

INSY 7310 Reference: Chapter 11 of Montgomery (7e) RSM Maghsoodloo

D. C. Montgomery (2009) provides a good description of Response Surface Methodology (RSM) on pp. 417-434 with a very good practical Example 11.1 on p. 420. You should carefully study pp. 417-434 of Montgomery's 7th edition (pp. 408-422 of the 6th edition), where below I will provide detailed explanations of what may be difficult to comprehend.

The Path of Steepest Ascent (POSA)

For the Example 11.1, where the objective is to maximize the response, a 1st-order approximation to the true response surface (RS) $\eta = f(x_1, x_2)$ at the design center ($\xi_1 = 35$ Minutes, $\xi_2 = 155$ °F) was 1st obtained to be $\hat{y} = 40.444\bar{4} + 0.775x_1 + 0.325x_2$, which describes a plane in D-3. Note that the coded design variables x_1 and x_2 are related to the natural variables reaction time and temperature through the linear transformation $x_1 = (\xi_1 - 35)/5$ and $x_2 = (\xi_2 - 155)/5$. These last 2 transformations imply that the half-design spacing for both Time and Temperature were 5 units. The coefficients of the regression model $\hat{y} = 40.444\bar{4} + 0.775x_1 + 0.325x_2$ were obtained from $\hat{\beta} = \mathbf{C}(\mathbf{X}'\mathbf{Y})$, where the matrix $\mathbf{C} = (\mathbf{X}'\mathbf{X})^{-1} = (\mathbf{X}^T\mathbf{X})^{-1} =$

$$\begin{bmatrix} 1/9 & 0 & 0 \\ 0 & 1/4 & 0 \\ 0 & 0 & 1/4 \end{bmatrix} \text{ and } \mathbf{X}'\mathbf{Y} = \mathbf{X}^T\mathbf{Y} = \begin{bmatrix} 364 \\ 3.10 \\ 1.30 \end{bmatrix}. \text{ It is paramount to realize that we are}$$

assuming the experimenter is far from the optimum region, and therefore the true RS, η , can be well approximated by a plane (or 1st-order model) in 3 dimensional space. This further implies that a 2-level design can be used to estimate the slopes in the x_1 and x_2 directions. A contour of a surface is defined as those pairs of (x_1, x_2) values for which the model \hat{y} has the same constant value c , i.e., the equation

$$c = 40.444\bar{4} + 0.775x_1 + 0.325x_2$$

is a contour of the surface $\hat{y} = 40.444\bar{4} + 0.775x_1 + 0.325x_2$ for any fixed specified constant c . For example, for the constant $c = 45\%$ yield, we have the contour

$$45\% = 40.444\bar{4} + 0.775x_1 + 0.325x_2. \quad (30)$$

However, Eq. (30) simply represents the line $x_2 = 14.0171 - 2.38462x_1$ in D-2 with slope $-0.775/0.325 = -2.38462$ and ordinate-intercept equal to 14.0171. Further, if we increase yield to $c = 50\%$, we will obtain another contour with the same slope $-0.775/0.325$ but intercept at 29.40171. In other words, all the contours of the response surface $\hat{y} = 40.444\bar{4} + 0.775x_1 + 0.325x_2$ are parallel lines with slope equal to $-0.775/0.325$. The path of steepest ascent is along the line that is perpendicular to all the contours. Since this perpendicular line (i.e., the path of steepest ascent, denoted POSA) has a slope that is the negative reciprocal of the contours $c = 40.444\bar{4} + 0.775x_1 + 0.325x_2$, then the slope of the POSA is equal to $0.325/0.775$. This clearly shows that in order to move in the direction of the POSA for every 0.775 unit increase in the x_1 -direction we must increase the design variable x_2 in the amount of 0.325 unit. For example, if the increase in the x_1 direction is $\Delta x_1 = 3$, then $\Delta x_2 = (0.325/0.775) \times 3 = 1.258067$, i.e., if we increase the natural variable ξ_1 from 35 minutes to 50 minutes of reaction time, then the natural variable ξ_2 has to change from 155°F to 161.29033; then we are indeed moving the DC (Design Center) in the direction of the POSA. Note that this is consistent with Table 11.3 on page 423 of Montgomery (7e). In case y is an smaller-the-better type response, then the experimenter has to move the DC in the direction of path of steepest descent (POSD).

On the other hand, suppose our objective is to minimize the response y , for example, the porosity in aluminum die castings would be a measure that has to be minimized. However, we do not have information about the exact shape of the response surface, but we have determined that two process parameters $x_1 =$ Die Temperature, and $x_2 =$ "Multiplied Pressure at Stage 3" have a significant impact on the response y , i.e., the mean of the response surface (RS) may be some quadratic function of x_1 and x_2 as shown below.

$$\eta(x_1, x_2) = E(y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 \quad (31)$$

If the coefficients in the above quadratic form were known, then we could attempt to obtain the (relative) minimum point, $\mathbf{x}_0 = [x_1^0 \quad x_2^0]^T = [x_1^0 \quad x_2^0]'$ that minimizes the response surface given in equation (31). Such a procedure would consist of the following steps:

- (1)** Set all the first partial derivatives equal to zero, i.e., require that $\frac{\partial \eta}{\partial x_i} = 0$, $i = 1, 2, 3, \dots, k$,

where for the RS in Eq. (31) the value of $k = 2$. Then solve the above system of k equations

with k unknowns simultaneously for the stationary (critical, or optimal) point $\mathbf{x}_s = \mathbf{x}_0 = [x_1^0 \ x_2^0 \ \dots \ x_k^0]'$.

(2) Then obtain mixed-partials $\eta_{ij} = \frac{\partial^2 \eta}{\partial x_i \partial x_j}$ for all $i, j = 1, 2, \dots, k$. Our objective here is to

ascertain whether the RS has a point of relative (or) local minimum, maximum, or a saddle

point (i.e., minimax). Then evaluate the values of $\eta_{ij} = \frac{\partial^2 \eta}{\partial x_i \partial x_j}$ at $\mathbf{x}_s = [x_1^0 \ x_2^0 \ \dots \ x_k^0]'$.

(3) If the value of $\eta_{ii} = \frac{\partial^2 \eta}{\partial x_i^2}$ at $\mathbf{x}_s > 0$ for all $i = 1, 2, \dots, k$, and the corresponding $(\eta_{ij} |_{\mathbf{x}_s})$

$\times (\eta_{ij} |_{\mathbf{x}_s}) > \left(\frac{\partial^2 \eta}{\partial x_i \partial x_j} \Big|_{\mathbf{x}_s} \right)^2$ for $i \neq j$, then these conditions are sufficient to guarantee that \mathbf{x}_s

is at least a relative (or local) point of minimum. If the value of $\eta_{ii} = \frac{\partial^2 \eta}{\partial x_i^2}$ at $\mathbf{x}_s < 0$ for all $i = 1,$

$2, \dots, k$, and the corresponding $(\eta_{ii} |_{\mathbf{x}_s}) \times (\eta_{jj} |_{\mathbf{x}_s}) > \left(\frac{\partial^2 \eta}{\partial x_i \partial x_j} \Big|_{\mathbf{x}_s} \right)^2$ for $i \neq j$, then \mathbf{x}_s is a local

point of maximum. If $\left(\frac{\partial^2 \eta}{\partial x_i^2} \Big|_{\mathbf{x}_s} \right) \times \left(\frac{\partial^2 \eta}{\partial x_j^2} \Big|_{\mathbf{x}_s} \right) < \left(\frac{\partial^2 \eta}{\partial x_i \partial x_j} \Big|_{\mathbf{x}_s} \right)^2$ for any $i \neq j$, then \mathbf{x}_s is a saddle

point (or a minimax). If $\left(\frac{\partial^2 \eta}{\partial x_i^2} \Big|_{\mathbf{x}_s} \right) \times \left(\frac{\partial^2 \eta}{\partial x_j^2} \Big|_{\mathbf{x}_s} \right) = \left(\frac{\partial^2 \eta}{\partial x_i \partial x_j} \Big|_{\mathbf{x}_s} \right)^2$, then further investigation is

necessary. As examples, you can easily verify that the three response functions $\eta(x_1, x_2) =$

$x_1^2 + x_2^2, 1 - x_1^2 - x_2^2,$ and $x_1 x_2$ have global minimum, maximum, and saddle point at the

origin $\mathbf{x}_s = [0 \ 0]'$, respectively. The surfaces $x_1^2 + x_2^2$ and $1 - x_1^2 - x_2^2$ have the origin as their

critical point (because $\frac{\partial \eta}{\partial x_i} = 0$ for $i = 1, 2$ at the origin), but $\frac{\partial^2 \eta}{\partial x_1^2}, \frac{\partial^2 \eta}{\partial x_2^2},$ and $\frac{\partial^2 \eta}{\partial x_1 \partial x_2}$ all

vanish at the origin. However, upon further inspection it is obvious that the latter two

response functions have a global minimum and maximum at the origin, respectively.

In practice, the coefficients β_j and β_{ij} of the RS (31) are unknown and have to be estimated, but if the experimenter is running the process far from the optimal point $\mathbf{x}_s = \mathbf{x}_o$, then it is nearly impossible to obtain accurate estimates of β_j and β_{ij} , and it is advisable to move closer to $\mathbf{x}_s = \mathbf{x}_o$ in the direction of POSD (or POSA when maximizing y) before fitting a 2nd order model using regression analysis. In order to move the DC most rapidly toward the point of minimum, the experimenter has to determine the path of steepest descent (or ascent if y is an LTB type response). This will require fitting a 1st-order model in some region of the factor space far away from \mathbf{x}_o . Just as an example, suppose we use MLREG and obtain the fitted plane $\hat{y} = 21 - 2x_1 + 3x_2$ at the design center (0, 0). If this were a maximization problem, then the path of steepest ascent would consist of decreasing x_1 , say by one unit, but increasing x_2 by 1.5 units. That is to say, our next design center would be at (-1, 1.5). However, if we are minimizing the response, such as $y = \text{Porosity}$, then the path of steepest descent is to increase x_1 by 1 unit but decrease x_2 by 1.5 units, i.e., our next design center for the minimization problem would be at (1, -1.5).

The ANOVA Table 11.2 on Page 422 of Montgomery's 7th Edition (p. 410 of the 6th Edition)

Since this ANOVA table includes both the pure quadratic terms x_1^2 , x_2^2 , and the interaction term $x_{12} = x_1x_2$, then its corresponding 2nd-order regression model is given by

$$y = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_{11}x_1^2 + \beta_{22}x_2^2 + \beta_{12}x_1x_2 + \epsilon$$

The design matrix \mathbf{X} for the above model that pertains to Table 11.1 on page 421 of Montgomery (p. 409 of 6e) is given on the next page.

Note that this design matrix \mathbf{X} has 4 factorial and 5 center points so that using Montgomery's notation $n_f = 4$, $n_c = 5$ and $n = 9$; thus \mathbf{X} is a 9×6 matrix. Further, columns x_1^2 and x_2^2 are identical implying that these two effects are hopelessly and completely aliased, and hence the rank of matrix \mathbf{X} , $R(\mathbf{X})$, is not 6 but its rank is $R(\mathbf{X}) = 5$. Therefore, attempts at

inverting the 6×6 matrix ($\mathbf{X}'\mathbf{X}$) will prove to be futile because its determinant is zero.

Consequently, we redefine the design matrix \mathbf{X} consisting of only 5 independent columns as follows:

$$\mathbf{X} = \begin{array}{c} \begin{array}{cccccc} x_0 & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \end{array} \\ \begin{array}{cccccc} 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ \hline 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{array} \end{array}, \quad \mathbf{Y} = \begin{array}{c} \begin{array}{cccccc} x_0 & x_1 & x_2 & x_1^2 = x_2^2 & x_1x_2 \end{array} \\ \begin{array}{c} 39.3 \\ 40.0 \\ 40.9 \\ 41.5 \\ \hline 40.3 \\ 40.5 \\ 40.7 \\ 40.2 \\ 40.6 \end{array} \end{array} \quad \mathbf{X} = \begin{array}{c} \begin{array}{cccccc} x_0 & x_1 & x_2 & x_1^2 = x_2^2 & x_1x_2 \end{array} \\ \begin{array}{cccccc} 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ \hline 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{array} \end{array}$$

Column 4 of the above Design-matrix, \mathbf{X} , now represents the joint effect of x_1^2 and x_2^2

$$\text{and } \mathbf{X}'\mathbf{Y} = \begin{bmatrix} 364 \\ 3.10 \\ 1.30 \\ 161.700 \\ -0.100 \end{bmatrix}. \text{ These lead to the regression model (using the } \mathbf{IM} = \mathbf{X}'\mathbf{X} \text{ given below)}$$

$$\hat{y} = 40.46 + 0.775 x_1 + 0.325 x_2 - 0.0350x^2 - 0.0250x_1x_2. \quad (32a)$$

$$\mathbf{IM} = \mathbf{X}'\mathbf{X} = \mathbf{X}^T\mathbf{X} = \begin{bmatrix} 9 & 0 & 0 & 4 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 \\ 4 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 4 \end{bmatrix}$$

$$\mathbf{C} = (\mathbf{X}'\mathbf{X})^{-1} = \begin{bmatrix} 0.20 & 0 & 0 & -0.20 & 0 \\ 0 & 0.25 & 0 & 0 & 0 \\ 0 & 0 & 0.25 & 0 & 0 \\ -0.2 & 0 & 0 & 0.45 & 0 \\ 0 & 0 & 0 & 0 & 0.25 \end{bmatrix}$$

Note that the exact definition of the information matrix, \mathbf{IM} , is the $[\text{COV}(\hat{\boldsymbol{\beta}})]^{-1} = (\mathbf{X}'\mathbf{X})/\sigma_{\epsilon}^2$ if the vector $\hat{\boldsymbol{\beta}}$ were the MLEs and n were very large. However, the LSQESTs in regression are also the MLEs. Thus, I am taking the liberty to refer to the $\mathbf{X}'\mathbf{X}$ matrix on the LHS as the \mathbf{IM} for convenience. The inverse, \mathbf{C} , of this oblique \mathbf{IM} matrix is also given on the bottom LHS.

Further, the information matrix, \mathbf{IM} , given above is not diagonal implying that the design matrix \mathbf{X} is not orthogonal. This is due to the fact that the $x_1^2 = x_2^2 = x^2$ column of \mathbf{X} is not orthogonal to the x_0 column. Therefore, I will make a simple (linear) transformation in \mathbf{X} to attain orthogonality. The revised orthogonal design matrix \mathbf{X} , denoted \mathbf{X}_0 , is given below.

$$\mathbf{X}_0 = \begin{matrix} & x_0 & x_1 & x_2 & x^2-4/9 & x_1x_2 \\ \begin{bmatrix} 1 & -1 & -1 & 5/9 & 1 \\ 1 & -1 & 1 & 5/9 & -1 \\ 1 & 1 & -1 & 5/9 & -1 \\ 1 & 1 & 1 & 5/9 & 1 \\ 1 & 0 & 0 & -4/9 & 0 \\ 1 & 0 & 0 & -4/9 & 0 \\ 1 & 0 & 0 & -4/9 & 0 \\ 1 & 0 & 0 & -4/9 & 0 \\ 1 & 0 & 0 & -4/9 & 0 \end{bmatrix}, \end{matrix}$$

The design matrix, \mathbf{X}_0 , on the LHS is the orthogonal representation of the design matrix. The orthogonal (diagonal) \mathbf{IM} is now given below. Note that every column of \mathbf{X}_0 is a contrast and any 2 columns are orthogonal, i.e., their dot product vanishes.

$$\mathbf{IM}_0 = (\mathbf{X}_0^T \mathbf{X}_0) = \begin{bmatrix} 9 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 20/9 & 0 \\ 0 & 0 & 0 & 0 & 4 \end{bmatrix} \rightarrow \mathbf{C}_0 = (\mathbf{IM}_0)^{-1} = \begin{bmatrix} 1/9 & 0 & 0 & 0 & 0 \\ 0 & 0.25 & 0 & 0 & 0 \\ 0 & 0 & 0.25 & 0 & 0 \\ 0 & 0 & 0 & 0.45 & 0 \\ 0 & 0 & 0 & 0 & 0.25 \end{bmatrix}$$

$$\mathbf{X}'_0 \mathbf{Y} = \begin{bmatrix} 364 \\ 3.10 \\ 1.30 \\ -0.07778 \\ -0.100 \end{bmatrix} \rightarrow \hat{\boldsymbol{\beta}} = \mathbf{C}_0 \times (\mathbf{X}'_0 \mathbf{Y}) = \begin{bmatrix} 364/9 \\ 3.10/4 \\ 1.30/4 \\ -0.035 \\ -0.10/4 \end{bmatrix}. \text{ Therefore, the orthogonal}$$

representation of the regression model is given by:

$$\hat{y} = 40.444\bar{4} + 0.775x_1 + 0.325x_2 - 0.0350(x^2 - 4/9) - 0.0250x_1x_2, \quad (32b)$$

where x^2 simultaneously represents the effect $x_1^2 + x_2^2$. In order to compute the net (or partial) contribution of each regressor to the overall SS_{REG} , we need to compute S_{1y} , S_{2y} , $S_{11y} = S_{22y}$ and S_{12y} . Below, I will compute one of these and you should verify the values of the rest.

$$S_{11y} = S_{22y} = 161.7 - \frac{(\sum_{i=1}^9 x_1^2)(\sum y)}{9} = 161.7 - \frac{4 \times 364}{9} = -0.07777778.$$
 Similarly, $S_{1y} = 3.10$, $S_{2y} = 1.30$, and $S_{12y} = -0.100$. Therefore, $SS_{REG} = 0.775 \times 3.10 + 0.325 \times 1.3 - 0.035 \times (-0.0777777) - 0.025 \times (-0.10) = 2.830222$. Note that the regression model in (32a) and its orthogonal representation (32b) have identical $\hat{\beta}_j$, and therefore, $SS_{REG}(x_1, x_2) = 0.775 \times 3.10 + 0.325 \times 1.3 = 2.8250$ (with 2 *df*), which is identical to the SS(due to linear effects) given by Montgomery in the first line of ANOVA Table 11.2 at the bottom of page 422. Since $SS_T = SS_{Total} = USS - CF = 14724.7800 - 14721.77777 = 3.0022222$ (with 8 *df*), then for the linear model of Eq. (30), $SS_{RES} = SS_T - SS_{REG}(x_1, x_2) = 3.0022222 - 2.8250 = 0.1772222$. In order to test for LOF, we need to 1st compute the SS(PE=Pure Error) from replications at the design center. $SS(PE) = 0.3^2 + 0.5^2 + 0.7^2 + 0.2^2 + 0.6^2 - 2.3^2/5 = 0.1720$ (with 4 *df*). Hence, $SS(LOF) = 0.17722222 - 0.1720000 = 0.00522222$. For your benefit, below I am providing the ANOVA Table that is more expanded than Table 11.2 on page 422 of Montgomery (p. 410 of 6e) when fitting a 1st-order model.

Augmented Table 11.2 of Montgomery

Source	<i>df</i>	SS	MS	F_0	<i>P-value</i>
Total	8	3.00222222			<i>p</i>
1 st -order Model	2	2.8250	1.4125	47.82132	0.0002057
Residuals	6	0.17722222	0.029537		
Pure Error	4	0.17200	0.0430		
LOF (= x_{12}, x^2)	2	0.00522222	0.0026111	0.060724	0.9419342

Montgomery further divides the 2-*df* LOF SS into 2 orthogonal components due to $x_1^2 + x_2^2 \leftrightarrow x^2$ (Pure Quadratic), and due to the interaction term x_1x_2 . To confirm his results, we use results from regression and proceed as follows: $\delta_{11}^2 = \hat{\beta}_{11}^2 / C_{44} = \frac{(-0.035)^2}{9/20} = 0.002722222 = -0.035 \times (-0.0777778) = \hat{\beta}_{11} \times S_{11y}$, which is identical to the SS(Pure Quadratic)

given at the bottom of page 422. We may also re-compute this SS(Pure Quadratic) using the fact the \mathbf{X}_0 matrix on page 40 of these notes clearly shows that the $x_1^2 - 4/9 = x_2^2 - 4/9 = x^2 - 4/9$ column is indeed a contrast and therefore $SS(x^2)$ is given by

$$SS_{\text{Contrast}} = \frac{(5 \times y_f. - 4 \times y_c.)^2}{4 \times 5^2 + 5 \times (-4)^2} = \frac{(5 \times 161.7 - 4 \times 202.3)^2}{4 \times 5^2 + 5 \times (-4)^2} = 0.002722222,$$

where by $y_f.$ we mean the sum of responses at the factorial portion of the design and $y_c.$ represents the subtotal at the center. Finally, the x_1x_2 column in the \mathbf{X}_0 matrix on page 40 of these notes shows that this column is also a contrast and thus $SS(\text{Interaction}) = SS(x_1x_2) = SS(x_{12}) = (39.3 - 40.0 - 40.9 + 41.5 + 0)^2/4 = 0.0025$. Note that due to orthogonality, $SS(x^2) + SS(x_1x_2) = 0.00522222 = SS(\text{LOF})$. Further, the LOF test in the ANOVA table on the previous page reflects the contributions of the quadratic terms, and as long as these quadratic contributions remain trivial, then we are far from the optimum region.

Before leaving 1st-order experimentation, we must assert that because the information

matrix, \mathbf{IM}_0 , is orthogonal, then $\sum_{j=1}^4 \delta_j^2 = \frac{0.775^2}{0.25} + \frac{0.325^2}{0.25} + \frac{(-0.035)^2}{0.45} + \frac{(-0.025)^2}{0.25} =$

$2.830222222 = SS_{\text{REG}} = SS(\text{Model})$, as was computed on page 41 of my notes. If a design matrix is oblique (i.e., not orthogonal) and cannot be orthogonalized by a linear transformation, then

most likely $\sum_{j=1}^k \delta_j^2 < SS_{\text{REG}}$.

NALYSIS OF SECOND ORDER SURFACE (Section 11.3 of Montgomery)

Consider the response surface $y = \eta + \epsilon$, where $\eta = E(y)$ and $\epsilon \sim N(0, \sigma_\epsilon^2)$, given in Eq. (11.4) near the bottom of page 425 (p. 413 of Montgomery's 6th edition). In order to comprehend axes translation followed by axes rotation, it will be easiest if we work with the specific response surface $\eta = E(y) = 8 - 18x_1 + 18x_2 + 5x_1^2 + 5x_2^2 - 8x_1x_2$. Then, for our example the parameter values are $\beta_0 = 8$, $\beta_1 = -18$, $\beta_2 = 18$, $\beta_{11} = \beta_{22} = 5$, and the interaction coefficient $\beta_{12} = -8$. Recall what we mean by the contours of a surface! These are the points

at which the surface η has the same constant value, say specifically $\eta = 10 = c$ (note that I could have selected any other feasible constant value). Further, the graph of η versus the independent variables x_1 and x_2 will be in 3-D, while the graph of the contour $8 - 18x_1 + 18x_2 + 5x_1^2 + 5x_2^2 - 8x_1x_2 = 10$ will be in 2-D. The obvious question that now arises 'is this last contour, with $\eta = c = 10$, an ellipse, a hyperbola, or just a straight line?'

To answer the above question, we must 1st determine the optimum nature of the surface η by obtaining its stationary point \mathbf{x}_o . Note that Montgomery uses \mathbf{x}_s for the location of the stationary point, but I prefer the subscript o (or O) to s (o = optimal; further, o is perhaps more universal than s). I will go thru the procedure W/O explanation as the optimization process by now should be self-explanatory.

$$\frac{\partial \eta}{\partial x_1} = -18 + 10x_1 - 8x_2, \text{ and } \frac{\partial \eta}{\partial x_2} = 18 + 10x_2 - 8x_1.$$

In order to find \mathbf{x}_o (assuming it exists), we must require that the above two partial derivatives to be zero at the optimum vector \mathbf{x}_o . This leads to a heterogeneous system of 2 equations with 2 unknowns shown below.

$$\begin{cases} 10x_1 - 8x_2 = 18 \\ -8x_1 + 10x_2 = -18 \end{cases} \longrightarrow \mathbf{x}_o = \begin{bmatrix} x_1 = 1 \\ x_2 = -1 \end{bmatrix}. \text{ To determine whether } \mathbf{x}_o \text{ is a point of minimum}$$

response, maximum response, or a saddle point (or minimax), we must examine the

$\partial^2 \eta / \partial x_i \partial x_j$, $i, j = 1, 2$ at \mathbf{x}_o . Since both $\partial^2 \eta / \partial x_1^2 = 10$, $\partial^2 \eta / \partial x_2^2 = 10 > 0$ and $\partial^2 \eta / \partial x_1 \partial x_2 = -8$, showing that $(\partial^2 \eta / \partial x_1^2) \times (\partial^2 \eta / \partial x_2^2) = 100 > (\partial^2 \eta / \partial x_1 \partial x_2)^2 = (-8)^2$, then \mathbf{x}_o is a point of minimum response and η is said to be strictly convex. Below, I will again summarize the

sufficient conditions for all types of optimality: **(1)** Point of (local) minimum response: $\frac{\partial \eta}{\partial x_i} = 0$

for all i , $\partial^2 \eta / \partial x_i^2 > 0$ for all i , and $(\partial^2 \eta / \partial x_i^2) \times (\partial^2 \eta / \partial x_j^2) > (\partial^2 \eta / \partial x_i \partial x_j)^2$ for all $i \neq j$

all evaluated at \mathbf{x}_o .

(2) Point of (local) maximum response: $\frac{\partial \eta}{\partial x_i} = 0$ for all i , $\partial^2 \eta / \partial x_i^2 < 0$ for all i , and

$(\partial^2 \eta / \partial x_i^2) \times (\partial^2 \eta / \partial x_j^2) > (\partial^2 \eta / \partial x_i \partial x_j)^2$ for $i \neq j$ all evaluated at \mathbf{x}_o and then η is called a

strictly concave surface.

(3) A saddle point : $\frac{\partial \eta}{\partial x_i} = 0$ for all i at \mathbf{x}_o , but $[(\partial^2 \eta / \partial x_i^2) \times (\partial^2 \eta / \partial x_j^2)]_{\mathbf{x}_o} <$

$[(\partial^2 \eta / \partial x_i \partial x_j)^2]_{\mathbf{x}_o}$ for at least one $i \neq j$.

If $(\partial^2 \eta / \partial x_i^2) \times (\partial^2 \eta / \partial x_j^2) = (\partial^2 \eta / \partial x_i \partial x_j)^2$, $i \neq j$, at \mathbf{x}_o , it will not be clear as to what type of optimum (if any) the surface η has at the exceptional point \mathbf{x}_o and further investigation is necessary. It is sometimes possible that no assessment can be made about the optimal nature of the RS (response surface). Note that a function is strictly convex (concave) iff the minimum (maximum) on any interval occurs at one of the end points.

Exercise 12. Identify the stationary points and their nature for the following 6

surfaces. (a) $\eta = 1 - x_1^2 - x_2^2$, (b) $\eta = x_1^2 + x_2^2$, (c) $\eta = x_1 x_2$, (d) $\eta = 1 - x_1^2 x_2^2$, (e) $\eta = x_1^2 x_2^2$, and (f) $\eta = x_1^3 x_2^2$.

Because our example surface $\eta = 8 - 18x_1 + 18x_2 + 5x_1^2 + 5x_2^2 - 8x_1x_2$ meets the criterion

(1) above, $\mathbf{x}_o = \begin{bmatrix} x_1 = 1 \\ x_2 = -1 \end{bmatrix}$ is a point of minimum response. To determine the global minimum

value of the response, we simply insert \mathbf{x}_o into the surface above η to obtain $\eta_o = 8 - 18 - 18 + 5 + 5 + 8 = -10$. Therefore, for our surface example, a contour of $\eta = -11.5$ does not exist

because $\eta = 8 - 18x_1 + 18x_2 + 5x_1^2 + 5x_2^2 - 8x_1x_2 \geq -10 = \eta_o$ for all vectors $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ in the

universe of 2-D. Note that for a surface whose exceptional point is one of minimum response, the objective will be to move in the direction of the path of steepest descent (not ascent).

Our next objective is to translate the (x_1, x_2) axes with origin at $(0, 0)$ to a new set of (X_1, X_2) axes whose origin is at \mathbf{x}_o . This translation will eliminate the two linear terms in our 2nd-order surface $\eta = 8 - 18x_1 + 18x_2 + 5x_1^2 + 5x_2^2 - 8x_1x_2$. Accordingly, we make the transformation $X_1 = x_1 - 1$ and $X_2 = x_2 + 1$ and substitute these into the surface equation η . In

matrix notation we have $\mathbf{X} = \mathbf{x} - \mathbf{x}_o = \begin{bmatrix} x_1 - 1 \\ x_2 + 1 \end{bmatrix}$. This eliminates the linear terms and reduces η

to:
$$\eta = -10 + 5X_1^2 + 5X_2^2 - 8X_1X_2. \quad (33)$$

Note that partial differentiation of equation (33) wrt $X_1 = x_1 - 1$ and $X_2 = x_2 + 1$ verifies the fact that in the translated coordinate system the optimal occurs at $\mathbf{X}_0 = [0 \quad 0]'$, and this in turn implies that a translation of axes to the point of optimum removes the linear terms from the model. Since the nature of a surface of the type (34) given below

$$\eta = \eta_0 + \lambda_{11} w_1^2 + \lambda_{22} w_2^2 = \eta_0 + \lambda_1 w_1^2 + \lambda_2 w_2^2 \quad (34)$$

is well known, our next objective is to rotate the (X_1, X_2) axes of the model (33) thru an angle θ into a (w_1, w_2) axes to force its interaction term, which is equal to $-8X_1X_2$, to zero. The equation of the RS in the rotated axis is given in Eq. (34). I will show the exact geometry in class that leads to the following orthogonal transformation.

$$\begin{cases} X_1 = w_1 \cos \theta - w_2 \sin \theta \\ X_2 = w_1 \sin \theta + w_2 \cos \theta \end{cases}. \text{ In matrix form this transformation can be written as } \mathbf{X} =$$

$$\mathbf{M}\mathbf{W}, \text{ where } \mathbf{X} = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}, \mathbf{M} = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}, \mathbf{W} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}, \text{ and } \mathbf{M} \text{ is called the rotation}$$

matrix.

Definition. A square matrix, \mathbf{B} , is orthogonal iff $\mathbf{B}^{-1} = \mathbf{B}^T = \mathbf{B}'$, i.e., a matrix is orthogonal iff its inverse is equal to its transpose.

Exercise 13. (a) Show that the above rotation matrix \mathbf{M} is indeed orthogonal. (b) Substitute the transformation $\mathbf{X} = \mathbf{M}\mathbf{W}$ into equation (33) and equate this to Eq. (34) in order to determine the angle of rotation θ such that the interaction term $\lambda_{12}w_1w_2 = 0$, and as a result show that our response surface equation reduces to $\eta = -10 + 9w_1^2 + w_2^2 = \eta_0 + 9w_1^2 + w_2^2$. Note that the value of $\eta_0 = -10$ stays in tact after the rotation of axes. (c) For the general surface $\eta = \eta_0 + \beta_{11}X_1^2 + \beta_{22}X_2^2 + \beta_{12}X_1X_2$ show that the coefficient of w_1w_2 is equal to $\lambda_{12} = [(\beta_{22} - \beta_{11})\sin(2\theta) + \beta_{12}\cos(2\theta)]/2$, and hence the angle of rotation, θ , must satisfy the equation

$$\tan(2\theta) = \frac{\beta_{12}}{\beta_{11} - \beta_{22}}. \quad (35)$$

Note that λ_1 and λ_2 should be selected such that the corresponding eigenvectors \mathbf{M}_1

and \mathbf{M}_2 result in the rotation matrix $\mathbf{M} = [\mathbf{M}_1 \quad \mathbf{M}_2] = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$.

In your development in part (c) of **Exercise 13** you will also observe that $\lambda_{11} = \lambda_1 =$

$$\beta_{11}\cos^2(\theta) + \beta_{22}\sin^2(\theta) + \beta_{12}\cos(\theta)\sin(\theta) = \frac{(\beta_{11} + \beta_{22}) + \beta_{11}\cos(2\theta) - \beta_{22}\cos(2\theta) + \beta_{12}\sin(2\theta)}{2}, \text{ and } \lambda_2 =$$

$$\lambda_{22} = \beta_{11}\sin^2(\theta) + \beta_{22}\cos^2(\theta) - \beta_{12}\cos(\theta)\sin(\theta) = \frac{(\beta_{11} + \beta_{22}) - \beta_{11}\cos(2\theta) + \beta_{22}\cos(2\theta) - \beta_{12}\sin(2\theta)}{2},$$

where $\sin(2\theta) = \beta_{12} / \sqrt{(\beta_{11} - \beta_{22})^2 + \beta_{12}^2}$ and I have made use of the trigonometric identities

$$\cos^2(\theta) = \frac{1 + \cos(2\theta)}{2} \text{ and } \sin^2(\theta) = \frac{1 - \cos(2\theta)}{2}; \text{ further for your info, } \sin(\theta_1 + \theta_2) =$$

$$\sin(\theta_1)\cos(\theta_2) + \cos(\theta_1)\sin(\theta_2), \text{ and } \cos(\theta_1 + \theta_2) = \cos(\theta_1)\cos(\theta_2) - \sin(\theta_1)\sin(\theta_2).$$

To determine what type of contours the surface “ $\eta - \eta_0 = \lambda_1 w_1^2 + \lambda_2 w_2^2$ ” has, or what curve the contour $\lambda_1 w_1^2 + \lambda_2 w_2^2 = \eta - \eta_0 = C_0$ represents, we need to examine the product $\lambda_1\lambda_2$.

Exercise 13(d). Use your results from part (c) to prove that $\lambda_1\lambda_2 = \beta_{11}\beta_{22} - (\beta_{12})^2/4$.

There are 3 possibilities for the product $\lambda_1\lambda_2 = \det(\mathbf{B}) = \beta_{11}\beta_{22} - (\beta_{12})^2/4$:

$$\text{(i) } \det(\mathbf{B}) = \lambda_1\lambda_2 > 0, \text{ (ii) } \lambda_1\lambda_2 = 0, \text{ (iii) } \lambda_1\lambda_2 < 0.$$

The Case of $\det(\mathbf{B}) = \lambda_1\lambda_2 = \beta_{11}\beta_{22} - (\beta_{12})^2/4 > 0$

Clearly in this case λ_1 and λ_2 must have the same signs. If C_0 has the opposite sign to those of λ_i 's, then such contours of η do not exist. On the other hand, if C_0 has the same sign as those of λ_i 's, then the contours of $\eta = \eta_0 + \lambda_1 w_1^2 + \lambda_2 w_2^2 = c$ represent ellipses centered around \mathbf{x}_0 .

The Case of $\det(\mathbf{B}) = \lambda_1\lambda_2 = \beta_{11}\beta_{22} - (\beta_{12})^2/4 = 0$

This case occurs iff either $\lambda_1 = 0$ or $\lambda_2 = 0$. Then the contours of η are simply parallel straight lines and this case generates the ridge system, described by Montgomery on p. 434 (pp. 422-423 of the 6th edition).

The Case of $\det(\mathbf{B}) = \lambda_1\lambda_2 = \beta_{11}\beta_{22} - (\beta_{12})^2 / 4 < 0$

The coefficients λ_1 and λ_2 must have opposite signs. If $C_0 \neq 0$, then the contours $\lambda_1 w_1^2 + \lambda_2 w_2^2 = C_0$ represent hyperbolas. If C_0 has the same sign as λ_1 , the symmetry axis of the hyperbolas coincides with w_1 , and vice a versa for w_2 . If $C_0 = 0$, then there are only 2 contour lines going thru the translated origin \mathbf{x}_0 .

TRANSLATION AND ROTATION OF AXES USING MATRIX ALGEBRA

Consider the following full quadratic fitted regression model for 3 independent

variables:
$$\hat{y} = \hat{\beta}_0 + \sum_{i=1}^3 \hat{\beta}_i x_i + \sum_{i=1}^3 \hat{\beta}_{ii} x_i^2 + \sum_{i=1}^2 \sum_{j>i} \hat{\beta}_{ij} x_i x_j, \quad (36)$$

where for simplicity and specificity I am letting $k = 3$ independent variables; this is unlike Montgomery's Model (11.4) on page 425 (p. 413 of the 6th edition) which is for general k . We first write model (36) in matrix form as $\hat{y} = \hat{\beta}_0 + \mathbf{x}'\hat{\boldsymbol{\beta}} + \mathbf{x}'\mathbf{B}\mathbf{x}$, (37)

where the vector $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$, $\hat{\boldsymbol{\beta}} = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \hat{\beta}_3 \end{bmatrix}$, and the 3×3 matrix $\mathbf{B} = \begin{bmatrix} \hat{\beta}_{11} & \hat{\beta}_{12}/2 & \hat{\beta}_{13}/2 \\ \hat{\beta}_{12}/2 & \hat{\beta}_{22} & \hat{\beta}_{23}/2 \\ \hat{\beta}_{13}/2 & \hat{\beta}_{23}/2 & \hat{\beta}_{33} \end{bmatrix}$.

To fully understand the relationship between (36) and (37), you should take a few minutes to insert the definitions of vector \mathbf{X} and matrix \mathbf{B} into (37) and show that Eq. (37) indeed reduces to (36). Further, you should note that all 3 terms on the RHS of (37) are indeed scalars.

Exercise 14. (a) Use partial differentiation with respect to x_i ($i = 1, 2, 3$) to show that the optimal solution of model (36) is given by the vector $\mathbf{x}_0 = -(\mathbf{B}^{-1}\hat{\boldsymbol{\beta}})/2$. (b) Verify the result of part (a) by vector partial differentiation of equation (37). (c) Use the results of part (b) to show that the optimal value of \hat{y} is given by $\hat{y}_0 = \hat{\beta}_0 + \mathbf{x}'_0\hat{\boldsymbol{\beta}}/2$. Note that the $\text{Trace}(\mathbf{B}) =$

$$\sum_{j=1}^k \lambda_j \text{ and the } \det(\mathbf{B}) = \prod_{j=1}^k \lambda_j, \text{ where it can be shown that } \lambda_j\text{'s are the eigenvalues (or}$$

characteristic roots) of the symmetric matrix \mathbf{B} .

1. TRANSLATION OF AXES TO \mathbf{x}_0

We 1st translate the coordinates $\mathbf{x}' = [x_1 \quad x_2 \quad x_3]$ to $\mathbf{X} = \mathbf{x} - \mathbf{x}_0$, where $\mathbf{x}_0 = -\frac{1}{2}\mathbf{B}^{-1}\hat{\boldsymbol{\beta}}$ is the stationary (or exceptional) point at which \hat{y} is optimized and clearly \mathbf{X} is also a $k \times 1$ vector ($k = 3$ for our example). Next, it is necessary to express \hat{y} in (37) in terms of the translated coordinates \mathbf{X} , and thus we substitute $\mathbf{x} = \mathbf{X} + \mathbf{x}_0$ into the vector equation (37). This will, after 6 algebraic steps, result in

$$\hat{y} = \hat{\beta}_0 + \frac{1}{2}\hat{\boldsymbol{\beta}}'\mathbf{x}_0 + \mathbf{X}'\mathbf{B}\mathbf{X} = \hat{y}_0 + \mathbf{X}'\mathbf{B}\mathbf{X} \quad (38)$$

Exercise (14d). Derive equation (38) according to my statement in the above paragraph.

Equation (38) clearly shows that if Y is an STB QCH (i.e., \mathbf{x}_0 is a point of minimum response), then for certain $\mathbf{X}'\mathbf{B}\mathbf{X} > 0$, i.e., the quadratic form $\mathbf{X}'\mathbf{B}\mathbf{X}$ is positive definite. On the other hand, if Y is an LTB type QCH (i.e., \mathbf{x}_0 is a point of maximum response), then for certain $\mathbf{X}'\mathbf{B}\mathbf{X} < 0$, i.e., the quadratic form $\mathbf{X}'\mathbf{B}\mathbf{X}$ is negative definite. If \mathbf{x}_0 is a saddle point (i.e., neither a point of minimum or maximum response), then the quadratic form $\mathbf{X}'\mathbf{B}\mathbf{X}$ is indefinite. An indefinite quadratic form can become positive for some vectors, \mathbf{X} , and negative for others, i.e., $-\infty < \mathbf{X}'\mathbf{B}\mathbf{X} < \infty$. Further, regardless of the nature of y , the critical value of \hat{y} occurs at $\mathbf{X}_0 = [0 \quad 0 \quad 0]'$. Put differently, the origin of the coordinate system (X_1, X_2, X_3) is now at the stationary point \mathbf{x}_0 , while that of (x_1, x_2, x_3) is at $(0, 0, 0)$.

Exercise 14(e). Substitute $\mathbf{x}_0 = -\frac{1}{2}\mathbf{B}^{-1}\hat{\boldsymbol{\beta}}$ in (38) to verify that $\mathbf{X}'\mathbf{B}\mathbf{X}$ must equal to zero at \mathbf{x}_0 , which again verifies that the optimum response occurs at $\mathbf{X}_0 = [0 \quad 0 \quad 0]'$.

Now, consider a contour of \hat{y} ; recall that all the values of \hat{y} on a contour are equal to the same constant, say c . Then, equation (38) shows that on this contour $c = \hat{y}_0 + \mathbf{X}'\mathbf{B}\mathbf{X}$.

Since c and \hat{y}_0 are both constants, then the functional form of any contour is given by

$$\mathbf{X}'\mathbf{B}\mathbf{X} = c - \hat{y}_0 = C_0 \quad (39)$$

where $C_0 = c - \hat{y}_0$ is also a constant. Equation (39) is called a quadratic form because its LHS

contains only terms of the type X_i^2 ($i = 1, 2, 3$) and $X_i X_j$ ($i \neq j$). Our next objective is to rotate the coordinates (X_1, X_2, X_3) in such a manner that the quadratic form in (39) has no cross-product terms $\hat{\beta}_{ij} X_i X_j$ ($i \neq j$). That is, we rotate the (X_1, X_2, X_3) axes such that the quadratic form $\mathbf{X}'\mathbf{B}\mathbf{X}$ transforms to the pure quadratic form $\sum_{i=1}^3 \lambda_i w_i^2$ in the (w_1, w_2, w_3) coordinate system. Then in the rotated coordinates, from equation (38) our model becomes

$$\hat{y} = \hat{y}_0 + \sum_{i=1}^3 \lambda_i w_i^2 \quad (40a)$$

2. ROTATION OF AXES to Pure Quadratic Forms

Since the nature of contours of the following pure quadratic form

$$\sum_{i=1}^3 \lambda_i w_i^2 = C_0 \quad (40b)$$

having no interaction terms, is well known, then our objective is to rotate \mathbf{X} into \mathbf{W} such that the rotated quadratic form has no cross-product terms $\lambda_{ij} w_i w_j$ and is as a result diagonalized. Accordingly, let \mathbf{M} be a 3×3 rotation matrix such that $\mathbf{M}\mathbf{X} = \mathbf{W}$, (or $\mathbf{W} = \mathbf{M}^{-1}\mathbf{X}$), where

$$\mathbf{M} = \begin{bmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{bmatrix}. \text{ It turns out that the rotation matrix } \mathbf{M} \text{ has to be an orthogonal}$$

matrix because otherwise the rotation will not accomplish the task of reducing the original quadratic form (38) to a diagonal form. Substituting $\mathbf{M}\mathbf{X}$ for \mathbf{X} into equation (39) results in $(\mathbf{M}\mathbf{X})'\mathbf{B}(\mathbf{M}\mathbf{X}) = C_0 \rightarrow \mathbf{W}'(\mathbf{M}'\mathbf{B}\mathbf{M})\mathbf{W} = \mathbf{W}'\boldsymbol{\lambda}\mathbf{W} = C_0$ (41)

In order to compare Eq. (41) with equation (40b), we write (40b) in matrix form:

$$C_0 = \sum_{i=1}^3 \lambda_i w_i^2 = \begin{bmatrix} w_1 & w_2 & w_3 \end{bmatrix} \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix} = \mathbf{W}'\boldsymbol{\lambda}\mathbf{W} \quad (42)$$

where $\boldsymbol{\lambda}$ is a 3×3 diagonal matrix. Comparing (41) with (42), we deduce that $\mathbf{W}'(\mathbf{M}'\mathbf{B}\mathbf{M})\mathbf{W}$

must equal to $\mathbf{W}'\boldsymbol{\lambda}\mathbf{W}$, and hence $\mathbf{M}'\mathbf{B}\mathbf{M} = \boldsymbol{\lambda}$ (43)

Eq. (43) shows that in matrix operations, the problem of axis rotation such that the interaction terms $\lambda_{ij}w_iw_j$ ($i \neq j$) vanish becomes one of choosing the 3×3 (in general, $k \times k$) rotation matrix \mathbf{M} in such a manner that $\mathbf{M}^T \mathbf{B} \mathbf{M}$ becomes a diagonal matrix $\hat{\lambda}$. This will require that \mathbf{M} to be an orthogonal matrix, i.e., \mathbf{M} must be constructed in such a manner that $\mathbf{M}^{-1} = \mathbf{M}' = \mathbf{M}^T$, or $\mathbf{M} \times \mathbf{M}' = \mathbf{I}_k$, where $k = 3$ for our example. Therefore, to put Eq. (11.5) on page 426 (415 of 6e) of Montgomery in the rotated form (11.9) on his p. 428 (416 of 6e), we must find an orthogonal $k \times k$ matrix such that

$$\mathbf{M}^T \mathbf{B} \mathbf{M} = \mathbf{M}' \mathbf{B} \mathbf{M} = \mathbf{M}^{-1} \mathbf{B} \mathbf{M} = \hat{\lambda} \rightarrow \mathbf{B} \mathbf{M} = \mathbf{M} \hat{\lambda} \quad (44)$$

Letting $\mathbf{M} = [\mathbf{M}_1 \quad \mathbf{M}_2 \quad \mathbf{M}_3]$, where \mathbf{M}_j 's are the 3×1 vectors near the bottom of page 49, we can rewrite equation (44) as $\mathbf{B} \mathbf{M} = \mathbf{B} [\mathbf{M}_1 \quad \mathbf{M}_2 \quad \mathbf{M}_3] = [\mathbf{B} \mathbf{M}_1 \quad \mathbf{B} \mathbf{M}_2 \quad \mathbf{B} \mathbf{M}_3] =$

$$= \mathbf{M} \hat{\lambda} = [\mathbf{M}_1 \quad \mathbf{M}_2 \quad \mathbf{M}_3] \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} = [\lambda_1 \mathbf{M}_1 \quad \lambda_2 \mathbf{M}_2 \quad \lambda_3 \mathbf{M}_3] \quad (45)$$

Eqs. (44) and (45) show that $\mathbf{M}' \mathbf{B} \mathbf{M}$ becomes the diagonal matrix $\hat{\lambda}$ iff we select λ_j 's and \mathbf{M}_j 's in such a manner that

$$\mathbf{B} \mathbf{M}_j = \lambda_j \mathbf{M}_j \quad \text{for all } j = 1, 2, 3, \dots, k \quad (46)$$

Equations of the form in (46) are called eigenvalue (or characteristic) equations; $\lambda_1, \lambda_2, \lambda_3, \dots$ are called the eigenvalues of the matrix \mathbf{B} , and \mathbf{M}_j ($j = 1, 2, 3, \dots$) are called its eigenvectors. To obtain the solutions \mathbf{M}_j , we rewrite Eq. (46) as

$$\mathbf{B} \mathbf{M}_j - \lambda_j \mathbf{M}_j = 0 \rightarrow (\mathbf{B} - \lambda_j \mathbf{I}_k) \mathbf{M}_j = 0 \quad (47)$$

Since \mathbf{M}_j 's cannot equal to the zero vector, then we must require that $(\mathbf{B} - \lambda_j \mathbf{I}_k) \mathbf{M}_j = 0$; but this is a homogeneous system of $k = 3$ equations with $k = 3$ unknowns m_{1j} , m_{2j} , and m_{3j} . The homogeneous system of equations in (47) has a nontrivial (i.e., \mathbf{M}_j not equal to the zero vector) iff the determinant of the coefficients, $\det(\mathbf{B} - \lambda_j \mathbf{I}_k)$, is zero. Therefore, in order to obtain the eigenvectors \mathbf{M}_j , we must 1st solve for λ_j 's from

$$|\mathbf{B} - \lambda_j \mathbf{I}_k| = \det(\mathbf{B} - \lambda_j \mathbf{I}) = 0$$

and then use Eq. (47) to obtain the eigenvectors \mathbf{M}_j of \mathbf{B} . It is necessary that these eigenvectors to be of unit length and perpendicular to each other so that the rotation matrix $\mathbf{M} = [\mathbf{M}_1 \quad \mathbf{M}_2 \quad \mathbf{M}_3]$ becomes orthogonal. To illustrate the above concepts, I will go thru

the detailed explanation of Montgomery's Example 11.2 on his pp. 428-434 (pp. 416-422 of the 6th edition).

From the computer output on page 431 (p. 419 of the 6th edition), we have:

For our surface example $\hat{y} = 79.940 + 0.994975x_1 + 0.515165x_2 - 1.37625x_1^2 - 1.00125x_2^2 +$

$0.2500x_1x_2$ and hence $\tan(2\theta) = \frac{\beta_{12}}{\beta_{11} - \beta_{22}} = \frac{0.25}{-1.37625 + 1.00125} = -2/3 \rightarrow 2\theta =$

-0.5880026044 Radians $\rightarrow \theta = -0.294001302$ Rad = -16.845033763 degrees. For the above

model, $\hat{\beta} = \begin{bmatrix} 0.994975 \\ 0.515165 \end{bmatrix}$, $\mathbf{x} = [x_1 \quad x_2]'$, and $\mathbf{B} = \begin{bmatrix} -1.37625 & 0.1250 \\ 0.1250 & -1.00125 \end{bmatrix}$,

and $\mathbf{B}^{-1} = \begin{bmatrix} -0.734946 & -0.09175354 \\ -0.09175354 & -1.0102064 \end{bmatrix}$. Further, Matlab computations give $\mathbf{x}_o =$

$-\mathbf{B}^{-1}\hat{\beta}/2 = \begin{bmatrix} 0.3892604 \\ 0.3058577 \end{bmatrix}$ and $\hat{y}_o = 80.21244$. This last optima can also be obtained thru

direct partial differentiation of \hat{y} with respect to x_1 and x_2 and requiring that both partial derivatives to be zero. Recall that our 1st task is to translate the (x_1, x_2) coordinate system to

the new origin at $\mathbf{x}_o = \begin{bmatrix} 0.3892604 \\ 0.3058577 \end{bmatrix}$. This is done thru the translation $\mathbf{X} = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \mathbf{x} - \mathbf{x}_o$

$= \begin{bmatrix} x_1 - 0.3892604 \\ x_2 - 0.3058577 \end{bmatrix}$. Note that the optimal value of y in the translated coordinate system now

occurs at $\mathbf{x}_o = \begin{bmatrix} X_1 = 0 \\ X_2 = 0 \end{bmatrix}$. So, in the new coordinate system the above model can be written as

$\hat{y} = 80.21244 - 1.37625X_1^2 - 1.00125X_2^2 + 0.25X_1X_2 = \hat{y}_o + \mathbf{X}'\mathbf{B}\mathbf{X}$. However, this last model in

(X_1, X_2) coordinates has the interaction term $0.25X_1X_2$, and the only transformation that removes this cross-product term is a rotation of the coordinate system (X_1, X_2) into the (w_1, w_2)

coordinates that will yield $\hat{y} = \hat{y}_o + \lambda_1 w_1^2 + \lambda_2 w_2^2$. This task is accomplished by the rotation

matrix \mathbf{M} thru the transformation $\mathbf{X} = \mathbf{M}\mathbf{W}$. As shown on pages 49-51 of these notes, we must

1st obtain the eigenvalues of the matrix \mathbf{B} by requiring that the $\det(\mathbf{B} - \lambda\mathbf{I}_2) = 0$, i.e., we must

require that we solve the following characteristic equation for λ .

$$|\mathbf{B} - \lambda \mathbf{I}_k| = \left| \begin{bmatrix} -1.37625 & 0.1250 \\ 0.1250 & -1.00125 \end{bmatrix} - \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix} \right| = \left| \begin{bmatrix} -1.37625 - \lambda & 0.125 \\ 0.125 & -1.00125 - \lambda \end{bmatrix} \right| =$$

$$(1.37625 + \lambda)(1.00125 + \lambda) - 0.015625 = \lambda^2 + 2.3775 \lambda + 1.36234531 = 0 \rightarrow$$

$\lambda_1 = -1.41409696$, and $\lambda_2 = -0.96340305$. I checked these eigenvalues with Matlab function $\text{eig}(\mathbf{B})$, and Matlab gave $\lambda_1 = -1.4140969547$ and $\lambda_2 = -0.9634030453$.

To obtain the eigenvector \mathbf{M}_1 , we have to insert $\lambda_1 = -1.4140970$ (6 decimal accuracy) into equation (47) and solve the resulting homogeneous system of 2 equations with 2

$$\text{unknowns, i.e., } (\mathbf{B} - \lambda_1 \mathbf{I}_k) \mathbf{M}_1 = \left(\begin{bmatrix} -1.37625 & 0.1250 \\ 0.1250 & -1.00125 \end{bmatrix} - \begin{bmatrix} -1.414097 & 0 \\ 0 & -1.414097 \end{bmatrix} \right) \begin{bmatrix} m_{11} \\ m_{21} \end{bmatrix}$$

$$= \begin{bmatrix} 0.037847 & 0.1250 \\ 0.1250 & 0.412847 \end{bmatrix} \times \begin{bmatrix} m_{11} \\ m_{21} \end{bmatrix}. \text{ The resulting homogeneous system is}$$

$$\begin{cases} 0.037847 m_{11} + 0.1250 m_{21} = 0 \\ 0.1250 m_{11} + 0.412847 m_{21} = 0 \end{cases}. \text{ Note that if the determinant of this system were not}$$

equal to zero, then the 2 equations would be inconsistent and there would be only a trivial solution $m_{11} = m_{21} \equiv 0$. However, recall that we computed both λ_1 and λ_2 in such a manner

$$\text{that would force the determinant of } (\mathbf{B} - \lambda_1 \mathbf{I}_k) = \begin{bmatrix} 0.037847 & 0.1250 \\ 0.1250 & 0.412847 \end{bmatrix} \text{ equal to zero. This}$$

is why λ_1 and λ_2 are called the characteristic roots of \mathbf{B} . Therefore, there are infinite number of solutions to the above system of 2 equations with 2 unknowns. Clearly, the 1st equation

requires that we select $m_{11} = -\frac{0.1250}{0.037847} \times m_{21}$. Now given a value of m_{21} , then we will find

the corresponding value of m_{11} . For example, suppose you specify $m_{21} = -1$, then $m_{11} = 3.3027756$. Similarly, using $(\mathbf{B} - \lambda_2 \mathbf{I}_k) \mathbf{M}_2 = \mathbf{0}$ you may verify that for this case the value of $m_{12} = 1$ and $m_{22} = 3.3027756$ will also be a possible solution. Note that the two vectors $\mathbf{M}_1 =$

$$\begin{bmatrix} 3.3027756 \\ -1 \end{bmatrix} \text{ and } \mathbf{M}_2 = \begin{bmatrix} 1 \\ 3.3027756 \end{bmatrix} \text{ are indeed orthogonal because } (\mathbf{M}_1^T) \times \mathbf{M}_2 \equiv (\mathbf{M}_2^T) \times \mathbf{M}_1 =$$

$$0, \text{ but the problem with this solution set is the fact that the matrix } \mathbf{M} = \begin{bmatrix} 3.3027756 & 1 \\ -1 & 3.3027756 \end{bmatrix}$$

is not an orthogonal matrix because its transpose given by $\mathbf{M}^T = \mathbf{M}' =$

$\begin{bmatrix} 3.3027756 & -1 \\ 1 & 3.3027756 \end{bmatrix}$ is not equal to its inverse. In fact the inverse of the matrix $\mathbf{M} =$

$\begin{bmatrix} 3.3027756 & 1 \\ -1 & 3.3027756 \end{bmatrix}$ is given by $\begin{bmatrix} 0.27735037 & -0.08397504 \\ 0.08397504 & 0.27735037 \end{bmatrix}$, which is obviously not

equal to $\mathbf{M}^T = \mathbf{M}'$. In order to make \mathbf{M} an orthogonal rotation matrix, i.e. such that $\mathbf{M}^{-1} = \mathbf{M}^T = \mathbf{M}'$, we must normalize each of its component \mathbf{M}_1 and \mathbf{M}_2 . This implies that both vectors \mathbf{M}_1

and \mathbf{M}_2 must be of unit length. Therefore, $\mathbf{M}_1 = \begin{bmatrix} 3.3027756 \\ -1 \end{bmatrix} / \sqrt{3.3027756^2 + (-1)^2} =$

$\begin{bmatrix} 0.957092 \\ -0.289784 \end{bmatrix}$, which is a unit vector in the w_1 direction. Further, the largest eigenvalue in

absolute value gives the direction of highest variation. Similarly, $\mathbf{M}_2 = \begin{bmatrix} 0.289784 \\ 0.957092 \end{bmatrix}$, which is a

unit vector in the w_2 direction. Further, note that now the rotation matrix $\mathbf{M} = [\mathbf{M}_1 \quad \mathbf{M}_2] =$

$\begin{bmatrix} 0.957092 & 0.289784 \\ -0.289784 & 0.957092 \end{bmatrix}$ is indeed orthogonal because $\mathbf{M} \times \mathbf{M}^T =$

$\begin{bmatrix} 0.95709203 & 0.28978415 \\ -0.28978415 & 0.95709203 \end{bmatrix} \times \begin{bmatrix} 0.95709203 & -0.28978415 \\ 0.28978415 & 0.95709203 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \mathbf{I}_2$ because

$\mathbf{M}^{-1} = \mathbf{M}^T$. I also used the Matlab function `[EIGVEC, lamda]= eig(B)`, which gave the results

$\text{EIGVEC} = \begin{bmatrix} 0.9570920265 & 0.2897841487 \\ -0.2897841487 & 0.9570920265 \end{bmatrix}$, and $\lambda = \begin{bmatrix} -1.4140969547 & 0 \\ 0 & -0.9634030453 \end{bmatrix}$.

Note that these eigenvalues and eigenvectors do not completely agree with those of Montgomery's on page 432 (pp. 420-422 of the 6th edition). Although, it is somewhat arbitrary as to which eigenvalue and eigenvector we designate as 1 and 2, I have intentionally selected

$\lambda_1 = -1.4140969547$ such that the resulting rotation matrix $\mathbf{M} = \begin{bmatrix} \text{Cos}\theta & -\text{Sin}\theta \\ \text{Sin}\theta & \text{Cos}\theta \end{bmatrix} =$

$\begin{bmatrix} 0.95709203 & 0.28978415 \\ -0.28978415 & 0.95709203 \end{bmatrix}$, where $\theta = -16.845033763$ degrees. Then, according to my

above designated results the relationship between the two coordinates (w_1, w_2) and (x_1, x_2) is

$$\mathbf{W} = \mathbf{M}^{-1}\mathbf{X} = \mathbf{M}^{-1}(\mathbf{x} - \mathbf{x}_0) =$$

$$\begin{bmatrix} 0.95709203 & -0.28978415 \\ 0.28978415 & 0.95709203 \end{bmatrix} \begin{bmatrix} x_1 - 0.3892604 \\ x_2 - 0.3058577 \end{bmatrix} \text{ or } \mathbf{W} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} =$$

$$\begin{bmatrix} 0.95709203 & -0.28978415 \\ 0.28978415 & 0.95709203 \end{bmatrix} \begin{bmatrix} x_1 - 0.3892604 \\ x_2 - 0.3058577 \end{bmatrix}. \text{ Therefore, the relationship between the}$$

(w_1, w_2) and (x_1, x_2) coordinates are $w_1 = 0.95709203x_1 - 0.28978415x_2 - 0.28392527$, and $w_2 = 0.28978415x_1 - 0.95709203x_2 - 0.40553550$.

To check on the validity of these 2 last relationships, suppose we wish to calculate the response at $(x_1 = 2, x_2 = 1)$. Substituting $x_1 = 2$ and $x_2 = 1$ into the model $\hat{y} = 79.940 + 0.994975x_1 + 0.515165x_2 - 1.37625x_1^2 - 1.00125x_2^2 + 0.2500x_1x_2$ yields $\hat{y}(2, 1) = 76.43886454\%$. At $(x_1 = 2, x_2 = 1)$ the coordinates w_1 and w_2 are $w_1 = 1.34047462934036$ and $w_2 = 1.13112482720609$. To determine if in the (w_1, w_2) coordinates the value of the response is also equal to 76.43886454%, we use Eq. (40a) to compute:

$$\begin{aligned} \hat{y} &= \hat{y}_0 + \mathbf{X}'\mathbf{B}\mathbf{X} = \hat{y}_0 + (\mathbf{M}\mathbf{W})'\mathbf{B}(\mathbf{M}\mathbf{W}) = \hat{y}_0 + \mathbf{W}'(\mathbf{M}'\mathbf{B}\mathbf{M})\mathbf{W} = \hat{y}_0 + \mathbf{W}'\boldsymbol{\lambda}\mathbf{W} \\ &= \hat{y}_0 + \sum_{i=1}^2 \lambda_i w_i^2 = 80.2124357 - 1.4140970 w_1^2 - 0.9634030453 w_2^2 \\ &= 80.2124357 - 1.4140970 \times 1.34047463^2 - 0.9634030453 \times 1.13112483^2 \\ &= 76.43886454\% \text{ (Check!).} \end{aligned}$$

Exercise 15. Use Eq. (35), that shows $\tan 2\theta = \frac{\beta_{12}}{\beta_{11} - \beta_{22}}$, to obtain the angle of

rotation for the Example 11.2 of Montgomery. (b) Then, use the equations $\lambda_1 = \beta_{11} \cos^2 \theta + \beta_{22} \sin^2 \theta + \beta_{12} \cos \theta \sin \theta$, and $\lambda_2 = \beta_{11} \sin^2 \theta + \beta_{22} \cos^2 \theta - \beta_{12} \cos \theta \sin \theta$ to re-compute the

eigenvalues of the matrix $\mathbf{B} = \begin{bmatrix} -1.37625 & 0.1250 \\ 0.1250 & -1.00125 \end{bmatrix}$. Determine why Montgomery's

expressions for w_i on page 422 will yield almost the same exact answer for \hat{y} at $(x_1 = 2, x_2 = 1)$.

(c) Draw the 95% contour of \hat{y} (i.e., $0.95 \times \hat{y}_0$) clearly indicating the two coordinate axes (X_1, X_2) and (w_1, w_2) .

By now the reader may have diagnosed that the quadratic form $\mathbf{X}'\mathbf{B}\mathbf{X}$ is positive definite iff all the eigenvalues of \mathbf{B} strictly exceed zero, in which case the matrix \mathbf{B} is said to be positive definite. The quadratic form $\mathbf{X}'\mathbf{B}\mathbf{X}$ is negative definite iff all the eigenvalues of \mathbf{B} are negative, in which case \mathbf{B} is said to be negative definite. The quadratic form $\mathbf{X}'\mathbf{B}\mathbf{X}$ is said to be indefinite iff some eigenvalues of \mathbf{B} are positive and the rest are negative. Note that for $\mathbf{X}'\mathbf{B}\mathbf{X}$ to be indefinite, \mathbf{B} must have at least one positive eigenvalue and at least one negative eigenvalue. As long as this last statement is true, then some eigenvalues can be zero. For Montgomery's Example 11.2, the quadratic form $\mathbf{X}'\mathbf{B}\mathbf{X} = -1.37625 X_1^2 - 1.00125 X_2^2 + 0.25X_1X_2 = -1.37625(X_1^2 + 0.72752044 X_2^2 - 0.18165304X_1X_2) = -1.37625[(X_1 - 0.09082652X_2)^2 + 0.719271 X_2^2]$, which shows $\mathbf{X}'\mathbf{B}\mathbf{X} < 0$ unless both X_1 & $X_2 = 0$, i.e., $\mathbf{X}'\mathbf{B}\mathbf{X}$ is negative definite.

Bonus HW3. Let \mathbf{B} be a real symmetric $k \times k$ matrix with orthogonal eigenvectors $\mathbf{M}_1, \mathbf{M}_2, \dots, \mathbf{M}_k$, i.e., the rotation matrix $\mathbf{M} = [\mathbf{M}_1 \quad \mathbf{M}_2 \quad \dots \quad \mathbf{M}_k]$ with eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_k$. Prove that $\mathbf{M}^{-1} = \mathbf{M}^T$ and further all \mathbf{M}_j 's must be of unit length.

Exercise 16. Consider the quadratic response surface $y = 60 + 28x_1 - 28x_3 + 5x_1^2 + 6x_2^2 + 7x_3^2 - 2\sqrt{2}x_1x_2 + \epsilon = \eta + \epsilon$. (a) Determine if the response is one of Min, Max, or saddle point (or minimax) type and obtain \mathbf{x}_0 and y_0 . (b) Then obtain its canonical form $y = y_0 + \sum_{i=1}^3 \lambda_i w_i^2 + \epsilon$ and verify that your answer is indeed correct by computing y at $\mathbf{x} = [-1 \quad 2 \quad 1]^T$ from both the RS equation and its canonical form. (c) Repeat parts (a) and the 1st part of part (b) for the RS $\eta = (165 + 24\sqrt{54}) + (8\sqrt{54} - 30)x_1 - (80 + 6\sqrt{54})x_2 - 5x_1^2 + 10x_2^2 - 2\sqrt{54}x_1x_2$, and draw the contour of this surface whose value is $\eta = c \equiv 30$.

Summary of RSM

1. In real-life situations, the experimenter has no knowledge (except for either minimizing or maximizing the response) what type of quadratic surface underlies the response y in the region of factor space. Assuming that the present DC is far from optimum, s/he must conduct a 1st-order experiment at the present operating

conditions of x_1, x_2, x_3, \dots . If a 1st-order good fit is not obtained, then the experimenter must decrease spacing until a good fit is obtained and at least one linear coefficient (i.e., slope) is statistically significant at the nominal value of 5%. If the experimenter is very far from the optimum, then a 1st-order good-fit is possible but the linear coefficients will not be significant, in which case the experimenter must increase design spacing in order to obtain a good 1st-order fit with at least one significant linear coefficient. If a good-fit and significant slope(s) are obtained, then the experimenter must move the DC in the direction of the POSA (or POSD). This procedure should continue until no longer a 1st-order good fit with significant coefficients can be obtained (or the experimenter can follow the procedure outlined in Table 11.3 on p. 423 of Montgomery). Bear in mind that near the optimum region, the slopes in all directions become very small relative to pure quadratic coefficients.

2. Once the experimenter suspects that the last DC is near the optimum region, then a full quadratic model must be fit with the same design spacing of the last 1st-order experiment. Assuming that the full quadratic model is a good fit with some significant quadratic coefficients, then the design spacing must be increased so that a better picture of the RS is attained.
3. Once a 2nd-order model with good fit is obtained in Step 2 above, then the experimenter must proceed to use the procedure that I have outlined on pp. 36-54 of these notes to arrive at the stationary point \mathbf{x}_s and its optimum value of \hat{y}_o .

Simultaneously Analyzing and then Optimizing Multiple Responses

Reference: (Section 11.3.4 of Montgomery, pp. 435-439)

Many response surface problems involve the simultaneous optimizations of two or more responses. For example, see table 11.6 of Montgomery atop page 429 (p. 417 of the 6th edition) where 3 simultaneous responses (y_1 = yield, y_2 = viscosity, and y_3 = molecular weight) were measured from each experimental unit at all 4 factorial, 5 center, and 4 axial design points ($N = 13$); it will be shown that $n_c = 8$ center points will make the $k = 2$ CCD 2nd-order

orthogonal. Through RSM the response variable $y_1 = \text{yield}$ was optimized with optimum value $\hat{y}_{10} = 80.21244$, reaction time at $\xi_{10} = 86.9463$ minutes and temperature at $\xi_{20} = 176.5293^\circ\text{F}$, i.e., $\xi_0 = [86.9463 \quad 176.5293]'$. This optimal solution would be exactly correct if the three responses were independent; unfortunately the correlation coefficient $r_{13} = 0.475201$ is significant at the 5.1% level ($P\text{-value} = 0.050389$) and hence it is very doubtful that y_1 and y_3 are independent. The problem now is how to select the levels of reaction time (ξ_1) and process temperature (ξ_2) as to optimize all 3 QCHs (quality characteristics) simultaneously when the responses are not independent, where in this experiment y_1 is LTB with only an LSL, viscosity is a nominal dimension with specs 65 ± 3 poise (or centipoise which denotes Dyne-seconds/cm²), i.e., $62 \leq y_2 \leq 68$ and molecular weight (MOW) is apparently considered an STB QCH with a single USL = 3400, i.e., $0 < y_3 \leq 3400$; I am not sure what the units of MOW is? Montgomery uses the notation Mn, which could stand for grams/mol but I am not certain? As the author mentions (see p. 437, p. 424 of the 6th edition), this multiple response optimization can now be solved as a constrained optimization problem as follows: Max y_1 ; subject to: $62 \leq y_2 \leq 68$ & $0 < y_3 \leq 3400$. As D. C. Montgomery states the Design-Expert software gives the optimal solution through a search routine as $\xi_{10} = 83.5$ minutes, $\xi_{20} = 177.1^\circ\text{F}$, & $\hat{y}_{10} = 79.5\%$; or reaction time $\xi_{10} = 86.6$ minutes, $\xi_{20} = 172.25^\circ\text{F}$ & and the optimum value of $\hat{y}_{10} = 79.5\%$. Examining the contours of y_2 & y_3 in Figure 11.16 on page 436 of Montgomery (p. 425 of the 6th edition), it is not quite clear what the optimum values of y_2 & y_3 are. Thus, I will use the regression functions in the middle of page 435 (p. 423 of the 6th edition) to estimate the optima \hat{y}_{20} and \hat{y}_{30} . At $\xi_{10} = 83.5$, $\xi_{20} = 177.1$, $\hat{y}_{20} \cong -9030.74 + 13.393(83.5) + 97.708(177.1) - 0.0275(83.5)^2 - 0.26757(177.1)^2 - 0.05(83.5 \times 177.1) = 68.3577$ as opposed to 67.5 from Figure 11.16 neither of which are desirable because the ideal target for viscosity is 65. The value of $\hat{y}_{30} \cong -6308.8 + 41.025(83.5) + 35.473(177.1) = 3399.0558$ barely satisfies the constraint $0 < y_3 \leq 3400$; Figure 11.16 of Montgomery gives roughly $\hat{y}_{30} = 3350$. Similarly, the other stationary point ($\xi_{10} = 86.6$, $\xi_{20} = 172.25$) gives $\hat{y}_{20} \cong 68.39778 > \text{USL}$ and $\hat{y}_{30} \cong 3354.1893$, which is not exactly in the mid range of [3200, 3400]. It seems that y_1 has been optimized but y_2 and y_3 barely meet constraints and may not have been optimized. Further, it

is not clear to this author whether MOW (molecular weight) is an STB QCH or a nominal dimension. The constraint $y_3 \leq 3400$ on page 437 (p. 424 of the 6th edition) indicates that y_3 may be an STB QCH but Montgomery's statement in the middle of page 438, $3200 \leq \text{MOW} \leq 3400$, would imply that y_3 is a nominal dimension with specs: 3300 ± 100 .

As pointed by Montgomery, in the middle of p. 436 (near the bottom of page 423 of 6e), when there are more than 3 responses to optimize simultaneously, the above procedure becomes awkward, and it is not clear to this author that the design expert software did find the best operating conditions of time and temperature for all 3 QCHs. Thus, Derringer and Suich (JQT, Vol. 12, pp. 214-219; 1980) proposed a *desirability function* that simultaneously optimizes several responses whose quality specifications are given.

Their general optimization approach consists of identifying the levels of one or more factors (or independent variables, or process inputs) that will simultaneously optimize at least two correlated response variables which are functions of the same (but not necessarily all) factors. The responses are generally in different units (e.g., % conversion, lbs, amount of material removed, psi, out-of-round, etc). Each response is first converted to a unit-less desirability value using its proper desirability function, d , whose domain is the interval $[0, 1]$, where 0 implies complete undesirability and 1 implies perfect desirability. We first give the definitions by Derringer and Suich (1980) below.

(1) The response Y is an STB Type QCH

Generally the ideal target, $T = y_t$, is zero and there is only a single USL denoted by $U = y_u = \text{USL}$; then a unit's desirability function is defined as

$$d_i = \begin{cases} 1, & y_i \leq T \\ [(U - y_i) / (U - T)]^f, & T \leq y_i \leq U \\ 0, & y_i > U \end{cases} \quad (48a)$$

If the ideal target $T = 0$, then the above equation reduces to

$$d_i = \begin{cases} 1, & y_i = 0 \\ [(U - y_i) / U]^f, & 0 \leq y_i \leq U \\ 0, & y_i > U \end{cases} \quad (48b)$$

where r is a constant whose most common value is 1 (in which case d is a linear function of y)

but can range within the open interval $(0, \infty)$. If r lies in the open-interval $(0, 1)$, then $\frac{d}{dy_i} d_i <$

0 and $d^2 d_i / dy_i^2 < 0$ so that d_i is strictly concave. When $r > 1$, $dd_i / dy_i < 0$ but $d^2 d_i / dy_i^2 > 0$ so that d_i is convex [see Figure 11.17(b) on page 438 of Montgomery, p. 426 of the 6th edition]. Therefore, when $r > 1$, a smaller desirability value is obtained for a y_i far from the ideal target than when $0 < r < 1$ for the same y_i .

(2) The response Y is an NTB Type QCH

Generally the ideal target, $T = y_t$, is different from zero and there is both a single LSL denoted by $L = y_L$ and an USL denoted by $U = y_u$; then a unit's desirability function is defined

$$d_i = \begin{cases} 0, & y_i < L \\ [(y_i - L) / (T - L)]^{r_1}, & L \leq y_i \leq T \\ [(U - y_i) / (U - T)]^{r_2}, & T \leq y_i \leq U \\ 0, & y_i > U \end{cases}; \text{ Most commonly, the weights} \quad (49)$$

$r_1 = r_2 = r$, and $U - L$ is the spread of the acceptable range $L \leq y_i \leq U$, i.e., if a unit's dimension is outside the interval $[L, U]$, then that item is considered nonconforming to specs.

(3) The response Y is an LTB Type QCH

Generally the ideal target, T , is infinity and there is only a single LSL denoted by $L = y_L = \text{LSL}$; then a unit's desirability function is defined as

$$d_i = \begin{cases} 0, & y_i \leq L \\ [(y_i - L) / (T - L)]^r, & L \leq y_i \leq T \\ 1, & y_i > T \end{cases} \quad (50)$$

Note that it will be impossible to define a desirability function for an LTB type QCH where $T = \infty$. Thus, the target is generally a maximum value that is difficult to achieve in practice. There may be a typo in the middle of p. 438 (at the bottom of page 426 of Montgomery's 6th Ed.) because $y_1 = \text{"yield"}$ is an LTB type QCH and hence must have an $\text{LSL} = L = 70$.

After individual desirability values are computed for all m responses (in our example m

= 3), they are converted to an overall desirability defined below

$$D(\text{at FLC}_j) = D_j = (d_1 \times d_2 \times \dots \times d_m)^{1/m} \quad (51)$$

Note that D_j at the j^{th} **FLC** is simply the geometric average of the m individual desirability's at that **FLC**. As an example, again consider Table 11.6 (p.429) of Montgomery where at the first **FLC**: y_1 (yield) = 76.5% (L = 70% and the target T = 80%), $y_2 = 62$ (viscosity Specs:65±3), and $y_3 = 2940$ (MOW Specs: 3200 ≤ y_3 ≤ 3400). The d_i values for run number 1 are $d_1 = [(76.5 - 70) / (80 - 70)] = 0.65$; $d_2 = (62-62)/3 = 0$, and $d_3 = 0$ because $y_3 = 2940 < L = 3200 \rightarrow D(\text{at FLC}_1) = D_1 = (d_1 \times d_2 \times d_3)^{1/3} = 0$. I used MS Excel to compute the values of D_2 through D_{13} , where the corresponding computations are tabulated below (and the corresponding Excel file is on my website). Unfortunately, all $D_j = 0$ for $j = 1, 2, \dots, 13$; In such situations there are two alternatives:

The Desirability Function Values for Table 11.6 on p. 429 of Montgomery

$y_1 = \text{yield (LSL = 70), T = 80}$; $y_2 = \text{Viscosity (62 < } y_2 < 68)$; $y_3 = \text{Molecular Weight (3200 < } y_3 < 3400)$

Run No.	ξ_1 (time)	ξ_2 (Temp)	y_1	d_1	y_2	d_2	y_3	d_3	$D_j=(d_1 d_2 d_3)^{1/3}$
1	80.0000	170.0000	76.50	0.65	62	0	2940	0	0
2	80.0000	180.0000	77.00	0.7	60	0	3470	0	0
3	90.0000	170.0000	78.00	0.8	66	0.66667	3680	0	0
4	90.0000	180.0000	79.50	0.95	59	0	3890	0	0
5	85.0000	175.0000	79.90	0.99	72	0	3480	0	0
6	85.0000	175.0000	80.30	1	69	0	3200	0	0
7	85.0000	175.0000	80.00	1	68	0	3410	0	0
8	85.0000	175.0000	79.90	0.99	70	0	3290	0.9	0
9	85.0000	175.0000	79.80	0.98	71	0	3500	0	0
10	92.0711	175.0000	78.40	0.84	68	0	3360	0.4	0
11	77.9289	175.0000	75.60	0.56	71	0	3020	0	0
12	85.0000	182.0711	78.50	0.85	58	0	3630	0	0
13	85.0000	167.9289	77.00	0.7	57	0	3150	0	0

(1) Compute an overall desirability index, D , that is weighted sum of individual d_i 's, i.e.,

$$D_j = \sum_{i=1}^m w_i d_i, \text{ where } \sum_{i=1}^m w_i \equiv 1. \text{ As an example, suppose we assign a weight of 0.50 to yield,}$$

0.35 to viscosity, and 0.15 to MOW (generally the weights must be assigned according to the importance of the QCHs that are being optimized). Then, the value of $D_1 = 0.50(0.65) = 0.325$, $D_2 = 0.35$, $D_3 = 0.6333$, ..., $D(\text{FLC}_{13}) = D_{13} = 0.35$, and run number 3 would give the maximum

overall desirability so that $\xi_0 = [90 \quad 170]^T$ and $\mathbf{y}_0 = [78 \quad 66 \quad 3680]^T$ and $D_0 = 0.63333$.

Unfortunately, the location of the stationary point ξ_0 heavily depends on the assigned weights w_i 's and most often it is not clear what set of weights would lead to the true stationary point.

In this example if we assign $w_1 = 0.60$, $w_2 = 0.20$ and $w_3 = 0.20$, then $\xi_0 = [85 \quad 175]^T$ and $\mathbf{y}_0 = [79.9 \quad 70 \quad 3290]^T$ so that $y_{20} = 70$ is outside the required specs $62 \leq y_2 \leq 68$. Thus, it is generally best to use the desirability index based on the geometric average proposed by Derringer and Suich (1980) unless the experimenter is certain about the relative importance of all the responses.

(2) Estimate y_i from a regression model and estimate the corresponding d_i ($i = 1, 2, \dots, m$) and D_j . Such a procedure led to the optimal solutions given near the bottom of page 438 (p. 427 of the 6th edition) of Montgomery. However, for $\xi_{10} = 86.5$ and $\xi_{20} = 170.5$ on p. 438 of Montgomery, my Excel file gives $D_0 = 0.8571$ versus the reported value of 0.822 by the Design-Expert software. I surmise that the discrepancy is in the way the specs are assigned to y_3 because I am certain about $L_1 = 70$, $62 \leq y_2 \leq 68$, and the fact that I used slightly different models for y_2 & y_3 . In my Excel file I assigned an ideal target of $T_3 = 3300$ to y_3 with $LSL_3 = 3200$ and $U_3 = 3400$, while the Design-Expert software may have just used the constraint $y_3 \leq 3400$. Further, for $\xi_{10} = 82$ and $\xi_{20} = 178.8$, my Excel file yields $D_0 = 0$ not close to $D = 0.792$ reported by Montgomery. This last discrepancy is due to the fact that Montgomery used a full-quadratic model for y_2 (on p. 435) and only a linear model for y_3 , while I used Minitab's Best-Subset to identify the best models for y_2 & y_3 . Both models are given in my Desirability Excel file. Further, I asked one of our Ph.D. students (MS. Yang) to write a set of Lingo codes to obtain the true optimal solution. Her program yielded $\xi_{10} = 87.00$ and $\xi_{20} = 170.1760$ with $D_0 = 0.99018$, but unfortunately she did not use the best fitted models in her program. This is probably why my Excel solution, $\xi_{10} = 86.76101$ and $\xi_{20} = 170.32625$, does not match hers.

If direct optimization via regression is not the objective, then $D = (d_1 \times d_2 \times \dots \times d_m)^{1/m}$ can still be used as the response in ANOVA to determine which factors most significantly influence D and then ascertain what **FLC** is best to attain the maximum desirability. Similarly, D can be used as the response in a control chart with the intention that the LCL_D will alarm that a

process may be well below an acceptable desirability level and the UCL_D can be used to stop a process and look for assignable causes that are improving desirability and ensure that those causes are perpetuated into the process. The following exercise is an example from a factorial experiment from two of my colleagues (C. W. Curtis in Chemical Engineering & J. N. Hool of ISE), where D must be used to locate the best FLC for the process.

Exercise 17. The objective is to convert coal and plastic-waste to energy expressed in %. Three factors Temperature (A at 2 levels 400C and 430), Time (B at 30 minutes and 60) and Catalyst (Z & NZ) may impact %conversion but two other responses $y_1 = \%Gas$ and $y_2 = \%HX$ (HX may stand for Hydrogen Oxide) are also emitted and measured along with %conversion. Both y_2 & y_3 are LTB type QCHs, which I am assigning $L_2 = 20\%$, $L_3 = 30\%$ and ideal targets of $T_2 = 75\%$ and $T_3 = 95\%$, respectively, while y_1 ($=\%Gas$) is an STB type QCH with an ideal target, T_1 , of zero and I am assigning an upper limit of $U_1 = 40\%$. The data for the factorial experiment with two replicates are provided below.

Data from C. W. Curtis & J. N. Hool

	$U_1=40$	$w_1=0.1$	$L_2=20$	$w_2=0.3$	$w_3=0.6$	$L_3=30\%$		
A	B	C	$y_1 = \%Gas$	$y_1 = \%Gas$	$y_2 = \%HX$	$y_2 = \%HX$	$y_3 = \%Conv$	$y_3 = \%Conv$
-1	-1	-1	20.700	17.700	16.990	16.010	36.190	35.210
-1	-1	1	23.900	21.500	10.180	8.620	32.090	31.110
-1	1	-1	20.500	19.900	6.090	4.110	26.180	24.620
-1	1	1	22.600	21.600	7.140	5.860	29.910	27.090
1	-1	-1	20.400	18.800	23.590	21.610	43.540	40.860
1	-1	1	29.100	27.900	24.830	22.570	53.370	50.830
1	1	-1	25.400	23.600	70.550	68.850	95.680	92.720
1	1	1	38.000	36.200	56.920	55.080	94.940	91.260

(a) Using $r=1$, and the weights $w_1 = 0.10$, $w_2 = 0.30$, and $w_3 = 0.60$, use $D_j = \sum_{i=1}^m w_i d_i$ to

compute the values of D at both replicates and use ANOVA to determine which effects have a significant impact on D. What FLC should the process be operating at? ANS: $SS(\text{Total}) = 1.676441024$, $SS(\text{ABC}) = 0.013250707$. (b) Use Eq. (51) to compute the D values at each replicate for each run (1 through 8); then average the two D's and obtain the optimal condition based on \bar{D}_j .

Designs for Fitting Response Surfaces (Section 11.4 of Montgomery)

Definition. A design is said to be orthogonal iff the $\mathbf{IM} = (\mathbf{X}^T\mathbf{X})$ is a diagonal matrix. All resolution III 2^{k-p} FFDs (fractional factorial designs) with n_c center points are orthogonal. This was illustrated when I discussed the Example 11.1 of Montgomery's 7th edition on pp. 420-425 (pp. 405-423 of 6e).

Another example of a 1st-order orthogonal design (OD) is the simplex, which is a modification of a fractional replicate of the 2^k when the experimenter can assume that the interaction between x_i and x_j ($i \neq j$) is practically nonexistent. However, For $k = 2$ factors, the $\frac{1}{2}$ fraction reduces to 2 runs providing only one degree of freedom to study the effects x_1 and x_2 , and hence another design point has to be added to the points $(-1, -1)$ and $(1, -1)$ that is orthogonal to both and such that $\mathbf{X}'\mathbf{X} = 3\mathbf{I}_3$. Hence, the coordinates of the vertices for $k = 2$ are at $(0, \sqrt{2})$, $(-\sqrt{3}/2, -1/\sqrt{2})$, and $(\sqrt{3}/2, -1/\sqrt{2})$. Therefore, the design matrix for $k =$

2 simplex is given by $\mathbf{X} = \begin{bmatrix} 1 & 0 & \sqrt{2} \\ 1 & -\sqrt{3}/2 & -1/\sqrt{2} \\ 1 & \sqrt{3}/2 & -1/\sqrt{2} \end{bmatrix}$. Note that the distance d of all 3 points

$(0, \sqrt{2})$, $(-\sqrt{3}/2, -1/\sqrt{2})$, and $(\sqrt{3}/2, -1/\sqrt{2})$ to the design center $(0, 0)$ is equal to $d = \sqrt{k} = \sqrt{2}$; further, every column except \mathbf{x}_0 is a contrast, the matrix \mathbf{X} is 1st-order orthogonal, the distance between any 2 design points (DPs) is $\sqrt{2N} = \sqrt{6}$, and $\mathbf{X}'\mathbf{X}$ is indeed equal to $3\mathbf{I}_3$, which implies $\mathbf{X}^{-1} = \mathbf{X}^T/(k+1)$. Further, simplex designs are appropriate only for constructing 1st-order models and should be avoided for use when the required model must have 2nd-order regressors. Note that the angle that any two adjacent points subtends with $(0, 0)$ is equal to $\theta = \arccos(-1/k) = 120$ degrees.

The $k = 3$ simplex design matrix is given by $\mathbf{X} = \begin{bmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$, which is a

2_{III}^{3-1} FFD with the generator $g = ABC$ and contrast function value equaling 1; again every column is a contrast and \mathbf{X} is 1st-order orthogonal. The distance of all 4 points $(1, -1, -1)$, $(-1,$

1, -1), (-1, -1, 1), (1, 1, 1) to the design center (0, 0, 0) is equal to $d = \sqrt{k} = \sqrt{3}$, and the distance between any 2 DPs is $\sqrt{2N} = \sqrt{8}$; further, the $\mathbf{IM} = \mathbf{X}'\mathbf{X} = 4\mathbf{I}_4$ so that $\mathbf{X}^{-1} = \mathbf{X}'/(k+1)$. The angle that any side (or any two adjacent points) subtends with the origin is equal to $\theta = \text{Cos}^{-1}(-1/k) = \text{arccosine}(-1/k)$, which is equal to 109.4712 degrees for $k = 3$ independent (or design) variables, and is equal to 120 degrees for $k = 2$. Thus, $\text{Cos}(\theta) = -1/k$ for all k .

None of the Simplex designs can be made 2^{nd} -order orthogonal because they do not provide sufficient df to study all quadratic effects and the interaction column x_1x_2 cannot be made orthogonal to the x_1 -column no matter how many center points, n_c , is used. For example, if we select $n_c = 3$ for the $k = 2$ Simplex, then the \mathbf{IM} matrix, as illustrated below will have only rank 4 no matter how many center points are used. Further, only three parameters can be estimated and PE has 2 df . Note that there are also two things wrong with the \mathbf{IM}_c because its rank is equal to 4 as anticipated [instead of 6 and hence the $\det(\mathbf{IM}_c) = 0$] due to the fact that there are two linear dependencies amongst the 6 columns: (1) $C_2/\sqrt{2} + C_6 \equiv 0$, (2) $C_3 + C_4/\sqrt{2} - C_5/\sqrt{2} \equiv 0$. This again should illustrate the fact that Simplex designs are appropriate only for 1^{st} -order modeling and should be avoided as a 2^{nd} -order design.

$$\mathbf{X} = \begin{matrix} & \mathbf{x}_0 & \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_1^2 & \mathbf{x}_2^2 & \mathbf{x}_1\mathbf{x}_2 \\ \begin{bmatrix} 1 & 0 & \sqrt{2} & 0 & 2 & 0 \\ 1 & -\sqrt{3}/2 & -1/\sqrt{2} & 1.5 & 0.5 & \sqrt{3}/2 \\ 1 & \sqrt{3}/2 & -1/\sqrt{2} & 1.5 & 0.5 & -\sqrt{3}/2 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \end{matrix}$$

Note that $\mathbf{x}_1 + \mathbf{x}_1\mathbf{x}_2 = 0$ and $\mathbf{x}_1^2 - \mathbf{x}_2^2 = 0$. Thus the rank of \mathbf{X} is $6 - 2 = 4$. This simply confirms the very fact that the design matrix on the LHS has 4 distinct points and hence it has a rank of 4 and not 6. Thus, only 3 effects x_1 , x_2 & either x_{11} or x_{22} can be studied.

$$\mathbf{IM}_c = (\mathbf{X}'_c \mathbf{X}_c) = \begin{bmatrix} 6 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & -3/\sqrt{2} \\ 0 & 0 & 3 & -3/\sqrt{2} & 3/\sqrt{2} & 0 \\ 0 & 0 & -3/\sqrt{2} & 3 & 0 & 0 \\ 0 & 0 & 3/\sqrt{2} & 0 & 3 & 0 \\ 0 & -3/\sqrt{2} & 0 & 0 & 0 & 1.5 \end{bmatrix} \rightarrow \det(\mathbf{IM}_c) = 0$$

Exercise 18. Obtain a simplex design for $k = 4$. Hint: Start with the $k = 3$ simplex and add one row and one column to retain orthogonality. Then rescale some of the vectors such that the distance of all 5 design points to the origin is $d = \sqrt{4} = \sqrt{k} = 2$ and your **IM** must equal to $\mathbf{X}'\mathbf{X} = 5\mathbf{I}_5$. This implies the added 5th point has to have dimension $\mathbf{P}_5 = [1 \ 0 \ 0 \ 0 \ 2]$, and hence the 5th input variable $\mathbf{x}_5 = [-0.5 \ -0.5 \ -0.5 \ -0.5 \ 2]^T$. The distance between any 2 DPs must be $\sqrt{2N} = \sqrt{10}$. Obtain the angle θ that any side (or any two adjacent points) subtends with the origin in radians and then in degrees. Note that $\cos(\theta) = \mathbf{P}_i'\mathbf{P}_j / (|\mathbf{P}_i| \times |\mathbf{P}_j|)$, where $\mathbf{P}_i'\mathbf{P}_j$ represents the dot product of any 2 of the 5 points in the design matrix and $|\mathbf{P}_i| \times |\mathbf{P}_j| = 4$ when $k = 4$.

DESIGNS FOR FITTING A SECOND ORDER MODEL

The most commonly used designs for 2^{nd} -order models in RSM are the Central Composite designs (CCDs). These are shown on pages 440-445 of Montgomery (429-435 of 6th edition) for 2 and 3 independent variables. A CCD for k factors consists of a $2^k = n_f$ factorial plus $n_a = 2k$ axial points located the same distance d from the origin $(0, 0, \dots, 0)$ as the factorial points. The choice of d is not arbitrary and 1st and foremost should be selected in such a manner that the CCD becomes rotatable. We now define a rotatable design.

Rotatability: A design is said to be rotatable iff the

$$V[\hat{y}(\mathbf{x})] = V(\mathbf{x}\hat{\boldsymbol{\beta}}) = \mathbf{x}'\mathbf{COV}(\hat{\boldsymbol{\beta}})\mathbf{x} = \mathbf{x}'[(\mathbf{X}'\mathbf{X})^{-1}\sigma_{\epsilon}^2]\mathbf{x} = (\mathbf{x}'\mathbf{C}\mathbf{x})\sigma_{\epsilon}^2$$

is the same for all vectors \mathbf{x} of the factor space that are of equal distance to the design center $(0, 0, \dots, 0)$. Such a design when rotated about $(0, 0, \dots, 0)$ will not alter the $V[\hat{y}(\mathbf{x})]$. A CCD becomes rotatable if the distance of axial points from $(0, 0, \dots, 0)$, d , is selected according to $d = (n_f)^{1/4} = (2^k)^{1/4} = 2^{k/4}$. Note that most authors use α for the distance d of the axial points to the origin, but I would refrain from such usage because α is almost universally used for the LOS of a statistical test. Thus, my notation d is used herein for Montgomery's α . Further, you must be cognizant of the fact that a CCD is not in general rotatable unless d is selected according to $d = (n_f)^{1/4}$.

Figure 11.20 on page 441 of Montgomery (p. 429 of 6th edition) shows the CCD for $k =$

2 and $k = 3$ independent design variables x_1 , x_2 and x_3 . For $k = 2$, the factorial portion of the CCD is simply a 2^2 factorial, which is automatically 1st-order orthogonal and rotatable. However, in order to study quadratic effects of a response surface, we must augment our 2^2 factorial with the $n_a = 4 = 2 \times k$ axial points $(d, 0)$, $(0, d)$, $(-d, 0)$, and $(0, -d)$. Then, the choice of $d = (n_f)^{1/4} = (4)^{1/4} = \sqrt{2}$ makes this CCD also rotatable. Before I show that such a CCD is indeed rotatable, you should note that all the $n_f + n_a = 8$ points now are of equal distance from the origin. This is due to the fact that, for example, the distance of the factorial point $(x_1 = -1, x_2 = 1)$ to the origin $(0, 0)$ is given by $\sqrt{(-1)^2 + 1^2} = \sqrt{2}$, and similarly the distance to the origin is $\sqrt{2}$ for the remaining 3 factorial points. Further, the 8 points lying on a circle provide 7 *df*, 5 of which can be used to study the effects x_1 , x_2 , x_{11} , x_{22} , and the interaction $x_1x_2 = x_{12}$.

Designs for which all of its points (with the exception of its center points) are of equal distance to the origin are called equiradial.

Therefore, the rotatable CCD for $k = 2$ is also an equiradial design because all of its 8 design points lie on the circle of $\sqrt{2}$ radius. I will now show that the $k = 2$ CCD with $d = \sqrt{2}$ but zero center points is not rotatable. Note that I am using the general regression notation of $\mathbf{x}_{11} = \mathbf{x}_1^2$, etc. The $\mathbf{IM} = \mathbf{X}'\mathbf{X}$ matrix listed below clearly shows the $k = 2$ CCD is not 2nd-order

\mathbf{x}_0	\mathbf{x}_1	\mathbf{x}_2	\mathbf{x}_{11}	\mathbf{x}_{22}	$\mathbf{x}_1\mathbf{x}_2$	
1	-1	-1	1	1	1	Factorial Region
1	-1	1	1	1	-1	
1	1	-1	1	1	-1	
1	1	1	1	1	1	
1	$-\sqrt{2}$	0	2	0	0	\rightarrow
1	0	$-\sqrt{2}$	0	2	0	Axial Region
1	$\sqrt{2}$	0	2	0	0	
1	0	$\sqrt{2}$	0	2	0	
1	0	$\sqrt{2}$	0	2	0	

$$\mathbf{IM} = \begin{bmatrix} 8 & 0 & 0 & 8 & 8 & 0 \\ 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 8 & 0 & 0 & 0 \\ 8 & 0 & 0 & 12 & 4 & 0 \\ 8 & 0 & 0 & 4 & 12 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 \end{bmatrix}$$

orthogonal, and even if we make the \mathbf{x}_{11} and $\mathbf{x}_2^2 = \mathbf{x}_{22}$ columns contrasts, the \mathbf{IM} will not

become a diagonal matrix. Therefore, when $n_c = 0$, the $k = 2$ CCD is not an orthogonal design. Further, the \mathbf{IM} matrix is indeed singular because $\text{Col4} + \text{Col5} = 2 \times \text{Col1}$, and hence its rank is 5 not 6. Further, in order to prove that the $k = 2$ CCD W/O center points is not rotatable, we need to show that for any 2 arbitrary points, \mathbf{P}_1 and \mathbf{P}_2 , in the (x_1, x_2) coordinate plane of equal distance to $(0, 0)$, the $V[\hat{\mathbf{y}}(\mathbf{P}_1)] = [\mathbf{P}_1'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{P}_1]\sigma_\epsilon^2 \neq [\mathbf{P}_2'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{P}_2]\sigma_\epsilon^2$. Let $\mathbf{P}_1 = (-1, 2)$ and $\mathbf{P}_2 = (1/2, \sqrt{19/4})$ both of which are exactly a distance of $d = \sqrt{5}$ from the origin. Then $\mathbf{x}_1 = [1 \ -1 \ 2 \ 1 \ 4 \ -2]^T$, but because $(\mathbf{X}'\mathbf{X})^{-1}$ is singular, the $V[\hat{\mathbf{y}}(x_1)] = [\mathbf{x}_1'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_1]\sigma_\epsilon^2$ cannot be computed. However, it can easily be shown that $n_c = 8$ center points will make a $k = 2$ CCD 2nd-order orthogonal. I will next show that if we add an $n_c > 1$ center points to the $k = 2$ CCD, then it will become rotatable. The corrected design matrix with $N = n_f + n_a + n_c = 4 + 4 + 8$

	x_0	x_1	x_2	$x_{11} - \bar{X}_{11}$	$x_{22} - \bar{X}_{22}$	x_1x_2	
$\mathbf{X}_{\text{corr}} =$	1	-1	-1	1/2	1/2	1	Factorial Region
	1	-1	1	1/2	1/2	-1	
	1	1	-1	1/2	1/2	-1	
	1	1	1	1/2	1/2	1	
	1	$-\sqrt{2}$	0	3/2	-1/2	0	Axial Region
	1	0	$-\sqrt{2}$	-1/2	3/2	0	
	1	$\sqrt{2}$	0	3/2	-1/2	0	
	1	0	$\sqrt{2}$	-1/2	3/2	0	
	1	0	0	-1/2	-1/2	0	Design Center
	1	0	0	-1/2	-1/2	0	
	1	0	0	-1/2	-1/2	0	
	1	0	0	-1/2	-1/2	0	
	1	0	0	-1/2	-1/2	0	
	1	0	0	-1/2	-1/2	0	
	1	0	0	-1/2	-1/2	0	
	1	0	0	-1/2	-1/2	0	

= 16 points is given above, where $\bar{x}_{11} = \bar{x}_{22} = 8/16 = 1/2$. You will show later that the choice of $n_c = 8$ makes this also a 2^{nd} -order orthogonal design but orthogonality is not a necessary condition for rotatability. The \mathbf{X}_{corr} matrix is now 2^{nd} -order orthogonal because the corrected \mathbf{IM} (listed below) is diagonal and has a rank of 6. Note that the corrected design matrix for the $k = 2$ CCD with $n_c = 8$ center is now a diagonal matrix; further, $V(\hat{\beta}_j)$ for $j = 1, 2, 3, 4$, and 5 is minimized for the orthogonal design relative to a corresponding oblique design with n_c

$$\mathbf{IM}_C = \mathbf{X}'_{\text{corr}} \mathbf{X}_{\text{corr}} = \begin{matrix} & x_0 & x_1 & x_2 & x_1^2 & x_2^2 & x_1 x_2 \\ \begin{bmatrix} 16 & 0 & 0 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 8 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 \end{bmatrix} \end{matrix}$$

different from 8 center points. For example, for $n_c = 8$ center points the $V(\hat{\beta}_j) = 0.125 \sigma_{\epsilon}^2$ for $j = 1, 2, 3, 4$ and $V(\hat{\beta}_5) = 0.25 \sigma_{\epsilon}^2$, while for $k = 2$ CCD with $n_c = 6$ center points $V(\hat{\beta}_j) = (0.125, 0.125, 0.1354, 0.1354, 0.25) \sigma_{\epsilon}^2$, respectively. We now check on rotatability of our \mathbf{X}_{corr} . Again let $\mathbf{P}_1 = (-1, 2)$ and $\mathbf{P}_2 = (1/2, \sqrt{19/4})$ both of which are exactly a distance of $d = \sqrt{5}$ from the $(0, 0)$. Then $\mathbf{x}_{1C} = [1 \quad -1 \quad 2 \quad 1/2 \quad 3.5 \quad -2]^T$, which yields $V[\hat{\mathbf{y}}(\mathbf{x}_1)] = [\mathbf{x}_{1C}'(\mathbf{X}'_{\text{corr}}\mathbf{X}_{\text{corr}})^{-1} \mathbf{x}_{1C}] \sigma_{\epsilon}^2 = 3.25 \sigma_{\epsilon}^2$, and $\mathbf{x}_{2C} = [1 \quad 1/2 \quad \sqrt{19/4} \quad -1/4 \quad (19/4 - 1/2) \quad \sqrt{19/16}]^T$, which yields $V[\hat{\mathbf{y}}(\mathbf{x}_{2C})] = 3.25 \sigma_{\epsilon}^2$. Matlab was used in these computations.

Exercise 19. Compute the $V[\hat{\mathbf{y}}(\mathbf{x})]$ at the points $\mathbf{P}_3 = (x_1 = \sqrt{3}, x_2 = \sqrt{2})$ and $\mathbf{P}_4 = (x_1 = 0, x_2 = \sqrt{5})$ for the above CCD and draw conclusions.

Exercise 20. Assume that the value of n_c in the above $k = 2$ CCD is not known to you. Prove that the only value of n_c that makes the corrected design matrix, \mathbf{X}_{corr} , orthogonal is $n_c = 8$ and hence $N = 16$. (b) Show that the $k = 2$ CCD with $n_c = 2$ is rotatable but not 2^{nd} -order

orthogonal.

Exercise 21. Show that a 3^2 design is orthogonal but is not equiradial and not rotatable. Hint: First transform the coordinates $(0, 1, 2)$ to $(-1, 0, 1)$ and then proceed as I did for the case of $k = 2$ CCD.

Montgomery provides the Table 16-8 in his 3rd Ed. (borrowed from “Multifactor Experimental Designs for Exploring Response Surfaces’ by Box and Hunter, Annals of Mathematical Statistics, vol. 28, 1957) that lists the required number of center points for a CCD to become orthogonal and the value of the axial distance d that makes the design rotatable. I am summarizing a part of that Table below, where N = the total number of design points

Table 16-8 of Montgomery’s 3rd Edition on his page 546

$k =$	2	3	4	5	2^{5-1}	6	2^{6-1}
n_f	4	8	16	32	16	64	32
n_a	4	6	8	10	10	12	12
n_c	8	9	12	17	10	24	15
N	16	23	36	59	36	100	59
d	$\sqrt{2}$	$2^{0.75}$	2.00	$2^{1.25}$	2.00	$2^{1.5}$	$(32)^{0.25}$

needed for (near) orthogonality. Note that the CCD matrix in Table 11.6 atop page 429 (p. 417 of Montgomery’s 6th ed.) is not 2nd-order orthogonal because its $n_c = 5$ and the needed n_c for orthogonality is 8 but the design is indeed rotatable. It turns out that all designs that are equiradial and 2nd-order orthogonal are not necessarily rotatable. One such example is the Box-Behnken design with $n_c = 4$ center points, which is equiradial and 2nd-order orthogonal but not rotatable. Further, if a 2nd-order design is both 2nd-order orthogonal and rotatable, then it seems that $V(\hat{\beta}_j)$ for $j > 0$ and $V(\hat{y})$ are minimized.

Other Designs

There are many other RSDs only some of which are orthogonal and rotatable. For $k = 2$ regressors, we can use either 4, 5, or 6 equi-spaced points on a unit circle. The problem with $n_a = 4$ axial points on a unit circle (called a $k = 4$ polygon denoted \mathbf{P}_4) is that the interaction

term cannot be studied because $x_1x_2 = 0$ for all 4 rows of the design matrix. Further, any attempt to obtain an n_c to make this design 2^{nd} -order orthogonal will be futile as there does not exist an N for which the design becomes 2^{nd} -order orthogonal. However, if the experimenter is certain that the two factors x_1 and x_2 do not interact and does not care about orthogonality and rotatability, then this circular design can be used with 4 to 6 center points to study the linear effects (x_1, x_2) and the pure quadratic effects (x_1^2, x_2^2) . The corrected design matrix for a polygon, **P4**, with the 4 points (1, 0), (0, 1), (-1, 0), (0, -1) and $n_c = 6$ center points is given below.

$$\mathbf{P4} = \begin{array}{c} \begin{array}{cccccc} x_0 & x_1 & x_2 & x_{11} - \bar{X}_{11} & x_{22} - \bar{X}_{22} & x_1x_2 \end{array} \\ \left[\begin{array}{cccccc} 1 & 1 & 0 & .80 & -.2 & 0 \\ 1 & 0 & 1 & -.2 & .80 & 0 \\ 1 & -1 & 0 & .80 & -.20 & 0 \\ 1 & 0 & -1 & -.2 & .80 & 0 \\ \hline 1 & 0 & 0 & -.2 & -.2 & 0 \\ 1 & 0 & 0 & -.2 & -.2 & 0 \\ 1 & 0 & 0 & -.2 & -.2 & 0 \\ 1 & 0 & 0 & -.2 & -.2 & 0 \\ 1 & 0 & 0 & -.2 & -.2 & 0 \\ 1 & 0 & 0 & -.2 & -.2 & 0 \end{array} \right] \end{array}$$

Note that the $\text{Rank}(\mathbf{P4}) = 5$ so that the $(\mathbf{P4}'\times\mathbf{P4})^{-1}$ exists only if we remove the x_1x_2 column, and then, it will be a 5×5 non-orthogonal matrix.

Montgomery provides two other equiradial designs on page 444 (p. 432 of his 6th edition). An equiradial hexagon is a polygon with 6 equal sides each of which subtends an angle of $2\pi/6 = 60$ degrees with the origin. The (x_1, x_2) coordinates for the 6 points on a unit circle are (1, 0), $(1/2, \sqrt{3}/2 = \sqrt{0.75})$, $(-1/2, \sqrt{3}/2)$, (-1, 0), $(-1/2, -\sqrt{3}/2)$, and $(1/2, -\sqrt{3}/2)$. This design is 1st-order orthogonal with or W/O any center points, but needs more than one center point to become 2^{nd} -order orthogonal and rotatable. I now derive the necessary value of n_c for a hexagon to attain 2^{nd} -order orthogonality and rotatability. We assume $n_c > 1$ so that $N = 6 + n_c$. The 2^{nd} -order design matrix for N points is given atop next page. Note that every column in **P6** is orthogonal to any other column with the exception

of pure quadratic $x_{11} - \bar{x}_{11}$ and $x_{22} - \bar{x}_{22}$ columns. The dot product of columns (3) and (4) of **P6** is given by: $(-6/N)(1 - 3/N) + 4(0.25 - 3/N)(0.75 - 3/N) + n_c(9/N^2)$. To attain 2nd-order orthogonality, we must require that the dot product $(\mathbf{x}_{11} - \bar{\mathbf{X}}_{11})'(\mathbf{x}_{22} - \bar{\mathbf{X}}_{22})$ becomes zero, i.e., we must require that $(-6/N)(1 - 3/N) + 4(0.25 - 3/N)(0.75 - 3/N) + n_c(9/N^2) = 0$. This last equation reduces to $N(N - 12) = 0$, and hence $N = 12$, which yields $n_c = 6$. With $n_c = 6$ center points, the **IM** for the orthogonal Hexagon is given below. The $V(\hat{\beta}_j)$ for $j > 0$ is smaller for $n_c = 6$ than any other number of center points.

	\mathbf{x}_0	\mathbf{x}_1	\mathbf{x}_2	$\mathbf{x}_{11} - \bar{\mathbf{X}}_{11}$	$\mathbf{x}_{22} - \bar{\mathbf{X}}_{22}$	$\mathbf{x}_1 \mathbf{x}_2$
Circle	1	1	0	$1 - 3/N$	$-3/N$	0
	1	.5	$\sqrt{.75}$	$.25 - 3/N$	$.75 - 3/N$	$\sqrt{.75}/2$
	1	-.5	$\sqrt{.75}$	$.25 - 3/N$	$.75 - 3/N$	$-\sqrt{.75}/2$
	1	-1	0	$1 - 3/N$	$-3/N$	0
	1	-.5	$-\sqrt{.75}$	$.25 - 3/N$	$.75 - 3/N$	$\sqrt{.75}/2$
	1	.5	$-\sqrt{.75}$	$.25 - 3/N$	$.75 - 3/N$	$-\sqrt{.75}/2$
P6 =						
Center	1	0	0	$-3/N$	$-3/N$	0
	1	0	0	$-3/N$	$-3/N$	0

	1	0	0	$-3/N$	$-3/N$	0

$$\mathbf{IM} = (\mathbf{P6})'(\mathbf{P6}) = \begin{bmatrix} 12 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.75 \end{bmatrix}$$

Next, I will show that the Hexagon is also rotatable. Accordingly, let $\mathbf{P}_1 = (2, 0)$ and $\mathbf{P}_2 = (1, \sqrt{3})$ be two points in the (x_1, x_2) plane both of whose distances to the design center $(0, 0)$ is equal to $d = 2.00$. Then $\mathbf{x}_{1c} = [1 \ 2 \ 0 \ 4 - 0.25 \ 0 - 0.25 \ 0]'$ and $\mathbf{x}_{2c} = [1 \ 1 \ \sqrt{3} \ 1 - 0.25$

$3-0.25 \sqrt{3}]'$. Matlab Computations give $V[\hat{y}(x_1)] = 10.8333333 \sigma_{\epsilon}^2$. I emphasize that in order to attain rotatability, we do not need to make the design 2nd-order orthogonal, neither is it absolutely necessary to make it equiradial. However, note that making the above design 2nd-order orthogonal does yield $V[\hat{y}(x_2)] = [\mathbf{x}_{1c}'(\mathbf{X}'_{\text{corr}}\mathbf{X}_{\text{corr}})^{-1}\mathbf{x}_{1c}] \sigma_{\epsilon}^2 = 10.8333333 \sigma_{\epsilon}^2$, i.e., smaller $V(\hat{\beta}_j)$ for $j > 0$.

Exercise 22. Validate the rotatability of the Hexagon design with $n_c = 4$ center points by computing the $V[\hat{y}(x)]$ at $P_3 = (\sqrt{2}, -\sqrt{2})$ and $P_4 = (-0.50, \sqrt{15/4})$.

Exercise 23. Repeat the analysis, that was performed above for a Hexagon, also for a Pentagon design matrix.

Exercise 24. Study section 11.4.3 on pages 446-450 of Montgomery (pp. 436-439 of 6e) but you will not be tested on the contents of this section.

I am not sure what is exactly accomplished by orthogonal blocking from the analytical standpoint except for the fact that the experimenter is forced to use blocking in the design because of time and/or resource constraints. I can easily generate the blocks orthogonally according to the definitions given near the bottom of page 446 (p. 436 of Montgomery's 6th edition) and repeated below.

- (1) A 2nd-order design blocks orthogonally if each block is 1st-order orthogonal
- (2) The number of runs in each block is proportional to the SS of the variable levels in different columns of the blocks.

However, I did not find the design matrices in different blocks of matrix **D** atop page 448 (p. 436 of the 6th edition) to be 2nd-order orthogonal. Furthermore, the 2nd-order $k = 2$ and $k = 3$ CCDs listed in Table 11.11 on page 450 (p. 438 of Montgomery's 6th edition) are not 2nd-order orthogonal.

Mixture Designs (Section 11.6, pp. 466-476)

Mixture designs have widespread applications in Textile Engineering, Chemical Engineering and Chemistry, Food Industry, Soft-Drink Industry, oil refinery, Asphalt Technology, etc, etc. Cornell (1990) reports a mixture experiment from Textile Industry in which 3

components (x_1 = the ingredient amount of Polyethylene by volume, x_2 = the amount of Polystyrene by volume, and x_3 = the ingredient amount of Polypropylene by volume) were mixed in order to make fiber that will be spun into yarn for draperies. The primary objective was to produce fiber of elongation y , measured in Kgs of force applied, that had maximum elasticity. The 1st order of business is for the reader to bear in mind that the three proportion variables x_1 , x_2 and x_3 (by volume) are not independent because the manufactured batch of fiber consists of only 3 components (and nothing else), and therefore, the sum of the 3 proportions $x_1 + x_2 + x_3$ must equal to 1, i.e., if the mixture consists of p components, then the mixture design (MD) must

satisfy the constraint $\sum_{j=1}^p x_j = 1$. Then, unlike classical regression where the p regressors were

assumed independent, in MDs the p components of the mixture are not independent, but exactly $p - 1$ of them are independent. For example, in the textile experiment under consideration, the experimenter has the freedom to specify $x_1 = 35\%$ (by volume), $x_3 = 40\%$, but now the value of x_2 is automatically determined to be 25%. Such a mixture is said to be complete because it consists of all 3 possible ingredients.

Secondly, if $x_1 = x_2 = x_3 = 0$, then no mixture can be made and the corresponding fiber elongation, y , must be identically equal to zero. Therefore, a linear mixture model cannot have a y -intercept term β_0 and is given by

$$y_i = \sum_{j=1}^p \beta_j x_{ij} + \epsilon_i \quad (52)$$

Again, please note that the value of the y -intercept $\beta_0 = 0$ so that $y = 0$ when all the x_j 's are zero, and the linear model (52) is used only when the factor space is far from the optimum region.

Thirdly, pure quadratic terms such as x_1^2 , x_2^2 , ..., x_p^2 are practically nonexistent

in MDs because $x_p^2 = x_p(1 - x_1 - x_2 - \dots - x_{p-1}) = x_p - \sum_{j=1}^{p-1} x_p x_j$. For the textile example under

consideration, $x_2^2 = x_2(1 - x_1 - x_3) = x_2 - x_1 x_2 - x_2 x_3$. This implies that the quadratic effects in MDs are expressed as $x_1 x_2$, $x_1 x_3$, ..., $x_1 x_{p-1}$, $x_2 x_3$, ..., $x_{p-1} x_p$. Therefore, the quadratic model for a

MD is given by

$$y_i = \sum_{j=1}^p \beta_j x_{ij} + \sum_{j=1}^{p-1} \sum_{k>j}^p \beta_{jk} x_{ij} x_{ik} + \epsilon_i \quad (53)$$

The two models in (52) and (53), specially model (53), are the most commonly used MDs. However, there are also cubic models which are listed in the middle of page 469 (p. 447 of Montgomery 6th edition): the full cubic (11.26) and the special cubic (11.28). I would venture to claim that over 66% of all MD models encountered in practice are of the shape given by Eqs. (52) & (53). There are basically two types of MDs:

(1) The Simplex Lattice, and (2) The Simplex Centroid MD.

THE SIMPLEX LATTICE MIXTURE DESIGN

A $\{p, m\}$ lattice MD consists of a simplex, discussed in section 11.6 of Montgomery (11-5 of 6e), but with the following restriction on the x_j 's, $j = 1, 2, \dots, p$, and $x_j = 0/m, 1/m, 2/m, 3/m, 4/m, \dots, m/m$, where $2 \leq m \leq p$ and larger values of m lead to more design points. Some of the cases for $p = 3$ and 4 lattices are given in Figures 11.40 on p. 468 of Montgomery (Figures 11.34 on page 446 of 6th edition). I will work out the design aspects for the case of $p = 4$ simplex lattice MD, which is not given in Figures 11.40 on page 468 of Montgomery. The $\{4, 4\}$ simplex lattice design points are obtained from the following fractions:

$x_j = 0/4, 1/4, 2/4, 3/4, 4/4$. The corresponding design points are listed below.

Pure blends: (1, 0, 0, 0), (0, 1, 0, 0), (0, 0, 1, 0), (0, 0, 0, 1)	→	4 Points
Binary blends: (1/4, 3/4, 0, 0)	→	${}_4P_2 = 12$ Points
Binary (of-equal) blends: (1/2, 1/2, 0, 0)	→	${}_4C_2 = 6$ Points
Tri blends : (1/4, 1/4, 1/2, 0)	→	$({}_4C_3) \times {}_3C_2 = 12$ Points
Complete (or full) blend : (1/4, 1/4, 1/4, 1/4)	→	1 Point
		Total = 35 Points

The complete blend (1/4, 1/4, 1/4, 1/4) is also called the centroid of the lattice MD. Note that the simplex lattice has a centroid only in the case of $\{p, p\}$ lattice. Next we try to outline the proof that in general a simplex lattice MD has a total of ${}_{(p+m-1)}C_m = (p+m-1)!/[m!(p-1)!]$ design points. For the case of $\{4, 4\}$ simplex lattice we showed above that there are 35 design points. To prove that $35 = {}_7C_4$, we proceed as follows: $35 = 7 \times 5 = 7 \times 6 \times 5 / 3! = (7 \times 6 \times 5) \times 4! / (3! \times 4!) =$

$$7! / (3! \times 4!) = \binom{7}{4} = \binom{p+m-1}{m} = {}_7C_4.$$

Exercise 25. Perform a complete analysis of the $\{4, 3\}$ and $\{5, 4\}$ simplex lattice MD as

I did above for the {4, 4} case.

THE SIMPLEX CENTROID MIXTURE DESIGN

Unlike the {p, m} lattice, all simplex centroid MDs have a centroid given by the complete mixture (1/p, 1/p, ..., 1/p). All centroid MDs have design points consisting of pure blends, binary of equal blends, tri of equal blends, quad blends of equal proportions, ..., (1/p, 1/p, ..., 1/p). Below, I will work out the case of p = 4 components simplex centroid.

Pure blends: (1, 0, 0, 0), ..., (0, 0, 0, 1) → 4 Points

Binary blends: (1/2, 1/2, 0, 0) → 6 Points

Tri blends : (1/3, 1/3, 1/3, 0) → 4 Points

Centroid: (1/4, 1/4, 1/4, 1/4) → 1 Point

Total = 15

Note that the blending (1/3, 1/2, 1/6, 0) is not a point for the centroid design because of unequal proportions. The total number of design

points, in general, for a centroid MD is given by ${}_pC_1 + {}_pC_2 + {}_pC_3 + \dots + {}_pC_p = \sum_{j=1}^p {}_pC_j = \sum_{j=0}^p {}_pC_j - 1$

= $2^p - 1$. For p = 4, $2^4 - 1 = 15$ as counted above.

Simplex MD's are generally constructed in such a manner as to minimize the $V(\hat{\beta})$, although I am not sure that which of the two structured MD's (Simplex Lattice or Centroid) yield smaller variance for the same comparable designs. Further, a D-optimal design is one whose determinant of matrix $\mathbf{C} = (\mathbf{X}'\mathbf{X})^{-1}$ is minimum (or nearly minimum). For example, the covariance matrix for the {3, 2} simplex mixture design with n = 1 response is given below with determinant value of 4096.

$$(\mathbf{X}'\mathbf{X})^{-1} =$$

x1	x2	x3	x1x2	x1x3	x2x3
1.0	0.0	0.0	-2.0	-2.0	0.0
0.0	1.0	0.0	-2.0	0.0	-2.0
0.0	0.0	1.0	0.0	-2.0	-2.0
-2.0	-2.0	0.0	24.0	4.0	4.0
-2.0	0.0	-2.0	4.0	24.0	4.0
0.0	-2.0	-2.0	4.0	4.0	24.0

While if we construct an unstructured MD such as

$$\mathbf{X} =$$

x1	x2	x3	x1x2	x1x3	x2x3
0.7	0.3	0	0.21	0	0
0	0.35	0.65	0	0	0.2275
0.3	0.4	0.3	0.12	0.09	0.12
0.5	0.5	0	0.25	0	0
0.333333	0.333333	0.333333	0.111111	0.111111	0.111111
0.25	0.5	0.25	0.125	0.0625	0.125

The determinant of the corresponding covariance matrix $\text{COV}(\hat{\beta}) / \sigma_{\epsilon}^2 = \mathbf{C}_U$ explodes to 59267346867.3616000.

.

Exercise 26. Perform a complete analysis of the $p = 5$ simplex centroid MD as I did above for the $p = 4$ case.

As an example of MD application, consider the Example 11.5 on pages 469-472 (448-450 of Montgomery's 6th edition). Assuming that we are close to the optimum region, the fitted quadratic model is of the type given in equation (53) and can further be expressed as

$$y_i = \sum_{j=1}^6 \beta_j x_{ij} + \epsilon_i, \quad (54)$$

where $x_4 = x_1x_2$, $x_5 = x_1x_3$, $x_6 = x_2x_3$, and $i = 1, 2, 3, \dots, 15$. If we now form the LSF for the model of (54) as

$$L(\beta) = \sum_{i=1}^n \epsilon_i^2 = \sum_{i=1}^n (y_i - \beta_1 x_{i1} - \dots - \beta_6 x_{i6})^2$$

and partially differentiate wrt β_j ($j = 1, 2, \dots, 6$), we will obtain a set of 6 normal equations with 6 unknowns, but with the constraint $x_1 + x_2 + x_3 \equiv 1$. In order to use standard regression packages by Minitab or SAS, it is best 1st to invoke this constraint into model (54) and proceed as though it were a regular regression model. That is to say,

$$y_i = \beta_1 x_1 + \beta_2 x_2 + \beta_3 (1 - x_1 - x_2) + \beta_4 x_4 + \beta_5 x_5 + \beta_6 x_6 + \epsilon_i. \quad (55)$$

However, model Eq. (55) is equivalent to

$$\begin{aligned} y_i &= \beta_3 + (\beta_1 - \beta_3) x_1 + (\beta_2 - \beta_3) x_2 + \beta_4 x_4 + \beta_5 x_5 + \beta_6 x_6 + \epsilon_i \\ &= b_0 + b_1 x_1 + b_2 x_2 + b_4 x_4 + b_5 x_5 + b_6 x_6 + \epsilon_i \end{aligned} \quad (56)$$

where $b_0 = \beta_3$, $b_1 = \beta_1 - \beta_3$, $b_2 = \beta_2 - \beta_3$, and $b_j = \beta_j$ for $j = 4, 5, 6$.

I actually used Matlab and fitted the model (56) to the data of Example 11.5 on pp. 469-470 of Montgomery (pp. 448-450 of 6e) and obtained the following model and the corresponding **IM** Listed below.

$$\mathbf{IM} = \mathbf{X}'\mathbf{X} = \begin{bmatrix} 15 & 5 & 5 & 0.75 & 0.75 & 0.75 \\ 5 & 3.5 & 0.75 & 0.375 & 0.375 & 0 \\ 5 & 0.75 & 3.5 & 0.375 & 0 & 0.375 \\ 0.75 & 0.375 & 0.375 & 0.1875 & 0 & 0 \\ 0.75 & 0.375 & 0 & 0 & 0.1875 & 0 \\ 0.75 & 0 & 0.375 & 0 & 0 & 0.1875 \end{bmatrix}.$$

$(\mathbf{X}'\mathbf{Y})^T = [203.1 \quad 71.7 \quad 57.5 \quad 11.475 \quad 12.675 \quad 7.875]$, and

$$\hat{y} = (\mathbf{X}'\mathbf{X})^{-1}(\mathbf{X}'\mathbf{Y}) = 16.4 - 4.7x_1 - 7.0x_2 + 19.0x_1x_2 + 11.40x_1x_3 - 9.60x_2x_3 \quad (57)$$

However, the above model (57) is identical to the one given in the middle of page 470 (p. 448 of Montgomery's 6th edition), which I will illustrate below. Recall the constraint $x_1 + x_2 + x_3 = 1$. We simply multiply the value of $\hat{b}_0 = 16.40$ in (57) by $1 = x_1 + x_2 + x_3$ and simplify the resulting equation.

$$\begin{aligned} \hat{y} &= 16.4(x_1 + x_2 + x_3) - 4.7x_1 - 7.0x_2 + 19.0x_1x_2 + 11.40x_1x_3 - 9.60x_2x_3 \\ &= 11.70x_1 + 9.40x_2 + 16.4x_3 + 19.0x_1x_2 + 11.40x_1x_3 - 9.60x_2x_3. \end{aligned} \quad (58)$$

This last Eq. (58) is indeed identical to the mixture model in the middle of page 470 (p. 448 of Montgomery's 6th edition). The advantage of model (57) over this last mixture model (58) is that (57) is in the format of the classical regression model and hence we can use regression theory from Chapter 10 to arrive at the proper ANOVA Table. WE 1st rewrite model (58) in the classical regression format, as before in Eq. (57)

$$\hat{y} = 16.4 - 4.7x_1 - 7.0x_2 + 19.0x_1x_2 + 11.40x_1x_3 - 9.60x_2x_3, \quad (57)$$

where $\hat{\beta}_0 = 16.4$, $\hat{\beta}_1 = -4.7$, ..., $\hat{\beta}_5 = -9.60$. The regression model in (57) clearly shows that

the Model SS must carry 5 *df* and is computed from $SS(\text{REG}) = \sum_{j=1}^5 \hat{\beta}_j S_{jy}$, where $S_{1y} = \sum_{i=1}^{15} x_{i1}y_i -$

$$(\sum x_1)(\sum y) / 15 = 71.7 - 5(203.10) / 15 = 4.00, S_{2y} = -10.20, S_{3y} = 1.320, S_{4y} = 2.520, \text{ and } S_{5y} =$$

–2.280. Therefore, $SS(\text{REG}) = \sum_{j=1}^5 \hat{\beta}_j S_{jy} = 128.29600 = SS_{\text{Model}}$ with 5 *df*. As usual, $USS = 2884.830$ with 15 *df*, $CF = (\sum y)^2/15 = 2749.9740$ with 1 *df*, and hence the $SS_{\text{Total}} = SS_T = USS - CF = 134.8560$ with 14 *df*. As a result, $SS_{\text{RES}} = 6.56$ with $14 - 5 = 9$ *df*.

Note that the value of SS_{RES} can also be computed directly from $SS_{\text{RES}} = SS_{\text{PE}} = (11^2 + 12.4^2 - 23.4^2/2) + (15^2 + 14.8^2 + 16.1^2 - 45.9^2/3) + (8.8^2 + 10^2 - 18.8^2/2) + (10^2 + 9.7^2 + 11.8^2 - 31.5^2/3) + (16.8^2 + 16^2 - 32.8^2/2) + (17.7^2 + 16.4^2 + 16.6^2 - 50.7^2/3) = 0.98 + 0.98 + 0.72 + 2.58 + 0.32 + 0.98 = 6.56$ with 9 *df*, which checks exactly with $SS_{\text{Total}} - SS_{\text{Model}} = 134.8560 - 128.2960$.

To obtain the ANOVA table, we need to examine the break-down of the Model SS into separate orthogonal components. However, due to the constraint $x_1 + x_2 + x_3 = 1$ and the fact that the $\mathbf{X}'\mathbf{X}$ is not a diagonal matrix, it will be impossible to obtain five 1-*df* SS's that will sum to SS_{Model} , i.e., an orthogonal breakdown of SS_{Model} as given in Eq. (57) into 5 additive components does not exist. Therefore, in mixture designs the appropriate procedure is to obtain sequential SS's due to linear, quadratic, and cubic effects. The sequential $SS_L = SS(x_1, x_2, x_3)$ is obtained by fitting the regression model $\hat{y} = a_0 + a_1 x_1 + a_2 x_2 = 15.794545 - 0.80 x_1 - 5.963636 x_2$ which results in $SS_L = -0.80 \times S_{1y} - 5.963636 \times S_{2y} = 57.6291$. Thus, the extra SS due to adding the quadratic effects $x_1 x_2$, $x_1 x_3$ and $x_2 x_3$ is given by $SS_Q = SS_{\text{Model}} - SS_L = 128.296 - 57.6291 = 70.66691$. The ANOVA Table is summarized below. As discussed earlier, the

ANOVA Table for the Example 11.5 of Montgomery on his page 470

Source	<i>df</i>	SS	MS	F_0	<i>P-Value</i>
Total	14	134.856			
x_1, x_2, x_3	2	57.62909	28.81455	39.53215	0.0 ⁴ 34873
Quadratic	3	70.66691	23.55564	32.31718	0.0 ⁴ 37865
Pure Error	9	6.56	0.728889		

eventual objective in mixture designs is to optimize the response y in the feasible region of the factor space $0 \leq x_j \leq 1, j = 1, 2, \dots, p$. You must bear in mind that an x_j can never be negative

nor can it ever exceed 1. We may optimize either model (57) or (58). I will attempt to obtain the exceptional point \mathbf{x}_0 for the mixture model (58) again listed below.

$$\hat{y} = 11.70x_1 + 9.40x_2 + 16.4x_3 + 19.0x_1x_2 + 11.40x_1x_3 - 9.60x_2x_3 \quad (58)$$

and in an assignment you will be asked to follow suite for the model (57). Recall that the objective is to maximize the elongation of the fiber formulation under the constraint $x_1 + x_2 + x_3 = 1$. Before invoking this constraint into our model, we must observe that the coefficients of both x_1x_2 and x_1x_3 are positive (i.e., these 2 combinations produce synergistic blending and will increase elongation), while the coefficient of x_2x_3 is negative so that this combination will produce antagonistic blending, i.e., the interaction x_2x_3 will decrease the response y .

To start the optimization procedure, we 1st invoke the constraint $x_2 = 1 - x_1 - x_3$ into model (58). This will yield the model

$$\hat{y} = 9.40 + 21.30x_1 - 2.6x_3 + 2x_1x_3 - 19x_1^2 + 9.60x_3^2. \quad (59)$$

Partial differentiations will yield

$$\frac{\partial \hat{y}}{\partial x_1} = 21.3 + 2x_3 - 38x_1 \longrightarrow \frac{\partial^2 \hat{y}}{\partial x_1^2} = -38.00$$

$$\frac{\partial \hat{y}}{\partial x_3} = -2.6 + 2x_1 + 19.2x_3 \longrightarrow \frac{\partial^2 \hat{y}}{\partial x_3^2} = 19.20$$

We may as well stop this maximization procedure right here because \mathbf{x}_0 is a point of maximum response only if

$$\left. \frac{\partial \hat{y}}{\partial x_1} \right|_{\mathbf{x}_0} = 0, \quad \left. \frac{\partial^2 \hat{y}}{\partial x_3^2} \right|_{\mathbf{x}_0} < 0, \text{ and } \left(\left. \frac{\partial^2 \hat{y}}{\partial x_1^2} \right|_{\mathbf{x}_0} \right) \left(\left. \frac{\partial^2 \hat{y}}{\partial x_3^2} \right|_{\mathbf{x}_0} \right) > \left(\left. \frac{\partial^2 \hat{y}}{\partial x_1 \partial x_3} \right|_{\mathbf{x}_0} \right)^2.$$

But the above required 2nd and 3rd conditions do not hold for the model (59), and the solution $x_1 = 0.56456$, $x_2 = 0.35883$, $x_3 = 0.07661$ yielding $\hat{y} = 15.31296$ is simply a saddle point (or a local optimum) and not necessarily a global maximum. This implies that our response function, \hat{y} in (59), is not strictly concave over the entire range of factor space $\{x_j \mid 0 \leq x_j \leq 1, j = 1, 2, 3\}$.

This fact can be verified by the 3 eigenvalues of the matrix

$$\mathbf{B} = \begin{bmatrix} 0 & 9.5 & 5.7 \\ 9.5 & 0 & -4.8 \\ 5.7 & -4.8 & 0 \end{bmatrix}$$

which are $\lambda_1 = -13.5681$, $\lambda_2 = 9.5607$, and $\lambda_3 = 4.0074$ and hence the surface is not concave or convex. Therefore, resort has to be made to other means. Below I will provide the step-by-step procedure as to how I would proceed in order to obtain the global optimum solution for a response surface such as

$$\hat{y} = 11.70x_1 + 9.40x_2 + 16.4x_3 + 19.0x_1x_2 + 11.40x_1x_3 - 9.60x_2x_3 \quad (58)$$

subject to the 7 constraints $0 \leq x_j \leq 1$, $j = 1, 2, 3, 4, 5, 6$ and $x_1 + x_2 + x_3 = 1$.

Step 1. Equation (58) clearly shows that the interaction ($-9.60x_2x_3$) is indeed antagonistic, i.e., unless either $x_2 = 0$, or $x_3 = 0$, the term ($-9.60x_2x_3$) always decreases the response value \hat{y} for all $0 < x_j < 1$, $j = 2, 3$. Therefore, the global optimum must occur either at $x_2 = 0$, or at $x_3 = 0$, but we do not know which one and have to try both possibilities.

Step 2. First, try $x_2 = 0$. Then the problem reduces to maximizing the objective function $y = 11.7x_1 + 16.4x_3 + 11.4x_1x_3$ subject to the 4 constraints $0 \leq x_j \leq 1$, $j = 1, 3, 5$ and $x_1 + x_3 = 1$.

Step 3. Invoke this last constraint into the objective function, which reduces it to $y = 16.4 + 6.7x_1 - 11.4x_1^2$. Then set dy/dx_1 to zero and determine the sign of d^2y/dx_1^2 : $dy/dx_1 = 6.7 - 22.8x_1$, $d^2y/dx_1^2 = -22.8 < 0$, which is the necessary condition for \mathbf{x}_0 to be the point of maximum response. Setting $dy/dx_1 = 0$ and solving the resulting equation yields $\mathbf{x}_0 = [0.29386 \quad 0 \quad 0.70614]'$ and the corresponding $\hat{y}_0 = 17.38443$. The text by R. H. Myers and D. C. Montgomery (Wiley, ISBN: 0-471-58100-3) reports the stationary point $[0.20 \quad 0 \quad 0.80]'$ with the corresponding $\hat{y}_0 = 17.28400$. Thus my solution is just a bit better than the one that they guesstimated by simply observing the contours of the response surface. The question now arises "how do we know for certain that $\mathbf{x}_0 = [0.29386 \quad 0 \quad 0.70614]'$ does yield the global maximum? To answer this question, we must also try $x_3 = 0$, as in step 4.

Step 4. Putting $x_3 = 0$ in the model (58) results in the objective function $y = 11.7x_1 + 9.4x_2 + 19x_1x_2$ subject to 4 more constraints $0 \leq x_j \leq 1$, $j = 1, 2, 4$ and $x_1 + x_2 = 1$. Proceeding as

in **Step 3** above, we obtain $\mathbf{x}_o = [0.56053 \quad 0.43947 \quad 0]^T$ with $\hat{y}_o = 15.36961$, which is much less than the optimum result of 17.38443 obtained in **step 3**. Therefore, there is no point (x_1, x_2, x_3) in the region of the factor space that will yield a response larger than $\hat{y}_o = 17.38443$ Kg, and hence $\mathbf{x}_o = [0.29386 \quad 0 \quad 0.70614]^T$ is the global optimum solution.

Before I close this section, the reader must be cognizant of the fact that the simplex lattice MD in the Example 11.5 of Montgomery (Example 11-3 of 6e) is a saturated design for the fitted model (58). This is due to the fact that the design matrix of the $\{3, 2\}$ lattice provides 6 **FLCs** and hence only 5 *df* for studying effects and the model already contains 5 independent effects. Hence, there are no *df* left to test the model for the LOF. The need for testing of LOF leads to the augmentation of simplex MDs.

Exercise 27. Repeat the above procedure to obtain the optimal solution for the model (58).

Augmenting Simplex Designs with Axial (or Interior) Runs In Order to Study Higher-Order Effects

Both the simplex-lattice and simplex-centroid designs have nearly all their points on the boundaries of the simplex, except for the centroid which is in the interior of the simplex when the design includes the point $(1/p, 1/p, \dots, 1/p)$. All centroid simplexes have a centroid by their definition, but only the $\{p, p\}$ simplex lattice has the centroid as an interior point. As R. H. Myers and D. C. Montgomery (1995, pp. 551-560, Wiley Publications, ISBN: 0-471-58100-3) report on the $\{3, 3\}$ simplex lattice which has ${}_5C_3 = 10$ design points, 3 of which are pure blends, 6 are binary blends of the type $(1/3, 2/3, 0)$, and only one interior point namely the centroid $(1/3, 1/3, 1/3)$. Therefore, as they suggest, the distribution of information occurs in the ratio of 3:6:1. To improve on this ratio, i.e., we need to augment this design with additional interior points. Further, they recommend that these interior points should be halfway between a vertex such as $(1, 0, 0)$ and the centroid $(1/3, 1/3, 1/3)$. Since the point $(2/3, 1/6, 1/6)$ is exactly a distance of $d = (1/6)^{1/2}$ from both $(1, 0, 0)$ and $(1/3, 1/3, 1/3)$, then the 3 augmented interior points for the $\{3, 3\}$ simplex lattice are $(2/3, 1/6, 1/6)$, $(1/6, 2/3, 1/6)$ and $(1/6, 1/6, 2/3)$. This augmented design will enhance the amount of information in the interior to the

ratio of 3:6:4. Further, if the lattice does not have a centroid, such as {4, 3}, then the centroid $(1/4, 1/4, 1/4, 1/4)$ must be added before augmenting the design with further interior points of equal distance to a vertex and the center. Below I am providing an example of an augmented MD borrowed from the Example 11.2 on pages 553-558 of Myers and Montgomery (1995).

Their experiment is a chemical etching process on the backs of silicon wafers in the semiconductor industry. The etching solution is a mixture of 3 acids A, B, and C. The experimenters objective was to study how the composition of the 3 acids in the mixture would affect the etching rate y . The final objective was to determine the mixture composition of the 3 acids that yielded an etching rate of at least 750. The MD used was a {3, 2} lattice augmented with 4 interior points $(2/3, 1/6, 1/6)$, $(1/6, 2/3, 1/6)$, $(1/6, 1/6, 2/3)$ and $(1/3, 1/3, 1/3)$. The design layout is provided in Table 2, where the value of $N = 14$. At first glance, it seems that the design matrix in Table 2 provides 9 df for studying the full cubic model (11.27) given in the middle of page 469 of Montgomery (p. 447 of 6th edition). Unfortunately, it is not

Table 2 [The {3, 2} augmented lattice MD]

Run	x_1 (Acid A)	x_2 (Acid B)	x_3 (Acid C)	Etch Rate y
1	1	0	0	540, 560
2	0	1	0	330, 350
3	0	0	1	295, 260
4	1/2	1/2	0	610
5	0	1/2	1/2	330
6	1/2	0	1/2	425
7	2/3	1/6	1/6	710
8	1/6	2/3	1/6	640
9	1/6	1/6	2/3	460
10	1/3	1/3	1/3	800, 850

possible to obtain a regression model with the regressors $x_1, x_2, x_3, x_4 = x_1x_2, x_5 = x_1x_3, x_6 = x_2x_3, x_7 = x_1x_2x_3, x_8 = x_1x_2(x_1 - x_2), x_9 = x_1x_3(x_1 - x_3),$ and $x_{10} = x_2x_3(x_2 - x_3)$. This is due to the fact that there are 2 constraints: $x_1 + x_2 + x_3 = 1$ and $x_1x_2(x_1 - x_2) + x_2x_3(x_2 - x_3) = x_1x_3(x_1 - x_3)$. Note that

the 2nd constraint is valid only for this case, i.e., in general $x_1x_2(x_1 - x_2) + x_2x_3(x_2 - x_3) \neq x_1x_3(x_1 - x_3)$. Further, Minitab will not even allow the inclusion of all 3 regressors x_1, x_2, x_3 simultaneously and will notify you that x_3 is 100% correlated with x_1 and x_2 . Therefore, I obtained the following model from Minitab

$$\hat{y} = 276.0725 + 272.5x_1 + 62.5x_2 + 642.8704x_4 + 27.8704x_5 + 67.8704x_6 + 9243.3333x_7 - 775.0x_8 + 980.0x_9. \quad (60)$$

I proceeded to write a Matlab program to obtain the regression function and the corresponding ANOVA table, which are listed on below.

$$\hat{y} = 548.573x_1 + 338.573x_2 + 276.073x_3 + 642.870x_4 + 27.870x_5 + 67.870x_6 + 9243.333x_7 - 775x_8 + 980x_9. \quad (61)$$

Note that model (61) indeed reduces exactly to (60) if we replace the 3rd term x_3 with $1 - x_1 - x_2$. Model (61) clearly shows that the entire model will carry 8 *df*, and residuals will have 5 *df* because the SS_{Total} has 13 *df*. My ANOVA Table from the Matlab program is summarized in Table 3.

ANOVA Table 3

Source	<i>df</i>	SS	MS	F_0	<i>P-Values</i>
Total	13	478821.42857			
x_1, x_2, x_3	2	133755.00	66877.50	93.3285	0.000110
Quadratic	3	229364.8548	76454.9516	106.694	0.0 ⁵ 5944
Special Cubic	1	107877.7918	107877.7918	150.5450	0.0 ⁵ 6364
Full Cubic	2	4240.87302	2120.43651	2.9591	0.146024
Residuals	5	3582.90895	716.5818		
Pure Error	4	2262.5000	565.625		
LOF	1	1320.40895	1320.40895	2.33442	0.201262

I used the software Lingo6 to obtain the optimal solution for the model (61) with the results $x_0 = [0.39816 \quad 0.35963 \quad 0.24221]'$ with $\hat{y}_0 = 838.7422 > 750$. Therefore, if the etching solution is made with roughly 40% acid A, 36% acid B, and 24% acid C, then more than 75% etching rate will be attained. The Lingo codes are also available on my website.

Exercise 28. Three different motor fuels x_1 , x_2 and x_3 can be blended to form gasoline.

The objective was to identify the blend that maximized MPG performance. An augmented simplex design was used to study the blending properties of the 3 fuels, and the results are shown in Table 4.

Table 4

Run	x_1	x_2	x_3	MPG, y
1	1	0	0	23.5, 24.8
2	0	1	0	24.1, 24.3
3	0	0	1	22.8, 23.1
4	1/2	1/2	0	25.1
5	0	1/2	1/2	27.8
6	1/2	0	1/2	27.6
7	2/3	1/6	1/6	26.8
8	1/6	2/3	1/6	25.9
9	1/6	1/6	2/3	24.5
10	1/3	1/3	1/3	24.8, 23.9, 24.5

(a) Fit only a linear model and test it for LOF. By hand calculations, verify the value of $SS(REG)$.

Show all your work! (b) Next, fit a quadratic model and test it for LOF. (c) Finally fit a full cubic model and determine if this model improves the one in (b) to be used for optimization. Identify the regressor(s) that account for the LOF. (d) Determine the optimal condition \mathbf{x}_0 and the corresponding value of \hat{y}_0 .

The student version of Lingo6 can be downloaded from www.lindo.com/

Evolutionary Operation (Section 11.7 of Montgomery; Section 11-6 of 6e)

RSM (response surface methodology) is an optimization technique for research laboratory on a small scale, while EVOP's (Evolutionary Operation's) objective is exactly the same but on a large scale, i.e., on a manufacturing floor. Therefore, the objective of EVOP is to

identify the optimal conditions of an unknown RS (Response Surface) in a real-plant operations.

For the sake of illustration, consider the Example 11.7 on pp. 477-480 (pp. 454-458 of Montgomery's 6th edition). Here, the objective of EVOP is to attain the maximum process yield, y , by running the process at optimum levels of x_1 = operating temperature (factor A), and x_2 = operating pressure (factor B).

The EVOP procedure generally uses a 2^k factorial design with a center point that is run exactly once. For our example, $k = 2$ factors, and therefore, there are 5 design points as shown in Figure 11.48 and Table 11.22 on page 477 (p. 455 of Montgomery's 6th edition). Thus, our response variable, y , is % process yield with current operating design center (DC) at $x_1 = 250$ °F, and $x_2 = 145$ psi, where the design spacing for both process variables is 10 units.

The primary objective of EVOP is to determine if the current operating conditions no longer optimize the response y , i.e., the current DC is no longer near optimum conditions. This determination is made ASA an effect becomes statistically significant at the 5% level, suggesting a change in process operating conditions is needed. It is then said that one phase has been completed. Each phase of EVOP consists of several cycles n , where n_p denotes the cycle at which a phase is completed (and the subscript p stands for phase). On the average, each phase consists of $n_p = 3$ to 6 cycles. If the process is actually being run near the optimum conditions and optimum process conditions do not change much with time, then the value of n_p can be very large.

I now provide you with notations that will be used throughout these notes, which is mostly consistent with the literature. Let $y_i(n)$ be the observation at the i^{th} design point and n^{th} cycle, where $n = 1, 2, 3, 4, \dots, n_p$ and only for two regressors the value of $i = 1, 2, 3, 4, 5$. Accordingly, a reference to page 477 (p. 455 of Montgomery's 6th) will reveal that $y_1(1) = 84.5\%$, $y_2(1) = 84.2\%$, $y_3(1) = 84.9\%$, $y_4(1) = 84.5\%$, and $y_5(1) = 84.3\%$. Similarly, the observations for the 2nd cycle, given in Table 11.23 on page 478 (p. 456 of Montgomery 6th edition), are $y_1(2) = 84.9\%$, $y_2(2) = 84.6\%$, $y_3(2) = 85.9\%$, $y_4(2) = 83.5\%$, and $y_5(2) = 84.0\%$. I have made and provided an EVOP Calculation Sheet for $k = 2$ process parameters on my website, which you may download for future use.

We now proceed to compute the average effects of A, B, and A×B. Figure 11-48 on page 477 (p. 455 of Montgomery's 6th edition) clearly shows that the total temperature (x_1) effect is given by the sum of the two contrasts $(\bar{y}_4 - \bar{y}_2) + (\bar{y}_3 - \bar{y}_5)$, and thus the average effect of A is given by

$$\bar{x}_1 = \bar{A} = \frac{1}{2} [(\bar{y}_4 - \bar{y}_2) + (\bar{y}_3 - \bar{y}_5)] = \frac{1}{2} (\bar{y}_3 + \bar{y}_4 - \bar{y}_2 - \bar{y}_5),$$

where the divisor 2 pertains to two contrasts. Similarly,

$$\bar{B} = \frac{1}{2} (\bar{y}_3 + \bar{y}_5 - \bar{y}_2 - \bar{y}_4), \text{ and } \overline{A \times B} = \frac{1}{2} (\bar{y}_3 + \bar{y}_2 - \bar{y}_4 - \bar{y}_5).$$

Since the variance of all the above 3 average effects are the same, we proceed first to compute

the $V(\bar{A}) = \frac{1}{4} \sum_{i=1}^4 V(\bar{y}_i) = V(\bar{y}) = \sigma_y^2/n$. We may further conclude that the $se(\bar{B}) = se(\overline{A \times B}) = se(\bar{A}) = \sigma_y / \sqrt{n}$, except for the change-in-the-mean (CIM) effect.

We have to be a bit more cautious about how to define the change in the mean response from the 2² peripheral points (2, 3, 4, and 5) to the DC, which is point (1). Note that the CIM determines the quadratic effect of x_1 and x_2 on y . It seems that at 1st glance the total effect from the design peripherals to the DC (design center) should be given by

$$\bar{y}_2 + \bar{y}_3 + \bar{y}_4 + \bar{y}_5 - 4\bar{y}_1 \quad (62)$$

and because there are 4 comparisons (or contrasts) in the expression (62), then the average CIM effect should be computed from $(\bar{y}_2 + \bar{y}_3 + \bar{y}_4 + \bar{y}_5)/4 - \bar{y}_1$. It should be intuitively apparent that the CIM effect must have a smaller variance than the \bar{A} , \bar{B} , and $\overline{A \times B}$ effects simply because (i) there are 5 means involved in the CIM effect versus 4 for the other 3 effects, (ii) the distance of the peripheral average $(\bar{y}_2 + \bar{y}_3 + \bar{y}_4 + \bar{y}_5)/4$ to the center \bar{y}_1 , for this example, is $\sqrt{(1/2)^2 + (1/2)^2} = \sqrt{0.5}$. That is, the distance of $(\bar{y}_2 + \bar{y}_3 + \bar{y}_4 + \bar{y}_5)/4$ to \bar{y}_1 is $\sqrt{0.5}$, as opposed to the average distance of $\bar{y}_3 + \bar{y}_4$ to $\bar{y}_2 + \bar{y}_5$, which is one unit for our example. Note that the $V[(\bar{y}_2 + \bar{y}_3 + \bar{y}_4 + \bar{y}_5)/4 - \bar{y}_1] = 1.25\sigma_y^2/n > V(\bar{A}) = V(\bar{B}) = V(\overline{A \times B})$. Thus, we have to find a divisor larger than 4 for the expression given in (62). Since

there are 5 means in the expression (62), George E. P. Box proposed a divisor of 5, i.e., the

average CIM effect is defined as $\overline{\text{CIM}} = 0.2(\bar{y}_2 + \bar{y}_3 + \bar{y}_4 + \bar{y}_5) - 0.8\bar{y}_1 =$

$$(\bar{y}_2 + \bar{y}_3 + \bar{y}_4 + \bar{y}_5 - 4\bar{y}_1)/5 = \frac{1}{5} \left[\sum_{i=2}^5 \bar{y}_i(n) \right] - \frac{4}{5} \bar{y}_1(n). \text{ Note that the } \overline{\text{CIM}} \text{ is also a measure}$$

of curvature in the RS and thus if the process is operating near optimum conditions, we should expect a higher yield at the DC than the peripherals. Therefore, this last definition George E.

P. Box is what we will be using as $\overline{\text{CIM}}$. The variance of the CIM effect is computed from

$$V[(\bar{y}_2 + \bar{y}_3 + \bar{y}_4 + \bar{y}_5 - 4\bar{y}_1)/5] = \frac{1}{25} [4V(\bar{y}) + 16V(\bar{y})] = 0.80\sigma_y^2/n. \text{ Perhaps}$$

it is more essential to detect a CIM more rapidly than other effects when the contrast for the CIM is positive. Note that for cycle $n = 1$, $SS_{\text{Model}} = 0.2880 = SS_A + SS_B + SS(A \times B) + SS(\text{CIM})$, where the contrast(CIM) = -0.02 .

Estimation of σ_y^2

The question now arises as to how we estimate σ_y ? Clearly, we need at least $n = 2$ cycles in order to estimate σ_y . One possible solution is, after $n = 1$ cycle, to obtain the values of S at the 5 design points, and average the 5 sample standard deviations. For the Example

11.7 of Montgomery, this leads to $S_i = 0.282843 = \sqrt{(-0.4)^2 / 2}$, 0.282843, 0.707111, 0.707111, 0.212132 and $\bar{S} = 0.43841$. Or we could use the pooled standard deviation from the 5 design

points for 2 cycles which is equal to $S_p = \sqrt{\frac{0.4^2 + 0.4^2 + 1^2 + (-1)^2 + (-0.3)^2}{2 \times 5}} = \sqrt{0.241000} =$

0.49092. However, the above estimation procedure is not used in EVOP because variability at the 5 FLCs may well be quite different, and as a result, G. E. P. Box suggested to use results from the field of Quality Control in order to estimate σ_y . To this end, let $W = R/\sigma$ be the relative range of a sample of size N drawn from a normal universe, where σ is the process standard deviation (i.e., a parameter) and R is the sample range (i.e., a random variable).

Then, $R = \sigma W$, and applying the expected-value operator to $R = \sigma W$ results in

$$E(R) = \sigma E(W) = \sigma d_2 \quad (63)$$

In Eq. (63), the values of $d_2 = E(W) = E(\text{Relative Range})$ have already been obtained in statistical literature for a normal universe using the SMD (sampling distribution) of R from a $N(\mu, \sigma^2)$ for different sample sizes $N \geq 2$ (see Table 5 below). The values of $d_2 = E(W)$ are also tabulated in every QC text book. I would recommend against the use of R in estimating σ_y when $N > 15$ because the SMD of R is very unstable for large sample sizes, i.e., one mild-outlier in the sample will unusually increase the data spread. Further, in the field of QC if the sampling design is unbalanced, then variation cannot be monitored with an R-chart.

Table 5 (The values of $d_2 = E(W)$ for $N = 2, 3, \dots, 15$)

N	2	3	4	5	6	7	8	9	10	11	12	13	14	15
d_2	1.128	1.693	2.059	2.326	2.534	2.704	2.847	2.970	3.078	3.173	3.258	3.336	3.407	3.472

To obtain the point estimate of σ_y , replace all 3 parameters in equation (63) with the corresponding point estimators, i.e.,

$$\bar{R} = \hat{\sigma}_{\text{Individuals}} \times d_2 \rightarrow \hat{\sigma} = \bar{R} / d_2, \text{ or } \hat{\sigma}_{\text{unit to unit}} = R / d_2 \quad (64)$$

In order to get the estimation procedure started for the EVOP, we 1st define $D_i(n) = \bar{y}_i(n-1) - y_i(n)$, $n = 2, 3, 4, \dots, n_p$ cycles; note that n must be at least 2 in order to compute the differences D_i , $i = 1, 2, 3, \dots, N$ and n_p stands for the cycle at which a phase has been completed. Recall that a phase is completed ASA at least one effect becomes statistically significant, i.e., n_p denotes the 1st cycle at which at least one effect exceeds its allowable Error Limits. For the Example 11.7 (11.5 on pp. 454-458 of Montgomery's 6e), the values of $D_i(n)$ are given below. $D_i(2)$: -0.40, -0.40, -1, 1, 0.30; $D_i(3)$: -0.30, 0.40, -1.20, -0.90, -1.05.

Second, we apply the operator Variance, V , to the $D_i(n) = \bar{y}_i(n-1) - y_i(n)$.

$$V[D_i(n)] = \frac{\sigma_y^2}{n-1} + \sigma_y^2 = \frac{n}{n-1} \sigma_y^2 \quad (65)$$

Eq. (63) also implies that an estimate of $V[D_i(n)]$ can be obtained from

$$\hat{V}[D_i(n)] = R_D^2 / d_{2,N}^2 \quad (66)$$

Combining equations (66) and (65) yields

$$\hat{V} [D_i(n)] = \frac{n}{n-1} \hat{\sigma}_y^2 = R_D^2 / d_{2,N}^2 \quad (67)$$

Eq. (67) now provides an estimate of σ_y provided below.

$$\hat{\sigma}_y = \left(\sqrt{\frac{n-1}{n}} \right) R_D / d_{2,N} = (f_{N,n}) R_D \quad (68)$$

where $f_{N,n} = \left(\sqrt{\frac{n-1}{n}} \right) / d_{2,N}$. For a 2^2 design, $N = 5$ points, while for a 2^3 design, $N = 9$ points (8 factorial plus one center point), and I am not certain what is exactly applicable to $N = 10$, but I will guess below. Perhaps, $N = 10$ pertains to a 2^3 factorial run in two blocks of 4 factorial points [(1), ab, ac, bc], [a, b, c, abc], and each block with one center point. Note that in this last block design $g = ABC$ is confounded with blocks and

$$\hat{\sigma}_y = \left[\sqrt{\frac{n-1}{n}} / d_{2,10} \right] R_D = (f_{10,n}) R_D$$

and R_D pertains to the range of all 10 differences. In such a block design it can be shown that $V(\text{Effect}) = \sigma_y^2 / (2n)$ and $V(\text{CIM}) = 0.40 \sigma_y^2 / n$. The values of $f_{N,n}$ are listed in Table 11.26 p. 480 (Table 11.21 atop page 458 of Montgomery's 6th edition) for $n = 2, 3, \dots, 10$ cycles and $N = 5, 9$, and 10 total design points. My preference is to use the designation $f_{N,n}$ for $\left(\sqrt{\frac{n-1}{n}} \right) / d_{2,N}$ rather than $f_{k,n}$ used in the literature, which may be somewhat confusing.

In order to better understand how to apply the above procedure to obtain a point estimate of σ_y , I will go thru the estimation procedure for both cycles $n = 2$ and 3 of Montgomery's Example 11.7. The data for cycle $n = 2$ is given in Table 11.23 of Montgomery on p. 478 (Table 11.18 on page 456 of 6e). This Table shows that the range of the differences $D_i(2)$ is equal to $1 - (-1) = 2.0$. Eq. (68) shows that $\hat{\sigma}_y = (f_{N,n}) R_D$ and Table 11.26 on p. 480 (Table 11.21 atop page 458 of Montgomery's 6e) shows that $f_{5,2} = 0.30$, and hence

$$\hat{\sigma}_y = 0.30 \times 2.0 = 0.60 = S_2.$$

The value of $f_{5,2}$ can also be obtained from $f_{5,2} = \left(\sqrt{\frac{1}{2}} \right) / 2.326 = 0.304$ (See Table 5 on p. 87 of my notes), or $\hat{\sigma}_y = 0.608$. For cycle $n = 3$, the data is given on page 478 (Table 11.19 on p. 456 of Montgomery's 6th edition), where $D_i(3) = 0.30, -0.40, 1.20,$

0.90, 1.05, and $R_D = 1.60$. The value of $f_{5,3} = (\sqrt{\frac{2}{3}})/2.326 = 0.35103$ and hence $\hat{\sigma}_y = 0.56165 = S_3$. Therefore, at the end of cycle 3, we must use $\bar{S} = (0.608 + 0.56165)/2 = 0.585$, in lieu of S , as an estimate of σ_y in computing the 95% error (or critical) limits for all the effects and CIM.

The general formula for \bar{S} is given by
$$\bar{S} = \frac{1}{n_p - 1} \sum_{n=2}^{n_p} S_n .$$

Since the Pressure effect (Factor B) is significant at the 5% level at the end of cycle 3, then one EVOP phase has been completed and the DC (Design Center) must be moved by examining the overall averages at the end of the n_p^{th} (3rd) cycle. Since point 3, ($x_1 = 255^\circ\text{F}$, $x_2 = 150$ psi) has the highest average yield of 85.80%, then a 2nd EVOP phase will have to commence with the DC at ($x_1 = 255^\circ\text{F}$, $x_2 = 150$ psi) and a spacing of 10 units. There is a typo in Montgomery's (7e) near the bottom of p. 479 about the DC of the next phase, where $x_2 = 255^\circ\text{F}$ not 225 as printed.

Exercise 29. The yield during the first 4 cycles of a chemical process is shown in the following table. The process parameters are $x_1 =$ percent concentration at levels 30, 31, and 32, and process temperature, x_2 at 140, 142, and 144 Fahrenheit . Analyze the data by the EVOP Method; you must complete calculations for all 4 cycles even if a phase is completed prior to cycle 4.

DP	(1)	(2)	(3)	(4)	(5)
Cycle					
1	60.7%	59.8	60.2	64.2	57.5
2	59.1	62.8	62.5	64.6	58.3
3	56.6	59.1	59.0	62.3	61.1
4	60.5	59.8	64.5	61.0	60.1