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Measurement Errors**

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Making Mixtures Robust to Noise Factors 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.

Key Words: Expected Quadratic Loss; Robust Design; Taguchi
Parameter Design

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 , $i=1, \dots, m$ 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:

$$\begin{aligned}
 Y &= \sum_{i=1}^m \beta_i X_i + \varepsilon, & \text{where } \sum_{i=1}^m X_i &= 1 \text{ and} \\
 Y &= \sum_{i=1}^m \beta_i X_i + \sum_{i < k} \beta_{ik} X_i X_k + \varepsilon, & \text{where } \sum_{i=1}^m X_i &= 1.
 \end{aligned} \tag{1}$$

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_i 's 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 an 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 , $j=1, \dots, n+p$) to the models (1) is fairly straightforward (Cornell, 1990). The full second-degree model in mixture variables and process variables is given by (2).

$$\begin{aligned}
Y = & \sum_{i=1}^m \beta_i X_i + \sum_{i < k} \sum_{i < k} \beta_{ik} X_i X_k + \sum_{j=1}^{n+p} z_j \left(\sum_{i=1}^m \alpha_{i(j)} X_i + \sum_{i < k} \sum_{i < k} \alpha_{ik(j)} X_i X_k \right) \quad (2) \\
& + \sum_{j \leq l} \sum_{j \leq l} z_j z_l \left(\sum_{i=1}^m \gamma_{i(jl)} X_i + \sum_{i < k} \sum_{i < k} \gamma_{ik(jl)} X_i X_k \right) + \varepsilon, \quad \text{where } \sum_{i=1}^m X_i = 1.
\end{aligned}$$

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 (Taguchi and Wu, 1985, 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*):

$$E(L) = MSE = (E_z(Y) - T)^2 + Var_z(Y) \quad (3)$$

Note that the expected value and variance of the response, denoted $E_z(Y)$ and $Var_z(Y)$ 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.

$$E(L) = E_z(Y) + 2\sqrt{Var_z(Y)} \quad (4)$$

$$E(L) = 2\sqrt{Var_z(Y)} - E_z(Y) \quad (5)$$

A number of different approaches to estimate the expected loss $E(L)$ or another measure of robustness have been proposed. Taguchi suggests running an experiment via the inner and outer array technique (Taguchi and Wu, 1985). 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 (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, $E(L)$ 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 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 $\mathbf{X} = (X_1, X_2, \dots, X_{m-1})$ and $\mathbf{z} = (z_1, \dots, z_{n+p})$. 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 generally as:

$$\min E(L(\mathbf{X}, \mathbf{z})) \quad (6)$$

subject to $g_q(\mathbf{X}, \mathbf{z}) \leq 0$ for $q = 1, \dots, c$,

where $E(L(\mathbf{X}, \mathbf{z}))$ 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:

$$g_1(\mathbf{X}) = -1 + \sum_{i=1}^{m-1} X_i, \quad g_{i+1}(\mathbf{X}) = -X_i \quad \text{for } i = 1, \dots, m-1, \text{ and}$$

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

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 techniques are available to solve this constrained nonlinear optimization problem. Typically the most efficient is to use 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:

$$\begin{aligned} \nabla E(L(X^*, z^*)) + \sum_{q=1}^c \lambda_q^* \nabla g_q(X^*) &= 0 \\ \lambda_q^* g_q(X^*) &= 0 \\ \lambda_q^* &\geq 0 \quad \text{for } q = 1, \dots, c, \quad \text{where } \nabla \text{ is the gradient operator.} \end{aligned} \quad (7)$$

Solving the above problem is accomplished by using a quadratic approximation to the Lagrangian function $E(L) + \sum_{q=1}^c \lambda_q^* g_q$. The routine “constr” in the Optimization toolbox of MATLAB[®] can be used to solve this problem. Note that c equals the number of constraints given in (6).

Let the mean and variance of the noise factors in the process equal $E(z_j) = \mu_j$ and $\text{Var}(z_j) = \sigma_j^2$, $j = 1, \dots, n$ respectively. Note that μ_j and σ_j^2 represent the mean and variability 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), though similar expressions for the general case are easily obtained. Using (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.

$$E_z(Y) = \sum_{i=1}^m \beta_i X_i + \sum_{i < k} \beta_{ik} X_i X_k, \quad \text{and} \quad (8)$$

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

Unfortunately solutions to (6) using this methodology are not guaranteed to converge to the global optimal unless $E(L(\mathbf{X}, \mathbf{z}))$ and all $g_q(X)$'s are convex. All the $g_q(X)$ constraints of the standard robust mixture problem are linear and thus convex, but

$E(L(\mathbf{X}, \mathbf{z}))$ is nonlinear and not convex in general. As a result, a number of starting positions should be tried.

Mixture experiments and mixing measurement errors

In many applications creating mixtures involves some mixing measurement error. We define mixing measurement error as errors that yield actual mixture proportions that are different than the desired proportions. Mixing 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, since in both cases the 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.

However, mixing measurement error is more complex than noise factors since, for mixture experiments, an error in the measurement for one component amount effects the relative proportion of all components. This is very important because in mixture experiments it is assumed that the relative proportion of the mixture variables influences the quality of the mixture.

Determining mixtures that are robust to mixing measurement errors under these assumptions can be done in a manner similar to that employed in the previous section. In the optimization problem represented by (6) an expression for the expected loss $E(L)$ is required. An appropriate expression for the expected loss under mixing measurement errors depends on the nature of the error. We assume the mixing measurement error arises

due to measurement errors in the mixture component amounts. 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 are $X_i = A_i / \sum_{i=1}^m A_i$ for $i = 1, \dots, m$. 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 (11) respectively.

$$X_i(rel) = A_i(1 + e_i) / \sum_{i=1}^n A_i(1 + e_i), \text{ for } i = 1, \dots, m. \quad (10)$$

$$X_i(abs) = (A_i + e_i) / \sum_{i=1}^n (A_i + e_i), \text{ for } i = 1, \dots, m. \quad (11)$$

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 mixing measurement error structure for all component proportions. As an example, Figure 1 shows the pattern of errors resulting from relative and absolute errors in the case of three mixture variables. The 27 points signify the mistaken component proportions that arise when all combinations of mixing errors $e_i = -err, 0, +err$ are considered for all three component proportions 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.

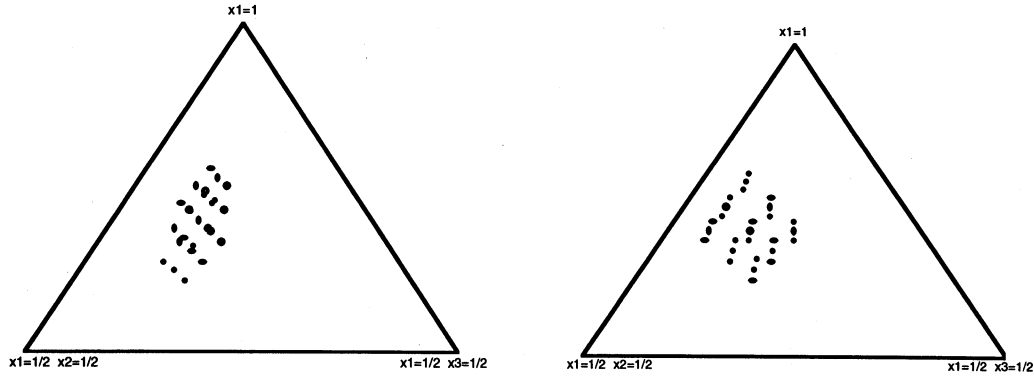


Figure 1: Mixing Measurement Error Plots
 relative errors ($err = .2$) on left, absolute errors ($err = .05$) on right,
 centered at $(X_1, X_2, X_3) = (0.7, 0.2, 0.1)$

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. Thus, since mixture problems depend only on the relative proportions of the various ingredients, 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. Unfortunately due to the interaction of errors the resultant effect of the mixing measurement error on the expected loss is complex and no simple closed form expression for the expected loss can be obtained. However, the expected loss 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, based on error patterns like those shown in Figure 1, a response model, and the probability of each point in the error pattern, $E_z(Y)$, $Var_z(Y)$ and thus $E(L)$ can be

estimated. The probability of any point in the error pattern is based on the probability density function of the measurement errors. In this article either normal, $e_i \sim N(0, \sigma_{e_i})$, 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 v 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 v^m points, where m equals the number of components subject to measurement error. As v increases the estimates become more accurate but the amount of work increases rapidly.

Fish Patties Texture Example

This application of mixtures 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 baking time z_1 (25 and 40 minutes), the oven temperature z_2 (375 and 425 degrees F), 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 (12) below. All terms given in (12) are significant at 5%.

$$\hat{Y} = 2.86X_1 + 1.11X_2 + 2.03X_3 - .99X_1X_2 - .85X_1X_3 \quad (12)$$

$$+ z_1(.44X_1 + .17X_2 + .19X_3 - .77X_1X_2) + z_2(.64X_1 + .2X_2 + .4X_3) + z_1z_3(.09X_1X_2)$$

subject to $X_1 + X_2 + X_3 = 1$, $0 \leq X_i \leq 1$ for $i=1, 2, 3$, and $z_j = \pm 1$ for $j=1, 2, 3$.

A contour plot of the value of expected response \hat{Y} , given by (12), for different mixture proportions and $z_3 = -1$, $z_1 = z_2 = 0$ is shown in Figure 2.

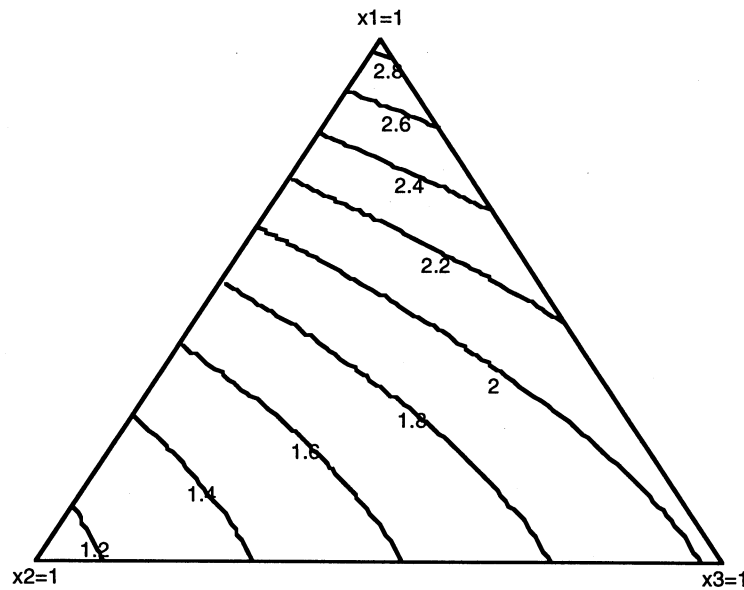


Figure 2: Contour Plot of Response \hat{Y} for $z_3 = -1$, $z_1 = z_2 = 0$

To introduce the notion of noise it is assumed that two of the process variable (z_1 and z_2) 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 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 from the previous sections.

Denote the mean and variance of the noise factors due to differences in customers as μ_j and σ_j^2 , respectively. In many situations both the mean and variance of the noise factors is out of the manufacturer's control. However, in the fish patties example, the frozen fish patties are sold with a recommended baking time and temperature. Thus, in the fish patties example we can presumably influence at least μ_1 and μ_2 . As a result, the means of the noise variables are variable in the optimization problem.

For simplicity of analysis in this example, 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. A perhaps more realistic analysis of the fish patties data where the means of the noise variables are allowed to vary yields optimal solutions all at $\mu_1 = \mu_2 = 1$. Since this value is at the boundary of our experimental region follow-up experiments should be run to verify the form of the response surface near that operating condition.

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 (12), (8) and (9):

$$E_{z_1, z_2}(Y) = 2.86X_1 + 1.11X_2 + 2.03X_3 - .99X_1X_2 - .85X_1X_3 \quad \text{and} \quad (13)$$

$$\begin{aligned} \text{Var}_{z_1, z_2}(Y) = \sigma_1^2 [.44X_1 + .17X_2 + .19X_3 - .77X_1X_2 + .09X_1X_2z_1]^2 \\ + \sigma_2^2 [.64X_1 + .2X_2 + .4X_3]^2 \end{aligned} \quad (14)$$

Figure 3 shows a contour plot of $\text{Var}_{z_1, z_2}(Y)$ as given by Equation (14). Note that since it is assumed that $\mu_1 = \mu_2 = 0$, Figure 2 shows contour plots for $E_{z_1, z_2}(Y)$ as well as \hat{Y} when $z_1 = z_2 = 0$.

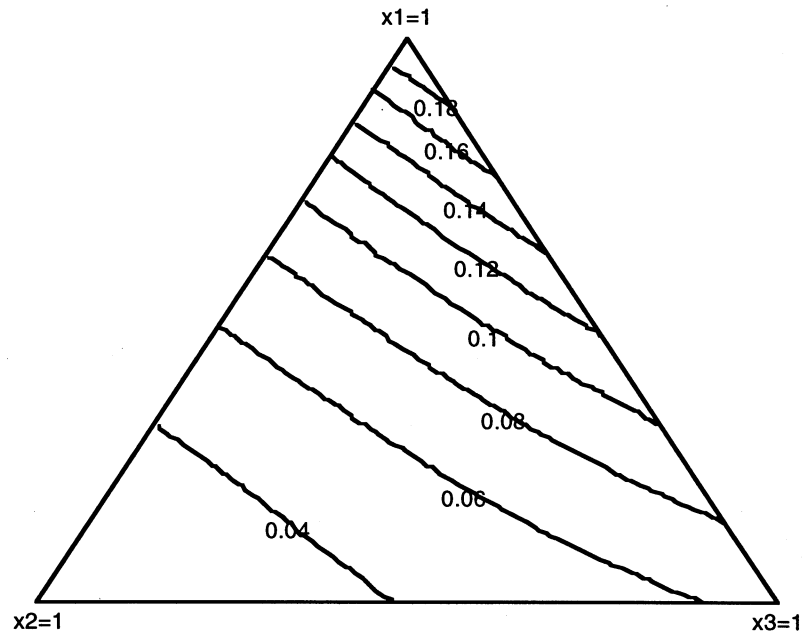


Figure 3: Contour Plot of $\text{Var}_{z_1, z_2}(Y)$ for $z_3 = -1$

Remembering that the target range for the average texture readings is between 2 and 3.5, 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 compromises 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 the X_1 , X_2 , X_3 and z_3 to

$$\text{minimize } E(L) = MSE = \left[E_{z_1, z_2}(Y) - T \right]^2 + Var_{z_1, z_2}(Y) \quad (15)$$

subject to $X_1 + X_2 + X_3 = 1$, $0 \leq X_i \leq 1$ for $i = 1, 2, 3$, and $-1 \leq z_3 \leq +1$,

with target value T and $E_{z_1, z_2}(Y)$ and $Var_{z_1, z_2}(Y)$ given by (13) and (14).

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 $z_3 = -1$.

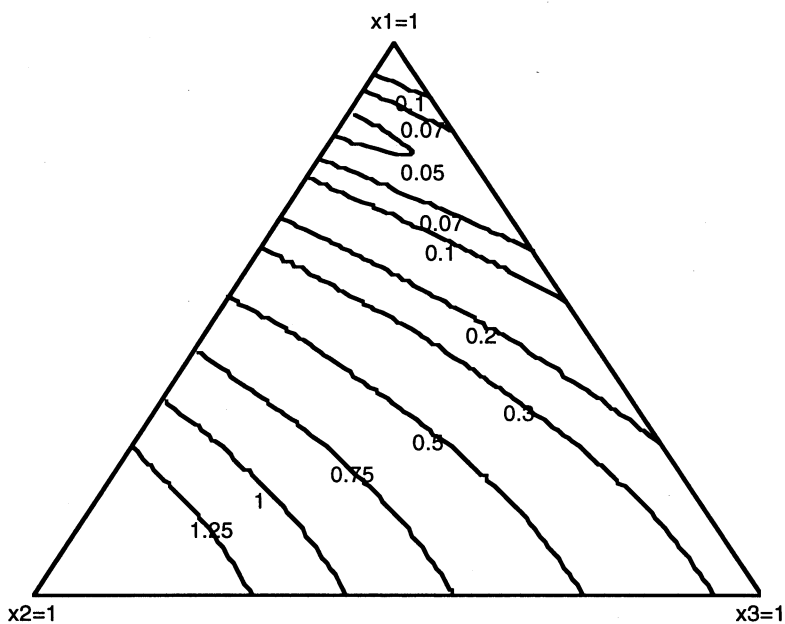


Figure 4: Contour Plot of MSE with $T = 2.5$, $z_3 = -1$

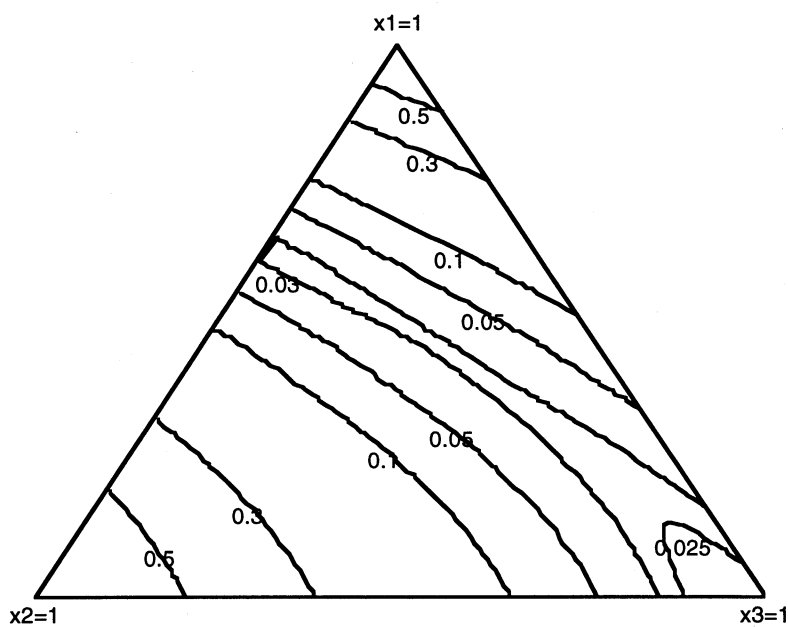


Figure 5: Contour Plot of MSE with $T = 2.0$, $z_3 = -1$

In this simple example, contour plots like Figures 4 and 5 would probably be sufficient to determine the optimal mixture proportions. However, when confronted with

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 for various target values. For example, when $T = 2.75$ the optimal robust mixture of fish is $(X_1, X_2, X_3) = (.9486, .0514, 0)$ with $z_3 = -1$, i.e., a mixture of about 95% mullet and 5% 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 given target value when $z_3 = -1$ and $z_1 = z_2 = 0$. For example, along the contour $\hat{Y} = 2.0$ 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: Robust Solution for Fish Patties Example

$$\mu_1 = \mu_2 = 0, \sigma_1^2 = \sigma_2^2 = 1/9$$

Target T	Optimal Solution (X_1, X_2, X_3)	z_1	<i>MSE</i>	Comparison <i>MSE</i> Range
2.00	(0, .0434, .9566)	-1	.0211	.0212 to .0299
2.25	(.7475, .2525, 0)	-1	.0306	.0367 to .0420
2.50	(.8523, .1477, 0)	-1	.0467	.0474 to .0535
2.75	(.9486, .0514, 0)	-1	.0595	.0604 to .0631
3.00	(1,0,0)	-1	.0866	N/A

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. The effect of mixing measurement error is investigated using the methodology discussed in the previous section.

Tables 2 and 3 show results obtained assuming uniform absolute and uniform relative errors respectively with a target texture value $T = 2.5$. 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.

Tables 2 and 3 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 (.8523, .1477, 0) under the given error model. For example, assuming a uniform absolute measurement error of 0.2, the mixture (.8523, .1477, 0) yields an *MSE* of 0.1047 which is substantially larger than that obtained with the optimal solution (.6984, 0, .3016). In this example the mixing measurement errors required to substantially change the solution are relatively large, but this need not always be the case.

Table 2: Solution to Fish Patties Example with Uniform Absolute Errors

$$\mu_1 = \mu_2 = 0, \sigma_1^2 = \sigma_2^2 = 1/9, T = 2.5$$

Error	Optimal Solution			Comparison no error solution <i>MSE</i>
	(X_1, X_2, X_3)	z_3	<i>MSE</i>	
0.0	(.8523, .1477, 0)	-1	.0467	.0467
0.05	(.8533, .1467, 0)	-1	.0519	.0519
0.1	(.7409, 0, .2591)	-1	.0574	.0679
0.2	(.6984, 0, .3016)	-1	.0694	.1047

Table 3: Solution to Fish Patties Example with Uniform Relative Errors
$$\mu_1 = \mu_2 = 0, \sigma_1^2 = \sigma_2^2 = 1/9, T = 2.5$$

Error	Optimal Solution			Comparison no error solution MSE
	(X_1, X_2, X_3)	z_3	MSE	
0.0	(.8523, .1477, 0)	-1	.0467	.0467
0.2	(.8564, .1436, 0)	-1	.0502	.0503
0.3	(.8382, .11, .0517)	-1	.0542	.0551
0.5	(.8086, .0532, .1382)	-1	.0637	.0735

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 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 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.

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Appendix

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

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

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