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Identifying Rising Ridge Behavior in Quadratic Response Surfaces

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Identifying rising ridge behavior in quadratic response surfaces

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Canonical analysis is a common method for exploring and exploiting fitted quadratic response surfaces. Much attention in canonical analysis is given to identifying ridge behavior in these surfaces in order to achieve optimal response at minimum cost. However, little attention has been given to classifying the identified ridge as a stationary ridge or a rising ridge. Knowing whether a ridge is stationary or rising is critical for making decisions about how to continue the response surface exploration or for setting process parameters. This article presents two methods that allow for identification, classification and confirmation of ridge behavior. The first method is based on linear regression and though easily implemented, can be imprecise. The second method is more precise and is based on a new parameterization of the canonical form. It uses nonlinear regression techniques that are becoming increasingly accessible through software packages.

1. Introduction

Traditional response surface methodology (Box and Wilson, 1951) advocates the fitting of a quadratic response surface in the latter stages of response surface exploration. Many textbooks such as Myers and Montgomery (1995, p. 217) and Box and Draper (1987, p. 332) suggest canonical analysis (see Section 2) of the fitted quadratic surface to determine if the surface has a minimum, a maximum, a saddle point, or some type of ridge system in the experimental region. The primary focus is on the identification of stationary ridge systems, where there is a line or plane of optimal or nearly optimal points. In this paper, methods are presented that not only identify ridge systems, but also classify them as stationary or rising.

A simple example can demonstrate the importance of both identifying as well as classifying a ridge system. Suppose that an experiment on the edge quality (1.0 is ideal) of a metal part involves two factors: (i) the feed rate; and (ii) the rotational speed of the cutting tool. The fitted surface for edge quality in Fig. 1 has a stationary ridge, such that any point on the line located at the top of the ridge (edge quality = 0.8), will have optimal edge quality.

In this example, increasing rotational speed costs vary little. Since increasing the feed rate increases throughput, the point shown by the star on the plot maximizes the edge quality while increasing the throughput. It is this ability to maximize both quality and productivity that makes the identification of a stationary ridge highly desirable.

If, instead, there were a rising ridge in the fitted surface for edge quality as shown in Fig. 2, the edge quality could only be maximized at one point in the experimental region. Thus, if maximum quality is to be achieved, the process must be run at the slowest feed rate (marked by the star on Fig. 2). In addition, the surface in Fig. 2, suggests that even higher edge quality could be achieved if the feed rate is reduced further indicating that more exploration of the surface may be needed if further improvements of edge quality are required. The example shows that being able to identify ridge behavior is not enough, one must also classify the ridge as stationary or rising in order to make well informed decisions about continued experimentation or setting process factors.

When more than three factors are involved, contour plots are difficult to make and an analytic technique like ridge analysis or canonical analysis is needed to study the characteristics of the fitted surface. Ridge analysis locates the optimal settings of the process factors at a fixed distance, r, from the center of the experimental design (see Hoerl (1985) for more details). Plots of the optimal settings and the optimal response as functions of r can be used to determine the nature of the response surface and the optimal settings in the experimental region. Peterson (1993) brought statistical inference into ridge analysis by constructing a guidance band for the optimal settings that is based on simultaneous confidence intervals around the optimal mean response at each value of r. He also generalized his method for use with response surfaces that are

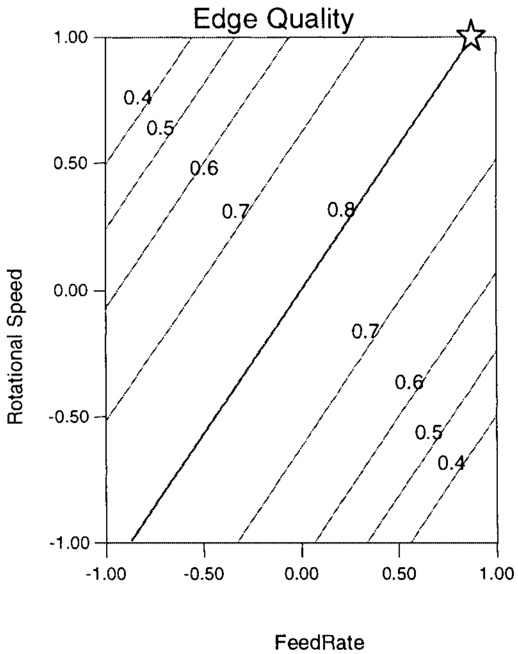

Fig. 1. A stationary ridge in edge quality.

not quadratic and have constraints, like those in mixture experiments.

The purpose of this paper is to use statistical inference in the context of canonical analysis, the other commonly used analytic technique for studying high dimensional quadratic response surfaces. Canonical analysis gets its name from the fact that it creates a canonical form for the following standard fitted quadratic surface model for the predicted response, $\hat{y}$, as a function of k factors:

$$\hat{y} = b_0 + \mathbf{x}'\mathbf{b} + \mathbf{x}'\mathbf{B}\mathbf{x}, \tag{1}$$

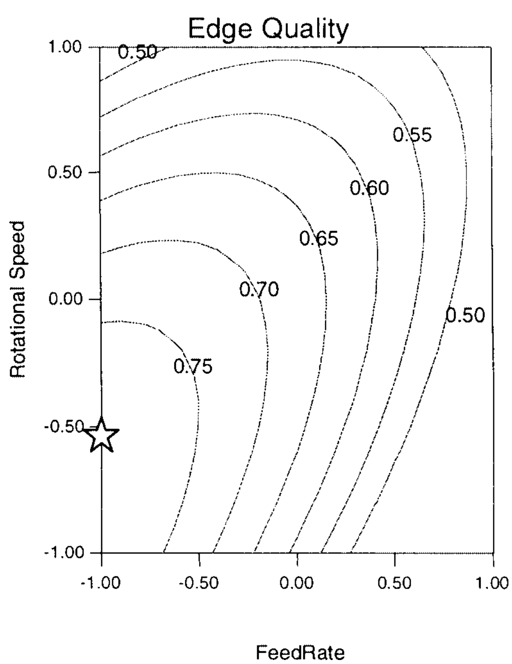

Fig. 2. A rising ridge in edge quality.

where $\mathbf{x} = (x_1, x_2, \ldots, x_k)'$ is a vector of k factors, $\mathbf{b} = (b_1, b_2, \ldots, b_k)'$ is a vector of coefficients for each of these factors, and

$$\mathbf{B} = \begin{bmatrix} b_{11} & \frac{1}{2}b_{12} & \ldots & \frac{1}{2}b_{1k} \\ \frac{1}{2}b_{12} & b_{22} & \ldots & \frac{1}{2}b_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{2}b_{1k} & \frac{1}{2}b_{2k} & \ldots & b_{kk} \end{bmatrix}, \tag{2}$$

is a matrix of the second-order coefficients.

Canonical analysis focuses on the signs and magnitudes of the eigenvalues of **B** in Equation (2) to determine the shape of the response surface. In particular, when all of the eigenvalues are positive, the stationary point of the fitted model is a minimum, whereas eigenvalues that are all negative indicate a maximum. If the eigenvalues have mixed signs, it indicates a saddle point. An eigenvalue of zero indicates the presence of a ridge in the surface.

Since response surface models are usually based on experimental data, the eigenvalues of the coefficient matrix, **B**, are subject to estimation error. This complicates the determination of the shape of the response surface. In the past, the focus of this literature has been on providing standard errors or confidence intervals for the eigenvalues. For example, Bisgaard and Ankenman (1996) introduce what they called the Double Linear Regression (DLR) method, based on a second linear regression in a rotated coordinate space, for obtaining approximate standard errors and subsequent confidence intervals for the eigenvalues. They go on to show that this method is equivalent to using the delta method used by Carter *et al.* (1990). Both sets of authors argue that if the confidence interval of one or more eigenvalues contains zero and all other eigenvalues are of the same sign, the true response surface may be a ridge. However, neither paper addresses the classification of the ridge as stationary or rising.

To determine if an identified ridge in a response surface is rising, there are two cases to consider. First, if the stationary point of the fitted quadratic surface is within the experimental region, then there is no suggestion of a rising ridge because there is no direction of improvement out of the experimental region. In this case, the DLR method of Bisgaard and Ankenman (1996) is sufficient since any identified ridge will be a stationary ridge. In the second case, the stationary point is outside the experimental region and the amount of rise in the ridge must be estimated. This paper provides two methods for testing for significant rise in an identified ridge with a stationary point outside the experimental region, and thus allows for the classification of such ridge systems. The first method, discussed in Section 4, is an extension of the DLR method and thus is based on linear regression. The second method, discussed in Section 5, is based on nonlinear regression and though somewhat more difficult to implement has improved precision. In the next two sections, the canonical form is reviewed and the steps for the identification, classification, and confirmation of a ridge system model are discussed.

2. The canonical form and rising ridges

The standard quadratic model in Equation (1) is in the coordinate system defined by the factors, $\mathbf{x} = (x_i, x_2, \ldots, x_k)'$. The *canonical* form of Equation (1) expresses the model in a new coordinate system defined by new factors denoted $\mathbf{z} = (z_1, z_2, \ldots, z_k)$. The new factors are linear combinations of the original factors, but the coordinate axes have been rotated to be aligned with the natural directions of the fitted quadratic surface. Figure 3 shows the same surface as Fig. 2, but also shows the new coordinate system that would be used for the canonical form of the edge quality response surface. The new factors, **z**, can be expressed as a function of the old factors, **x**, and the second-order coefficient matrix, **B**, as follows:

$$\mathbf{z} = (z_1, z_2, \ldots, z_k) = \mathbf{D}'\mathbf{x}, \tag{3}$$

where $\mathbf{D} = [\mathbf{d}_1, \mathbf{d}_2, \ldots, \mathbf{d}_k]$ is a matrix of normalized eigenvectors of **B** in Equation (2) such that $\mathbf{DD}' = \mathbf{D}'\mathbf{D} = \mathbf{I}$. For convenience, the eigenvectors will be ordered such that $\mathbf{d}_j$ is the eigenvector of **B** that corresponds to λ_j , the *j*th largest eigenvalue of **B** (i.e., $\lambda_j \geq \lambda_{j+1} \forall j$).

The canonical form of the fitted model in Equation (1) is then

$$\hat{y} = b_0 + \mathbf{z}'\boldsymbol{\phi} + \mathbf{z}'\boldsymbol{\Lambda}\mathbf{z}, \tag{4}$$

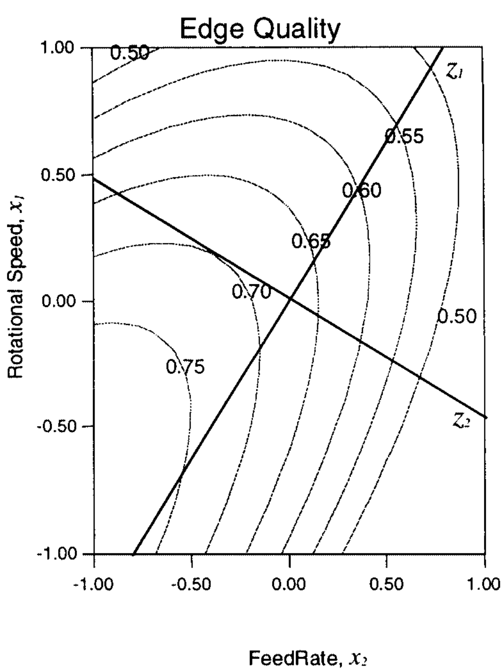

Fig. 3. A rising ridge with the A-canonical axes.

where $\boldsymbol{\phi} = (\phi_1, \phi_2, \ldots, \phi_k)' = \mathbf{D}'\mathbf{b}$ and $\boldsymbol{\Lambda} = \mathbf{D}'\mathbf{B}\mathbf{D} = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_k)$. By observing that the second-order coefficient matrix in this model, Λ, is a diagonal matrix, it can be seen that the rotation of the coordinate system has had the effect of eliminating the interaction terms.

Equation (4) is called the A-canonical form (Box and Draper, 1987, p. 333) and is usually used for interpreting a quadratic response surface when the stationary point is outside the experimental region. The coordinates of the estimated stationary point, $\mathbf{x}_s$, can be calculated by $\mathbf{x}_s = -\mathbf{B}^{-1}\mathbf{b}/2$. The alternative B-canonical form is used when the stationary point is inside the experimental region. The B-canonical form not only rotates the axes, but also relocates the origin of the new coordinate system to the estimated stationary point of the response surface thus eliminating the first-order terms. Since the focus of this paper is the classification of rising ridges, which are indicated only when the stationary point is outside the experimental region, only the A-canonical form in Equation (4) will be considered in this article.

The canonical form shows why the eigenvalues determine the shape of the response surface. In Equation (4), they are the curvature terms that will dominate the linear terms far from the origin. Thus, if all the curvature terms are positive (negative), then the surface must have a global minimum (maximum) at the stationary point. Eigenvalues of mixed signs will produce saddle shaped surfaces that do not contain ridges of optimal values and will not be considered. Also, since a surface with a finite minimum is simply a mirror image of a surface with a finite maximum, only maximization of a surface with a finite maximum will be discussed directly. The discussion can be easily modified for minimization of a surface with a finite minimum.

Quadratic surfaces with ridges have at least one eigenvalue equal to zero. For example, if the first eigenvalue, λ_1, is zero and all other eigenvalues are negative, then there will be no curvature along the z_1 axis, resulting in a ridge in the response surface with the top of the ridge being the z_1 axis (a line). If ϕ_1, the linear coefficient related to z_1, is zero, the ridge will be stationary (flat along the ridge). However, if ϕ_1 is nonzero, the ridge will increase along that axis in one direction or the other creating a rising ridge.

Similarly, if the first two eigenvalues are zero and the others are negative, the surface will have a ridge with a plane (containing the z_1 and z_2 axes) at the top. This two-dimensional ridge may or may not be rising. To have a two-dimensional stationary ridge, both curvature coefficients λ_1 and λ_2 and both linear coefficients ϕ_1 and ϕ_2 must be zero and all other eigenvalues must be negative. If the curvature coefficients are zero, but one or both of the linear coefficients are nonzero, then the ridge is rising. The canonical formulation chooses the direction of the z_2 axis to be the direction with the most (negative) curvature and the direction of the z_1 axis to be orthogonal to the z_2 axis. If there is no curvature on this plane, the directions chosen for the

z_1 and z_2 axes are arbitrary. However, if the ridge is rising there will a direction of steepest ascent on the plane.

Finding the direction of steepest ascent is a familiar problem in response surface methodology. The formula for the fitted response on the top of a two-dimensional ridge as a function of z_1 and z_2 is

$$\hat{y}\,|z_3, z_4, \ldots, z_k = \text{constant} + \phi_1 z_1 + \phi_2 z_2.$$

The vector of steepest ascent on the ridge is ∇, the gradient vector with respect to z_1 and z_2. The gradient vector is $\nabla = (\phi_1,\ \phi_2)'$ and its length is $\sqrt{\phi_1^2 + \phi_2^2}$, which is the change in the response per unit along this vector. The length of ∇ measures the steepest ascent of the ridge.

The arguments above can be generalized to a g-dimensional ridge (i.e., $\lambda_1 = \lambda_2 = \cdots = \lambda_g = 0$). By induction, to have a g-dimensional stationary ridge, the first g eigenvalues and their associated linear coefficients must all be zero. If the ridge is rising, the vector of steepest ascent is $\nabla = (\phi_1,\ \phi_2, \ldots,\ \phi_g)'$ and the steepest ascent is

$$\phi_{\nabla} = \sqrt{\sum_{i=1}^{g} \phi_i^2}.$$

Since there is no curvature on the top of the ridge, the response is constant in any direction on the hyperplane that is orthogonal to the vector of steepest ascent. There will be $g - 1$ such directions.

3. Ridge identification, classification, and confirmation

When dealing with a specific data set, three steps are needed to study the ridge behavior of a multi-dimensional quadratic response surface. They are identification, classification, and confirmation of the ridge. Identification is where g, the dimension of the ridge is determined. If g is greater than zero, then a ridge has been identified. Classification determines if the identified ridge is rising or stationary. In the last step, the full quadratic model is reduced to the form of a stationary or rising ridge to confirm that the reduced model fits sufficiently well.

The first step is ridge identification and this can be accomplished using the DLR method. This method is described in detail in Section 4 and the formula for the confidence intervals for the eigenvalues is given in Equation (6). If there are g eigenvalues whose confidence intervals contain zero, then there is reason to suspect a g-dimensional ridge.

The second step, classification of the ridge, is more difficult. If a g-dimensional ridge has been identified, then the surface has a ridge with a hyperplane (containing the z_1–z_g axes) at the top. Since there is no curvature on the top of the ridge, the directions of the z_1 and z_g axes are not meaningful. If z_g is reoriented so as to be parallel to the vector of steepest ascent, the response will be constant along the other $g - 1$ axes, which can be chosen arbitrarily provided each axis is orthogonal to all other axes. In order to determine if a ridge is rising, two models are compared. One is a g-dimensional stationary ridge and the other is the same model, except that it includes an additional linear term in the reoriented z_g. The linear coefficient ϕ_g from this term estimates the steepest ascent on the ridge. An extra sum of squares test can be used to determine if estimating the direction and rise in the ridge significantly improves the fit of the model. If it does, the ridge should be classified as rising.

Table 1 shows a general ANOVA table for an extra sum of squares test for testing a model reduction (Bates and Watts, 1988, p. 103). In the table, n is the number of observations. The degrees of freedom used in the larger model is p_L. The degrees of freedom used in the reduced model is p_R. The regression sums of squares accounted for by the larger and reduced models after correcting for the mean are denoted SS_L and SS_R, respectively. The total corrected sum of squares is denoted SS_T and the residual sum of squares from the larger model is SS_E. The critical F value for comparison is F^α with $p_L - p_R$ and $n - p_L$ degrees of freedom where $100(1-\alpha)\%$ is the desired confidence level.

To test for a rising ridge, the extra sum of squares test is used where the larger model is a g-dimensional rising ridge. The reduced model is a g-dimensional stationary ridge. The null hypothesis is that the ridge is stationary. If the test statistic in Table 1, F_X, is larger than F^α with $p_L - p_R$ and $n - p_L$ degrees of freedom, then the null hypothesis is rejected and the rising ridge model should be used. If the null hypothesis is not rejected, then it can be reasonably assumed that the surface is a stationary ridge. This test classifies the ridge.

The third and final step is a confirmation that the chosen model is a close fit. Since both the rising ridge model and the stationary ridge model are reduced forms of the full canonical model in Equation (4), another extra sum of squares test can be used for the confirmation. In the confirmation step, the full model in Equation (4) is the larger model and the model chosen in the classification step

Table 1. The ANOVA table for the extra sum of squares test

Source	*Sum of squares*	*Degrees of freedom*	*Mean square*	F-*Ratio*
Reduced model	SS_R	$\nu_R = p_R - 1$	$S_R^2 = SS_R/\nu_R$	
Extra parameters	$SS_X = SS_L - SS_R$	$\nu_X = p_L - p_R$	$s_X^2 = SS_X/\nu_X$	$F_X = S_X^2/S_E^2$
Error	SS_E	$\nu_E = n - p_L$	$S_E^2 = SS_E/\nu_E$	
Total, corrected	SS_T	$n - 1$		

(either rising or stationary ridge) is the reduced model. The null hypothesis is that the chosen model is correct. If F_X is larger than F^α with $p_L - p_R$ and $n - p_L$ degrees of freedom, then the null hypothesis is rejected and the existence of a g-dimensional ridge in the response surface is in doubt. Otherwise, the null hypothesis is not rejected and the chosen model is a reasonable model for the surface.

The two different methods for constructing and fitting the stationary and rising ridge models are presented in the next two sections. The first method, presented in Section 4, is based on linear regression and assumes that the $k - g$ canonical axes that are not on the top of the ridge are fixed by Equation (3). This method is easily implemented with a standard regression package, but it suffers some imprecision due to fixing of the canonical axes. The second method, in Section 5, is based on nonlinear regression and is more precise than the first method since it allows the directions of all canonical axes to be re-estimated for each fitting. The second method is relatively easily implemented if one has software that handles both manipulation of symbolic matrices and nonlinear regression. Such software is becoming more common (e.g., Mathematica®), but is still not as accessible as linear regression software.

4. Fitting ridge models with linear regression

As previously mentioned, Bisgaard and Ankenman (1996) provided a linear regression method, called the DLR method, for obtaining approximate standard errors of the eigenvalues of **B**. This method can identify ridges, but does not address the classification or confirmation of the ridge. In this section, the DLR method is modified to include these steps.

The DLR method is simple in concept and execution. After the standard quadratic model of Equation (1) is fit to the data with linear regression, the experimental design is re-expressed in terms of the A-canonical variables, **z**, defined in Equation (3). In this coordinate system, linear regression is again used to fit the following full second-order model to the data

$$\hat{y} = b_0^* + \mathbf{z}'\mathbf{b}^* + \mathbf{z}'\mathbf{B}^*\mathbf{z}, \tag{5}$$

where $\mathbf{b}^* = (b_1^*, b_2^*, \ldots, b_k^*)'$ and

$$\mathbf{B}^* = \begin{bmatrix} b_{11}^* & \frac{1}{2}b_{12}^* & \cdots & \frac{1}{2}b_{1k}^* \\ \frac{1}{2}b_{12}^* & b_{22}^* & \cdots & \frac{1}{2}b_{2k}^* \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{2}b_{1k}^* & \frac{1}{2}b_{2k}^* & \cdots & b_{kk}^* \end{bmatrix}.$$

The ith pure quadratic coefficient, b_{ii}^*, is equal to λ_i, the ith eigenvalue of **B** and the interaction coefficient, b_{ij}^*, is zero for all $i \neq j$, so $\mathbf{B}^* = \mathbf{\Lambda}$. Thus, after fitting Equation (5) to the data, the standard error, $se(b_{ii}^*)$, provided by linear regression techniques for b_{ii}^* is an approximate standard error for the ith eigenvalue (see the Appendix for details). Note that for $se\left(b_{ii}^*\right)$ to be correctly calculated by a regression program, all interaction terms must be in the model during fitting even though they will have coefficients that are nearly zero. The approximate $100(1-\alpha)\%$ confidence interval for the ith eigenvalue is:

$$\lambda_i \pm t_{1-\alpha/2,n-p}se(b_{ii}^*), \tag{6}$$

where n is the number of observations, p is the number of parameters in the model, and $t_{1-\alpha/2,n-p}$ is the $1-\alpha/2$ quantile of Student's t-distribution with $n-p$ degrees of freedom.

Since all the eigenvalues are tested, adjustment for multiple comparisons might be considered. The Bonferroni adjustment replaces $t_{1-\alpha/2,n-p}$ in Equation (6) with $t_{1-\alpha/2k,n-p}$, for k eigenvalues. Assuming the surface is to be maximized and all significant eigenvalues are negative, a g-dimensional ridge is identified if the confidence intervals for $\lambda_1, \lambda_2, \ldots, \lambda_g$ all contain zero.

To classify the ridge with the extra sum of squares test, models for a stationary ridge (the reduced model) and a rising ridge (the larger model) must be constructed. The model for a g-dimensional stationary ridge has no interaction terms and no terms involving $z_1, z_2, \ldots, z_g$ and is

$$\hat{y} = b_0^* + \sum_{i=g+1}^{k} z_i b_i^* + \sum_{i=g+1}^{k} z_i^2 b_{ii}^*. \tag{7}$$

When fitting the full model in Equation (5), the interactions had no effect on the predicted response since their coefficients were estimated to be zero. These terms were included to represent the

$$\binom{k}{2}$$

degrees of freedom that were used to determine the directions of the canonical axes. Including them in the regression for the full model allowed $se(b_{ii}^*)$ to be correctly calculated in a standard linear regression output. In the reduced model, there is no guarantee that these interaction coefficients will be zero. Including nonzero interaction terms violates the hypothesis of the stationary ridge, so they must be removed when fitting Equation (7). The model in Equation (7) has a total of $2(k-g)+1$ parameter estimates. Although not explicitly in the linear model, an additional

$$\binom{k}{2} - \binom{g}{2},$$

degrees of freedom are needed to estimate the directions of the canonical axes that are not on the ridge. The number of degrees of freedom needed to determine the direction of the canonical axes will be explained more thoroughly in Section 5. Thus, for the extra sum of squares test, the number of degrees of freedom for the stationary ridge model is

$$p_R = 1 + 2k - 2g + \binom{k}{2} - \binom{g}{2}. \tag{8}$$

The rising ridge model (the larger model in the extra sum of squares test) must also be constructed. For the rising ridge, the $k-g$ canonical axes with significant curvature are preserved. The gth canonical axis is redirected to coincide with the vector of steepest ascent on the ridge and the other $g-1$ canonical axes are eliminated. A new rotation matrix is defined as $\mathbf{D}_{\nabla} = (\mathbf{d}_{\nabla}, \mathbf{d}_{g+1}, \ldots, \mathbf{d}_k)$, where the new canonical axis is the normalized gradient vector

$$\mathbf{d}_{\nabla} = \frac{\sum_{i=1}^{g} \phi_i \mathbf{d}_i}{\phi_{\nabla}},$$

where

$$\phi_{\nabla} = \sqrt{\sum_{i=1}^{g} \phi_i^2}.$$

The rising ridge model can now be fit using the definition $\mathbf{z} = (z_{\nabla}, z_{g+1}, \ldots, z_k) = \mathbf{D}'_{\nabla}\mathbf{x}$. The model does not include any interactions or a curvature term for z_{∇} and thus the rising ridge model is:

$$\hat{y} = b_0^* + z_{\nabla}\phi_{\nabla} + \sum_{i=g+1}^{k} z_i b_i^* + \sum_{i=g+1}^{k} z_i^2 b_{ii}^*, \quad (9)$$

where ϕ_{∇} is the steepest ascent on the ridge. To estimate the directions of the $k-g+1$ axes,

$$\binom{k}{2} - \binom{g-1}{2}$$

degrees of freedom are used. The number of degrees of freedom needed for the rising ridge model is then

$$p_{\mathrm{L}} = 2 + 2(k-g) + \binom{k}{2} - \binom{g-1}{2}. \quad (10)$$

Using the extra sum of squares test in Table 1 for classification of the ridge, the regression sums of squares from Equations (7) and (9) are used as SS_{R} and SS_{L} respectively. The residual and total corrected sum of squares from Equation (9) are SS_{E} and SS_{T} respectively. The degrees of freedom for the reduced and larger models are given in Equations (8) and (10), respectively.

This test will allow the ridge to be classified as stationary or rising, however, a more precise test is presented in the next section. The primary problem with the linear regression method just described is that the direction of the last $k-g$ canonical axes are not reoriented for the fitting of Equations (7) and (9). Thus, there may be a stationary ridge model that fits better than Equation (7) and a rising ridge model that fits better than Equation (9). In the nonlinear method presented in Section 5, the directions of these canonical axes are re-estimated for each model assuring that each model fits the data as closely as possible.

The confirmation step requires no more model fitting. It only requires another extra sum of squares test where the full model in Equation (5) is used as the larger model and the model chosen in the classification step is the reduced model. The regression, residual, and total corrected sum of squares from the fitting of Equation (5) are SS_{L}, SS_{E} and SS_{T}, respectively. The number of degrees of freedom needed for the full model is

$$p_{\mathrm{L}} = 1 + 2k + \binom{k}{2}.$$

If the ridge has been classified as rising, then the regression sum of squares from fitting Equation (9) is used as SS_{R} and the degrees of freedom calculated in Equation (10) are used as p_{R} instead of p_{L}. If the ridge is classified as stationary, then SS_{R} is taken from fitting Equation (7) and p_{R} from Equation (8). Since the linear regression method does not necessarily find the best fitting model with the stationary or rising ridge form, the F statistic, F_{X}, calculated in this test may be somewhat inflated. Thus, if the test fails to reject the chosen ridge model, then it is reasonable to conclude that the chosen ridge model clearly fits the data. However, if the test rejects the chosen model, there is still some chance that that model would fit if the canonical axes were reoriented. In this case, the nonlinear method in Section 5 should be used for confirmation.

5. Fitting ridge models with nonlinear regression

In this section, a parameterization is presented which allows each of the models (full, stationary ridge, and rising ridge) needed for ridge classification and confirmation to be written as a nonlinear regression model. Each nonlinear model contains parameters related to the directions of the canonical axes and thus will allow the canonical axes to be re-estimated for each fitting.

Since the coordinate system of the A-canonical form is obtained by rotation, polar coordinates will be used to parameterize the unit vectors in $\mathbf{D}$. Elementary rotation matrices, sometimes called the Givens matrix (Seber, 1977, p. 314) will be the basis of the parameterization. In two dimensions, the full model in Equation (4) can be written as:

$$\hat{y} = \beta_0 + (x_1, x_2)\mathbf{D}\begin{pmatrix}\phi_1 \\ \phi_2\end{pmatrix} + (x_1, x_2) \times \mathbf{D}\begin{bmatrix}\lambda_1 & 0 \\ 0 & \lambda_2\end{bmatrix}\mathbf{D}'\begin{pmatrix}x_1 \\ x_2\end{pmatrix}, \quad (11)$$

where

$$\mathbf{D} = \begin{bmatrix}\cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta)\end{bmatrix}.$$

The nonlinear model in (11) has six parameters, $(b_0, \phi_1, \phi_2, \theta, \lambda_1, \lambda_2)$. This parameterization does not remove all ambiguity because any multiple of an eigenvector is still an eigenvector and thus there are four possible sign patterns for the eigenvectors in the matrix $\mathbf{D}$: $(\mathbf{d}_1, \mathbf{d}_2)$, $(-\mathbf{d}_1, \mathbf{d}_2)$,

$(\mathbf{d}_1, -\mathbf{d}_2)$, $(-\mathbf{d}_1, -\mathbf{d}_2)$. Each of these matrices will be valid eigenvector matrices, but will have a different value for the parameter θ. In response surface applications, the signs of the eigenvectors are unimportant since it does not matter which direction along the canonical axis is called positive. Ultimately the sign of the eigenvector, $\mathbf{d}_i$, will change only the sign, (but not the magnitude) of the linear coefficient, ϕ_i.

The parameterization used above can be readily generalized to k dimensions by expressing the rotation matrix $\mathbf{D}'$ as a function of a vector $\boldsymbol{\theta}$. The matrix function will be denoted $\mathbf{D}'(\boldsymbol{\theta})$. To produce such a parameterization, $\mathbf{D}'(\boldsymbol{\theta})$ is decomposed into

$$\binom{k}{2}$$

possible $k \times k$ Givens matrices, each of which represents one of the

$$\binom{k}{2}$$

planar rotations necessary to realign the coordinate axes from the original $\mathbf{x}$ axes to the canonical $\mathbf{z}$ axes. Each of these rotation matrices will include a parameter θ_{qr}, which defines the angle of rotation in the plane containing the qth and rth coordinate axes, where $q < r$. Each Givens matrix looks like an identity matrix in all rows except q and r. The (q, q) and (r, r) elements are $\cos(\theta_{qr})$ and the (q, r) and (r, q) elements are $\sin(\theta_{qr})$ and $-\sin(\theta_{qr})$, respectively. All other elements in the two rows are zero. For example, in three dimensions, $\mathbf{D}'(\boldsymbol{\theta})$ is decomposed as

$$\mathbf{D}'(\boldsymbol{\theta}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta_{23}) & \sin(\theta_{23}) \\ 0 & -\sin(\theta_{23}) & \cos(\theta_{23}) \end{bmatrix} \begin{bmatrix} \cos(\theta_{13}) & 0 & \sin(\theta_{13}) \\ 0 & 1 & 0 \\ -\sin(\theta_{13}) & 0 & \cos(\theta_{13}) \end{bmatrix} \times \begin{bmatrix} \cos(\theta_{12}) & \sin(\theta_{12}) & 0 \\ -\sin(\theta_{12}) & \cos(\theta_{12}) & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Since the determinant of any product of Givens matrices must be equal to one and many orthogonal matrices have a determinant of -1, any sign pattern for the eigenvectors in $\mathbf{D}(\boldsymbol{\theta})$ such that the determinant of $\mathbf{D}(\boldsymbol{\theta})$ is one can be used. Other parameterizations for orthogonal matrices are given in Pinheiro and Bates (1996). In Section 4, it was suggested that estimation of the directions of the canonical axes reduce the degrees of freedom available for estimating the error. It is the estimation of the rotation angles that cause the loss of these degrees of freedom.

If the order and signs of the eigenvectors are fixed, the reparameterization is a one-to-one transformation from $(b_0, b_1, b_2, \ldots, b_k \vdots b_{11}, b_{12}, \ldots, b_{1k} \vdots b_{22}, b_{23}, \cdots, b_{2k} \vdots \cdots \vdots b_{kk})$ to a new parameter set:

$$\xi' = \big(b_0, \phi_1, \phi_2, \ldots, \phi_k \vdots \theta_{12}, \theta_{13}, \ldots, \theta_{1k} \vdots \theta_{23}, \theta_{24}, \ldots, \theta_{2k} \vdots \cdots \vdots \theta_{k-1,k} \vdots \lambda_{(1)}, \lambda_{(2)}, \ldots, \lambda_{(k)}\big), \tag{12}$$

with the implied relationships $\boldsymbol{\phi} = \mathbf{D}'(\boldsymbol{\theta})\mathbf{b}$ and $\mathbf{BD}(\boldsymbol{\theta}) = \mathbf{D}(\boldsymbol{\theta})\boldsymbol{\Lambda}$. The parameters in Equation (12) can be estimated directly using nonlinear regression by fitting the following model to the data:

$$\hat{y} = b_0 + \mathbf{x}'\mathbf{D}(\boldsymbol{\theta})\boldsymbol{\phi} + \mathbf{x}'\mathbf{D}(\boldsymbol{\theta})\boldsymbol{\Lambda}\mathbf{D}'(\boldsymbol{\theta})\mathbf{x}. \tag{13}$$

Standard methods of estimation and inference from nonlinear regression (Seber and Wild, 1989, p. 191) can be applied to any subset of the parameters in Equation (12) after fitting Equation (13).

Box and Draper (1987, p. 359) introduced the concept of directly fitting the canonical form of a quadratic response surface with nonlinear regression. However, unlike the model in Equation (13), the parameterizations that they used were tailored to each individual example and are not easily generalized to higher dimensions. Although the function in Equation (13) is easily generalized, it can be extremely cumbersome when expressed as an algebraic function of the angles in $\boldsymbol{\theta}$. In order to create this model for more than two dimensions, a software package, such as Mathematica® that handles both symbolic matrix multiplication and nonlinear regression analysis is recommended.

To apply a nonlinear regression algorithm to Equation (13), starting estimates are required for the parameters. Accurate starting values for the angles $\boldsymbol{\theta} = (\theta_{12}, \ldots, \theta_{k-1,k})'$ can be difficult to find, but are not so important since the parameters are confined to a finite range. Starting values of $\pi/4$ for all angles will work in most cases. Since they are not important, the signs of the eigenvectors can be determined during convergence by the starting estimates and the algorithm. The absolute value of the least-squares estimates for the first order coefficients, $\boldsymbol{\phi} = (\phi_1, \phi_2, \ldots, \phi_k)'$, is known from the relationship, $\boldsymbol{\phi} = \mathbf{D}'(\boldsymbol{\theta})\mathbf{b}$. However, the signs of these estimates depend on the signs of the eigenvectors, which are not known before convergence. Thus, the best starting values for all first-order coefficients is zero, halfway between the two possible values. The eigenvalues of $\mathbf{B}$ and the constant b_0 from fitting the original model in Equation (1) can be used as starting values since they do not depend on the signs of the eigenvectors.

The model reduction for a stationary ridge is easily implemented in the nonlinear model of Equation (13) by setting $\lambda_j = \phi_j = 0 \quad \forall_j \le g$. However, when these parameters are set to zero, the model is constant on the g-dimensional hyperplane at the top of the ridge and thus none of the

$$\binom{g}{2}$$

angles on the ridge can be estimated. Because the rotations of $\mathbf{z} = \mathbf{D}'(\boldsymbol{\theta})\mathbf{x}$ are done in sequence, it is not easy to determine which rotations are in that g-dimensional space. However, if any given angle is set to zero, then the Givens matrix which contains that angle will be the identity matrix which can be placed anywhere in the sequence of rotations and is therefore effectively on the top of the ridge. Thus, the

$$\binom{g}{2}$$

angles θ_{ij}, where i and j are less than or equal to g, can be set to zero. To fit a g-dimensional stationary ridge, the model in Equation (13) is refit after setting

$$\lambda_j = \phi_j = \theta_{ij} = 0 \quad \forall i < j \le g. \tag{14}$$

For refitting, the previous estimates of the constant, the nonzero angles, the linear coefficients and eigenvalues can be used as starting estimates.

To construct a rising ridge model, only a single linear term, the rise in the ridge, must be added back into the model. With the g curvature terms removed and a single linear term in the model, the direction of the gth canonical axis will be redirected during refitting to coincide with the vector of steepest ascent on the ridge. Thus $\phi_g = \phi_\nabla$, the rise in the ridge. There will still be $g-1$ dimensions on the ridge that are orthogonal to the vector of steepest ascent. The model will be constant in these $g-1$ dimensions and thus

$$\binom{g-1}{2}$$

angles will not be estimable. To fit a g-dimensional rising ridge, the model in Equation (13) is fit with the following reductions:

$$\lambda_g = \lambda_j = \phi_j = \theta_{ij} = 0 \quad \forall i < j \le g-1. \tag{15}$$

After refitting the nonlinear stationary and rising ridge models, the same tests for classification and confirmation that were described in Section 4 can be performed. Since the estimates of the angles are explicitly in the nonlinear models, the degrees of freedom for each model is simply the number of parameters in that model. These are identical to the values suggested for degrees of freedom for a stationary and rising ridge model in Section 4 (see Equations (8) and (10)).

6. An example

Data from Box and Draper (1987, p. 362) is used as an example. Table 2 provides the design and the data. The experiment involved three factors x_1, x_2, and x_3. The goal is to maximize the response y. The experiment was run in four blocks and thus, in addition to the standard second-order model in Equation (1), three block parameters are also estimated. Thus, all models will have an additional three degrees of freedom. The estimated stationary point is $\mathbf{x}_s = -\mathbf{B}^{-1}\mathbf{b}/2 = (25.8, 15.5, 18.5)'$ which is well outside the experimental region so either a stationary or a rising ridge is a possibility.

After fitting the model in Equation (1), the eigenvector matrix is found to be

$$\mathbf{D} = \begin{bmatrix} -0.297 & 0.737 & 0.612 \\ 0.888 & 0.447 & -0.104 \\ -0.350 & 0.513 & -0.784 \end{bmatrix}.$$

Table 2. The data for the small reactor experiment

Run	*Block*	x_1	x_2	x_3	y
1	1	−1	−1	1	40.0
2	1	1	−1	−1	18.6
3	1	−1	1	−1	53.8
4	1	1	1	1	64.2
5	1	0	0	0	53.5
6	1	0	0	0	52.7
7	2	−1	−1	−1	39.5
8	2	1	−1	1	59.7
9	2	−1	1	1	42.2
10	2	1	1	−1	33.6
11	2	0	0	0	54.1
12	2	0	0	0	51.0
13	3	$-\sqrt{2}$	0	0	43.0
14	3	$\sqrt{2}$	0	0	43.9
15	3	0	$-\sqrt{2}$	0	47.0
16	3	0	$\sqrt{2}$	0	62.8
17	3	0	0	$-\sqrt{2}$	25.6
18	3	0	0	$\sqrt{2}$	49.7
19	4	$-\sqrt{2}$	0	0	39.2
20	4	$\sqrt{2}$	0	0	46.3
21	4	0	$-\sqrt{2}$	0	44.9
22	4	0	$\sqrt{2}$	0	58.1
23	4	0	0	$-\sqrt{2}$	27.0
24	4	0	0	$\sqrt{2}$	50.7

Table 3. The estimated eigenvalues and their approximate 95% confidence intervals

Parameter	*Estimate*	*Standard error*	*95% C.I. by the DLR method*
λ_1	1.711	0.543	(0.51, 2.91)
λ_2	−0.097	0.543	(−1.29, 1.10)
λ_3	−10.489	0.543	(−11.69, −9.29)

Table 4. The sums of squares for the different models

Model	*Equation numbers*	*Regression sum of squares*	*Degrees of freedom used in model*	*Residual sum of squares*
Stationary ridge (linear)	(7)	2199.02	8	872.89
Rising ridge (linear)	(9)	2965.47	10	106.44
Stationary ridge (nonlinear)	(13), (14)	2366.27	8	705.64
Rising ridge (nonlinear)	(13), (15)	2994.29	10	77.62
Full model	(1)	3032.94	13	38.97

The model in Equation (5) is fit with linear regression. The approximate 95% confidence intervals (without Bonferroni adjustment) for the eigenvalues are calculated using Equation (6) and are provided in Table 3. These confidence intervals suggest that the surface may be a saddle point since it appears that $\lambda_1 > 0$, $\lambda_2 \approx 0$, $\lambda_3 < 0$. However, since λ_1 is relatively small, it is reasonable to continue to investigate the possibility that a two-dimensional ridge may exist in this response surface with a maximum on the plane containing the first and second canonical axes. When fitting the full model in Equation (5), the first-order coefficients are $\phi_1 = 1.25$, $\phi_2 = 6.81$, and $\phi_3 = -6.33$. The new rotation matrix for the rising ridge model in the linear regression method is then

$$\mathbf{D}_{\nabla} = \begin{bmatrix} 0.667 & 0.612 \\ 0.600 & -0.104 \\ 0.441 & -0.784 \end{bmatrix}.$$

The sums of squares for the different models are shown in Table 4 and total corrected sum of squares is 3071.91. The residual sum of squares for any model is the total corrected sum of squares minus the regression sum of squares for that model. The classification and confirmation tests are shown for both linear and nonlinear methods in Table 5.

The conclusion from the linear model is that there is no stationary ridge, but that a two-dimensional rising ridge cannot be confirmed since the confirmation test rejects the rising ridge model when compared to the full model. The nonlinear method is able to find a rising ridge model that fits better than the linear method and the confirmation test suggests that a two-dimensional rising ridge is a reasonable model for this response surface. The conclusion is that this surface may be a rising ridge and that further investigation of the response in the direction of the steepest ascent may prove worthwhile for increasing the response.

Table 5. Classification and confirmation F-tests

Hypothesis	F-*critical* ($\alpha = 0.05$)	F_X	*Conclusion*
Classification (linear)	3.74	50.40	Reject stationary ridge
Confirmation (linear)	3.20	3.81	Cannot confirm the rising ridge
Classification (nonlinear)	3.74	56.64	Reject stationary ridge
Confirmation (nonlinear)	3.20	2.18	Confirms the rising ridge

7. Conclusions

After a ridge has been identified in a quadratic response surface, it is important to determine if the ridge is rising or stationary. Two methods of fitting stationary and rising ridge models are proposed, one using linear regression and the other using nonlinear regression. Using either method, tests are suggested for classifying and confirming that a response surface has: (i) no ridge; (ii) a stationary ridge; or (iii) a rising ridge. The linear regression method is accessible with any regression program. The nonlinear method is more difficult to implement, but improves the precision of the model fitting.

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Appendix

The standard error of the eigenvalues from the DLR method

Suppose that for a given experiment, there is a single response, y, and k explanatory variables denoted $\mathbf{x} = (x_i, x_2, \ldots, x_k)'$. If there are n observations, the design matrix, $\mathbf{X}_\mathrm{D}$, is an $n \times k$ matrix such that the (i, j) element of $\mathbf{X}_\mathrm{D}$ is the level of x_j in the ith observation. The design matrix written in the canonical variables $\mathbf{z} = (z_1, z_2, \ldots, z_k)'$ is simply $\mathbf{Z}_\mathrm{D} = \mathbf{X}_\mathrm{D}\mathbf{D}$. The model matrix for fitting Equation (5) with linear regression is an $n \times p$ matrix as follows: $\mathbf{Z} = [\mathbf{1}, \mathbf{z}_1, \ldots, \mathbf{z}_k, \mathbf{z}_{12}, \ldots, \mathbf{z}_{(k-1)k}, \mathbf{z}_{11}, \ldots, \mathbf{z}_{kk}]$, where $p = (k+1)(k+2)/2$, $\mathbf{1}$ is a column of n ones, $\mathbf{z}_1, \ldots, \mathbf{z}_k$ are the k columns of the rotated design matrix, $\mathbf{Z}_\mathrm{D}$, and the other $k(k+1)/2$ columns are generated through element-by-element multiplication of all possible pairs of columns of $\mathbf{Z}_\mathrm{D}$. Thus for any $r = 1, 2, \ldots, k$ and $s = r, r+1, \ldots, k$, $\mathbf{z}_{rs}$ is generated by the element-by-element multiplication of $\mathbf{z}_r$ and $\mathbf{z}_s$. Assuming independent and identically distributed $N(0, \sigma^2)$ errors, $se(b^*_{ii})$, is the square root of the ith diagonal element of the lower $k \times k$ submatrix of $s^2(\mathbf{Z}'\mathbf{Z})^{-1}$, where s^2 is the residual variance. The approximate standard error for λ_i is then $se(b^*_{ii})$.

Biography

Bruce E. Ankenman is an Associate Professor in the Department of Industrial Engineering and Management Sciences at the McCormick School of Engineering at Northwestern University. He received a Bachelors of Electrical Engineering and Applied Physics from Case Western Reserve University. He received a Masters of Manufacturing Systems Engineering and a Ph.D. in Industrial Engineering from University of Wisconsin-Madison. Before graduate school, he worked as a design engineer in the automotive industry for 5 years. His current research interests include response surface methodology, design of experiments, robust design, experiments involving variance components and dispersion effects, and experimental design for simulation experiments. He is the chair of the Quality Statistics and Reliability Section of INFORMS, is on the Editorial Board for *IIE Transactions: Quality and Reliability Engineering*, and is an Associate Editor for *Naval Research Logistics*.

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