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Dynamic multiple responses by ideal solution analysis

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Abstract

High technology industry must continuously improve product quality and multiple correlated product quality characteristics must be assessed simultaneously due to product complexity. While many Taguchi method applications have addressed a state system problem, dynamic multi-response problems have seldom been examined. This study presents a novel optimization procedure for dynamic multiple responses based on Taguchi's parameter design. The signal to noise (SN) ratio and system sensitivity are used to assess the performance of each response. Principal component analysis is then performed on the SN values and system sensitivity values to obtain a set of uncorrelated components. The optimization direction for each component is also determined based on the corresponding variation mode chart. Finally, the relative closeness to the ideal solution resulting from the technique for order preference by similarity to ideal solution is determined as an overall performance index for multiple responses. A case study obtained from biological reduction of an ethyl acetoacetate process demonstrates the effectiveness of the proposed procedure.
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1. Introduction

Stringent global competition demands continuously elevating product quality. Off-line quality control and robust design have been widely implemented throughout industry to upgrade product quality. As a major proponent of the philosophy of robust design, Taguchi focused on information of both the mean and variability of a quality characteristic using the signal to noise (SN) ratio. In doing so, the optimal factor/level combination obtained from the Taguchi method can be determined to simultaneously reduce the quality variation and bring the mean close to the target value. Despite its widespread industrial applications, the Taguchi method can only be used for optimizing single-response problems. Cases involving dynamic multi-response problems have rarely been seen. However, industry has increasingly emphasized developing procedures capable of simultaneously optimizing the dynamic

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multi-response problems in light of the increasing complexity of modern product design. Furthermore, moderate or high correlations among these responses may incur difficulty in optimizing multiple responses simultaneously. Accordingly, developing optimization procedure of dynamic multiple responses must consider the correlations among these responses to accurately depict the multi-response performances in a dynamic system.

This study develops a novel multi-response optimization procedure for a dynamic system that can resolve the correlation problems among responses and reduce the computational complexity. The SN ratio and system sensitivity are used to assess the performance of each response. Principal component analysis (PCA) is then performed on SN values and system sensitivity values to obtain a set of uncorrelated principle components, which are linear combinations of the original responses. Additionally, the variation mode chart is plotted to interpret the variation mode (or principal component variation) resulting from PCA. Based on engineering requirements, engineers can determine the optimization direction for each principal component using the variation mode chart. Finally, technique for order preference by similarity to ideal solution (TOPSIS) is adopted to derive the overall performance index (OPI) for multiple responses. The optimal factor/level combination is determined with the maximum OPI value and therefore, simultaneously reduces the quality variation and brings the mean to the target value. Results obtained from the biological reduction of an ethyl acetoacetate process experiment demonstrate the effectiveness of the proposed procedure.

2. Literature review

2.1. Dynamic system

The feasibility of optimizing a dynamic system has received increasing attention in recent years (Wasserman, 1998). A dynamic system differs from a state system in that the former contains signal factors to achieve the target performance or express the intended output. The response varies with the level of the signal factor. For example, signal factors may be the steering angle in the steering mechanism of an automobile or the speed control setting of a fan. The signal factors are selected by engineers to enhance product functions and enhance manufacturing flexibility.

A dynamic system ideally assumes that a linear form exists between the response and the signal factor. The ideal function can be expressed as follows:

$$Y = \beta M + \varepsilon \tag{1}$$

where Y denotes the response of a dynamic system, M represents the signal factor, β is the slope or system sensitivity, and ε denotes the random error.

Wasserman (1996) indicated that since various control factor/level combinations influence both β and ε, Eq. (1) should be modified as follows:

$$Y = \beta(\mathbf{d})M + \varepsilon(\mathbf{d}) \tag{2}$$

where $\beta(\mathbf{d})$ reflects the system sensitivity under a certain control condition, $\mathbf{d}$. $\varepsilon(\mathbf{d})$ represents the random errors under $\mathbf{d}$, and $\varepsilon(\mathbf{d})$ is assumed to possess a normal distribution with a mean of zero and a variance of $\sigma^2(\mathbf{d})$. Taguchi used the SN ratio and system sensitivity as performance measures in a dynamic system to assess the robustness of a process. The SN ratio and system sensitivity are as follows:

$$SN = 10 \log_{10} \frac{\beta^2}{\sigma^2}, \tag{3}$$

$$S = 10 \log_{10} \beta^2, \tag{4}$$

where S represents the system sensitivity in a dynamic system. Phadke and Dehnad (1988) assumed that the quality loss varies with the input signals. The desired response of the product, $g^*(M)$, can be represented as a function of M. They also defined the quadratic loss through $g^*(M)$. For any given M, the quadratic loss can be expressed as follows:

$$Q(M) = \int_y k[y - g^*(M)]^2 \, dF(y/M)$$
$$= kE_{y/M}[\{y - g^*(M)\}^2] \tag{5}$$

where y denotes the quality characteristic value, M represents the signal factor, and k is a constant. The corresponding expected total loss, $\overline{Q}$, can be expressed as

$$\overline{Q}(z,S) = k[\{B(z,S) - 1\}^2 E\{g^{*^2}\}] + \sigma^2(z,S) \qquad (6)$$

where $\sigma^2(z,S)$ denotes the mean square value of e, $B(z,S)$ is defined as a ratio of the actual slope (or system sensitivity) to the ideal slope, z represents the control factors and S is the scaling factor in a dynamic system.

Eq. (6) reveals that the quality loss is affected by two components. The first component represents the system sensitivity of the output response as deviated from the ideal system sensitivity and the other component represents the variation in the quality characteristics. Taguchi suggested that simultaneously adjusting the actual slope β to the ideal slope β_0 and reducing the quality variation can minimize the total quality loss.

2.2. Multiple responses optimization

Most of the previous optimization methods for multi-response problems focused on a state system. Many Taguchi practitioners have adopted engineering knowledge to resolve multi-response optimization problems. For example, Phadke (1989) combined engineering knowledge with relevant experience to optimize three responses, i.e., surface, wafer thickness, and deposition rate, in a very-large-scale integrated (VLSI) circuit-manufacturing process. Other techniques, such as Logothetis and Haigh (1988), Elsayed and Chen (1993), Chang and Shivpuri (1995), Ames et al. (1997), Tong and Su (1997), Su and Tong (1997) and Antony (2000), either utilized SN ratios for each response to create new composite indices or applied mathematical algorithms to optimize a state multi-response problem. Despite their contributions, the above multi-response optimization methods share the following limitations:

1. The optimal factor/level combination for multiple responses is determined based on pure engineering experience and the correlations among responses are not considered. Owing to that the engineer's judgment often leads to uncertainty during decision making, different engineers may produce conflicting results when addressing the same problem.

2. These procedures are developed based on the linear programming technique or other complicated mathematical algorithms. Therefore, making them impractical for most engineering applications.

2.3. Principal component analysis

Hotelling (1933) initially developed PCA to explain the variance–covariance structure of a set of variables by linearly combining the original variables. The PCA technique can account for most of the variation of the original p variables via k uncorrelated principal components, where $k \leqslant p$. Restated, let $\mathbf{x} = x_1, x_2, \ldots, x_p$ be a set of original variables with a variance–covariance matrix $\boldsymbol{\Sigma}$. Through the PCA, a set of uncorrelated linear combinations can be obtained as the following matrix:

$$\mathbf{Y} = \mathbf{A^T x} \qquad (7)$$

where $\mathbf{Y} = (Y_1, Y_2, \ldots, Y_P)^T$, Y_1 is called the first principal component, Y_2 is called the second principal component and so on; $\mathbf{A} = (a_{ij})_{P \times P}$ and $\mathbf{A}$ is an orthogonal matrix with $\mathbf{A^T A = I}$. Therefore, $\mathbf{x}$ can be expressed as follows:

$$\mathbf{x} = \mathbf{AY} = \sum_{j=1}^{p} \mathbf{A}_{.j} Y_j \qquad (8)$$

where $\mathbf{A}_{.j} = [a_{1j}, a_{2j}, \ldots, a_{pj}]^T$ is the jth eigenvector of $\boldsymbol{\Sigma}$.

Variation mode chart (Yang, 1996) is an effective means of analyzing variation mode (or principal component variation) obtained from PCA. Analyzing this chart can provide further insight into the different variation types for each variation mode. Therefore, the portion of variation contributed by original variables $(x_1, x_2, \ldots, x_p)$ in each mode can be obtained. The calculation process for establishing a variation mode chart is given as follows.

Let $\mathbf{z}_j = \mathbf{A}_{.j} Y_j = [a_{1j}, a_{2j}, \ldots, a_{pj}]^T, Y_j = [z_{1j}, z_{2j}, \ldots, z_{pj}]^T$, Eq. (8) can be rewritten as follows:

$$\mathbf{x} = \mathbf{z}_1 + \mathbf{z}_2 + \cdots + \mathbf{z_p} \qquad (9)$$

where $\mathbf{z}_j$ is a product of a random scalar Y_j and a deterministic vector $\mathbf{A}_{.j}$; $\mathbf{z}_j$ can be defined as a geometrical variation mode. The mean, varianceand standard deviation of z_{ij} are given as follows:

$$E(z_{ij}) = E(a_{ij} \times Y_j) = a_{ij}E(Y_j) = 0, \qquad (10)$$

$$\text{Var}(z_{ij}) = \text{Var}(a_{ij} \times Y_j) = a_{ij}^2\text{Var}(Y_j) = a_{ij}^2\lambda_j, \quad (11)$$

$$\sigma(z_{ij}) = |a_{ij}|\sqrt{\lambda_j}, \qquad (12)$$

where λ_j is the variance of Y_j, representing the eigenvalue of the jth principal component. Fig. 1 plots the variation mode chart based on a three-sigma zone ($u \pm 3\sigma$) that describes the pattern and magnitude for each variation mode. In this figure, the solid line denotes the variation extent limit (VEL$_1$), which is equal to $3\sigma(z_{ij})$ as shown in Eq. (13). The dotted line denotes the variation extent limit (VEL$_2$), which is equal to $-3\sigma(z_{ij})$ as shown in Eq. (14):

$$\text{VEL}_1(z_j) = \left(3a_{1j}\sqrt{\lambda_j}, \ldots, 3a_{pj}\sqrt{\lambda_j} \right), \qquad (13)$$

$$\text{VEL}_2(z_j) = \left(-3a_{1j}\sqrt{\lambda_j}, \ldots, -3a_{pj}\sqrt{\lambda_j} \right). \qquad (14)$$

The following example, including four variables $\mathbf{x} = (x_1, x_2, x_3, x_4)$, illustrates how to use a variation mode chart to characterize the exact pattern and magnitude of a variation mode. In this example, assume that the eigenvalue $\lambda_1 = 33.62$ and $A_{.1} = (0.503, 0.332, -0.455, -0.656)$. The VEL$_1(z_1) = (8.75, 5.77, -7.91, -11.4)$ and the VEL$_2(z_1) = (-8.75, -5.77, 7.91, 11.4)$ are accordingly obtained using Eqs. (13) and (14). Thus, the variation mode chart for the mode 1 is presented in Fig. 2.

Clearly, when x_1 and x_2 vary in the positive direction, x_3 and x_4 vary in the negative direction. As x_1 moves in the positive direction up to 8.75, x_2 moves in the positive direction up to 5.77, x_3 and x_4
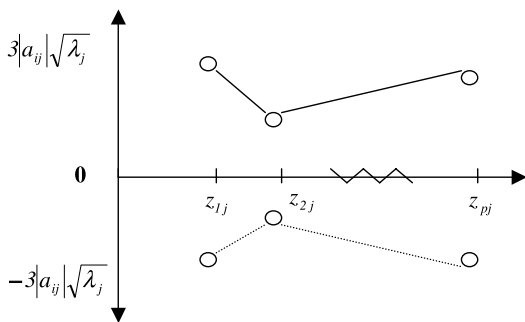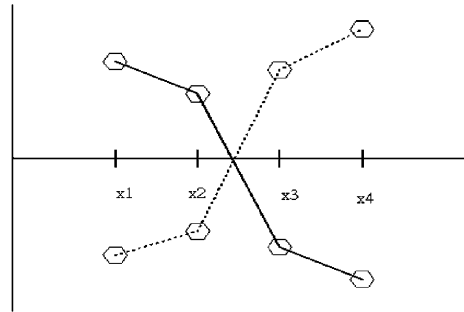

Fig. 1. Variation mode chart.

Fig. 2. An example of variation mode chart.

move in the negative direction up to 7.91 and 11.4, respectively. If responses x_1 and x_2 are more important than responses x_3 and x_4, the principal component score is determined as a larger value is desired. In this case, optimizing (or maximizing) the principal component increases response x_1 and x_2 by 8.75 and 5.77, respectively, and decreases x_3 and x_4 by 7.91 and 11.4, respectively. Whereas responses x_3 and x_4 are more important than responses x_1 and x_2, the principal component score is determined as a smaller value is desired. In this case, optimizing (or minimizing) the principal component decreases responses x_1 and x_2 by 8.75 and 5.77, respectively and increases x_3 and x_4 by 7.91 and 11.4, respectively. Therefore, analysis of variation mode chart can provide further insight into the variation pattern of various variables. Doing so can facilitate the reduction of the origins of variable variations.

2.4. TOPSIS

Hwang and Yoon (1981) developed TOPSIS to assess the alternatives before multiple attributes decision-making. TOPSIS simultaneously considers the distances to the ideal solution and negative ideal solution regarding each alternative and selects the most relative closeness to the ideal solution as the best alternative. That is, the best alternative is the nearest one to the ideal solution and the farthest one from the negative ideal solution. The procedure of TOPSIS is summarized as follows:

1. Establish an alternative performance matrix.

The structure of the alternative performance matrix is expressed as follows:

$$\mathbf{D} = \begin{array}{c} \\ A_1 \\ A_2 \\ \cdot \\ A_i \\ \cdot \\ A_m \end{array} \begin{array}{cccccc} X_1 & X_2 & \dots & X_j & \dots & X_n \\ \left[\begin{array}{cccccc} x_{11} & x_{12} & \dots & x_{1j} & \dots & x_{1n} \\ x_{21} & x_{22} & \dots & x_{2j} & \dots & x_{2n} \\ \cdot & \cdot & \dots & \cdot & \dots & \cdot \\ x_{i1} & x_{i2} & \dots & x_{ij} & \dots & x_{in} \\ \cdot & \cdot & \dots & \cdot & \dots & \cdot \\ x_{m1} & x_{m2} & \dots & x_{mj} & \dots & x_{mn} \end{array} \right] \end{array} \tag{15}$$

where A_i denotes the possible alternatives, $i = 1, \ldots, m$; X_j represents attributes relating to alternative performance, $j = 1, \ldots, n$; and x_{ij} is the performance of A_i with respect to attribute X_j.

2. Normalize the performance matrix.

The normalized performance matrix can be obtained using the following transformation formula:

$$r_{ij} = \frac{x_{ij}}{\sqrt{\sum_{i=1}^{m} x_{ij}^2}} \tag{16}$$

where r_{ij} represents the normalized performance of A_i with respect to attribute X_j. The matrix form of r_{ij} is given as follows:

$$\mathbf{R} = [r_{ij}] \tag{17}$$

where $i = 1, \ldots, m$ and $j = 1, \ldots, n$.

3. Multiply the performance matrix by its associated weights.

Each column of matrix $\mathbf{R}$ is multiplied by weights associated with each attribute. The weighted performance matrix $\mathbf{V}$ is obtained as follows:

$$\mathbf{V} = \begin{bmatrix} w_1 r_{11} & w_2 r_{12} & \cdot & w_j r_{1j} & \cdot & w_n r_{1n} \\ w_1 r_{21} & w_2 r_{22} & \cdot & w_j r_{2j} & \cdot & w_n r_{2n} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ w_1 r_{i1} & w_2 r_{i2} & \cdot & w_j r_{ij} & \cdot & w_n r_{in} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ w_1 r_{m1} & w_2 r_{m2} & \cdot & w_j r_{mj} & \cdot & w_n r_{mn} \end{bmatrix}$$

$$= \begin{bmatrix} v_{11} & v_{12} & \cdot & v_{1j} & \cdot & v_{1n} \\ v_{21} & v_{22} & \cdot & v_{2j} & \cdot & v_{2n} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ v_{i1} & v_{i2} & \cdot & v_{ij} & \cdot & v_{in} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ v_{m1} & v_{m2} & \cdot & v_{mj} & \cdot & v_{mn} \end{bmatrix} \tag{18}$$

where w_j represents the weight of attribute X_j and v_{ij} represents the weighted normalized performance of A_i with respect to X_j for $i = 1, \ldots, m$ and $j = 1, \ldots, n$.

4. Determine the ideal and negative ideal solutions.

The ideal value set V^+ and the negative ideal value set V^- are determined as follows:

$$\mathbf{V}^+ = \{(\max v_{ij} \,|\, j \in \mathbf{J}) \text{ or } (\min v_{ij} \,|\, j \in \mathbf{J}'), \\ i = 1, 2, \ldots, m\} = \{v_1^+, v_2^+, \ldots, v_n^+\},$$

$$\mathbf{V}^- = \{(\min v_{ij} \,|\, j \in \mathbf{J}) \text{ or } (\max v_{ij} \,|\, j \in \mathbf{J}'), \\ i = 1, 2, \ldots, m\} = \{v_1^-, v_2^-, \ldots, v_n^-\},$$

where

$$\mathbf{J} = \{j = 1, 2, \ldots, n \,|\, v_{ij}, \text{ a larger response is desired}\}$$

$$\mathbf{J}' = \{j = 1, 2, \ldots, n \,|\, v_{ij}, \text{ a smaller response is desired}\}$$

5. Calculate the separation measures.

The separation of each alternative from the ideal solution (S_i^+) is given as follows:

$$S_i^+ = \sqrt{\sum_{j=1}^{n} (v_{ij} - v_j^+)^2}. \tag{19}$$

The separation of each alternative from the negative ideal solution (S_i^-) is as follows:

$$S_i^- = \sqrt{\sum_{j=1}^{n} (v_{ij} - v_j^-)^2}. \tag{20}$$

The alternative definitions of $S_i^+ = \sum_{j=1}^{n} |v_{ij} - v_j^+|$ and $S_i^- = \sum_{j=1}^{n} |v_{ij} - v_j^-|$ can also be utilized to replace Eqs. (19) and (20).

6. Calculate the relative closeness to the ideal solution and rank the preference order.

The relative closeness C_i to the ideal solution can be expressed as follows:

$$C_i = \frac{S_i^-}{S_i^+ + S_i^-} \tag{21}$$

where the C_i value lies between 0 and 1. The closer the C_i value is to 1 implies a higher priority of the ith alternative.

3. Proposed procedure

This study proposes an optimization procedure for multiple responses in a dynamic system based on Taguchi's parameter design. Because multiple responses always contain moderate or high correlations among each other, the PCA is initially performed on the SN values and system sensitivity obtained from each response to integrate the dimension of multiple responses to a smaller number of uncorrelated components. The variation mode charts for components obtained from PCA are then utilized to investigate the variation pattern of various integrated responses. Finally, TOPSIS is utilized to determine the optimal factor/level combination for multiple responses. The proposed procedure for optimizing multi-response problems includes the following seven steps:

Step 1. Calculate the SN ratio and system sensitivity for each response.

The SN ratio and system sensitivity can be obtained using Eqs. (3) and (4).

Step 2. Conduct the PCA on normalized SN ratio and system sensitivity.

The SN ratio and system sensitivity for each response is normalized by the following formula:

$$\frac{SN_{ij} - \overline{SN_j}}{S_{SN_j}},\tag{22}$$

$$\frac{S_{ij} - \overline{S_j}}{S_{S_j}},\tag{23}$$

where SN_{ij} denotes the SN ratio of the jth response under the ith experimental run; $\overline{SN_j}$ and S_{SN_j} represent the mean and standard deviation of SN ratios for the jth response, respectively. S_{ij} denotes the system sensitivity of the jth response under the ith experimental run; $\overline{S_j}$ and S_{S_j} represent the mean and standard deviation of system sensitivity for the jth response, respectively. The eigenvalues and eigenvectors for each principal component are obtained after conducting PCA on normalized SN ratio and system sensitivity.

Step 3. Determine the number of principal components retained and establish the variation mode

charts for SN ratio and system sensitivity, respectively.

Some principal components are selected for further analysis based on (1) the significance of the linear correlation between the responses and principal components. (2) the cumulative variation of the responses accounted for by the selected principal components. The corresponding variation mode charts for SN ratio and system sensitivity are also established using Eqs. (13) and (14).

Step 4. Determine the optimization direction of the selected principal components.

The optimization direction of each selected principal component is determined according to the variation mode chart. When more than one principal component is selected for further analysis, the first principal component initially determines the optimization direction. Thereafter, the optimization direction of the second principal component is determined, and so on for the remaining selected components.

Step 5. Conduct TOPSIS to obtain the OPI for the selected principal component scores.

According to the optimization direction of the selected principal components of SN ratio and system sensitivity obtained from Step 4, TOPSIS is then employed to obtain an OPI. Thus, the experimental runs are treated as alternatives; the selected principal components are treated as attributes and quality performance matrices associated with SN ratio and system sensitivity are formed. The weighted quality performance matrices can be obtained using Eqs. (15)–(18), where weights are the eigenvalues associated with each principal component. If a larger value is desired, the ideal and negative ideal solutions representing the maximum and minimum principal component scores of all experimental runs are expressed in Eqs. (24) and (25). Whereas a smaller value is desired, the ideal and negative ideal solution representing the minimum and maximum principal component scores of all experimental runs are expressed in Eqs. (26) and (27). Correspondingly, the OPI values (or C_i values for $i = 1, \ldots, m$) under each experimental run are derived using Eqs. (19)–(21).

$$v_j^+ = \max\{v_{1j}, v_{2j}, \ldots, v_{mj}\}, \tag{24}$$

$$v_j^- = \min\{v_{1j}, v_{2j}, \ldots, v_{mj}\}, \tag{25}$$

$$v_j^+ = \min\{v_{1j}, v_{2j}, \ldots, v_{mj}\}, \tag{26}$$

$$v_j^- = \max\{v_{1j}, v_{2j}, \ldots, v_{mj}\}. \tag{27}$$

Step 6. Determine the optimal factor/level combination.

The main effects on OPI for SN ratio and system sensitivity are determined based on C_i values. Thus, the corresponding diagrams plot the factor effect on OPI. The optimal factor/level combination producing the maximum OPI value is determined based on Taguchi's two-stage optimization procedure. That is, initially, minimize the system variation based on the diagrams of SN ratio. The adjustment factor, significantly affecting to system sensitivity and insignificantly affecting to SN ratio, is then determined based on the diagrams of system sensitivity and SN ratio. Therefore, we can simultaneously reduce quality variation and bring the actual output values on the target values using adjustment factor.

4. Illustrative example

A biological reduction of the ethyl 4-chloro acetoacetate processes for the production of an optically pure compound was used to demonstrate the effectiveness of the proposed optimization method. The Industrial Technology Research Institute at Taiwan performed this illustrative example. S-4-Chloro-3-hydroxybutyric acid ethyl ester (S-CHBE) is a widely used chiral synthon used for synthesizing various optically active compounds such as antihypertensive drugs, HMG-CoA reductase inhibitors and antibiotics (Patel et al., 1992). The compound can be produced by adding ethyl 4-chloro acetoacetate to baker's yeast (Ushio et al., 1991). The reaction produces S-CHBE (a desired-form product) with a small amount R-CHBE (a non-desired-form product). When carefully controlled, the S-CHBE forming enzymes are more active than the R-CHBE and ultimately produce a higher optical purity.

Therefore, the following two optimized responses were determined:

1. For the S-CHBE (y_S) concentration: a larger response is desired.
2. For the R-CHBE (y_R) concentration: a smaller response is desired.

Since altering the substrate concentration will affect both responses y_S and y_R, the substrate concentration was considered a signal factor (M) in the experiment. Additionally, the freshness of the yeast was then considered a noise factor. Throughout the brainstorm analysis and pre-test experiments, eight control factors were selected for optimization. Tables 1 and 2 display these factors and their corresponding levels.

The L_{18} orthogonal array was employed in this experiment. Six observations were made for both y_S and y_R under each experimental combination based on the previous planning experiment. The experimental data was analyzed by strictly following the proposed procedure. Table 3 displays the experimental observations, SN ratios and system sensitivity for each response resulted from Taguchi's SN ratio formula. Tables 4–7 display the eigenvalues and eigenvectors arising from PCA for SN ratios and system sensitivity, respectively, conducted by employing SAS statistical software package (many other statistical soft packages such as SPSS, Minitab or STATISTICA can also be used to conduct PCA).

Both two principal components are retained for SN ratio and system sensitivity according to Tables 4–7, since the first one principal component for SN ratio and system sensitivity only account for 68% and 65% of the variation of the original variables. Two principal components are uncorrelated and can account for 100% of the variation of original variables. Table 8 and Fig. 3 display the variation mode of the first principal component for SN ratio and system sensitivity. Table 9 and Fig. 4 display the variation mode of the second principal component for SN ratio and system sensitivity. Clearly, the directions of variation mode for responses S-CHBE and R-CEBE associated with SN ratio are consistent and the directions of variation mode for responses S-CHBE and

Table 1
Factors and their corresponding levels

Factor		Level		
		Level 1	Level 2	Level 3
Signal factor	Substrate concentration (%)	1	3	5
Noise factor	Batch of yeast (N)	First lot	Second lot	
Control factors	Type of cap (A)	Sponge	Aluminum	
	Shaking rate (B)	140 rpm	170 rpm	200 rpm
	Glucose conc. (C)	0.2%	0.6%	1%
	Yeast addition (D)	Fluctuate level 1	Fluctuate level 2	Fluctuate level 3
	Conc. of enzyme inhibitor (E)	Fluctuate level 1	Fluctuate level 2	Fluctuate level 3
	pH of reaction solution (F)	7.5	8.0	8.5
	Buffer concentration (G)	0.3 M	0.4 M	0.5 M
	Yeast preculture time (H)	1 hour	2 hours	3 hours

Table 2
The fluctuating factor/level

Substrate concentration (%)		1	3	5
Yeast addition (D)	Level 1	40%	80%	120%
	Level 2	60%	100%	140%
	Level 3	80%	120%	160%
Conc. of enzyme inhibitor (E)	Level 1	1.0 ml/l	1.2 ml/l	1.4 ml/l
	Level 2	1.2 ml/l	1.4 ml/l	1.6 ml/l
	Level 3	1.4 ml/l	1.6 ml/l	1.8 ml/l

Table 3
Experimental observations, SN ratio and system sensitivity

Ex. no.	Control factor								SN ratio		System sensitivity	
L_{18}	A	B	C	D	E	F	G	H	S	R	S	R
1	1	1	1	1	1	1	1	1	0.81	−2.21	−6.87	−19.65
2	1	1	2	2	2	2	2	2	5.81	1.30	−7.48	−18.28
.	.	.	.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.	.	.	.
17	2	3	2	1	3	1	2	3	3.82	2.56	−8.68	−24.51
18	2	3	3	2	1	2	3	1	5.55	0.48	−7.38	−19.63

R-CHBE associated with system sensitivity are opposite in the first principal component. Therefore, the first principal component is determined, as a larger value desired integrated response. Doing so, the SN ratios of both responses can be enhanced, the response value for S-CHBE can be increased and the response value for R-CHBE can be decreased simultaneously, these conforming the engineering requirement, when optimizing the first principal component. Whereas, the directions of variation mode for responses S-CHBE and R-CHBE associated with SN ratio are opposite and the directions of variation mode for responses S-CHBE and R-CHBE associated with system sensitivity are consistent in the second principal component. Since the selected optimization direction of the second principal component cannot comfort the engineering requirement for responses

Table 4
The eigenvalues and explained percentage of variation for SN ratios

Compo-nents	Eigen-value	Differ-ence	Percent-age	Cumulative percentage
First component	1.35723	0.714450	0.678613	0.67861
Second component	0.64277	–	0.321387	1.00000

Table 5
The eigenvectors of principal components for SN ratio

Response	First component	Second component
S-CHBE	0.707107	0.707107
R-CHBE	0.707107	−0.707107

Table 6
The eigenvalues and explained percentage of variation for sensitivity

Compo-nents	Eigen-value	Differ-ence	Percent-age	Cumulative percentage
First component	1.30626	0.612512	0.653128	0.65313
Second component	0.69374	–	0.346872	1.00000

Table 7
The eigenvectors of principal components for system sensitivity

Response	First component	Second component
S-CHBE	0.707107	0.707107
R-CHBE	−0.707107	0.707107

S-CHBE and R-CHBE in SN ratio and system sensitivity simultaneously, we must determine the optimization direction by trading off between these two responses. Because the S-CHBE is more important than R-CHBE, the second principal component is determined, as a larger value desired

Table 8
The variation mode for SN ratio

The first principal component					
SN ratio	+	–	System sensitivity	+	–
S-CHBE	2.47	−2.47	S-CHBE	2.42	−2.42
R-CHBE	2.47	−2.47	R-CHBE	−2.42	2.42

Table 9
The variation mode for system sensitivity

The second principal component					
SN ratio	+	–	System sensitivity	+	–
S-CHBE	1.70	−1.70	S-CHBE	1.77	−1.77
R-CHBE	−1.70	1.70	R-CHBE	1.77	−1.77

integrated response. In this case, increasing the SN ratio of response S-CHBE by 1.70 can decrease the SN ratio of NU by 1.70 and increase the system sensitivity of responses S-CHBE and R-CHBE by 1.77 simultaneously.

Table 10 lists the OPI values, which are measures of relative closeness to the ideal solution for SN ratio and system sensitivity resulting from TOPSIS. Accordingly, the response diagram on OPI values for SN ratio and system sensitivity is established as shown in Figs. 5 and 6. According to Tables 11 and 12 and Figs. 5 and 6, the following results can be obtained:

1. The trends of factors A and F are consistent on SN ratio and system sensitivity. Accordingly, the optimal level is determined with the larger SN ratio for factors A and F.
2. For factors B, C, E and G, the effect on SN ratio is larger than on system sensitivity. Therefore, the optimal level is determined with the larger SN ratio for these factors.
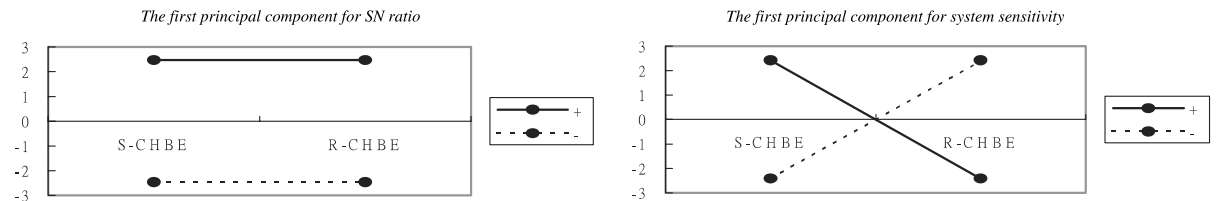

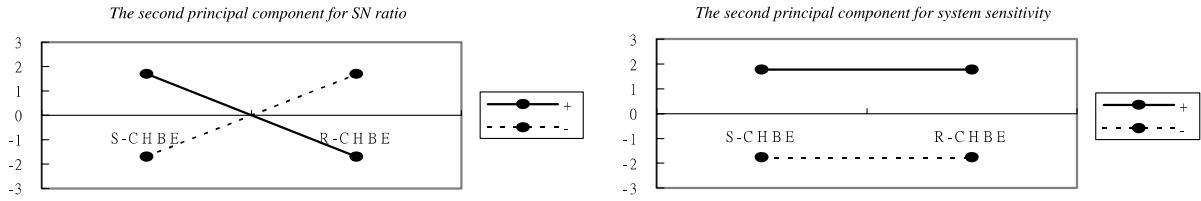Fig. 3. The variation mode chart for the first principal component.

Fig. 4. The variation mode chart for the second principal component.

Table 10
The overall performance index for SN ratio and system sensitivity

Ex. no.	OPI for SN ratio	OPI for system sensitivity
1	0.65	0.30
2	0.50	0.79
.	.	.
.	.	.
17	0.50	0.65
18	0.56	0.75

3. For factors D and H, the effect on system sensitivity is larger than on SN ratio. Therefore, the optimal level is determined with the larger system sensitivity for these two factors.

Base on the above analysis, the optimal factor/level combination is determined as $A_1B_3C_2D_1E_2$-$F_2G_2H_1$. Factor H is considered as an adjustment factor, since this factor significantly affects to the system sensitivity and insignificant affects to the SN ratio. Note that using the alternative S_i^+ and S_i^-, the same optimal factor/level combination will also be obtained.

The predicted SN ratio and system sensitivity based on significant factors for S-CHBE and R-CHBE under the optimal factor/level combination are calculated and compared with that of the starting factor–level to confirm the reproducibility. For S-CHBE, factors B, D, E and F are significant effects on SN ratio and factors A, D, E, F and H are significant effects on system sensitivity. For R-CHBE, factors B, E, F and H are significant effects on SN ratio and factors A, B, C, D and E are significant effects on system sensitivity. Accordingly, the predicted SN ratio and system sensitivity for S-CHBE and R-CHBE are calculated as follows:

The SN ratio for S-CHBE is

$$\eta_{\text{opt}} = \bar{\eta} + (\eta_{B_3} - \bar{\eta}) + (\eta_{D_1} - \bar{\eta}) + (\eta_{E_2} - \bar{\eta}) + (\eta_{F_2} - \bar{\eta}) = 5.347.$$

The SN ratio for R-CHBE is

$$\eta_{\text{opt}} = \bar{\eta} + (\eta_{B_3} - \bar{\eta}) + (\eta_{E_2} - \bar{\eta}) + (\eta_{F_2} - \bar{\eta}) + (\eta_{H_1} - \bar{\eta}) = 3.411.$$
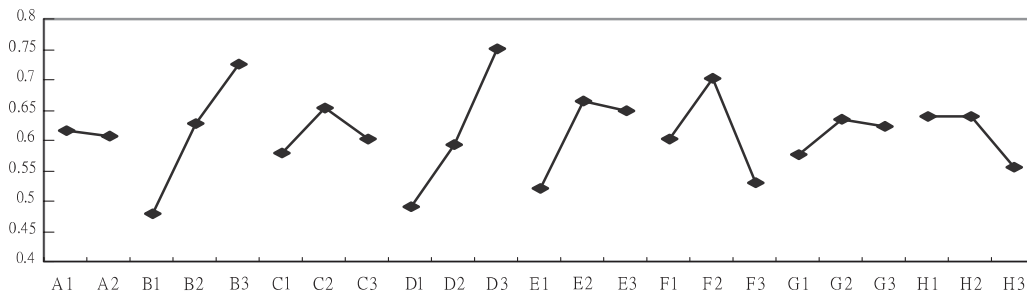

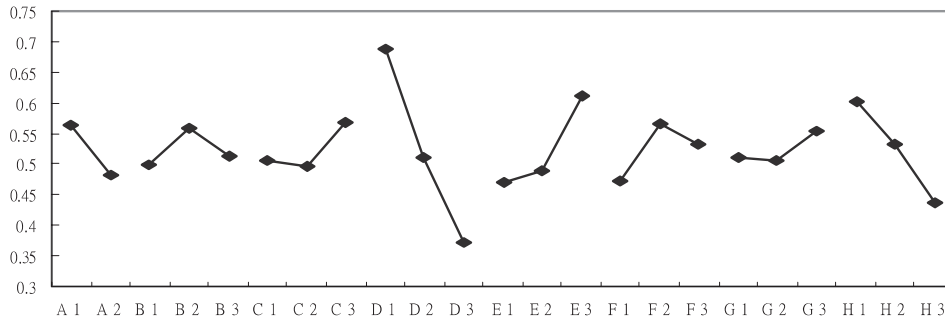Fig. 5. Response diagram for SN ratio.

Fig. 6. Response diagram for system sensitivity.

Table 11
Response table for SN ratio

Factors	Level 1	Level 2	Level 3	Difference
A	0.62	0.61		0.01
B	0.48	0.63	0.73	0.25
C	0.58	0.65	0.60	0.07
D	0.49	0.59	0.75	0.26
E	0.52	0.67	0.65	0.15
F	0.60	0.70	0.53	0.17
G	0.58	0.64	0.62	0.06
H	0.64	0.64	0.56	0.08

Table 12
Response table for system sensitivity

Factors	Level 1	Level 2	Level 3	Difference
A	0.56	0.48		0.08
B	0.50	0.56	0.51	0.06
C	0.51	0.50	0.57	0.07
D	0.69	0.51	0.37	0.32
E	0.47	0.49	0.61	0.14
F	0.47	0.57	0.53	0.09
G	0.51	0.51	0.55	0.05
H	0.60	0.53	0.44	0.17

Meanwhile, the system sensitivity for S-CHBE is

$$\eta_{\text{opt}} = \bar{\eta} + (\eta_{A_1} - \bar{\eta}) + (\eta_{D_1} - \bar{\eta}) + (\eta_{E_2} - \bar{\eta}) + (\eta_{F_2} - \bar{\eta})$$
$$+ (\eta_{H_1} - \bar{\eta}) = -6.078.$$

The system sensitivity for R-CHBE is

$$\eta_{\text{opt}} = \bar{\eta} + (\eta_{A_1} - \bar{\eta}) + (\eta_{B_3} - \bar{\eta}) + (\eta_{C_2} - \bar{\eta})$$
$$+ (\eta_{D_1} - \bar{\eta}) + (\eta_{E_2} - \bar{\eta}) = -22.257.$$

Table 13 summarizes the computations of the predicted SN values and system sensitivity values

for both responses and compares with the starting level, $A_1B_3C_2D_2E_2F_2G_2H_1$. Table 13 reveals that the predicted SN ratio and system sensitivity both on S-CHBE and R-CHBE are significant improved except the SN ratio for S-CHBE is slightly lower than the starting level. This finding confirms that the optimal factor/level combination can be reproduced and the proposed procedure for optimizing dynamic multiple responses can efficiently enhance the product/process quality.

5. Conclusion

This study utilizes the PCA to simplify the dynamic multi-response problems and determines the optimization direction by using the variation mode chart. The optimal factor/level combination is also determined based on the OPI for multiple responses obtained from TOPSIS. A case study in which the biological reduction of the ethyl 4-chloro acetoacetate processes for the production of an optically pure compound is optimized confirms the effectiveness of the proposed procedure.

The proposed procedure has the following merits:

1. The multi-response optimization direction is difficult to determine when optimizing response individually, since moderate or high conflicting exits among the optimization factor/level combination for theses responses, especially in dynamic system in light of considering the effects of SN ratio and system sensitivity on the dynamic system simultaneously. The OPI

Table 13
Summary of the computations for the proposed procedure and starting level

| | Factor/level | Predicted values | | | |
| | | SN ratio | | System sensitivity | |
		S-CHBE	R-CHBE	S-CHBE	R-CHBE
The proposed procedure	$A_1B_3C_2D_1E_2F_2G_2H_1$	5.347	3.411	**−6.078**	**−22.257**
Starting level	$A_1B_3C_2D_2E_2F_2G_2H_1$	**6.814**	3.411	−6.587	−19.574

obtained from TOPSIS can eliminate these conflicts. Furthermore, the TOPSIS simultaneously considers the ideal and negative ideal solution to obtain an overall performance index. Therefore, the OPI cannot be dominated by the best or the worst quality characteristics.

2. The proposed procedure transforms the correlated multiple responses into uncorrelated components through PCA, thereby simplifying the optimization process. Therefore, the more responses the more efficiently this proposed procedure can get.

3. The proposed procedure can also resolve the multi-response problems in a static system with some modification.

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