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인공신경망을 이용한 로버스트설계에 관한 연구*

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Robust Parameter Design Based on Back Propagation Neural Network

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■ Abstract ■

Since introduced by Vining and Myers in 1990, the concept of dual response approach based on response surface methodology has widely been investigated and adopted for the purpose of robust design. Separately estimating mean and variance responses, dual response approach may take advantages of optimization modeling for finding optimum settings of input factors. Explicitly assuming functional relationship between responses and input factors, however, it may not work well enough especially when the behavior of responses are poorly represented. A sufficient number of experimentations are required to improve the precision of estimations. This study proposes an alternative to dual response approach in which additional experiments are not required. An artificial neural network has been applied to model relationships between responses and input factors. Mean and variance responses correspond to output nodes while input factors are used for input nodes. Training, validating, and testing a neural network with empirical process data, an artificial data based on the neural network may be generated and used to estimate response functions without performing real experimentations. A drug formulation example from pharmaceutical industry has been investigated to demonstrate the procedures and applicability of the proposed approach.

Keywords : Robust Parameter Design, Dual Response Approach, Back-Propagation Neural Networks, Response Surface Methodology

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1. Introduction

Since introduced by Taguchi in the 1980s, the concept of robust parameter design (RPD) gained a considerable amount of attention from quality engineers and researchers to realize a process insensitive to external noises which are often major sources of process variability. His approach and principles have widely been considered innovative and efficient for the purpose of process optimization. On the other hand, much debate and controversy have also been generated about the implementation and the technical nature of data analysis. Providing a more statistically sound and efficient approach to data analysis, Vining and Myers [14] suggested a dual response approach to RPD by combining Taguchi's philosophy and response surface methodology (RSM). A dual response approach may offer considerable modeling flexibility by providing 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. Readers are referred to Myers and Montgomery [6] for further discussion on the advantages of mean and variance modeling for process optimization. However, it may not work well enough especially when the behavior of responses are poorly represented. A second-order polynomial model is mostly assumed for estimating response functions in RSM and it is often the case that the behavior of mean or variance responses may not be described well by a plausible 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 [15]. For example, Subramanian et al. [13] argued that the prediction of a pharmaceutical response based on a second-order polynomial equation often results in the poor estimation of optimal drug formulation. In addition, it is not unusual to observe that certain assumptions underlying dual response approach are not justified. One may find many studies suggesting remedies to rectify these problems. For example, Park and Cho [7] proposed a robust design scheme with contaminated and non-normal data. More recently, Pickle et al. [8] and Robinson et al. [9] investigated a semi-parametric approach to RPD with the presence of unusual curvatures in the underlying function.

Despite 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 obvious that a better estimation of response functions may be attained by conducting a large enough number of experimental runs. In practice, however, it is often the case that engineers may have to make decisions only with a limited number of experiments mainly due to cost and/or time constraints. Under such circumstances, Shi et al. [11] suggested the use of 'happenstance data' gathered during the course of production and stored in the data repository of the company. They also argued that happenstance data can be used to model the functional relationships if coupled with effective and proper data-mining techniques. The motivation of this study is to propose an alternative approach to RPD on the basis of happenstance data. Back-propagation neural network (BPNN) models are constructed and validated using happenstance, historical or experimental data. Predicting responses of interest at well-designed process settings based on BPNN models, a usual RSM can be applied to estimate mean and variance responses for the purpose of RPD. The remainder of this manuscript is organized as follows : Section 2 briefly introduces the basic concept of BPNN and previous studies related to the application of neural network to RPD. The proposed RPD procedure based on BPNN is presented in Sections 3 followed by an illustrative example in Section 4. Conclusions follow in the last section.

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 [1]. 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 et al. [10], which is based on a gradient-descent optimization technique. 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 (i.e., differences between the estimated and desired output). Once trained, the network can be used for any input vectors from the the region of interest which is called the "generalization property" of the network.

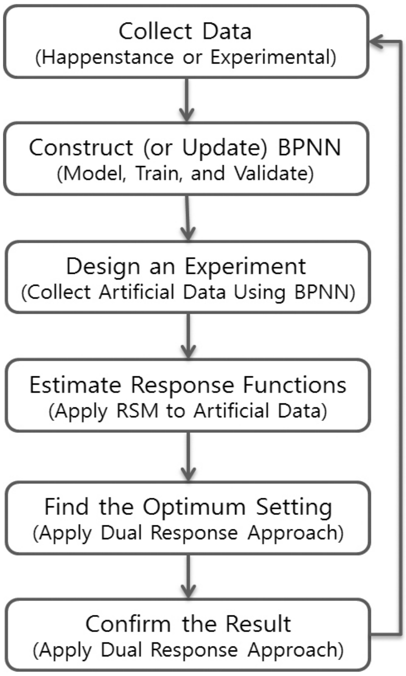
One may find a great number of studies on the application of ANNs to engineering design problems especially when there is no formal underlying theory for the solution. For the purpose of this study, it should be enough to briefly review previous studies directly related to applying ANNs to the RPD problem. Su and Hsieh [12] attempted to apply the ANNs to RPD with dynamic quality characteristics, and Ma and Su [5] extended their research by employing a multiple objective evolutionary algorithm. However, they have adopted the signal-to-noise (SN) ratio, which is a much-debated performance measure. Chang [2] employed ANNs combined with simulated annealing to solve multiple response parameter design problems based on the desirability function. Most recently, Chang and Chen [3] investigated the same problem by adapting genetic algorithm instead of simulated annealing. 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 [14], a dual response approach to RPD may offer considerable modeling flexibility by separately modeling mean and variance responses. The authors were unable to locate previous researches applying ANNs to dual response approach except for Koksoy and Yalcinoz [4], where a Hopfield neural network is employed to find the optimum settings of input factors. This study employs the BPNN for estimating the relationship between input factors and responses of interest.

3. Proposed RPD Procedure

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, mean and standard deviation responses are obtained at each design point from well-designed settings based on the prediction from the BPNN. The predicted data may further be used to model the functional relationships by applying a usual RSM technique. Finally, a dual response optimization model for RPD is established to find the optimum settings of input factors. The overall procedure of the proposed approach is depicted in <Figure 1>.

3.1 Modeling Input-Response Relationship

In this stage, a BPNN is constructed to model



〈Figure 1〉 Proposed Approach

the relationship between input factors and responses of interest. Happenstance, historical or experimental data may be collected to be fed into the model and train the BPNN. Values of input factors and corresponding responses of process mean and variance are assigned to input nodes and output nodes, respectively. Thus, the number of input nodes is equivalent to the number of input factors while the BPNN has 2 output nodes. Constructing a BPNN model is complicated since many training parameters are involved in the training process. Readers are referred to Rumelhart et al. [10] for detailed procedures for constructing a BPNN model.

3.2 Predicting Dual Responses

A well-trained BPNN may now be used to predict the responses for any settings of input factors from the feasible solution space due to the generalization property. Designing an experiment around the region of further investigation within the feasible solution space, predicted responses for process mean and variance may be obtained using the BPNN. A usual RSM may be applied to estimate the input-response relationship in a functional form (e.g., a second-order polynomial model) based on the artificial data using BPNN. In a dual response approach, response functions for mean and standard deviation are expressed as follows :

$$\hat{\mu}(x) = a_0 + \sum_{i=1}^{k} a_i x_i + \sum_{i=1}^{k} a_{ii} x_i^2 + \sum\sum_{i<j}^{k} a_{ij} x_i x_j \quad (1)$$

$$\hat{\sigma}(x) = b_0 + \sum_{i=1}^{k} b_i x_i + \sum_{i=1}^{k} b_{ii} x_i^2 + \sum\sum_{i<j}^{k} b_{ij} x_i x_j \quad (2)$$

where $\hat{\mu}(x)$ and $\hat{\sigma}(x)$ represent the estimated response functions for mean and standard deviation expressed in terms of input vector x, respectively. The estimated coefficients are denoted by a and b.

3.3 Optimization

An RPD optimization model can now be established based on the estimated response functions given in equations (1) and (2). For example, Vining and Myers [14] proposed an optimization model for the nominal-the-best type (N-type) quality characteristics as follows :

$$\begin{aligned} &\text{Min } \hat{\sigma}(x) \\ &\text{s.t. } \hat{\mu}(x) = \tau \end{aligned} \quad (3)$$

where τ represents the target value of the quality characteristic. Various formulations and optimization schemes have been suggested in the literature, and interested readers may refer to Koksoy and Yalcinoz [4]. It is most desirable that optimum setting of input factors should be verified through confirmation experiments.

4. Illustrative Example

To demonstrate the proposed procedure for RPD based on happenstance data, an illustrative example from a pharmaceutical process is investigated. Subramanian et al. [13] studied the formulation of Cytarabine Liposomes by using ANNs. Three input factors are drug/lipid molar ratio (X_1), PC/Chol (Phosphatidylcholine /Cholesterol) 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 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. Now suppose that the target of PDE is 83.5, i.e., τ = 83.5, and the standard deviation needs to be minimized as well. It is found that the optimum may be obtained in the neighborhood of 1 : 13 of X_1, 60 : 40 of X_2, and 2mL of X_3 by applying a usual RSM to the original data set. In the conventional approach, another set of experimental runs needs to be conducted within a smaller experimental region to trace the optimum solution with a higher precision. On the other hand, the proposed approach suggests constructing a BPNN based on the original data set instead of performing costly and time-consuming experiments. We have considered 15 candidates for network architecture given in <Table 1> and the structure 3-7-4-2 shown in <Figure 2> yields the least mean squared error. Further, the Lavenberg-Marquardt searching method works best among the 13 learning rules considered in this study as shown in <Table 2>. Completing the training process, the BPNN was tested against another set of data provided for the purpose of validation. It has been found that the BPNN estimates the mean response pretty well while it was impossible to evaluate the performance of estimating the SEM responses since they are not provided. A neural network toolbox in Matlab R2012a is used to construct the BPNN.

〈Table 1〉 Mean Squared Error of Candidate Network Architecture

Structure	MSE
3-1-2	0.26174
3-2-2	0.23868
3-3-2	0.20549
3-4-2	0.13200
3-5-2	0.07623
3-6-2	0.04050
3-7-2	0.01204
3-8-2	0.04250
3-7-1-2	0.12237
3-7-2-2	0.14457
3-7-3-2	0.00150
3-7-4-2	3.327×10^{-28}
3-7-5-2	6.539×10^{-28}
3-7-6-2	4.344×10^{-25}
3-7-7-2	2.022×10^{-25}

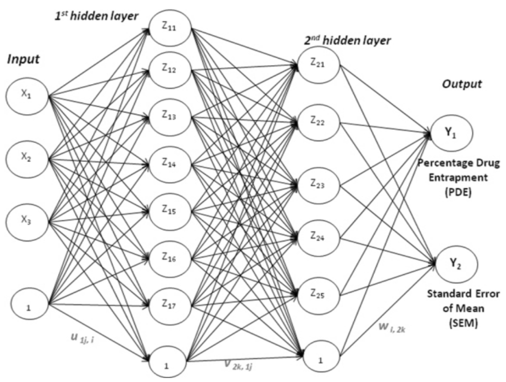
Note) * Learning rate = 0.1.
** Maximum number of iterations = 50.000.

〈Table 2〉 Performance of Learning Rules

Rules	MSE	Epoch	Time
traingd	1.97×10^{-4}	10,000	448
traingdm	9.99×10^{-6}	6880	293
traingda	9.79×10^{-6}	334	14
traindx	7.78×10^{-6}	126	5
trainbr	5.60×10^{-6}	6	1
trainc	9.60×10^{-6}	147	19
traincgp	9.87×10^{-6}	38	2
traincgb	5.82×10^{-6}	29	1
trainlm	1.89×10^{-6}	1	1
trainoss	9.25×10^{-6}	27	2
trainr	9.95×10^{-6}	83	29
trainrp	1.02×10^{-5}	98	4
trainscg	9.92×10^{-6}	11	2

Note) * Learning Rules from MATLAB Toolbox.

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. Mean and SEM responses at each deign point are obtained using the BPNN shown in <Figure 2>. The coded values of the input factors are shown in <Table 3>, and the predicted responses are summarized in <Table 4>. Note that the experiment is designed inside the range of interest given in Subramanian et al. [13].



〈Figure 2〉 BPNN Model for the Example

〈Table 3〉 Coded Values of Input Factors

Coded values	Actual values		
	X_1	X_2	X_3
-1	1 : 12	55 : 45	1.5
0	1 : 13	60 : 40	2.0
1	1 : 14	65 : 35	2.5

〈Table 4〉 Predicted Responses Using BPNN

Run	X_1	X_2	X_3	Mean	SEM
1	-1	-1	-1	83.079	2.086
2	0	-1	-1	84.803	1.943
3	1	-1	-1	84.666	1.798
4	-1	0	-1	83.543	1.632
5	0	0	-1	81.580	1.386
6	1	0	-1	79.786	1.165
7	-1	1	-1	78.619	1.041
8	0	1	-1	77.267	0.996
9	1	1	-1	76.255	1.124
10	-1	-1	0	79.799	2.192
11	0	-1	0	83.075	2.086
12	1	-1	0	84.699	1.967
13	-1	0	0	83.934	1.717
14	0	0	0	83.294	1.599
15	1	0	0	81.919	1.428
16	-1	1	0	78.488	0.995
17	0	1	0	78.453	1.020
18	1	1	0	78.347	1.103
19	-1	-1	1	65.073	2.027
20	0	-1	1	72.997	1.975
21	1	-1	1	79.654	1.938
22	-1	0	1	76.007	1.194
23	0	0	1	79.398	1.095
24	1	0	1	80.255	1.182
25	-1	1	1	74.968	0.447
26	0	1	1	74.774	0.502
27	1	1	1	75.917	0.674

Applying RSM to the predicted data using BPNN shown in <Table 4>, the response functions for the mean and standard deviation can be estimated as follows :

$$\begin{aligned}\hat{\mu}(x) = &\ 83.363 + x_1 - 1.375x_2 - 2.809x_3 \\ &- 2.694x_2^2 + 3.076x_3^2 - 1.885x_1x_2 \\ &+ 2.026x_1x_3 + 2.362x_2x_3 \\ \hat{\sigma}(x) = &\ 1.507 - 0.053x_1 - 0.562x_2 - 0.11x_3 \\ &- 0.223x_3^2 + 0.085x_1x_2 \\ &- 0.067x_1x_3 - 0.138x_2x_3\end{aligned}$$

Note that the response function of standard deviation is obtained using SEM values. Using the estimated response functions above, an RPD optimization model can be established. Solving the RPD optimization model given in equation (3), the optimum setting of input variables is found to be (-1.0, -1.0, 0.846) in coded unit at which the mean and standard deviation are 83.5 and 1.569, respectively. The optimum solution has been obtained with Response Optimizer in MINITAB 15.0. The result needs to be validated by conducting a confirmation experiment to see if the desired responses are obtained.

5. Conclusions

In this article, a dual response approach to RPD is proposed by employing a BPNN model 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. Then, mean and standard deviation responses are obtained at each design point from well-designed settings based on the prediction from the BPNN. The predicted data may further be used to model the functional relationships. Finally, a dual response model for

RPD is established to find the optimum settings of input factors using the estimated response functions. An illustrative example demonstrates the proposed approach. Since the optimum setting of input variables is obtained based on artificial data in the proposed approach, its performance is highly dependent upon the accuracy of the neural network. Even if the accuracy may be greatly improved by collecting process data for an extensive period of time, it is highly recommended to validate the results by performing confirmation experiments.

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