Chapter 11. Supplemental Text Material

S11-1. The Method of Steepest Ascent

The method of steepest ascent can be derived as follows. Suppose that we have fit a first-order model

$$\hat{y} = \hat{\beta}_0 + \sum_{i=1}^{k} \hat{\beta}_i x_i$$

and we wish to use this model to determine a path leading from the center of the design region **x** = **0** that increases the predicted response most quickly. Since the first–order model is an unbounded function, we cannot just find the values of the *x*'s that maximize the predicted response. Suppose that instead we find the *x*'s that maximize the predicted response at a point on a hypersphere of radius *r*. That is

$$\text{Max } \hat{y} = \beta_0 + \sum_{i=1}^{k} \hat{\beta}_i x_i$$

subject to

$$\sum_{i=1}^{k} x_i^2 = r^2$$

The can be formulated as

$$\text{Max } G = \beta_0 + \sum_{i=1}^{k} \hat{\beta}_i x_i - \lambda\left[\sum_{i=1}^{k} x_i^2 - r^2\right]$$

where λ is a LaGrange multiplier. Taking the derivatives of *G* yields

$$\frac{\partial G}{\partial x_i} = \hat{\beta}_i - 2\lambda x_i \quad i - 1,2,\cdots,k$$

$$\frac{\partial G}{\partial \lambda} = -\left[\sum_{i=1}^{k} x_i^2 - r^2\right]$$

Equating these derivatives to zero results in

$$x_i = \frac{\hat{\beta}_i}{2\lambda} \quad i = 1,2,\cdots,k$$

$$\sum_{i=1}^{k} x_i^2 = r^2$$

Now the first of these equations shows that the coordinates of the point on the hypersphere are proportional to the signs and magnitudes of the regression coefficients (the quantity 2λ is a constant that just fixes the radius of the hypersphere). The second equation just states that the point satisfies the constraint. Therefore, the heuristic description of the method of steepest ascent can be justified from a more formal perspective.

S11-2. The Canonical Form of the Second-Order Response Surface Model

Equation (11-9) presents a very useful result, the **canonical form** of the second-order response surface model. We state that this form of the model is produced as a result of a translation of the original coded variable axes followed by rotation of these axes. It is easy to demonstrate that this is true.

Write the second-order model as

$$\hat{y} = \hat{\beta}_0 + \mathbf{x}'\hat{\beta} + \mathbf{x}'\mathbf{B}\mathbf{x}$$

Now translate the coded design variable axes **x** to a new center, the stationary point, by making the substitution $\mathbf{z} = \mathbf{x} - \mathbf{x}_s$. This translation produces

$$\begin{aligned}
\hat{y} &= \hat{\beta}_0 + (\mathbf{z} + \mathbf{x}_s)'\hat{\beta} + (\mathbf{z} + \mathbf{x}_s)'\mathbf{B}(\mathbf{z} + \mathbf{x}_s) \\
&= \left[\hat{\beta}_0 + \mathbf{x}_s'\hat{\beta} + \mathbf{x}_s'\mathbf{B}\mathbf{x}_s\right] + \mathbf{z}'\hat{\beta} + \mathbf{z}'\mathbf{B}\mathbf{z} + 2\mathbf{x}_s'\mathbf{B}\mathbf{z} \\
&= \hat{y}_s + \mathbf{z}'\mathbf{B}\mathbf{z}
\end{aligned}$$

because from Equation (11-7) we have $2\mathbf{x}_s'\mathbf{B}\mathbf{z} = -\mathbf{z}'\hat{\beta}$. Now rotate these new axes (**z**) so that they are parallel to the principal axes of the contour system. The new variables are $\mathbf{w} = \mathbf{M}'\mathbf{z}$, where

$$\mathbf{M}'\mathbf{B}\mathbf{M} = \Lambda$$

The diagonal matrix Λ has the eigenvalues of **B**, $\lambda_1, \lambda_2, \cdots, \lambda_k$ on the main diagonal and **M** is a matrix of normalized eigenvectors. Therefore,

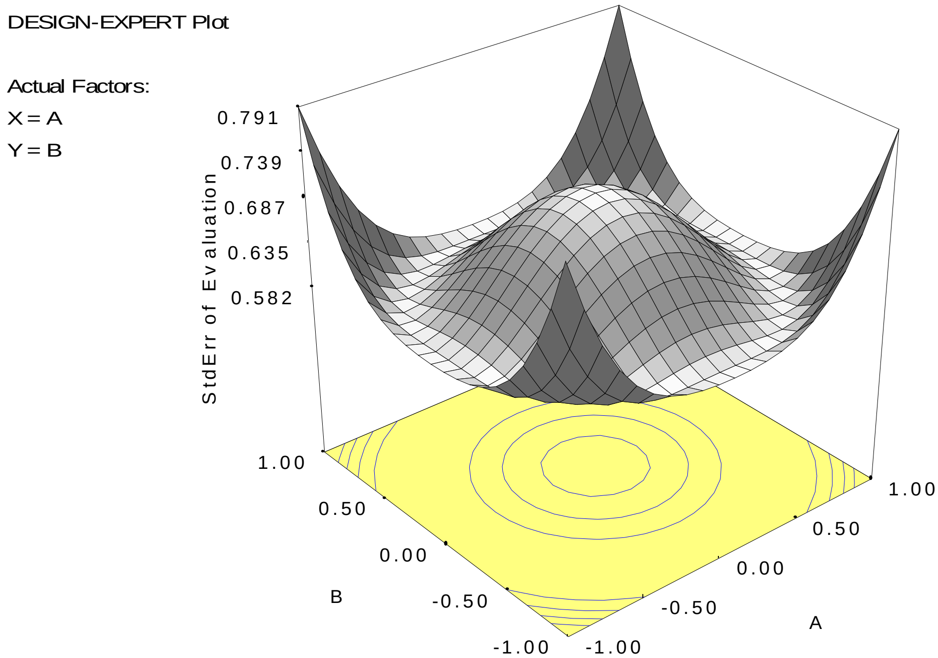
$$\begin{aligned}
\hat{y} &= \hat{y}_s + \mathbf{z}'\mathbf{B}\mathbf{z} \\
&= \hat{y}_s + \mathbf{w}'\mathbf{M}'\mathbf{B}\mathbf{M}\mathbf{z} \\
&= \hat{y}_s + \mathbf{w}'\Lambda\mathbf{w} \\
&= \hat{y}_s + \sum_{i=1}^{k} \lambda_i w_i^2
\end{aligned}$$

which is Equation (11-9).

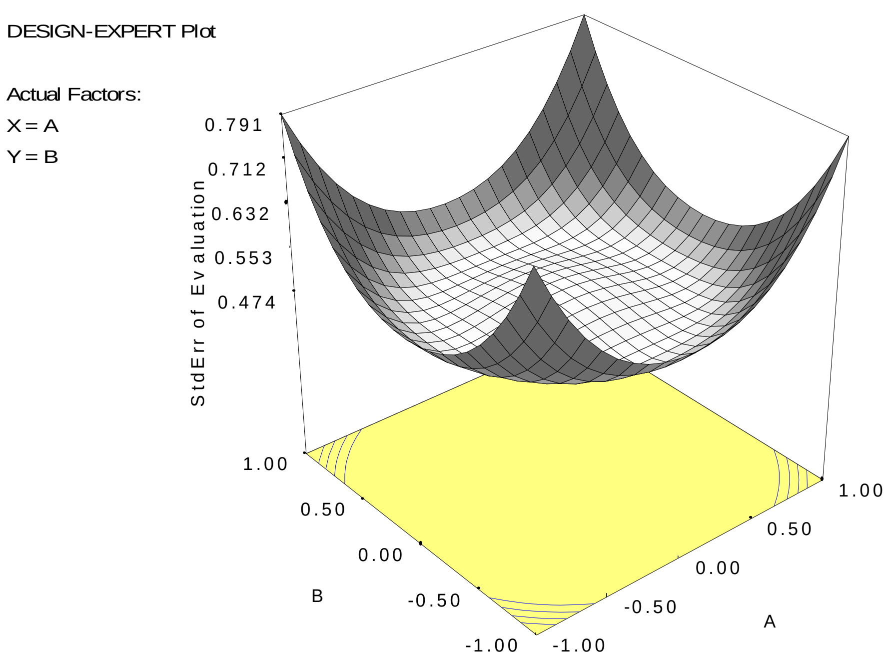
S11-3. Center Points in the Central Composite Design

In section 11-4,2 we discuss designs for fitting the second-order model. The CCD is a very important second-order design. We have given some recommendations regarding the number of center runs for the CCD; namely, $3 \le n_c \le 5$ generally gives good results.

The center runs serves to stabilize the prediction variance, making it nearly constant over a broad region near the center of the design space. To illustrate, suppose that we are considering a CCD in $k = 2$ variables but we only plan to run $n_c = 2$ center runs. The following graph of the standardized standard deviation of the predicted response was obtained from Design-Expert:



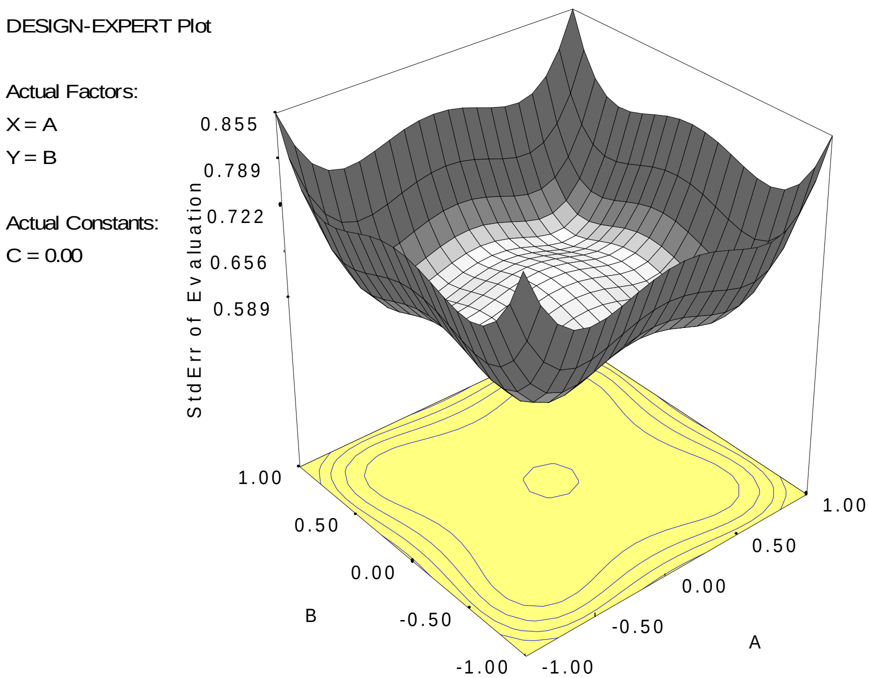
Notice that the plot of the prediction standard deviation has a large "bump" in the center. This indicates that the design will lead to a model that does not predict accurately near the center of the region of exploration, a region likely to be of interest to the experimenter. This is the result of using an insufficient number of center runs. Suppose that the number of center runs is increased to $n_c = 4$. The prediction standard deviation plot now looks like this:



Notice that the addition of two more center runs has resulted in a much flatter (and hence more stable) standard deviation of predicted response over the region of interest.
The CCD is a spherical design. Generally, every design on a sphere must have at least one center point or the $\mathbf{X}'\mathbf{X}$ matrix will be singular. However, the number of center points can often influence other properties of the design, such as prediction variance.

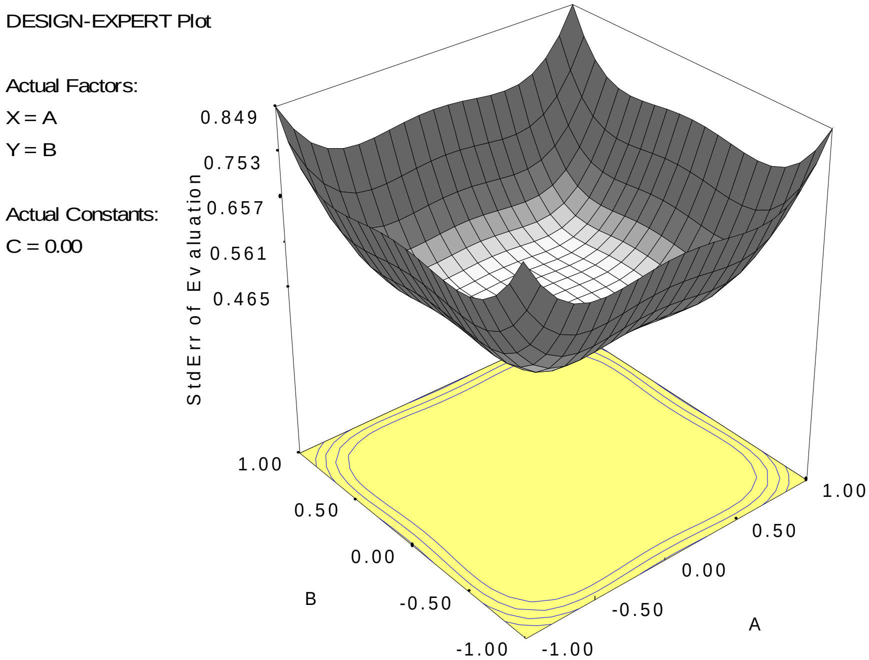
S11-4. Center Runs in the Face-Centered Cube

The face-centered cube is a CCD with $\alpha = 1$; consequently, it is a design on a cube, it is not a spherical design. This design can be run with as few as $n_c = 0$ center points. The prediction standard deviation for the case k = 3 is shown below:



Notice that despite the absence of center points, the prediction standard deviation is relatively constant in the center of the region of exploration. Note also that the contours of constant prediction standard deviation are not concentric circles, because this is not a rotatable design.

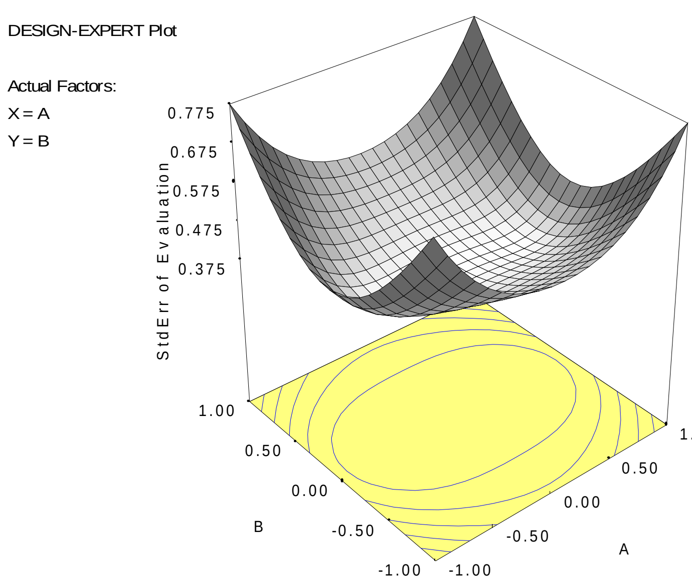
While this design will certainly work with no center points, this is usually not a good choice. Two or three center points generally gives good results. Below is a plot of the prediction standard deviation for a face-centered cube with two center points. This choice work very well.



S11-5. A Note on Rotatability

Rotatability is a property of the prediction variance in a response surface design. If a design is rotatable, the prediction variance is constant at all points that are equidistant from the center of the design.

What is not widely known is that rotatability depends on both the design and the model. For example, if we have run a rotatable CCD and fit a **reduced** second-order model, the variance contours are no longer spherical. To illustrate, below we show the standardized standard deviation of prediction for a rotatable CCD with $k = 2$, but we have fit a reduced quadratic (one of the pure quadratic terms is missing).



Notice that the contours of prediction standard deviation are not circular, even though a rotatable design was used.