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Development of Dual Response Approach using Artificial Intelligence for Robust Parameter Design

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Abstract. Prediction process of parameters in robust design is very important. If the prediction results is fairly precise then the quality improvement process will economize time and reduce cost. Dual response approach based on response surface methodology has widely investigated. Separately estimating mean and variance responses, dual response approach may take advantages of optimization modeling for finding optimum setting of input factors. A sufficient number of experimentations are required to improve the precision of estimations. This research recommended an alternative dual response approach without performing experiments. A hybrid neural network-genetic algorithm has been applied to model relationships between responses and input factors. Mean and variance responses conform to output nodes while input factors are used for input nodes. Using empirical process data, process parameter can be predicted without performing real experimentations. A genetic algorithm has been applied to obtain the input factors optimum setting. An example has been studied to demonstrate the procedures and applicability of the proposed approach.

1. Introduction

Robust design is an important engineering design methods for quality improvement. It can reduce manufacturing cost and design cycle time. Robust design is a cost-effective methodology for determining the optimal settings of control factors that make the product performance more sensitive to the effects of noise factors [1]. Robust parameter design (RPD) is a method to determine the optimal conditions of input variables so that give the optimal response. RPD introduced by Taguchi. He suggested the use of orthogonal array and SN (signal-to-noise) ratio using the inner array to factors beyond the control and outer factors for noise factor. The combination of the best design parameters are determined by minimizing the SN ratio. Besides the average value endeavored to achieve the desired target by identifying adjustment factors [2].

Offering a more statistically sound and efficient approach to data analysis, a dual response approach to RPD by combining Taguchi's philosophy and response surface methodology (RSM) was suggested [3]. A dual response approach may offer considerable modeling flexibility by giving an estimate of process mean and standard deviation at any point of interest. Separately modeling response functions for process mean and variance, an engineer can gain insights on the relationship between input variables and responses [4-7].

A second-order polynomial model is mostly assumed for predicting response functions in RSM and it is often the case that the behaviour of mean or variance responses may not be described well by a reasonable second-order polynomial model. In practice, the fitting and predictive performances of low-order polynomial models and especially of the process variance response are very poor when the relationship between the input factors and the quality characteristic of the process is highly nonlinear and noisy [8]. For example, there is disputed that the prediction of a pharmaceutical response based on a second-order polynomial equation often produces in the poor estimation of optimal drug formulation [9].

Inspite of the criticisms centering around RPD based on RSM, therefore, data collected from well-design experiments produce valuable information for modeling and predicting functional relationships. It is also clear that a better estimation of response functions may be achieved by conducting a large enough number of experimental runs. Engineers may have to make decisions only with a limited number of experiments mainly due to cost and/or time constraints. Under such circumstances, an argumet states that the use of experimental data gathered during the course of production and stored in the data repository of the company. They also suggested that happenstance data can be used to model the functional relationships if coupled with effective and proper data-mining techniques [4-7].

The back propagation model, which was originally proposed by Rumelhart in 1986, is able to effectively deal with prediction and optimization problems [10]. In 1994, Liao and Chen have tried to observe Back Propagation Neural Network model to predict and optimize creep feed grinding process. They found that the result better than the regression method's result [11]. Further, a Hopfield neural network approach was proposed to solve dual response systems problems [12]. The authors found that this approach is capable for minimizing multi-objective functions.

To simplify, the main problem is how to predict the optimal parameters with limited number of experimental run. This study want to propose an alternative RPD approach on the basis of happenstance (experimental) data. Then we will try to construct, train and simulate hybrid Back Propagation Neural Network–Genetic Algorithm models based on happenstance data.

The remaining parts of this paper are organized as follows. In Section 2, we describe briefly the basic theory of BPNN and GA. The proposed RPD procedure based on BPNN-GA is presented in Section 3. In Section 4, the proposed procedure is applied to a case study. Finally, the conclusions are presented in Section 5.

2. Literature Review

As a functional abstraction of the biologic neural structures of the central nervous system, artificial neural networks (ANNs) operate as black-box, model-free, and adaptive tools to capture and learn significant structures in data [13]. Their computing abilities have been proven in many fields including prediction, estimation, optimization, pattern recognition, and so on. One of the most widely used ANNs is the neural network based on the simple error back propagation training algorithm suggested by Rumelhart, which is based on a gradient-descent optimization technique [10]. A typical ANN consists of three types of layers-input, hidden, and output layers - each of which has various interconnected nodes called neurons. A neuron receives one or more input signals and provides output signal after processing input signals based on the transfer function. The output signal is transferred to connecting neurons in varying intensities depending on connection weights. In the supervised learning of the network, the network is presented with training data set, each consisting of an input vector from an input space and a desired output corresponding to the input. According to the defined learning algorithm, the network adjusts its parameters so that the errors between the estimated and desired output are minimized. The BPNN algorithm iteratively adjusts the connection weights to minimize the sum of squared residual. Once trained, the network can be used for any input vectors from the the region of interest [4-7].

One may find a great number of studies on the application of ANNs to engineering design problems especially when there is no formal underlying theory for the solution. For the purpose of this study, it should be enough to briefly review previous studies directly related to applying ANNs to the RPD problem. Su and Hsieh attempted to apply the ANNs to RPD with dynamic quality characteristics [14], and Ma and Su extended their research by employing a multiple objective evolutionary algorithm [15]. However, they have adopted the signal-to-noise (SN) ratio, which is a much debated performance measure. Chang (2008) employed ANNs combined with simulated annealing to solve multiple response parameter design problems based on the desirability function [16]. Most recently, Chang and Chen investigated the same problem by adapting genetic algorithm instead of simulated annealing [17]. The desirability function is quite useful for compromising among multiple objectives. Strictly speaking, however, these studies may not be classified as one of the RPD studies because the standard variation response has not been considered. As pointed out by Vining and Myers, a dual response approach to RPD may offer considerable modeling flexibility by separately modeling mean and variance responses [3]. Arungpadang & Kim Young Jin have constructed and validated BPNN models based on happenstance data [4-7]. This study have applied RSM to estimate mean and variance responses for the purpose of RPD.

There still exist some limitation when BPNN is trained since it often gets trapped in a local minimum because the use of gradient descent [14]. Research combining NN and GA began to appear around 1988s. The primary direction involve using the GA want to improve the performance of NNs through finding optimal NN architecture or parameter setting as an alternative to BPNN for optimizing the network [18].

The combination of NN and GA has been used for integrated process modeling and optimization. The hybrid NN-GA technique is a powerful method for process modeling and optimization that is better than other techniques such as response surface methodology, particularly for complex process models.

The authors were unable to locate previous researches applying Neural Network and Genetic Algorithm to dual response approach. Ozcelik and Erzurumlu have tried to use Anova, GA and NN in warpage optimization of plastic injection molding [19]. Then, the hybrid BPNN and GA for optimization of injection was applied in molding process parameters [20]. In 2011, Chang and Chen have developed a neuro–genetic approach to optimize parameter design of dynamic multi response experiments [17]. But those researches above and others similar cannot be classified as the dual response approach. That is the baseline why this study will employ the BPNN and GA for estimating the relationship between input factors and responses of interest.

3. The Proposed Procedures

The proposed approach consists of three stages: First, happenstance (or experimental) data are collected to construct a BPNN to represent the input-response relationship, based on which mean and standard deviation responses may be predicted for a given setting of input factors within the feasible solution space. Second, after population initializing then fitness computation and scaling, GA's procedures have applied. Finally, optimum parameter set are obtained based on mean and standard deviation response. The overall procedure of the proposed approach is depicted in Figure 1.

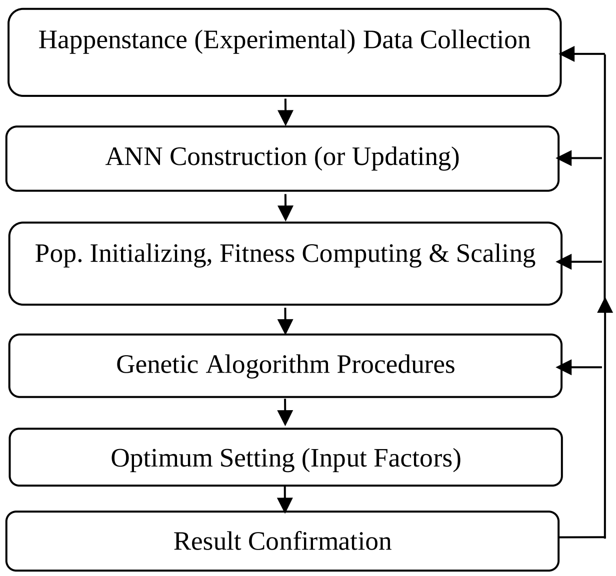

Figure 1. Proposed Approach

3.1 Construct and Training BPNN

Determine experimental data used for training and testing the BPNN model. Establish the network architecture (input, hidden, and output layers). Search the optimal network architecture and confirm that the network is not overfitted. Convert the experimental input and output data to number within the range [-1 1]. The purpose of normalization is performed to avoid mismatch in the influence of some input values to the network weights and biases. Then, train the network using the normalized data by utilizing a Levenberg-Marquardt training function.

3.2 Population Initializing, Fitness Computation and Scaling

Adjust the initial generation index to zero, the population number and the number of independent variables. Generate a random initial population. Every individual has vector entries with certain lengths which are divided into many segments. Next, the performance of the solution vector in the current population is computed by using a fitness function. Convert the solution vector to be a number between -1 and 1. Then, the vector is entered as an input vector to the training process to obtain the corresponding outputs. After that, scale the raw fitness scores to values in a range that is appropriate for the selection function. In the GA, the selection function applies the scaled fitness values to pick the parents for the next generation. The performance of the genetic algorithm is affected by the range of the scaled values. The scaling function employed in this algorithm based on the rank of each individual than its score. Lower raw scores have higher scaled values since the algorithm minimizes the fitness function.

3.3 Genetic Algorithm Process

Select the parents based on their scaled values by taking the selection function. The selection function specifies a higher probability of selection to individuals with higher scaled values. Each individual can be chosen more than once as a parent.

Options of reproduction specify how the GA produces children for the next generation from the parents. Elite count specifies the number of individuals with the best fitness values that are assured to withstand to the next generation. Arrange elite count to be a positive integer within the range (elite children). Crossover fraction decide the fraction of each population that are produced by crossover. The rest of individuals in the next generation are produced by mutation. Set crossover fraction to be a fraction between 0 and 1. Crossover allow the algorithm to extract the best genes from different individuals. That process occurs by choosing genes from a pair of individuals in the current generation and recombining them. The output is potentially superior children for the next generation. The probability is equal to crossover fraction. Mutation function performs small random changes. It gives genetic diversity and therewith increases the possibility to create individuals with better fitness values.

The recent population is replaced with the children to form the next generation since the reproduction is made. Next process is increment the generation index (Gen = Gen + 1). Then, repeat the fitness computation stage to increment of generation stage, until convergence is achieved. The algorithm stops if one of the following five conditions is met. They are fixed generations, fitness limit, time limit, stall generations or stall time limit. If the convergence criterion is achieved, the children with the highest ranking based on the fitness value are decide to be the optimal parameter set of population.

4. Ilustrative Example

An example from a pharmaceutical process is studied to illustrate the RPD proposed procedure based on happenstance data. An investigation of the formulation of cytarabine liposomes by using ANNs was carried out [9]. Three input factors are drug/lipid molar ratio (X_1), PC/Chol in percentage ratio of total lipids (X_2), and the volume of hydration medium (X_3). The output variable of interest is the percentage drug entrapment (PDE) of which mean and standard error of mean (SEM) are also provided. Three replications have been made at each factor setting. Note that SEM response may also be used in place of standard deviation (SD) response, since the standard deviation can be calculated as SEM multiplied by the square root of the number of replications. For the purpose of this study, experimental data provided may be considered happenstance data which are used to construct a BPNN. Figure 1 depicts the network architecture used for the example, and we found that Lavenberg-Marquard's searching method works well as the learning rule.

A 3^3 factorial experiment is now designed within the range of interest to estimate the response functions of process mean and SEM by applying RSM. A feed-forward BPNN was used to construct for PDE and SD estimation. Mean and SD responses at each design point are obtained using the model architecture shown in Figure 2.

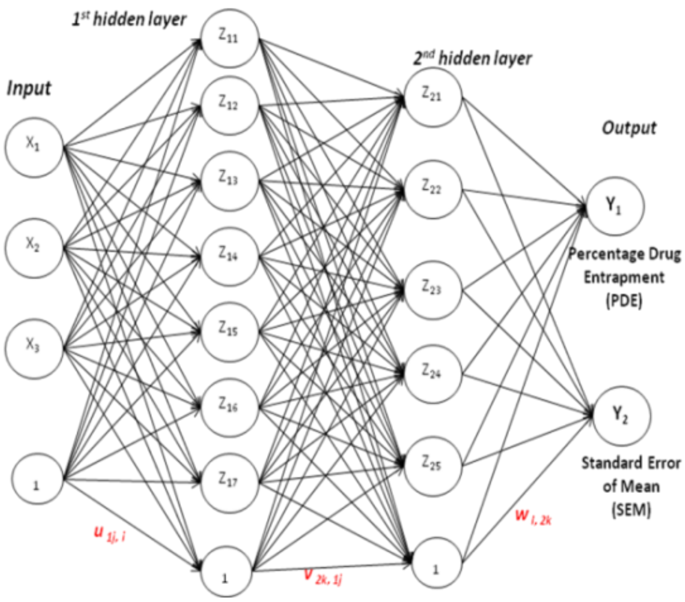

Figure 2. BPNN Model for the Example

A neural network and global optimization toolbox in Matlab7.11 is used to construct the BPNN-GA model. The network consists of three inputs, two hidden layers and two outputs. The coded values of the input factors are shown in Table 1.

Table 1. Coded Values of Input Factors

Coded values	Actual values		
	X_1	X_2	X_3
-1	1 : 7	50 : 50	1 mL
0	1 : 10	60 : 40	2 mL
1	1 : 13	70 : 30	3 mL

In the next step, BPNN-GA model is simulated to obtain the optimal parameter within the feasible solution space of the system. The values of the three control factors are set as continuous as fall in the range between -1 (lower bound value) and 1 (upper bound value). The operational conditions of GA are set as: population size, crossover fraction, number of generation, fitness scaling function, selection function, crossover function, mutation function and mutation probability. The display of coding in m-file then the running result windows from BPNN-GA model can be seen in Figure 3.

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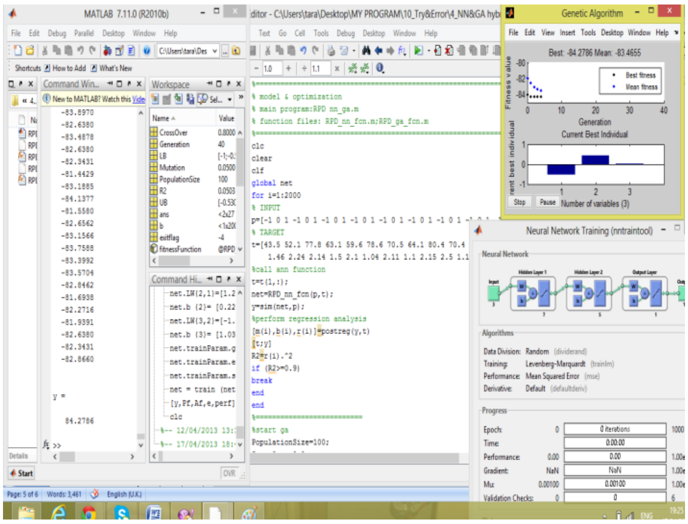

Figure 3. Matlab Implementation

All the estimation results describe in Table 2. This table list the predicted responses at the optimal parameter set (X_1, X_2, dan X_3). Every estimated value give its optimal parameter set. This table show to us that for some setting we can get the estimated mean value around 83.2284 (minimum value) to 85.0417 (maximum value).

Table 2. The predicted responses at the optimal parameter set

i	Pop	Gen	Estimated Value	X_1	X_2	X_3
1900	100	40	83.3301	**-1.0000**	**0.5000**	**0.4108**
	200		83.3297	-0.9998	0.4999	0.4104
	300		83.3238	-0.9994	0.4940	0.3967
	400		83.2883	-0.9914	0.4711	0.3692
	500		83.2284	-0.9841	0.4377	0.3881
	600		83.3235	-0.9999	0.4989	0.4236
2000	100	40	84.3687	-0.5311	0.5000	-0.0968
	200		84.3680	-0.5337	0.4979	-0.0953
	300		84.3675	-0.5351	0.4987	-0.0924
	400		84.2844	-0.5328	0.4292	-0.0036
	500		84.2540	**-0.5329**	**0.4930**	**0.0134**
	600		84.2708	-0.5362	0.4770	0.0079
2500	100	40	85.0417	-0.5300	0.0245	-0.5000
	200		85.0410	-0,5300	0.0296	-.0.5000
	300		85.0417	-0.5300	0.0244	-0.5000
	400		85.0416	-0.5300	0.0226	-0.5000
	500		82.3608	-0.8328	0.5000	-0.5000
	600		84.5788	**-0.5300**	**0.1567**	**-0.5000**

Table 3 describe the real value of parameter set (drug lipid, PC Chol and hydration volume) for some mean-SD value. Estimated SD value do not differ too much from one another.

Table 3. Optimum parameter set, estimated PDE value and estimated SD value

Estimated PDE Value	Drug Lipid	PC : Chol	Hydration Volume	Estimated SD Value
83.3301	**1 : 12**	62.5 : 37.5	2.2 mL	1.7904
84.2540	**1 : 12.41**	62.4 : 37.6	2.0 mL	1.7900
84.5788	**1 : 12.41**	60.8 : 39.2	1.75 mL	1.7897

For the purpose of benchmarking, this study conducted a comparison to previous researches related to this study. Table 4 demonstrate the comparison of these researches.

Table 4. BPNN-GA model compare to another study

	BPNN-GA	**Arungpadang & Kim Y.J. (2012)**	**Subramaniam (2004)**
Approach	**Dual**	**Dual**	**Singular**
Tools	**NN, GA**	**NN, RSM**	**NN, RSM**
Result	PDE : mean = 84.5%; standard deviation= 1.78. X_1= 1 : 12.41; X_2 = 60.8 : 39.2; X_3= 1.75	PDE : mean = 83.5%; standard deviation = 1.569. X_1= 1: 12; X_2 = 55 : 45; X_3= 2.424 mL.	PDE = 83.5%. X_1= 1: 13; X_2 = 60 : 40; X_3= 2 mL .

Note that BPNN-GA model can predict pretty well the mean and SD value. Its value not so different compare to the result of Arungpadang and Kim [4-7] and Subramaniam [9]. The result needs to be validated by conducting a confirmation experiment to see if the desired responses are obtained. The most important thing is BPNN-GA model gives an alternative method to solve and predict the optimal parameters in case with limited number of experimental run. So engineers can make decisions only with a limited number of experiments. They can reduce the total cost and shorten process time.

5. Conclusion and Further Study

In this article, a dual response approach to RPD is proposed by combining BPNN and GA to estimate the input-response relationship. The proposed approach consists of three stages. In the first stage, a BPNN is constructed to represent the input-response relationship based on happenstance data. After population initializing then fitness computation and scaling, GA's procedures have applied. Finally, optimum parameter set are obtained based on mean and standard deviation response. Some possibilities further researches are: (1) to find another procedures, another combination of procedures to enhance ability of this model, and (2) try to combine BPNN model to another AI methods.

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