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Research Article

Response surface designs using the generalized variance inflation factors

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using GVIF, the H310 design can be improved for the standard global optimality criteria of A, D, and E.

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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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2. Variance inflation factors

For our linear model $Y=X\beta+\varepsilon$, let D_X be the diagonal matrix with entries on the diagonal $D_X[i,i]=(X'X)_{i,i}^{-1/2}$. When the design has been standardized $X\rightarrow XD_X$, the VIFs are the

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VIFp=[SX-1]p,p=[DX-1(X′X)-1DX-1]p,p=(xp′xp)1/2det(Cp,p)det(X′X)

(xp′xp)1/2=det(Mp)det(X′X)

(1)

the ratio of the determinant of the idealized moment matrix Mp 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

VarM(β^j)=σ2∑i=1n(xij-x¯j)211-Rj2

where Rj2 is the square of the multiple correlation from the regression of the jth column of X=[xij] on the remaining columns as in Liao and Valliant (2012). The first term σ2/∑(xij-x¯j)2 is the model variance for β^j had the jth explanatory variable been orthogonal to the remaining variables. The second term 1/(1-Rj2) is a standard definition of the jthVIF as in Thiel (1971).

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3. Generalized variance inflation factors

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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],xp] that GVIF[xp|X[p]]=VIFp. 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 VIF=11-ρ2 with ρ the correlation coefficient as required. Fox and Monette (1992) suggested that X1 contains the variables which are of “simultaneous interest,” while X2 contains additional variables selected by the investigator. We will set X1 for the constant and main effects and set X2 the (optional) quadratic terms with values from X1.

Willan and Watts (1978) measured the effect of collinearity using the ratio of the volume of the actual joint confidence region for β^ to the volume of the joint confidence region in the fictitious orthogonal reference design. Their ratio is in the spirit of GVIF as det(X′X) is inversely proportional to the square of the volume of the joint confidence region for β^. They also introduced a measure of relative predictability and they note: “The existence of near linear relations in the independent variables of the actual data reduces the overall predictive efficiency by this factor.” For a simple case study, consider the simple linear regression model with n=4, x1=[-2,-1,1,2]′, and y=[4,1,1,4]′. The 95% prediction interval for x1=0 is 2.5±10.20. If the model also includes x2=[-2.(2)=(0,0) is 2.5±46.(arity introduc

For the (ension n×s, set

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R=D(1-1/2Is×s; (3)

with det

det(R)=det(X′X)det(X1′X1)det(X2′X2)=1GVIF(X2|X1);

equivalently,

det(R)=det(Ir×r-Br×sBs×r′)=det(Is×s-Bs×r′Br×s)

where Br×s=X1′X1-1/2(X1′X2)X2′X2-1/2.

In the case {r=p-1, s=1}, X2=xp is a n×1 vector and the partitioned design X=[X1,xp] has det(R)=1-[xp′X1X1′X1-1X1′xp]/xp′xp. From standard facts for the inverse of a partitioned matrix, for example, Myers (1990, p. 459), VIFp=[R-1]p,p=[D(p-1,1)-1(X′X)-1D(p-1,1)-1]p,p can be computed directly as

xp′xp1/2(X′X)p,p-1xp′xp1/2=xp′xpxp′xp-xp′X1X1′X1-1X1′xp=11-[xp′X1X1′X1-1X1′xp]/xp′xp=1det(R)=GVIF(X2|X1).

Table 1. CCD with parameter a, canonical index γX2, and GVIF

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We study the eigenvalue structure of M(r,s) in Appendix 1. Let {λ1≥λ2≥

≥λmin(r 2-1/2. It is

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

$$γX2=ρ12+ρ22$$

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 section, we compare the central composite design (CCD) X of Box and Wilson (1951) and the factorial design Z. The design points are shown in Table A1 of Appendix 2. Both designs are 9×6 and use the quadratic response model

$$y=β0+β1x1+β2x2+β11x12+β22x22+β12x1x2+ε.$$

The CCD design uses

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6. Larger designs (p=10)

We consider the quadratic response surface designs for

$$y=β0+β1x1+β2x2+β3x3+β11x12+β22x22+β33x32+β12x1x2+β13x1x3+β23x2x3+ε \quad (5)$$

with n responses and with X partitioned into X1|X2 with X1 the four lower order terms (r=4) and X2 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 these designs, the off-diagonal 4×6 array in R has only one non-zero singular value with its square the canonical index γX2. It follows that GVIF(X2|X1)=11-γX2.

Table 2. Hybrid designs H310, H311B, Box and Behnken BBD,and CCD

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Table the GVIF
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Let X be Table A6

for the quadratic response surface model (r=4 and s=6) as in Equation (5). Let α={α1≥…≥αr≥0} and β={β1≥…≥βr≥0} be the non-negative singular values of the off-diagonal array for RX and RZ, respectively. As αi≤βi(1≤i≤r) in Table 3, it follows that GVIF(X2|X1)≤GVIF(Z2|Z1) showing less collinearity between the lower and higher order terms for the BDD design.

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8. An improved H310 design

When the diagonal matrix Λr×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 X1′X1-1/2(X1′X2)X2′X2-1/2 has multiple positive singular values. The Frobenious norm for a rectangular matrix Ar×s is defined by ||A||F2=∑i=1r∑j=1saij2=trace(A′A). For a design matrix X, we extend the definition of the canonical index with γX2=||Λr×s||F2. Alternatively, γX2=trace(X2′X2-1(X2′X1)X1′X1-1(X1′X2)) as in Equation 7.

We examine, in detail, the H310 design matrix X11×10, Table A2 in Appendix 2, with our attention to the value of -0.1360 in row 2 for x3. In succession, we will replace the values {1.1736,0.6386,-0.9273,1.0000,1.2906,-0.1360} by a free parameter and use γX2 to determine an optimal value. For example, replacing the four entries which are

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Denote the “improved” H310 design as the H310 design with the value of $c6=-0.01264$. 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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The abnormality of the second row in H310 has been noted in Jensen (1998) who showed that the design is least sensitive to the second row of X, the row containing the value $c6=-0.1360$.

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Appendix 1

We study the eigenvalue structure of M(r,s). Let {λ1≥λ2≥...≥λmin(r,s)≥0} be the non-negative singular values of X1′X1-1/2(X1′X2)X2′X2-1/2.

As with the canonical correlation coefficients Eaton (1983), write the off-diagonal rectangular array Br×s of R as PΛQ′with P and Q orthogonal matrices and Λr×s the rectangular diagonal matrix with the non-negative singular values down the diagonal. Set

$$L=Pr\times r0r\times s0s\times rQs\times s.$$

For notational convenience, we assume r≤s. The matrix L is orthogonal and transforms R→L′RL into diagonal matrices:

$$Ir\Lambda r\times s\Lambda s\times r'Is=Ir[SVr\times r|0r\times (s-r)][SVr\times r|0r\times (s-r)]'Is$$

(A1)

with Λr×s=[SVr×r|0r×(s-r)] where SVr×r is the diagonal matrix of the non-negative singular values. Since L is orthogonal, this transformation has not changed the eigenvalues. To compute the determinant of R, convert the matrix in Equation 6 into an upper diagonal matrix by Gauss Elimination on Λs×r′. This changes r of the 1′s on the

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Appendix 2

Table A1. The lower order matrix for the CCD with center run with a=2, n=9 and the lower order matrix for the factorial design with center run n=9

Display Table

Table A2. The lower order matrix for the hybrid (H310) design of Roquemore (1976) with center run, n=11

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Table A3. The lower order matrix for the hybrid (H311B) design of Roquemore (1976) with center run, n=11

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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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Table A7. The Lower order matrix for the small composite design of Hartley (1959) (SCD) for α=1.732 with center run, n=11

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