Middle-East Journal of Scientific Research 11 (12): 1623-1627, 2012
ISSN 1990-9233

DOI: 10.5829/idosi.mejsr.2012.11.12.1653

A Comparative Optimization of Textile Systems Using Response Surface and Parametric Dual Modeling Methods

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Abstract: In this study, a Comparison between response surface and parameter dual methodologies for optimization of multilamellar liposomes from Soya lecithin with 75% phosphatidylcholine in textile system were carried out and the behavior of liposomes in dye-bath at different temperature, time, Sodium Sulphate, pH and concentration (five factors) were considered using a standard Central Composite Design (CCD) matrix in both cases to produce representative data. The results of optimization method for the data of recent published research article which was only based on general mean function shows that the estimation of optimal factor values through new methodology of parameter dual is more efficient.

Key words: Response surface and parameter dual methodologies . central composite design . liposomes . wool dyeing . color strength (K/S)

INTRODUCTION

There are a number of potential approaches to directly modeling the mean and variance as a function of the control factors. A general approach is to assume that the underlying functional forms for the mean and variance models can be expressed parametrically. Assuming a d point design with n_i replicates at each location (i = 1, 2, …, d), the point estimators of the process mean and variance, $\overline{y}_i$ and s_i^2, respectively, forms the data for the dual response system. Since the purpose of this article is to demonstrate the utility of a hybrid approach (combining a parametric and nonparametric approach to modeling) for robust design, we will consider an "off the shelf" model for the mean. An "off the shelf" model for the process mean is linear in the model parameters and can be written as:

Means model:

$$\overline{y}_i = x_i'\beta + g^{1/2}(x_i^{*\prime};\gamma)\varepsilon_i \qquad (1)$$

where x_i' and $x_i^{*\prime}$ are 1×k and 1×l vectors of means model and variance model regressors, respectively, expanded to model form, β and γ are k×1 and m×1 vectors of mean and variance model parameters, respectively, g is the underlying variance function and ε_I denotes the random error for the mean function. The ε_i are assumed to be uncorrelated with mean zero and variance of one. Note that the model terms for the i^{th} observation in the means model are denoted by x_i' while the model terms for the variance model are denoted by $x_i^{*\prime}$. This allows for the fact that the process mean and variance may not depend on the same set of regressors.

Similar to the modeling of the mean, various modeling strategies have been utilized for estimating the underlying variance function. Bartlett and Kendall [1] demonstrated that if the errors are normal about the mean model and if the design points are replicated, the variance can be modeled via a log-linear model with the d sample variances utilized for the responses. A great deal of work has also been done using generalized linear models for estimating the variance function. Although not an exhaustive list, the reader is referred to Box and Meyer [2], Aitkin [3], Grego [4], and Myers and Montgomery [5]. As mentioned previously, since the purpose of this manuscript is to demonstrate the utility of a hybrid approach to modeling, we choose an "off the shelf" approach to variance modeling. The log-linear model proposed by Bartlett and Kendall [20] is a popular one [6, 7] and and is written explicitly as:

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Variance model:

$$\ln(s_i^2) = g^*(X_i^*) + \eta_i = X_i^*\gamma + \eta_i \quad (2)$$

where η_i denotes the model error term whose expectation is assumed to be zero and whose variance is assumed constant across the d design points.

Assuming the model forms for the mean and variance given in (1) and (2), the model parameters are estimated using the following Estimated Weighted Least Squares (EWLS) algorithm.

Step 1: Fit the variance model, $\ln(s_i^2) = X_i^*\gamma + \eta_i$, via Ordinary Least Squares (OLS), obtaining $\hat{\gamma}^{(OLS)} = (X^{*\prime}X^*)^{-1} X^* y^*$ where y^* is the d×1 vector of log transformed sample variances.

Step 2: Use $\hat{\sigma}_i^2 = \exp(X_i^{*\prime}\hat{\gamma}^{(OLS)})$ as the estimated variances to compute the d×d estimated variance-covariance matrix for the means model,

$$\hat{V} = \mathrm{diag}(\hat{\sigma}_1^2, \hat{\sigma}_2^2, \ldots, \hat{\sigma}_d^2).$$

Step 3: Use $\hat{V}^{-1}$ as the estimated weight matrix to fit the means model, yielding $\hat{\beta}^{(EWLS)} = (X'\hat{V}^{-1}X)^{-1}X'\hat{V}^{-1}\bar{y}$ where $\bar{y}$ denotes the d×1 vector of sample averages.

The algorithm above yields the following estimates of the process mean and variance functions:

Estimated process mean:

$$\hat{E}[y_i]^{(EWLS)} = x_i'\,\hat{\beta}^{(EWLS)} \quad (3)$$

Estimated process variance:

$$\hat{\mathrm{Var}}[y_i]^{(OLS)} = \exp(x_i^{*\prime}\hat{\gamma}^{(OLS)}) \quad (4)$$

Therefore, A purely parametric approach involves the user specifying functional forms for both the mean and variance functions. In what could be considered an off-the shelf parametric model, the user assumes a known linear model for the process mean and a known log-linear relationship for the variance.

$$\bar{y}_i = h(x_i) + g^{1/2}(z_i\gamma)\varepsilon_i = x_i'\beta + g^{1/2}(x_i^{*\prime};\gamma)\varepsilon_i \quad (5)$$

$$\ln(s_i^2) = g^*(x_i^*) + \eta_i = x_i^{*\prime}\gamma + \eta_i \quad (6)$$

The iterative analysis begins with an initial Ordinary Least Squares (OLS) fit to the mean and then uses gamma regression to fit an exponential function to the squared OLS residuals. The mean and variance model parameters are re-estimated via Estimated Weighted Least Squares (EWLS) and the entire iterative process continues until convergence of the parameter estimates in the means model. At convergence, these mean and variance model estimates are the maximum likelihood estimates provided that the errors are normally distributed. Valid inferences from such an analysis depend heavily on the assumption that the specified forms of h and g are sufficient across the entire range of the data. If h and g are misspecified, any inferences from the analysis become suspect. Assuming the model forms for the mean and variance given in (5) and (6), the model parameters are estimated using the Estimated Weighted Least Squares (EWLS) algorithm for mean model and Ordinary Least Square (OLS) for Variance model. The algorithm above yields the following estimates of the process mean and variance functions.

Estimated process mean:

$$\hat{E}(y_i)^{EWLS} = x_i'\hat{\beta}$$

Estimated process variance:

$$\hat{V}(y_i)^{(ols)} = \exp(x_i^{*\prime}\hat{\gamma}^{(ols)})$$

Once estimates of the mean and variance have been calculated, the goal becomes finding the operating conditions for the control factors such that the mean is as close as possible to the target while maintaining minimum process variance. This is often accomplished via minimization of an objective function such as the Squared Error Loss (SEL):

$$SEL = E(y(x) - T)^2 = \{E(y(x) - T\}^2 + V[y(x)]$$

where T denotes the target value for the process mean. Minimization can be accomplished via non-linear programming using a method such as the generalized reduce gradient or the Nelder-Mead simplex algorithm. Note that the determined set of optimal operating conditions is highly dependent on quality estimation of both the mean and variance functions.

Misspecification of the forms of either the mean or variance models can have serious implications in process optimization.

MATERIALS AND METHODS

The wool fabric with plain woven structure from 48/2 Nm yarns was supplied by Iran Merino. The fabric was scoured with 1% anionic detergent VEROLAN-NBO (supplied by Rodulf) at 708C for 45 min and then washed with tap water and dried at room temperature. Industrial grade of aluminium sulphate was used for mordanting of wool samples. Soya lecithin (containing 75% phosphatidylcholine) with phase transition temperature (Tc) of 2188C was gifted by Lipoid (Germany). Madder was prepared from Yazd providence of Iran. The reflectance spectra of the dyed samples were recorded on an ACS Spectra Sensor II integrated with an IBM-PC. The wash-fastness of the liposomes treated madder-dyed fabric were measured according to ISO150-C01. For light-fastness measurements, the samples were exposed to the daylight for 7 days according to the daylight ISO 105-B01 and changes in the color (fading) were assessed by the blue scale. Also the dry and wet rub fastness of the samples evaluated according to ISO 105-X12. The sample pictures were taken with Philips XL30 SEM with 34000. The drop absorbency of the fabric samples was also measured by dropping of water droplet from 1 cm on the fabric surface on the glass by a small syringe. The time of complete absorption of the water droplets on the fabric surface was recorded and the mean value of 20 replicates was reported. Dyeing The mordanted wool samples were steeped in the dye bath with liquor-to-goods ratio of 40 : 1 that was prepared by 2% o.w.f. of extracted dye at pH 2-4 (acetic acid) with different concentrations of freshly prepared MLV liposomes (0, 1, 2, 3% o.w.f.). Dyeing was started at room temperature and then raised 28C/min to the final desired temperature including 75, 85 and 958C. The dyeing was carried out with liposomes and without liposomes in various times of 30, 45 and 60 min. The samples were rinsed with tap water and dried at room temperature. The amount of reflectance was selected at the maximum wavelength and the K/S value which is of the type "the larger the better" was calculated according to the Kubelka-Munk equation:

$$K/S = (1-R)^2 / 2R$$

Once the data are collected, our goal is to fit a model to estimate the true relationship between the explanatory variables and response. For the response problem, we may use regression techniques to model the relationships between the explanatory variables and the responses. However, in fact, the fits obtained by the regression techniques in the univariate case are equivalent to the fits obtained by the multivariate regression techniques, including the parametric, nonparametric and semi parametric methods. Therefore, in this study, For the response variables, suppose the true relationship between the k explanatory variables, $x_{1i}, x_{2i}, \ldots, x_{ki}$ and the response, y, i=1,..., n, is $y_i = f(x_{1i}, x_{2i}, \ldots, x_{ki}) + \varepsilon_i$, where the function f represents the true relationship, n is the sample size and ε_i represents a random error term

Table 1: Design matrix of experiments and results of the runs

Sample	Zirconium oxychloride	Temperature	Citric acid	Formic acid	X1	X2	M
1	10.30	95.0	12.80	5.65	1.7	0.5	1.20
2	10.30	77.0	12.80	10.35	2.6	0.7	1.65
3	4.00	86.0	9.55	8.00	2.2	1.2	1.70
4	5.60	95.0	12.80	10.35	3.2	1.8	2.50
5	10.30	95.0	6.30	5.65	1.5	0.5	1.00
6	7.95	101.14	9.55	8.00	1.5	0.5	1.00
7	5.60	95.0	6.30	10.35	2.3	1.0	1.65
8	11.90	86.0	9.55	8.00	1.8	0.9	1.35
9	7.95	86.0	15.02	8.00	1.8	0.8	1.30
10	5.60	77.0	12.80	5.65	2.1	1.3	1.70
11	7.95	86.0	9.55	8.00	2.5	1.0	1.75
12	7.95	86.0	9.55	8.00	1.5	0.4	0.95
13	7.95	86.0	9.55	8.00	1.4	0.5	0.95
14	7.95	86.0	4.08	8.00	2.7	1.5	2.10
15	5.60	77.0	6.30	5.65	2.9	1.0	1.95
16	7.95	86.0	9.55	8.00	1.3	0.5	0.90
17	7.95	70.86	9.55	8.00	2.0	0.6	1.30
18	7.95	86.0	9.55	11.95	1.7	0.7	1.20
19	10.30	77.0	6.30	10.35	2.0	0.5	1.25
20	7.95	86.0	9.55	4.05	2.5	0.7	1.60
21	7.95	86.0	9.55	8.00	1.2	0.5	0.85

Table 2: ANOVA for response surface methodology

Source	Sum of square	DF	Mean square	F value	Sig
Model	1.230	3	0.410	2.66	0.0814 (Not significant)
X1	0.510	1	0.510	3.28	0.0879
X4	0.036	1	0.036	0.23	0.6350
X4X4	0.069	1	0.069	4.46	0.0498
Residual	2.630	17	0.150		
Lack of fit	1.900	13	0.180	0.81	0.6587
Total	3.860	20	-		

Table 3: Analysis of variance of parameter model

	Df	Sum. Sq	Mean. Sq	F. value	Pr. F.
X1	1	2.00E-05	2.00E-05	0.00037	0.98483
X2	1	0.12462	0.12462	1.89513	0.18758
x3	1	0.01789	0.01789	0.27209	0.60908
x4	1	0.00092	0.00092	0.014	0.9073
Residuals	16	1.05213	0.06576	NA	NA

Table 4: Estimates of the model parameters

	Estimate	Std..Error	T value	Probability
(Intercept)	4.10640	2.59944	1.57972	0.16525
x1	5.28657	8.55476	0.61797	0.55931
x2	-3.73090	8.40389	-0.44395	0.67264
x3	-10.88841	6.01406	-1.81049	0.12019
x4	-11.57946	8.56543	-1.35188	0.22515
x1.x1	3.84247	2.48712	1.54495	0.17331
x1.x2	-8.66034	7.46944	-1.15944	0.29033
x1.x3	-0.00276	1.95430	-0.00141	0.99892
x1.x4	-0.96834	3.12422	-0.30995	0.76709
x2.x2	2.33854	7.07644	0.33047	0.75228
x2.x3	4.78325	4.77934	1.00082	0.35555
x2.x4	7.49969	7.46997	1.00398	0.35415
x3.x3	4.17161	2.15817	1.93293	0.10143
x3.x4	2.16444	1.96273	1.10277	0.31238
x4.x4	2.85402	2.5029	1.14029	0.29763

Table 5: Analysis of variance of response y-bar

	Df	Sum.Sq	Mean.Sq	F.value	Probability
x1	1	1.37437	1.37437	5.66958	0.05469
x2	1	0.03744	0.03744	0.15444	0.70791
x3	1	0.01712	0.01712	0.07062	0.79933
x4	1	0.07599	0.07599	0.31349	0.59581
x1.x1	1	0.50307	0.50307	2.07527	0.19978
x1.x2	1	0.42856	0.42856	1.76792	0.23195
x1.x3	1	0.02641	0.02641	0.10894	0.75258
x1.x4	1	0.1097	0.1097	0.45255	0.52617
x2.x2	1	0.00593	0.00593	0.02447	0.88083
x2.x3	1	0.2351	0.2351	0.96984	0.36275
x2.x4	1	0.24314	0.24314	1.00299	0.35525
x3.x3	1	0.83507	0.83507	3.44486	0.11284
x3.x4	1	0.29497	0.29497	1.21682	0.31225
x4.x4	1	0.3152	0.3152	1.30025	0.29763
Residuals	6	1.45447	0.24241	NA	NA

from the process assumed to be independently identically distributed with mean zero and constant variance s_{i2}. Consequently,

$$E(y_i \mid x_{li},\dots,x_{ki}) = \mu_i = f(x_{1i}, \dots, x_{ki})$$

is the true mean response function. It should be noted that the function f may be a different function of the same k repressors for the response.

A CCD was conducted with a total of 21 design points, including 4^2 runs in the factorial region, augmented with six axial runs and two center runs (Table 1).

Using the second-order polynomial parametric method to model of response to obtain the optimal fitted value y (x) at location x. The final fitted second-order models for the responses by RSM are given in Table 2. For the response y, the final fitted models include one terms: $x_4 x_4$. The natural independent variables are transformed into the coded variables within the range of [0,1].

Where the results of analysis variance and estimates of parameters for parameter model are given in Table 3 and 4, respectively.

However, the results of analysis of variance of response y-bar are given in Table 5.

Table 6: Results on model comparisons of OLS and RSM

Method	SEL	R^2	R^2_{adj}	PRESS	Y_{hat}
RSM	0.150	0.319	0.199	5.192	1.723
OLS	0.139	0.416	0.210	4.887	1.806

?The best value is bold

RESULTS ON MODEL COMPARISONS

During the modeling stage, Table 6 shows the numerical results for model comparisons of RSM and OLS for the response respectively. Table 6 shows that OLS has smaller, often substantially smaller, SEL than RSM across of the response. Table 6 shows that OLS has smaller, often substantially smaller, s^2 and larger, substantially larger, R^{adj} than RSM across of the response. OLS has larger R^2 than RSM in of the response. OLS has smaller PRESS than RSM in the response.

OPTIMIZATION RESULTS

During the optimization stage, the desirability function method is used to obtain the best compromise of the response. In the individual desirability function, the prespecified parameters are set as follows. The maximum (or minimum) of the observed data is used as the T value for response since they are not available. That is, in this example, T = 2.20. Since a CCD was utilized in the example, the solution vector x_s shall be constrained to be within the experimental region R, a hyper-circle in this 4-dimensional example. As mentioned previously, the natural independent variables are transformed into the coded variables within the range of [0, 1]. Therefore, the solution vector x_s is defined as $(x_1-0.5)^2+(x_2-0.5)^2+(x_3-0.5)^2 \le 0.5^2$ in the transformed experimental region. As mentioned earlier, using the second-order polynomial to parametrically model response to obtain the optimal fitted value y(x) at location x. The final fitted models are given in as well as the location where the simultaneous optimal solution is found. Based on the location they found using Design-Expert, the corresponding fitted values for the response is re-calculated by us as well as the desirability value D and given as follows. The RSM solution: x1 = 0.106, x2 = 0.913, x3 = 0.123, x4=0.062 and D=0.9271. We find the optimization solutions by the one different modeling Technique. The solutions we find by the OLS method are: x1=0.121, x2=0.889, x3=0.117, x4=0.081 and D=0.9365.

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