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ORIGINAL ARTICLE

A unique solution for principal component analysis-based multi-response optimization problems

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Abstract A procedure to find a unique solution for multi-response optimization problems based on indexing is presented. The procedure utilizes principal component analysis to map the original data to a new vector of component scores, transforming the original response variables into uncorrelated principal components. This process involves loadings that are the elements of the eigenvectors corresponding to the eigenvalues of response variables in the correlation matrix. It is shown that for a given eigenvalue λ, its corresponding eigenvectors are not unique, which could lead to different "optimal" parametric (factor-level) settings and will further mislead the process or product improvement strategy. The proposed indexing method will determine a unique optimal solution in the presence of $(2^p)(p!)$ combinations of eigenvectors.

Keywords Multi-response optimization · PCA · Indices · Eigenvector · Factor levels

1 Introduction

The objective of the robust design of experiments is to make a product and a process robust against the influence of uncontrollable factors. This objective can be achieved through parameter optimization and design of experiments. Parameter optimization and quality improvement based on the Taguchi method have shown high effectiveness and robustness and have been widely used in many areas. To meet the requirement of considering more than one quality characteristics in a real industrial process, the traditional single-response method has been expanded to multi-response optimization. Table 1 presents a typical multi-response experimental layout. Many approaches for multi-response optimization such as assigning weight to response variables [1], grey relational analysis [2], and multiple regression model [3] have been proposed in recent years.

Among these approaches, multi-response optimization based on principal component analysis (PCA) has gained more attention since it takes into account the possible correlations between response variables without increasing the computational complexity. Su and Tong [4] proposed the PCA-based multi-response robust design procedure and transformed a set of response variables to a set of uncorrelated principal components by applying PCA so that the number of responses is reduced and the optimal factor/level combination can be chosen based on these uncorrelated components. The detailed procedure of this approach is shown in "Section 2."

In the PCA-based multi-response optimization process [4], the components with eigenvalues larger than 1 are chosen to replace the original response variables. When more than one components with larger than 1 eigenvalues are selected, the tradeoffs are needed, but there is no standard method for selecting a feasible tradeoff solution. To overcome this shortcoming in the PCA-based method, Liao [5] proposed a weighted principal component analysis (WPCA)-based multi-response optimization approach which takes all the uncorrelated components into consideration in order to explain all the response variables. Each component is multiplied by a weight, which is the proportion of its corresponding variance over the total variance. The weights are used to emphasize the contribution of components based on their corresponding variation. All the weighted components are combined into one multi-response performance index (MPI) through summation,

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Table 1 Experimental data for multi-response optimization

Measurement combination no.	Factor level				Response			
	1st	2nd	⋯	k th	Y_1	Y_2	⋯	Yp
1	−	−	⋯	−	$y_{111}, y_{112}, \cdots, y_{11n}$	$y_{121}, y_{122}, \cdots, y_{12n}$	⋯	$y_{1p1}, y_{1p2}, \cdots, y_{1pn}$
2	+	−	⋯	−	$y_{211}, y_{212}, \cdots, y_{21n}$	$y_{221}, y_{222}, \cdots, y_{22n}$	⋯	$y_{2p1}, y_{2p2}, \cdots, y_{2pn}$
3	−	+	⋯	−	$y_{311}, y_{312}, \cdots, y_{31n}$	$y_{321}, y_{322}, \cdots, y_{32n}$	⋯	$y_{3p1}, y_{3p2}, \cdots, y_{3pn}$
4	+	+	⋯	−	$y_{411}, y_{412}, \cdots, y_{41n}$	$y_{421}, y_{422}, \cdots, y_{42n}$	⋯	$y_{4p1}, y_{4p2}, \cdots, y_{4pn}$
⋮	⋮	⋮		⋮	⋮	⋮		⋮
$m = 2^k$	+	+	⋯	+	$y_{m11}, y_{m12}, \cdots, y_{m1n}$	$y_{m21}, y_{m22}, \cdots, y_{m2n}$	⋯	$y_{mp1}, y_{mp2}, \cdots, y_{mpn}$

and the choice of optimal factor-level combination is based on the value of MPI. The main procedures for applying multi-response optimization based on WPCA are shown in "Section 2." This paper presents a detailed study and improvement over the WPCA-based method.

However, one of the challenges in PCA is how to interpret the principal components, and this problem also exists in principal component-based multi-response optimization procedures. Auer et al. [6] pointed out that PCA-based approach is meaningful only if none of the elements in eigenvectors is negative. In another study, Gauri et al. [7] discussed several problems with the PCA-based multi-response optimization approach, including the misleading results caused by the normalization of input data and different results obtained by using quality loss versus S/N ratio as input data. Moreover, different optimal solutions are obtained from using different statistical software packages.

In this paper, it is shown that each eigenvalue obtained from the application of PCA in multi-response optimization has a set of eigenvectors, and different eigenvectors corresponding to each eigenvalue will lead to different results. To solve this problem, a method for determining the optimal eigenvector combination is proposed. Once the optimal eigenvector combination is determined, these eigenvectors are used to calculate the multi-response performance indices, and then the optimal factor-level combination will be uniquely determined. "Section 2" presents the detailed procedures of multi-response optimization based on PCA and on WPCA. "Section 3" presents some details concerning the usage of quality loss or S/N ratio as input data. In "Section 4," the problem caused by one eigenvalue corresponding to more than one eigenvectors is stated and analyzed. To solve this problem, a method for determining the optimal eigenvector combination is proposed in "Section 5." To verify the proposed approach, a numerical example is given in "Section 6."

2 Multi-response optimization based on principal components

In the application of Taguchi's robust design experimentation, a 2^k factorial design problem with p response variables and n replicates per experiment (run) is given in Table 1.

In Table 1, y_{ijk} is the jth response of the ith measurement combination for the kth replication, $i=1,2,\ldots,m$, $j=1,2,\ldots,p$, and $k=1,2,\ldots,n$. The step-by-step procedures for executing PCA-based multi-response optimization and WPCA-based multi-response optimization are described below:

Step 1: Compute quality loss or S/N ratio for each response:

(a) Compute loss of the jth response in the ith measurement combination (L_{ij}) for the smaller-the-better case,

$$L_{ij} = c\left(\frac{1}{n}\sum_{k=1}^{n} y_{ijk}^2\right)$$

for the larger-the-better case,

$$L_{ij} = c\left(\frac{1}{n}\sum_{k=1}^{n} \frac{1}{y_{ijk}^2}\right)$$

and for the nominal-the-better case,

$$L_{ij} = c\left[\left(\frac{1}{n}\sum_{k=1}^{n} y_{ijk} - T_i\right)^2 + \frac{1}{n-1}\sum_{k=1}^{n}\left(y_{ijk} - \frac{1}{n}\sum_{k=1}^{n} y_{ijk}\right)^2\right]$$

(b) Compute S/N ratio of the jth response in the ith measurement combination (η_{ij}) for the smaller-the-better and the larger-the-better cases,

$$\eta_{ij} = -10\log_{10} L_{ij}$$

and for the nominal-the-better cases,

$$\eta_{ij} = 10\log_{10}\left[\frac{\left(\frac{1}{n}\sum_{k=1}^{n} y_{ijk}\right)^2}{\frac{1}{n-1}\sum_{k=1}^{n}\left(y_{ijk}-\frac{1}{n}\sum_{k=1}^{n} y_{ijk}\right)^2}\right]$$

Step 2: Normalize quality loss or S/N ratio of each response:

(a) If quality losses are used as input data, normalize quality loss for each response,

$$L_{ij}^{(N)} = \frac{L_{ij}-\min\{L_{1j}, L_{2j}, \dots, L_{mj}\}}{\max\{L_{1j}, L_{2j}, \dots, L_{mj}\}-\min\{L_{1j}, L_{2j}, \dots, L_{mj}\}}$$

(b) If S/N ratios are used as input data, normalize S/N ratio for each response,

$$\eta_{ij}^{(N)} = \frac{\eta_{ij}-\min\left\{\eta_{1j}, \eta_{2j}, \dots, \eta_{mj}\right\}}{\max\left\{\eta_{1j}, \eta_{2j}, \dots, \eta_{mj}\right\}-\min\left\{\eta_{1j}, \eta_{2j}, \dots, \eta_{mj}\right\}}$$

The normalized data are summarized in Table 2.

Step 3: Perform PCA on normalized data of Table 2 to identify the elements of the eigenvector corresponding to the lth largest eigenvalue $\lambda^{(l)}$

$$a_{l1}, a_{l2}, \dots, a_{lp}$$

and the lth component for the ith measurement combination (z_{il}):

$$z_{il} = a_{l1}L_{i1}^{(N)} + a_{l2}L_{i2}^{(N)} + \cdots + a_{lp}L_{ip}^{(N)}$$

or

$$z_{il} = a_{l1}\eta_{i1}^{(N)} + a_{l2}\eta_{i2}^{(N)} + \cdots + a_{lp}\eta_{ip}^{(N)}$$

Step 4: Transform normalized quality loss or normalized SN ratio into a Multi-response Performance Index (MPI) statistics:

(a) For multi-response optimization based on PCA, choose components with eigenvalue greater than 1 to replace the original responses and assign an index (Ω_l) to the eigenvector corresponding to the l th largest eigenvalue, as shown in Table 3.

(b) For multi-response optimization based on WPCA, the explained variance of each component is considered as weight (w_l),

$$w_l = \frac{\lambda^{(l)}}{\lambda^{(1)} + \lambda^{(2)} + \cdots + \lambda^{(p)}}$$

and all components are combined into one MPI, as shown in Table 4.

Step 5: Determine the optimal factor-level combination:

From the analysis of variance (ANOVA) of MPI, the factor-level combination corresponding to the optimal values of multi-response performance index Ω is chosen as the optimal result.

Reasons for choosing between quality loss or S/N ratio as input data and their effects on determining the optimal solution in the process of PCA- and WPCA-based multi-response optimization are presented in "Section 3."

3 Criterion for using quality loss or SN ratio as input data

It can be observed from the previous section that either quality losses or SN ratios are used as an input data for multi-response optimization analysis in the previous studies and applications. In the PCA-based multi-response optimization approach proposed by Su and Tong [4], they used quality loss as the input data. Meanwhile, Antony [8] performed PCA on normalized quality loss data in industrial experiments. The SN ratio, by contrast, is widely accepted and used as a performance measure, especially in engineering applications, since "it combines location and dispersion of a response variable in a single

Table 2 Normalized quality loss/SN ratio

Measurement combination no.	Factor level				Normalized quality loss/SN ratio			
	1st	2nd	⋯	k th	Y_1	Y_2	⋯	Y_p
1	–	–	⋯	–	$L_{11}^{(N)}$ or $\eta_{11}^{(N)}$	$L_{12}^{(N)}$ or $\eta_{12}^{(N)}$	⋯	$L_{1p}^{(N)}$ or $\eta_{1p}^{(N)}$
2	+	–	⋯	–	$L_{21}^{(N)}$ or $\eta_{21}^{(N)}$	$L_{22}^{(N)}$ or $\eta_{22}^{(N)}$	⋯	$L_{2p}^{(N)}$ or $\eta_{2p}^{(N)}$
3	–	+	⋯	–	$L_{31}^{(N)}$ or $\eta_{31}^{(N)}$	$L_{32}^{(N)}$ or $\eta_{32}^{(N)}$	⋯	$L_{3p}^{(N)}$ or $\eta_{3p}^{(N)}$
4	+	+	⋯	–	$L_{41}^{(N)}$ or $\eta_{41}^{(N)}$	$L_{42}^{(N)}$ or $\eta_{42}^{(N)}$	⋯	$L_{4p}^{(N)}$ or $\eta_{4p}^{(N)}$
⋮	⋮	⋮		⋮	⋮	⋮		⋮
m	+	+	⋯	+	$L_{m1}^{(N)}$ or $\eta_{m1}^{(N)}$	$L_{m2}^{(N)}$ or $\eta_{m2}^{(N)}$	⋯	$L_{mp}^{(N)}$ or $\eta_{mp}^{(N)}$

Table 3 Compute MPI for multi-response optimization based on PCA

Measurement combination no.	Factor level				Multi-response performance index (MPI)			
	1st	2nd	$\cdots$	k th	Ω_1 $\lambda^{(1)}>1$	Ω_2 $\lambda^{(2)}>1$	$\cdots$	Ω_h $\lambda^{(h)}>1$
1	–	–	$\cdots$	–	z_{11}	z_{12}	$\cdots$	z_{1h}
2	+	–	$\cdots$	–	z_{21}	z_{22}	$\cdots$	z_{2h}
3	–	+	$\cdots$	–	z_{31}	z_{32}	$\cdots$	z_{3h}
4	+	+	$\cdots$	–	z_{41}	z_{42}	$\cdots$	z_{4h}
$\vdots$	$\vdots$	$\vdots$		$\vdots$	$\vdots$	$\vdots$		$\vdots$
m	+	+	$\cdots$	+	z_{m1}	z_{m2}	$\cdots$	z_{mh}

performance measure, whereas other methods examine mean and variance as separate performance measures" and "SN ratios are always expressed in decibels" [3]. However, Gauri and Pal [7] pointed out that due to the replication variability, it is possible that two response variables are highly correlated whereas their SN ratios are not or two response variables have small correlation, but their SN ratios result in a significant correlation coefficient. If this happens, applying PCA on SN ratios will mislead the optimization result since PCA provides an orthogonal transformation based on correlation analysis.

Su and Tong [4] applied PCA in the multi-response optimization first; they designed a procedure to transform response variables into uncorrelated components which are used for determining the optimal factor-level combination. In this procedure, the quality loss for each response at each experimental trail is computed, and PCA is performed on the basis of the normalized quality losses. After the original response variables are transferred into a set of principal components, the original experimental values are projected into the new coordinate system related to these components and denoted as the multi-response performance index (MPI). The components with eigenvalues larger than "one" are kept to replace the original response variables. In the final step of determining the optimal factor-level combination, they treated the factor-level combination with the largest MPI value as the best solution, which has little or nothing to do with the theoretical basis and could lead to an unreasonable solution. According to Taguchi, the value of a loss function increases as the quality characteristic moves away from a target. When the quality characteristic is equal to a target value, the cost of deviating from a target value is zero [9]. Therefore, the optimal factor-level combination should be determined based on the smallest MPI value when quality losses are used as the input data, rather than the largest MPI value as stated by Su and Tong [4].

On the contrary, the S/N ratio measures the level of a desired signal associated with the level of its background noise, and thus, a higher value of the S/N ratio indicates more useful information compared to false data. Therefore, when the S/N ratio of quality loss is used as the input data instead of quality loss, the factor-level combination with the largest multi-response performance index should be considered as the optimal one. In the following sections, S/N ratio is used as preferential input data as discussed by [3].

"Section 4" presents the reasons for different eigenvectors leading to different optimal results in the principal component-based multi-response optimization problem.

4 Choice of eigenvectors in WPCA-based multi-response optimization

Gauri and Pal [7] pointed out that different software packages may lead to a different optimal factor-level combination by applying the same principal component-based methods on a same data set. The reason for this problem is due to different eigenvectors obtained by different software packages corresponding to a same eigenvalue. Suppose matrix $\boldsymbol{A}$ has an eigenvector $\boldsymbol{v}$ with its corresponding eigenvalue λ,

Table 4 Compute MPI for multi-response optimization based on WPCA

Measurement combination no.	Factor level				Multi-response performance index
	1st	2nd	$\cdots$	kth	Ω
1	–	–	$\cdots$	–	$\Omega_1=w_1z_{11}+w_2z_{12}+\cdots+w_pz_{1p}$
2	+	–	$\cdots$	–	$\Omega_2=w_1z_{21}+w_2z_{22}+\cdots+w_pz_{2p}$
3	–	+	$\cdots$	–	$\Omega_3=w_1z_{31}+w_2z_{32}+\cdots+w_pz_{3p}$
4	+	+	$\cdots$	–	$\Omega_4=w_1z_{41}+w_2z_{42}+\cdots+w_pz_{4p}$
$\vdots$	$\vdots$	$\vdots$		$\vdots$	$\vdots$
m	+	+	$\cdots$	+	$\Omega_m=w_1z_{m1}+w_2z_{m2}+\cdots+w_pz_{mp}$

$\boldsymbol{A}\boldsymbol{v} = \lambda \boldsymbol{v}$

.

Obviously, if $\boldsymbol{v}$ is multiplied by any real number p, $p\boldsymbol{v}$ is also an eigenvector of $\boldsymbol{A}$ corresponding to the eigenvalue of λ,

$\boldsymbol{A}(p\boldsymbol{v}) = \lambda(p\boldsymbol{v})$

.

Because the functions for computing eigenvectors of a matrix include vector normalization in most software packages, the eigenvectors obtained in different software are unit vectors differing in +/− sign. Therefore, the eigenvectors' differences are with respect to their sign, while the absolute values of elements in the eigenvectors are the same. In order to discuss the effect of eigenvectors with different signs in the process of determining optimal solution, a mathematical inference is shown in the following section.

4.1 Problem due to eigenvectors with different signs

Suppose we have a 2^2 experiment with two response variables as given in Table 5.

The eigenvectors and eigenvalues for the data of Table 5 are obtained from the PCA and are shown in Table 6, where $\begin{bmatrix} a_{11} \\ a_{12} \end{bmatrix}$ is the eigenvector corresponding to the eigenvalue λ_1, and $\begin{bmatrix} a_{21} \\ a_{22} \end{bmatrix}$ is the eigenvector corresponding to the eigenvalue λ_2.

Based on the eigenvectors and eigenvalues above, the multi-response performance indices Ω are calculated as shown in Table 7, where $w_1 = \frac{\lambda_1}{\lambda_1+\lambda_2}$ and $w_2 = \frac{\lambda_2}{\lambda_1+\lambda_2}$ are the weights corresponding to the first component and the second component, respectively.

When $\begin{bmatrix} a_{11} \\ a_{12} \end{bmatrix}$ is an eigenvector of eigenvalue λ_1, $\begin{bmatrix} -a_{11} \\ -a_{12} \end{bmatrix}$ is also the eigenvector corresponding to the same eigenvalue λ_1. Therefore, the calculation of multi-response performance indices will be performed based on the eigenvectors $\begin{bmatrix} -a_{11} \\ -a_{12} \end{bmatrix}$ and $\begin{bmatrix} a_{21} \\ a_{22} \end{bmatrix}$ which will lead to a new set of multi-response performance indices Ω', as shown in Table 8.

Without loss of generality, assume that in Table 7, $\Omega_1 = \max\{\Omega_1, \Omega_2, \Omega_3, \Omega_4\}$, which means that combination 1 is the optimal solution, and consequently $\Omega_1 > \Omega_2$, where

$$
\begin{aligned}
&\Omega_1 - \Omega_2 = (w_1 e_{11} + w_2 e_{12}) - (w_1 e_{21} + w_2 e_{22}) > 0 \\
&\frac{1}{\lambda_1+\lambda_2}\left(\lambda_1\left\{a_{11}\left[\eta_{11}^{(N)} - \eta_{21}^{(N)}\right] + a_{12}\left[\eta_{12}^{(N)} - \eta_{22}^{(N)}\right]\right\}\right. \\
&\left. + \lambda_2\left\{a_{21}\left[\eta_{11}^{(N)} - \eta_{21}^{(N)}\right] + a_{22}\left[\eta_{12}^{(N)} - \eta_{22}^{(N)}\right]\right\}\right) > 0
\end{aligned} \tag{1}
$$

Also,

$$
\begin{aligned}
&\Omega_1' - \Omega_2' = (-w_1 e_{11} + w_2 e_{12}) - (-w_1 e_{21} + w_2 e_{22}) \\
&= \frac{1}{\lambda_1+\lambda_2}\left(\lambda_1\left\{-a_{11}\left[\eta_{11}^{(N)} - \eta_{21}^{(N)}\right] - a_{12}\left[\eta_{12}^{(N)} - \eta_{22}^{(N)}\right]\right\} + \lambda_2\left\{a_{21}\left[\eta_{11}^{(N)} - \eta_{21}^{(N)}\right] + a_{22}\left[\eta_{12}^{(N)} - \eta_{22}^{(N)}\right]\right\}\right)
\end{aligned}
$$

Then,

$$
\begin{aligned}
&\left(\Omega_1' - \Omega_2'\right) - (\Omega_1 - \Omega_2) \\
&= [(-w_1 e_{11} + w_2 e_{12}) - (-w_1 e_{21} + w_2 e_{22})] - [(w_1 e_{11} + w_2 e_{12}) - (w_1 e_{21} + w_2 e_{22})] \\
&= \frac{-2\lambda_1\left\{a_{11}\left[\eta_{11}^{(N)} - \eta_{21}^{(N)}\right] + a_{12}\left[\eta_{12}^{(N)} - \eta_{22}^{(N)}\right]\right\}}{\lambda_1+\lambda_2}
\end{aligned} \tag{2}
$$

Table 5 A 2^2 experimental design model with two response variables

Measurement combination no.	Factor levels		Normalized response S/N ratio	
	A	B	Y_1	Y_2
1	–	–	$\eta_{11}^{(N)}$	$\eta_{12}^{(N)}$
2	–	+	$\eta_{21}^{(N)}$	$\eta_{22}^{(N)}$
3	+	–	$\eta_{31}^{(N)}$	$\eta_{32}^{(N)}$
4	+	+	$\eta_{41}^{(N)}$	$\eta_{42}^{(N)}$

Table 6 Eigenvectors and eigenvalues obtained through performing PCA on data in Table 5

	PC1	PC2
	a_{11}	a_{21}
	a_{12}	a_{22}
Eigenvalue	λ_1	λ_2

Since $\lambda_1+\lambda_2$ in Eq. 1 is positive, the numerator of Eq. 1 is positive, but $\lambda_1\{a_{11}[\eta_{11}^{(N)}-\eta_{21}^{(N)}]+a_{12}[\eta_{12}^{(N)}-\eta_{22}^{(N)}]\}$ is not necessarily negative or zero. Thus, Eq. 2 is not necessarily positive or zero, which means that $\Omega_1^{'}-\Omega_2^{'}$ is not necessarily larger or equal to $\Omega_1-\Omega_2$. Therefore, when Ω_1 is larger than Ω_2, $\Omega_1^{'}$ may be smaller than $\Omega_2^{'}$, which leads to a different optimal solution.

The reason for the eigenvectors +/− signs affecting the choice of optimal factor-level combination is: The opposite direction of eigenvector alters the information of relative magnitude of original data points. This is demonstrated from a two-response example in an intuitive perspective. A two-response example of experimental results with different eigenvectors leading to different MPI is given next, and the problem caused by eigenvectors in opposite signs is demonstrated in an intuitive perspective.

4.2 Experimental design example

An example of an experimental design with four factors and nine runs experiment is given in Table 9.

In the application of the PCA-based multi-response optimization method proposed by Su and Tong (1997), the eigenvector of the first principal component [0.707, 0.707] corresponding to the eigenvalue λ_1 is chosen.

The multi-response optimization indices Ωs are calculated through

$$\Omega_i = 0.707Y_{i1} + 0.707Y_{i2}$$

which are the depicted points on Fig. 1 after the transformation of the original data points (*).

Obviously, the point corresponding to the largest Ω value is the 7th point, and its corresponding factor-level combination should be chosen as the optimal solution.

[0.707, 0.707] is the eigenvector for PC1 with eigenvalue λ_1 and so is [−0.707, −0.707]. Now, the direction of the new axis after performing PCA is horizontal opposite, and the Ω' value is calculated through:

$$\Omega_i{}' = -0.707Y_{i1}-0.707Y_{i2}$$

which are the depicted points on Fig. 2 after the transformation of the original data points (*).

Now, it can be seen that the point corresponding to the largest Ω' value is the 1st point, and its corresponding factor-level combination should be chosen as the optimal solution, which is different from what we obtained based on the eigenvector [−0.707, −0.707].

"Section 5" presents a method for finding a unique optimal solution through assigning indices.

5 Method for determining a unique optimal solution

In this section, a method for determining the optimal eigenvector combination is presented. A procedure for selecting a combination of eigenvectors which represents a new coordinate axes, such that the projections of original data in the new coordinate system preserves the original information as much as possible is developed. The original information is identified as relative magnitudes, as discussed in "Section 5.1." In a two-response problem, the normalized S/N ratios for each response are shown on the fourth and fifth column of Table 10.

The PCA is applied on the normalized S/N ratios, and the projections of original data in the new coordinate system are shown on the last two columns of Table 10. If $\eta_{11}^{(N)}>\eta_{21}^{(N)}$ and $\eta_{12}^{(N)}<\eta_{22}^{(N)}$, it is expected that $e_{11}>e_{21}$ and $e_{12}<e_{22}$ after axes rotation.

To achieve this objective, the idea of indexing is introduced. For each response variable, the values of experimental data are sorted in an ascending order and index 1 is assigned to the smallest value, index 2 is assigned to the second smallest value, and so on. Similarly, indices are assigned to the projection of original data points (after performing the PCA) in the new coordinate system. The sum of the absolute differences (SAD) of each pair of indices (indices of original data and

Table 7 Multi-response performance indices computed for the data of Tables 5 and 6

Measurement combination no.	Factor levels		Principal component		Multi-response performance index
	A	B	PC1	PC2	Ω
1	−	−	$e_{11}=a_{11}\eta_{11}^{(N)}+a_{12}\eta_{12}^{(N)}$	$e_{12}=a_{21}\eta_{11}^{(N)}+a_{22}\eta_{12}^{(N)}$	$\Omega_1=w_1e_{11}+w_2e_{12}$
2	−	+	$e_{21}=a_{11}\eta_{21}^{(N)}+a_{12}\eta_{22}^{(N)}$	$e_{22}=a_{21}\eta_{21}^{(N)}+a_{22}\eta_{22}^{(N)}$	$\Omega_2=w_1e_{21}+w_2e_{22}$
3	+	−	$e_{31}=a_{11}\eta_{31}^{(N)}+a_{12}\eta_{32}^{(N)}$	$e_{32}=a_{21}\eta_{31}^{(N)}+a_{22}\eta_{32}^{(N)}$	$\Omega_3=w_1e_{31}+w_2e_{32}$
4	+	+	$e_{41}=a_{11}\eta_{41}^{(N)}+a_{12}\eta_{42}^{(N)}$	$e_{42}=a_{21}\eta_{41}^{(N)}+a_{22}\eta_{42}^{(N)}$	$\Omega_4=w_1e_{41}+w_2e_{42}$

Table 8 Multi-response performance indices based on the new set of eigenvectors

Measurement combination no.	Factor levels		Principal component		Multi-response performance index
	A	B	PC1	PC2	Ω'
1	–	–	$-e_{11}=-a_{11}\eta_{11}^{(N)}-a_{12}\eta_{12}^{(N)}$	e_{12}	$\Omega'_1=-w_1e_{11}+w_2e_{12}$
2	–	+	$-e_{21}=-a_{11}\eta_{21}^{(N)}-a_{12}\eta_{22}^{(N)}$	e_{22}	$\Omega'_2=-w_1e_{21}+w_2e_{22}$
3	+	–	$-e_{31}=-a_{11}\eta_{31}^{(N)}-a_{12}\eta_{32}^{(N)}$	e_{32}	$\Omega'_3=-w_1e_{31}+w_2e_{32}$
4	+	+	$-e_{41}=-a_{11}\eta_{41}^{(N)}-a_{12}\eta_{42}^{(N)}$	e_{42}	$\Omega'_4=-w_1e_{41}+w_2e_{42}$

components after PCA projection) is obtained first (see step 4 of "Section 5.1"), then the minimal SAD gives the optimal eigenvector combination. It should be noted that the minimum of SAD preserves the maximum characteristics of the original response values. Then, the eigenvectors corresponding to the minimum SAD are used to calculate the multi-response performance indices in which the identification of optimal factor-level combination is based (steps 4 and 5 in Section 2).

5.1 Indexing procedure

This section presents an indexing procedure in five steps for an input data, which could be the normalized quality loss or normalized S/N ratio, of a p response and m trail experiment. By comparison of the effect of different sets of eigenvectors (having different combinations of +/− signs), a set of eigenvectors among 2^p sets which leads to an optimal solution is identified.

Step 1: Calculate the variance of each response variable:

The components obtained through PCA are arranged in a descending order of their eigenvalues (which is the contribution of the component's explanation of their variances). In order to increase the efficiency of comparison, the response variables Y_1, Y_2, …, Y_p are sorted in a descending order of their corresponding variances; $\sigma^2_{Y_1}, \sigma^2_{Y_2}, \ldots, \sigma^2_{Y_p}$.

Let

$$Y^{(1)} = Y_{l_1},\ Y^{(2)} = Y_{l_2},\ \ldots,\ Y^{(p)} = Y_{l_p}$$

where $l_1, l_2, \ldots, l_p$=1, 2, …, p, $l_1 \neq l_2 \neq \cdots \neq l_p$, and $\sigma^2_{Y^{(1)}} \geq \sigma^2_{Y^{(2)}} \geq \cdots \geq \sigma^2_{Y^{(p)}}$. Now, $Y^{(1)}, Y^{(2)}, \ldots, Y^{(p)}$ form the original coordinate system, as shown in Table 11. Where $Y^{(1)}$ is called the first axis, $Y^{(2)}$ is called the second axis, and so on.

After the indices are assigned for data points of the new coordinate system, the indices are compared within the same columns. For example, the calculation of differences between $Y^{(1)}$ indices and first principal component indices and between $Y^{(2)}$ indices and the second principal component indices … are needed. Consequently, many unnecessary comparisons between all possible combinations are reduced.

Step 2: Assign indices 1, 2, 3, …, m to $y_{1l_1}, y_{2l_1}, y_{3l_1}, \ldots, y_{ml_1}$, such that

$$i^{(0)}_{il_1} = k,\ i = 1, 2, 3, \ldots, m,\ k = 1, 2, 3, \ldots, m$$

Table 9 Experiment for four factors, with two response variables

Measurement combination no.	Factor level				S/N ratio of responses	
	A	B	C	D	Y_1	Y_2
1	1	1	1	1	1	1.5
2	1	2	2	2	3	2
3	1	3	3	3	4	4
4	2	1	2	3	6	5
5	2	2	3	1	5.5	2
6	2	3	1	2	2.5	3
7	3	1	3	2	6.5	6
8	3	2	1	3	2	1
9	3	3	2	1	5	5.5

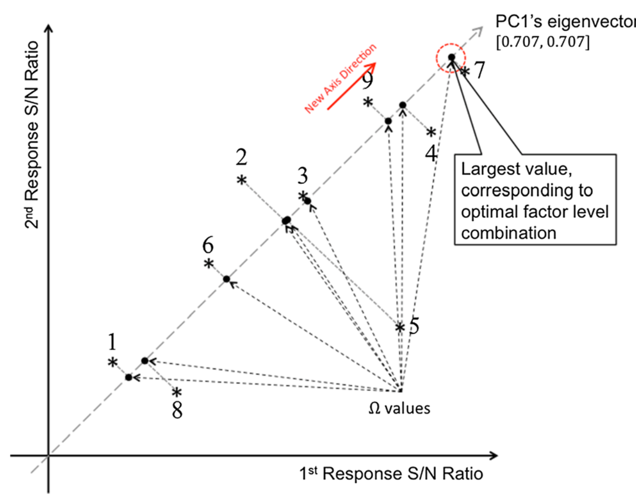
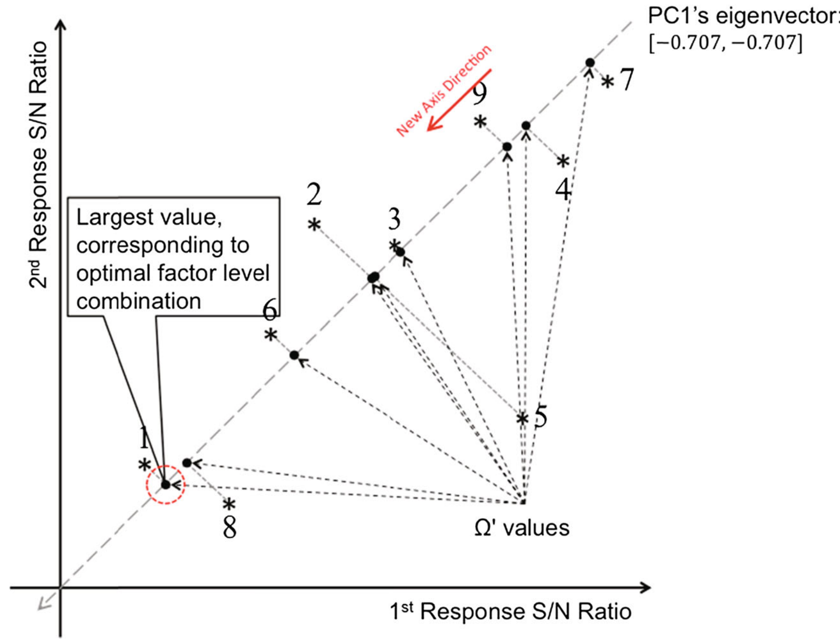


Fig. 1 Multi-response performance indices for the data in Table 9 with eigenvector [0.707,0.707]

Fig. 2 Multi-response performance indices for the data of example in Table 9 with eigenvector [−0.707,–0.707]



Therefore, y_{il_1} is the kth largest value among the m points on response $Y^{(1)}$, index $i_{ij}^{(0)}=k$,,where $i=1, 2, 3, \ldots, m$, $j=l_1, l_2, l_3, \ldots, l_p$, $k=1, 2, 3, \ldots, m$, as shown in Table 12.

Step 3: After performing PCA on the data, p eigenvectors are obtained:

$$\boldsymbol{v}_1 = \begin{pmatrix} v_{11} \\ v_{12} \\ \vdots \\ v_{1p} \end{pmatrix}, \boldsymbol{v}_2 = \begin{pmatrix} v_{21} \\ v_{22} \\ \vdots \\ v_{2p} \end{pmatrix}, \cdots, \boldsymbol{v}_p = \begin{pmatrix} v_{p1} \\ v_{p2} \\ \vdots \\ v_{pp} \end{pmatrix}$$

and their corresponding eigenvalues are: $\lambda_1, \lambda_2, \ldots, \lambda_p$, with $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$.

Step 4: For the new coordinate system with $(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \cdots \quad \boldsymbol{v}_p)$ axes, project original data points onto a new coordinate system, as shown in Table 13.

Next, assign indices 1, 2, 3, …, m to $z_{1j}^{(1)}, z_{2j}^{(1)}, \ldots, z_{mj}^{(1)}$, such that

$$i_{ij}^{(1)} = k,\ i = 1, 2, 3, \ldots, m,\ j = 1, 2, 3, \ldots, p,\ k = 1, 2, 3, \ldots, m$$

Table 10 A 2^k experimental design with two response variables

Measurement combination no.	Factor levels		Normalized S/N ratio		Principal components	
	A	B	Y_1	Y_2	PC1	PC2
1	–	–	$\eta_{11}^{(N)}$	$\eta_{12}^{(N)}$	e_{11}	e_{12}
2	–	+	$\eta_{21}^{(N)}$	$\eta_{22}^{(N)}$	e_{21}	e_{22}
⋮	⋮	⋮	⋮	⋮	⋮	⋮

Therefore, $z_{ij}^{(1)}$ is the k th largest value in the j th column of Table 13. The indices are shown as in Table 14.

Then, calculate the differences between each pair of indices; a pair of indices consisting of one from the original data and its corresponding index from rotated data. Then, find the sum of the absolute differences of the pairs as follows:

$$d_{01} = \left| i_{1l_1}^{(0)} - i_{11}^{(1)} \right| + \left| i_{2l_1}^{(0)} - i_{21}^{(1)} \right| + \cdots + \left| i_{ml_1}^{(0)} - i_{m1}^{(1)} \right| + \left| i_{1l_2}^{(0)} - i_{12}^{(1)} \right| + \cdots + \left| i_{ml_p}^{(0)} - i_{mp}^{(1)} \right|$$

Then, new coordinate system axes are updated to $(-\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \cdots \quad \boldsymbol{v}_p)$, and the difference between the indices of each pair (original data and rotated data) is calculated:

Table 11 Response variables sorted according to the variance

Experiment combination no.	Factor levels				Original coordinate system			
	A	B	C	…	$Y^{(1)}$	$Y^{(2)}$	…	$Y^{(p)}$
1	1	1	1	…	y_{1l_1}	y_{1l_2}	…	y_{1l_p}
2	2	1	1	…	y_{2l_1}	y_{2l_2}	…	y_{2l_p}
3	3	2	1	…	y_{3l_1}	y_{3l_2}	…	y_{3l_p}
m	3	3	3	…	y_{ml_1}	y_{ml_2}	…	y_{ml_p}
Variance					$\sigma^2_{Y^{(1)}} \geq \sigma^2_{Y^{(2)}} \geq \cdots \geq \sigma^2_{Y^{(p)}}$			

Table 12 Indices for original coordinate system

Experiment combination no.	Factor levels				Original coordinate system			
	A	B	C	…	$Y^{(1)}$	$Y^{(2)}$	…	$Y^{(p)}$
1	1	1	1	…	$i^{(0)}_{1l_1}$	$i^{(0)}_{1l_2}$	…	$i^{(0)}_{1l_p}$
2	2	1	1	…	$i^{(0)}_{2l_1}$	$i^{(0)}_{2l_2}$	…	$i^{(0)}_{2l_p}$
3	3	2	1	…	$i^{(0)}_{3l_1}$	$i^{(0)}_{3l_2}$	…	$i^{(0)}_{3l_p}$
m	3	3	3	…	$i^{(0)}_{ml_1}$	$i^{(0)}_{ml_2}$	…	$i^{(0)}_{ml_p}$

$$d_{02} = \left|i^{(0)}_{1l_1} - i^{(2)}_{11}\right| + \left|i^{(0)}_{2l_1} - i^{(2)}_{21}\right| + \cdots + \left|i^{(0)}_{ml_1} - i^{(2)}_{m1}\right| + \left|i^{(0)}_{1l_2} - i^{(2)}_{12}\right| + \cdots + \left|i^{(0)}_{ml_p} - i^{(2)}_{mp}\right|$$

This step is repeated for all combinations of eigenvectors with different +/− signs.

Step 5: The minimal d_{0h}, where h=1, 2, …, 2^p from the comparisons of the original data set with the 2^p eigenvector sets is identified, and its corresponding eigenvector coordinate system is chosen as the optimal eigenvector combination. This optimal eigenvector combination is used for determining the optimal factor-level combination in the WPCA multi-response optimization method.

5.2 Mathematical programming form

Now, the above procedures are stated in mathematical programming model. Let

Table 14 Indices for new coordinate system with axes $(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \cdots \quad \boldsymbol{v}_p)$

Experiment combination no.	Factor levels				Original coordinate system			
	A	B	C	…	$Y^{(1)}$	$Y^{(2)}$	…	$Y^{(p)}$
1	1	1	1	…	$i^{(1)}_{11}$	$i^{(1)}_{12}$	…	$i^{(1)}_{1p}$
2	2	1	1	…	$i^{(1)}_{21}$	$i^{(1)}_{22}$	…	$i^{(1)}_{2p}$
3	3	2	1	…	$i^{(1)}_{31}$	$i^{(1)}_{32}$	…	$i^{(1)}_{3p}$
m	3	3	3	…	$i^{(1)}_{m1}$	$i^{(1)}_{m2}$	…	$i^{(1)}_{mp}$

$$\boldsymbol{Y} = \begin{pmatrix} y_{11} & y_{12} & \cdots & y_{1p} \\ y_{21} & y_{22} & \cdots & y_{2p} \\ \vdots & \vdots & & \vdots \\ y_{m1} & y_{m2} & \cdots & y_{mp} \end{pmatrix}_{m\times p} \tag{3}$$

$$\boldsymbol{V}_0 = (\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \cdots \quad \boldsymbol{v}_p) = \begin{pmatrix} v_{11} & v_{21} & \cdots & v_{p1} \\ v_{12} & v_{22} & \cdots & v_{p2} \\ \vdots & \vdots & & \vdots \\ v_{1p} & v_{2p} & \cdots & v_{pp} \end{pmatrix}_{p\times p} \tag{4}$$

$$\boldsymbol{I}_0 = \begin{pmatrix} i^{(0)}_{1l_1} & i^{(0)}_{1l_2} & \cdots & i^{(0)}_{1l_p} \\ i^{(0)}_{2l_1} & i^{(0)}_{2l_2} & \cdots & i^{(0)}_{2l_p} \\ \vdots & \vdots & & \vdots \\ i^{(0)}_{ml_1} & i^{(0)}_{ml_2} & \cdots & i^{(0)}_{ml_p} \end{pmatrix}_{m\times p} \tag{5}$$

The process of determining the optimal eigenvector combination is to find the matrix $\boldsymbol{X}$, such that Minimize $d = \left|i^{(0)}_{1l_1} - i_{11}\right| + \cdots + \left|i^{(0)}_{ml_1} - i_{m1}\right| + \left|i^{(0)}_{1l_2} - i_{12}\right| + \cdots + \left|i^{(0)}_{ml_p} - i_{mp}\right|$ subject to

$$\boldsymbol{X} = \begin{pmatrix} x_{11} & 0 & \cdots & 0 \\ 0 & x_{22} & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & x_{pp} \end{pmatrix}_{p\times p} \tag{6}$$

$$\begin{aligned} &x_{ii} = -1,\ 1, \quad i = 1, 2, \ldots, p \\ &\boldsymbol{V} = \boldsymbol{V}_0\boldsymbol{X} \end{aligned} \tag{7}$$

Table 13 New coordinate system with axes $(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \cdots \quad \boldsymbol{v}_p)$

New coordinate system with axes $(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \cdots \quad \boldsymbol{v}_p)$								
Exp. no.	Factor levels				Axis			
	A	B	C	…	1	2	…	p
1	1	1	1	…	$z^{(1)}_{11}=(y_{11}, y_{12}, \cdots, y_{1p})\boldsymbol{v}_1$	$z^{(1)}_{12}=(y_{11}, y_{12}, \cdots, y_{1p})\boldsymbol{v}_2$	…	$z^{(1)}_{1p}=(y_{11}, y_{12}, \cdots, y_{1p})\boldsymbol{v}_p$
2	2	1	1	…	$z^{(1)}_{21}=(y_{21}, y_{22}, \cdots, y_{2p})\boldsymbol{v}_1$	$z^{(1)}_{22}=(y_{21}, y_{22}, \cdots, y_{2p})\boldsymbol{v}_2$	…	$z^{(1)}_{2p}=(y_{21}, y_{22}, \cdots, y_{2p})\boldsymbol{v}_p$
⋮	⋮	⋮	⋮		⋮	⋮		⋮
m	3	3	3	…	$z^{(1)}_{m1}=(y_{m1}, y_{m2}, \cdots, y_{mp})\boldsymbol{v}_1$	$z^{(1)}_{m2}=(y_{m1}, y_{m2}, \cdots, y_{mp})\boldsymbol{v}_2$	…	$z^{(1)}_{mp}=(y_{m1}, y_{m2}, \cdots, y_{mp})\boldsymbol{v}_p$

Table 15 S/N ratios for four response variables with their corresponding variances

Measurement combination no.	Factor levels				Response S/N ratio $\boldsymbol{Y}$				Normalized response S/N ratio $\boldsymbol{Y}_N$			
	A	B	C	D	$Y^{(1)}$ SR_AP	$Y^{(2)}$ SR_P	$Y^{(3)}$ FC-P	$Y^{(4)}$ FC_AP	$Y^{(1)}$ SR_AP	$Y^{(2)}$ FC_P	$Y^{(3)}$ FC-AP	$Y^{(4)}$ SR_P
1	1	1	1	1	−0.2567	4.8825	12.3958	11.7005	0.3465	0.3051	0.0000	0.8981
2	1	2	2	2	−1.6557	2.2702	11.7005	12.0412	0.2743	0.0000	0.2348	0.6953
3	1	3	3	3	7.9588	6.1961	13.9794	12.3958	0.7708	1.0000	0.4792	1.0000
4	2	1	2	3	−6.9661	−6.6891	12.3958	12.0412	0.0000	0.3051	0.2348	0.0000
5	2	2	3	1	11.7005	5.0362	11.7005	12.0412	0.9641	0.0000	0.2348	0.9100
6	2	3	1	2	−3.6369	2.3837	13.5556	12.7654	0.1719	0.8140	0.7339	0.7041
7	3	1	3	2	−0.8279	4.4370	12.0412	12.0412	0.3170	0.1495	0.2348	0.8635
8	3	2	1	3	−4.5577	5.6799	12.3958	13.1515	0.1244	0.3051	1.0000	0.9599
9	3	3	2	1	12.3958	5.0362	12.0412	11.7005	1.0000	0.1495	0.0000	0.9100
Variance					52.2074	15.6919	0.6282	0.2328	0.1393	0.1209	0.1106	0.0945

$$\boldsymbol{Z} = \boldsymbol{YV} = \begin{pmatrix} z_{11} & z_{12} & \cdots & z_{1p} \\ z_{21} & z_{22} & \cdots & z_{2p} \\ \vdots & \vdots & & \vdots \\ z_{m1} & z_{m2} & \cdots & z_{mp} \end{pmatrix}_{m\times p} \tag{8}$$

$$\boldsymbol{I} = \begin{pmatrix} i_{11} & i_{12} & \cdots & i_{1p} \\ i_{21} & i_{22} & \cdots & i_{2p} \\ \vdots & \vdots & & \vdots \\ i_{m1} & i_{m2} & \cdots & i_{mp} \end{pmatrix}_{m\times p} \tag{9}$$

where $\boldsymbol{I}$ is calculated based on $\boldsymbol{Z}$, and $i_{kh}=m$, where z_{kh} is the mth largest value in the hth column in $\boldsymbol{Z}$, $k=1, 2, \ldots, m$, $h=1, 2, \ldots, p$, and $i_{kh}=1, 2, \ldots, m$

$$\boldsymbol{I}_\Delta = \boldsymbol{I}_0 - \boldsymbol{I}$$
$$= \begin{pmatrix} i_{11}^{(0)}-i_{11} & i_{12}^{(0)}-i_{12} & \cdots & i_{1p}^{(0)}-i_{1p} \\ i_{21}^{(0)}-i_{21} & i_{22}^{(0)}-i_{22} & \cdots & i_{2p}^{(0)}-i_{2p} \\ \vdots & \vdots & & \vdots \\ i_{m1}^{(0)}-i_{m1} & i_{m2}^{(0)}-i_{m2} & \cdots & i_{mp}^{(0)}-i_{mp} \end{pmatrix}_{m\times p} \tag{10}$$

6 Numerical example

To verify the proposed method in "Section 5," an experimental design example is developed in this section. The example is based on an injection-molding process for friction properties of fiber-reinforced polybutylene terephthalate carried out by Fung and Kang [10]. Four response variables, FC_P, FC_AP, SR_P, and SR_AP, are studied in this example: the S/N ratio and normalized S/N ratio for the smaller the better are calculated first. Then, in order to determine the optimal eigenvector combination, the variance of each response variable is calculated, and the response variables are ordered according to their corresponding variances to form the original coordinate system, as demonstrated in Table 15. Based on Eq. 3, the input matrix $\boldsymbol{Y}$ for non-normalized S/N ratio data and $\boldsymbol{Y}_N$ for normalized S/N ratio data are demonstrated in Table 15.

Next, the indices are assigned to the original input data, and based on Eq. 5, the original index matrices for non-normalized S/N ratio data and normalized S/N ratio data are

Table 16 PCA coefficients for the new coordinate system with axes $(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad \boldsymbol{v}_4)$

Data in new coordinate system with axes $(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad \boldsymbol{v}_4)$								
Experiment combination no.	Factor levels				Axis			
	A	B	C	D	1	2	3	4
1	1	1	1	1	1.1510	−6.1074	−14.7344	7.6633
2	1	2	2	2	−1.0801	−4.1524	−14.2554	8.2560
3	1	3	3	3	9.2766	−4.5944	−16.6425	8.1651
4	2	1	2	3	−9.2047	2.3238	−15.2506	8.3199
5	2	2	3	1	12.3915	−2.0772	−14.5460	8.6427
6	2	3	1	2	−2.9209	−5.0889	−16.1592	8.3707
7	3	1	3	2	0.4546	−5.9010	−14.4891	8.0861
8	3	2	1	3	−2.6246	−8.4623	−14.9290	8.8467
9	3	3	2	1	13.0474	−1.8240	−14.8072	8.2515

Table 17 Comparison of difference between indices of original data and the rotated data

Input data: S/N ratio		Input data: normalized S/N ratio	
Eigenvector combinations	d	Eigenvector combinations	d
$(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	90	$(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	132
$(-\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	128	$(-\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	104
$(\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	84	$(\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	108
$(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	56	$(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	134
$(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	104	$(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	126
$(-\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	122	$(-\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	80
$(-\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	94	$(-\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	106
$(-\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	142	$(-\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	98
$(\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	50	$(\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	110
$(\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	98	$(\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	102
$(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	70	$(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	128
$(-\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	88	$(-\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad \boldsymbol{v}_4)$	82
$(-\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	136	$(-\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	74
$(-\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	108	$(-\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	100
$(\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	64	$(\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	104
$(-\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	102	$(-\boldsymbol{v}_1 \quad -\boldsymbol{v}_2 \quad -\boldsymbol{v}_3 \quad -\boldsymbol{v}_4)$	76

$$\boldsymbol{I}_0 = \begin{pmatrix} 6 & 5 & 5 & 1 \\ 4 & 2 & 1 & 3 \\ 7 & 9 & 9 & 7 \\ 1 & 1 & 6 & 4 \\ 8 & 6 & 2 & 5 \\ 3 & 3 & 8 & 8 \\ 5 & 4 & 3 & 6 \\ 2 & 8 & 7 & 9 \\ 9 & 7 & 4 & 2 \end{pmatrix}$$

and

$$\boldsymbol{I}_{0N} = \begin{pmatrix} 6 & 5 & 1 & 5 \\ 4 & 1 & 3 & 2 \\ 7 & 9 & 7 & 9 \\ 1 & 6 & 4 & 1 \\ 8 & 2 & 5 & 6 \\ 3 & 8 & 8 & 3 \\ 5 & 3 & 6 & 4 \\ 2 & 7 & 9 & 8 \\ 9 & 4 & 2 & 7 \end{pmatrix}$$

respectively.

Table 18 Optimal eigenvector combinations for data in Table 15

Optimal eigenvector combination								
	Input data: S/N ratio				Input data: normalized S/N ratio			
	PC1	PC2	PC3	PC4	PC1	PC2	PC3	PC4
	0.9358	−0.3486	0.0334	0.0396	0.7083	0.3845	−0.1910	0.5603
	0.3517	0.9330	−0.0562	−0.0514	−0.3664	0.6105	−0.6770	−0.1866
	−0.0060	0.0454	0.9623	−0.2680	−0.5189	0.4204	0.5107	0.5415
	−0.0215	0.0769	0.2640	0.9612	0.3080	0.5502	0.4944	−0.5983
Eigenvalue	58.2589	9.7439	0.6456	0.1118	0.2097	0.1590	0.0713	0.0253

Table 19 Multi-response performance indices for data in Table 15

Measurement combination no.	Factor levels				MPI	
	A	B	C	D	Input: S/N ratio	Input: normalized S/N ratio
1	1	1	1	1	1.9914	0.4674
2	1	2	2	2	−0.1795	0.3853
3	1	3	3	3	8.6806	0.6563
4	2	1	2	3	−7.9718	−0.0174
5	2	2	3	1	10.9442	0.7764
6	2	3	1	2	−1.5885	0.2937
7	3	1	3	2	1.3705	0.4563
8	3	2	1	3	−0.8702	0.4074
9	3	3	2	1	11.4659	0.7780

Then, PCA is applied. From Eq. 4, the principal components eigenvector matrices for non-normalized S/N ratio data and normalized S/N ratio data are obtained as

$$\boldsymbol{V}_0 = (\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad \boldsymbol{v}_4) = \begin{pmatrix} 0.9358 & 0.3486 & -0.0334 & 0.0396 \\ 0.3517 & -0.9330 & 0.0562 & -0.0514 \\ -0.0060 & -0.0454 & -0.9623 & -0.2680 \\ -0.0215 & -0.0769 & -0.2640 & 0.9612 \end{pmatrix}$$

and

$$\mathrm{V}_{0\mathrm{N}} = (\mathrm{v}_1 \quad \mathrm{v}_2 \quad \mathrm{v}_3 \quad \mathrm{v}_4) = \begin{pmatrix} -0.7083 & -0.3845 & -0.1910 & -0.5603 \\ 0.3664 & -0.6105 & -0.6770 & 0.1866 \\ 0.5189 & -0.4204 & 0.5107 & -0.5415 \\ -0.3080 & -0.5502 & 0.4944 & 0.5983 \end{pmatrix}$$

respectively.

Now, considering the non-normalized S/N ratios as input data, the original data points are projected onto the new coordinate system $(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad \boldsymbol{v}_4)$. From Eqs. 7, 8, and 9, and as demonstrated in Table 13, a new coordinate system $\boldsymbol{Z}=\boldsymbol{YZ}$ with axes $(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad \boldsymbol{v}_4)$ are obtained as shown on Table 16:

Then, the indices of data in new coordinate system with axes $(\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \boldsymbol{v}_3 \quad \boldsymbol{v}_4)$ are assigned, and from Eq. 10, the index matrix is obtained:

$$\boldsymbol{I} = \begin{pmatrix} 6 & 2 & 6 & 1 \\ 4 & 6 & 9 & 5 \\ 7 & 5 & 1 & 3 \\ 1 & 9 & 3 & 6 \\ 8 & 7 & 7 & 8 \\ 2 & 4 & 2 & 7 \\ 5 & 3 & 8 & 2 \\ 3 & 1 & 4 & 9 \\ 9 & 8 & 5 & 4 \end{pmatrix}$$

and from Eq. 10, the difference between indices of the original data (non-normalized) and indices of rotated data is calculated:

$$\boldsymbol{I}_\Delta = \boldsymbol{I}_0 - \boldsymbol{I} = \begin{pmatrix} 0 & 3 & -1 & 0 \\ 0 & 4 & -8 & -2 \\ 0 & 4 & 8 & 4 \\ 0 & 8 & 3 & -2 \\ 0 & -1 & -5 & -3 \\ 1 & -1 & 6 & 1 \\ 0 & 1 & -5 & 4 \\ -1 & 7 & 3 & 0 \\ 0 & -1 & -1 & -2 \end{pmatrix}$$

Table 20 Optimal factor-level combinations for example in Table 15

Factor level						
Factors	Input: S/N ratio			Input: normalized S/N ratio		
	Level 1	Level 2	Level 3	Level 1	Level 2	Level 3
A	3.4975	0.4613	3.9887	0.5030	0.3509	0.5472
B	−1.5366	3.2982	6.1860	0.3021	0.5230	0.5760
C	−0.1558	1.1049	6.9984	0.3895	0.3820	0.6297
D	8.1338	−0.1325	−0.0538	0.6739	0.3784	0.3488
Optimal Factor/Level Combination	A3-B3-C3-D1			A3-B3-C3-D1		

Then, the sum of absolute difference between indices of the original data and indices of rotated data is calculated:

$d = 90$

Similarly, the above procedures are continued for all combinations of eigenvectors with different +/− signs and also for the normalized S/N ratios as the input data. The differences of data index between original data and rotated data for non-normalized and normalized S/N ratios are shown in Table 17.

From the smallest value of d, the optimal eigenvector combinations for the case with S/N ratio as input data and for the case with normalized S/N ratio as input data are determined as shown in Table 18.

Once the optimal eigenvector combination is determined, following the steps 4 and 5 in "Section 2," the multi-response performance indices (MPIs) and then the optimal factor-level combinations are obtained as shown in Tables 19 and 20.

Table 20 shows that both cases, with the S/N ratio as input data and with the normalized S/N ratio as input data, lead to the same result. The optimal factor-level combination for this example is at level 3 for factors A, B, and C and at level 1 for factor D.

7 Conclusions

In the process of performing principal component analysis for a multi-response optimization problem, eigenvalues and eigenvectors are computed for transforming the original response variables into uncorrelated principal components. However, for each eigenvalue, there are more than one eigenvectors corresponding to it, and different choices of eigenvector will lead to different multi-response performance indices, which consequently lead to different factor-level combinations. To improve the multi-response optimization method based on PCA, a new approach for determining the optimal eigenvector combination is proposed. The procedure for this approach is based on comparison of assigned indices and determination of a set of eigenvectors which represents the new coordinate axes, such that the relative magnitudes of the projections of data in the new coordinate system have minimal total difference between each pair of indices (the original data and the rotated ones). Based on the proposed method, only one combination of eigenvectors leads to a unique optimal factor-level combination in a multi-response optimization.

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