

Comparison of Parametric and Nonparametric Approaches in Robust Parameter Design (A Case Study in Textile Systems)

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Abstract: Robust Parameter Design (RPD) is an engineering methodology intended as a cost effective approach for improving the quality of products and processes. An essential component of robust parameter design involves the assumption of well estimated models for the process mean and variance. In this study, researchers examine the effect of three factors, temperature, time and liposome on the results of color strength (K/S) in dyeing process of wool fibers by application two different methods, namely; parametric and nonparametric to modeling a dual response surface (mean and variance) and then optimize this process in both methods within the robust design setting. Comparing the results suggest the relative superiority of nonparametric method in terms of SEL.

Key words: Liposome, wool dyeing, color strength (K/S), central composite design, genetic algorithm, Iran

INTRODUCTION

In the mid 1980, Japanese quality consultant Genichi Taguchi popularized a cost efficient approach to quality improvement known as Robust Parameter Design (RPD). The goal RPD is to determine levels of the control factors which cause the response to be robust to changes in the levels of the noise variables. Variation in the process which results from uncontrollable fluctuations in the noise factors can be summarized by taking the sample variance of the points in the noise factor space at each of the control factor setting. The process can be made robust to the variation associated with the noise factors by choosing the factor combination of the control factors corresponding to the smallest sample variance. It is often the case that the levels of the noise factors are unobservable not only in the process but also in a controlled experimental setting. In these situations, replications at the control factor setting provide the researcher with an idea of process variability and the approach to robust design is the same namely to choose the factor combination in the control factor space which corresponds to the smallest sample variance. It is these types of situations which will be the focus of this study. Instead of using only the sample variances for describing the underlying process variance, Vining and Myers (1990) introduced a dual model response surface approach to RPD in which it is assumed that both the mean and variance can be described by separate parametric regression models. Optimal control factor settings are then found using constrained optimization (constrained estimated mean and minimized process variance with respect to control factor settings).

If one or both models are misspecified by the researcher, the estimates may be highly biased and consequently the optimal control factor settings may be misspecified. Vining and Bohn (1998) (henceforth referred to as VB) point out that traditional parametric models are often inadequate particularly when modeling the variance and suggest the use of nonparametric techniques for modeling the variance.

In this study, researchers examine the effects of three important factors in dyeing process of wool fibers, namely; temperature, time and liposome on the results of color strength (K/S) as response variable. To this purpose, researchers modeling the mean and variance of this process with a dual model response surface by using of both parametric and nonparametric methods and then obtain operating conditions of this process where the process variance is minimized and the process mean achieves a given target value. The Central Composite Design (CCD) is used for the experimental plan and to produce representative data. The results of both methods are compared in terms of SEL. Researchers also use of a more flexible and efficient optimization routine the Genetic Algorithm (GA) for determining optimal control factor settings.

Researchers note that commercial liposome recently were incorporated into textile auxiliaries, mainly for wool dyeing (Corderch *et al.*, 1999). This is a clean technology that has already been adapted by some textile industries. These are additional benefits for material weight yield during subsequent spinning. These improved smoothness and mechanical properties of the dyed textiles and showed a clear reduction in the contamination load of the dye-baths (Leeder, 1986). Use of liposome as

an auxiliary in wool dyeing can be related to the bilayer structure of lipids from the Cell Membrane Complex (CMC) of wool that is similar to the liposome and the action of this morphological fraction of the fiber in wool processing. A wool fiber includes of cuticle and cortical cells held together by the CMC and forms the continuous phase in the keratin. This phase contains a small amount of lipid material. Diffusion properties of wool fibers are influenced by the lipid structure of the intercellular spaces that could act as solvents for hydrophobic chemical. The dyes diffuse with ease into swollen regions such as the CMC (intercellular diffusion) rather than through the cuticle cells (transcellular diffusion).

Last few years, several studies have related the potential application of liposome in wool dyeing. Meza have investigated liposome as doer in wool dyeing with acid (De la Maza *et al.*, 1993, 1995a, b; 1997) disperse metal complex dyes. Also they have worked on the effects of commercially available liposome as a simple additive. Recently, they used an optimized mixture of commercial liposome and cationic surfactant to improve leveling property. In the previous research, the influence of temperature on stability of Multilamellar Liposome (MLV) in wool dyeing was studied and it was found that the presence of 1% owf (on weight of fabric) of liposome at 85°C could improve the dye exhaustion of Irgalan Blue FBL on wool fabric. It has also reported that the wash fastness properties of dyed samples with liposome have also improved. There is no report on using liposome in wool dyeing with natural dyes. Therefore, researchers try to prepare and produce MLV from Soya lecithin with 75% phosphatidylcholine and study the influence of liposome in dye bath at different and concentration during wool dyeing with madder as a most famous natural dye.

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 70°C 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 (T_c) of -18°C 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.

Liposomes preparation: MLV liposomes were prepared following the thin film hydration method. A lipid film was formed by removing the organic solvent with rotary

evaporation (with temperature of bath being 35-40°C and 30 rpm) from a chloroform solution containing Soya lecithin. Aqueous phase containing distilled water was added to the lipid film. The solution was shaken by hand to deliver the lipid from the walls of flask and disperse large lipid aggregates, glass beads were added to facilitate dispersions. The milky suspension was agitated at 40°C to obtain a complete emulsion. This means that the lipid extensively hydrated and MLV liposomes formed (Montazer *et al.*, 2006).

Preparation for dyeing: Before dyeing, the wool samples should be cleaned to prepare the samples free from the impurities. Therefore, the samples are scoured in first step and then dyed later. Also, the dyestuff should be ready for process too. Researchers can extract dyestuff from the natural collected madder.

Scouring: The samples were scoured in a bath containing 1 g L⁻¹ anionic detergent, 1 mL L⁻¹ ammonia (pH = 8.5) in 70°C for 45 min with liquor-to-goods ratio (L:G) of 40:1. The samples were then rinsed with warm water (60°C) and tap water and then dried at room temperature.

Dyestuff extraction: For extraction of dyestuff the madder were steeped in water solution for 24 h and then heated at 70°C for 20 min and the solution was then passed through the filter. The filtered solution was transferred to a glassing flask. The solution of dye was concentrated by removing the water with rotary evaporation.

Mordanting: The scoured samples (L:G = 40:1) were steeped in the mordant bath prepared with 20% owf of aluminium sulphate with pH = 4.5-5.8 (adjusted by acetic acid).

Mordanting of sample was started at room temperature and the temperature was raised for 2°C min⁻¹ to boil and heated for 60 min. The samples were rinsed with tap water and dried at room temperature.

Dyeing: The mordanted wool samples were steeped in the dye bath with liquor-to-goods ratio of 40:1 that was prepared by 2% owf of extracted dye at pH 4.5-5.5 (acetic acid) with different concentrations of freshly prepared MLV liposome (1, 2, 3% owf).

Dyeing was started at room temperature and then raised 2°C min⁻¹ to the final desired temperature. The dyeing was carried out with liposome 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:

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

$$\text{Variance model: } \ln(s_i^2) = g^*(X_i^*) + \eta_i = X_i^* \gamma + \eta_i \quad (2)$$

Parametric approach: Given the data from a crossed array, 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 ($i = 1, 2, \dots, d$) the point estimators of the process mean and variance y_i and S_i^2 , respectively form the data for the dual response system. Since, the purpose of this study is to demonstrate the utility of a hybrid approach (combining a parametric and nonparametric approach to modeling) for robust design researchers 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:

$$\text{Means model: } \bar{y}_i = x_i' \beta + g^{1/2}(x_i^*; \gamma) \varepsilon_i \quad (1)$$

Where x_i' and x_i^* are $1 \times k$ and $1 \times l$ vectors of means and variance model regressors, respectively expanded to model form β and γ are $k \times 1$ and $l \times 1$ vectors of mean and variance model parameters respectively, g is the underlying variance function and 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^* . 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 (1946) 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 sample variances utilized for the responses. A great deal of study 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 (1986), Aitkin (1987), Grego (1993), Lee and Nelder (2003) and Myers *et al.* (2005). As mentioned before since, the purpose of this study is to demonstrate the utility of a hybrid approach to modeling researchers choose an off the shelf approach to variance modeling. The log-linear model proposed by Bartlett and Kendall (1946) is a popular one (Vining and Myers, 1990; Myers and Montgomery, 2002) and is written explicitly as:

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 Eq. 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 $\hat{\gamma}^{(OLS)} = (x^{*'} x^*)^{-1} x^{*'} y^*$ where y^* is the $d \times 1$ vector of log transformed sample variances
- Step 2: Use $\hat{\sigma}_i^2 = \exp(x_i^{*'} \hat{\gamma}^{(OLS)})$ as the estimated variances to compute the $d \times d$ estimated variance covariance matrix for the means model $\hat{V} = \text{diag}(\hat{\sigma}_1^2, \hat{\sigma}_2^2, \dots, \hat{\sigma}_d^2)$
- 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 $d \times 1$ vector of sample averages

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

$$\text{Estimated process mean: } \hat{E}[y_i]^{(EWLS)} = x_i' \hat{\beta}^{(EWLS)} \quad (3)$$

$$\text{Estimated process variance: } \hat{\text{Var}}[y_i]^{(OLS)} = \exp(x_i^{*'} \hat{\gamma}^{(OLS)}) \quad (4)$$

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.

Any control factor which influences the expression in Eq. 4 is known as a dispersion factor. Any control factor that does not influence the expression in Eq. 4 but does influence the expression in Eq. 3 is known as an adjustment factor. When both dispersion and adjustment factors are present, the robust design problem can be approached in a two step fashion. Specifically, levels of the dispersion factors are chosen so as to minimize the estimated process variance in Eq. 4 and then the levels of the adjustment factors are chosen so as to bring the estimated process mean in Eq. 3 to a desired level. If only dispersion factors are present and these factors also influence the process mean, the researcher is left with finding the levels of the control factors that yield a desirable trade-off between low variance and a deviation

from the targeted mean. This is often accomplished via minimization of an objective function such as the Squared Error Loss (SEL):

$$SEL = E[y(x) - T]^2 = \{E[y(x)] - T\}^2 + Var[y(x)] \quad (5)$$

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. The SEL approach is also useful when adjustment factors are present but are not strong enough to bring the mean to the targeted value. 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.

Nonparametric approach: Situations may arise in which the user cannot explicitly state parametric forms for the dual model. In these situations, parametric specifications may result in serious bias of the estimated mean and/or variance. To prevent the bias induced by parametric model misspecification, VB and Anderson-Cook and Prewitt (2005) (henceforth referred to as AP) suggest the use of nonparametric regression for estimating the process mean and variance. Expressing the dual model where the mean and variance functions (h and g*, respectively) are assumed to have unknown but smooth forms, researchers have:

$$\text{Model mean : } \bar{y}_i = h(x'_i) + g^{1/2}(x'^*_i) \varepsilon_i$$

$$\text{Variance model: } \ln(s_i^2) = +g^*(x'^*_i) + \eta_i$$

Similar to parametric regression, estimators are linear combinations of the response values \bar{y}_i and (s_i^2) however the weighting schemes in some nonparametric regression methods assign more weight to observations closest to the point of prediction x_0 . The nonparametric fits are more flexible than the parametric fits as they are not confined to the users specified form. This enables the nonparametric approach to more adequately fit processes whose underlying models have more complicated forms than those expressed by the linear models in Eq. 1 and 2. Several fitting techniques have been proposed in the nonparametric regression literature such as kernel regression (Nadaraya, 1964; Watson, 1964; Priestley and Chao, 1972; Gasser and Muller, 1984) local polynomial models (Fan and Gijbels, 1996) spline based smoothers and series-based smoothers (Ruppert *et al.*, 2003). VB first applied nonparametric smoothing in the RPD setting by

using the Gasser-Muller estimator for the dual response problem. AP continued with this idea by using the Nadaraya-Watson estimator and Local Polynomial Regression (LPR) the method used in this research. LPR is a popular class of nonparametric smoothing methods and is particularly appealing in response surface applications due to its robustness to biased estimates at the boundary of the design space. LPR is essentially a Weighted Least Squares (WLS) problem where the weights are given by a kernel function. The polynomial form of the local polynomial fit can be of order one or greater and researchers focus on degree $p = 1$, Local Linear Regression (LLR) in this study.

For the multiple regressor case at point $x_0 = (x_{01}, x_{02}, \dots, x_{0k})$ where prediction is desired researchers define the kernel function as:

$$K(\bar{x}_0 - \bar{x}_i) = \frac{1}{b^k} \prod_{j=1}^k K\left(\frac{\bar{x}_{0j} - \bar{x}_{ij}}{b}\right) \quad (6)$$

Where $\bar{x}_i = (x_{i1}, x_{i2}, \dots, x_{ik})$, $K(\bar{x}_{0j} - \bar{x}_{ij} / b)$ is a univariate kernel function b is the bandwidth. When estimating both the mean and variance nonparametrically a different kernel function may be used for the mean than for the variance since the regressors effecting the mean do not necessarily effect the variance. The choice of kernel function is not crucial to the performance of the estimator (Simonoff, 1996). Thus for convenience researchers will use the simplified Gaussian kernel $K(u) = e^{-u^2}$.

The smoothness of the estimated function is controlled by the bandwidth b . Since, the coding of variables in response surface designs typically involves centering and scaling the units are comparable in all directions. Thus, it is reasonable to use the same bandwidth b , in all dimensions as expressed in Eq. 6. The choice of bandwidth is critical and the literature is rich with bandwidth selection methods (Härdle, 1990; Härdle *et al.*, 2004). Typically, the bandwidth is chosen to minimize some optimality criteria such as MSE. Mays *et al.* (2001) introduce a penalized cross-validation technique PRESS** for choosing an appropriate bandwidth. The approach chooses the bandwidth as the value b that minimizes PRESS** defined as:

$$PRESS^{**} = \frac{PRESS}{d - \text{trace}(H^{(LLR)}) + (d - (k + 1)) \frac{SSE_{max} - SSE_b}{SSE_{max}}}$$

Where SSE_{max} is the largest error sum of squares over all possible bandwidth values, SSE_b is the error sum of squares associated with a particular bandwidth value b , k is the number of regressors and the prediction error sum of squares PRESS is given by:

$$PRESS = \sum_{i=1}^d (y_i - \hat{y}_{i,-i})^2$$

where, $\hat{y}_{i,-i}$ denotes the estimated response obtained by leaving out the i th observation when estimating at location x_i . The LLR smoother matrix $H^{(LLR)}$ is defined as:

$$H^{(LLR)} = \begin{bmatrix} h_1^{(LLR)} \\ h_2^{(LLR)} \\ \vdots \\ h_d^{(LLR)} \end{bmatrix}$$

Where h_i defined in the study. MBS show that PRESS** performs well by guarding against very small and very large bandwidths.

The nonparametric estimate of the dual model is found by first estimating the underlying variance function and then using the estimated variances as weights an Estimated Weighted Local Linear Regression (EWLLR) fit is found for the mean. For more information regarding weighted LLR the reader is referred to Lin and Carroll (2000). Expressions for the fits are provided as:

$$\begin{aligned} \text{Estimated process mean: } \hat{E}(y_0)^{(EWLLR)} &= x_0' \hat{\beta}^{(EWLLR)} = x_0' \\ & (x_0' W_0 X)^{-1} x_0' W_0 \bar{y} = h_0^{(EWLLR)} \bar{y} \end{aligned} \quad (7)$$

$$\begin{aligned} \text{Estimated process variance: } \hat{\text{Var}}(y_0)^{(LLR)} &= \exp(x_0' \hat{\gamma}^{(LLR)}) \\ &= \exp \left[x_0' (x_0' W_0 X)^{-1} x_0' W_0 y^* \right] = \exp(h_0^{(LLR)} y^*) \end{aligned} \quad (8)$$

Regarding notation for the means fit $h_0^{(EWLLR)} = X_0' (X' W_0 X)^{-1} X' W_0$:

$$W_0 = \left\langle \sqrt{h_{0i}^{(KER)}} \right\rangle \hat{V}^{-1} \left\langle \sqrt{h_{0i}^{(KER)}} \right\rangle$$

Where $\left\langle \sqrt{h_{0i}^{(KER)}} \right\rangle$ the diagonal matrix containing the square roots of the kernel weights associated with x_0 . $\left\langle \sqrt{h_{0i}^{(KER)}} \right\rangle = \text{diag} \left(\sqrt{h_{01}^{(KER)}}, \sqrt{h_{02}^{(KER)}}, \dots, \sqrt{h_{0d}^{(KER)}} \right)$ with:

$$h_{0i}^{(KER)} = \frac{K(x_0, \bar{x}_i)}{\sum_{i=1}^d K(x_0, \bar{x}_i)}$$

And \hat{V} is the estimated variance-covariance matrix:

$$\hat{V} = \text{diag}(\hat{\sigma}_1^2, \hat{\sigma}_2^2, \dots, \hat{\sigma}_d^2)$$

Regarding notation for the variance fit:

$$h_0^{(LLR)} = x_0' (x_0' W_0 x_0)^{-1} x_0' W_0$$

and W_0 is the diagonal matrix containing the kernel weights associated with x_0 . Under the assumption of normality of \bar{y} and y^* the estimates of $E[y_0]$ and $\text{Var}[y_0]$ given by Eq. 7 and 8 are the local maximum likelihood estimates of Fan *et al.* (1995).

Similar to the parametric approach to robust design once estimates of the mean and variance functions have been calculated a squared error loss approach will be used for process optimization. Unfortunately, most of the analytic optimization methods suggested for the parametric approach are based on gradient techniques which require continuous functions with derivatives for the estimated mean and variance functions. Since, the mean and variance estimates from nonparametric methods do not result in closed form expressions, these optimization routines are no longer applicable. VB utilize a simplex search based on the AMOEBA algorithm (Vetterling *et al.*, 1992) which does not require the calculation of derivatives however simplex methods tend to be time consuming and often find local as opposed to global optima (Haupt and Haupt, 2004). Therefore, researchers advocate the use of Genetic Algorithms (GA) for optimization.

The GA, originally developed by Holland (1975) has become a popular optimization technique. It is especially useful for optimizing functions that do not have known parametric forms as it does not require derivatives to find the optimal solutions. Instead, the GA is based on the principles of genetics and uses evolutionary concepts such as selection, crossover and mutation to find the optimal solutions. Furthermore, GA uses an intelligent sequential search strategy which enables the user to find global not local solutions more efficiently. Thus, researchers will use the GA for process optimization.

Parametric vs. nonparametric: Parametric and nonparametric approaches to modeling each possess positive and negative attributes. The parametric method is superior if the true, underlying functions can be adequately expressed parametrically and if the user correctly specifies the parametric forms. However, if either of the models is misspecified the estimates may be highly biased and optimal control factor settings may be miscalculated. On the other hand if the user has no idea about the true form of the underlying functions nonparametric methods offer a nice alternative. Nonparametric methods can provide superior fits by capturing structure in the data that a misspecified parametric model cannot. However, nonparametric

methods were originally developed for situations with large sample sizes whereas a main underpinning of RSM is the use of cost efficient experimental designs (i.e., small sample sizes). In small sample settings, nonparametric fitting techniques may fit irregularities in the data too closely thereby creating estimated mean and variance functions that are highly variable. Consequently, optimization may be based on non-reproducible idiosyncrasies in the data.

Experimental design: The Central Composite Design (CCD) is used for experimental plan with three factors, temperature (A), time (B) and liposomes amount (C) on the results of color strength (K/S). The ranges of these factors are shown in Table 1 and details of this design are showed in Table 2.

In Table 2, x_1 - x_3 are the coded variables that represents temperature, time and liposomes amount, respectively and y_i , $i = 1, 2, 3$ denotes the amounts of color strength (K/S).

Five levels of each factor are involved in this design. The coded and natural levels are given by the following:

	-1.6820	-1.0000	0.000	1.000	-1.6820
x_1	70.00	75.00	82.50	90.00	95.00
x_2	20.00	30.00	45.00	60.00	70.00
x_3	0.32	1.00	2.00	3.00	3.68

Table 1: Ranges of factors

Factors	Name	Units	Lower limit	Upper limit
A	Temperature	c	75	90
B	Time	min	30	60
C	Liposomes	mg mL ⁻¹	1	3

Table 2: Central composite design for dyeing of wool with madder

Run number	x_1	x_2	x_3	y_1	y_2	y_3	y	s
1	-1.000	-1.000	-1.000	7/05	7/57	10/30	8.31	1/75
2	1.000	-1.000	-1.000	25/10	22/60	24/18	23.96	1/26
3	-1.000	1.000	-1.000	14/40	13/66	16/46	14.84	1/45
4	1.000	1.000	-1.000	24/80	22/25	24/47	23.94	1/22
5	-1.000	-1.000	1.000	8/27	7/04	9/50	9.27	1/23
6	1.000	-1.000	1.000	21/43	23/75	23/55	22.91	1/29
7	-1.000	1.000	1.000	18/79	16/00	18/63	17.81	1/57
8	1.000	1.000	1.000	21/54	22/77	23/64	22.65	1/06
9	-1.682	0.000	0.000	10.15	10/33	7/48	9.32	1/60
10	1.682	0.000	0.000	23/18	23/75	20/92	22.56	1/43
11	0.000	-1.682	0.000	19/26	16/62	19/41	18.43	1/57
12	0.000	1.682	0.000	23/25	25/19	25/38	24.61	1/18
13	0.000	0.000	-1.682	19/22	16/95	19/67	18.62	1/46
14	0.000	0.000	1.682	21/67	21/60	19/43	20.90	1/27
15	0.000	0.000	0.000	20/00	22/18	19/61	20.60	1/39
16	0.000	0.000	0.000	21/79	19/88	19/43	20.37	1/25
17	0.000	0.000	0.000	20.94	22/28	19/60	20.94	1/34
18	0.000	0.000	0.000	20/06	20/03	22/43	20.84	1/38
19	0.000	0.000	0.000	20/07	22/30	19/72	20.70	1/40
20	0.000	0.000	0.000	19/36	21/19	21/83	20.79	1/28

RESULTS AND DISCUSSION

In order to use parametric approach to analyze the experiments shown in Table 2. Researchers consider a first order model for the log transformed variance model and a second order model for the mean. Table 3 and 4 shows the resulting ANOVA tables for the process variance and mean.

Considering target value 30 (K/S) in SEL objective function and using the estimated mean and variance functions as shown in Table 3 and 4, researchers obtain in parametric approach by GA algorithm the optimal factor settings of A = 95°C, B = 20 min, C = 0.51 mg mL⁻¹ which has an estimated SEL of 14.9 (a predicted response of 26.4 and a predicted process variance of 1.88). As Table 1 shows the computed adjusted R-squared in variance model is low (0.42). Therefore, this model cannot be a proper enough one. This may be reason for using the nonparametric approach in the data of Table 2.

In nonparametric approach, researchers need to specify a three-dimensional kernel function and bandwidth vector. Researchers consider product kernels because of the cuboidal design region and use the same kernel, $K_1(x) = K_2(x) = K_3(x)$ and the same bandwidth $b_1 = b_2 = b_3$ for each factor. Using PRESS**, researchers obtain a bandwidth of 0.31 for both variance and means models. In this approach researchers obtain by GA algorithm and considerin targe t-value 30 (K/S) in SEL objective function the optimal factor setting of A = 95°C, B = 20 min, C = 0.32 mg mL⁻¹ which has an estimated SEL of 4.9 (a predicted response of 28.2 and a predicted

Table 3: ANOVA table for the log transformed variance model

Analysis of variance					
Sources	df	Sum sq.	Mean sq.	F-value	Pr (>F)
x ₁	1	0.137787	0.137787	9.6635	0.006757**
x ₂	1	0.051640	0.051640	3.6217	0.075180
x ₃	1	0.047213	0.047213	3.3112	0.087568
Error	16	0.228135	0.014258	-	-
Parameter estimates					
Variables	Estimate	SE	t-value	Pr (> t)	
(Intercept)	1.42176	0.09736	14.604	1.14e-10***	
x ₁	-0.33607	0.10811	-3.109	0.00676**	
x ₂	-0.20574	0.10811	-1.903	0.07518	
x ₃	-0.19672	0.10811	-1.820	0.08757	

Multiple R²: 0.5091; Adjusted R²: 0.4171; F-statistic: 5.532 on 3 and 16 df; p-value: 0.008439

Table 4: ANOVA table for the mean model

Analysis of variance					
Source	df	Sum sq.	Mean sq.	F-value	Pr (>F)
x ₁	1	140.397	140.397	254.1559	1.944e-08 ***
x ₂	1	21.818	21.818	39.4957	9.088e-05***
x ₃	1	0.668	0.668	1.2086	0.2973671
x ₁ .x ₂	1	15.439	15.439	27.9487	0.0003542 ***
x ₁ .x ₃	1	2.587	2.587	4.6827	0.0557359
x ₂ .x ₃	1	0.094	0.094	0.1695	0.6892641
x ₁ .x ₁	1	30.266	30.266	54.7894	2.310e-05***
x ₂ .x ₂	1	0.199	0.199	0.3597	0.5620303
x ₃ .x ₃	1	1.832	1.832	3.3168	0.0985818
Residuals	10	5.524	0.552		
Parameter estimates					
Variables	Estimate	SE	t value	Pr (> t)	
(Intercept)	-4.733	2.342	-2.021	0.070859	
x ₁	53.441	4.387	12.181	2.54e-07***	
x ₂	14.547	4.355	3.340	0.007487**	
x ₃	10.344	4.353	2.377	0.038841*	
x ₁ .x ₂	-21.065	3.971	-5.305	0.000345***	
x ₁ .x ₃	-8.827	3.970	-2.224	0.050388	
x ₂ .x ₃	1.726	3.952	0.437	0.671567x ₁ .x ₁	
	-22.422	3.005	-7.461	2.16e-05***	
x ₂ .x ₂	1.290	3.004	0.429	0.676780	
x ₃ .x ₃	-5.470	3.003	-1.821	0.098582	

Multiple R²: 0.9748; Adjusted R²: 0.952; F-statistic: 42.9 on 9 and 10 df; p-value: 8.134e-07

process variance of 1.12). The dual model response surface approach to RPD has been shown to study well when the variance of response is not constant over the experimental region and can be successfully modeled using regression methods.

One drawback however is that optimization depends too heavily on the assumption of well estimated models for the process mean and variance and it is often the case that user specified parametric models are not flexible enough to adequately model the process mean and variance. VB and AP suggest the use of nonparametric smoothing when the user is unable to specify the explicit forms for the mean and/or variance functions.

Using the dying process data shown in Table 2 to compare the parametric and nonparametric approaches researchers find that the nonparametric approach performs best in terms of SEL.

CONCLUSION

The optimization based on the nonparametric approach recommends control factor setting which result in the estimated mean being closer to target as well as the smallest estimate of process variance.

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