

The Use of Hodges-Lehmann Estimator in Multiple Response Optimization with Replication

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Abstract The development of an approximation model for the true response surface is needed in Response Surface Methodology. In multiple response optimization (with replication), the sample mean is widely used to calculate the mean value at each design point of every quality characteristic before the model fitting. However, the existence of outliers may have certain effects on the sample mean. Thus, the Hodges-Lehmann estimator, a robust estimator, is proposed in place of the sample mean in this paper. A summary of the properties and advantages of the Hodges-Lehmann estimator will be given together with an example from the literature to illustrate the computation of this proposal.

Keywords Response surface methodology; Hodges-Lehmann estimator; Optimization; Generalized reduced gradient.

1 Introduction

In multiple response optimization, researchers seek to optimize the mean responses of p quality characteristics simultaneously to find an optimal setting. Generally, there are two types of multiple response optimization: multiple response optimization without replication (non replication or single observation) and multiple response optimization with replication. Researchers like Castillo et al. [1], Derringer and Suich [2] and others contributed to the development of multiple response optimization (non replication). Table 1 is the general form of an experimental design for a multiple response approach (non replication) with p quality characteristics, m design points, k coded process settings and single observation (non replication) at each design point.

Table 1 General Form of an Experimental Design for a Multiple Response Approach (non replication).

Design Point	Coded Process Settings				Quality Characteristics				
	x_1	x_2	...	x_k	1	2	...	p	
1	-1	-1	...	-1	Y_{11}	Y_{21}	...	Y_{p1}	
2	0	-1	...	-1	Y_{12}	Y_{22}	...	Y_{p2}	
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	
m	1	1	...	0	Y_{1m}	Y_{2m}	...	Y_{pm}	

On the other hand, Fogliatto and Albin [3] considered a multiple response approach with replication in their paper. In their experimental design, there are more than one observation at each design point of every quality characteristic. Table 2 is the general form of an experimental design for a multiple response approach (with replication) with p quality characteristics, m design points, k coded process settings and n replications at each design point of every quality characteristic.

Table 2 General Form of an Experimental Design for a Multiple Response Approach (with replication).

Design Point	Coded Process Settings				Quality Characteristic 1				Quality Characteristic 2				...	Quality Characteristic p			
					Replication				Replication					Replication			
	x_1	x_2	...	x_k	1	2	...	n	1	2	...	n		1	2	...	n
1	-1	-1	...	-1	Y_{111}	Y_{112}	...	Y_{11n}	Y_{211}	Y_{212}	...	Y_{21n}		Y_{p11}	Y_{p12}	...	Y_{p1n}
2	0	-1	...	-1	Y_{121}	Y_{122}	...	Y_{12n}	Y_{221}	Y_{222}	...	Y_{22n}		Y_{p21}	Y_{p22}	...	Y_{p2n}
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮		⋮	⋮	⋮	⋮
m	1	1	...	0	Y_{1m1}	Y_{1m2}	...	Y_{1mn}	Y_{2m1}	Y_{2m2}	...	Y_{2mn}		Y_{pm1}	Y_{pm2}	...	Y_{pmn}

The sample mean was used by Fogliatto and Albin [3] to find the mean value at each design point of every quality characteristic before they fitted models for the p quality characteristics.

Hampel et al. [4] pointed out that many empirical datasets have typically 10% outliers. The existence of outliers may be due to some sporadic variation, copying/recording/typing error, computation error, observation that is not part of the population being studied, etc. It is well known that the existence of outliers may have certain effects or influence on the sample mean. In addition, Abu-Shawiesh and Abdullah [5] stated that when the underlying assumptions under which the statistical procedure was developed are slightly incorrect or not met, the traditional measures may not give accurate results. In order to overcome the influential of outliers, robust estimators seem to be an alternative for solving the above problems. Abu-Shawiesh and Abdullah [5] and Alloway and Raghavachari [6] applied a robust estimator, which is known as the Hodges-Lehmann estimator (a.k.a. HL.E.), to control charts. Here, we propose to replace the sample mean by HL.E. as an estimate for the location parameter.

In the next section, the HL.E. and its properties will be given together with its advantages. Next, a data set in the literature will be used to illustrate the computation of the HL.E. Finally, conclusions will be drawn regarding this proposal.

2 The Hodges-Lehmann Estimator

In 1963, Hodges and Lehmann [7] proposed the HL.E. as an estimator for the point of symmetry θ of a continuous and symmetric distribution. Initially, the HL.E. is a nonparametric estimator based on the Wilcoxon signed-rank statistic. However, Lehmann [8] showed later

that this estimator belongs to the class of robust R-estimators. The computations of the HL.E. follow four steps:

Let Y_1, Y_2, \dots, Y_n be a random sample obtained from some distribution, which is continuous and symmetrical about θ . Then,

- (i) Compute

$$M = \frac{n(n+1)}{2} \quad (1)$$

- (ii) Compute the Walsh averages,

$$W_r = \frac{Y_i + Y_j}{2} \quad (2)$$

where $r = 1, 2, \dots, M$ and $i \leq j = 1, 2, \dots, n$.

- (iii) Reorder the Walsh averages in ascending order, that is

$$W_{(1)} \leq W_{(2)} \leq \dots \leq W_{(M)} \quad (3)$$

- (iv) The HL.E. for the point of symmetry θ of a continuous and symmetric distribution is defined as:

$$\text{HL.E.} = \text{median} \{W_{(1)}, W_{(2)}, \dots, W_{(M)}\} \quad (4)$$

or

$$\text{HL.E.} = \begin{cases} W_{(k+1)} & \text{if } M \text{ is odd} \\ (W_{(k)} + W_{(k+1)})/2 & \text{if } M \text{ is even} \end{cases} \quad (5)$$

where

$$k = \begin{cases} (M-1)/2 & \text{if } M \text{ is odd} \\ M/2 & \text{if } M \text{ is even} \end{cases}$$

In addition to the above computations of the HL.E., the main properties of this estimator are given below:

- (i) The asymptotic relative efficiency of the HL.E. relative to the sample mean is 0.955 if the underlying distribution is Normal (Gaussian). However, the asymptotic relative efficiency of the HL.E. is often greater than unity if the underlying distribution is non-normal (Lehmann [8]). Alloway and Raghavachari [6] stated that the asymptotic properties of the HL.E. are impressive,
- (ii) The asymptotic relative efficiency for the HL.E. is the same as the Wilcoxon signed-rank test and it is asymptotically normally distributed. Besides that, it is robust against gross errors (Hodges [9]),
- (iii) The HL.E. has a breakdown point of 29%, which is high enough for most purposes (Hampel [10]), and
- (iv) The HL.E. is unbiased and translation invariant (Abu-Shawiesh and Abdullah [5]).

Besides having good properties, Abu-Shawiesh and Abdullah [5] gave an advantage of the HL.E., that is: it should give reasonable results for distributions in the neighborhood of the Normal (Gaussian) distribution. In addition, Alloway and Raghavachari [6] mentioned that the performances of robust estimators are often better than traditional measures for heavy tailed distributions and the HL.E. properties are reasonable and easy to explain to users. Details concerning of the HL.E. can be found in Hodges and Lehmann [7].

3 Example

This example is a food-processing case study taken from Fogliatto and Albin [3], which have three control factors: the processing time (x_1 – in mins), the processing temperature (x_2 – in °F) and the type of beef (x_3 – natural or restructured). Fogliatto and Albin [3] stated that x_3 is a qualitative control factor which should have been treated as a fixed block effect. In order to overcome this problem, they considered x_3 as a quantitative factor and defined as an integer variable when searching for the optimum settings. This consideration will also be applied in this paper. In addition, we also assume that x_1 and x_2 are allowed to vary within the limits in the experimental design (that is, $-1 \leq x_1 \leq 1$ and $220 \leq x_2 \leq 265$) since they are quantitative factors. This example considered three responses that are related to the food product and they are: the cohesiveness of beef cubes, the fibrousness of the meat and the flaking of the meat. According to Fogliatto and Albin [3], evaluation of these three responses were performed by the Spectrum Method, a quantitative descriptive analysis technique and measured using a 15-point continuous scale. Thus, these three responses are dimensionless. Table 3 is the data set plus the sample mean, the H.L.E., upper bounds, target values and lower bounds of the respective responses.

In Table 3, we see that there are four replications at each design point of all the three responses. Hence, $n = 4$. In order to help readers to understand better about the computations of H.L.E., the first design point of Cohesiveness will be used. Let $Y_1 = 7$, $Y_2 = 10.5$, $Y_3 = 9.3$ and $Y_4 = 10.3$, the computations follow the description in the previous section:

- (i) Compute

$$M = \frac{n(n+1)}{2} = \frac{4(5)}{2} = 10$$

- (ii) Compute the Walsh averages, $W_r = \frac{Y_i + Y_j}{2}$ where

$$r = 1, 2, \dots, 10 \text{ and } i \leq j = 1, 2, \dots, 4.$$

Thus,

$$\begin{aligned} W_1 &= \frac{Y_1 + Y_1}{2}; & W_2 &= \frac{Y_1 + Y_2}{2}; & W_3 &= \frac{Y_1 + Y_3}{2}; & W_4 &= \frac{Y_1 + Y_4}{2}; & W_5 &= \frac{Y_2 + Y_2}{2}; \\ &= 7.00 & &= 8.75 & &= 8.15 & &= 8.65 & &= 10.50 \\ W_6 &= \frac{Y_2 + Y_3}{2}; & W_7 &= \frac{Y_2 + Y_4}{2}; & W_8 &= \frac{Y_3 + Y_3}{2}; & W_9 &= \frac{Y_3 + Y_4}{2}; & W_{10} &= \frac{Y_4 + Y_4}{2} \\ &= 9.90 & &= 10.40 & &= 9.30 & &= 9.80 & &= 10.30 \end{aligned}$$

- (iii) Reorder the Walsh averages in ascending order, that is

$$\begin{aligned} W_1 &= 7.00; & W_2 &= 8.15; & W_3 &= 8.65; & W_4 &= 8.75; & W_5 &= 9.30; \\ W_6 &= 9.80; & W_7 &= 9.90; & W_8 &= 10.30; & W_9 &= 10.40; & W_{10} &= 10.50 \end{aligned}$$

(iv) Since $M = 10$ is even, $k = \frac{10}{2} = 5$, then

$$\text{H.L.E.} = \frac{W_{(5)} + W_{(6)}}{2} = \frac{9.30 + 9.80}{2} = 9.55$$

The computations for the rest of the design points of all responses repeat the whole procedure as illustrated above and the H.L.E. are given in Table 3.

Table 3 The Food-Processing Data.

Design Point	Control Factors			Responses								
				Cohesiveness			Fibrousness			Flaking		
	X_1	X_2	X_3	Data	S.M.	H.L.E.	Data	S.M.	H.L.E.	Data	S.M.	H.L.E.
1	-1	225	-1	7,10,5, 9,3,10,3	9.275	9.550	6,8,10,8, 9,5,10,5	9.400	9.750	6,8,10,8, 9,3,10,8	9.425	9.675
2	1	220	-1	9,8,11, 9,8,10,3	10.225	10.175	9,8,11,5, 9,8,11	10.525	10.525	9,8,11,5, 9,8,11	10.525	10.525
3	-1	265	1	3,3,2,9, 2,3,5	2.925	3.000	3,5,3, 2,3,5	3.000	3.125	3,5,2,5, 3,3,2,5	2.950	2.950
4	1	250	1	2,5,5,3, 3,5,3,5	3.700	3.500	2,5,6, 3,8,3,8	4.025	3.800	2,3,3,5, 3,3	2.950	3.000
5	-1	220	-1	7,8,5,3, 9,5,8,3	7.725	7.925	6,5,5,5, 9,3,8,5	7.450	7.450	6,8,6, 9,5,8,5	7.700	7.700
6	1	220	1	3,2, 2,2,3	2.325	2.225	3,2,5, 2,2,3	2.450	2.450	3,2,5, 2,2,3	2.450	2.450
7	-1	250	1	3,3,3,3, 2,2	2.650	2.650	3,3,3,8, 2,2	2.775	2.775	3,3,2, 2,2	2.325	2.000
8	-1	250	-1	10,10, 9,5,9,8	9.825	9.850	10,10, 8,8,9,6	9.600	9.700	10,10, 9,5,10	9.875	10.000
	Upper Bound			15			15			15		
	Target Value, T			8.0			3.4			6.0		
	Lower Bound			0			0			0		

In this paper, we fit the three responses with linear models (since this data set only has eight design points) for the sample mean and the H.L.E. Model selection procedures in SPSS, version 7.5.2, that is, Stepwise, Backward and Forward will be employed here. We use the default settings in SPSS, namely, the probability of F for entry is 0.05 and for removal is 0.10. For each model selection procedure, models for the sample mean and the H.L.E. of the three responses will be obtained. In order to make this study meaningful, the adjusted R squared value will be used to choose the best models. For example, SPSS give 3 models for the sample mean of the response, Flaking, when the Backward procedure is used. Thus, we will choose the model with the highest adjusted R squared value among the 3 models before proceeding to the optimization.

3.1 Model Selection Procedure: Stepwise

Let $\hat{\omega}_{1,S.M.}$ denotes the fitted model for the sample mean of the response, Cohesiveness; $\hat{\omega}_{2,S.M.}$ denotes the fitted model for the sample mean of the response, Fibrousness; $\hat{\omega}_{3,S.M.}$ denotes the fitted model for the sample mean of the response, Flaking; $\hat{\omega}_{1,H.L.E.}$ denotes the fitted model for the H.L.E. of the response, Cohesiveness; $\hat{\omega}_{2,H.L.E.}$ denotes the fitted model

for the H.L.E. of the response, Fibrousness and $\hat{\omega}_{3,\text{H.L.E.}}$ denotes the fitted model for the H.L.E. of the response, Flaking. The best models for the sample mean and the H.L.E. of the three responses are, respectively:

$$\hat{\omega}_{1,\text{S.M.}} = 6.081 - 3.181x_3 \quad (6)$$

$$\hat{\omega}_{2,\text{S.M.}} = 6.153 - 3.091x_3 \quad (7)$$

$$\hat{\omega}_{3,\text{S.M.}} = 6.025 - 3.356x_3 \quad (8)$$

$$\hat{\omega}_{1,\text{H.L.E.}} = 6.109 - 3.266x_3 \quad (9)$$

$$\hat{\omega}_{2,\text{H.L.E.}} = 6.197 - 3.159x_3 \quad (10)$$

$$\hat{\omega}_{3,\text{H.L.E.}} = 6.038 - 3.438x_3 \quad (11)$$

Table 4 shows the R squared and adjusted R squared values for (6), (7), (8), (9), (10) and (11) when the Stepwise procedure is used. Table 4 clearly indicates that the adjusted R squared values for (6) and (9), (7) and (10), and (8) and (11) are close to each other.

Table 4 R Squared and Adjusted R Squared Values for (6), (7), (8), (9), (10) and (11).

Model	R squared	Adjusted R squared
(6)	0.946	0.937
(7)	0.923	0.910
(8)	0.950	0.942
(9)	0.957	0.949
(10)	0.927	0.915
(11)	0.948	0.939

As mentioned in an earlier part of this section, these 3 responses are dimensionless. Hence, minimization the Total Deviation will be used as optimization criterion. The Total Deviation is defined as:

$$\text{Total Deviation} = \sum_{i=1}^3 |\hat{\omega}_i - T_i| \quad (12)$$

In addition, the Generalized Reduced Gradient algorithm in the “Solver” option in Microsoft Excel is used to minimize the Total Deviation and to find the optimal settings of this example. Two types of minimization have been carried out separately, that is, minimize

$$\sum_{i=1}^3 |\hat{\omega}_{i,\text{S.M.}} - T_i| \text{ and } \sum_{i=1}^3 |\hat{\omega}_{i,\text{H.L.E.}} - T_i|$$

when x_3 is fitted as 1 and -1 together with the constraints

$$(-1 \leq x_1 \leq 1, 220 \leq x_2 \leq 265 \text{ and } 0 \leq \text{responses} \leq 15).$$

Table 5 summarizes the optimization of the sample mean and the H.L.E. by using the Stepwise procedure. When $x_3 = 1$, the use of the sample mean leads to the optimal setting $(x_1, x_2, x_3) = (*, *, 1)$ with Total Deviation = 8.7690 while the H.L.E. also leads to the same optimal setting $(x_1, x_2, x_3) = (*, *, 1)$ with Total Deviation = 8.9190 where an insignificant

control factor is denoted by “*”. This is because models (6), (7), (8), (9), (10) and (11) only involve the constant and x_3 . The choice of levels for x_1 and x_2 must be based on economic considerations and on technical knowledge of the process. The use of the sample mean and the HL.E. again shared the same optimal setting when $x_3 = -1$ with almost comparable Total Deviations. Generally, these two estimators produce almost identical result in term of the Total Deviation when the Stepwise procedure is employed.

Table 5 Comparison of the Optimal Settings for the sample mean and the HL.E.

x_3	Estimator	Optimal Settings	Cohesiveness	Fibrousness	Flaking	Total Deviation
1	sample mean	(*, *, 1)	2.9000	3.0620	2.6690	8.7690
	HL.E.	(*, *, 1)	2.8430	3.0380	2.6000	8.9190
-1	sample mean	(*, *, -1)	9.2620	9.2440	9.3810	10.4870
	HL.E.	(*, *, -1)	9.3750	9.3560	9.4760	10.8070

Note: an insignificant control factor is denoted by “*”.

Figure 1 gives the Microsoft Excel spreadsheet after the spreadsheet implementation used for models (9), (10) and (11) when $x_3 = 1$.

3.2 Model Selection Procedure: Backward

We repeat the whole analysis again but now with the use of the Backward procedure. The best models for the sample mean and the HL.E. of the three responses are, respectively:

$$\hat{\omega}_{1,S.M.} = -5.450 + 0.780x_1 + 0.04938x_2 - 3.808x_3 \quad (13)$$

$$\hat{\omega}_{2,S.M.} = -5.819 + 0.925x_1 + 0.05138x_2 - 3.771x_3 \quad (14)$$

$$\hat{\omega}_{3,S.M.} = -3.752 + 0.719x_1 + 0.04192x_2 - 3.903x_3 \quad (15)$$

$$\hat{\omega}_{1,HL.E.} = -4.451 + 0.642x_1 + 0.04514x_2 - 3.821x_3 \quad (16)$$

$$\hat{\omega}_{2,HL.E.} = -5.208 + 0.820x_1 + 0.04889x_2 - 3.792x_3 \quad (17)$$

$$\hat{\omega}_{3,HL.E.} = -4.225 + 0.764x_1 + 0.04402x_2 - 4.014x_3 \quad (18)$$

Table 6 shows the R squared and adjusted R squared values for (13), (14), (15), (16), (17) and (18) when the Backward procedure is used. From Table 6, the adjusted R squared values for (13) and (16), (14) and (17), and (15) and (18) are close to each other.

The “Solver” option will be used again here with the same information (including constraints, minimize

$$\sum_{i=1}^3 |\hat{\omega}_{i,S.M.} - T_i| \quad \text{and} \quad \sum_{i=1}^3 |\hat{\omega}_{i,HL.E.} - T_i|$$

separately) except that equations (13), (14), (15), (16), (17) and (18) would replace equations (6), (7), (8), (9), (10) and (11). Table 7 summarizes the optimization of the sample mean and the HL.E. when Backward procedure is used. Table 7 clearly indicate that both the sample mean and the HL.E. lead to the same optimal settings when $x_3 = 1$ and $x_3 = -1$ with almost comparable Total Deviations.

The screenshot shows an Excel spreadsheet with the following data:

Fitted Regression Functions				
b0	b1	b2	b3	
6.109	0.000	0.000	-3.266	
6.197	0.000	0.000	-3.159	
6.038	0.000	0.000	-3.438	

Factor Levels	Responses	Constraints	
		Lower Bound	Upper Bound
x1 *	Cohesiveness	2.8430	Cohesiveness 0 15
x2 *	Fibrousness	3.0380	Fibrousness 0 15
x3 1.0000	Flaking	2.6000	Flaking 0 15

Total Deviation		8.9190
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Figure 1 Microsoft® Excel® Implementation.

Table 6 R Squared and Adjusted R Squared Values for (13), (14), (15), (16), (17) and (18).

Model	R squared	Adjusted R squared
(13)	0.987	0.978
(14)	0.977	0.960
(15)	0.980	0.965
(16)	0.987	0.977
(17)	0.970	0.948
(18)	0.979	0.964

Table 7 Comparison of the Optimal Settings for the sample mean and the H.L.E.

x_3	Estimator	Optimal Settings	Cohesiveness	Fibrousness	Flaking	Total Deviation
1	sample mean	(1, 265, 1)	4.6077	4.9507	4.1728	6.7702
	H.L.E.	(1, 265, 1)	4.3321	4.7759	4.1903	6.8535
-1	sample mean	(-1, 220, -1)	8.4416	8.3306	8.6544	8.0266
	H.L.E.	(-1, 220, -1)	8.6588	8.5198	8.7094	8.4880

3.3 Model Selection Procedure: Forward

The use of the Forward procedure in this example produces the same models for the sample mean, the H.L.E., R squared and adjusted R squared values as the Stepwise procedure. Thus, the Forward procedure as a model selection procedure will give exactly the same results (optimal settings, responses and Total Deviations) as the Stepwise procedure for this example.

4 Conclusion

Although the use of the Hodges-Lehmann estimator in this paper does not show any improvement over the sample mean, it manages to show that the Hodges-Lehmann estimator can still give comparable results as the sample mean when no outliers exist. In addition, this robust estimator will give more accurate results than the sample mean when outliers exist or the underlying assumptions are slightly incorrect (or not met). Thus, the Hodges-Lehmann estimator is very helpful especially to those practitioners who are inexperienced in detecting outliers. We do admit that the computations of the Hodges-Lehmann estimator are slightly more complicated than that for the sample mean but the use of existing technologies (such as computers and programmable calculators) can overcome this difficulty easily. As highlighted by Alloway and Raghavachari [6], the more efficient estimators tend to involve more work.

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