Making Mixtures Robust to Noise and Mixing Measurement Errors

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Mixture experiments involve the mixing or blending of two or more ingredients to form an end product. Typically, the quality of the end product is a function of the relative proportions of the ingredients and other extraneous process factors such as heat or time. When some of the process variables are either uncontrollable or difficult to control (i.e., noise variables) the goal of a mixture experiment should be to find the mixture amounts and process settings that lead to a product of high quality that is also robust to the noise. Due to the nature of mixture experiments this leads to a constrained optimization problem. This article discusses setting up an appropriate objective function and provides techniques for determining the robust mixture proportions. It is also shown that under certain conditions mixing measurement errors can be handled in the same way.

Introduction

MANY products involve mixing various components. Paint, plastic, bread, and fruit punch are good examples. In such circumstances it is of interest to determine what component proportions lead to desirable results in terms of some quality characteristics such as yield or texture. Let X_i, $i = 1, 2, \ldots, m$ represent the proportions of the m components, where $\sum_{i=1}^{m} X_i = 1$, and let Y represent the output quality characteristic of interest. In this case, due to the constraint on the proportions, the feasible region of mixtures is a simplex (e.g. a triangle for three components and a tetrahedron for four components).

The goal of a mixture experiment is find a model for the response Y in terms of the mixture proportions. Scheffé (1958) developed canonical polynomials of various orders to model the mixture response. His first-degree and second-degree models are given below:

$$Y = \sum_{i=1}^{m} \beta_i X_i + \epsilon$$

$$Y = \sum_{i=1}^{m} \beta_i X_i + \sum\sum_{i<k} \beta_{ik} X_i X_k + \epsilon. \qquad (1)$$

The error term ϵ is assumed to be $N(0, \sigma^2)$ and independent of the mixture variables. Cubic and special cubic models have also been determined. See Cornell (1990) for more information regarding these models and mixture experiments in general. The models (1) do not contain intercept terms (β_0) and squared terms ($\beta_{ii} X_i^2$); using the constraint that the sum of the X_is equals unity, models containing such terms can always be reduced to those given in (1).

In many mixture problems there are also process variables. A process variable is a factor in a experiment, other than the mixture variables, such as heat, that may influence the quality of the end product. The addition of process factors (z_j, $j = 1, \ldots, n + p$) to the models (1) is fairly straightforward (Cornell (1990)). The full second-degree model in mixture variables and process variables is given by (2).

$$Y = \sum_{i=1}^{m} \beta_i X_i + \sum\sum_{i<k}^{m} \beta_{ik} X_i X_k$$

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$$+ \sum_{j=1}^{n+p} z_j \left(\sum_{i=1}^{m} \alpha_{i(j)} X_i + \sum \sum_{i<k} \alpha_{ik(j)} X_i X_k \right) \quad (2)$$
$$+ \sum \sum_{j \le l}^{n+p} z_j z_l \left(\sum_{i=1}^{m} \gamma_{i(jl)} X_i + \sum \sum_{i<k}^{m} \gamma_{ik(jl)} X_i X_k \right)$$
$$+ \epsilon.$$

Given a model like (1) or (2), an appropriate experimental design (Cornell (1990)) and some experimental results, regression methods are used to estimate the model parameters (β, α, γ). The fitted response surface shows the tradeoffs involved with various mixture levels. The goal in the traditional analysis of a mixture experiment is to determine the mixture proportions and process settings that yield the best response. The best response could be, for example, the maximum yield, or a target texture.

In many mixture problems some process variables should be treated as noise variables since they are either uncontrollable or difficult to control during regular production or when the customer uses the product. In addition, mixing measurement errors may be present that result in mixture proportions that are different than the intended proportions. Mixing measurement errors can arise due to errors in measuring the mixture component amounts (for example, when the product is mixed by the customer). In the presence of noise variables and/or mixing measurement errors the objective of the analysis of the experiment should change. In the philosophy of Taguchi's parameter design (see, e.g., Taguchi and Wu (1980) and Ross (1988)) rather than determine the mixture that yields the best response, it is desirable to determine the mixture proportions and process settings that yield a high quality product that is also relatively unaffected by the inherent variability in the noise variables and the actual mixture proportions. In other words, the objective becomes one of finding a mixture that is robust to changes in the noise factors and/or mixing measurement errors.

This article is organized in the following manner. First, methods for determining mixture proportions robust to noise factors are discussed. The next section turns to the effect of mixing measurement errors, and shows that assuming no error during the experiment, mixing measurement error can be handled in a similar manner as noise factors. Finally, these mixture experiment analysis techniques are illustrated through a re-analysis of the fish patties texture data given in Cornell (1990). The example uses the original data, but assumes that two of the original process variables are noise factors and introduces the possibility of mixing measurement error.

Mixture Experiments and Noise Factors

When designing a robust product there are two goals that may be competing against one another. An optimal or near optimal response (maximum, minimum, or target) is desired, along with little variation in the response due to variation in the noise factors. This sort of multiple objective is common in response surface problems. Myers and Montgomery (1995) suggest three possible approaches to handle multiple objectives: graphical optimization, mathematical programming, and simultaneous optimization. To design robust mixtures, all three approaches are feasible, although either graphical optimization or simultaneous optimization are probably most appropriate. The graphical approach involves building a model for both the average response and the variability in the response and using overlaid contour plots to determine good choices for the mixture proportions. Clearly, this approach is only feasible when the number of mixture and process variables is small, say no greater than three or four of each. Simultaneous optimization is a very generally applicable method that involves combining the two objectives together into one objective using either explicit or implicit weights. Many different methods of doing this have been proposed. Using a loss function is a popular approach (Ross (1988)). In the loss function approach to robust design, the goal is to minimize the expected loss that arises due to the uncontrollable variability in the noise variables. The appropriate form of the loss function depends on many factors including the nature of the response Y. When the response Y has a target value T, a quadratic loss function is frequently used. A quadratic loss function is appealing since the expected value of the quadratic loss $L = (Y - T)^2$ is the mean squared error (MSE) of the response Y, (MSE(Y)):

$$E_{\mathbf{z}}(L) = \text{MSE}(Y)$$
$$= (E_{\mathbf{z}}(Y) - T)^2 + \text{Var}_{\mathbf{z}}(Y). \quad (3)$$

Note that the expected value and variance of the response, denoted $E_{\mathbf{z}}(Y)$ and $\text{Var}_{\mathbf{z}}(Y)$ respectively, are determined based on the variability in the noise factors that occurs during regular production or when the customer uses the product.

The best choice for the loss function is not obvious in most cases, and alternatives are possible.

For the smaller-the-better case the response could be rescaled so that $Y > 0$ and the loss function defined as $L = Y^2$, whereas for the larger-the-better case the loss functions $L = 1/Y^2$ or $L = \exp(-Y)$ are common. Alternatives, such as Expressions (4) and (5) for the smaller-the-better and larger-the-better cases respectively have been suggested by Myers and Montgomery (1995) and are easier to use.

$$E_{\mathbf{z}}(L) = E_{\mathbf{z}}(Y) + 2\sqrt{\mathrm{Var}_{\mathbf{z}}(Y)} \quad (4)$$

$$E_{\mathbf{z}}(L) = 2\sqrt{\mathrm{Var}_{\mathbf{z}}(Y)} - E_{\mathbf{z}}(Y). \quad (5)$$

A number of different approaches to estimate the expected loss $E_{\mathbf{z}}(L)$ or another measure of robustness have been proposed. Taguchi and Wu suggest running an experiment via the inner and outer array technique (Taguchi and Wu (1980)). The inner and outer array method involves running an experiment for all combinations of control (mixture and process) and noise levels of interest. However, as pointed out by Shoemaker, Tsui, and Wu (1991), the inner-outer array methodology is often inefficient, since it requires many trials and provides estimates of many higher-order terms that are very unlikely to have any significant effect on the solution. An alternative is to combine the control and noise variables in a single array and to work directly with the resulting response surface to approximate a prediction model for the loss or other joint measure of robustness (see Welch, Yu, Kang, and Sacks (1990)). Note both techniques assume that during the experiment the noise factors are controllable and can be set to the desired levels. An alternative when the noise factors are always uncontrollable but measurable is to use an observational study.

For mixture problems we can estimate the expected loss, $E_{\mathbf{z}}(L)$ given by (3), (4), (5) or another loss function, from a fitted model such as (2) using the Welch et al. (1990) approach. To determine robust mixture proportion settings we wish to minimize the expected loss subject to the constraint on the mixture proportions $\sum_{i=1}^{m} X_i = 1$, and any other application specific constraints. In all mixture problems, one of the mixture variables can always be eliminated through the constraint equation $X_m = 1 - \sum_{i=1}^{m-1} X_i$. Also, without loss of generality the process/noise variables can all be rescaled so that they range between -1 and $+1$. Let $\mathbf{X} = (X_1, X_2, \ldots, X_{m-1})$ and $\mathbf{z} = (z_1, \ldots, z_{n+p})$. Assume that the first n process variables are noise factors, whereas the remaining p variables are controllable process variables. The resulting constrained minimization problem can be written as:

$$\begin{aligned} &\text{minimize } E_{\mathbf{z}}(L(\mathbf{X}, \mathbf{z})) \\ &\text{subject to } g_q(\mathbf{X}, \mathbf{z}) \le 0 \quad \text{for } q = 1, \ldots, c, \end{aligned} \quad (6)$$

where $E_{\mathbf{z}}(L(\mathbf{X}, \mathbf{z}))$ is the expected loss function with the expectation taken over the n noise variables in $\mathbf{z}$, and the constraints for the standard mixture problem are:

$$\begin{aligned} g_1(\mathbf{X}) &= -1 + \sum_{i=1}^{m-1} X_i \\ g_{i+1}(\mathbf{X}) &= -X_i \qquad \text{for } i = 1, \ldots, m-1 \\ g_{j+m}(\mathbf{z}) &= z_j - 1 \end{aligned}$$

and

$$g_{j+m+p}(\mathbf{z}) = -z_j - 1 \qquad \text{for } j = n+1, \ldots, n+p,$$

plus any additional constraints specific to the application. Additional constraints on the mixture proportions and/or the process variables may arise, for example, due to cost considerations, physical constraints, or prior experience with the process.

A number of standard optimization techniques are available to solve this constrained nonlinear optimization problem (see Luenberger (1989)). For example, direct application of the popular generalized reduced gradient (GRG) method is feasible. A more efficient approach, in this case due to the linear constraints, utilizes the Karush-Kuhn-Tucker (KKT) conditions (Luenberger (1989)). The KKT conditions use Lagrange multipliers and stipulate that a solution X^*, Z^* to (6) must satisfy:

$$\begin{aligned} &\nabla E_{\mathbf{z}}(L(\mathbf{X}^*, \mathbf{z}^*)) + \sum_{q=1}^{c} \lambda_q^* \nabla g_q(\mathbf{X}^*, \mathbf{z}^*) = 0 \\ &\lambda_q^* g_q(\mathbf{X}^*, \mathbf{z}^*) = 0 \\ &\lambda_q^* \ge 0 \quad \text{for } q = 1, \ldots, c, \end{aligned} \quad (7)$$

where ∇ is the gradient operator.

Solving the above problem is accomplished by using a quadratic approximation to the Lagrangian function $E(L) + \sum_{q=1}^{c} \lambda_q^* g_q$, and iteratively improving the solution. We used the routine "constr" in the Optimization toolbox of MATLAB®. Note that c equals the number of constraints given in (6). Unfortunately, solutions to (6) are not guaranteed to converge to the global optimal unless $E_{\mathbf{z}}(L(\mathbf{X}, \mathbf{z}))$ and all $g_q(\mathbf{X}, \mathbf{z})$s are convex. All the $g_q(\mathbf{X}, \mathbf{z})$ constraints of the standard robust mixture problem are linear and thus convex, but $E_{\mathbf{z}}(L(\mathbf{X}, \mathbf{z}))$ is nonlinear and not convex in general. As a result, a number of different starting positions should be tried.

To derive an expression for $E_{\mathbf{z}}(L(\mathbf{X}, \mathbf{z}))$ let the mean and variance of the noise factors in the process equal $E(z_j) = \mu_j$ and $\text{Var}(z_j) = \sigma_j^2$, $j = 1, \ldots, n$, respectively. Note that μ_j and σ_j^2 represent the mean and variance of the noise factor present during regular operation of the process, which is not necessarily the same as the mean and variance of the noise factors in the experiment. Then, from (2), it is possible to derive closed form expressions for the expected value and variance of Y. For example, assuming $\mu_1 = \mu_2 = 0$, gives equations (8) and (9).

$$E_{\mathbf{z}}(Y) = \sum_{i=1}^{m} \beta_i X_i + \sum_{i<k} \beta_{ik} X_i X_k, \tag{8}$$

and

$$\begin{aligned}\text{Var}_{\mathbf{z}}(Y) &= \sum_{j=1}^{n} \sigma_j^2 \left(\sum_{i=1}^{m} \alpha_{i(j)} X_i + \sum_{i<k} \alpha_{ik(j)} X_i X_k \right)^2 \\ &+ \sum_{j<l} \sigma_j^2 \sigma_l^2 \left(\sum_{i=1}^{m} \gamma_{i(jl)} X_i + \sum_{i<k} \gamma_{ik(jl)} X_i X_k \right)^2 \\ &+ \sum_{j=1}^{n} 2\sigma_j^2 \left(\sum_{i=1}^{m} \gamma_{i(jj)} X_i + \sum_{i<k} \gamma_{ik(jj)} X_i X_k \right)^2 . \end{aligned} \tag{9}$$

Similar expressions for the general case are long, but easily obtained. Using expressions for $E_{\mathbf{z}}(Y)$ and $\text{Var}_{\mathbf{z}}(Y)$, like (8) and (9), an explicit expression for the expected loss given by (3), (4), or (5) can be written which then specifies the minimization problem (6) to be solved.

Generally, the optimization variables in (6) are the m-1 independent mixture proportions X_1, X_2, $\ldots$, X_{m-1}, and the levels of the p process variables $z_{n+1}, \ldots, z_{n+p}$. However, in some circumstances, the means, or some subset of the means, of the noise factors $\mu_1, \ldots, \mu_n$ are also controllable, leaving the variance of the noise as uncontrollable. In this situation, the optimization problem given in (6) can be adapted by adding constraints that keep the means of the noise factors in the range -1 to $+1$, and by allowing the controllable means to be optimization variables.

Mixture Experiments and Mixing Measurement Errors

In many applications, creating mixtures involves some mixing measurement error. We define any error that yields actual mixture proportions that are different than the desired proportions as a mixing measurement error. Mixing measurement errors can arise through imprecise measurement of the component amounts or simple carelessness. In this article it is assumed that during regular production, or when the customer mixes the components, some mixing error may occur, but negligible mixing error occurs during the experiment. Under these conditions, the response model (2) derived from the experimental results is unaffected by the mixing error. This scenario is realistic when experiments are performed with greater care than is feasible during regular production or when the customer mixes the product. Assuming negligible errors during the experiment, the effect of mixing measurement error is similar to the effect of noise factors. In both cases our goal is to determine which mixture proportions are robust to the uncontrollable variability, be it due to noise, or due to mixing errors in actual production.

Two types of measurement errors in the component amounts are considered in this article. In engineering metrology (Sirohi and Radha-Krishna (1980, p. 30)) measurement errors are specified as either relative (i.e., proportional to component amounts) or absolute in size. Let A_i represent the desired amount of component i used in the mixture. Then, ideally the mixture proportions that drive the response Y are $X_i = A_i / \sum_{j=1}^{m} A_j$ for $i = 1, 2, \ldots, m$. Using this notation, relative errors result in actual component amounts of the form $A_i(1 + e_i)$, whereas absolute errors yield actual component amounts of the form $A_i + e_i$, where e_i equals the error made in the mixture amount for component i. Relative or absolute measurement errors in the component amounts yield mixing measurement error in the actual component proportions as given by equation (10) and equation (11) respectively,

$$X_i(\text{rel}) = \frac{A_i(1 + e_i)}{\sum_{j=1}^{m} A_j(1 + e_j)}, \quad \text{for } i = 1, \ldots, m \tag{10}$$

$$X_i(\text{abs}) = \frac{(A_i + e_i)}{\sum_{j=1}^{m} (A_j + e_j)}, \quad \text{for } i = 1, \ldots, m. \tag{11}$$

As illustrated by expressions (10) and (11) for both relative and absolute measurement error, errors in any one component amount, or a combination of component amounts, leads to errors in the component proportions for all mixture variables with non-zero proportions. Thus measurement error in any one or more component amounts yields a correlated

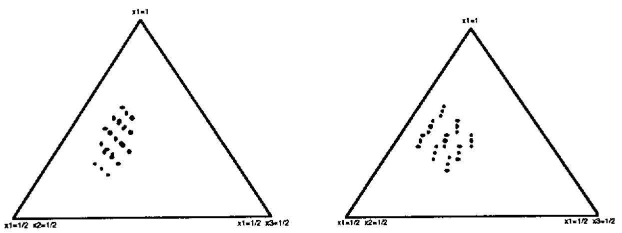

FIGURE 1. Mixing Measurement Error Plots. a) Relative Errors (err = 0.2) and b) Absolute Errors (err = 0.05). Both Centered at $(X_1, X_2, X_3) = (0.7, 0.2, 0.1)$.

mixing measurement error structure for all component proportions. As an example, Figure 1 shows the pattern of actual component proportions resulting from relative and absolute measurement errors in the case of three mixture variables. The 27 points signify the actual component proportions that arise when all combinations of mixing errors $e_i = -\text{err}$, 0, $+\text{err}$ are considered for all three mixture components and the desired component amounts are $A = (0.7, 0.2, 0.1)$. Note that in Figure 1 only the upper quarter of the feasible region is shown to aid the visual display.

For relative measurement errors, expression (10) is appropriate for all mixture proportions. However, for realism, the absolute measurement error model (11), must be adjusted when some component proportions are close to zero. In this article it is assumed that no measurement error is possible for components that have recommended amounts equal to zero. In other words, if a component is absent from the desired mixture it will not be added in error, and negative component amounts are not tolerated. As a result, in the extreme case that the recommended mixture contains only one component, mixing error has no effect. Notice that the mixing measurement error patterns change based on the type of error assumed, the size of errors, and on the desired mixture amounts.

To evaluate the robustness of a design to mixing measurement error, the expected loss is still an appropriate measure. However, now the expected loss used in (6) is taken over the mixing measurement error rather than the noise. Denote this expected loss over the mixing measurement error as:

$$E_e(L) = (E_e(Y) - T)^2 + \text{Var}_e(Y), \qquad (12)$$

where $E_e(Y)$ and $\text{Var}_e(Y)$ are the expected response and variance of the response under the given measurement error model. Unfortunately, due to the interaction of measurement errors, the effect of the mixing measurement errors is complex and no simple closed form expression for $E_e(L)$ can be obtained. However, $E_e(Y)$ and $\text{Var}_e(Y)$, and thus $E_e(L)$ can be approximated by evaluating the response model (2) at a number of carefully chosen mixture proportions that simulate the mixing measurement error pattern. For example, assuming the points in the relative error plot of Figure 1 approximate the effect of measurement error on true component proportions, simple estimates of $E_e(Y)$ and $\text{Var}_e(Y)$ are:

$$\widehat{E}_e(Y) = \sum_{i=1}^{r} \pi_i Y_i, \qquad (13)$$

and

$$\widehat{\text{Var}}_e(Y) = \sum_{i=1}^{r} \pi_i \left(Y_i - \widehat{E}_e(Y)\right)^2, \qquad (14)$$

where Y_i and π_i are the corresponding response and relative probability of each of the points, and r equals the number of points used to approximate the measurement error pattern. The relative probability of any point in the error pattern is based on the probability density function of the measurement errors. In this article, either normal $e_i \sim N(0, \sigma^2_{E_i})$, or uniform, $e_i \sim U(-a_i, a_i)$ is assumed, although other distributions could be used if supported by prior knowledge or data. There are a number of ways the simulated error pattern can be generated. Random points from the distribution of the measurement errors may be chosen. Alternatively ν representative points from each of the measurement error distributions could be used. Using the representative points methodology the effect of mixing measurement error is estimated from ν^m points, where m equals the number of components subject to measurement error. As ν increases the estimates become more accurate but the amount of work increases rapidly.

Fish Patties Texture Example

The fish patties texture example is discussed in more detail in Cornell (1990). The problem is to produce the best fish patties from a combination of three possible fish species, namely mullet (X_1), sheepshead (X_2), and croaker (X_3). The response or quality variable of interest Y is the average texture readings measured in grams of force $(\times 10^{-3})$ required to puncture the patty surface. Ideally, the patty is not too soft nor too firm. The target average texture value T lies between 2.0 and 3.5. The experiment also involves three process variables: the oven temperature z_1 (375 and 425 degrees F), the oven baking time z_2 (25 and 40 minutes), and the deep frying time z_3 (25 and 40 seconds). The process variables were all rescaled so that the two process levels used correspond to -1 and $+1$. The experimental results are given in Cornell (1990, p. 359) and are reproduced in the Table A1 in the Appendix. The experimental design included a complete inner and outer array for all permutations of the mixture proportions (1, 0, 0), (1/2, 1/2, 0), and (1/3, 1/3, 1/3), and two levels for each of the process/noise variables. Thus there are $(3 + 3 + 1)2^3 = 56$ runs.

Cornell (1990) fits the full second-order model (2) and determines the significant parameters. Refitting the response based on the identified significant parameters yields response equation (15) below. All terms given in (15) are significant at 5%.

$$\begin{aligned}\widehat{Y} &= 2.86X_1 + 1.11X_2 + 2.03X_3 \\ &\quad - 0.99X_1X_2 - 0.85X_1X_3 \\ &\quad + z_1(0.44X_1 + 0.17X_2 + 0.19X_3 - 0.77X_1X_2) \\ &\quad + z_2(0.64X_1 + 0.2X_2 + 0.4X_3) + z_1z_3(0.09X_1X_2) \\ &\text{subject to} \quad X_1 + X_2 + X_3 = 1, \quad 0 \le X_i \le 1 \\ &\quad \text{for } i = 1,2,3, \text{ and } z_j = \pm 1 \text{ for } j = 1,2,3.\end{aligned} \tag{15}$$

A contour plot of the value of estimated response $\widehat{Y}$, given by (15), for different mixture proportions and $z_3 = -1$, $z_1 = z_2 = 0$ is shown in Figure 2.

To introduce the notion of noise it is assumed that two of the process variables (z_1 and z_1) are outside of the control of the manufacturer. This would happen, for example, if the fish patties are deep fried by the manufacturer and sold frozen, with the final baking

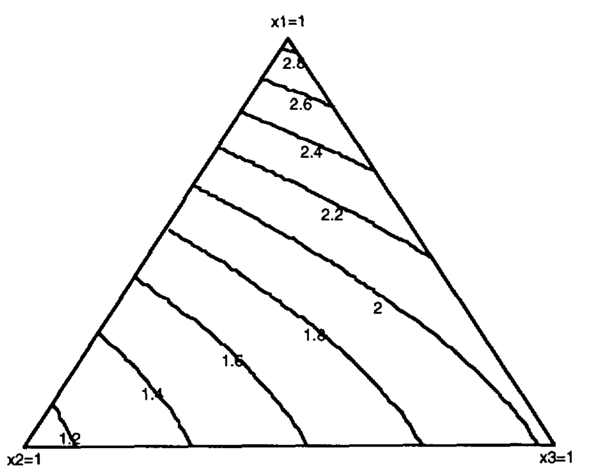

FIGURE 2. Contour Plot of Response $\widehat{Y}$ for $z_3 = -1$, $z_1 = z_2 = 0$.

of the fish patties to be performed by customers. The fish patties are packaged with a suggested temperature and baking time, but due to variations in ovens and in customers, the recommended time and temperature are not always used. Thus, for this example, $m = 3$, $n = 2$, and $p = 1$ following the notation given previously.

Denote the mean and variance of the noise factors due to differences in customers as μ_j and σ_j^2, respectively. For simplicity of analysis in this example, we initially assume that the recommended baking time and temperature are 32.5 minutes and 400 degrees respectively. This baking time and temperature are midway between the two levels used in the experiment (i.e., they correspond to $z_1 = z_2 = 0$). Also assume that on average the baking recommendations are followed by the customers (i.e., $\mu_1 = \mu_2 = 0$, however, some variation about the recommended values is expected). Assuming $\sigma_1^2 = \sigma_2^2 = 1/9$ yields a standard deviation of 1/3 for which the interval -1 to $+1$ represents a six-sigma span. Notice that this noise variability refers to the expected variability in the customers, given in terms of the rescaled noise variable, and not (necessarily) to the variability of the noise factors used in the experiment. In addition it is assumed that the covariance between all noise factors is zero, although the addition of a covariance term in the analysis is straight-forward.

When the design of the experiment is under our control, Taguchi (1986, p. 109) recommends setting the levels of the noise variables so that the variability of the noise factors in the experiment equal the variability of the noise factors in the real world. In this example this advice was not followed since the original experiment was designed to analyze the problem considering only process variables and not noise variables. The noise levels chosen would correspond to $\sigma_1^2 = \sigma_2^2 = 1$, which was deemed too large to be reasonable in this example.

Using the assumptions: $\mu_1 = \mu_2 = 0$ and $\sigma_1^2 = \sigma_2^2 = 1/9$, we derive from (15), (8), and (9):

$$\begin{aligned}E_{z_1,z_2}(\widehat{Y}) &= 2.86X_1 + 1.11X_2 + 2.03X_3 \\ &\quad - 0.99X_1X_2 - 0.85X_1X_3 \end{aligned} \tag{16}$$

$$\begin{aligned}\mathrm{Var}_{z_1,z_2}(\widehat{Y}) &= \sigma_1^2[0.44X_1 + 0.17X_2 + 0.19X_3 \\ &\quad - 0.77X_1X_2 + 0.09X_1X_2z_3]^2 \\ &\quad + \sigma_2^2[0.64X_1 + 0.2X_2 + 0.4X_3]^2. \end{aligned} \tag{17}$$

Figure 3 shows a contour plot of $\mathrm{Var}_{z_1,z_2}(\widehat{Y})$ as

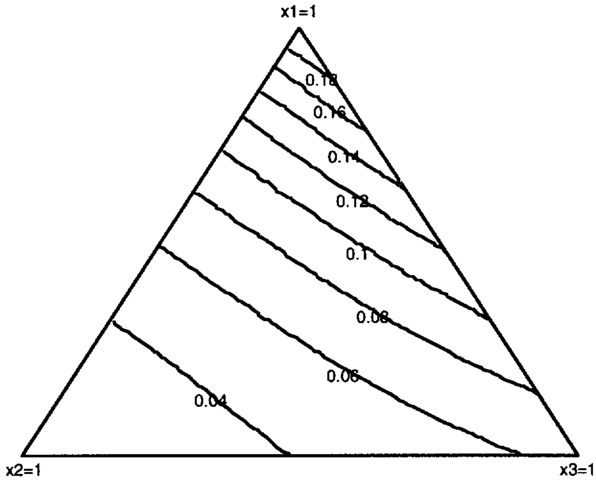

FIGURE 3. Contour Plot of $\text{Var}_{z_1,z_2}(\widehat{Y})$ for $z_3 = -1$.

given by equation (17). Note that assuming $\mu_1 = \mu_2 = 0$, Figure 2 shows contour plots for $\widehat{E}_{z_1,z_2}(\widehat{Y})$ as well as $\widehat{Y}$ when $z_1 = z_2 = 0$.

Remembering that the target range for the average texture readings is between 2 and 3.5, for this small example a graphical solution approach can be attempted based on Figures 2 and 3. Figure 2 suggests that mixture points near the $X_1 = 1$ vertex are best, whereas Figure 3 shows that the variability in the solution is reduced as the $X_2 = 1$ vertex is approached. Making a compromise between these conflicting goals is difficult using the graphical approach although the tradeoff is evident.

The simultaneous optimization approach suggests that the most robust design minimizes the $E(L)$ or MSE subject to the mixture constraints. Thus, our optimization problem is to find X_1, X_2, X_3, and z_3 that

$$\begin{aligned} \text{minimize } E_{z_1,z_2}(L) &= \text{MSE} \qquad (18) \\ &= \left[E_{z_1,z_2}(\widehat{Y}) - T\right]^2 + \text{Var}_{z_1,z_2}(\widehat{Y}) \\ \text{subject to } \quad & X_1 + X_2 + X_3 = 1, \\ & 0 \le X_i \le 1 \\ & \text{for } i = 1, 2, 3, \text{ and } -1 \le z_3 \le 1, \end{aligned}$$

with target value T, and $E_{z_1,z_2}(\widehat{Y})$ and $\text{Var}_{z_1,z_2}(\widehat{Y})$ given by (16) and (17).

Since in this example the number of mixture components is small, graphical displays are easily created and can be very informative. Contour plots of the MSE for various mixture proportions and target values T are given in Figures 4 and 5. An approximate optimal solution can be determined by finding the feasible mixture that lies on the contour of smallest MSE. Additional considerations, such as cost, could at this point also be considered. In this example, $z_3 = -1$ always leads to the best MSE values. As a result, all contour plots are shown for $z_3 = -1$.

In this simple example, contour plots like Figure 4 and Figure 5 would probably be sufficient to determine the optimal mixture proportions. However, when confronted by more mixture components and/or process variables a numerical technique is essential. The robust mixture design problem can be solved using the methodology presented in previous sections. Results obtained using the KKT conditions solution approach given by (7), are shown in Table 1

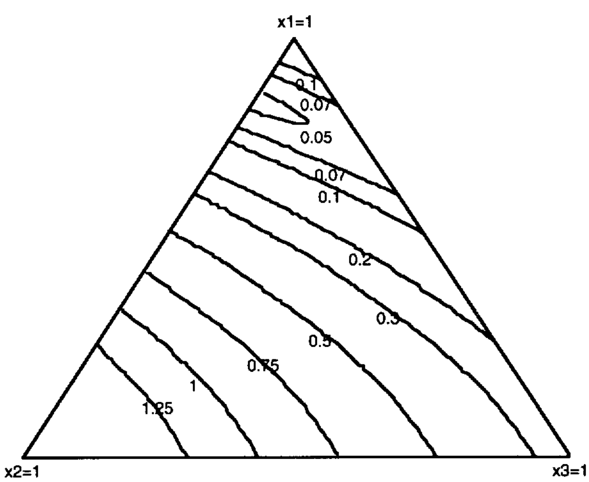

FIGURE 4. Contour Plot of MSE with $T = 2.5$, $z_3 = -1$.

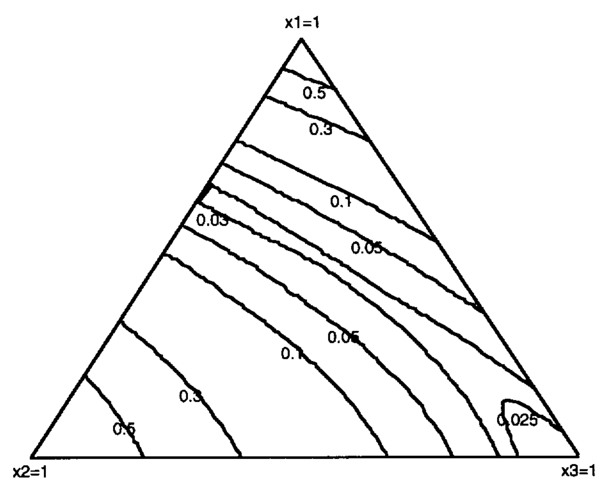

FIGURE 5. Contour Plot of MSE with $T = 2.0$, $z_3 = -1$.

TABLE 1. Robust Solution for Fish Patties Example
$\mu_1 = \mu_2 = 0$, $\sigma_1^2 = \sigma_2^2 = 1/9$

Target	Optimal Solution			Comparison
T	(X_1, X_2, X_3)	z_3	MSE	MSE Range
2.00	(0, 0.043, 0.957)	−1	0.0211	0.0212 to 0.0299
2.25	(0.747, 0.253, 0)	−1	0.0306	0.0367 to 0.0420
2.50	(0.852, 0.148, 0)	−1	0.0467	0.0474 to 0.0535
2.75	(0.949, 0.051, 0)	−1	0.0595	0.0604 to 0.0631
3.00	(1, 0, 0)	−1	0.0866	N/A

for various target values. For example, when $T = 2.5$ the optimal robust mixture of fish is $(X_1, X_2, X_3) = (0.852, 0.148, 0)$ with $z_3 = -1$ (i.e., a mixture of about 85% mullet and 15% sheepshead and a 25 second deep frying time). These optimal robust settings are somewhat different than the optimal mixture proportions when considering only the mean response. Using only the mean response criteria any mixture proportion along a contour line in Figure 2 is equally good. However, when looking at MSE these solutions are not equivalent. To show the influence of the noise variables on the optimal solution to this problem, Table 1 also shows the range of MSE values obtained along contours of a given target value when $z_3 = -1$ and $z_1 = z_2 = 0$. For example, along the contour $\widehat{Y} = 2.0$ in Figure 2 the resultant MSE values range from a low of 0.0212 to a high of 0.0299. Table 1 shows that ignoring the effect of noise factors can lead to solutions having substantially larger MSE values than the optimal solution.

Table 1 gives the optimal fish patty mixtures assuming an average oven temperature and baking time of 400 degrees and 32.5 minutes respectively. However, in the fish patties example, the fish is sold frozen with a recommended baking time and temperature. As a result, assuming the customers pay some attention to the recommendations, the means of the noise factors (oven temperature and baking time) could be considered design variables to be optimized. Assuming that the recommendations are followed on average, the optimization problem is expanded to allow μ_1 and μ_2 as optimization variables, and additional constraints are added to restrict μ_1 and μ_2 to the standardized range of −1 to +1. Making these changes to (6), the derived optimal solutions are shown in Table 2. Table 2 shows that the best recommended cooking temperature and time are at the upper limits of our experience, namely 425 degrees and 40 minutes respectively. Since these values fall at the edges of our experimental region it would be prudent to check these results with a follow-up study to verify the form of the response surface near the proposed optimal mixture.

Now consider the addition of mixing measurement error in the fish patties example. Mixing measurement error could occur, for example, if the amounts of the different fish species are not very carefully controlled during regular production. In this scenario we would like to determine a formula for fish patties that yields textures that are robust to changes in the fish proportions that arise due to the measurement error. The effect of mixing measurement error is investigated using the methodology discussed in the previous section. To focus the discussion, our analysis is restricted to the case where $\mu_1 = \mu_2 = 0$ and the target texture T equals 2.5. Generating similar results for other situations is a straightforward extension of the procedure outlined below and in the previous section.

Table 3 and Table 4 show results obtained assuming uniform absolute and uniform relative errors respectively. For simplicity, it was assumed that the same error structure holds for all mixture components. Different error levels or models for each component could be easily incorporated. These results are generated by using representative points that divide the measurement error distributions into seven groups of equal probability. This approach was found to be effective, since it assured reasonable coverage of the measurement error densities while restricting the number of required numerical calculations.

To illustrate this solution procedure consider the absolute errors case with the mixing errors e_i ranging uniformly from −0.1 to 0.1. Let the desired component amounts of the three mixture variables be (A_1, A_2, A_3), and without loss of generality, assume that the A_is have been rescaled to equal the desired component proportions (i.e., $\sum A_i = 1$). Under this scenario the distribution of the actual com-

TABLE 2. Robust Solution for Fish Patties Example with Control Over Noise Means, $\sigma_1^2 = \sigma_2^2 = 1/9$

Target	Optimal Solution			
T	(X_1, X_2, X_3)	(μ_1, μ_2)	z_3	MSE
2.00	(0, 0.549, 0.451)	(1, 1)	1	0.013
2.25	(0, 0.331, 0.669)	(1, 1)	−1	0.016
2.50	(0, 0.112, 0.888)	(1, 1)	1	0.020
2.75	(0.172, 0, 0.828)	(1, 1)	−1	0.028
3.00	(0.753, 0.247, 0)	(1, 1)	−1	0.036

TABLE 3. Solution for Fish Patties Example with Uniform Absolute Errors, $\mu_1 = \mu_2 = 0$, $\sigma_1^2 = \sigma_2^2 = 1/9$, $T = 2.5$

	Optimal Solution			Comparison
Error	(X_1, X_2, X_3)	z_3	MSE	no error solution MSE
0.0	(0.852, 0.148, 0)	−1	0.0467	0.0467
0.05	(0.853, 0.147, 0)	−1	0.0519	0.0519
0.1	(0.741, 0, 0.259)	−1	0.0574	0.0679
0.2	(0.698, 0, 0.302)	−1	0.0694	0.1047

TABLE 4. Solution for Fish Patties Example with Uniform Relative Errors, $\mu_1 = \mu_2 = 0$, $\sigma_1^2 = \sigma_2^2 = 1/9$, $T = 2.5$

	Optimal Solution			Comparison
Error	(X_1, X_2, X_3)	z_3	MSE	no error solution MSE
0.0	(0.852, 0.148, 0)	−1	0.0467	0.0467
0.2	(0.856, 0.144, 0)	−1	0.0502	0.0503
0.3	(0.838, 0.110, 0.052)	−1	0.0542	0.0551
0.5	(0.809, 0.053, 0.138)	−1	0.0637	0.0735

ponent amounts for each component is uniform between $A_i - 0.1$ and $A_i + 0.1$, and the true component proportions are given by (11). The consequences of this measurement error structure on the robustness of any particular desired mixture blend is estimated by using seven representative values for each mixture component. The seven representative values are determined by dividing the uniform distribution into seven regions of equal probability, and taking the conditional expected value for each group

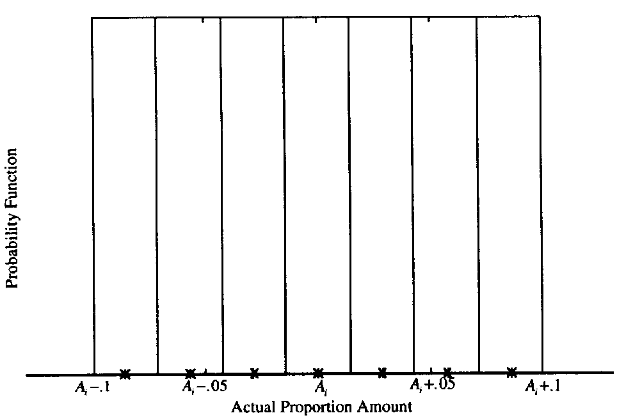

FIGURE 6. Uniform Distribution Divided into 7 Groups of Equal Probability "*" Denote the Representative Component Amounts Utilized: $A_i + e_i$.

as the representative value. The seven representative values are denoted by "*"s in Figure 6. Thus, for a component amount $A_i = 0.3$, the representative components amounts used are 0.214, 0.243, 0.271, 0.3, 0.329, 0.357, and 0.386. Based on each combination of representative component amounts for each fish species the true component proportions given by (11) are used in (15) to derive a corresponding response, denoted Y_i. Then from (12), (13) and (14) $E_e(L)$ can be estimated. Note that since the error structure is divided into regions of equal probability all π_is in (13) and (14) equal $1/r$, where r, in this example, equals $7^3 = 343$.

More accurate estimates can be obtained by using more representative values. However, for the fish patties example, using more than seven representative values for each component did not change the solution substantially.

Table 3 and Table 4 show that the change in optimal mixtures can be substantial if the mixing measurement error is large. The comparison column gives the MSE of the no error solution (0.852, 0.148, 0) under the given error model. For example, assuming a uniform absolute measurement error of 0.2, the mixture (0.852, 0.148, 0) yields an MSE of 0.1047 which is substantially larger than that obtained with the optimal solution (0.698, 0, 0.302). In this example the mixing measurement errors required to substantially change the solution are relatively large, but this need not always be the case.

The numerical solutions given by solving (6) provide optimal mixture proportions for the given problem. However, it is typically prudent to also explore the feasible region to get a sense of the tradeoffs involved with different mixture proportions. At this stage, qualitative factors, or quantitative factors not included in the formal problem statement, can be considered. For problems with few variables, like the fish patties example, this is fairly straightforward through examination of plots like Figure 4. In problems with larger numbers of mixture variables, the numerical solution can be used to focus the follow-up graphical exploration on those mixtures close to the numerically optimal mixture.

Conclusions

In this article mixtures subject to noise factors and/or mixing measurement error are analyzed. Under uncontrollable variation such as noise or mixing measurement error, mixtures that are robust to this variation are desired. Using the methodology presented in this article, optimal robust mixture blends

TABLE A1. Average Texture Reading for Fish Patties

Process Variables			Mixture Composition						
z_1	z_2	z_3	(1, 0, 0)	(0, 1, 0)	(0, 0, 1)	$(\frac{1}{2}, \frac{1}{2}, 0)$	$(\frac{1}{2}, 0, \frac{1}{2})$	$(0, \frac{1}{2}, \frac{1}{2})$	$(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$
−1	−1	−1	1.84	0.67	1.51	1.29	1.42	1.16	1.59
1	−1	−1	2.86	1.10	1.60	1.53	1.81	1.50	1.68
−1	1	−1	3.01	1.21	2.32	1.93	2.57	1.83	1.94
1	1	−1	4.13	1.67	2.57	2.26	3.15	2.22	2.60
−1	−1	1	1.65	0.58	1.21	1.18	1.45	1.07	1.41
1	−1	1	2.32	0.97	2.12	1.45	1.93	1.28	1.54
−1	1	1	3.04	1.16	2.00	1.85	2.39	1.60	2.05
1	1	1	4.13	1.30	2.75	2.06	2.82	2.10	2.32

can be found using constrained nonlinear optimization. The effect of noise variables and/or mixing measurement error is dependent on the variability of the noise factors, the magnitude of the measurement errors, and the response model. An example, given to illustrate the effect of this analysis on the optimal mixture proportions, shows that the influence of noise and/or mixing measurement error can be substantial.

Appendix

The 56 experimental data points for the fish patties example from Cornell (1990) are reproduced in Table A1.

Acknowledgments

This research was supported, in part, by the Natural Sciences and Engineering Research Council of Canada and the Manufacturing Research Council of Ontario. The authors would like to thank John Cornell, Greg Piepel, the Editor, and anonymous referees for their constructive suggestions. MATLAB® is a registered trademark of The MathWorks.

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Key Words: *Loss Functions, Robust Design, Taguchi Methods.*