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Research Article

Response surface designs using the generalized variance inflation factors

Diarmuid O'Driscoll & Donald E. Ramirez | Guohua Zou (Reviewing Editor)

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Response surface designs are a mainstay in applied statistics. The variance inflation factors VIF are a measure of collinearity for a single variable in a linear regression model. The generalization to subsets of variables is the generalized variance inflation factor GVIF. This research introduces GVIF as a penalty measure for extending a linear response model to a response surface with the included quadratic terms. The methodology is demonstrated with case studies, and, in particular, it is shown that using GVIF, the H310 design can be improved for the standard global optimality criteria of A, D, and E.

1. Introduction

We consider a linear regression $Y=X\beta+\varepsilon$ with X a full rank $n\times p$ matrix and $L(\varepsilon)=N(0,\sigma^2 I_n)$. The variance inflation factor VIF, Belsley (1986), measures the penalty for adding one non-orthogonal additional explanatory variable to a linear regression model, and they can be computed as a ratio of determinants. The extension of VIF to a measure of the penalty for adding a subset of variables to a model is the generalized variance inflation factor GVIF of Fox and Monette (1992), which will be used to study response surface designs, in particular, as the penalty for adding the quadratic terms to the model.

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previous columns with the entries in the off-diagonal elements of the pth row and pth column of $X'X$ all zeros. Denote by M_p the idealized moment matrix

$$M_p = \begin{bmatrix} X_{[p]}'X_{[p]} & 0_{p-1} \\ 0_{p-1}' & x_p'x_p \end{bmatrix}.$$

The VIFs are the diagonal entries of $S_X^{-1} = D_X^{-1}(X'X)^{-1}D_X^{-1}$. It remains to note that the inverse, S_X^{-1}, can be computed using cofactors $C_{i,j}$. In particular,

$$\mathrm{VIF}_p = [S_X^{-1}]_{p,p} = [D_X^{-1}(X'X)^{-1}D_X^{-1}]_{p,p} = (x_p'x_p)^{1/2}\frac{\det(C_{p,p})}{\det(X'X)}(x_p'x_p)^{1/2} = \frac{\det(M_p)}{\det(X'X)} \quad (1)$$

the ratio of the determinant of the idealized moment matrix M_p to the determinant of the moment matrix $X'X$. This definition extends naturally to subsets and is discussed in the next section.

For an alternate view of the how collinearities in the explanatory variables inflate the model variances of the regression coefficients when compared to a fictitious orthogonal reference design, consider the formula for the model variance

$$\mathrm{Var}_M(\hat{\beta}_j) = \frac{\sigma^2}{\sum_{i=1}^{n}(x_{ij}-\bar{x}_j)^2}\frac{1}{1-R_j^2}$$

where R_j … e jth column
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$$M(r,s)=\begin{bmatrix} X_1'X_1 & 0_{r\times s} \\ 0_{s\times r} & X_2'X_2 \end{bmatrix}.$$

Following Equation 1, to measure the effect of adding X_2 to the design X_1, that is for $X_2|X_1$, we define the generalized variance inflation factor as

$$\mathrm{GVIF}(X_2|X_1)=\frac{\det(M(r,s))}{\det(X'X)}=\frac{\det(X_1'X_1)\det(X_2'X_2)}{\det(X'X)} \quad (2)$$

as in Equation 10 of Fox and Monette (1992), who compared the sizes of the joint confidence regions for β for partitioned designs and noted when $X=[X_{[p]},x_p]$ that $\mathrm{GVIF}[x_p|X_{[p]}]=\mathrm{VIF}_p$. Equation 2 is in the spirit of the efficiency comparisons in linear inferences introduced in Theorems 4 and 5 of Jensen and Ramirez (1993). A similar measure of collinearity is mentioned in Note 2 in Wichers (1975), Theorem 1 of Berk (1977), and Garcia, Garcia, and Soto (2011). For the simple linear regression model with $p=2$, Equation 2 gives $\mathrm{VIF}=\frac{1}{1-\rho^2}$ with ρ the correlation coefficient as required. Fox and Monette (1992) suggested that X_1 contains the variables which are of “simultaneous interest,” while X_2 contains additional variables selected by the investigator. We will set X_1 for the constant and main effects and set X_2 the (optional) quadratic terms with values from X_1.

Willan and Watts (1978) measured the effect of collinearity using the ratio of the volume … nt confiden… s in the spirit of GVIF … the joint confiden… tability and they not… les of the actual d… mple case study, c… , and $y=$ $[4,1,1$ … lso includes $x_2=[$ … $2)=(0,0)$ is $2.5\pm46.$ … arity introduc…

For the … ension $n\times s$, set

and denote the canonical moment matrix as

$$R = D_{(r,s)}(X'X)D_{(r,s)} = \begin{bmatrix} I_{r\times r} & (X_1'X_1)^{-1/2}(X_1'X_2)(X_2'X_2)^{-1/2} \\ (X_2'X_2)^{-1/2}(X_2'X_1)(X_1'X_1)^{-1/2} & I_{s\times s} \end{bmatrix}; \quad (3)$$

with determinant

$$\det(R) = \frac{\det(X'X)}{\det(X_1'X_1)\det(X_2'X_2)} = \frac{1}{GVIF(X_2|X_1)};$$

equivalently,

$$\det(R) = \det(I_{r\times r} - B_{r\times s}B_{s\times r}') = \det(I_{s\times s} - B_{s\times r}'B_{r\times s})$$

where $B_{r\times s} = (X_1'X_1)^{-1/2}(X_1'X_2)(X_2'X_2)^{-1/2}$.

In the case $\{r=p-1,\ s=1\}$, $X_2 = x_p$ is a $n\times 1$ vector and the partitioned design $X=[X_1, x_p]$ has $\det(R) = 1-[x_p'X_1(X_1'X_1)^{-1}X_1'x_p]/x_p'x_p$. From standard facts for the inverse of a partitioned matrix, for example, Myers (1990, p. 459), $VIF_p = [R^{-1}]_{p,p} = [D_{(p-1,1)}^{-1}(X'X)^{-1}D_{(p-1,1)}^{-1}]_{p,p}$ can be computed directly as

$$(x_p'x_p)^{1/2}(X'X)^{-1}_{p,p}(x_p'x_p)^{1/2} = \frac{x_p'x_p}{x_p'x_p - x_p'X_1(X_1'X_1)^{-1}X_1'x_p} = \frac{1}{1-[x_p'X_1(X_1'X_1)^{-1}X_1'x_p]/x_p'x_p} = \frac{1}{\det(R)} = GVIF(X_2|X_1).$$

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(4)

For the partitioning X=[Xr|Xs], the canonical moment matrix, Equation 3, has the identity matrices Ir, Is down the diagonal and off-diagonal array X1′X1-1/2X1′X2X2′X2-1/2. For the quadratic model y=β0+β1x+β2x2 and partitioning X=[1,x|x2], we have

$$R=10\rho101\rho2\rho1\rho21.$$

From Equation 4, GVIF(x2|1,x)=(1-λ2)-1 where λ=ρ12+ρ22 is the unique positive singular value of [ρ1,ρ2]′. Denote

$$\gamma X2=\rho12+\rho22$$

as the canonical index with GVIF(x2|1,x)=11-γX2=1det(R). Surprisingly, many higher order designs also have the off-diagonal entry of the canonical moment matrix with a unique positive singular value with GVIF(X2|X1)=11-γX2 with the collinearity between the lower order terms and the upper order terms as a function of the canonical index γX2.

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5. Central composite and factorial designs for quadratic models (p=6)

In this se … d Wilson (1951) a … of Appendix 2. Both …

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then $\rho_1=\rho_2=2/10$, $\gamma_{X2}=8/10$, and $GVIF(X_2|X_1)=5$. Surprisingly, the classical choice of $a=2$ gives the largest value for $GVIF(X_2|X_1)$, that is the worst value, indicating the greatest collinearity between the lower and higher order terms, as noted in O'Driscoll and Ramirez (in press).

6. Larger designs (p=10)

We consider the quadratic response surface designs for

$$y=\beta_0+\beta_1x_1+\beta_2x_2+\beta_3x_3+\beta_{11}x_1^2+\beta_{22}x_2^2+\beta_{33}x_3^2+\beta_{12}x_1x_2+\beta_{13}x_1x_3+\beta_{23}x_2x_3+\varepsilon \quad (5)$$

with n responses and with X partitioned into $X_1|X_2$ with X_1 the four lower order terms ($r=4$) and X_2 the six quadratic terms ($s=6$). Four popular designs are given in Appendix 2. They are the hybrid designs (H310 and H311B) of Roquemore (1976) Tables A2 and A3, the Box and Behnken (1960) (BBD) design Table A4, and the CCD of Box and Wilson (1951) Table A5.

For each design, we compute the 10×10 canonical moment matrix. It is striking that, for all th… singular value wi… $1-\gamma_{X2}$.

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Table 2 reports that the design H310 is the most conditioned with respect to the GVIF with the least amount of collinearity between the lower and higher order terms.

7. More complicated designs with ordered singular values

Let X be the minimal design of Box and Draper (1974) BDD with $n=11$ from Table A6, and let Z be the small composite design of Hartley (1959) SCD with $n=11$ from Table A7 for the quadratic response surface model ($r=4$ and $s=6$) as in Equation (5). Let $\alpha=\{\alpha_1\geq\ldots\geq\alpha_r\geq0\}$ and $\beta=\{\beta_1\geq\ldots\geq\beta_r\geq0\}$ be the non-negative singular values of the off-diagonal array for RX and RZ, respectively. As $\alpha_i\leq\beta_i(1\leq i\leq r)$ in Table 3, it follows that $GVIF(X_2|X_1)\leq GVIF(Z_2|Z_1)$ showing less collinearity between the lower and higher order terms for the BDD design.

8. An improved H310 design

When the diagonal matrix $\Lambda_{r\times s}$ in Equation 6 in Appendix 1 has only one non-zero entry, we have denoted the square of this value the canonical index. We extend this definition to the case when $X_1'X_1^{-1/2}(X_1'X_2)X_2'X_2^{-1/2}$ has multiple positive singular

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in Table 4. The sixth entry of c_6=-0.1360 was not optimal with $\gamma X2$=0.8181 with cmin=-0.01264, a magnitude value smaller.

Table 4. Optimal values cmin for $\gamma X2$

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Denote the "improved" H310 design as the H310 design with the value of c_6=-0.01264. The "improved" H310 also has a unique positive singular value for the off-diagonal of R with its square the canonical index $\gamma X2$. All of the standard design criteria favor the "improved" H310 design over the H310 design, which was originally constructed based on the rotatability criterion to maintain equal variances for predicted responses for points that have the same distance from the design center. As usual $A(X)=tr((X'X)^{-1})$, $D(X)=det((X'X)^{-1})$, and $E(X)=max\{eigenvalues\ of\ (X'X)^{-1}\}$. The small relative changes Δ in the design criteria are shown in Table 5 in Column 4.

Table 5. Design criteria for the "improved" H310 with Δ the relative change

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have used GFIV to study standard quadratic response designs. The H310 design of Roquemorer (1976) was shown not to be optimal with respect to GFIV and an “improved” H310 design was introduced which was favored over H310 using the standard design criteria A, D, and E.

Additional information

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Notes on contributors

Diarmuid O’Driscoll

Diarmuid O’Driscoll is the head of the Mathematics and Computer Studies Department at Mary Immaculate College, Limerick. He was awarded a Travelling Studentship for his MSc at University College Cork in 1977. He has taught at University College Cork, Cork Institute of Technology, University of Virginia, and Frostburg State University. His research interests are in mathematical education, errors in variables regression, and design criteria

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Appendix 1

We study the eigenvalue structure of $M(r,s)$. Let $\{\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{\min(r,s)} \geq 0\}$ be the non-negative singular values of $X_1'X_1^{-1/2}(X_1'X_2)X_2'X_2^{-1/2}$.

As with the canonical correlation coefficients Eaton (1983), write the off-diagonal rectangular array $B_{r\times s}$ of R as PAQ' with P and Q orthogonal matrices and $\Lambda_{r\times s}$ the

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$$GVIF(X_2|X_1)=\prod_{i=1}^{\min(r,s)}\frac{1}{1-\lambda_i^2}.$$

The singular values of $R_{12}=(X_1'X_1)^{-1/2}(X_1'X_2)(X_2'X_2)^{-1/2}$ are the non-negative square roots of the eigenvalues of $\Lambda'\Lambda$ denoted by

$$\mathrm{eigvals}(\Lambda'\Lambda)=\mathrm{eigvals}((Q'R_{12}'P)(P'R_{12}Q))=\mathrm{eigvals}((X_1'X_1)^{-1}(X_1'X_2)(X_2'X_2)^{-1}(X_2'X_1)). \quad \text{(A2)}$$

If the trace of the inverse of the matrix in Equation 6 is required, then we note that

$$\begin{bmatrix} I_r & \Lambda_{r\times s} \\ \Lambda_{s\times r}' & I_s \end{bmatrix}^{-1}=\begin{bmatrix} (I_r-\Lambda_{r\times s}\Lambda_{s\times r}')^{-1} & -\Lambda_{r\times s}(I_s-\Lambda_{s\times r}'\Lambda_{r\times s})^{-1} \\ -\Lambda_{s\times r}'(I_r-\Lambda_{r\times s}\Lambda_{s\times r}')^{-1} & (I_s-\Lambda_{s\times r}'\Lambda_{r\times s})^{-1} \end{bmatrix}$$

with trace given by $\mathrm{tr}((L'RL)^{-1})=|r-s|+2\sum_{i=1}^{\min(r,s)}\frac{1}{1-\lambda_i^2}$.

Appendix 2

Table A1. The lower order matrix for the CCD with center run with a
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Table A4. The lower order matrix for the Box and Behnken (1960) design (BBD) with center run, n=13

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Table A5. The lower order matrix for the Box and Wilson (1951) CCD for α=1.732 with center run, n=15

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Table A6. The lower order matrix for the Box and Draper (1974) minimal design (BDD) with center run, n=11

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