Available online at www.sciencedirect.com
ScienceDirect
Computers & Industrial Engineering 54 (2008) 879–888
computers & industrial engineering
www.elsevier.com/locate/caie

Neural network-based simulation metamodels for predicting probability distributions

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Received 16 August 2005; received in revised form 14 August 2006; accepted 29 August 2007
Available online 4 November 2007

Abstract

Simulation is an important tool for supporting decision-making under uncertainty, particularly when the system under consideration is too complex to evaluate analytically. The amount of time required to generate large numbers of simulation replications can be prohibitive, however, necessitating the use of a simulation metamodel in order to describe the behavior of the system under new conditions. The purpose of this study is to examine the use of neural network metamodels for representing output distributions from a stochastic simulation model. A series of tests on a well-known simulation problem demonstrate the ability of the neural networks to capture the behavior of the underlying systems and to represent the inherent uncertainty with a reasonable degree of accuracy.

Keywords: Neural networks; Simulation; Metamodels; Percentiles

1. Introduction

Decision makers are often faced with determining a choice of action based on uncertainty. In manufacturing and service industries, these decisions can be enhanced by the use of "what if" scenarios for the system in question. These scenarios involve stochastic systems such as production lines, inventory management, and customer service facilities where the behavior of operators, suppliers, and customers is not known with certainty. In particular, a decision maker may be interested in the likelihood that a stochastic system will produce an output that lies within a specified range of possible values. For example, she may wish to determine the likelihood that a particular set of process inputs will generate revenues greater than some fixed amount, or she may wish to determine the inputs necessary to ensure an 80% chance that the process will be completed within a particular range of target dates.

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0360-8352/$ - see front matter
doi:10.1016/j.cie.2007.08.012

The need to assess the likelihood of observing outputs within a given range of values is also common in other application areas which frequently make use of computer simulation models. In an environmental setting, for example, water quality is often judged by the concentration of contaminants such as phosphorous or nitrates. Modeling the distribution of such concentrations, based on the application of new management practices in a watershed, can help to determine the likelihood that contaminant levels will actually exceed an acceptable value. Similarly, it would be useful for a computer network administrator to be able to predict the likelihood that a change in policy could lead to denial of service, and it would help call center staffing to be able to predict the likelihood that a new staffing plan would result in a shortage of employees and a corresponding increase in blocked calls.

The complexity of such problems is enhanced not only by the stochastic nature of the underlying system, but also by the interdependencies inherent in such systems. For very simplified systems, it may be possible to identify the distribution of potential outcomes and then to use the theoretical cumulative distribution function (CDF) to determine the likelihood of seeing values within given ranges. For many realistic systems, however, a tool such as simulation may be necessary to characterize the system's behavior. If a simulation model that accurately represents the underlying system can be developed, then multiple replications of that model can be used to generate an empirical representation of the system's output distribution for each combination of input parameters. Each empirical output distribution may then be analyzed as a surrogate for the actual process output, in order to support the decision-making process.

Particularly complex processes will often necessitate very complex simulations in order to accurately represent their behavior. Such simulations can require a significant amount of time to generate even a single replication; thus if large numbers of replications are necessary to characterize system behavior, it may simply be too expensive to use the actual simulation model. In such situations, a simulation metamodel may be a more appropriate choice for analyzing the behavior of the system. The purpose of this research study is to characterize the ability of neural network-based simulation metamodels to predict the output probability distribution that results from multiple replications of a stochastic simulation.

2. Artificial neural networks (ANN) as simulation metamodels

A simulation model is typically created to represent the relationship between a system's output (some response variable, y) and its set of input variables ($\mathbf{x} = \{x_1, x_2, x_k\}$, for some $k \geqslant 1$). A metamodel is a mathematical function that can be used to approximate such a simulation model. If the actual functional relationship, $y = f(x_1, x_2, \ldots, x_k)$, is not known then an appropriate function ($\hat{f}$) must be selected (or constructed) and its parameters estimated based on empirical data (Banks, Carson, & Nelson, 1996). Friedman and Pressman (1988) discuss several advantages that simulation metamodels offer researchers: simplified models, enhanced exploration and interpretation of the model, sensitivity analysis, optimization, and a better understanding of both the interrelationships among the variables and the behavior of the system.

Artificial neural networks (ANN) are a specific example of a tool that can be used for simulation metamodeling. An artificial neural network effectively acts as a tool for non-linear regression. It consists of a number of simple, highly interconnected processing elements or nodes and incorporates the ability to process information by a dynamic response of these nodes and their connections to external inputs (Freeman & Skapura, 1991; Haykin, 1998).

The method of using ANN for metamodels was introduced by Hurrion (1992). Donohue, Houck, and Myers (1993) evaluated regression metamodels by modeling a Jackson network. Padgett and Roppel (1992) gave a general overview and discussion of potential uses of ANN for simulation modeling. Pierreval (1992) and Pierreval and Huntsinger (1992) modeled simplified manufacturing shops as stochastic pattern recognition and classification problems, and used neural approximation to model a continuously valued deterministic simulation system. In Kilmer and Smith (1993), a classical (s, S) inventory problem was used to show the improvement of ANN over first- and second-order linear regression models.

Other applications of neural networks for simulation metamodeling include an emergency department simulation (Kilmer, Smith, Tunasar, & Shuman, 1995), an economic analysis of risky projects (Badiru & Sieger, 1998), an optimum Kanban allocation procedure (Hurrion, 1997; Savsar & Choueiki, 2000), a job shop system