The Performance of Optimum Response Surface Methodology Based on MM-Estimator

Habshah Midi, Mohd Shafie Mustafa, Anwar Fitrianto

Abstract — The Ordinary Least Squares (OLS) method is often used to estimate the parameters of a second-order polynomial response surface methodology (RSM) model whereby a face-centered composite design of experiment is considered. The parameters of the model are usually estimated using the OLS technique. Nevertheless, the classical OLS suffers a huge set back in the presence of a typical observations that we often call outliers. In this situation, the optimum response estimator is not reliable as it is based on the OLS which is not resistant to outliers. As an alternative, we propose using a robust MM-estimator to estimate the parameters of the RSM and subsequently the optimum response is determined. A numerical example and simulation study are presented to assess the performance of the optimum response-MM based, denoted as Optimum-MM. The numerical results signify that the Optimum-MM is more efficient than the Optimum-OLS.

Keywords — Response Surface Model (RSM), Ordinary Least Squares (OLS), Outliers, MM-estimator.

I. INTRODUCTION

Response Surface Methodology (RSM) is a well known tool in process and product development using design of an experiment. The RSM consists of statistical and mathematical techniques developed in 1950s for the purpose of determining optimization that are used to improve existing product in an industry. It is designed with a product of process involving functional relationship between the values of some measurable response variables, y and a set of experimental factors (input variables) denoted by $x_1, x_2, ..., x_k$. The RSM has wide applications in a variety of real problems from diversified areas such as engineering, food manufacturing, biological sciences, chemical sciences, etc.

The optimum response *y* is determined after a model that relate between the set of independent variables and the response variable is established.

In general, such a relationship is unknown but can be approximated by a low-degree polynomial model of the form

$$y = f'(x)\beta + \varepsilon \tag{1}$$

where $x = (x_1, x_2, ..., x_k)', f(x)$ is a vector function of p elements, β is a vector of constant coefficients, and ε is an error term. Khuri and Mukhopadhyay (2010) stated that model (1) provides an adequate representation of the response.

In most RSM problem, two important models are commonly used either a first-order or a second-order model.

The regression coefficients of the model are often estimated using the method of Ordinary Least Squares (OLS). The OLS method gives good parameter estimates when the responses are normally distributed and no outliers in the data set. Nonetheless, in real practice, many distributions of the response variable is (considerably) not normal which is due to the presence of outlier. Outliers occur very frequently in real data, and they often go unnoticed because nowadays much data is processed by computer without careful inspection or screening. Yohai (1987) stated that a small fraction of outlier or even one outlier may have significant effect on the OLS estimates. Subsequently, the determination of the optimum response is not reliable as it is based on the OLS which is not resistant to outliers [5, 8].

Robust regression methods are recommended to be used, to remedy this problem (Maronna, 2006, Rousseeuw & Leroy, 1987). Furthermore, Montgomomery et al. (2001) shown that robust regression methods can help the practitioners to identify possible outliers.

The aim of this paper is to investigate the effect of outliers on the optimum yield response. Since the OLS is not outliers resistant, the alternative robust technique called MM-estimator (Maronna, 2006) which has a very high breakdown point is used to estimate the model parameters and subsequently obtain the optimum response. The performances of the Optimum-MM and Optimum-OLS techniques are assessed based on numerical examples and simulations study.

II. USING A CENTRAL COMPOSITE DESIGN IN SECOND-ORDER MODEL

Mohd Shafie Mustafa is with the Institute for Mathematical Research, University Putra Malaysia, 43400 UPM Serdang, Selangor, MALAYSIA (phone: +603-89466817; fax: +603-89437958; e-mail: shafie@math.upm.edu.my).

Habshah Midi is with the Deputy Dean of Faculty of Science, University Putra Malaysia, 43400 UPM Serdang, Selangor, MALAYSIA (e-mail: habshah@science.upm.edu.my).

Anwar Fitrianto is with the Mathematics Department, Faculty of Science, University Putra Malaysia, 43400 UPM Serdang, Selangor, MALAYSIA (e-mail: anwarfitrianto@gmail.com).

In general, the model (1) is used to describe the response surface *f*.

A polynomial model is usually a sufficient approximation in a small region of the response surface. Therefore, depending on the approximation of vector function *f*, either first-order or second-order models are used. Furthermore, a second-order model is useful in approximating a portion of the true response surface with parabolic curvature. The second-order includes all linear terms, plus all quadratic terms and all cross-product terms are given as

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum\sum_{i<j} \beta_{ij} x_i x_j + \varepsilon$$
$$= \beta_0 + x_i'\beta + x_i'\beta x_i + \varepsilon_{ij} \tag{2}$$

where $x = (x_1, x_2, ..., x_k)'$, $\beta = (\beta_1, \beta_2, ..., \beta_k)'$, ε is a random error and assumed to be independent with $N(0, \sigma^2)$.

The number of parameters in model (2) must contain at least $p = 1 + 2k + ½k(k\text{-}1)$ distinct design point, where k is a number of control variables. In addition, Myers et al. (2009) stated that the design must involve at least three levels of each design variable to estimate the pure quadratic terms. The design setting are usually coded of each factor in each experiment so that zero represents the center point, and +1 and -1 represent the upper and lower of the factor, respectively. For the *i*th factor, such coded levels x_i are obtained as

$$x_i = \frac{(\xi_i - \bar{\xi})}{\Delta\xi} \tag{3}$$

where x_i is the coded unit, ξ_i is the natural value of the *i*th independent variable, and $\bar{\xi}$ is the mean of the natural unit.

The coded values were calculated according to the following equation:

$$x_i = \frac{\xi_i - (\text{high level} + \text{low level})/2}{(\text{high level} + \text{low level})/2} \tag{4}$$

There are many designs available for fitting a second-order model. The central composite design (CCD) is the most frequently used design for fitting a second-order response surface. It was first introduced by Box and Wilson (1951). It consists of factorial points, axial points, and central points. In the construction of CCD, Khuri and Mukhopadhyay (2010) pointed out that this design consists of the following three features:

i. A complete (or a fraction of) 2^k factorial design whose factors' levels are coded as -1, 1. This is called the factorial portion.
ii. An axial portion consisting of $2k$ points arranged so that two points are chosen on the axis of each control variable at a distance of α from the design centre (chosen as the point at the origin of the coordinates system).
iii. A chosen number, n_0 of center points.

III. OPTIMIZATION OF A SECOND-ORDER MODEL

Consider a second-order response surface equation model as

$$\hat{y} = \beta_0 + x'\beta_* + x'Bx \tag{5}$$

where $x = (x_1, x_2, ..., x_k)'$, $\beta = (\beta_1, \beta_2, ..., \beta_k)'$, and B is a symmetric matrix of order k x k whose *i*th diagonal element is β_{ii} (i = 1,2, … , k) and its (i,j)th off-diagonal element is $\frac{1}{2}\beta_{ij}$ (i,j = 1, 2, … , k; $i \neq j$).

The stationary point is determined by first differentiating $\hat{y}$ with respect to x as follows:

$$\frac{\partial \hat{y}}{\partial x} = b + 2\hat{B}x \tag{6}$$

and, set the derivative to be equals to 0, the stationary point (x_0) can be obtained

$$x_0 = -\frac{1}{2}\hat{B}^{-1}b \tag{7}$$

where;

$$b = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix}, \quad \hat{B} = \begin{bmatrix} \hat{\beta}_{11} & \hat{\beta}_{22}/2 & \cdots & \hat{\beta}_{1q}/2 \\ & \hat{\beta}_{22} & \cdots & \hat{\beta}_{2q}/2 \\ & & \ddots & \vdots \\ sym. & & & \hat{\beta}_{qq}/2 \end{bmatrix}$$

b is a (q x 1) vector of the first-order regression coefficients and B is a (q x q) symmetric matrix.

In result, the predicted response value at stationary point can be calculated as

$$\hat{y}(x) = \beta_0 + x'\beta_* + x'Bx \tag{8}$$

IV. REGRESSION ESTIMATOR BASED ON MM-ESTIMATION

The Ordinary Least Squares (OLS) method is often used to estimate the parameters of the model. However, it can be adversely affected by outliers [2, 16]. As an alternative, MM-estimator which has a very high breakdown point is used to estimate the parameters of the model. The MM-estimator is one of the robust regression techniques tend to dampen the effect of the outliers. The MM-estimator was originally proposed by Yohai in 1987. Yohai (1987) defined the MM-estimator as a three-stage procedure:

i. an initial regression estimate is computed which is consistent robust and with high breakdown point but not necessarily efficient.
ii. an M-estimate of the errors scale is computed using residuals based on the initial estimate.
iii. an M-estimate of the regression parameters based on a proper redescending psi-function, ρ is computed.

For a given ψ function equals to ρ', the MM parameter estimates are defined as any solution of;

$$\frac{1}{n}\sum_{t=1}^{n}\psi\left(\frac{Y_t - X_t'\beta}{\hat{\sigma}_s}\right)X_t = 0 \qquad (11)$$

where Y_t be the response variable and X_t the p-vector of covariates observed for $t = 1,2,\ldots,n$.

In the following, a step-by-step procedure for optimum-MM and optimum-OLS are presented based on RSM:

Step 1: Building an appropriate second-order response surface model for each response and compute the regression coefficients of the second-order model (2) using the RSM based on OLS and RSM based on MM-estimator.

Step 2: Next, the adequacy of the second-order model is tested, which can be assessed from the analysis of variance (ANOVA) table.

Step 3: Perform the canonical analysis. The canonical analysis is performed to determine the location and the nature of the stationary point of the second-order model. The stationary point is then be referred as the center point of the new region of interest.

V. NUMERICAL EXAMPLES

In this section, a numerical example is presented to investigate the performance of the proposed optimum-MM. The optimization of xanthan gum production by X. campestric in 18 batches of experiments was obtained from an experiment conducted by Psomas et al. (2007).

There are two response variables observed in his experiment which are xanthan gum (y_1) and biomass (y_2) production while the predictor variables or input factors are agitation rate (x_1), temperature (x_2), and time of cultivation (x_3), using a face centered composite design of experiments. In this article, we only focus on xanthan gum production (y) as a response variable.

To see the effect of outliers on the optimum-OLS and the optimum-MM, we purposely modify (contaminated) the xanthan dataset in this experiment. The objective of this experiment is to search for an optimal setting and optimal yield (response) that can achieve the target with maximum optimum of xanthan gum production with and without contaminated data.

Table 1: The Xanthan Gum Production Data

Run	Agitation rate (x_1)	Temperature (x_2)	Time (x_3)	x_1	x_2	x_3	y
1	100	25	24	-1	-1	-1	0.278 (27.8)
2	600	25	24	1	-1	-1	0.375
3	100	35	24	-1	1	-1	0.141
4	600	35	24	1	1	-1	0.333
5	100	25	72	-1	-1	1	0.315
6	600	25	72	1	-1	1	0.692
7	100	35	72	-1	1	1	0.279
8	600	35	72	1	1	1	0.699 (69.9)
9	100	30	48	-1	0	0	0.215
10	600	30	48	1	0	0	0.486 (48.6)
11	350	25	48	0	-1	0	0.583
12	350	35	48	0	1	0	0.569
13	350	30	24	0	0	-1	0.348 (34.8)
14	350	30	72	0	0	1	0.511
15	350	30	48	0	0	0	0.503 (50.3)
16	350	30	48	0	0	0	0.467
17	350	30	48	0	0	0	0.453
18	350	30	48	0	0	0	0.475 (47.5)

Table 1 presents the data set taken from Psomas et al. (2007) experiments which contains three independent variables in coded and uncoded form according to the experimental design and the response (xanthan gum production) for all experiments.

The coded values of independent factors were calculated as follows;

Agitation rate: $x_1 = \frac{\xi_{i1}-350}{250}$

Temperature: $x_2 = \frac{\xi_{i2}-30}{5}$

Time: $x_3 = \frac{\xi_{i3}-48}{24}$

In this article, the second order response surface models (OLS and MM-estimator) are fitted using S-Plus 6.2 Professional software.

A. The Estimated Coefficients

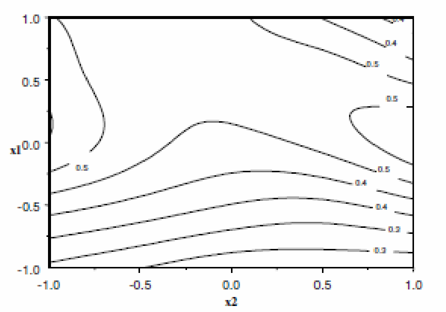
A second order polynomial model was fitted to the production of xanthan gum data. Table 2 presents the estimated regression coefficients, interactive terms, quadratic terms and probability values (p-values) based on the OLS and the MM-estimator. The analysis was done using the coded values. Psomas et al. (2007) stated that when the regression model is determined with coded values of the variables, the size of each coefficient gives a direct measurement of the importance of each effect.

Thus, the second-order model is appropriate for xanthan dataset. Coefficients with p-values larger than 0.05 are considered not significant and are not included in the model. It is important to point out that when a higher order (square and interaction factor) was significant, the linear factor must follow the later (Montgomery et al, 2001).

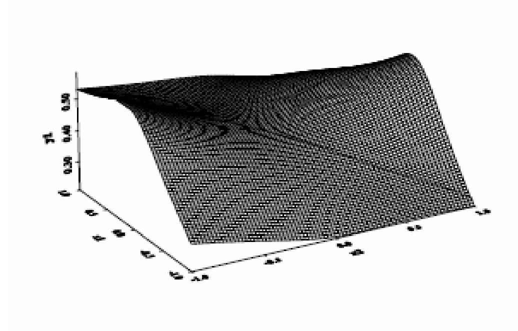
The results of Table 2 show that at $\alpha = 0.05$, all coefficients based on OLS are significant. Two interaction factors of MM-estimator are not significant. But, after the deletion of factor $x_1 * x_2$ and $x_2 * x_3$ and recomputed the estimates for the second time, all the coefficients are significant.

Table 2**:** Estimated coefficient for Xanthan data using OLS (A) and MM (B)

Term	Coefficient	SE coefficient	*t*-value	*p*-value
(A) OLS estimator				
Constant				
x_1	0.4779	0.0081	58.6629	0.0000
x_2	0.1357	0.0065	20.7211	0.0000
x_3	-0.0222	0.0065	-3.3899	0.0095
$x_1 * x_1$	0.1021	0.0065	15.5904	0.0000
$x_2 * x_2$	-0.1309	0.0126	-10.4013	0.0000
$x_3 * x_3$	0.0946	0.0126	7.5228	0.0001
$x_1 * x_2$	-0.0519	0.0126	-4.1219	0.0033
$x_1 * x_3$	0.0173	0.0073	2.3560	0.0462
$x_2 * x_3$	0.0635	0.0073	8.6726	0.0000
	0.0188	0.0073	2.5608	0.0336
(B) MM-estimator				
Constant				
x_1	0.4776	0.0073	65.0315	0.0000
x_2	0.1356	0.0071	19.1892	0.0000
x_3	-0.0222	0.0080	-2.7930	0.0234
$x_1 * x_1$	0.1024	0.0080	12.8637	0.0000
$x_2 * x_2$	-0.1302	0.0112	-11.5877	0.0000
$x_3 * x_3$	0.0948	0.0112	8.4367	0.0000
$x_1 * x_2$	-0.0523	0.0112	-4.6584	0.0016
$x_1 * x_3$	0.0172	0.0082	2.0897	0.0700
$x_2 * x_3$	0.0635	0.0082	7.7117	0.0001
	0.0187	0.0094	1.9864	0.0822

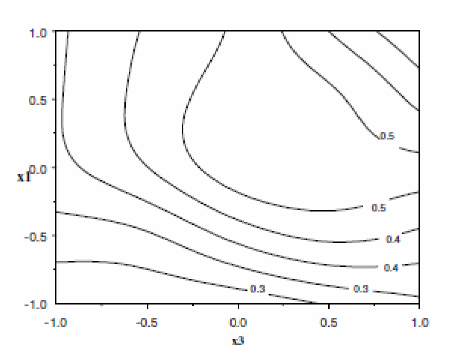


(a) Contour Plot

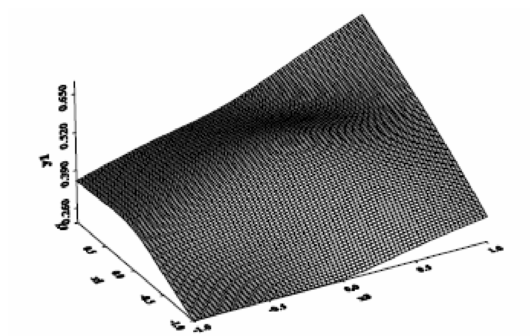


(b) Response Surface

Figure 1: The effect on Agitation Rate versus Temperature and Their Mutual effect on the Xanthan Dataset

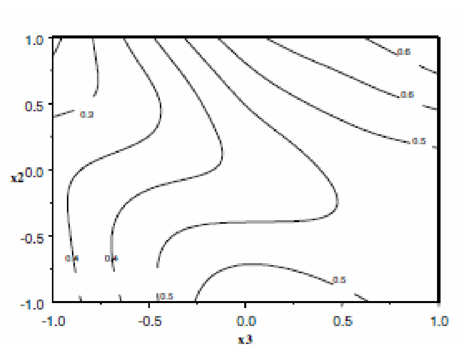


(a) Contour Plot

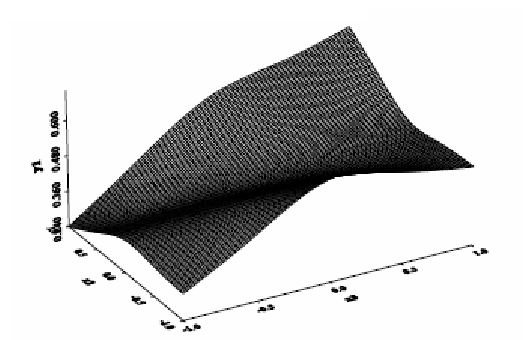


(b) Response Surface

Figure 2: The effect on Agitation Rate versus Time and Their Mutual effect on the Xanthan Dataset



(a) Contour Plot



(b) Response Surface

Figure 3: The effect on Temperature versus Time and Their Mutual effect on the Xanthan Dataset

The geometric nature of the second-order function is displayed in figs. 1-3. The response surfaces of figure 1 shows that an increase of agitation rate and temperature simultaneously yields in a minimax production of xanthan gum production for both estimators. On the other hand, the effect of agitation rate and time in figure 2 indicates that the maximum yields production of xanthan. Furthermore, the increase of temperature and time shows that the contour of response surface is a minimax effect of xanthan production. These indications for both the RSM based OLS and the RSM based MM-estimator supported by the numerical results in the table 4.

Table 3 summarizes the corresponding analysis of variance results. Of some concern was the size of the F statistics for the lack of fit test. When using the RSM based on OLS, all the contribution of factors are significant and there is no indication of lack-of- fit, evidenced by large *p* values for the lack-of-fit test, which equals to 0.555.

Similar to the OLS method, the RSM based on MM-estimator also suggesting no evidence of lack-of-fit in the model.

Table 3: Analysis of variance for xanthan production using OLS (A) and MM (B)

Source	df	SS	MS	F	*p*
(A) OLS estimator					
Regression	9	0.4073	0.0453	105.51	0.000
Residual error	8	0.0034	0.0004		
Lack-of-fit	5	0.0021	0.0004	0.95	0.555
Pure error	3	0.0013	0.0004		
Total	17	0.4107			
(B) MM-estimator					
Regression	9	0.4062	0.0451	80.6	0.000
Residual error	8	0.0045	0.0006		
Lack-of-fit	5	0.0032	0.0006	1.42	
Pure error	3	0.0013	0.0004		
Total	17	0.4107			

The optimum response based on MM and OLS are then computed and the results are exhibited in Table 4. The results of Table 4 shows that when there is no outlier, the OLS method leads to the optimal setting (x_1, x_2, x_3) = (0.8744,-0.1115, 1.4983), which results in optimum yields equals to 0.615. In this situation, the performance of the MM estimator is fairly closed to the OLS, with optimal setting (x_1, x_2, x_3) = (0.8914,0.1171,1.5201) and optimal yield equals to 0.6146.

Table 4: The optimum response for xanthan data

Factor	Optimum-OLS setting	Optimum-MM setting
x_1 (Agitation rate)	0.8744	0.8914
x_2 (Temperature)	-0.1115	0.1171
x_3 (Time)	1.4983	1.5201
Optimum Response	0.6150	0.6146

B. Analysis on modified (contaminated) xanthan dataset

To see the effect of outliers on the Optimum-MM and Optimum-OLS, we purposely modify (contaminated) the response of xanthan gum production data. Three design points (factorial point, axial point, and central point) each with two contaminated point (in parenthesis and bold) are shown in Table 1. The variables x_1, x_2, and, x_3 are centred and rescaled similar to the earlier data. As mentioned in section A, coefficients with p-values larger than 0.05 are considered not significant and are not included in the model. Thus, for contaminated data, all the coefficients using the RSM based on OLS are not significant. However, the coefficients using the RSM based on MM are significant.

The RSM based on OLS and the RSM based on MM-estimator were then applied to the data and the results of the optimum responses are exhibited in Table 5.

It can be observed from Table 5 that in the presence of outliers in the data set, the OLS based method failed to determine the optimal settings and optimal response due to the insignificant of all variables in the model. In the event that the optimal response is obtained, the result is very misleading. However, using MM-estimator, the results are closed to the results as in the clean dataset. It is interesting to note that the MM based method is only slightly affected by the outliers. Other results' examples are consistent and not reported here due to space constraint.

VI. Simulation Studies

In this section, a series of Monte Carlo simulation study are performed for comparison of the Optimum-MM and the Optimum-OLS with and without contaminated data using a face-centered composite design of experiment. A second-order polynomial model was fitted and the optimum conditions were estimated.

The responses are randomly generated based on the following function

$$Y_t = \beta_0 + \beta_1 (X_1)_t + \beta_2 (X_2)_t + \beta_3 (X_3)_t + \beta_{11}(X_1^2)_t + \beta_{22}(X_2^2)_t + \beta_{33}(X_3^2)_t + \beta_{12}(X_1 X_2)_t + \beta_{13}(X_1 X_3)_t + \beta_{23}(X_2 X_3)_t + \varepsilon_t \quad (10)$$

To generate the Y values, first we fixed the values of variables x_1, x_2, and, x_3 are centred and rescaled from the natural variables so that $x_i \in [-1,1]$ and the parameter coefficient, β equal to 1. The errors, ε_t are generated from a normal distribution with mean zero and variance 0.3. In this regards, 1000 simulated values were generated for each model with 18 design points.

In order to check how the presence of contaminated data affects the estimators, two contaminated data $(Y_{4,i}, Y_{10,i})$ were observed. The 4th and 10th data points are replaced with their corresponding y values increased by 100 units.

The optimum responses for xanthan gum production data with and without contamination are shown in Table 6 and Table 7. As can be expected, for clean data, the results (Table 6) clearly indicate that the RSM based on OLS method performed better than the RSM based on MM-estimator since it has less biased, smaller SE and RMSE. The OLS and MM based technique are fairly closed to each other in this regard.

It is interesting to see that the optimum-MM has smaller RMSE than the optimum-OLS in the presence of outliers. On the other hand, the performance of optimum-OLS is very poor.

Table 5: Optimum response for contaminated data

Design Point	Method	Optimal Setting = (x_1, x_2, x_3)	Optimum Response = y
Factorial Point	OLS	(-0.1698,-0.1822, -0.1726)	-2.9365
	MM	(0.5585,0.0963, 1.1696)	0.5733
Axial Point	OLS	-	-
	MM	(0.8721,-0.0732, 1.1909)	0.5971
Center Point	OLS	-	-
	MM	(0.9231,0.1149, 1.6017)	0.6160

'-' indicate that the optimum cannot be estimated

Table 6: Estimation the Optimum response for clean data

Method	Optimum-OLS	Optimum-MM
Bias	-0.084438	-0.114096
SE	0.015252	0.052209
RMSE	0.48966	1.65493

Table 7: Estimation the Optimum response for contaminated dataset

Method	Optimum-OLS	Optimum-MM
Bias	-49.418853	-5.974056
SE	0.161975	0.951636
RMSE	48.688756	30.486846

VII. CONCLUSION

This article clearly shows that the performance of the optimum-MM to estimate the optimal setting and optimal response is comparable to the optimum-OLS when no outlier(s) in a data set. However, the optimum-OLS is very sensitive to the presence of outliers. On the other hand, the optimum-MM is very reliable as it is outlier resistant. Hence, in the presence of outlier(s) it is recommended to use the optimum-MM to estimate the optimal response.

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