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Nash-Sutcliffe Efficiency Approach for Quality Improvement

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Abstract

Robust parameter design is an effective tool to obtain the best operating conditions of a given system. Because of its practicability and usefulness, the widespread applications of robust design techniques provide major quality improvements. In fact, evaluating the quality performance of the fitted response model could be a way to reach the possible perfect quality. This study focuses on the model quality performance criterion and presents a new optimization approach based on Nash-Sutcliffe efficiency (NSE). The proposed approach is configured on optimizing the fitted NSE response surface for the "target is best" case. Furthermore, this study provides a reference in which NSE model performance criterion is used and modeled by response surface approach for the first time in the field of quality improvement. The main advantage of the proposed approach is to allow the practitioners evaluating the model quality performance by maximizing the fitted NSE response surface which acts as a measure of model efficiency. The procedure and the validity of the proposed approach are illustrated on a popular example, the *printing process study*.

Keywords

Robust parameter design, dual response surface, Nash-Sutcliffe efficiency.

1. Introduction.

Robust parameter design (RPD) was introduced by Taguchi (1986) to make the system as robust as possible to undesirable fluctuations in the system's performance. RPD, along with Taguchi's philosophy, has received considerable attention for more than thirty years in different industrial fields. However, his experimental methodology and analysis techniques have been exposed to a lot of criticism from the statistical community – e.g., Box (1985) and Vining and Myers (1990). Consequently, new methodologies have been proposed based on these criticisms. Vining and Myers (1990) conducted one of the earliest research attempts to develop an alternative tool for off-line quality, and discussed a procedure constructed by combining response surface methodology (RSM) and the some effective properties of Taguchi's RPD. RSM, first presented by Box and Wilson (1951), is an effective procedure for modeling a possible process relationship between a quality characteristic and design factors to determine the optimal operating conditions.

Vining and Myers (1990) presented the dual response surface (DRS) approach which is configured by separately fitting response surfaces of the system mean and variance. Thereby, DRS meet the primary goal of RPD by optimizing primary response subject to a pre-defined value of secondary response. This novel approach to RSM has become sound and is widely quoted in the current literature. Further improvement for the DRS problem was carried out by Del Castillo and Montgomery (1993) which proposed using nonlinear programming based on inequality constraints. Subsequently, the concept of the relaxing the zero bias assumption is handled by Lin and Tu (1995) and Copeland and Nelson (1996). Lin and Tu (1995) focused on the process bias along with the variability and proposed minimizing the MSE criterion. A slightly different version of the MSE criterion, based on considering how far the mean can be located from its target, is discussed by Copeland and Nelson (1996). Further work has been conducted by Köksoy and Doganaksoy (2003). They proposed an alternative formulation based on joint optimization of the mean and standard deviation responses under no constraints or minimally constrained. Following these articles, some studies examining the DRS problem can be listed as follows: Shoemaker et al. (1991), Lucas (1994), Kim and Lin (1998), Fan (2000), Köksoy (2005), Köksoy and Fan (2012), Zeybek and Köksoy (2016, 2018), Zeybek (2018).

MSE and its general normalization version, NSE, are the two most widely used criteria for the model efficiency. MSE is dependent on the estimated variable and its values vary on the interval $[0, \infty)$. However, MSE has some shortcomings such as it can be very large in magnitude depending on the units of the predicted values. It is also difficult to compare models for different systems or in different formats. On the other hand, NSE can be interpreted as a comparative ability of a model with regards to a baseline model, so it acts a measure of model performance (Gupta et al., 2009). Therefore, especially in hydrological modelling, climatology, and image quality assessment, NSE criterion is an effective alternative to MSE since it is dimensionless, being scaled onto the interval $(-\infty, 1]$. The general applications of the NSE can be found in the papers of Murphy (1988), Weglarzyk (1998), Gupta et al. (2009), Zhong and Dutta, (2015).

This paper focuses on a NSE criterion based quality improvement approach and provides a reference in which fitted NSE model performance criterion response surface is used for the first time in a robust parameter design. To make an improvement of the performance of the process design, NSE criterion is modeled by response surface approach and configured on the optimizing for the "target is best" case. Since the fitted NSE response surface is used as an objective function in the optimization, the best operating conditions are determined by maximizing the model quality performance criterion. So, the practitioners obtain the criterion to be precise and interpret the value assigned to the quality criterion of the system mean and variance estimates.

The remainder of this manuscript is divided into three sections as follows: A brief overview of NSE criterion is presented in the next section. Section 3 presents the proposed approach. The proposed approach is applied on the basis of a popular example *printing process* study, before the paper finally ends with a conclusion.

2. Overview of NSE criterion

Suppose a set of data in the form of $(x_{1i}, x_{2i}, \dots, x_{mi}, y_i, i = 1, \dots, n)$ where y_i is the response variable affected by the independent variables x_j $(j = 1, \dots, m)$. Then, a statistical model such as $\hat{y} = f(x_1, x_2, \dots, x_m)$ can be created to predict the values of the response variable.

As a measure for the model performance, NSE criterion is introduced by Nash and Sutcliffe (1970). NSE better reflects to desirable and undesirable features of the interested model and increases as the quality of the model increases. NSE can be defined in the following form,

$$NSE = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \quad (1)$$

where $\bar{y} = \frac{\sum_{i=1}^{n} y_i}{n}$ is the mean of the observed values of the response. This formula can be applied directly to the original data on any model. It has a range from $-\infty$ to 1. The value 1 indicates the desirability perfect quality and practitioners seek for an NSE value close to 1. A negative NSE signs the unacceptable model performance. In optimization, NSE is subject to maximization.

3. The proposed approach

Consider a quality characteristic y depends on k controllable coded factors, $x_1, x_2, \ldots, x_k$. Suppose that the constructed design has n-design points, each replicates r times, where y_{ij} represents the j^{th} response at the i^{th} design point, $j = 1, \ldots, r$ and $i = 1, \ldots, n$. Thus, the fitted mean and standard deviation response surfaces, $\hat{\mu}(x)$ and $\hat{\sigma}(x)$, can be modeled by,

$$\hat{\mu}(x) = \hat{\gamma}_0 + \sum_{i=1}^{k} \hat{\gamma}_i x_i + \sum_{i=1}^{k} \hat{\gamma}_{ii} {x_i}^2 + \sum\nolimits_{i<t}^{k} \sum \hat{\gamma}_{it} x_i x_t \tag{2}$$

and

$$\hat{\sigma}(x) = \hat{\delta}_0 + \sum_{i=1}^{k} \hat{\delta}_i x_i + \sum_{i=1}^{k} \hat{\delta}_{ii} {x_i}^2 + \sum\nolimits_{i<t}^{k} \sum \hat{\delta}_{it} x_i x_t \tag{3}$$

where $\hat{\gamma} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{w}_{\boldsymbol{\mu}}$ and $\hat{\delta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{w}_{\sigma}$. The vectors of the sample mean and standard deviation $\mathbf{w}_{\boldsymbol{\mu}} = (\bar{y}_1, \bar{y}_2, \ldots, \bar{y}_n)'$ and $\mathbf{w}_{\sigma} = (s_1, s_2, \ldots, s_n)'$ are obtained from sample mean and standard deviation for each design point. And, $\mathbf{X}$ denotes the design matrix.

For the purposes of constructing NSE response surface based on Equation (1), first, the values of NSE for each design point are determined by the following proposed formula,

$$NSE_i = 1 - \frac{\left(\bar{y}_i - \hat{\mu}_i(x)\right)^2}{(\bar{y}_i - \bar{\bar{y}})^2} \tag{4}$$

where $\bar{\bar{y}} = \frac{\sum_{i=1}^{n} \bar{y}_i}{n}$ is the overall mean of the replicated responses. Here, $\hat{\mu}_i(x)$ represents the estimated mean response of the replicated responses for each design point and is obtained using Equation (2).

Finally, the fitted NSE modeled by a second-order response surface is proposed as follows,

$$\widehat{NSE}(x) = \hat{\alpha}_0 + \sum_{i=1}^{k} \hat{\alpha}_i x_i + \sum_{i=1}^{k} \hat{\alpha}_{ii} {x_i}^2 + \sum\nolimits_{i<t}^{k} \sum \hat{\alpha}_{it} x_i x_t \tag{5}$$

where $\hat{\gamma} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{w}_{\mathbf{NSE}}$, and the vector of the $\mathbf{w}_{\mathbf{NSE}} = (NSE_1, NSE_2, \ldots, NSE_n)'$ is obtained from the designed data using Equation (4) for each design point. $\mathbf{X}$ denotes the design matrix. A general scheme for constructing of the proposed NSE response surface modeling is illustrated in Table 1.

Table 1. General scheme for the proposed NSE response modeling

Design point	**Controllable factors**				**Response (replicated r times)**						
i	x_1	x_2	…	x_k	y_1	y_2	…	y_r	$\bar{y}_i$	$\hat{\mu}_i(x)$	NSE_i
1	x_{11}	x_{12}		x_{1k}	y_{11}	y_{12}		y_{1r}	$\bar{y}_1$	$\hat{\mu}_1(x)$	NSE_1
2	x_{21}	x_{22}		x_{2k}	y_{21}	y_{22}		y_{2r}	$\bar{y}_2$	$\hat{\mu}_2(x)$	NSE_2
3	x_{31}	x_{32}		x_{3k}	y_{31}	y_{32}		y_{3r}	$\bar{y}_3$	$\hat{\mu}_3(x)$	NSE_3
…	…	…		…	…	…		…	…	…	…
n	x_{n1}	x_{n2}		x_{nk}	y_{n1}	y_{n2}		y_{nr}	$\bar{y}_n$	$\hat{\mu}_n(x)$	NSE_n

The regular DRS optimization assigns the best operating conditions, subject to an additional constraint $(\boldsymbol{x}^* \in R)$, which defines the experimental region, i.e., $-1 \leq x_i \leq 1$, $i = 1, \ldots, k$ for cuboidal designs and $\mathbf{x}'\mathbf{x} \leq \rho^2$ for spherical designs, where ρ is the design radius. Therefore, for the "target is best" case, the optimization of the proposed NSE response modeling is suggested based on maximizing $\widehat{NSE}(x)$ given by Equation (5) under an additional constraint of the experiment, such as spherical or cuboidal. In addition, NSE has a range from $-\infty$ to 1 where 1 indicates the desirability perfect quality and negative NSE signs the unacceptable model performance. Therefore, for the purposes of determining the best operating conditions with a desirable quality performance, an additional constraint should be added such that $0 \leq \widehat{NSE}(x) \leq 1$.

4. Example: Printing process study

The proposed NSE based quality improvement approach is illustrated by a well-known printing process study example from Box and Draper (1987). A 3^3 factorial design with three replicates, see Table 2, is performed to examine the effect of speed (x_1), pressure (x_2), and distance (x_3) on the ability of a printing machine (y) to apply colored inks to package labels. The fitted response surfaces for the process mean and standard deviation were obtained by Vining and Myers (1990) as follows:

$$\hat{\mu}(x) = 327.6 + 177.0x_1 + 109.4x_2 + 131.5x_3 + 32.0x_1^2 - 22.4x_2^2 - 29.1x_3^2 + 66.0x_1x_2 + 75.5x_1x_3 + 43.6x_2x_3 \quad (6)$$

$$\hat{\sigma}(x) = 34.9 + 11.5x_1 + 15.3x_2 + 29.2x_3 + 4.2x_1^2 - 1.3x_2^2 + 16.8x_3^2 + 7.7x_1x_2 + 5.1x_1x_3 + 14.1x_2x_3 \quad (7)$$

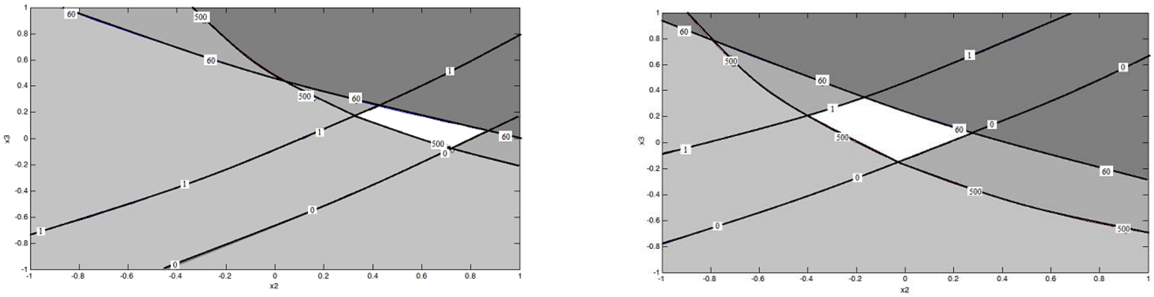
Thus, for the purposes of constructing NSE response surface given by Equation (5), first, the estimated values of the mean $\hat{\mu}_i(x)$, $i = 1, \dots, n$, are obtained using Equation (6), and then the values of NSE for each design point (NSE_i ,$i = 1, \dots, n$) are determined using Equation (4), see Table 2. When the NSE_i values are examined, it is obvious that the design points 6, 9, 16, and 19 have negative NSE which indicates that unacceptable model performance. However, the remaining design points have NSE values greater than zero, generally around 0.90, i.e., quality performance is good. Finally, the fitted NSE response surface is obtained as follows,

$$\widehat{NSE}(x) = 1.59 - 0.56x_1 - 0.57x_2 + 0.63x_3 - 0.77x_1^2 - 0.53x_2^2 - 0.65x_3^2 - 0.77x_1x_2 + 1.25x_1x_3 + 0.98x_2x_3 \quad (8)$$

Table 2. The printing process study.

i	x_1	x_2	x_3	y_1	y_2	y_3	$\bar{y}_i$	s	$\hat{\mu}_i(x)$	NSE_i
1	-1	-1	-1	34	10	28	24.00	12.49	75.30	0.97
2	0	-1	-1	115	116	130	120.33	8.39	78.80	0.95
3	1	-1	-1	192	186	263	213.67	42.83	146.30	0.56
4	-1	0	-1	82	88	88	86.00	3.46	97.50	1.00
5	0	0	-1	44	178	188	136.67	80.41	167.00	0.97
6	1	0	-1	322	350	350	340.67	16.17	300.50	-1.39
7	-1	1	-1	141	110	86	112.33	27.57	74.90	0.97
8	0	1	-1	259	251	259	256.33	4.62	210.40	0.38
9	1	1	-1	290	280	245	271.67	23.63	409.90	-9.33
10	-1	-1	0	81	81	81	81.00	0.00	116.80	0.98
11	0	-1	0	90	122	93	101.67	17.67	195.80	0.80
12	1	-1	0	319	376	376	357.00	32.91	338.80	0.82
13	-1	0	0	180	180	154	171.33	15.01	182.60	0.99
14	0	0	0	372	372	372	372.00	0.00	327.60	0.40
15	1	0	0	541	568	396	501.67	92.50	536.60	0.97
16	-1	1	0	288	192	312	264.00	63.50	203.60	-0.42
17	0	1	0	432	336	513	427.00	88.61	414.60	0.99
18	1	1	0	713	725	754	730.67	21.08	689.60	0.99
19	-1	-1	1	364	99	199	220.67	133.82	100.10	-0.65
20	0	-1	1	232	221	266	239.67	23.46	254.60	0.96
21	1	-1	1	408	415	443	422.00	18.52	473.10	0.77
22	-1	0	1	182	233	182	199.00	29.44	209.50	0.99
23	0	0	1	507	515	434	485.33	44.64	430.00	0.89
24	1	0	1	846	535	640	673.67	158.21	714.50	0.99
25	-1	1	1	236	126	168	176.67	55.51	274.10	0.50
26	0	1	1	660	440	403	501.00	138.94	560.60	0.90
27	1	1	1	878	991	1161	1010.00	142.45	911.10	0.98

An effective way as a starting point to solve a DRS problem is graphical methods which provide to examine the location of the optimal operating conditions by superimposing the contour plots for the interested responses. Figure 1 display the overlaid contour plots of this printing process example. In generating these plots, in line with the assumptions of Köksoy and Doganaksoy (2003), a mean value greater than 500 and standard deviation less than 60 are considered. Since only two values of the factors can be used at a time in these plots, the value of x_1 is fixed at 0.5 and 1. Then the constructed plots are illustrated in Figure 1. The white area shows the operating region where process requirements about mean and standard deviation, and NSE criterion are met. When the contour plots are examined, it is obvious that a large value than 0.5 needs to be set for x_1 to meet all process requirements adequately. And, the levels of the x_2 and x_3 need to be changed in reverse directions in order to continue to meet the all requirements simultaneously.



(a) (b)

Figure 1. Contour plots for the NSE, mean and standard deviation response surfaces; (a) $x_1: 0.5$, (b) $x_1: 1$

The printing process study requires such a problem that the target is 500 and the desired standard deviation is less than 60; but, in the papers based on relaxing zero bias optimization; e.g., Lin and Tu (1995) and Köksoy and Doganaksoy (2003), this value is taken as 45. Note that, these values are used in previous studies. In line with the mentioned information about printing process data, the optimal factor settings are obtained by maximizing the following optimization problem,

$$\begin{aligned} &\text{maximizing} \quad \widehat{NSE}(x) \\ &\text{such that} \quad 0 \le \widehat{NSE}(x) \le 1 \qquad \boldsymbol{x}^* \in R \end{aligned}$$

For the experimental region, $\boldsymbol{x}^* \in R$, cuboidal region, $-1 \le x_i \le 1,\ i = 1,2,3$, is examined. On the other hand, two different cases are considered for the constraints related to the system requirements:

i. *zero bias assumption* : $\hat{\mu}(x) = 500$ and $\hat{\sigma}(x) \le 60$
ii. *relaxing zero bias assumption* : $494 < \hat{\mu}(x) \le 500$ and $\hat{\sigma}(x) \le 45$

Table 3 illustrates the results obtained from the proposed approach and existing methods for cuboidal region. In Table 3, while the proposed approach - Case 1 indicates the optimization is conducted under zero bias assumption with the constraints such that $\hat{\mu}(x) = 500$ and $\hat{\sigma}(x) \le 60$, Case 2 represents the relaxing zero bias assumption under the constraints such that $494 < \hat{\mu}(x) \le 500$ and $\hat{\sigma}(x) \le 45$.

Table 3. A comparative study for the printing process example under $-1 \le x_i \le 1,\ i = 1,2,3$

	$\mathbf{x}^*$	$\hat{\boldsymbol{\mu}}$	$\hat{\boldsymbol{\sigma}}$	$\widehat{\boldsymbol{NSE}}$
Proposed approach (Case 1)	$(0.7335, -0.0136, 0.1513)$	500.00	50.65	1.00
Proposed approach (Case 2)	$(1.000, -0.1010, -0.1095)$	496.12	44.87	0.19
Vining and Myers (1990)	$(0.6140, 0.2280, 0.1000)$	500.00	51.77	Unknown
Lin and Tu (1995)	$(1.000, 0.0700, -0.2500)$	494.44	44.43	Unknown
Köksoy and Doganaksoy (2003)	$(1.000, 0.085, -0.2540)$	495.99	44.62	Unknown

For the Case 1, the optimal design point turns out to be $\mathbf{x}^* = (0.7335, -0.0136, 0.1513)$, where $\hat{\mu} = 500$, $\hat{\sigma} = 50.65$, and the resulting $\widehat{NSE} = 1$. The optimal solution obtained by the proposed approach hits the target with a desirable quality performance. And, the proposed approach provides a reduction about %10 in terms of the estimated standard deviation compared with the Vining and Myers (1990) approach. On the other hand, for the Case 2, the optimal design points is obtained as $\mathbf{x}^* = (1.000, -0.1010, -0.1095)$, where $\hat{\mu} = 496.12$, $\hat{\sigma} = 44.87$, and the resulting $\widehat{NSE} = 0.19$. It is obvious that, although there is a decline in the performance of desirable quality, the quality performance is still above zero, i.e., not in the range of unacceptable model performance. In fact, this decline can be explained by the relaxing zero bias assumption about the mean. The proposed approach for the Case 2 has the smallest bias but somewhat large standard deviation compared with the results of Lin and Tu (1995) and Köksoy and Doganaksoy (2003). However, it is important to point that, as Köksoy and Fan (2012) and Zeybek and Köksoy (2016) indicated, the results from different approaches cannot be compared in a straightforward manner since the methods differ in terms of their optimizaiton criteria. On the other hand, if we make a comparison in context of the additional information they provide about the process, using the proposed approach has some advantages. Unlike the existing methods, the proposed approach provides an additional information such as a measure of model performance and this information allows the estimation of which operating conditions offer the perfect quality.

5. Conclusion

The constrained optimization algorithms based quality technologies have received considerable attention in recent years for the quality improvement. In particular, researchers have sought to understand the extent of the quality of the obtained best operating conditions from different quality improvement approaches. This manuscript has presented an effective methodology that quantifies the quality performance of the model acts as a measure of model efficiency.

The NSE criterion a widely used criteria for the model efficiency, thus adapting this criterion in the field of quality improvement not only provides a wide range of engineering information about the system, but also offers a comprehensive solution to the quality engineering. This proposed strategy is constructed on modeling NSE criterion by response surface and using it as an objective function in the optimization to make an improvement of the performance of the process design. Furthermore, the proposed approach is an improvement from the perspective of the best operating conditions which are determined by maximizing the model quality performance criterion. In the future, an efficient technique for the multi-response process optimization based on NSE criterion could be taken into account.

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