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Dual response surface methodology: Applicable always?

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Abstract. Quality improvement experiments always aim to reduce the process variances and simultaneously to achieve the target mean value. Locating the optimal process parameters is the fundamental problem in quality engineering to achieve the goal. Dual response surface methodology is generally used to reach the goal for replicated measures. This article focuses that dual response surface methodology may *not* always applicable to analyze replicated responses. This technique sometimes may mislead to locate the optimal process parameters. An example illustrates this point.

1. Introduction

Experimental designs are widely used in quality improvement techniques (Taguchi [16], Myers et al. [13]). Response surface methodology (RSM) is generally used to locate the optimal process parameters to achieve the target mean value assuming homogeneous variances (Khuri and Cornell [8]; Box and Draper [2]). RSM derives the model between the response (y) and a number of input variables (x_i's). Generally, a second order model is used to derive the empirical relationship, based on ordinary least squares method, assuming observations are independent and homogeneous variances.

Quality engineers and practitioners have noticed that process variability is also an important factor to reach the target mean. Thus, they focus on process variability along with the target mean. Evidence shows that the equal variation assumption may not be practically valid always (Myers et al. [13, Table 2.7, p.26]). Indeed, when the variances for all observations are not equal, classical response surface methodology can be misleading. The principal aim in an industrial process is to find operating condition that achieves the target value for the mean of a process characteristic, and simultaneously minimizes the process variability. The pioneering work has been credited to Taguchi [16], who developed a package of tools which were viewed unfavorably by many researchers and practitioners due to lack of statistical foundation (Nair et al. [14]).

Recently, the dual response surface (DRS) approach which was first introduced by Myers and Carter [12], popularized by Vining and Myers [17], has received a great deal of attention in response to its attempt to tackle such a nonequal variance problem (Del Castillo [5], Copeland and Nelson [3], Kim and Lin [9]). Basically, the DRS approach builds two empirical models–one for the mean, and one for the standard deviation, and then optimizes one of these responses subject to an appropriate constraint on the other's value. In practice, the two separate models give the analyst a more scientific understanding of the total process, and thus allow them to see what levels of the control factors can lead to satisfactory values of the response as well as the variance.

This article focuses that DRS approach may *not* always applicable for analyzing multiple observations. DRS approach may sometimes mislead to locate the optimal level combinations of process parameters. An

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example illustrates this point clearly. The structure of this paper is organized as follow. A short summary of DRS approach is given in Section 2. Section 3 describes gamma and log-normal models with constant variance. Section 4 presents anlysis of a real example. Section 5 concludes the article.

2. DRS approach

The DRS approach consists of roughly three stages: first stage–data collection (design of experiment), second stage–model building, and the third stage–optimization. Consider the situation in which a response y depends on k variables, coded x_1, x_2,..., x_k. The true response function is unknown so we shall approximate it over a limited experimental region by a polynomial representation. If a first order model, $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + ... + \beta_k x_k + e$, suffers lack of fit arising from the existence of surface curvature, we might then wish to fit, by least squares, a quadratic response of the form

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum^{k} \sum_{i<j}^{k} \beta_{ij} x_i x_j + e.$$

Again, such a model works well when the variance of the response is relatively small and stable (a constant value), but when the variance of y is non-constant, classical response surface methodology could be misleading.

Vining and Myers [17] used the DRS approach, and proposed an ingenious method to tackle such a problem. They modeled both the location effect (w_μ) and the dispersion effect (w_σ) as separate responses. Namely,

$$\begin{aligned} w_\mu &= \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum^{k} \sum_{i<j}^{k} \beta_{ij} x_i x_j + e_\mu, \\ w_\sigma &= \gamma_0 + \sum_{i=1}^{k} \gamma_i x_i + \sum_{i=1}^{k} \gamma_{ii} x_i^2 + \sum^{k} \sum_{i<j}^{k} \gamma_{ij} x_i x_j + e_\sigma. \end{aligned}$$

They fit second order models to both of the responses and then optimize the two fitted response surface models simultaneously. Specifically, they optimize one fitted response subject to an appropriate constraint on the value of the other fitted response using the Lagrangian multiplier approach. Based on the fitted DRS models, many optimization schemes have been proposed by many researchers (Vining and Myers [17], Del Castillo [5], Copeland and Nelson [3], Kim and Lin [9]). Note that the optimization results may not be trusted if models built in the second stage of DRS approach do not reflect the true model very well.

3. Log-normal and gamma model

In regression models for positive observations analysis can often be based on either the log-normal or the gamma model (Firth [6], McCullagh and Nelder [11], Myers et al. [13]). There is a well known correspondence between multiplicative regression models and additive models of their logarithms. In classical linear models, it is assumed that the variance of the response (Y) is constant over the entire range of parameter values. When the variance increases with the mean we may consider a model with the constant coefficient of variation $Var(Y) = \sigma^2 \mu_Y^2$, where σ is the coefficient of variation of Y and $\mu_Y = E(Y)$. In generalized linear models (GLMs; McCullagh and Nelder [11]) the gamma model satisfies the mean and variance relationship above. For small σ, the variance-stabilizing transformation, $Z = \log(Y)$, has approximate moments $E(Z) = \log \mu_Y - \sigma^2/2$ and $Var(Z) \simeq \sigma^2$.

If the systematic part of the model is multiplicative on the original scale, and hence additive on the log scale, then

$$Y_i = \mu_{Y_i} \epsilon_i \quad (i = 1, 2, ..., n) \tag{1}$$

with $\eta_i = \log \mu_{Y_i} = x_i^t \beta = \beta_0 + x_{i1}\beta_1 + ... + x_{ip}\beta_p$ and $\{\epsilon_i\}$'s are independent identically distributed (IID) with $E(\epsilon_i) = 1$. In GLMs μ_{Y_i} is the scale parameter and $Var(\epsilon_i) = \sigma^2$ is the shape parameter. Then

$$Z_i = \log Y_i = \mu_{Z_i} + \delta_i \quad (i = 1, 2, ..., n) \tag{2}$$

with $\mu_{Z_i} = \beta_0 + E(\log \epsilon_i) + x_{i1}\beta_1 + ... + x_{ip}\beta_p$ and $\{\delta_i = \log \epsilon_i - E\{\log(\epsilon_i)\}\}$'s are IID with $E(\delta_i) = 0$.

Conversely, if Y_i follows a log-normal distribution, i.e. $Z_i \sim N(\mu_{Z_i}, \sigma^2)$ then

$$\mu_{Y_i} = E(\exp Z_i) = \exp(\mu_{Z_i} + \sigma^2/2) \neq \exp(\mu_{Z_i}).$$

Thus, with the exception for the intercept term, the remaining parameters $\beta_1, \beta_2, ..., \beta_p$ can be estimated either from the constant coefficient of variation model (1) or linear model for the transformation of the original data to log scale (2). The intercept parameters in models (1) and (2) are not the same, but they will often be unimportant in practice (Myers et al. [13, p. 169]).

Firth [6] gave a comparison of the efficiencies of the maximum-likelihood (ML) estimators from gamma model (the constant coefficient of variation model) when the errors are in fact log-normal with those of the log-normal model when the errors have a gamma distribution. He concluded that the ML estimators from the gamma model perform slightly better under reciprocal misspecification. For small σ^2 it is likely to be difficult to discriminate between Normal-theory linear models for $\log Y$ and gamma-theory multiplicative models for Y.

Below we analyze an example based on both the log-normal and gamma models as described above. Both the analyses show identical results and variance of the response is constant.

4. Roman catapult experiment

Luner [10] presented an experimental setup of data for the Roman catapult. This is an ideal experiment to illustrate DRS approach. The aim of the catapult experiment is to deliver a projectile to a designated target (80 inches) with a high degree of accuracy and precision. A second order central composite design with three factors is used for the catapult experiment. Factors are arm length (x_1), stop angle (x_2), and pivot height (x_3). The model matrix, factors and the responses are given in Luner [10, pp. 695–698]. For ready reference, experimental layout and resulting responses (outcomes) are reproduced in Appendix (Table 2).

Table 1: Results for mean with constant variance models ((1) and (2)) of Catapult data from log-normal and gamma fit

		log-normal model				gamma model			
	Covar.	estimate	*s.e.*	t	P-value	estimate	*s.e.*	t	P-value
Mean model	Const.	4.29	0.03	167.57	0.00	4.31	0.02	173.91	0.00
	x_1	0.19	0.03	6.02	0.00	0.19	0.03	6.27	0.00
	x_2	0.02	0.03	0.62	0.54	0.02	0.03	0.85	0.40
	x_3	0.25	0.03	8.03	0.00	0.25	0.03	8.36	0.00
	x_2x_3	−0.08	0.04	−2.01	0.05	−0.08	0.04	−1.91	0.06
Const. Var model	Const.	−3.24	0.19	−16.96	0.00	−3.31	0.19	−17.35	0.00
AIC				486.2				482.6	

Luner [10] analyzed the catapult data using dual response surface approach. He derived mean model using the group means as responses rather than using all the data by weighted least squares regression analysis, and thus a second order mean model was fitted. Weighted least squares method was used to remove the heteroscedasticity in the data set. For variance, a second order standard deviation model was fitted using the group standard deviations as responses rather than using all the data by simple least squares regression analysis. It has not been verified that whether the data is homoscedastic or not. Sometimes a simple transformation is sufficient to remove the heteroscedasticity in the data. Das and Lee [4] pointed that it is better to analyze the original data rather than transformed statistics.

Here we analyze the catapult data using the constant coefficient of variation model (i.e., gamma model (1)), and linear model for the transformation of the original data to log scale (i.e., log-normal model (2)). The selected models have the smallest Akaike information criterion (AICs) value in each class. Because AIC selects a model which minimizes the predicted squared error loss (Hastie et al. [7, p. 203]), it is not necessary that *all* the selected effects are significant. We retain some insignificant effects in the model in order to respect the marginality rule, namely that when an interaction term is significant all related lower-order interactions and main effects should be included in the model (Nelder [15]). We fit both of the models ((1) and (2)), analysis is given in Table 1.

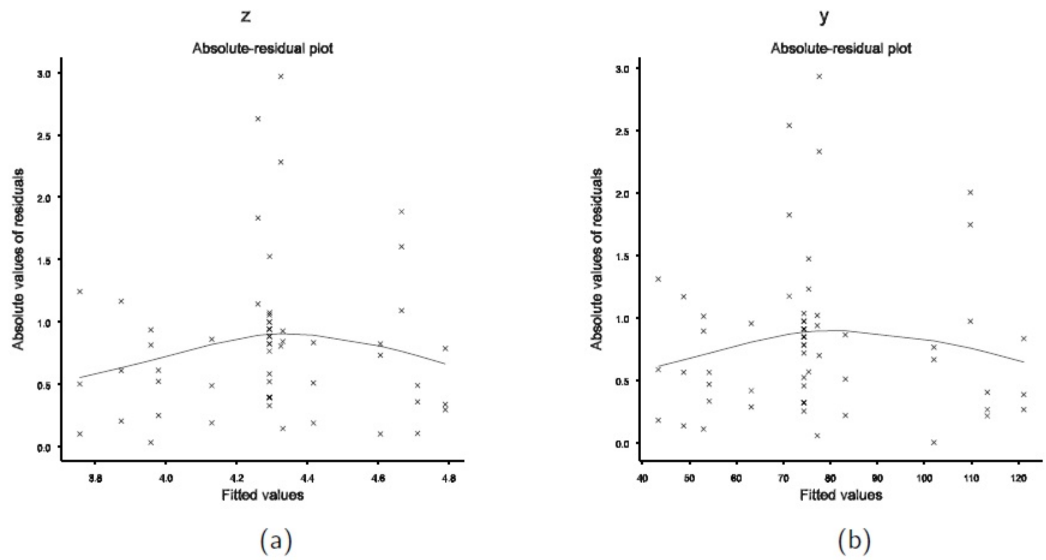

Figure 1: The Absolute residual plots with respect to fitted values for the constant variance models of (a) log-normal and (b) gamma for catapult data

In Figures 1(a) and 1(b), we plot the absolute values of residuals with respect to fitted values for log-normal and gamma fitted models (Table 1), respectively. If the transformation or gamma model with constant variance are satisfactory, they should have a flat running means. Here both the plots show flat running means, an indication that variance is constant, so that the simple log transformation or gamma model with constant variance is sufficient to remove heteroscedasticity. In Figures 2(a) and 2(b), we plot the normal probability plot of the mean model for log-normal and gamma fitted models (Table 1), respectively. Figures 2(a) and 2(b) do not show any systematic departures, indicating no lack of fit of our final selected models. Even though the estimates and their standard errors (in Table 1) are identical in both the models, satisfying Firth's [6] conjecture, but the *AIC* (in Table 1) shows that gamma model gives a better fit, which is also clear from plots (Figures 1(b) and 2(b)).

The following are the *main* differences of our analysis from Luner [10]:

1. Luner found that the response projectile length has a non-constant variance, but according to our analysis it has constant variance ($e^{-3.31} = 0.0365$; from gamma fitted model, using log-link).
2. Our mean model ($e^{4.31+0.19x_1+0.02x_2+0.25x_3-0.08x_2x_3}$; from gamma fitted model, using log-link) is very simple than the Luner's mean model.
3. We have no variance model (i.e., no one factor is significant), but Luner's variance model is very complicated (i.e., many factors are significant).

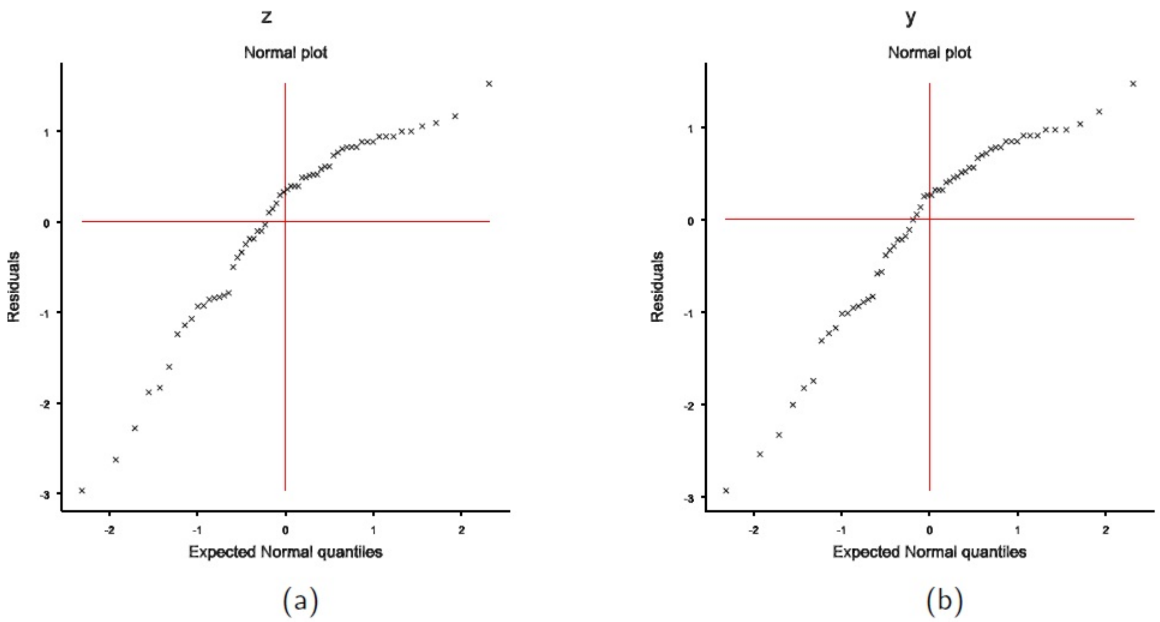

Figure 2: The Normal probability plots for mean for the constant variance models of (a) log-normal and (b) gamma for catapult data

4. In our mean model only x_1, x_3, and x_2x_3 are significant, but in Luner's mean model x_1, x_3, x_1^2, x_1x_3 and x_2x_3 are significant.
5. From our analysis, optimal settings of the process parameters can be easily determined, but it is very difficult from Luner's model.
6. Our optimal settings (for example, $x_1 = 0.3$, $x_2 = 0.5$ and $x_3 = 0.0$, target mean = 79.997, variance = 0.0365) of the process parameters are completely different from Luner's model.

5. Concluding remarks

DRS approach is always recommended to analyze multiple responses for deriving mean and variance models (Vining and Myers [17]). The Roman catapult data has been modeled via log-normal and gamma models (Section 3). Proper modeling is very crucial in any optimization problem such as dual response surface technique. Practitioners need to use all possible data analysis technique before finalizing the selected model, and the selected model is to be verified with proper model checking tools. Analysis of original responses is more better, rather than summarizing statistics such as sample mean and sample variance (Box [1], Das and Lee [4]). We have seen that analysis of sample means results inefficient analysis to classify insignificant factors as significant, and vice versa. It is seen that efficient analysis may give better fitted model of the data set. Here it is observed that simple log transformation is sufficient to remove the heteroscedasticity *but* it is not always true (Myers et al. [13, Table 2.7, p. 36]). For quality improvement data analysis, identification of important process factors are very important, so that the use of efficient statistical method is crucial. Practitioners need to examine whether variances may be stabilized or not. Thus, for completely stabilized variance model, DRS approach may mislead the proper selection of optimal level combination of process parameters, resulting poor quality of product.

Appendix

Table 2: Experimental Layout and Responses conducted by Luner [10] for the Roman Catapult Data

Trail No.	Run order	x_1	x_2	x_3	Rep. 1	Rep. 2	Rep. 3
1	20	−1	−1	−1	39	34	42
2	9	−1	−1	1	80	71	91
3	11	−1	1	−1	52	44	45
4	14	−1	1	1	97	68	60
5	15	1	−1	−1	60	53	68
6	10	1	−1	1	113	104	127
7	13	1	1	−1	78	64	65
8	1	1	1	1	130	79	75
9	7	−1.682	0	0	59	51	60
10	4	1.682	0	0	115	102	117
11	19	0	−1.682	0	50	43	57
12	18	0	1.682	0	88	49	43
13	12	0	0	−1.682	54	50	60
14	8	0	0	1.682	122	109	119
15	6	0	0	0	87	78	89
16	5	0	0	0	86	79	85
17	17	0	0	0	88	81	87
18	3	0	0	0	89	82	87
19	2	0	0	0	86	79	88
20	16	0	0	0	88	79	90

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