시뮬레이션과 RSM을 이용한 시스템 최적화 과정에서 공통난수 활용에 따른 분산 분석

Analysis of Variance for Using Common Random Numbers When Optimizing a System by Simulation and RSM

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Abstract

When optimizing a complex system by determining the optimum condition of the system parameters of interest, we often employ the process of estimating the unknown objective function, which is assumed to be a second order spline function. In doing so, we normally use common random numbers for different set of the controllable factors resulting in more accurate parameter estimation for the objective function. In this paper, we will show some mathematical result for the analysis of variance when using common random numbers in terms of the regression error, the residual error and the pure error terms. In fact, if we can realize the special structure of the covariance matrix of the error terms, we can use the result of analysis of variance for the uncorrelated experiments only by applying minor changes.

Key Words: Simulation Optimization, Common Random Numbers, Analysis of Variance

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I. Introduction

Simulation is a modeling or an analyzing tool for complex systems. It involves the construction of a descriptive model that explains the operations of a system, in order to quantitatively analyze the relationship between the system components. Simulation also involves sampling the experiments based on sound statistical theory, since the behavior of some system components is assumed to be random.

Many different approaches have been developed for finding an optimum condition of a system with random behavior using simulation experiments. A good discussion on the different optimization methods using the simulation experiments can be found on Park and Lee[2] and Yang and Lee[5]. Among the several optimization methods, we are focusing on the Response Surface Methodology(RSM)[7,10,15,17,19]. RSM is defined as the functional approach where we are approximating the system behavior of interest as a second order spline function with respect to the controllable factors. The controllable factors are often called as the decision variables. This approach was first adopted in simulation optimization problems by Smith[19] and was later extended by Daugherty & Turnquist[10], and Park[3,17].

In the process of estimating the objective function, which is unknown but is assumed to be a second order spline function, we use common random numbers for different set of the decision variables, resulting in more accurate parameter estimation for the objective function. Obviously, more accurate parameter estimation will give us more accurate optimum solution to the system of interest.

Early research on simulation experiments used common random numbers for comparing the alternatives. By using common random numbers we can compare the alternatives by performing simulation experiments under almost identical conditions so that we can obtain relative results, that is the difference of responses between alternatives, efficiently. Conway[8] discussed the importance of common random numbers when we perform simulation experiments for comparing alternatives. Fishman[12] adopted the strategy and investigated the theoretical background of it when he tried to compare the mean responses of the alternatives through simulation experiments.

The strategy of using common numbers looked promising in reducing the variance of the estimated response function in the study by Cooley and Houck[9], Tew and Wilson [20], Schruben and Margolin [18] and Nozari, et. al., [16]. However, a few research has been devoted to use common random numbers in order to reduce the variance of the parameter estimator for the unknown objective function in RSM[9,17,18,20], since it is complicated to analyze the effect of using common random numbers.

The primary goal of this paper is to analyze the impact of using common random numbers and show some mathematical result for the analysis of variance(ANOVA) in terms of the regression error, the residual error and the pure error terms. The analysis of variance is the key for the regression significance test and the lack of fit test in the process of estimating the response function with RSM type simulation optimization.

This paper is organized as follows. In section II, after the introduction in this section, we will give some general discussion on the simulation optimization problem using correlated experiments with RSM, which was described in Park[3,17], Kwon[1] and Yang and Lee[5]. The major result of using common random numbers in the process of analysis of variance is given in section III. Finally, some comments and the possible future research topics will be included in section IV. Also, the proofs for the major results discussed in Section III will be explained in detail in the Appendix.

II. Correlated Simulation Experiments

The RSM approach for simulation optimization problems begins with performing a set of simulation experiments over the settings of controllable factors, or equivalently the decision variables. The batch means or the expected values of several numbers of repetitive simulation experimental results of the system performance measure of interest are assumed to be unimodal in terms of the decision variables of the system. Then, we approximate the unknown expected value of the system performance measure as a second order linear function.

The general description and the formal setting of the RSM process for the simulation optimization problem were described in detail by Park[3,4,17].

Consider the general linear model of

$$Y = X'b + \varepsilon . \qquad (1)$$

Here in model (1), Y is the vector of n simulation outputs consisting of Y_i, $i=1,2,...,n$. Here, Y_i is computed as the average of m batch means $Y_{i1}, Y_{i2}, \dots, Y_{im}$ at design point i. Also, b is the parameter vector of $b_0, b_1, \dots, b_k$, $b_{11}, \dots, b_{k-1,k}$ and ε is the n dimensional observation error vector.

$$X' = \begin{bmatrix} 1 & x_{11} & x_{21} & \dots & x_{p-1,1} \\ 1 & x_{12} & x_{22} & \dots & x_{p-1,2} \\ \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \\ 1 & x_{1n} & x_{2n} & \dots & x_{p-1,n} \end{bmatrix} \qquad (2)$$

is an experimental design matrix augmented by the vector of 1, x_{ij}, $i,j=1,2,\dots,k$, $i<j$, and x_j^2, $j=1,2,\dots,k$, where k is the number of the decision variables, p is the number of parameters in the model.

In the usual regression analysis, we perform the regression significance test using regression sum of squares. The regression significance test is used to tell whether the regression equation is actually meaningful. We also performs the lack of fit test using residual sum of square. The lack of fit test tells whether the fitted model is properly describe the regression model.

Table 1 depicts the usual ANOVA table with unweighted regression analysis with independent simulation outputs.

In Table 1, T is $\Sigma_{i=1}^{n}\Sigma_{j=1}^{m}(Y_{ij}-Y_i)^2$ where Y_{ij} is the j-th simulation batch mean on the i-th design point, and Y_i is the average of Y_{ij}, $j=1,2,\dots,m$ batches.

Table 1. ANOVA table for unweighted regression

source	degree of freedom	sum of sqaures
regression	$p-1$	$\beta' X' Y - n\overline{Y^2}$
residual	$n-p$	$Y'Y - \beta' X' Y$
total	$n-1$	$Y'Y - n\overline{Y^2}$
pure error	$(m-1)n$	T/m

Suppose that we can correlate Y_l and Y_m through performing simulation experiments at design points $\underline{x}^l$ and $\underline{x}^m$ using common random numbers. Then we will perform weighted regression for estimating b in regression model (1), assuming that the simulation output vector of Y is correlated with the covariance matrix of $\sigma^{*2}R$. Here, σ^{*2} is the estimated common variance of Y_l and Y_m, and R is the estimated correlation coefficient matrix between Y_l and Y_m, $l, m = 1, 2, \ldots, n$.

The following is the normal weighted regression process to estimate b in model (1). First, compute R^{-1}. Second, compute $P^{-1} = W\sqrt{\Lambda}\,W$, where $P^{-1}P^{-1} = R^{-1}$ and W is the eigenvector of R^{-1}. Also, Λ is the diagonal matrix consisting of the eigenvalues of R^{-1}. Third, transform X' and Y to $Q' = P^{-1}X'$, $Z = P^{-1}Y$. Finally, estimate b by $\beta = (QQ')^{-1}Q'Z$.

Table 2 shows the usual ANOVA table for the weighted regression analysis[11].

Table 2. ANOVA table for weighted regression

source	degree of freedom	sum of sqaures
regression	$p-1$	$\beta' Q' Z - n\overline{Z^2}$
residual	$n-p$	$Z'Z - \beta' Q' Z$
total	$n-1$	$Z'Z - n\overline{Z^2}$
pure error	$(m-1)n$	$\Sigma_{i=1}^{n}\Sigma_{j=1}^{m}(Y_{ij} - \bar{Y}_i)^2/m$

III. The ANOVA Table for Special Covariance Structure using Common Random Numbers

Suppose that we can correlate Y_l and Y_m through simulation experiments at design points $\underline{x}^l$ and $\underline{x}^m$ using common random numbers for each design point. Also, let us assume that, as a result of using common random numbers, the covariance matrix V of the error terms $\varepsilon = (\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n)$ is found to be a special form with the diagonal elements being σ^2 and all the off-diagonal elements being $\rho\sigma^2$, $0 < \rho < 1$.

If we formally describe the special structure of V, then we can write as

$$V = \sigma^2(1-\rho)I_n + \sigma^2\rho J_n, \quad 0 < \rho < 1,$$

where $\sigma^2\rho$ is the common correlation coefficient for ε_l and ε_m, $l \neq m$,

$\sigma^2 = Var(\varepsilon_l)$, $l=1,2,..,n$, I_n is an n x n identity matrix, and J_n is n by n matrix of all the elements being 1. (3)

Then, the best estimator for b is known as

$$\beta = (XX')^{-1}X'Y \quad (4)$$

and the covariance matrix as

$$Cov(\beta) = (XV^{-1}X')^{-1} \quad (5)$$

or $(XV^{-1}X')^{-1} = (1-\rho)\sigma^2(XX')^{-1}$ (6)

except element (1,1) which is for β_0.

Note that equations (4) and (5) are from Lewis and Odell[13]. Equation (6) was proved by Schruben and Margolin[18] when we have design matrix X' being orthogonally blockable. However, Park[4] proved that equation(6) is still valid when design matrix X' is not orthogonally blockable but is of general form.

As we described in section II, we may perform the regression test and the lack of fit test using the terms in Table 2 of weighted regression for this correlated simulation outputs. However, it is possible to employ the usual regression test and the lack of fit test with the terms in ANOVA table for uncorrelated simulation outputs with minor change, if the covariance structure can be assumed as a special one as equation(3). Table 3 shows the ANOVA table when the covariance structure V with equation(3) can be assumed. The individual terms in Table 3 will be proved in the Appendix.

Table 3. ANOVA table for covariance structure of V in equation (3)

source	degree of freedom	sum of sqaures
regression	$p-1$	$(\beta' X' Y - n\overline{Y}^2)/(1-\rho)$
residual	$n-p$	$(Y'Y - \beta' X' Y)/(1-\rho)$
total	$n-1$	$(Y'Y - n\overline{Y}^2)/(1-\rho)$
pure error	$(m-1)n$	T/m

In Table 3, T is defined same as that of Table 2. Table 3 shows that the terms in the ANOVA table with weighted regression for this special case can be derived from the results with unweighted regression, when we can reasonably assume that the simulation outputs are specially correlated. In other words, we can still use the ANOVA table with unweighted regression by making minor adjustments. We also assumes that ρ, the common correlation coefficient, is between 0 and 1, which were shown in many real situations[17,18].

If ρ is close to 1, where the simulation outputs at different experimental points are closely correlated, then the sum of square terms for the regression and for the residual become very large. In this case, we can test the significance and the lack of fit for the regression equation more easily. On the other hand, if ρ is close to 0, then it is not much beneficial to use common random numbers in terms of the regression significance test and the lack of fit test.

Apparently, it is critical to test if we have realized the covariance matrix for the error terms ε not being significantly departed from a special structure V as in equation (3). The test procedure can be found in Morrison[14].

IV. Conclusion and Further Research Topic

We have presented the impact of using common random numbers for the regression test and the lack of fit test in the process of estimating the parameters of the objective function in RSM. The major result obtained in section III revealed that if we use common random numbers for estimating the parameters of the unknown objective function, we can still have the sum of square terms with a minor modification from the results of uncorrelated simulation experiments.

The result obtained in this paper is very helpful to the simulation experimenters using common random numbers, since they can still utilize the sum of square terms for independent simulation experiments.

Finally, it may be interesting to investigate the impact of using antithetic random numbers in the process of RSM approach for simulation optimization problems. Not many researches have been done for this topic yet.

Appendix

Let $Y^{+} = [Y_{11}, \ldots, Y_{1m}, Y_{21}, \ldots, Y_{n1}, \ldots, Y_{nm}]$ be the vector of individual batch means, where Y_{ir} is the r-th batch mean at design point i in experimental design matrix of equation(2). Also, define Y be the vector of n simulation outputs consisting of Y_i, $i=1,2,\ldots,n$. Here, Y_i is computed as the average of m batch means $Y_{i1}, Y_{i2}, \ldots, Y_{im}$ at design point i.

Suppose that we perform weighted regression for the model defined in equation (1) where X' is defined as equation (2) and b is defined as the parameter vector of $b_0, b_1, \ldots, b_k, b_{11}, \ldots, b_{k-1,k}$. Assume that the covariance matrix V is the form of equation (3).

Consider the transformation for performing weighted regression, $Q' = P^{-1}X'$, $Z = P^{-1}Y$, $Z^{+} = (P^{-1} \otimes I_m)Y^{+}$, where $PP = V$, and $\otimes$ is the notation for Kronecker product.

Theorem:

The sum of square terms resulting from weighted regression are

(1) Regression sum of square:

$$SS_R = \sum_{i=1}^{n}(Z_i^{*} - \overline{Z})^2 = \sum_{i=1}^{n}(Y_i^{*} - \overline{Y})^2/(1-\rho) \quad \text{(A1)}$$

with $p-1$ d.o.f.(degree of freedom)

(2) Residual sum of square:

$$SS_L = Z'Z - \beta' QZ = (Y'Y - Y^{*'}Y)/(1-\rho) \quad \text{(A2)}$$

with $n-p$ d.o.f.

(3) Error sum of square:

$$SS_E = (1/m)\sum_{i=1}^{n}\sum_{r=1}^{m}(Y_{ir} - Y_i)^2 \quad \text{(A3)}$$

with $n(m-1)$ d.o.f., and
$E(SS_E) = \sigma^2$.

Note:

$$Y^* = X'\beta,\ Z^* = P^{-1}Y^*$$

$$\overline{Y} = (1/n)\sum_{i=1}^{n} Y_i,\ \overline{Z} = (1/n)\sum_{i=1}^{n} Z_i$$

Proof:

(1) Regression sum of square

Without loss of generality, let us assume that $\sigma^2 = 1$. Since V is symmetric, so are V^{-1} and P^{-1}, where $V^{-1} = P^{-1}P^{-1}$.

Let $V^{-1} = (a-g)I_n + gJ_n$ and

$$a = (1+(n-2)\rho)/((1+(n-1)\rho)(1-\rho))$$

$$g = -\rho/((1+(n-1)\rho)/(1-\rho)),\ \rho \neq 0. \quad \text{(A4)}$$

from the Appendix in Park[4].

Since V^{-1} has the form of $(a-g)I_n + gJ_n$, P^{-1} should have the form of $(c-d)I_n + dJ_n$.

Here, I_n and J_n is defined in equation (3).

Solving for c and d, noting that

$$c^2 + (n-1)d^2 = a$$
$$2cd + (n-2)d = g \quad \text{(A5)}$$

we have

$$c = (1-n^{-1})[(1+(n-1)\rho)/h]^{1/2} + (1/n)[(1-\rho)/h]^{1/2}$$
$$d = (-1/n)[(1+(n-1)\rho)/h]^{1/2} + (1/n)[(1-\rho)/h]^{1/2} \quad \text{(A6)}$$

where $h = 1 + (n+2)\rho - (n-1)\rho^2$. (A7)

Now,

$$\begin{aligned} SS_R &= \sum_{i=1}^{n}(Z_i^* - \overline{Z})^2 \\ &= \sum_{i=1}^{n}[(c-d)Y_i^* + d(Y_1^* + \ldots + Y_n^*) - (c-d)\overline{Y} - nd\overline{Y}]^2 \\ &= \sum_{i=1}^{n}[(c-d)Y_i^* - (c-d)\overline{Y}]^2 \\ &= (c-d)^2\sum_{i=1}^{n}(Y_i^* - \overline{Y})^2 \\ &= \sum_{i=1}^{n}(Y_i^* - \overline{Y})^2/(1-\rho) \end{aligned} \quad \text{(A8)}$$

Note:

$$\begin{aligned} \overline{Z} &= (1/n)\sum_{i=1}^{n} Z_i \\ &= (1/n)\sum_{i=1}^{n}[(c-d)Y_i + d(Y_1 + \ldots + Y_n)] \\ &= (1/n)(c-d)n\overline{Y} + (1/n)dn^2\overline{Y} \\ &= (c-d)\overline{Y} + nd\overline{Y} \end{aligned}$$

$$d\,(Y_1^* + \ldots + Y_n^*) = nd\overline{Y}$$

(2) Residual sum of square

$$\begin{aligned} SS_L &= Z'Z - \beta'QZ \\ &= Y'V^{-1}Y - \beta'XP^{-1}P^{-1}Y \\ &= Y'V^{-1}Y - Y^{*\prime}V^{-1}Y \end{aligned} \quad \text{(A9)}$$

The first term becomes

$$Y' V^{-1} Y = Y' \cdot [(a-g) I_n + bJ_n] \cdot Y$$
$$= \sum_{i=1}^{n} Y_i \cdot [a Y_i + g(Y_1 + \ldots + Y_n - Y_i)]$$
$$= \sum_{i=1}^{n} (a Y_i Y_i - g Y_i Y_i)$$
$$+ g(Y_1 + \ldots + Y_n)(Y_1 + \ldots + Y_n)$$
$$= (a-g) Y' Y - n^2 (\rho / h) \overline{Y^2}$$
$$= (1-\rho)^{-1} Y' Y - (n^2 \rho / h) \overline{Y^2} \quad \text{(A10)}$$

where h is given in equation (A7).
Similarly, the second term becomes

$$Y^{*'} V^{-1} Y = (1-\rho)^{-1} Y^{*'} Y - (n^2 \rho / h) \overline{Y^2}. \quad \text{(A11)}$$

Finally, we have

$$SS_L = (Y' Y - Y^{*'} Y)/(1-\rho) \quad \text{(A12)}$$

(3) Error sum of square

We know that

$$\sum_{i=1}^{n} \sum_{r=1}^{m} (Z_{ir} - Z_i)^2 / (nm(m-1)) \quad \text{(A13)}$$

is the best estimator for σ^2.
Consider

$$\sum_{i=1}^{n} \sum_{r=1}^{m} (Z_{ir} - Z_i)^2$$
$$= (Z^+ - Z\otimes 1)' (Z^+ - Z\otimes 1)$$
$$= [(P^{-1}\otimes I) Y^+ - (P^{-1}\otimes I)(Y\otimes 1)]'$$
$$\cdot [(P^{-1}\otimes I) Y^+ - (P^{-1}\otimes I)(Y\otimes 1)]$$
$$= Y^{+'} (P^{-1}\otimes I)' (P^{-1}\otimes I) Y^+$$
$$- (Y\otimes 1)' (P^{-1}\otimes I)' (P^{-1}\otimes I) Y^+$$
$$- Y^{+'} (P^{-1}\otimes I)' (P^{-1}\otimes I)(Y\otimes 1)$$
$$+ (Y\otimes 1)' (P^{-1}\otimes I)(P^{-1}\otimes I)(Y\otimes 1)$$
$$= Y^{+'} (V^{-1}\otimes I) Y^+ - (Y\otimes 1)' (V^{-1}\otimes I) Y^+$$
$$- Y^{+'} (V^{-1}\otimes I)(Y\otimes 1)$$
$$+ (Y\otimes 1)' (V^{-1}\otimes I)(Y\otimes 1)$$
$$= Y^{+'} (V^{-1}\otimes I)(Y^+ - Y\otimes 1)$$
$$- (Y\otimes 1)' (V^{-1}\otimes I)(Y^+ - Y\otimes 1)$$
$$= (Y^{+'} - Y\otimes 1)' (V^{-1}\otimes I)(Y^+ - Y\otimes 1)$$
$$= a \sum_{i=1}^{n} \sum_{r=1}^{m} (Y_{ir} - Y_i)^2$$
$$+ g \sum_{i=1}^{n} \sum_{\substack{j=1 \\ i \neq j}}^{n} \sum_{r=1}^{m} (Y_{ir} - Y_i)(Y_{jr} - Y_j)$$
$$\text{(A14)}$$

Note:
I : m x m unit matrix
1 : 1 x m matrix of 1's.
We know that

$$(nm(m-1))^{-1} E \left[\sum_{i=1}^{n} \sum_{r=1}^{m} (Z_{ir} - Z_i)^2 \right]$$
$$= [a/(nm(m-1))] E \left[\sum_{i=1}^{n} \sum_{r=1}^{m} (Y_{ir} - Y_i)^2 \right]$$
$$+ [g(n-1)/(nm(m-1))] \cdot$$
$$E \left[\sum_{i=1}^{n} \sum_{\substack{j=1 \\ i \neq j}}^{n} \sum_{r=1}^{m} (Y_{ir} - Y_i)(Y_{jr} - Y_j) \right] = \sigma$$
$$\text{(A15)}$$

where a, g, h are defined in equation(A4) and (A7).
Suppose

$$[nm(m-1)]^{-1} E \left[\sum_{i=1}^{n} \sum_{r=1}^{m} (Y_{ir} - Y_i)^2 \right]$$
$$= \tau^2 \neq \sigma^2,$$
$$\text{(A16)}$$

then,

$$(nm\ (m-1))^{-1}E\ [\ \sum_{i=1}^{n}\ \sum_{r=1}^{m}(Z_{ir}-Z_i)^2]$$
$$=a\tau^2+g(n-1)\rho\ \tau^2=\ \tau^2\neq\sigma^2$$

(A17)

Thus, if and only if

$$[nm(m-1)\ ]^{-1}\ E\ [\ \sum_{i=1}^{n}\ \sum_{r=1}^{m}(Y_{ir}-Y_i)^2]$$
$$=\sigma^2,$$
$$[nm(m-1)\ ]^{-1}\ E\ [\ \sum_{i=1}^{n}\ \sum_{r=1}^{m}(Z_{ir}-Z_i)^2]$$
$$=\sigma^2. \quad \text{(A18)}$$

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