped to the Kohonen network. In addition, the local density of data is also reflected by the map: areas of the input data space which are represented by more data are mapped to a larger area of the network.

Each node of the map is defined by a vector w_{ij} whose elements are adjusted during the training. The basic training algorithm is quite simple; 1) select an object from the training set, 2) find the node which is closest to the selected data (i.e. the distance between w_{ij} and the training data is a minimum), 3) adjust the weight vectors of the closest node and the nodes around it in a way that the w_{ij} move towards the training data, 4) repeat from step 1 for a fixed number of repetitions. The amount of adjustment in step 3 as well as the range of the neighborhood decreases during the training. This ensures that there are coarse adjustments in the first phase of the training, while fine tuning occurs during the end of the training.

This form of training has the effect of organizing the ‘map’ of the output nodes such that different areas of the map will respond to different input patterns. Hence, the Kohonen network has self-organizing properties and is capable of recognition. Application examples of the Kohonen network include recognition of images and speech signals (SDL Component Suite, 2008). The next section focuses on the most common type of network which is the feedforward artificial neural network (FANN) that has also been implemented in this work.

2.2 Feedforward Artificial Neural Network (FANN)

The most popular neural network architecture is the feedforward neural network. Figure 2.4 shows typical feedforward neural network architecture. The previous sections have circumstantially touched on this topic. The network consists of an input layer, a number of hidden layers and an output layer. The output and hidden layer are made up of a number of nodes. However, the input layer is essentially a direct link to the inputs of the first hidden layer (Gomm et al., 1993). An individual node in the network can be described by Equation 2.1.

As mentioned in previous sections, the activation functions can be hard limiter, threshold logic, sigmoidal or tanh functions. Sigmoidal activation function for the nodes in the hidden layer and output layers are the most common choice. The outputs of each node in a layer are connected to the inputs of all of the nodes in the subsequent layer. Data flows through the network in only one direction only from input to output hence it is called feedforward neural network.

Nowadays, feedforward network is not only applied as single network or "best" network but also a few improvements and modifications have been made in order to further enhanced the network performance especially in terms of the ability to generalize the model and minimizing model's error (Zhang, 1999). The next section explains about training methods in feedforward neural network and the following section elaborates on bootstrap re-sampling methods, stacked neural network and also their applications in modeling and control. Other types of networks are recurrent network, radial basis function (RBF) network, B-spline network and so on.

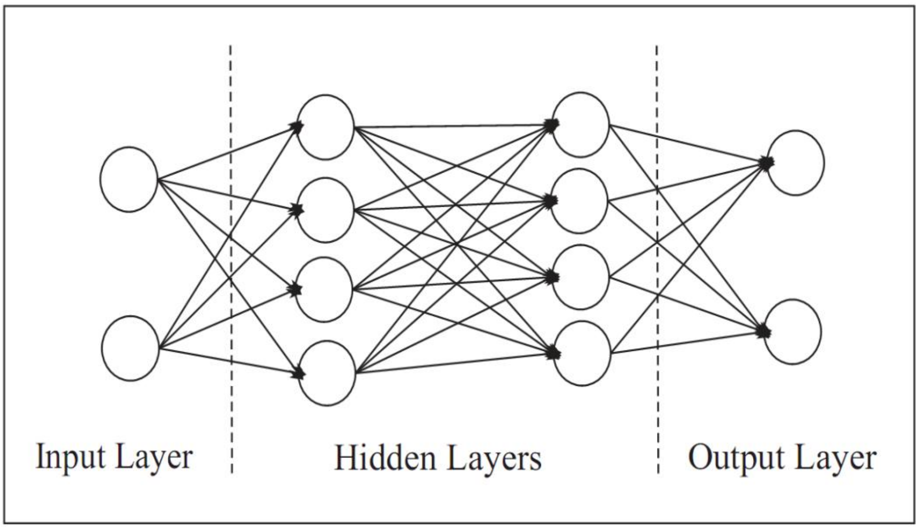


Figure 2.4: A Multi-layer Feedforward Neural Network

Neural networks have also gone through a revolution in their applications when improvements to the neural network such as bootstrap re-sampling method and multiple neural networks are introduced. The goal of introducing these improved methods for neural network is mainly to tackle problems such as lack of generalization capability and also phenomena called overfitting and underfitting. These drawbacks are usually encountered within the neural networks. Despite of their differences, these methods possess similar mathematical concept especially the one that is used in training. Training is an important step in developing neural network models. Model robustness is primarily related to the learning or training methods and the amount and representativeness of the training data. In other words,training is one of the methods that enable neural network to learn about the dynamic of a process in order to be able to generalize the process.

2.2.1 Training Paradigms in Feedforward Artificial Neural Network

The goal of the neural network training/learning process is to find the set of weight values that will cause the output from the neural network to match the actual target values as closely as possible. There are several issues involved in designing and training a feedforward neural network: 1) Selecting how many hidden layers to use in the network, 2) Deciding how many neurons to use in each hidden layer, 3) Finding a globally optimal solution that avoids local minima, 4) Converging to an optimal solution in a reasonable period of time, 5) Validating the neural network to test for over fitting.

Learning in neural network is achieved by adjusting the modifiable connection weights between the units as shown in Figure 2.5. As shown in Figure 2.5, a set of neural networks is trained by adjusting weights and number of hidden neurons in the system. The resulting output from the training process is compared with the targeted output value. The process continues until the resulting output from the system and the targeted output are matched. The moment both outputs are synchronized, the neural networks are considered as well trained and the process proceeds to the testing and validation steps.

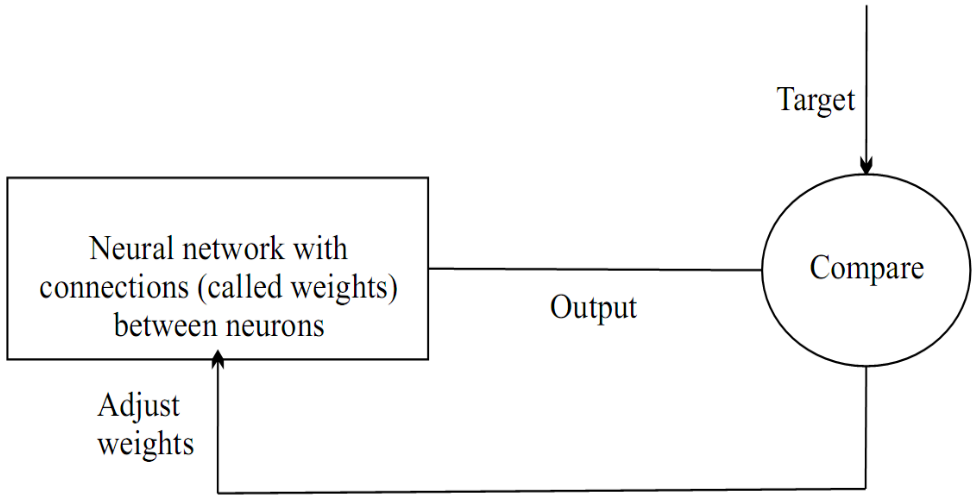

Target
Neural network with connections (called weights) between neurons
Compare
Output
Adjust weights

Figure 2.5: Basic Neural Network Training Method

Learning in neural networks is a problem of finding a set of connection weights which would enhance the ability of neural networks to store experiential knowledge; hence the learned knowledge can be used to achieve the desired response in the future. Up to now, there are various choices of learning algorithms available, and they can be classified into three main classes; supervised learning, reinforcement or graded learning and unsupervised learning. A supervised learning algorithm adjusts the strength or weights of the inter-neuron connections according to the difference between the desired and actual network outputs corresponding to a given input. Thus, supervised learning requires a “teacher” or “supervisor” to provide desired or target output signals.

Backpropagation (BP) algorithm is one of the notable supervised learning algorithms. This approach basically refers to an external agent like computer program that totally monitors the input and output vector pairs and adjusts the weights in such a way that matches each network output with its target value. Other commonly used supervised learning algorithms are Levenberg-Marquardt and gradient descent method. Reinforcement learning algorithm is also similar to the supervised learning except that the desired output is not provided. It employs a critic only to evaluate the goodness of the neural network output corresponding to a given output. Genetic algorithm (GA) is an example of the reinforcement learning algorithm.

Unsupervised learning on the contrary, uses only the input vector for network training and the network regulates its own weights without the benefits of knowing what particular output to assign for a given input. During training, only input patterns are presented to the neural network which automatically adapts the weights of its connections to cluster the input patterns into groups with similar features. Kohonen Rule for training Kohonen network is one example of unsupervised learning and also Carpenter-Grossberg Adaptive Resonance Theory (ART) algorithm.

2.2.2 Levenberg- Marquardt (LM) Training Paradigm

Levenberg-Marquardt is a virtual standard in nonlinear optimization which significantly outperforms gradient descent and conjugate gradient methods. It is a pseudo-second order method which means that it works with only function evaluations and gradient information but it estimates the Hessian matrix using the sum of outer products of the gradients (Roweis, 2005) . The technique that