



Received: 22 December 2014
Accepted: 15 May 2015
Published: 14 June 2015

*Corresponding author: Donald E. Ramirez, Department of Mathematics, University of Virginia, Charlottesville, VA 22904, USA
E-mail: der@virginia.edu

Reviewing editor:
Guohua Zou, Chinese Academy of Sciences, China

Additional information is available at the end of the article

STATISTICS | RESEARCH ARTICLE

Response surface designs using the generalized variance inflation factors

Diarmuid O'Driscoll¹ and Donald E. Ramirez^{2*}

Abstract: We study response surface designs using the generalized variance inflation factors for subsets as an extension of the variance inflation factors.

Subjects: Mathematics & Statistics; Science; Statistical Computing; Statistical Theory & Methods; Statistics; Statistics & Probability

Keywords: variance inflation factors; generalized variance inflation factors; response surface designs

1. Introduction

We consider a linear regression $\mathbf{Y} = \mathbf{X}\beta + \epsilon$ with \mathbf{X} a full rank $n \times p$ matrix and $\mathcal{L}(\epsilon) = N(\mathbf{0}, \sigma^2 \mathbf{I}_n)$. 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.

2. Variance inflation factors

For our linear model $\mathbf{Y} = \mathbf{X}\beta + \epsilon$, let \mathbf{D}_X be the diagonal matrix with entries on the diagonal $\mathbf{D}_X[i, i] = (\mathbf{X}'\mathbf{X})_{ii}^{-1/2}$. When the design has been standardized $\mathbf{X} \rightarrow \mathbf{X}\mathbf{D}_X$, the *VIFs* are the diagonal entries of the inverse of $\mathbf{S}_X = \mathbf{D}_X(\mathbf{X}'\mathbf{X})\mathbf{D}_X$. That is, the *VIFs* are the ratios of the actual variances for

ABOUT THE AUTHORS

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. In 2014, he was awarded a Teaching Heroes Award by the National Forum for the Enhancement of Teaching and Learning (Ireland).

Donald E. Ramirez is a full professor in the Department of Mathematics at the University of Virginia in Charlottesville, Virginia. He received his PhD in Mathematics from Tulane University in New Orleans, Louisiana. His research is in harmonic analysis and mathematical statistics. His current research interests are in statistical outliers and ridge regression.

PUBLIC INTEREST STATEMENT

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*.

the explanatory variables to the “ideal” variances had the columns of \mathbf{X} been orthogonal. Note that we follow Stewart (1987) and do not necessarily center the explanatory variables.

For our linear model $\mathbf{Y} = \mathbf{X}\beta + \epsilon$, view $\mathbf{X} = [\mathbf{X}_{[p]}, \mathbf{x}_p]$ with \mathbf{x}_p the p^{th} column of \mathbf{X} and $\mathbf{X}_{[p]}$ the matrix formed by the remaining columns. The variance inflation factor VIF_p measures the effect of adding column \mathbf{x}_p to $\mathbf{X}_{[p]}$. For notational convenience, we demonstrate VIF_p with the last column p . An ideal column would be orthogonal to the previous columns with the entries in the off-diagonal elements of the p^{th} row and p^{th} column of $\mathbf{X}'\mathbf{X}$ all zeros. Denote by \mathbf{M}_p the idealized moment matrix

$$\mathbf{M}_p = \begin{bmatrix} \mathbf{X}'_{[p]}\mathbf{X}_{[p]} & \mathbf{0}_{p-1} \\ \mathbf{0}'_{p-1} & \mathbf{x}'_p\mathbf{x}_p \end{bmatrix}.$$

The VIF s are the diagonal entries of $\mathbf{S}_X^{-1} = \mathbf{D}_X^{-1}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{D}_X^{-1}$. It remains to note that the inverse, \mathbf{S}_X^{-1} , can be computed using cofactors \mathbf{C}_{ij} . In particular,

$$\begin{aligned} VIF_p &= [\mathbf{S}_X^{-1}]_{p,p} = [\mathbf{D}_X^{-1}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{D}_X^{-1}]_{p,p} \\ &= (\mathbf{x}'_p\mathbf{x}_p)^{1/2} \frac{\det(\mathbf{C}_{p,p})}{\det(\mathbf{X}'\mathbf{X})} (\mathbf{x}'_p\mathbf{x}_p)^{1/2} = \frac{\det(\mathbf{M}_p)}{\det(\mathbf{X}'\mathbf{X})} \end{aligned} \tag{1}$$

the ratio of the determinant of the idealized moment matrix \mathbf{M}_p to the determinant of the moment matrix $\mathbf{X}'\mathbf{X}$. 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

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

where R_j^2 is the square of the multiple correlation from the regression of the j^{th} column of $\mathbf{X} = [x_{ij}]$ on the remaining columns as in Liao and Valliant (2012). The first term $\sigma^2 / \sum (x_{ij} - \bar{x}_j)^2$ is the model variance for $\hat{\beta}_j$ had the j^{th} explanatory variable been orthogonal to the remaining variables. The second term $1/(1 - R_j^2)$ is a standard definition of the j^{th} VIF as in Thiel (1971).

3. Generalized variance inflation factors

In this section, we introduce the $GVIF$ s as an extension of the classical variance inflation factors VIF from Equation 1. For the linear model $\mathbf{Y} = \mathbf{X}\beta + \epsilon$, view $\mathbf{X} = [\mathbf{X}_1, \mathbf{X}_2]$ partitioned with \mathbf{X}_1 of dimension $n \times r$ usually consisting of the lower order terms and \mathbf{X}_2 of dimension $n \times s$ usually consisting of the higher order terms. The idealized moment matrix for the (r, s) partitioning of \mathbf{X} is

$$\mathbf{M}_{(r,s)} = \begin{bmatrix} \mathbf{X}'_1\mathbf{X}_1 & \mathbf{0}_{r \times s} \\ \mathbf{0}'_{s \times r} & \mathbf{X}'_2\mathbf{X}_2 \end{bmatrix}.$$

Following Equation 1, to measure the effect of adding \mathbf{X}_2 to the design \mathbf{X}_1 , that is for $\mathbf{X}_2|\mathbf{X}_1$, we define the *generalized variance inflation factor* as

$$GVIF(\mathbf{X}_2|\mathbf{X}_1) = \frac{\det(\mathbf{M}_{(r,s)})}{\det(\mathbf{X}'\mathbf{X})} = \frac{\det(\mathbf{X}'_1\mathbf{X}_1) \det(\mathbf{X}'_2\mathbf{X}_2)}{\det(\mathbf{X}'\mathbf{X})} \tag{2}$$

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 $\mathbf{X} = [\mathbf{X}_{[p]}, \mathbf{x}_p]$ that $GVIF[\mathbf{x}_p|\mathbf{X}_{[p]}] = VIF_p$. 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 $VIF = \frac{1}{1-\rho^2}$ with ρ the correlation coefficient as required. Fox and Monette (1992) suggested that \mathbf{X}_1 contains the variables which are of “simultaneous interest,” while \mathbf{X}_2 contains additional variables selected by the investigator. We will set \mathbf{X}_1 for the constant and main effects and set \mathbf{X}_2 the (optional) quadratic terms with values from \mathbf{X}_1 .

Willan and Watts (1978) measured the effect of collinearity using the ratio of the volume of the actual joint confidence region for $\hat{\beta}$ to the volume of the joint confidence region in the fictitious orthogonal reference design. Their ratio is in the spirit of *GVIF* as $\det(\mathbf{X}'\mathbf{X})$ is inversely proportional to the square of the volume of the joint confidence region for $\hat{\beta}$. 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 $n = 4$, $\mathbf{x}_1 = [-2, -1, 1, 2]'$, and $\mathbf{y} = [4, 1, 1, 4]'$. The 95% prediction interval for $x_1 = 0$ is 2.5 ± 10.20 . If the model also includes $\mathbf{x}_2 = [-2.001, -1.001, 1.001, 2.001]'$, then the 95% prediction interval for $(x_1, x_2) = (0, 0)$ is 2.5 ± 46.02 demonstrating the loss of predictive efficiency due to the collinearity introduced by \mathbf{x}_2 .

For the (r, s) partition of $\mathbf{X} = [\mathbf{X}_1, \mathbf{X}_2]$ with \mathbf{X}_1 of dimension $n \times r$ and \mathbf{X}_2 of dimension $n \times s$, set

$$\mathbf{D}_{(r,s)} = \begin{bmatrix} (\mathbf{X}'_1\mathbf{X}_1)^{-1/2} & \mathbf{0} \\ \mathbf{0} & (\mathbf{X}'_2\mathbf{X}_2)^{-1/2} \end{bmatrix},$$

and denote the canonical moment matrix as

$$\begin{aligned} \mathbf{R} &= \mathbf{D}_{(r,s)}(\mathbf{X}'\mathbf{X})\mathbf{D}_{(r,s)} \\ &= \begin{bmatrix} \mathbf{I}_{r \times r} & (\mathbf{X}'_1\mathbf{X}_1)^{-1/2}(\mathbf{X}'_1\mathbf{X}_2)(\mathbf{X}'_2\mathbf{X}_2)^{-1/2} \\ (\mathbf{X}'_2\mathbf{X}_2)^{-1/2}(\mathbf{X}'_2\mathbf{X}_1)(\mathbf{X}'_1\mathbf{X}_1)^{-1/2} & \mathbf{I}_{s \times s} \end{bmatrix}; \end{aligned} \tag{3}$$

with determinant

$$\det(\mathbf{R}) = \frac{\det(\mathbf{X}'\mathbf{X})}{\det(\mathbf{X}'_1\mathbf{X}_1)\det(\mathbf{X}'_2\mathbf{X}_2)} = \frac{1}{GVIF(\mathbf{X}_2|\mathbf{X}_1)};$$

equivalently,

$$\det(\mathbf{R}) = \det(\mathbf{I}_{r \times r} - \mathbf{B}_{r \times s}\mathbf{B}'_{s \times r}) = \det(\mathbf{I}_{s \times s} - \mathbf{B}'_{s \times r}\mathbf{B}_{r \times s})$$

$$\text{where } \mathbf{B}_{r \times s} = (\mathbf{X}'_1\mathbf{X}_1)^{-1/2}(\mathbf{X}'_1\mathbf{X}_2)(\mathbf{X}'_2\mathbf{X}_2)^{-1/2}.$$

In the case $\{r = p - 1, s = 1\}$, $\mathbf{X}_2 = \mathbf{x}_p$ is a $n \times 1$ vector and the partitioned design $\mathbf{X} = [\mathbf{X}_1, \mathbf{x}_p]$ has $\det(\mathbf{R}) = 1 - [\mathbf{x}'_p\mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^{-1}\mathbf{X}'_1\mathbf{x}_p]/(\mathbf{x}'_p\mathbf{x}_p)$. From standard facts for the inverse of a partitioned matrix, for example, Myers (1990, p. 459), $VIF_p = [\mathbf{R}^{-1}]_{p,p} = [\mathbf{D}_{(p-1,1)}^{-1}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{D}_{(p-1,1)}^{-1}]_{p,p}$ can be computed directly as

$$\begin{aligned} (\mathbf{x}'_p\mathbf{x}_p)^{1/2}(\mathbf{X}'\mathbf{X})^{-1}_{p,p}(\mathbf{x}'_p\mathbf{x}_p)^{1/2} &= \frac{\mathbf{x}'_p\mathbf{x}_p}{\mathbf{x}'_p\mathbf{x}_p - \mathbf{x}'_p\mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^{-1}\mathbf{X}'_1\mathbf{x}_p} \\ &= \frac{1}{1 - [\mathbf{x}'_p\mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^{-1}\mathbf{X}'_1\mathbf{x}_p]/(\mathbf{x}'_p\mathbf{x}_p)} \\ &= \frac{1}{\det(\mathbf{R})} = GVIF(\mathbf{X}_2|\mathbf{X}_1). \end{aligned}$$

We study the eigenvalue structure of $\mathbf{M}_{(r,s)}$ in Appendix 1. Let $\{\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{\min(r,s)} \geq 0\}$ be the non-negative singular values of $(\mathbf{X}'_1\mathbf{X}_1)^{-1/2}(\mathbf{X}'_1\mathbf{X}_2)(\mathbf{X}'_2\mathbf{X}_2)^{-1/2}$. It is shown in Appendix 1 that an alternative formulation for *GVIF* is

$$GVIF(\mathbf{X}_2|\mathbf{X}_1) = \prod_{i=1}^{\min(r,s)} (1 - \lambda_i^2)^{-1}. \tag{4}$$

4. Quadratic model with $p = 3$

For the partitioning $\mathbf{X} = [\mathbf{X}_r|\mathbf{X}_s]$, the canonical moment matrix, Equation 3, has the identity matrices $\mathbf{I}_r, \mathbf{I}_s$ down the diagonal and off-diagonal array $(\mathbf{X}'_1\mathbf{X}_1)^{-1/2}\mathbf{X}'_1\mathbf{X}_2(\mathbf{X}'_2\mathbf{X}_2)^{-1/2}$. For the quadratic model $y = \beta_0 + \beta_1x + \beta_2x^2$ and partitioning $\mathbf{X} = [\mathbf{1}, \mathbf{x}|\mathbf{x}^2]$, we have

$$\mathbf{R} = \begin{bmatrix} 1 & 0 & \rho_1 \\ 0 & 1 & \rho_2 \\ \rho_1 & \rho_2 & 1 \end{bmatrix}.$$

From Equation 4, $GVIF(\mathbf{x}^2|\mathbf{1}, \mathbf{x}) = (1 - \lambda^2)^{-1}$ where $\lambda = \sqrt{\rho_1^2 + \rho_2^2}$ is the unique positive singular value of $[\rho_1, \rho_2]'$. Denote

$$\gamma_x^2 = \rho_1^2 + \rho_2^2$$

as the *canonical index* with $GVIF(\mathbf{x}^2|\mathbf{1}, \mathbf{x}) = \frac{1}{1 - \gamma_x^2} = \frac{1}{\det(\mathbf{R})}$. Surprisingly, many higher order designs also have the off-diagonal entry of the canonical moment matrix with a unique positive singular value with $GVIF(\mathbf{X}_2|\mathbf{X}_1) = \frac{1}{1 - \gamma_x^2}$ with the collinearity between the lower order terms and the upper order terms as a function of the canonical index γ_x^2 .

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

In this section, we compare the central composite design (CCD) \mathbf{X} of Box and Wilson (1951) and the factorial design \mathbf{Z} . The design points are shown in Table B1 of Appendix 2. Both designs are 9×6 and use the quadratic response model

$$y = \beta_0 + \beta_1X_1 + \beta_2X_2 + \beta_{11}X_1^2 + \beta_{22}X_2^2 + \beta_{12}X_1X_2 + \varepsilon.$$

The CCD traditionally uses the value $a = \sqrt{2}$ in four entries, while the factorial design uses the value $a = 1$. To study the difference in the designs with these different values, we computed the *GVIF* to compare the “orthogonality” between the lower order terms \mathbf{X}_1 of dimension 9×3 and the higher order quadratic terms \mathbf{X}_2 of dimension 9×3 . The off-diagonal $\mathbf{B}_{3 \times 3}$ entry of \mathbf{R} from Equation 3 in Section 3 has the form

$$\mathbf{B}_{3 \times 3} = \begin{bmatrix} \rho_1 & \rho_2 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Table 1. CCD with parameter a , canonical index γ_x^2 , and *GVIF*

a	γ_x^2	$GVIF(\mathbf{X}_2 \mathbf{X}_1)$
0.000	0.44444	1.800
1.000	0.80000	5.000
1.500	0.8858	8.758
$\sqrt{2}$	0.8889	9.000
1.750	0.8514	6.729
∞	0.44444	1.800

with $\rho_1 = \rho_2 = \frac{2}{3} \frac{2+\alpha^2}{\sqrt{8+2\alpha^2}}$, canonical index $\gamma_X^2 = \rho_1^2 + \rho_2^2$ and $GVIF(\mathbf{X}_2|\mathbf{X}_1) = \frac{1}{1-\gamma_X^2}$ as in the quadratic model case with $p = 3$ shown in the Section 4. For Table 1, if $\alpha = 1$, then $\rho_1 = \rho_2 = 2/\sqrt{10}$, $\gamma_X^2 = 8/10$, and $GVIF(\mathbf{X}_2|\mathbf{X}_1) = 5$. Surprisingly, the classical choice of $\alpha = \sqrt{2}$ gives the largest value for $GVIF(\mathbf{X}_2|\mathbf{X}_1)$, 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

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

with n responses and with \mathbf{X} partitioned into $[\mathbf{X}_1|\mathbf{X}_2]$ with \mathbf{X}_1 the four lower order terms ($r = 4$) and \mathbf{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 B2 and B3, the Box and Behnken (1960) (*BBD*) design Table B4, and the CCD of Box and Wilson (1951) Table B5.

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 \mathbf{R} has only one non-zero singular value with its square the canonical index γ_X^2 . It follows that $GVIF(\mathbf{X}_2|\mathbf{X}_1) = \frac{1}{1-\gamma_X^2}$.

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 \mathbf{X} be the minimal design of Box and Draper (1974) *BDD* with $n = 11$ from Table B6, and let \mathbf{Z} be the small composite design of Hartley (1959) *SCD* with $n = 11$ from Table B7 for the quadratic response surface model ($r = 4$ and $s = 6$) as in Equation (5). Let $\alpha = \{\alpha_1 \geq \dots \geq \alpha_r \geq 0\}$ and $\beta = \{\beta_1 \geq \dots \geq \beta_r \geq 0\}$ be the non-negative singular values of the off-diagonal array for \mathbf{R}_X and \mathbf{R}_Z , respectively. As $\alpha_i \leq \beta_i (1 \leq i \leq r)$ (Table 3), it follows that $GVIF(\mathbf{X}_2|\mathbf{X}_1) \leq GVIF(\mathbf{Z}_2|\mathbf{Z}_1)$ showing less collinearity between the lower and higher order terms for the *BDD* design.

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

Design	n	r	γ_X^2	$GVIF(\mathbf{X}_2 \mathbf{X}_1)$
<i>H310</i>	11	4	0.8199	5.553
<i>H311B</i>	11	4	0.9091	11.00
<i>BBD</i>	13	4	0.9231	13.00
<i>CCD</i>	15	4	0.9333	15.00

Table 3. Singular values for off-diagonal array of \mathbf{R} for *BDD* and *SCD* with *GVIF*

	BDD		SCD
	0.9017		0.9535
$\alpha =$	0.3424	$\beta =$	0.6325
	0.3424		0.6325
	0.1877		0.6325
<i>GVIF</i> =	7.114		50.93

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 $(\mathbf{X}'_1\mathbf{X}_1)^{-1/2}(\mathbf{X}'_2\mathbf{X}_2)(\mathbf{X}'_2\mathbf{X}_2)^{-1/2}$ has multiple positive singular values. The Frobenius norm for a rectangular matrix $\mathbf{A}_{r \times s}$ is defined by $\|\mathbf{A}\|_F^2 = \sum_{i=1}^r \sum_{j=1}^s a_{ij}^2 = \text{trace}(\mathbf{A}'\mathbf{A})$. For a design matrix \mathbf{X} , we extend the definition of the *canonical index* with $\gamma_X^2 = \|\Lambda_{r \times s}\|_F^2$. Alternatively, $\gamma_X^2 = \text{trace}((\mathbf{X}'_2\mathbf{X}_2)^{-1}(\mathbf{X}'_2\mathbf{X}_1)(\mathbf{X}'_1\mathbf{X}_1)^{-1}(\mathbf{X}'_1\mathbf{X}_2))$ as in Equation 7.

We examine, in detail, the H310 design matrix $\mathbf{X}_{11 \times 10}$, Table B2 in Appendix 2, with our attention to the value of -0.1360 in row 2 for \mathbf{x}_3 . 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 γ_X^2 to determine an optimal value. For example, replacing the four entries which are 1.1736 with c_1 , we calculate the minimum value for $\gamma_X^2 = 0.8199$ with $c_1 = 1.1768$ denoted c_{\min} in Table 4. These values are within the four digit accuracy of the data. We performed a similar calculation with c_2 using the four entries which are 0.6386; with c_3 with the four entries which are -0.9273 ; with c_4 with the eight entries which are 1; and with c_5 with the single entry 1.2906. The original design has $\gamma_X^2 = 0.8199$. The entries in the H310 design are given to four significant digits. With this precision, the original design is nearly optimal with respect to the canonical index γ_X^2 for the first five entries in Table 4. The sixth entry of $c_6 = -0.1360$ was not optimal with $\gamma_X^2 = 0.8181$ with $c_{\min} = -0.01264$, a magnitude value smaller.

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 \mathbf{R} with its square the canonical index γ_X^2 . 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 $A(\mathbf{X}) = \text{tr}((\mathbf{X}'\mathbf{X})^{-1})$, $D(\mathbf{X}) = \det((\mathbf{X}'\mathbf{X})^{-1})$, and $E(\mathbf{X}) = \max\{\text{eigenvalues of } (\mathbf{X}'\mathbf{X})^{-1}\}$. The small relative changes Δ in the design criteria are shown in Table 5 in Column 4.

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 \mathbf{X} , the row containing the value $c_6 = -0.1360$.

Table 4. Optimal values c_{\min} for γ_X^2

Design entries						c_{\min}	γ_X^2
c_1	0.6386	-0.9273	1	1.2906	-0.1360	1.1768	0.8199
1.1736	c_2	-0.9273	1	1.2906	-0.1360	0.6356	0.8199
1.1736	0.6386	c_3	1	1.2906	-0.1360	-0.9303	0.8199
1.1736	0.6386	-0.9273	c_4	1.2906	-0.1360	0.9975	0.8199
1.1736	0.6386	-0.9273	1	c_5	-0.1360	1.2880	0.8199
1.1736	0.6386	-0.9273	1	1.2906	c_6	-0.0126	0.8181

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

	$c_6 = -0.1360$	$c_6 = -0.01264$	Δ
A	2.697	2.688	0.33%
D	0.1552×10^{-6}	0.1542×10^{-6}	0.64%
E	0.8611	0.8512	1.15%
γ_X^2	0.8199	0.8181	0.22%

9. Conclusions

The *VIF* measure the penalty for adding a non-orthogonal variable to a linear regression. The *VIF* can be computed as a ratio of determinant as in Equation 1. A similar ratio criterion was studied by Fox and Monette (1992) to measure the effect of adding a subset of new variables to a design and they dubbed it the generalized variance inflation factor *GVIF*, Equation 2. We have noted the relationship between *GVIF* and the singular values of the off-diagonal array in the canonical moment matrix and have used *GFIV* to study standard quadratic response designs. The *H310* design of Roquemor (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*.

Funding

The authors received no direct funding for this research.

Author details

Diarmuid O'Driscoll¹

E-mail: diarmuid.odriscoll@mic.ul.ie

Donald E. Ramirez²

E-mail: der@virginia.edu

¹ Department of Mathematics and Computer Studies, Mary Immaculate College, Limerick, Ireland.

² Department of Mathematics, University of Virginia, Charlottesville, VA, 22904, USA.

Citation information

Cite this article as: Response surface designs using the generalized variance inflation factors, Diarmuid O'Driscoll & Donald E. Ramirez, *Cogent Mathematics* (2015), 2: 1053728.

References

Belsley, D. A. (1986). Centering, the constant, first-differencing, and assessing conditioning. In E. Kuh & D. A. Belsley (Eds.), *Model reliability* (pp. 117–153). Cambridge: MIT Press.

Berk, K. (1977). Tolerance and condition in regression computations. *Journal of the American Statistical Association*, 72, 863–866.

Box, G. E. P., & Behnken, D. W. (1960). Some new three-level designs for the study of quantitative variables. *Technometrics*, 2, 455–475.

Box, M. J., & Draper, N. R. (1974). On minimum-point second order design. *Technometrics*, 16, 613–616.

Box, G. E. P., & Wilson, K. B. (1951). On the experimental attainment of optimum conditions. *Journal of the Royal Statistical Society, Series B*, 13, 1–45.

Eaton, M. L. (1983). *Multivariate statistics*. New York, NY: Wiley.

Fox, J., & Monette, G. (1992). Generalized collinearity diagnostics. *Journal of the American Statistical Association*, 87, 178–183.

Garcia, C. B., Garcia, J., & Soto, J. (2011). The raise method: An alternative procedure to estimate the parameters in presence of collinearity. *Quality and Quantity*, 45, 403–423.

Hartley, H. O. (1959). Smallest composite design for quadratic response surfaces. *Biometrics*, 15, 611–624.

Jensen, D. R. (1998). Principal predictors and efficiency in small second-order designs. *Biometrical Journal*, 40, 183–203.

Jensen, D. R., & Ramirez, D. E. (1993). Efficiency comparisons in linear inference. *Journal of Statistical Planning and Inference*, 37, 51–68.

Liao, D., & Valliant, R. (2012). Variance inflation in the analysis of complex survey data. *Survey Methodology*, 38, 53–62.

Myers, R. (1990). *Classical and modern regression with applications* (2nd ed.). Boston, MA: PWS-Kent.

O'Driscoll, D., & Ramirez, D. E. (in press). *Revisiting some design criteria* (under review).

Roquemor, K. G. (1976). Hybrid designs for quadratic response surfaces. *Technometrics*, 18, 419–423.

Stewart, G. W. (1987). Collinearity and least squares regression. *Statistical Science*, 2, 68–84.

Thiel, H. (1971). *Principles of econometrics*. New York, NY: Wiley.

Wichers, R. (1975). The detection of multicollinearity: A comment. *Review of Economics and Statistics*, 57, 366–368.

Willan, A. R., & Watts, D. G. (1978). Meaningful multicollinearity measures. *Technometrics*, 20, 407–412.

Appendix 1

We study the eigenvalue structure of $\mathbf{M}_{(r,s)}$. Let $\{\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{\min(r,s)} \geq 0\}$ be the non-negative singular values of $(\mathbf{X}'_1 \mathbf{X}_1)^{-1/2} (\mathbf{X}'_1 \mathbf{X}_2) (\mathbf{X}'_2 \mathbf{X}_2)^{-1/2}$.

As with the canonical correlation coefficients Eaton (1983), write the off-diagonal rectangular array $\mathbf{B}_{r \times s}$ of \mathbf{R} as $\mathbf{P}\mathbf{A}\mathbf{Q}'$ with \mathbf{P} and \mathbf{Q} orthogonal matrices and $\mathbf{A}_{r \times s}$ the rectangular diagonal matrix with the non-negative singular values down the diagonal. Set

$$\mathbf{L} = \begin{bmatrix} \mathbf{P}_{r \times r} & \mathbf{0}_{r \times s} \\ \mathbf{0}_{s \times r} & \mathbf{Q}_{s \times s} \end{bmatrix}.$$

For notational convenience, we assume $r \leq s$. The matrix \mathbf{L} is orthogonal and transforms $\mathbf{R} \rightarrow \mathbf{L}'\mathbf{R}\mathbf{L}$ into diagonal matrices:

$$\begin{bmatrix} \mathbf{I}_r & \mathbf{A}_{r \times s} \\ \mathbf{A}'_{s \times r} & \mathbf{I}_s \end{bmatrix} = \begin{bmatrix} \mathbf{I}_r & [\mathbf{S}\mathbf{V}_{r \times r} | \mathbf{0}_{r \times (s-r)}] \\ [\mathbf{S}\mathbf{V}'_{r \times r} | \mathbf{0}'_{r \times (s-r)}] & \mathbf{I}_s \end{bmatrix} \quad (A1)$$

with $\Lambda_{r \times s} = [SV_{r \times r} | 0_{r \times (s-r)}]$ where $SV_{r \times r}$ is the diagonal matrix of the non-negative singular values. Since \mathbf{L} is orthogonal, this transformation has not changed the eigenvalues. To compute the determinant of \mathbf{R} , convert the matrix in Equation 6 into an upper diagonal matrix by Gauss Elimination on $\Lambda'_{s \times r}$. This changes r of the 1's on the diagonal in rows $r + 1$ to $r + r$ into $1 - \lambda_i^2$, and thus $\det(\mathbf{R}) = \prod_{i=1}^{\min(r,s)} (1 - \lambda_i^2)$ with

$$GVIF(\mathbf{X}_2 | \mathbf{X}_1) = \prod_{i=1}^{\min(r,s)} \frac{1}{1 - \lambda_i^2}.$$

The singular values of $\mathbf{R}_{12} = (\mathbf{X}'_1 \mathbf{X}_1)^{-1/2} (\mathbf{X}'_1 \mathbf{X}_2) (\mathbf{X}'_2 \mathbf{X}_2)^{-1/2}$ are the non-negative square roots of the eigenvalues of $\Lambda' \Lambda$ denoted by

$$\begin{aligned} \text{eigvals}(\Lambda' \Lambda) &= \text{eigvals}((\mathbf{Q}' \mathbf{R}'_{12} \mathbf{P}) (\mathbf{P}' \mathbf{R}_{12} \mathbf{Q})) \\ &= \text{eigvals}((\mathbf{X}'_1 \mathbf{X}_1)^{-1} (\mathbf{X}'_1 \mathbf{X}_2) (\mathbf{X}'_2 \mathbf{X}_2)^{-1} (\mathbf{X}'_2 \mathbf{X}_1)). \end{aligned} \tag{A2}$$

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

$$\begin{bmatrix} \mathbf{I}_r & \Lambda_{r \times s} \\ \Lambda'_{s \times r} & \mathbf{I}_s \end{bmatrix}^{-1} = \begin{bmatrix} (\mathbf{I}_r - \Lambda_{r \times s} \Lambda'_{s \times r})^{-1} & -\Lambda_{r \times s} (\mathbf{I}_s - \Lambda'_{s \times r} \Lambda_{r \times s})^{-1} \\ -\Lambda'_{s \times r} (\mathbf{I}_r - \Lambda_{r \times s} \Lambda'_{s \times r})^{-1} & (\mathbf{I}_s - \Lambda'_{s \times r} \Lambda_{r \times s})^{-1} \end{bmatrix}$$

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

Appendix 2

Table B1. The lower order matrix for the CCD with center run with $a = \sqrt{2}$, $n = 9$ and the lower order matrix for the factorial design with center run $n = 9$

Central composite design			Factorial design		
1	x_1	x_2	1	x_1	x_2
1	1	1	1	1	1
1	1	-1	1	1	-1
1	-1	1	1	-1	1
1	-1	-1	1	-1	-1
1	a	0	1	1	0
1	$-a$	0	1	-1	0
1	0	a	1	0	1
1	0	$-a$	1	0	-1
1	0	0	1	0	0

Table B2. The lower order matrix for the hybrid (H310) design of Roquemore (1976) with center run, $n = 11$

1	x_1	x_2	x_3
1	0	0	1.2906
1	0	0	-0.1360
1	1	1	0.6386
1	1	-1	0.6386
1	-1	1	0.6386
1	-1	-1	0.6386
1	1.1736	0	-0.9273
1	-1.1736	0	-0.9273
1	0	1.1736	-0.9273
1	0	-1.1736	-0.9273
1	0	0	0

Table B3. The lower order matrix for the hybrid (H311B) design of Roquemore (1976) with center run, $n = 11$

1	x_1	x_2	x_3
1	0	0	2.4495
1	0	0	-2.4495
1	2.1063	0.7507	1
1	2.1063	-0.7507	-1
1	-2.1063	-0.7507	1
1	-2.1063	0.7507	-1
1	0.7507	2.1063	-1
1	0.7507	-2.1063	1
1	-0.7507	-2.1063	-1
1	-0.7507	2.1063	1
1	0	0	0

Table B4. The lower order matrix for the Box and Behnken (1960) design (BBD) with center run, $n = 13$

1	x_1	x_2	x_3
1	1	1	0
1	1	-1	0
1	1	0	1
1	1	0	-1
1	-1	1	0
1	-1	-1	0
1	-1	0	1
1	-1	0	-1
1	0	1	1
1	0	1	-1
1	0	-1	1
1	0	-1	-1
1	0	0	0

Table B5. The lower order matrix for the Box and Wilson (1951) CCD for $\alpha = 1.732$ with center run, $n = 15$

1	x_1	x_2	x_3
1	1	1	1
1	1	-1	-1
1	-1	1	-1
1	-1	-1	1
1	1.732	0	0
1	-1.732	0	0
1	0	1.732	0
1	0	-1.732	0
1	0	0	1.732
1	0	0	-1.732
1	0	0	0

Table B6. The lower order matrix for the Box and Draper (1974) minimal design (BDD) with center run, $n = 11$

1	x_1	x_2	x_3
1	1	-1	-1
1	-1	1	-1
1	-1	-1	1
1	-1	-1	-1
1	0.1925	0.1925	-1
1	0.1925	-1	0.1925
1	-1	0.1925	0.1925
1	-0.2912	1	1
1	1	-0.2912	1
1	1	1	-0.2912
1	0	0	0

Table B7. The Lower order matrix for the small composite design of Hartley (1959) (SCD) for $\alpha = 1.732$ with center run, $n = 11$

1	x_1	x_2	x_3
1	1	1	1
1	1	1	-1
1	1	-1	1
1	1	-1	-1
1	-1	1	1
1	-1	1	-1
1	-1	-1	1
1	-1	-1	-1
1	1.732	0	0
1	-1.732	0	0
1	0	1.732	0
1	0	-1.732	0
1	0	0	1.732
1	0	0	-1.732
1	0	0	0



© 2015 The Author(s). This open access article is distributed under a Creative Commons Attribution (CC-BY) 4.0 license.

You are free to:

Share — copy and redistribute the material in any medium or format

Adapt — remix, transform, and build upon the material for any purpose, even commercially.

The licensor cannot revoke these freedoms as long as you follow the license terms.

Under the following terms:

Attribution — You must give appropriate credit, provide a link to the license, and indicate if changes were made.

You may do so in any reasonable manner, but not in any way that suggests the licensor endorses you or your use.

No additional restrictions

You may not apply legal terms or technological measures that legally restrict others from doing anything the license permits.



Cogent Mathematics (ISSN: 2331-1835) is published by Cogent OA, part of Taylor & Francis Group.

Publishing with Cogent OA ensures:

- Immediate, universal access to your article on publication
- High visibility and discoverability via the Cogent OA website as well as Taylor & Francis Online
- Download and citation statistics for your article
- Rapid online publication
- Input from, and dialog with, expert editors and editorial boards
- Retention of full copyright of your article
- Guaranteed legacy preservation of your article
- Discounts and waivers for authors in developing regions

Submit your manuscript to a Cogent OA journal at www.CogentOA.com

