A Mathematical Model Based on Principal Component Analysis for Optimization of Correlated Multiresponse Surfaces

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Abstract

Optimization of multiple quality characteristics (or response variables) is more complicated than optimization of a single one since we face different units, importance and optimality directions. In most real situations there are correlated responses that make conclusion more difficult. If correlations among quality characteristics are ignored, engineering designer may miss finding design variable settings which simultaneously improved the quality of all the responses. In this work optimization of multiple correlated responses was studied and a novel mathematical model was proposed based on Principal Component Analysis (PCA) to optimize correlated multiresponse problems. The proposed method is also demonstrated by two numerical examples from the literature to confirm the efficiencies.

Keywords: Multiple Response Surface (MRS), correlated responses, mathematical programming, Principal Component Analysis (PCA)
1. INTRODUCTION

Setting of controllable input variables to meet a required specification of quality characteristic (or response variable) in a process is one of the common problems in the process quality control. But generally there are more than one quality characteristics in the process and the experimenter attempts to optimize all of them simultaneously. Since response variables are different in some properties such as scale, measurement unit, type of optimality and their preferences, there are different approaches in model building and optimization of multiresponse surface problems. Moreover, when correlations among the responses are ignored, the determined levels for inputs variables will not improve the quality of all of the responses simultaneously. Due to the interrelation among response variables, all fitted surfaces and optimization approaches may lead into imprecise results. It is also considerable point that when two responses are highly correlated, the problem can be reduced to a problem in which only one of them can be considered. On the other hand, if two responses have negligible correlation, the problem could be analyzed separately for each response. However, when the responses have meaningful (not highly) correlation, analysts must apply some other approach that simultaneously meet several output considering their interrelation.

In this work, Multiple Response Surface (MRS) optimization problem with correlation of responses are considered to make explicit conclusion and a novel mathematical model was proposed based on Principal Component Analysis (PCA) to obtain uncorrelated responses. This paper is organized as follows, in the next section we review some earlier works in multiresponse optimization (MRO). In Section 3 a summary of PCA method is introduced and in Section 4 the proposed approach and related models and methods are described. The representative examples are studied in Section 5 and finally, Section 6 gives some conclusions and mention considerable points for future researches.

2. LITERATURE REVIEW

MRO problems have been studied in several areas from different aspects. We can categorize all viewpoints in the literature into three general categories: (1) Desirability viewpoints: in this category, researchers try to aggregate information of each response and get one response. Then optimization is performed on single objective called total desirability function. (2) Priority based methods: some cases have responses with different importance, in such problem, we must consider most important response for optimization and if solutions were not unique, then find the best solution by comparing the status of other responses for alternative solutions and foresaid steps is repeated till considering all of the responses and finding a unique optimal solution. (3) Loss function: in this category, based on loss function (represented by Taguchi) all of the response values are aggregated and converted to a single one. Wide range of researches, have been studied to develop and generalize Taguchi loss function with respect to special trait of its cases. Some earlier works in multiresponse optimization are: Derringer and Suich (1980) ap-
plied a desirability function to optimize multi-response problems in a static experiment. Del Castillo et al. (1996) demonstrated the use of modified desirability functions for optimizing a multi-response problem. Layne (1995) presented a procedure that simultaneously considers three functions -- the weighted loss function, the desirability function, and a distance function -- to determine the optimum parameter combination. Hence, it will lead to the conflict by making the necessary compromise for the results of the three methods to determine the optimum parameters’ settings. Logothetis and Haigh (1988) also optimized a process with five responses by utilizing the multiple regression technique and the linear programming approach. These two methods are also computationally complex and, therefore, are difficult to apply on the shop floor. Pignatiello (1993) utilized a variance component and a squared deviation-from-target to form an expected loss function to optimize a multiple response problem. This method is difficult to implement. The first reason is that a cost matrix must be initially obtained, and the second reason is that it needs more experimental data. Ariles-León (1996-1997) presented a method, which is based on the notions of a standardized loss function with specification limits, to optimize a multi-response problem. However, only the nominal-the best (NTB) characteristic is suitable for this approach, which may limit the capability of this approach. Ames et al. (1997) presented a quality loss function approach in response surface models to deal with a multi-response problem. The basic strategy is to describe the response surfaces with experimentally derived polynomials, which can be combined into a single loss function by using known or desired targets. Next, minimizing the loss function with respect to process inputs locates the best operating conditions. Lai and Chang (1994) proposed a fuzzy multi-response optimization procedure to search for an appropriate combination of process parameter settings. Bashiri and Hejazi (2009) used Multiple Attribute Decision Making (MADM) methods such as VIKOR, PROMETHEE II (Preference Ranking Organization Method for Enrichment Evaluation II), ELECTRE III (ELimination Et Choix Traduisant la REalité III) and TOPSIS (Technique for Order Preference by Similarity to an Ideal Solution) in converting multi-response to single response in order to analyze the robust experimental design. The main advantages of their method was to consider standard deviation that contributed to robust experimental design and also because of fitting only one response regression function, the proposed method decreased statistical error. Hsieh (2006) used neural networks to estimate relation between control variables and responses. Tong et al. (1997) developed a multi-response signal-to-noise (MRSN) ratio, which integrates the quality loss for all responses to solve the multi-response problem. The conventional Taguchi method can be applied based on MSRN and the optimum factor/level combination can be obtained. Su and Tong (1997) also proposed a principle component analysis approach to optimize a multi-response problem. Initially, the quality loss of each response is standardized; principle component analysis is then applied to transform the primary quality responses into fewer quality responses. Finally, the optimum parameter combination can be obtained by maximizing the summation standardized quality loss. Su and Tong’s (1997) research is based on Taguchi method and proposed approach have no efficiency when the number of components is greater than one. Tong and Su (1997) proposed a procedure, which applied fuzzy set theory to MADM to optimize a multi-responses problem. Although their method can reduce the uncertainty in determining each response’s weight, it is still too computationally complicated to be practically
used. Tong et al. (2007) use VIKOR methods in converting Taguchi criteria to single response and then find regression model and related optimal setting. Chiao and Hamada (2001) considered experiments with correlated multiple responses whose means, variances, and correlations depend on experimental factors. Analysis of these experiments consists of modeling distributional parameters in terms of the experimental factors and finding factor settings which maximize the probability of being in a specification region, i.e., all responses are simultaneously meeting their respective specifications. Kazemzadeh et al. (2008) proposed a general framework for multiresponse optimization problems based on goal programming and studied some existing works and some types of related decision makers and attempts to aggregate all of characteristics in to one approach. Shah et al. (2004) illustrate the seemingly unrelated regressions (SUR) method for estimating the regression parameters that it can be useful when response variables in MRS problem are correlated and can lead to a more precise estimate of the optimum variable setting. Tong et al. (2005) also consider correlation of responses and use PCA and TOPSIS method to find the best variable setting. This method cannot determine the desired direction of components after the linear transformation. Antony (2000) used PCA in combination of Taguchi’s method. The proposed approach has obvious limitations since it is assumed that only those of components whose eigenvalues greater than one can be selected to form final response variables so if the problem has more than one components with such characteristic then their method could not be applied. Tong et al. (2005) and Wang (2007) determined the optimization direction of each component on the basis of the corresponding variation mode chart. Furthermore, Tong et al. (2005) and Wang (2007) use TOPSIS to find an overall performance index as a criterion for optimizing the multiple quality characteristics. Hejazi et al. (2011) aggregated multiple responses using goal programming method and assumed several correlated response variables with probabilistic important weights. They solved the stochastic model by some deterministic equivalents. A summary of correlated Multiresponse optimization methods and a comparison between them are represented in Table 1.

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 $k \leq p$. Restated, let $x = x_1, x_2, \ldots, x_p$ be a set of original variables with a variance-covariance matrix $\Sigma$. Through the PCA, a set of uncorrelated linear combinations can be obtained in the following matrix:

$$ Y = A^T x $$

Where $Y = (Y_1, Y_2, \ldots, Y_p)^T$, $Y_1$ is called the first principal component, $Y_2$ is called the second principal component and so on; $A = (a_{ij})_{p \times p}$ and $A$ is an orthogonal matrix with $A^T A = I$. Therefore, $X$ can also be expressed as follows:
<table>
<thead>
<tr>
<th>Method</th>
<th>Solution</th>
<th>Location effect</th>
<th>Dispersion effect</th>
<th>Interaction effect</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Su and Tong (1997)</td>
<td>●</td>
<td>●</td>
<td>●</td>
<td></td>
<td>Application of PCA only in Taguchi method (More efficient with single Principal Component (PC)), Analyzing by factor plot.</td>
</tr>
<tr>
<td>Tong et al. (2005)</td>
<td>●</td>
<td>●</td>
<td>●</td>
<td></td>
<td>Analyzing by variation mode chart.</td>
</tr>
<tr>
<td>Ribeiro et al. (2010)</td>
<td>●</td>
<td>●</td>
<td>●</td>
<td></td>
<td>Use first PC and optimize the response surfaces.</td>
</tr>
<tr>
<td>Proposed method</td>
<td>●</td>
<td>●</td>
<td>●</td>
<td>●</td>
<td>Allowing different weight (importance) of responses, no limitation for number of components, no Limitation to use Taguchi design, gives Pareto optimum in mathematical model. Considers correlation before regressing the response surfaces.</td>
</tr>
</tbody>
</table>
2.8 Mathematical Model Based on Principal Component Analysis for Optimization of Correlated Multiresponse Surfaces

\[ X = AY = \sum_{j=1}^{p} A_j Y_j \]  

(2)

Where \( A_j = [a_{1j}, a_{2j}, \ldots, a_{pj}]^T \) is the \( j \)th eigenvector of \( \Sigma \). Consequently, the secondary variables have following characteristics (Timm, 2002):

1. \( \sum_{j=1}^{p} a_{ij}^2 = 1 \quad \forall i = 1, \ldots, p \) 

(3)

2. \( \sum_{i=1}^{p} a_{ik} a_{jk} = 0 \quad \forall i, j | i \neq j \) 

(4)

3. Each secondary variable can be obtained from a linear combination of original variables.

4. The first secondary variable covers maximum deviation existing in original variables.

\[ Var(Z_1 = p_1^T Y) = p_1^T \Sigma p_1 \] would be maximized subject to the constraint that \( p_1^T p_1 = 1 \). It was shown that the characteristic vector associated with the largest root of the following equation is the optimal solution for \( p_1 \) and the largest root \( \lambda_1 \) is the variance of \( Z_1 \).

\[ |\Sigma - \lambda I| = 0 \]  

(5)

5. The \( k^{th} \) secondary variable covers maximum deviation which is not covered by \( k-1^{th} \) one.

If the solution of Equation (5) is expressed as \( A = (\lambda_1, \lambda_2, \ldots, \lambda_p) \) such that \( \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_p \), the \( k^{th} \) component would be the characteristic vector associated to \( \lambda_k \).

6. Secondary variables are independent.

4. PROPOSED METHOD

In this paper a mathematical model is developed to find the best combination of variables setting in order to optimize response surfaces. To reach this objective, after running the experiments, related results are gathered and then by means of PCA, uncorrelated components are calculated. These components are new responses and are replaced as experiments responses (observed results). Since after calculation of components, the desired direction of optimization is missed (because of the linear combination of original variables), it is necessary to find optimization direction for each component. For solving this problem the best results of each response, will be calculated by a linear programming and it will be used as a goal for modeling the final objective function. The summary of proposed method is as following steps:

1. Collecting experiments data (responses vs. control variables).

2. Computing uncorrelated responses by PCA (each component is a response).
3. Finding relation function between control variables and new responses by RSM.
4. Optimize of the multiple response surfaces in terms of control variable as decision variables and find optimum value of each component.
5. Find optimum responses by inverting the PCA relations.

These steps are also drawn as a flowchart in Figure 1.

Note that we could consider standard deviations of each response as separated responses, if robustness was important. The next section contains the mathematical formulations and related parameters.

4.1 Mathematical model

In this section, a mathematical program to analyze correlated multiresponse problem has been developed based on PCA. The optimization model has multiple objectives and can be written as follows (Appendix A gives a summarized definition of parameters required to express the model):

\[
\min \text{imize } z = g_j(x) - PC^*_j \quad \forall j = 1, \ldots, n
\]  
(6)

\[
\min \text{imize } k
\]  
(7)

Subject to:

\[
\left| \frac{h_j(\text{PC}) - Y^*_j}{d_j} \right| < kz \quad \forall j = 1, \ldots, n
\]  
(8)

\[
L_i \leq x_i \leq u_i ; \quad \forall i = 1, \ldots m
\]  
(9)

![Figure 1. Proposed method in flowchart view](image-url)
In order to solve this multi-objective model some vector optimization method could be applied to convert multiple objectives to single one. For this purpose Global Criterion method was used to convert first objective set in Equation (6) and then by phasing the model, objectives in Equations (6) and (7) will be analyzed in two stages.

4.2 Global criterion (L_p-metric method) approach

This method allows one to transform a multi-objective optimization problem into a single-objective problem. The function traditionally used in this method is distance.

Through the distance to a referent objective method, the multi-objective method can be written as follows:

\[
\text{Optimize} \ [\text{minimize/maximize}]
\]

\[
F'(x) = \left[ \sum_{i=1}^{n} w_i \left| \frac{Z_i - f_i(x)}{Z_i} \right| \right]^{-1/p}
\]

Where \(Z_i\) is the optimum value of problem objective function when only \(i\)th objective was considered and \(w_i\) is a value representing importance of each objective (Donoso and Fabregat, 2007). In this study GC method was applied to convert problem into single objective form. Now the constraints and objective in the model are explained. First objective function set in Equation (6) represents distance between each response surface and its goal. The next objective function in Equation (7) is put to minimize difference between original responses and their related goals (best observed value). Constraint set in Equation (8) ensures that each response has a minimum difference from its best value. In this set, the normalized distance was used and \(k\) is an arbitrary constant parameter that helps to have feasible solution region. The less values of \(k\) result into a better final solution, but with less values of \(k\), if the model did not have a feasible solution, the analyst must increase \(k\) to find a feasible region. This constraint is used to specify desired optimization direction for each real response. The model could be solved in two stages: the first stage solves the model with second objective only to find the best value of \(k\) that ensure existence of a feasible solution, then second stage applies optimal value of \(k\) obtained from first stage to optimize the first objective function (Equation (6)). At the end, constraint set in Equation (9) represents specific region for each controllable variable. In the next section, some numerical examples are represented to show efficiency of the proposed model.

5. NUMERICAL EXAMPLES

In this section, proposed method is applied to analyze two cases. In addition, the results have been compared with other existing methods.
5.1 Case 1

Tong et al. (2005) attempted to improve the quality of the chemical-mechanical polishing process of copper thin film. Five controllable factors with three levels were considered in an L\textsuperscript{18} orthogonal array. Three response variables for this process are as follows:
1. Removal rate (RR): a larger value is desired.
2. Non-uniformity (NU): a smaller value is desired.
3. TaN/Cu selectivity: a larger value is desired.

Table 2 displays the experimental design and results. Three Signal to Noise (SN) ratios from Taguchi formula are considered as responses.

According to the proposed method, initially response values must be made uncorrelated by PCA. Table 3 displays statistical results for PCA performed by MINITAB software.

After performing PCA, three uncorrelated responses (components) have been determined. The component values (new responses) are shown in Table 4. According to Table 3, converted responses are as follows:

\[ f_1(Y) = PC_1 = 0.449 \cdot RR + 0.882 \cdot NU + 0.145 \cdot TaN \]
\[ f_2(Y) = PC_2 = -0.887 \cdot RR + 0.459 \cdot NU - 0.044 \cdot TaN \]
\[ f_3(Y) = PC_3 = -0.106 \cdot RR - 0.109 \cdot NU + 0.988 \cdot TaN \]

Next step in proposed method will be conducted by forming response surfaces between factors and new responses.

After converting responses by PCA, for each component (Principal Component, PC), the response surface must be obtained by regression models. Following equations (performed by Design Expert 7.1.1 software), represent regression functions between PCs and controllable variables.

\[ g_1 = PC_1 = 0.242 + 3.464 \cdot A + 1.758 \cdot B - 1.879 \cdot D \]
\[ g_2 = PC_2 = -61.457 + 0.207 \cdot A + 0.587 \cdot B + 4.08 \cdot C + 4.178 \cdot D - 1.28 \cdot AD - 0.713 \cdot BC - 1.34 \cdot CD \]
\[ g_3 = PC_3 = 7.4398 + 0.9254 \cdot B + 0.408 \cdot C \]

Now in the final step, according to parameter definition described in Section 5, we use optimization model with following variables:

\[ Y^* = (65, -8, 25) \]
\[ d = (8.71, 14.62, 4.35) \]
\[ h_1 = RR = 0.449 \cdot PC_1 - 0.887 \cdot PC_2 - 0.106 \cdot PC_3 \]
\[ h_2 = NU = 0.882 \cdot PC_1 + 0.459 \cdot PC_2 - 0.109 \cdot PC_3 \]
\[ h_3 = TaN = 0.145 \cdot PC_1 - 0.044 \cdot PC_2 + 0.988 \cdot PC_3 \]
\[ PC^* = (15.28467, -57.1427, 11.09801) \]

By forming mathematical model and solving it (by LINGO software), it is found that optimal setting for controllable variables are: \( X = (3, 3, 3, 2.16, 1) \). It is considerable point that after solving model in first stage, optimal value of \( k \) equals to 2.1048. Table 5 displays final results that contains the values of objective function (Z), control variables (A: E), prediction of responses (RR, NU, TaN) and related components (PCs).
In Tong et al. (2005) it is found that the optimal solution are obtained from variation mode chart and also because of highest priority, only one response was considered; but in the proposed method, we find the best solutions by systematic approach and also by considering multiple solution which could have different priorities. About TaN response variable, it should be stated in Tong et al. (2005), TaN has positive coefficient in all components so the optimization of multiresponse problem does not have undesired effects on this response.

### Table 2. Experimental observations and Signal to Noise (SN) ratio

<table>
<thead>
<tr>
<th>Experiment number</th>
<th>Controllable variables (Factors)</th>
<th>SN Ratio for each response</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A</td>
<td>B</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>7</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>8</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>9</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>10</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Max</td>
<td>56.39</td>
<td></td>
</tr>
<tr>
<td>Min</td>
<td>47.68</td>
<td></td>
</tr>
<tr>
<td>Range</td>
<td>8.71</td>
<td></td>
</tr>
</tbody>
</table>

### Table 3. Principal Component Analysis: RR, NU, TaN

<table>
<thead>
<tr>
<th>Variable</th>
<th>PC1</th>
<th>PC2</th>
<th>PC3</th>
<th>Eigen analysis of the Covariance Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>RR</td>
<td>0.449</td>
<td>-0.887</td>
<td>-0.106</td>
<td>Eigen value 20.939 3.820 1.216</td>
</tr>
<tr>
<td>NU</td>
<td>0.882</td>
<td>0.459</td>
<td>-0.099</td>
<td>Proportion 0.806 0.147 0.047</td>
</tr>
<tr>
<td>TaN</td>
<td>0.145</td>
<td>-0.044</td>
<td>0.988</td>
<td>Cumulative 0.806 0.953 1.000</td>
</tr>
</tbody>
</table>

### Table 4. Component values after PCA

<table>
<thead>
<tr>
<th>Experiment number</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>...</th>
<th>10</th>
<th>11</th>
<th>12</th>
<th>13</th>
<th>...</th>
<th>16</th>
<th>17</th>
<th>18</th>
</tr>
</thead>
<tbody>
<tr>
<td>PC1</td>
<td>3.55</td>
<td>2.86</td>
<td>0.53</td>
<td>...</td>
<td>2.02</td>
<td>-1.62</td>
<td>6.84</td>
<td>3.21</td>
<td>...</td>
<td>9.57</td>
<td>5.96</td>
<td>15.17</td>
</tr>
<tr>
<td>PC2</td>
<td>-54.9</td>
<td>-55.2</td>
<td>-57.5</td>
<td>...</td>
<td>-54</td>
<td>-56.7</td>
<td>-54.9</td>
<td>-57.5</td>
<td>...</td>
<td>-56.9</td>
<td>-60.4</td>
<td>-57</td>
</tr>
<tr>
<td>PC3</td>
<td>9.21</td>
<td>9.94</td>
<td>12.49</td>
<td>...</td>
<td>10.71</td>
<td>10.11</td>
<td>11.20</td>
<td>8.92</td>
<td>...</td>
<td>10.54</td>
<td>9.84</td>
<td>10.68</td>
</tr>
</tbody>
</table>

### Table 5. Optimum values from mathematical model -- Case 1

<table>
<thead>
<tr>
<th>Variable</th>
<th>Z</th>
<th>PC1</th>
<th>PC2</th>
<th>PC3</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>Prediction value</th>
</tr>
</thead>
<tbody>
<tr>
<td>RR</td>
<td>1.79</td>
<td>11.84</td>
<td>-61.26</td>
<td>11.44</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>2.16</td>
<td>1</td>
<td>58.44</td>
</tr>
<tr>
<td>NU</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>1</td>
<td>-18.92</td>
</tr>
<tr>
<td>TaN</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>1</td>
<td>15.72</td>
</tr>
</tbody>
</table>

Tong et al. (2005)
5.2 Case 2

Su and Tong (1997), studied a case that involves improving a hard disk drive’s quality, and an experiment was performed to determine the effects of design parameters on the responses. The four desired responses are:

1. PW: 50% pulse width (STB, Smaller-The-Better);
2. HFA: high-frequency amplitude (LTB, Larger-The-Better);
3. OW: over write (LTB);
4. PS: peak shift (STB).

Optimal settings could, it was hoped, be found such that a low variability for the responses could be achieved. Table 6 lists experimental factors and their alternative levels. The standard array $L_{18}$ was selected for the experiment.

According to Equations (3) and (4), the model parameters have been obtained as shown in following equations:

$$PC_1 = 0.565 \ W + 0.514 \ HFA - 0.4 \ OW + 0.508 \ PS$$
$$PC_2 = 0.203 \ W - 0.001 \ HFA + 0.866 \ OW + 0.457 \ PS$$
$$PC_3 = -0.070 \ W + 0.806 \ HFA + 0.288 \ OW - 0.512 \ PS$$
$$PC_4 = -0.797 \ W + 0.293 \ HFA - 0.088 \ OW + 0.521 \ PS$$

After computing converted response variables, RSM should conducted on the PCs and factors. Following equations shows response surfaces for this case:

$$g_1 = -0.71 + 0.45 A - 0.85 B + 1.78 C + 1.74 D + 1.36 E + 0.081 F + 0.11 G + 0.059 H + 0.38 AB + 0.32 AC - 0.27 AD - 0.68 AE + 0.079 AF - 0.45 CD + 0.50 CE - 0.26 CF$$
$$g_2 = -2.72 + 2.73 A + 0.26 B - 0.97 C + 2.18 D + 2.14 E - 0.91 F - 0.33 G + 0.4 H - 0.11 AB + 0.49 AC - 1.18 AD - 1.03 AE - 0.31 AF - 0.33 CD - 0.30 CE + 0.50 CF$$
$$g_3 = -3.01 + 3.09 A - 2.82 B + 0.93 C - 1.68 D + 4.78 E - 0.25 AB + 0.41 AC - 0.31 AE + 0.29 BC + 0.99 BD - 1.16 BE + 0.61 CD + 0.45 CE - 1.01 DE + 0.62 B2 - 0.22 C2$$
$$g_4 = -1.40 + 1.32 A - 0.38 B - 0.10 C + 0.72 D + 0.29 E + 0.32 F + 0.12 AB - 0.23 AD - 0.38 AE - 0.22AF + 0.064 BC - 0.089 CD + 0.075 CE - 0.082 CF$$

---

**Table 6. Experiment results (normalized data (Case study 2))**

<table>
<thead>
<tr>
<th>Factors</th>
<th>Responses (Normalized loss function)</th>
<th>PW (50% pulse width)</th>
<th>HFA (high-frequency amplitude)</th>
<th>OW (over write)</th>
<th>PS (peak shift)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A 1</td>
<td>B 1</td>
<td>C 1</td>
<td>D 1</td>
<td>E 1</td>
<td>F 1</td>
</tr>
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The same calculations as the previous case must be applied to find model requirements; so we cede more discussions and only give parameter values as follows:

\[ Y^* = (1, 1, 1, 1) \]
\[ d = (1, 1, 1, 1) \]
\[ h_1 = PW = 0.565 \text{PC}_1 + 0.203 \text{PC}_2 - 0.07 \text{PC}_3 - 0.797 \text{PC}_4 \]
\[ h_2 = HFA = 0.514 \text{PC}_1 - 0.001 \text{PC}_2 + 0.806 \text{PC}_3 + 0.293 \text{PC}_4 \]
\[ h_3 = OW = -0.4 \text{PC}_1 + 0.866 \text{PC}_2 + 0.288 \text{PC}_3 - 0.088 \text{PC}_4 \]
\[ h_4 = PS = 0.508 \text{PC}_1 + 0.457 \text{PC}_2 - 0.512 \text{PC}_3 + 0.521 \text{PC}_4 \]
\[ PC^* = (1.65, 1.53, 0.72, -0.187) \]

After solving model in first stage, we found \( k = 2.99 \). Detailed results are shown in Table 7 to confirm the model solutions.

Su and Tong (1997) used single principal component to aggregate the multiple response problems and consideration of correlation was not clear. Also they explained that use of more than single PC entails difficulties on conclusion and analyzing, since the trade off of PCs must be considered. In their method, \( \Omega \) value must be maximized in order to gain the best responses values. Consider the first eigenvalue, after computing the \( \Omega \) equation, if related coefficients do not have the same signs, the problem would be more difficult to solve. Assume that there were both negative and positive coefficients for responses in \( \Omega \) equation; in this case, maximization or minimization of the \( \Omega \) gives no assurance for optimization of all of the response values because, the maximization of \( \Omega \) tries to minimize those responses that have negative coefficient (see into \( OW \) in case 2). Hence using the single PC could disorder the aggregation. The proposed method, on one hand, used maximum number of PC resulting better representation of original data without losing information, and on other hand, there is no limitation in form of eigenvector (any sign for each coefficient in eigenvector will be allowed and analyzable). The comparison of the proposed method and Su research are summarized as follows:

1. We applied one of the most popular methods for aggregating the multiple responses (desirability function, distance function and Taguchi loss function).
2. Usage of the PCA in our method was directly related to uncorrelating the response vectors.
3. Although we applied the PCA and optimized the PC values, similar to Su and Tong’s (1997) research, it was contemplated that the direction of the optimality remains unchanged.
4. Our proposed method, optimize the objective function in continuous space.
5. Consideration of different degree of important for each response was allowed by our aggregation function but in Su and Tong’s (1997) research, it is possible that the coefficients of the each response in omega equation had not compatibility with its importance.

Table 8 shows the final results of proposed method in comparison to other approaches in literature.

The less value of the EDG (Euclidian Distance to Goal values) results into better response variables. The proposed method has significant differences in comparison to other studies.
6. CONCLUSION

In this study we proposed a novel mathematical model for optimization of multiple response models when responses are correlated. If optimization performed without considering correlation, the correlation between responses may be interacting, and thereupon Optimality may be lost in confirmation experiments. Because of this confliction, we applied PCA method to calculate uncorrelated components from correlated ones. We also studied two cases from literature to illustrate efficiency of the proposed method. At the end of the paper some benefits of the proposed method in comparison to other related approaches was given and results have been discussed.

References

A Mathematical Model Based on Principal Component Analysis for Optimization of Correlated Multiresponse Surfaces


Hotelling, H., 1933, Analysis of a complex of statistical variables into principal components, *Journal of Educational Psychology*, 24(7), 498-520.


Appendix A: Parameter Definition

The mathematical formulations will be expressed by following parameters:

\( Y_j \): Experimental responses (\( j = 1, \ldots, n \)).
\( Y_j^* \): Best observed value for \( j \)th response.
\( d_j \): Range of values for \( j \)th response.
\( X = x_1, x_2, \ldots, x_m \): Vector of experiment controllable variables.
\( (l_j, u_j) \): Lower & upper bound of \( j \)th controllable variable, \( j = 1, \ldots, m \).
\( PC_j \): Principal Component (\( j = 1, \ldots, n \)).

According to Equation (A1), it is known that:

\[
PC_j = f_j(Y_1, Y_2, \ldots, Y_n) \tag{A1}
\]

and

\[
Y_j = h_j(PC_1, PC_2, \ldots, PC_n) \tag{A2}
\]

And According to Equation (A2), it’s obvious that: \( h = f - 1 \).

\( PC_j^* = f_j(Y_1^*, Y_2^*, \ldots, Y_n^*) \)

\( g_j(X) \): Response surface (regression function) for \( PC_j \).
以主成份分析為基礎的數學模式找出相關性的多重反應曲面最佳化

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摘 要
多重品質特性 (或反應變數) 最佳化遠比單一因子的最佳化來得複雜，因為我們面臨不同單位、重要性與最佳化方向。在大多數真實情形下，反應是相關的，因此下結論變得困難。若把品質特性的相關性忽略，工程設計人員可能無法發現設計變數的設定可以同時改善所有反應的品質。本研究以多重相關性反應的最佳化為重點，並且提出一個以主成份分析為基礎的新的數學模式。並且利用兩個從文獻找來的範例說明所提出的方法有較好的效率。

關鍵詞：多重反應曲面、相關性反應、數學規劃、主成份分析

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