Chapter 1

Introduction

Over the past few decades, emphasis has increasingly been placed upon optimal process design, safe plant operation, better product quality, and higher profitability, in the chemical process industries (CPI). Nonlinear models are typically required for process control, process optimization, data rectification, state and parameter estimation, and prediction of process behavior. Development of such model is often a difficult task for processes that are complex or poorly understood. When the theoretical modeling is difficult, empirical, data-driven modeling provides a useful alternative.

In recent years, artificial neural networks (ANNs) have been proposed as a promising tool for identifying chemical process models from process data. Neural networks are very useful because of their ability to model complex nonlinear process, even when process understanding is limited. With their excellent nonlinear representational capabilities, neural networks have shown widespread applicability in a variety of fields, ranging from molecular modeling to stock market predictions. They have found exponentially increasing usage in a broad spectrum of science and engineering applications. In process control, neural networks provide an attractive alternative in modeling nonlinear systems and have activated their use in various control-related applications.

1.1 Artificial Neural Networks

Artificial neural network technology, a computational technique, is capable of representing any nonlinear mapping that exists between input-output variables. Neural networks are highly interconnected mathematical structures with the ability to learn, and consist of processing units called "neurons" arranged in different layers. The processing units are associated with simple localized computations and are massively connected in parallel with each other. Every connection has an associated parameter, called the "connection weight" or simply the "weight" representing the strength of the connection. These connection weights, together with the nonlinear computations within a neuron, and their massive interconnections, collectively give neural networks the ability to represent any nonlinear function.

The values of the connection weights are determined through a procedure called "training" or "learning". Training algorithms can be broadly classified into supervised and unsupervised training algorithm. In supervised training schemes, the networks are presented with some known examples of inputs and targets. The networks learn the knowledge underlying those data patterns and are capable of reproducing them when recalled. Networks properly trained are very good at interpolation and can also predict the outputs for data that were not used for training.

Neural networks emerged from attempts to develop mathematical models to simulate the functioning of the human brain. Interests in connectionist research deteriorated after the nineteen-seventies due to the limitations of the earlier models such as perceptron (Minsky and Papert, 1969). With the development of multilayer perceptrons and back propagation techniques (Rumelhart, Hinton, and William, 1986a) neural networks have come to the forefront once again. From their resurgence in the eighties, there has been exponential growth in the field of neural networks. Currently, there are many different types of networks and a number of training algorithms for the various types of networks.

Neural networks learn from examples to provide excellent representation between input-output variables. The ability to learn from examples gives neural networks the capability of modeling complex nonlinear systems and this capability has motivated their use in many chemical engineering systems as well.

1.2 Modeling Approaches

Modeling of chemical processes has been generally considered as the first step to improve process control and management. Good process models are essential for the implementation of most advanced control algorithms. Indeed, developing a valid dynamic model of a process is often the major part of the work required to implement advanced control strategies. First principles modeling, in other words, white-box modeling or physical modeling is a traditional approach developing a model from first principles and estimating the values of the model parameters from process data. However, this procedure is often difficult and/or costly because the process may not be well understood or is too complex to model. Furthermore, this method is computationally demanding and requires simplifying assumptions that degrade its accuracy, but are necessary in order to make it solvable for a real time application.

An alternative approach is empirical modeling methods that rely on process data to develop input-output relationships. Artificial neural networks (ANNs) have shown great promise for such modeling task (Bhat and McAvoy, 1990; MacMurray and Himmelblau, 1995). ANNs consist of interconnected processing elements or nodes, which have basis functions and activation functions inside, that learn directly from process data and require minimal prior process knowledge. Their universal approximation capabilities (Hornik, Stinchcombe, and White, 1989) make them good candidates for modeling any nonlinear chemical process. These models have the advantages of high accuracy, short development time, and the ability to adapt to changing process conditions. Their fast execution times make them ideal for real-time process optimization. They have the limitation of being only as good as the data used to generate them (Baratti, Vacca, and Servido, 1995). Therefore, a model developed with process data that do not span a wide operating region can have limited utility.

Gray-box modeling is the other approach that compensates the weak points of white-box modeling and black-box modeling. It can be defined as a suitable combination of them, but at this moment little is known about what is suitable and what is not. In this work, neural networks are used to model chemical processes as a black-box modeling tool. Literatures concerning to the neural network modeling are provided in the next chapter.

1.3 Control Systems

Industrial processes are often nonlinear and due to the lack of robust nonlinear modeling techniques, such systems have been controlled using linear systems principles. Although linear controllers such as PID controllers are the major controllers in the plants, their ability in regulating the nonlinear systems is limited in the narrow operating range. They performed poorly when the systems are operated out of the limited ranges and are highly nonlinear. To improve the control of nonlinear systems a number of nonlinear controller design techniques were developed. Methods ranging from ad hoc strategies, to process specific algorithms, to nonlinear model based techniques - in conjunction with nonlinear programming - were developed. Due to its efficiency and development, nonlinear control techniques have shown promise for higher economic incentives and have started to appear in the industries. Review regarding various nonlinear controllers and control strategies is given in the literature (Bequette, 1991).

Developments in the area of artificial intelligence (AI) have also been making a large impact in the field of the chemical process control. Artificial neural networks is a branch in AI, their ability to provide excellent nonlinear models has offered a promise in the improvement of process modeling and control of nonlinear systems (Hunt et al., 1992). They can learn not only plant models but also plant inverse models, which can be used as nonlinear controllers. According to the previous works, neural networks were implemented in many control strategies, for examples, robust control, predictive control, inverse-model-based control, adaptive control, etc. Researches concerning the neural network application in process control are reviewed in the next chapter.

1.4 Research Objectives

The objectives of this research are as follows:

1. To study the use of the neural networks especially multilayer feedforward networks for identification of a front-end acetylene hydrogenation system.

2. To study the use of the neural networks for function approximation in order to improve the control performance of the Generic Model Control (GMC).

3. To study the use of the neural networks as a nonlinear controller in the Nonlinear Internal Model Control (NIMC).

1.5 Scope of the Research Work

Multilayer feedforward networks with one hidden layer are investigated in this research. Error back-propagation and Levenberge-Marquardt algorithms are used to train the networks. Sigmoid function is the activation function used in hidden layer and output layer neurons. The sum-squared error is the performance index used to select the well-trained neural network. An acetylene hydrogenation system and a Continuous Stirred Tank Reactor (CSTR) are nonlinear systems employed in this research. Advanced control techniques: Generic Model Control (GMC) and Nonlinear Internal Model Control (NIMC) are studied.

The research work can be divided into three parts as follows:

1. **The application of neural networks for system identification**: The industrial front-end acetylene hydrogenation system is studied. The plant data are used to train and test the neural networks.

2. **The application of neural networks for function approximation**: The neural network is trained to approximate function f in the GMC formulation. The control performance of the GMC with the neural network approximator is compared to the control performance of the GMC with a state estimator derived from mass balance.

3. **The application of neural networks for advanced control**: The neural networks are trained to learn the forward and the inverse model of the CSTR. The models obtained are implemented in the NIMC configuration as a process model and the nonlinear controller, respectively.

The control performance of GMC and NIMC are evaluated with disturbance rejection and set point tracking in nominal case and in the presence of plant-model mismatches. Programs based on MATLAB version 5.2 and neural network toolbox (as given in Appendix A) are written to formulate neural network models and control techniques.

1.6 Organization of the Thesis

The contents in this thesis can be categorized into eight chapters. Chapter 2 presents the literature review in the applications of neural networks in process control including three subsections: chemical process modeling with neural networks, neural network application in control techniques and neural network application in other related applications. Chapter 3 describes the neural network fundamentals consisting of the origin and development of neural networks, types of neural networks, multilayer feedforward network architecture, functions of a neuron, and backpropagation algorithm, respectively. Chapter 4 introduces the forward and inverse modeling together with the procedure in applying the neural networks for system identification. The application of multilayer feedforward networks for system identification of an acetylene hydrogenation system is illustrated in Chapter 5. Chapter 6 provides an application of neural network for function approximation in GMC control. The application of neural network as a nonlinear controller in NIMC configuration is presented in Chapter 7. Finally, the conclusions and recommendations for the future work are given in the last chapter.