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On the Dual Response System

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1. Introduction

The purpose of this paper is to give a confidence region of a stationary point for a primary response y_p under the constraints that the secondary response y_s takes on some specified or desirable value. Engineers and scientists frequently need to analize dual response data. When studying a chemical reaction for instance, for each setting of group of "input" variables determining the reaction conditions, not one but a number of "output" variables or responses may be measured. The author studies the case when only two responses arise, one is the primary response, the other is the secondary response. We want to know the confidence region of the optimum stationary point for the primary response under the constraint that the secondary response takes some desirable value.

2. Dual response problem

Let the models be denoted by

$$y_{pi}=\beta_0+\sum_{i=1}^{k}\beta_l x_{li}+\sum_{i=1}^{k}\beta_{ll}x_{li}+\sum_{j>m=1}^{k}\sum^{k}\beta_{lm}x_{li}x_{mj}+\varepsilon_{pi} \quad i=1,2,\cdots\cdots,n_1$$

$$y_{si}=\gamma_0+\sum_{i=1}^{k}\gamma_l x_{li}+\sum_{i=1}^{k}\gamma_{ll}x_{li}+\sum_{j>m=1}^{k}\sum^{k}\gamma_{lm}x_{li}x_{mi}+\varepsilon_{si} \quad j=1,2,\cdots\cdots,n_2$$

If we assume that ε_{pi}'s are i.i.d. normal $(0,\sigma_p^2)$, ε_{si}'s are i.i.d. normal $(0,\sigma_s^2)$ and $\mathrm{cov}(\varepsilon_{pi},\varepsilon_{si})=0$, then the coefficients can be estimated by least squares method, as

$$\begin{aligned}\hat\beta&=(\hat\beta_0,\hat\beta_1,\cdots\cdots,\hat\beta_k,\hat\beta_{11},\hat\beta_{22},\cdots\cdots,\hat\beta_{kk},\hat\beta_{12},\hat\beta_{13},\cdots\cdots,\hat\beta_{k-1,k})\\&=(b_0,b_1,\cdots\cdots,b_k,b_{11},b_{22},\cdots\cdots,b_{kk},b_{12},b_{13},\cdots\cdots,b_{k-1,k})\\&=(X_p'X_p)^{-1}\ X_p'Y_p\end{aligned}$$

and

$$\begin{aligned}\hat\gamma&=(\hat\gamma_0,\hat\gamma_1,\cdots\cdots,\hat\gamma_k,\hat\gamma_{11},\hat\gamma_{22},\cdots\cdots,\hat\gamma_{kk},\hat\gamma_{12},\hat\gamma_{13},\cdots\cdots,\hat\gamma_{k-1,k})\\&=(c_0,c_1,\cdots\cdots,c_k,c_{11},c_{22},\cdots\cdots,c_{kk},c_{12},c_{13},\cdots\cdots,c_{k-1,k})\\&=(X_s'X_s)^{-1}\ X_sY_s,\end{aligned}$$

where

$$X_p=\begin{pmatrix} 1, x_{11}, \cdots\cdots, x_{k1}, x_{11}^2, \cdots\cdots, x_k^2, x_{11}x_{21}, \cdots\cdots, x_{k-1,1}x_{k1} \\ 1, x_{12}, \cdots\cdots, x_{k2}, x_{12}^2, \cdots\cdots, x_{k2}^2, x_{12}x_{22}, \cdots\cdots, x_{k-1,2}x_{k2} \\ \cdots\cdots \qquad \cdots\cdots \qquad \cdots\cdots \\ 1, x_{1n_1}, \cdots\cdots, x_{kn_1}, x_{1n_1}^2, \cdots\cdots, x_{kn_1}^2, x_{1n_1}x_{2n_1}, \cdots\cdots, x_{k\ 1,n_1}x_{kn_1} \end{pmatrix}$$

$$Y_p'=(y_{p1}, y_{p2}, \cdots\cdots, y_{pn_1}),$$

X_s and Y_s are similar matrices.

It is well known result that the variance-covariance matrices are the following form;

$$\mathrm{Cov}(\hat{\beta})=(X_p'X_p)^{-1}\sigma_p^2,\quad \mathrm{Cov}(\hat{\gamma})=(X_s'X_s)^{-1}\sigma_s^2 \tag{2.1}$$

Note that X_p and X_s may or may not be equal matrices.

So let the fitted models be

$$\hat{y}_p=b_0+\mathbf{x}'\mathbf{b}+\mathbf{x}'B\mathbf{x}$$

$$\hat{y}_s=c_0+\mathbf{x}'\mathbf{c}+\mathbf{x}'C\mathbf{x}$$

where

$$\mathbf{b}'=(b_1, b_2, \cdots\cdots, b_k)$$

$$\mathbf{c}'=(c_1, c_2, \cdots\cdots, c_k)$$

$$\mathbf{x}'=(x_1, x_2, \cdots\cdots, x_k)$$

$$B=\begin{pmatrix} b_{11}, \frac{b_{12}}{2}, \cdots\cdots, \frac{b_{1k}}{2} \\ b_{22}, \cdots\cdots, \frac{b_{2k}}{2} \\ \vdots \quad \vdots \\ sym. \qquad b_{kk} \end{pmatrix}$$

$$C=\begin{pmatrix} c_{11}, \frac{c_{12}}{2}, \cdots\cdots, \frac{c_{1k}}{2} \\ c_{22}, \cdots\cdots, \frac{c_{2k}}{2} \\ \vdots \quad \vdots \\ sym. \qquad c_{kk} \end{pmatrix}$$

The solution proposed and discussed in the sequel is to find the conditions on $\mathbf{x}$ which optimize (maximize or minimize) $\hat{y}_p$ subject to $\hat{y}_s=k$, where k is some desirable or acceptable value of the secondary response. Using Lagrangian multipliers,

$$L=b_0+\mathbf{x}'\mathbf{b}+\mathbf{x}'B\mathbf{x}-\mu(c_0+\mathbf{x}'\mathbf{c}+\mathbf{x}'C\mathbf{x}-k) \tag{2.2}$$

we require solutions for $\mathbf{x}$ in the set of equations

$$\frac{\partial L}{\partial \mathbf{x}}=0. \tag{2.3}$$

This result is in the following;

$$(B-\mu C)\mathbf{x}=\frac{1}{2}(\mu\mathbf{b}-\mathbf{c}). \tag{2.4}$$

Myers and Carter (4) gave the following theorem.

Theorem. *Let* $\mathbf{x}_1$ *and* $\mathbf{x}_2$ *be distinct solutions to Equation* (2.4), *using* μ_1 *and* μ_2 *respectively and tet* $\hat{y}_{s1}=\hat{y}_{s2}$. *If the matrix* $(B-\mu C)$ *is negative definite, then* $\hat{y}_{p1}>\hat{y}_{p2}$. *If* $(B-\mu_1 C)$ *is positive definite, then* $\hat{y}_{p1}<\hat{y}_{p2}$. *In addition, if* $B-\mu_1 C$ *is negative definite, then* $B-\mu_2 C$

cannot be negative definite.

Consider the quadratic form with matrix given by $(B-\mu C)$, i.e.,

$$q=w'(B-\mu C)w.$$

Since B and C are symmetric real matrix, there exists a non-singular matrix S such that

$$S'BS=diag(\lambda_1, \lambda_2, \cdots\cdots, \lambda_k)$$

and

$$S'CS=I_k.$$

performing the transformation

$$w'=v'S',$$

we have

$$q=v'\text{diag}(\lambda_1-\mu,\ \lambda_2-\mu, \cdots\cdots, \lambda_k-\mu)v. \qquad (2.5)$$

The λ's are merely the eigenvalues of the real symmetric matrix

$$D_2^{(-\frac{1}{2})}Q'BQD_2^{(-\frac{1}{2})}=T. \qquad (2.6)$$

Here Q is the orthogonal matrix for which

$$Q'CQ=D_2$$

and D_2 is the diagonal matrix containing the eigenvalues of C. The matrix $D_2^{(-\frac{1}{2})}$ is a diagonal matrix containing the reciprocals of the square roots of the eigenvalues of C. From Equation (2.5), it is clear that we can insure negative definiteness of $B-\mu C$ if $\mu>\lambda_k$ (positive definite if $\mu<\lambda_1$) where λ_1, $\lambda_2, \cdots\cdots, \lambda_k$ are arranged in ascending order. So, it becomes appearent this indeed defines the working region for μ and, in fact any $\mu_i>\lambda_k$ yields $\mathbf{x}_i$ which gives rise to an absolute maximum $\hat{y}_{pi}$ (absolute minimum for $\mu_i<\lambda_1$) conditional on a surface of secondary rsponse given by

$$\hat{y}_{si}=c_0+\mathbf{x}'\mathbf{c}+\mathbf{x}'C\mathbf{x}$$

3. Confidence Region for the Constrainted Stationary Point

If the true stationary point is $\mathbf{x}_0=\mathbf{p}$

$$(B-\mu C)\ \mathbf{p}-\frac{1}{2}(\mu\mathbf{b}-\mathbf{c})=\delta \qquad (2.7)$$

may not be $(0, 0, \cdots\cdots, 0)'$, where δ is a $k\times 1$ vector.

$$\mathrm{E}(\delta)=$$

$$\mathrm{Cov}(\delta)=\mathrm{E}(\delta\delta')=\mathrm{V}_1\sigma_p^2+\mathrm{V}_2\sigma_s^2 \overset{\text{let}}{=} V. \qquad (2.8)$$

Since $\mathrm{Cov}(\beta)$ and $\mathrm{Cov}(\gamma)$ are known (Equation 2.1), we can calculate V.

The estimators of σ_p^2, σ_s^2 are in the following

$$\sigma_p^2=\frac{Y_p'Y_p-\hat{\beta}'X_p'Y_p}{\phi_1} \text{ with } \phi_1=n_1-\frac{k^2+3k+2}{2} \text{ d. f.},$$

$$\sigma_s^2=\frac{Y_s'Y_s-\hat{\gamma}'X_s'Y_s}{\phi_3} \text{ with } \phi_2=n_2\frac{k^2+3k+2}{2} \text{ d. f.}$$

Thus $\dfrac{\delta'V^{-1}\delta}{\phi_1+\phi_2}$ is distributed $F(k, n_1+n_2-\phi_1-\phi_2)$

Hence $100(1-\alpha)\%$ confidence region of the stationary point in the constrainted dual pesponse system is denoted by

$$\delta' V\delta \leq kF(k, n_1+n_2-\phi_1-\phi_2;\ \alpha).$$

Example Suppose we have the following data

x_1	x_2	y_p	y_s
−1	−1	52	13.9
1	−1	45	12.9
−1	1	30	13.1
1	1	46	13.6
−2	0	47	—
2	0	52	—
0	−2	49	—
0	2	54	—
−1.5	0	—	14.5
1.5	0	—	14.4
0	−1.5	—	14.6
0	1.5	—	15.9
0	0	44	11.9
0	0	42	15.8

with $n_1=n_2=10$.

Then we can calculate the followings

$$(X_p'X_p')^{-1}=\begin{pmatrix} 10, & 0, & 0, & 12, & 12, & 0 \\ & 12, & 0, & 0, & 0, & 0 \\ & & 12, & 0, & 0, & 0 \\ & & & 36, & 4, & 0 \\ & \text{sym.} & & & 36, & 0 \\ & & & & & 4 \end{pmatrix}^{-1}$$

$$=\begin{pmatrix} .3571, & 0, & 0, & -.2313, & -.1071, & 0 \\ & .0833, & 0, & 0, & 0, & 0 \\ & & .0833, & 0, & 0, & 0 \\ & & & .0703, & .0291, & 0 \\ & \text{sym.} & & & .0603, & 0 \\ & & & & & .25 \end{pmatrix}$$

$$(X_s'X_s)^{-1}=\begin{pmatrix} .4932, & 0, & 0, & -.2313, & -.2313, & 0 \\ & .1176, & 0, & 0, & 0, & 0 \\ & & .1176, & 0, & 0, & 0 \\ & & & .1854, & .0867, & 0 \\ & \text{sym.} & & & .1854, & 0 \\ & & & & & .25 \end{pmatrix}$$

$\sigma_p^2=36.33,\ \ \sigma_s^2=.8443$

$\hat{y}_p=41+1.5833\,x_1-.91667\,x_2+1.875\,x_1^2+2.375\,x_2^2+5.75\,x_1x_2$

$\hat{y}_s=11.464-.7647\,x_1+.2177\,x_2+1.0848\,x_1^2+1.4404\,x_2^2+.375\,x_1x_2$

$$T=\begin{pmatrix} .9979, & 0 \\ 0, & .8108 \end{pmatrix} \begin{pmatrix} .9187, & -.3949 \\ .3949, & .9187 \end{pmatrix} BQ'D_2^{(-\frac{1}{2})}=\begin{pmatrix} -.13264, & 1.45391 \\ 1.45391, & 2.88179 \end{pmatrix}.$$

The eigenvalues of T are $\lambda_1=-.7196$, $\lambda_2=3.4687$.

The working region of μ for maximizing $\hat{y}_p$ is $\mu>3.4687$.

For $\mu=4.1$, from Equation (2.4) the stationary point is $(-1.8555, -.5439)$.

From Equation (2.7) $\delta'=(d_1, d_2)$ is

$$d_1=-2.5727x_1+2.1063x_2-3.6281$$

$$d_2=2.1063x_1-3.5306x_2+1.9880.$$

$$Cov(\delta)=\begin{pmatrix} .0603x_1^2+.25x_2^2+.3500, & .2791x_1x_2 \\ & .25x_1^2+.0603x_2^2+.3500 \end{pmatrix} \sigma_p^2$$

$$+\begin{pmatrix} 3.1166x_1^2+4.2025x_2^2+.0294, & 5.6599x_1x_2 \\ & 4.2025x_1^2+3.1166x_2^2+.0294 \end{pmatrix} \sigma_s^2=V.$$

Hence the confidence region of this stationary point is in Fig. 1.

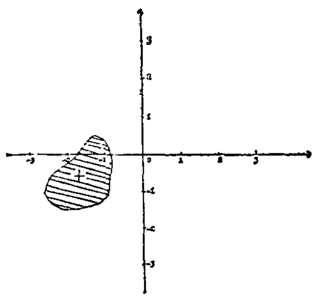

Fig. 1.

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