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Finding Cost-Effective Mixtures Robust to Noise Variables in Mixture-Process Experiments

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Abstract

In mixture experiments with process variables, we consider the case that some of process variables are either uncontrollable or hard to control, which are called noise variables. Given the such mixture experimental data with process variables, first we study how to search for candidate models. Good candidate models are screened by the sequential variables selection method and checking the residual plots for the validity of the model assumption. Two methods, which use numerical optimization methods proposed by Derringer and Suich (1980) and minimization of the weighted expected loss, are proposed to find a cost-effective robust optimal condition in which the performance of the mean as well as the variance of the response for each of the candidate models is well-behaved under the cost restriction of the mixture. The proposed methods are illustrated with the well known fish patties texture example described by Cornell (2002).

Keywords: Robust optimal condition for the several combined models, multiple responses surface methods, weighted expected loss.

1. Introduction

Mixture experiments involve combining ingredients or components of a mixture; subsequently, the response is a function of the proportions of components which is independent of the total amount of a mixture. In many mixture experiments, the product quality characteristics depend on the proportions of the components in the mixture as well as on the condition on the process variables. Process variables are factors in an experiment that are not mixture components but could affect the blending properties of the mixture ingredients. The model for the mixture experiments with process variables is called a combined model. We often use the product model between the canonical polynomial model for a mixture and process variables model as a combined model and then, the product design between the simplex-centroid design and the two level factorial design (or the central composite design) as a combined design.

In mixture experiments with process variables, some of the process variables cannot be controlled during the normal production or are set up by the customer when the customer uses the product. Thus they should be treated as noise variables. Steiner and Hamada (1997) and Myers *et al.* (2009) discussed how to make mixtures robust to noise errors. In practice, there might exist several good candidate models for the given mixture experimental data with process variables. Given such data, we first study how to find good candidate models. Then, we propose a strategy to find a cost-effective robust optimal condition in which the performance of the mean as well as the variance of the response

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for each of the candidate models is well-behaved under the cost restriction of the mixture. Section 2 discusses the model for mixture-process variable experiments with noise variables is discussed. Section 3 reviews the strategy for finding several good candidate models for the given experimental data. Section 4 proposes two methods to find a cost-effective robust optimal condition. The proposed methods are illustrated with the well-known fish patties texture example described by Cornell (2002) in Section 5.

2. Model for Mixture-Process Variable Experiments with Noise Variables

Suppose that there are q mixture components, c controllable process variables and n noise variables. Let x_i represent the proportions of the i^{th} component in the mixture, then

$$x_1 + x_2 + \cdots + x_q = 1, \quad x_i \geq 0, \ i = 1, 2, \ldots, q. \tag{2.1}$$

In addition, we have c controllable process variables $w_j,\ j = 1, \ldots, c$ and n noise variables z_k, $k = 1, \ldots, n$. Those process variables are coded to be $[-1, 1]$. Because of the restriction (2.1), the polynomial model over the experimental region for a mixture is reduced to the canonical polynomial model of the Scheffe type where the second-order model is

$$E(y) = \sum_{i=1}^{q} \beta_i x_i + \sum_{i<j}^{q} \beta_{ij} x_i x_j. \tag{2.2}$$

We consider the starting model as the product model between the mixture model and the process variables model. For example, in the case of the product model between the quadratic canonical model in the mixture variables and a model with both main effects and two-factor interaction in the process variables, the starting combined model can be written as

$$\begin{aligned} E(y) = &\sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q-1}\sum_{i<j}^{q} \beta_{ij} x_i x_j + \sum_{k=1}^{c}\left[\sum_{i=1}^{q} \alpha_{ik} x_i + \sum_{i=1}^{q-1}\sum_{i<j}^{q} \alpha_{ijk} x_i x_j\right] w_k \\ &+ \sum_{k=1}^{n}\left[\sum_{i=1}^{q} \alpha_{i(k)} x_i + \sum_{i=1}^{q-1}\sum_{i<j}^{q} \alpha_{ij(k)} x_i x_j\right] z_k + \sum_{k=1}^{c}\sum_{l=1}^{q}\left[\sum_{i=1}^{q} \gamma_{ikl} x_i + \sum\sum_{i<j} \gamma_{ijkl} x_i x_j\right] w_k z_l \\ &+ \sum\sum_{k<l}\left[\sum_{i=1}^{q} \delta_{ikl} x_i + \sum\sum_{i<j} \delta_{ijkl} x_i x_j\right] w_k w_l + \sum\sum_{k<l}\left[\sum_{i=1}^{q} \lambda_{ikl} x_i + \sum\sum_{i<j} \lambda_{ijkl} x_i x_j\right] z_k z_l. \end{aligned} \tag{2.3}$$

If only terms up to the cubic order interaction effects between mixture variables and process variables are included and the quartic order interaction effects are disregarded in the product model, the combined model is given as follows:

$$\begin{aligned} E(y) = &\sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q-1}\sum_{i<j}^{q} \beta_{ij} x_i x_j + \sum_{k=1}^{c}\left[\sum_{i=1}^{q} \alpha_{ik} x_i + \sum_{i=1}^{q-1}\sum_{i<j}^{q} \alpha_{ijk} x_i x_j\right] w_k \\ &+ \sum_{k=1}^{n}\left[\sum_{i=1}^{q} \alpha_{i(k)} x_i + \sum_{i=1}^{q-1}\sum_{i<j}^{q} \alpha_{ij(k)} x_i x_j\right] z_k + \sum_{k=1}^{n}\sum_{l=1}^{c}\left[\sum_{i=1}^{q} \gamma_{ikl} x_i\right] w_l z_k \\ &+ \sum\sum_{k<l}\left[\sum_{i=1}^{q} \delta_{ikl} x_i\right] w_k w_l + \sum\sum_{k<l}\left[\sum_{i=1}^{q} \lambda_{ikl} x_i\right] z_k z_l \end{aligned} \tag{2.4}$$

A candidate model for the proper model could be a subset model of the starting model whose terms are a subset of those in the starting model (2.3) or model (2.4).

It is initially assumed that noise variables are centered to have means of zeros and mutually independent. We derive models for both the mean response and its variance. The variance model is directly related to the slope in the direction of the noise variables. For the combined model given in (2.4), the mean response with respect to noise variables is

$$\begin{aligned} E_Z(Y) = &\sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q-1} \sum_{i<j}^{q} \beta_{ij} x_i x_j + \sum_{k=1}^{c} \left[\sum_{i=1}^{q} \alpha_{ik} x_i + \sum_{i=1}^{q-1} \sum_{i<j}^{q} \alpha_{ijk} x_i x_j \right] w_k \\ &+ \sum_{k=1}^{c-1} \sum_{l>k} \left[\sum_{i=1}^{q} \delta_{ikl} x_i \right] w_k w_l \end{aligned} \tag{2.5}$$

and the variance is

$$\begin{aligned} \mathrm{Var}_Z(Y) = &\sum_{k=1}^{n} \left[\sum_{i=1}^{q} \alpha_{i(k)} x_i + \sum_{i=1}^{q-1} \sum_{i<j} \alpha_{ij(k)} x_i x_j + \sum_{l=1}^{c} \left[\sum_{i=1}^{q} \gamma_{ikl} x_i \right] w_l \right]^2 \sigma_{z_k}^2 \\ &+ \sum_{k<l} \sum \left[\sum_{i=1}^{q} \lambda_{ikl} x_i \right]^2 \sigma_{z_k}^2 \sigma_{z_l}^2 + \sigma^2. \end{aligned} \tag{2.6}$$

The propagation of error (POE) is the estimate of standard deviation of the transmitted variability in the response, $\widehat{\mathrm{var}(Y)}^{1/2}$.

3. Finding Proper Combined Models

To find proper combined models which explain the experimental data well, we first find the reasonable starting model, and then proper models whose terms are a subset of those in the starting model. In order to find reasonable starting models, we construct a combined model mixture process fit summary table which is calculated based on the partitioning of the sequential regression sums of squares. We check the p-value of mixture order and process order and then, find the highest order whose p-values are less than 0.10, which determine the starting product model. An alternative method is to search for the product model whose adj-R^2 is the largest. For the given starting model, we use the all possible hierarchical subset regression search with adj-R^2 criterion, backward elimination method and the stepwise method to find several candidates for the proper model. Here the model reduction is done by term by term in order to respect the hierarchy of model terms. By inspecting studentized residual plots, we check the validity of several candidate models to screen ideal candidate models.

4. Cost Effective Parameter Design for Several Candidate Models

Suppose that several good candidate models are found for given mixture experimental data with process variables. Our goal is to find levels of the cost effective mixture components and controllable process variables that are robust to variations in noise variables while simultaneously providing an acceptable mean response for each of the candidate models. As a practical approach to find a cost-effective robust optimal condition, we propose to use multiple response optimization methods by assigning the model for the new response y_j to the j^{th} candidate model, and then, the cost of the mixture to be a linear function of the cost of the components of mixture. The first approach is to use numerical optimization methods proposed by Derringer and Suich (1980). Their procedure make use of desirability functions and convert the predicted response and POE for each candidate model into an individual desirability function that varies over [0, 1]. The geometrical mean of the linear desirability values is then maximized to find a robust optimal condition with cost restriction. The second approach is to assign weights to each candidate model and then, find a condition at which the weighted expected loss with respect to noise variables is minimized.

5. Case Study of Fish Patties Texture Example

We consider the fish patties texture example in Cornell (2002). In this example there are three mixture components, namely mullet x_1, sheepshead x_2 and croaker x_3 and three process variables, deep frying time w_1(25 and 40 seconds), oven temperatures z_1(375 and 425 degrees F) and oven baking time z_2(25 and 40 minutes). The response variable Y is the texture of patties which is measured by a compression test reading in grams of force required to initially puncture the surface of a patty. It is desirable that the average texture lies between 2 and 3.5 and the target value for the mean response is 2.75. It is assumed that two of the process variables z_1 and z_2 are noise variables since the fish patties are deep fried by the manufacturer and sold frozen, with the final baking of fish patties being done by customers. Thus, in this example $q = 3$, $c = 1$ and $n = 2$. We consider experimental data given in Cornell (2002) where the experimental design is the product design of a simplex-centroid in mixture variables and a 2^3 factorial in the process variables.

By checking the adj-R^2 value of mixture order and process order in the combined model mixture process fit summary table, the product model between the quadratic model in the mixture variables and a model with both main effects and two-factor interaction in the process variables is chosen as the starting model. Using the all possible hierarchical subset regression search with adj-R^2 criterion, we obtain the model with 31 terms, which is reduced to the following model, cand1 by applying a backward elimination method with the level of significance being 0.1;

$$\begin{aligned}\widehat{Y_1}(x,w,z) = {} & 2.86x_1 + 1.07x_2 + 2.00x_3 - 0.97x_1x_2 - 0.83x_1x_3 + 0.36x_2x_3 \\ & - 0.076x_1w_1 - 0.087x_2w_1 - 7.830E - 003x_3w_1 - 0.016x_1x_3w_1 \\ & + 0.49x_1z_1 + 0.17x_2z_1 + 0.24x_3z_1 - 0.80x_1x_2z_1 - 0.53x_1x_3z_1 \\ & + 0.71x_1z_2 + 0.26x_2z_2 + 0.40x_3z_2 - 0.66x_1x_2z_2 - 0.12x_1x_3z_2 \\ & - 0.058x_1w_1z_1 + 0.075x_1w_1z_2 - 0.054x_2w_1z_1 + 0.12x_3w_1z_1 - 0.034x_3w_1z_2 \\ & - 0.34x_1x_3w_1z_2 + 0.065x_1z_1z_2.\end{aligned}$$

We get the same model by applying a backward elimination method and the stepwise method to the starting model. If we disregard the quartic order interaction effects from the cand1 model and then, apply the backward elimination method to the resulting model, we obtain the following cand2 model;

$$\begin{aligned}\widehat{Y_2}(x,w,z) = {} & 2.86x_1 + 1.07x_2 + 2.00x_3 - 0.97x_1x_2 - 0.83x_1x_3 + 0.36x_2x_3 \\ & - 0.078x_1w_1 - 0.087x_2w_1 - 9.190E - 003x_3w_1 \\ & + 0.49x_1z_1 + 0.17x_2z_1 + 0.24x_3z_1 - 0.80x_1x_2z_1 - 0.53x_1x_3z_1 \\ & + 0.70x_1z_2 + 0.26x_2z_2 + 0.39x_3z_2 - 0.66x_1x_2z_2 \\ & - 0.068x_1w_1z_1 + 0.11x_3w_1z_1 + 0.065x_1z_1z_2.\end{aligned}$$

By checking the sequential p-value of mixture order and process order in the combined model mixture process fit summary table, the product model between the quadratic model in the mixture variables

Table 1: The performance of cand1, cand2, cand3 and GBM model

Model	adj-R^2	pred-R^2	Number of terms p
Cand1	.9769	.9559	27
Cand2	.9733	.9510	21
Cand3	.9645	.9477	16
GBM	.9505	.9308	14

and linear model in the process variables is chosen as the starting model. Using the all possible hierarchical subset regression search with adj-R^2 criterion, we obtain the following model:

$$\begin{aligned}\widehat{Y_3}(x,w,z) = {} & 2.86x_1 + 1.11x_2 + 2.03x_3 - 0.99x_1x_2 - 0.85x_1x_3 - 0.079x_1w_1 - 0.088x_2w_1 \\ & + 0.49x_1z_1 + 0.17x_2z_1 + 0.24x_3z_1 - 0.80x_1x_2z_1 - 0.53x_1x_3z_1 \\ & + 0.70x_1z_2 + 0.26x_2z_2 + 0.39x_3z_2 - 0.66x_1x_2z_2.\end{aligned}$$

The residual plots of cand1, cand2 and cand3 model are provided in Figure 1. For each of the candidate model the normal probability plot of the studentized residuals follows the linear pattern and the residual plot against the predicted values shows that the studentized residuals fall within a verified horizontal band centered around zero.

The example was also analyzed in Goldfarb *et al.* (2003). Their model is adapted to include x_3w_1 term to respect the hierarchy of model terms and the resulting model is called GBM. Table 1 summarizes the performance of cand1, cand2, cand3 and GBM model. Those three candidate models are superior to the GBM model with respect to adj-R^2 and pred-R^2 criterion.

Now we consider the proper model to be cand2 model. Using equations (2.5) and (2.6), we obtain the mean predicted response and the estimate of variance with respect to noise variables as

$$\begin{aligned}\widehat{E(Y_2)} = {} & 2.86x_1 + 1.07x_2 + 2.00x_3 - 0.97x_1x_2 - 0.83x_1x_3 + 0.36x_2x_3 \\ & - 0.078x_1w_1 - 0.087x_2w_1 - 9.190E - 003x_3w_1\end{aligned}$$

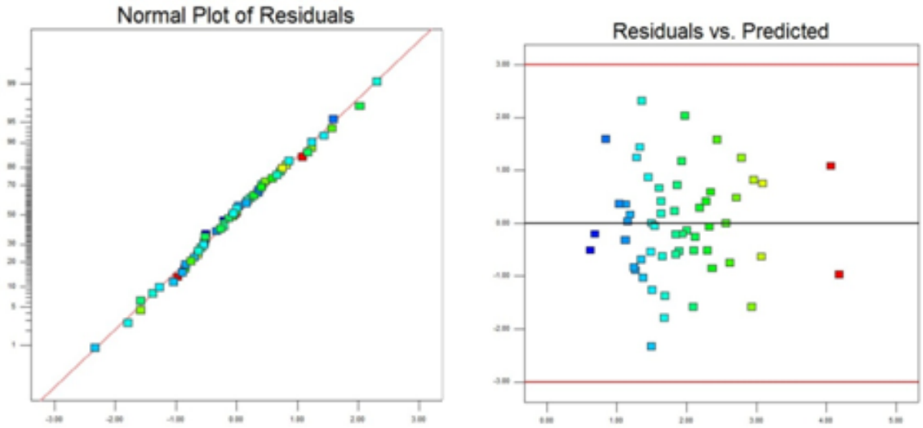
and

$$\begin{aligned}\widehat{\mathrm{Var}(Y_2)} = {} & (0.49x_1 + 0.17x_2 + 0.24x_3 - 0.80x_1x_2 - 0.53x_1x_3 - 0.068x_1w_1 + 0.11x_3w_1)^2\sigma^2_{z_1} \\ & + (0.70x_1 + 0.26x_2 + 0.39x_3 - 0.66x_1x_2)^2\sigma^2_{z_2} + (0.065x_1)^2\sigma^2_{z_1}\sigma^2_{z_2} + \widehat{\sigma^2}\end{aligned}$$

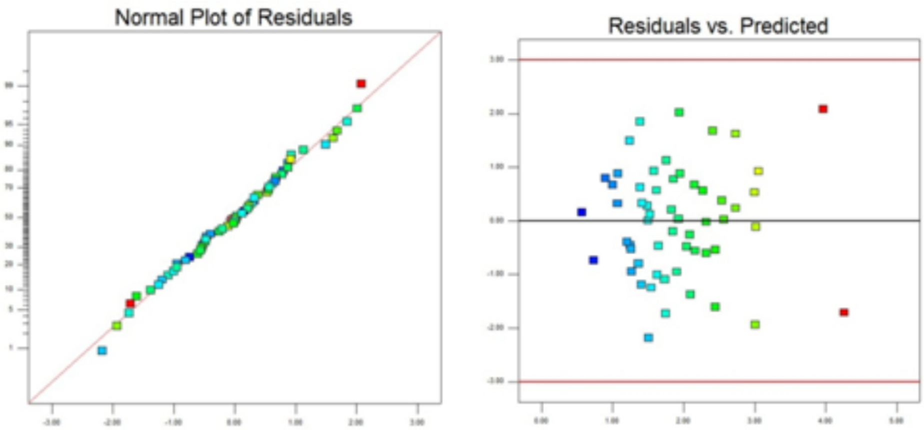
and then, $\widehat{\mathrm{sd}}(Y_2) = \widehat{\mathrm{var}(Y_2)}^{1/2}$. Similarly we get $\widehat{E(Y_1)}$, $\widehat{\mathrm{sd}}(Y_1)$, $\widehat{E(Y_3)}$ and $\widehat{\mathrm{sd}}(Y_3)$. It is known that unit price of mullet, sheepshead and croaker is ₩641, ₩892 and ₩768, respectively. The cost constraint is that the price of the mixture is less than 710. Thus the cost constraint mixture space is given as follows: $641x_1 + 892x_2 + 768x_3 \leq 710$.

Method 1. Simultaneous optimization proposed by Derringer and Suich.

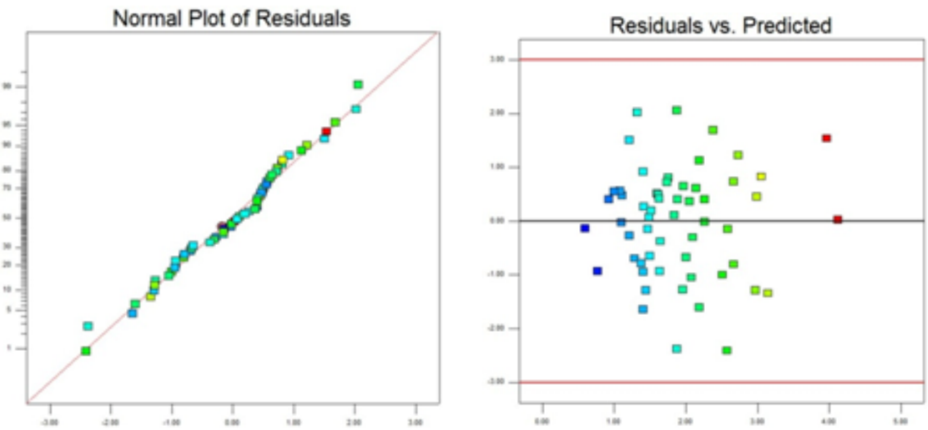
We assume that $\sqrt{\sigma^2_{z_1}} = 1/3$, $\sqrt{\sigma^2_{z_2}} = 1/3$ and $\widehat{\sigma^2}$ is the residual mean square obtained by fitting the response model. The range of the standard deviation over the design space of the mixture components and the controllable process variable is about (.15, .35) for the cand1 and cand2 model and (.17, .32) for the cand3 model. The acceptable range for the standard deviation could be taken as



(a) cand1 model



(b) cand2 model



(c) cand3 model

Figure 1: *Residual Plots*

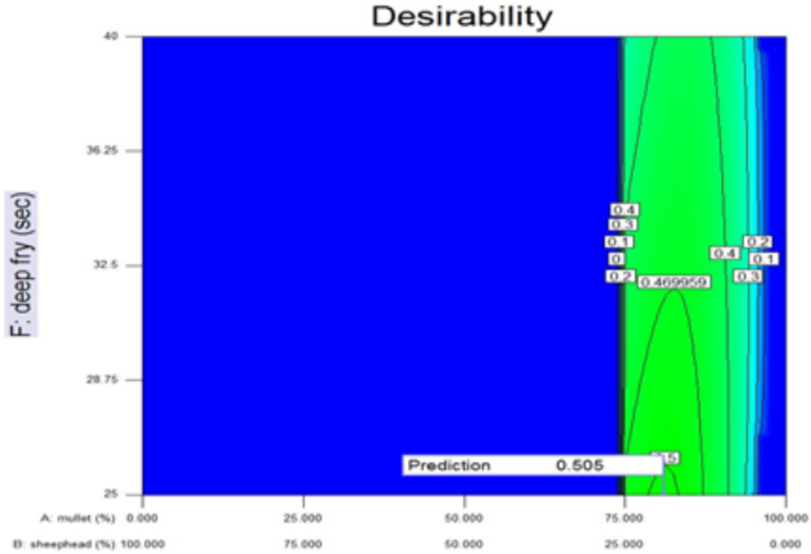


Figure 2: *Contour plots of the overall desirability D.*

(.15, .30). The individual linear desirability for the mean response is defined as

$$d = \begin{cases} 0, & y < 2.0, \\ \dfrac{y - 2.0}{3.5 - 2.0}, & 2.0 \le y \le 2.75, \\ \dfrac{3.5 - y}{3.5 - 2.0}, & 2.75 \le y \le 3.5, \\ 0, & y > 3.5 \end{cases}$$

and that for the standard deviation is defined as

$$d = \begin{cases} 1, & \text{sd} < 0.15, \\ \dfrac{0.3 - \text{sd}}{0.3 - 0.15}, & 0.15 \le \text{sd} \le 0.3, \\ 0, & \text{sd} > 0.3. \end{cases}$$

The routine fmincon in MATLAB was used to get a cost-effective robust optimal condition by maximizing the overall desirability D which is defined as a geometric mean of individual desirability of $\widehat{E(Y_j)}$, $\widehat{\text{sd}}(Y_j)$, $j = 1, 2, 3$ under the product space of the cost constraint mixture space and the space of controllable process variable w_1. A cost-effective robust optimal condition was found to be at $x_1 = .810$, $x_2 = .190$, $x_3 = 0$, $w_1 = -1$(time = 25 seconds) where the overall desirability $D = .505$, $\widehat{Y_1} = 2.452$, $\widehat{\text{sd}}(Y_1) = 0.225$, $\widehat{Y_2} = 2.453$, $\widehat{\text{sd}}(Y_2) = 0.241$, $\widehat{Y_3} = 2.456$, $\widehat{\text{sd}}(Y_3) = 0.243$.

Figure 2 present contour plots of the overall desirability D which helps to understand how to get robust optimal conditions graphically. Method 1 could be implemented easily using Design Expert 8.0

Method 2. Minimizing the weighted expected loss.

When the response has a target value 2.75 and a quadratic loss function is used, the expected loss is

$$E_Z(L) = E_Z(Y - 2.75)^2$$
$$= (E_Z Y - 2.75)^2 + \mathrm{Var}_z(Y).$$

A uniform weight is assigned to each of the candidate models and then the weighted expected loss is minimized in order to find a robust optimal condition whose performance is simultaneously good for each of the candidate model. The weighted expected loss is estimated by

$$\widehat{E_Z}(L) = \frac{1}{3}\left[\sum_{1}^{3}\left(\widehat{Y_i}(x, w) - 2.75\right)^2 + \widehat{\mathrm{Var}}(Y_i(x, w))\right].$$

The resulting constrained minimization problem is to the minimize $\widehat{E_Z}(L)$ subject to the cost constraint mixture space $641x_1 + 892x_2 + 768x_3 \leq 710$ and the space of controllable process variable $-1 \leq w_1 \leq 1$. The routine fmincon in MATLAB provides a cost-effective robust optimal condition by solving the above constrained minimization problem. A cost-effective robust optimal condition was found at $x_1 = .912$, $x_2 = .088$, $x_3 = 0$, $w_1 = -1$ where $\widehat{E_Z}(L) = .0753$, $\widehat{y_1} = 2.706$, $\widehat{\mathrm{sd}}(Y_1) = 0.265$, $\widehat{y_2} = 2.707$, $\widehat{\mathrm{sd}}(Y_2) = 0.277$, $\widehat{y_3} = 2.708$, $\widehat{\mathrm{sd}}(Y_3) = 0.279$.

The difference between two methods is that the former uses the scaled mean response and the scaled standard deviation by defining the desirability but the latter uses original values in the objective function, which end up with a different robust optimal condition.

6. Concluding Remarks

Given mixture experimental data with process variables where some of the process variables are noise variables, there might exist several good candidate models in practice. Two methods, which use numerical optimization methods proposed by Derringer and Suich (1980) and minimization of the weighted expected loss, are proposed to find a cost-effective robust optimal condition on mixture components and controllable process variables and illustrated with the fish patties texture example described by Cornell (2002). Depending on the preference of the scaling of the major terms in the objective function, one of two methods could be used.

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