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Simultaneous Optimization of Multiple Responses to the Combined Array

Yong-Man Kwon[1]

Abstract

In the Taguchi parameter design, the product-array approach using orthogonal arrays is mainly used. However, it often requires an excessive number of experiments. An alternative approach, which is called the combined-array approach, was suggested by Welch et al (1990) and studied by Vining and Myers (1990) and others. In these studies, only single response variable was considered. We propose how to simultaneously optimize multiple responses when there are correlations among responses.

Key Words and Phrases: Taguchi Parameter Design, Product-Array Approach, Combined-Array Approach, Simultaneously Optimize Multiple Responses

1 Introduction

Products and their manufacturing processes are influenced both by control factors that can be controlled by designers and by noise factors that are difficult or expensive to control such as environmental conditions. The basic idea of parameter design is to identify, through exploiting interactions between control factors and noise factors, appropriate settings of control factors that make the system's performance robust to changes in the noise factors. Parameter design is a quality improvement technique proposed by the Japanese quality expert Taguchi, which was described by Taguchi (1986, 1987), Kackar (1985) and others.

The control factors are assigned to an inner array, which is an orthogonal array. For each row in the inner array, the noise factors are assigned to an outer array, also an orthogonal array. Because the outer array is run for every row in the inner array, we call this setup a product array. A large number of experimental trials

[1]Associate Professor, Department of Computer Science and Statistics, Chosun University, Kwangju, 503-062, Korea

in Taguchi's product array may be required because the noise array is repeated for every row in the control array. There have been efforts for integrating Taguchi's important notion of heterogeneous variability the standard experimental design and modeling technology provided by response surface methodology. They combined control and noise factors in a single design matrix, which we call a combined array.

The combined array approach was first proposed by Welch et al (1990). The initial motivation of the combined array is the run-size saving. Related approaches were discussed by Vining and Myers (1990), Box and Jones (1992), etc. Treatment of the mean and variance responses via a constrained optimization was discussed in Vining and Myers (1990).

In many experimental situations, a number of responses are measured for a given setting of design variables. Khuri and Conlon (1981) introduced a procedure for the simultaneous optimization of multiple responses using a distance function.

In this paper we propose the simultaneous optimization measure of multiple responses to the combined array. One numerical example is given in Section 3.

2 Simultaneous Optimization of Multiple Responses

2.1 Multivariate Linear Model

Suppose the response y, depends on control variables (or factors) and noise variables. Let a set of control variables be denoted by $\underline{x} = (x_1, x_2, \cdots, x_l)'$ and a set of noise variables by $\underline{z} = (z_1, z_2, \cdots, z_m)'$. Suppose that all response functions in a multiresponse system depend on the same set of $\underline{x}$ and $\underline{z}$ and that they can be represented by second order models within a certain region of interest. Let N be the number of experimental runs and r be the number of response functions. The ith second order model is

$$y_i(\underline{x}, \underline{z}) = \beta_{i0} + \underline{x}'\underline{\beta}_i + \underline{x}'B_i\underline{x} + \underline{z}'R_i\underline{z} + \underline{z}'\underline{\gamma}_i + \underline{z}'D_i\underline{x} + \epsilon_i, \quad i = 1, 2, \cdots, r, \qquad (1)$$

where β_i is $l \times 1$, γ_i is $m \times 1$, $B_i' = B_i$ is $l \times l$, $R_i' = R_i$ is $m \times m$ and D_i is $m \times l$ which are vectors or matrices of unknown regression parameters, and ϵ_i is a random error associated with the ith response.

Equation (1) can be expressed in matrix notation as

$$\underline{y}_i = X\underline{\theta}_i + \underline{\epsilon}_i, \quad i = 1, 2, \cdots, r, \qquad (2)$$

in which $\underline{y}_i$ is an $N \times 1$ vector of observations on the ith response, X is an $N \times p$ full column rank matrix of known constants, $\underline{\theta}_i$ is the $p \times 1$ column vector of unknown regression parameters and ϵ_i is a vector of random errors associated with the ith response. We also assume that

$$E(\underline{\epsilon}_i) = \underline{0}, \; Var(\underline{\epsilon}_i) = \sigma_{ii}I_N, \; Cov(\underline{\epsilon}_i, \underline{\epsilon}_j) = \sigma_{ij}I_N \quad i, j = 1, 2, \cdots, r, \; i \neq j.$$

The $r \times r$ matrix whose (i,j)th element σ_{ij} is will be denoted by Σ. An unbiased estimator of Σ is given by

$$\widehat{\Sigma} = Y'[I_N - X(X'X)^{-1}X']Y/(N-p),$$

where $Y = (\underline{y}_1, \underline{y}_2, \cdots, \underline{y}_r)$, and I_N is an identity matrix of order $N \times N$. The r equations given in (2) may be written in a compact form

$$\underline{y} = \begin{bmatrix} \underline{y}_1 \\ \underline{y}_2 \\ \vdots \\ \underline{y}_r \end{bmatrix} = \begin{bmatrix} X & 0 & \cdots & 0 \\ 0 & X & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & X \end{bmatrix} \begin{bmatrix} \underline{\theta}_1 \\ \underline{\theta}_2 \\ \vdots \\ \underline{\theta}_r \end{bmatrix} + \begin{bmatrix} \underline{\epsilon}_1 \\ \underline{\epsilon}_2 \\ \vdots \\ \underline{\epsilon}_r \end{bmatrix} = Z\underline{\theta} + \underline{\epsilon}, \tag{3}$$

where $\underline{y}$ is $rN \times 1$, Z is $rN \times rp$, $\underline{\theta}$ is $rp \times 1$ and $\underline{\epsilon}$ is $rN \times 1$. The variance-covariance matrix of $\underline{\epsilon}$ is

$$Var(\underline{\epsilon}) = \Sigma \otimes I = \Omega,$$

where $\otimes$ is a symbol for the direct (or Kronecker) product of matrices.

The BLUE (best linear unbiased estimator) of $\underline{\theta}$ in (3) is

$$\widehat{\underline{\theta}} = (Z'\Omega^{-1}Z)^{-1}(Z'\Omega^{-1}\underline{y}) = (Z'Z)^{-1}Z'\underline{y}.$$

Thus, the BLUE of $\underline{\theta}$ is $\widehat{\underline{\theta}} = (\widehat{\underline{\theta}}_1', \widehat{\underline{\theta}}_2', \cdots, \widehat{\underline{\theta}}_r')'$ where $\widehat{\underline{\theta}}_i = (X'X)^{-1}X'\underline{y}_i$ is the least squares estimator of the $p \times 1$ vector of regression coefficients for the ith response model (see Huang (1970, p.188)). The variance-covariance of $\widehat{\underline{\theta}}$

$$Var(\widehat{\underline{\theta}}) = (Z'\Omega^{-1}Z)^{-1} = (X'X)^{-1}\Sigma.$$

The prediction equation for the ith response is given by

$$\widehat{y}_i(\underline{x}, \underline{z}) = \underline{g}'(\underline{x}, \underline{z})\widehat{\underline{\theta}}_i, \quad i = 1, 2, \cdots, r, \tag{4}$$

where $(\underline{x}', \underline{z}')'$ is the vector of coded input variables, $\underline{g}'(\underline{x}, \underline{z})$ is a vector of the same form as a row of the matrix X evaluated at the point $(\underline{x}, \underline{z})$. From (4) it follows that

$$Var[\widehat{y}_i(\underline{x}, \underline{z})] = \underline{g}'(\underline{x}, \underline{z})(X'X)^{-1}\underline{g}(\underline{x}, \underline{z})\sigma_{ii}, \quad i = 1, 2, \cdots, r,$$

$$Cov[\widehat{y}_i(\underline{x}, \underline{z}), \widehat{y}_j(\underline{x}, \underline{z})] = \underline{g}'(\underline{x}, \underline{z})(X'X)^{-1}\underline{g}(\underline{x}, \underline{z})\sigma_{ij}, \quad i, j = 1, 2, \cdots, r; i \neq j.$$

Hence,

$$Var[\widehat{\underline{y}}(\underline{x}, \underline{z})] = \underline{g}'(\underline{x}, \underline{z})(X'X)^{-1}\underline{g}(\underline{x}, \underline{z})\Sigma,$$

where $\widehat{\underline{y}}(\underline{x}, \underline{z}) = (\widehat{y}_1(\underline{x}, \underline{z}), \widehat{y}_2(\underline{x}, \underline{z}), \cdots, \widehat{y}_r(\underline{x}, \underline{z}))'$ is the vector of predicted responses at the point $(\underline{x}, \underline{z})$. An unbiased estimator of $Var[\widehat{y}_i(\underline{x}, \underline{z})]$ is given by

$$\widehat{Var}[\widehat{\underline{y}}(\underline{x}, \underline{z})] = \underline{g}'(\underline{x}, \underline{z})(X'X)^{-1}\underline{g}(\underline{x}, \underline{z})\widehat{\Sigma}.$$

2.2 Estimated Mean and Variance Models

Box and Jones (1992) modeled the mean and variance separately in a single response. But, we are interested in showing the estimated mean and variance response models in multiple responses.

The fitted ith second-order model in (4) can be rewritten as

$$\widehat{y}_i(\underline{x},\underline{z}) = b_{i0} + \underline{x}'\underline{b}_i + \underline{x}'\widehat{B}_i\underline{x} + \underline{z}'\widehat{R}_i\underline{z} + \underline{z}'\underline{r}_i + \underline{z}'\widehat{D}_i\underline{x}, \quad i = 1, 2, \cdots, r.$$

The noise variables $\underline{z}$ are not controllable and they are random variables. In the absence of other knowledge, $\underline{z}$ would be usually uniformly distributed over R_z.

Let $\widehat{m}_i(\underline{x})$ be the ith estimated mean response at an $\underline{x}$ averaged over the noise variables

$$\widehat{m}_i(\underline{x}) = \int_{R_z} \widehat{y}(\underline{x},\ \underline{z})p(\underline{z})d\underline{z}, \quad i = 1, 2, \cdots, r,$$

where $p(\underline{z})$ is a probability density function of $\underline{z}$ and $\underline{z}$ has a uniform distribution over $R_z(-1 \leq z \leq 1)$. Box and Jones (1992) showed that the ith estimated mean becomes

$$\widehat{m}_i(\underline{x}) = b_{i0} + \underline{x}'\underline{b}_i + \underline{x}'\widehat{B}_i\underline{x} + \frac{1}{3}tr\widehat{R}_i, \quad i = 1, 2, \cdots, r, \tag{5}$$

where $tr\widehat{R}_i$ is the trace of the matrix $\widehat{R}_i$. Let us write $\widehat{v}_i(\underline{x})$ for the ith mean square variation about the ith mean response

$$\widehat{v}_i(\underline{x}) = \int_{R_z} (\widehat{y}_i(\underline{x},\underline{z}) - \widehat{m}_i(\underline{x}))^2 p(\underline{z})d\underline{z}, \quad i = 1, 2, \cdots, r.$$

Let us call this measure the ith estimated variance, which becomes

$$\widehat{v}_i(\underline{x}) = \frac{1}{3}(\underline{r}_i + \widehat{D}\underline{x})'(\underline{r}_i + \widehat{D}\underline{x}) + \widehat{A}_i, \quad i = 1, 2, \cdots, r, \tag{6}$$

where $\widehat{A}_i = [4\Sigma_{j=1}^{m}(r_{jj}^i)^2 + 5\Sigma_{j=1}^{m-1}\Sigma_{k=j+1}^{m}(r_{jk}^i)^2]/45$ and r_{jk}^i is the jth row and kth column element of the matrix $\widehat{R}_i$.

From (5) the ith estimated mean can be rewritten as

$$\widehat{m}_i(\underline{x}) = \underline{h}'(\underline{x})\widehat{\underline{\theta}}_{0i}, \quad i = 1, 2, \cdots, r, \tag{7}$$

where $\underline{h}'(\underline{x}) = (1, x_1, \cdots, x_l, x_1^2, \cdots, x_l^2, x_1x_2, \cdots, x_{l-1}x_l, 1/3, \cdots, 1/3)$ and $\widehat{\underline{\theta}}_{0i} = (b_0^i, b_1^i, \cdots, b_l^i, b_{11}^i, \cdots, b_{ll}^i, b_{12}^i, \cdots, b_{(l-1)l}^i, r_{11}^i, \cdots, r_{mm}^i)'$ is a part of $\widehat{\underline{\theta}}_i$. From the fact that $\widehat{\underline{\theta}}_{0i}$ is a part of $\widehat{\underline{\theta}}_i$, the variance-covariance of $\widehat{\underline{\theta}}_0$ is given by

$$Var(\widehat{\underline{\theta}}_0) = (X'X)_0^{-1}\Sigma,$$

Where $\underline{\widehat{\theta}}_0 = (\underline{\widehat{\theta}}'_{01}, \underline{\widehat{\theta}}'_{02}, \cdots, \underline{\widehat{\theta}}'_{0r})'$, is $p \times p$, $(X'X)_0^{-1}$ is $q \times q$ where $p = (l+m+n)(l+m+2)/2$, and $q = (l+1)(l+2)/2 + m$. Here $(X'X)_0^{-1}$ is the $q \times q$ submatrix of $(X'X)^{-1}$. From (7) and above, we then have

$$Var[\underline{\widehat{m}}(\underline{x})] = \underline{h}'(\underline{x})(X'X)_0^{-1}\underline{h}'(\underline{x})\Sigma,$$

where $\underline{\widehat{m}}(\underline{x}) = (\widehat{m}_1(\underline{x}), \widehat{m}_2(\underline{x}), \cdots, \widehat{m}_r(\underline{x}))'$ is the vector of estimated mean responses at the point $\underline{x}$. An unbiased estimator of $Var[\underline{\widehat{m}}(\underline{x})]$ is given by

$$\widehat{Var}[\underline{\widehat{m}}(\underline{x})] = \underline{h}'(\underline{x})(X'X)_0^{-1}\underline{h}'(\underline{x})\widehat{\Sigma}. \quad (8)$$

2.3 The Proposed Measure

Let us find conditions on a set of control variables $\underline{x}$ which optimize a set of estimated mean responses $\underline{\widehat{m}}(\underline{x})$ subject to maintaining estimated variance responses $\underline{\widehat{v}}(\underline{x})$ within some specified upper bounds. If all the estimated mean $\underline{\widehat{m}}(\underline{x})$ attain their individual optimum values $\underline{\tau}$ at the same set $\underline{x}$ of operating conditions, then the problem of simultaneous optimization is obviously solved. This ideal optimum rarely occurs. In more general situations we might consider finding compromising conditions on the control variables that are somewhat favorable to all mean responses. Such deviation of the compromising conditions from the ideal optimum condition can be evalulated by means of a distance function which measures the distance of $\underline{\widehat{m}}(\underline{x})$ from $\underline{\tau}$.

Let $\underline{\tau}$ be the optimum (or target) value of $\underline{\widehat{m}}(\underline{x})$ over R_x and let $\underline{\tau} = (\tau_1, \tau_2, \cdots, \tau_r)$. We shall consider a constrained-optimization procedure for each response according to the Taguchi's three basic situations as follows.

1.nominal-is-best characteristics: target value of $\widehat{m_i}(\underline{x}) = \tau_i$ subject to $\widehat{v_i}(\underline{x}) \leq l_i$, where l_i is some upper bound on the variation,

2.larger-the-better characteristics: $Max_{\underline{x} \in R_x}\widehat{m_i}(\underline{x}) = \tau_i$ subject to $\widehat{v_i}(\underline{x}) \leq l_i$,

3.smaller-the-better characteristics: $Min_{\underline{x} \in R_x}\widehat{m_i}(\underline{x}) = \tau_i$ subject to $\widehat{v_i}(\underline{x}) \leq l_i$.

A distance function of $\underline{\widehat{m}}(\underline{x})$ for the target value $\underline{\tau}$ may be expressed as

$$D[\underline{\widehat{m}}(\underline{x}), \underline{\tau}] = [(\underline{\widehat{m}}(\underline{x}) - \underline{\tau})'\{Var[\underline{\widehat{m}}(\underline{x})]\}^{-1}(\underline{\widehat{m}}(\underline{x}) - \underline{\tau})]^{1/2}.$$

Using the estimate given in (8) for the variance-covariance matrix of $\underline{\widehat{m}}(\underline{x})$, we get a distance function

$$\left[\frac{(\underline{\widehat{m}}(\underline{x}) - \underline{\tau})'\widehat{\Sigma}^{-1}(\underline{\widehat{m}}(\underline{x}) - \underline{\tau})}{\underline{h}'(\underline{x})(X'X)_0^{-1}\underline{h}'(\underline{x})}\right]^{1/2}.$$

If the mean response $\underline{\widehat{m}}(\underline{x})$ takes on different degrees of importance, we can imply weights $w_1, w_2, \cdots, w_r$ where $0 < w_i < 1$ for each i and $\Sigma_{i=1}^{r} w_i = 1$. Then the distance function can be written as

$$\left[\frac{\{W(\underline{\widehat{m}}(\underline{x}) - \underline{\tau})\}'\widehat{\Sigma}^{-1}\{W(\underline{\widehat{m}}(\underline{x}) - \underline{\tau})\}}{\underline{h}'(\underline{x})(X'X)_0^{-1}\underline{h}'(\underline{x})}\right]^{1/2}, \quad (9)$$

where $W = \begin{bmatrix} w_1 & 0 & \cdots & 0 \\ 0 & w_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & w_r \end{bmatrix}$. From the constrained-optimization procedure and the distance measure of $\widehat{\underline{m}}(\underline{x})$ for the target value $\underline{\tau}$, we propose a simultaneous optimization of $\widehat{\underline{m}}(\underline{x})$ while constraining the estimated variance response $\widehat{v}_i(\underline{x})$ over the region of interest R_x. From (9), the proposed simultaneous-optimization measure can be written as

$$\begin{aligned} \underset{\underline{x}\in R_x}{Min}\ P_m(\underline{x}) &= \underset{\underline{x}\in R_x}{Min}\ \frac{\{W(\widehat{\underline{m}}(\underline{x})-\underline{\tau})\}'\widehat{\Sigma}^{-1}\{W(\widehat{\underline{m}}(\underline{x})-\underline{\tau})\}}{\underline{h}'(\underline{x})(X'X)_0^{-1}\underline{h}'(\underline{x})} \\ & \quad subject\ to\ \ \widehat{v}_i(\underline{x}) \le l_i, \quad i=1,2,\cdots,r. \end{aligned} \tag{10}$$

The P_m measure can be used without a prior knowledge about the estimated mean responses. It takes into consideration the variances and correlations of the estimated mean responses. If a simultaneous optimum value is much different from its corresponding individual optimum value, we may choose a bound on it and then reoptimize P_m. Also we may analyze P_m sequentially as the acceptable values for the estimated variance responses $l_1, l_2, \cdots, l_r$ are varied.

3 Numerical Example

In this section we give a numerical example, consisting of a multiresponse system of two response variables, y_1 and y_2, and two control variables, x_1 and x_2 and a noise variable z. The design is somewhat similar to the standard central composite design. The cube portion of the experimental arrangement is chosen to be a 2^3 design and star points are added only for the two control variables. The following Table 1 gives the factor levels and a set of hypothetical data. Each of the two responses was fitted to a second order regression model. The estimated response models by the method of least squares are given by

$$\begin{aligned} \widehat{y}_1(\underline{x},z) &= 76.00 - 12.37x_1 - 8.96x_2 - 7.22x_1^2 - 8.45x_2^2 \\ &\quad -8.11x_1x_2 + 5.38z^2 - 1.44z + 2.96x_1z - 1.86x_2z, \end{aligned} \tag{11}$$

$$\begin{aligned} \widehat{y}_2(\underline{x},z) &= 103.00 - 12.21x_1 + 6.68x_2 - 13.96x_1^2 - 8.50x_2^2 \\ &\quad -2.93x_1x_2 + 6.23z^2 - 1.38z + 1.75x_1z - 2.95x_2z. \end{aligned} \tag{12}$$

From (11) and (12), using the mean and variance response equation (5) and (6), the estimated mean and variance response models are given by

$$\widehat{m}_1(\underline{x}) = 77.79 - 12.37x_1 - 8.96x_2 - 7.22x_1^2 - 8.45x_2^2 - 8.11x_1x_2,$$

$$\widehat{m}_2(\underline{x}) = 105.08 - 12.21x_1 + 6.68x_2 - 13.96x_1^2 - 8.50x_2^2 - 2.93x_1x_2,$$

$$\widehat{v}_1(\underline{x}) = (-1.44 + 2.96x_1 - 1.86x_2)^2/3 + 2.57,$$

$$\widehat{v}_2(\underline{x}) = (-1.38 - 1.75x_1 - 2.95x_2)^2/3 + 3.45.$$

The region of interest R_x is given by the inequality $-1 \leq x_1, x_2 \leq 1$. The ranges for $\widehat{m_1}(\underline{x})$, $\widehat{m_2}(\underline{x})$, $\widehat{v_1}(\underline{x})$ and $\widehat{v_2}(\underline{x})$ over R_x are respectively, $32.68 \leq \widehat{m_1}(\underline{x}) \leq 83.25$, $66.66 \leq \widehat{m_2}(\underline{x}) \leq 109.65$, $2.57 \leq \widehat{v_1}(\underline{x}) \leq 15.63$ and $3.45 \leq \widehat{v_1}(\underline{x}) \leq 15.77$.

Suppose that the quality characteristics for y_1 and y_2 are the nominal-is-best characteristics and the larger-the-better characteristics. Let us assume that the target value of $\widehat{m}_1(\underline{x})$ is taken to be 75.00 and the target value of $\widehat{m}_2(\underline{x})$ is taken to be $Max_{\underline{x} \in R_x} \widehat{m}_2(\underline{x}) = 109.65$. The maximum acceptable values for $\widehat{v}_1(\underline{x})$ and $\widehat{v}_2(\underline{x})$ are $\widehat{v}_1(\underline{x}) \leq 4$ and $\widehat{v}_2(\underline{x}) \leq 4$, respectively. Assume it is of interest to obtain the target condition on the estimated mean response $\underline{\widehat{m}}(\underline{x})$ while constraining the variance response $\underline{\widehat{v}}(\underline{x})$.

We obtained the results of simultaneous optimization based on the minimization of the P_m measure over R_x. Table 2 indicates that the optimal setting for the constraint that $\widehat{v}_1(\underline{x}) \leq 4$, $\widehat{v}_2(\underline{x}) \leq 4$, $w_1 = 0.1$ and $w_2 = 0.9$ is $x_1 = -0.10$ and $x_2 = 0.18$ which produces a predicted value of 77.21, 107.14, 4.00 and 3.80 for $\widehat{m}_1(\underline{x})$, $\widehat{m}_2(\underline{x})$, $\widehat{v}_1(\underline{x})$ and $\widehat{v}_2(\underline{x})$ respectively.

<Table 1.> Experimental Design and Response Values

Run Number	x_1	x_2	z	y_1	y_2
1	-1	-1	-1	80.6	81.4
2	-1	-1	1	74.9	95.9
3	-1	1	-1	83.1	105.0
4	-1	1	1	71.2	103.0
5	1	-1	-1	66.8	74.0
6	1	-1	1	74.2	76.8
7	1	1	-1	38.1	81.2
8	1	1	1	36.8	76.9
9	-1.41	0	0	80.9	100.0
10	1.41	0	0	42.4	50.5
11	0	-1.41	0	73.4	71.2
12	0	1.41	0	45.0	101.0
13	0	0	0	77.4	102.0
14	0	0	0	74.6	104.0

<Table 2.> Simultaneous Optimization for P_m

Weight		Location of Optima		Simultaneous Optima			
w_1	w_2	x_1	x_2	$\widehat{m_1}(\underline{x})$	$\widehat{m_2}(\underline{x})$	$\widehat{v_1}(\underline{x})$	$\widehat{v_2}(\underline{x})$
0.1	0.9	-0.10	0.18	77.21	107.14	4.00	3.80
0.3	0.7	-0.03	0.29	74.92	106.68	4.00	3.56
0.5	0.5	-0.03	0.29	74.92	106.68	4.00	3.56
0.7	0.3	-0.03	0.29	74.92	106.68	4.00	3.56
0.9	0.1	-0.01	0.26	75.03	106.37	3.84	3.58

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