Comment on "A Note on Collinearity Diagnostics and Centering" by Velilla (2018)

Román Salmerón Gómez* **Catalina García García**† **Jose García Pérez**‡

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1 Introduction

Given the following basic model with n observations and m independent variables:

$$\mathbf{Y} = \mathbf{X} \cdot \boldsymbol{\beta} + \boldsymbol{\varepsilon}, \quad (1)$$

where $\mathbf{Y}$ is a vector $n \times 1$ that contains the observations of the dependent variable, $\mathbf{X}$ is a matrix $n \times m$ whose columns contain the observations of the independent variables and $\boldsymbol{\varepsilon}$ represents the random disturbance with $E(\boldsymbol{\varepsilon}) = 0$ and $cov(\boldsymbol{\varepsilon}) = \sigma^2 \boldsymbol{I}$ and the first column of matrix $\mathbf{X}$ is a vector of ones, that is, $\mathbf{X} = [\mathbf{1}\ \mathbf{X}_2 \dots \mathbf{X}_m]$, where $\mathbf{1} = (1\ 1 \dots 1)'_{n \times 1}$, several authors have contributed to the controversy surrounding the standardization of data when the model (1) presents a worrying degree of collinearity (Marquardt and Snee (1975), Smith and Campbell (1980), Marquardt (1980) Belsley et al. (1980), Belsley (1982), Vinod and Ullah (1981). Gunst (1984) noted that "one of the problems of centering data is to carefully consider whether it is important to detect collinearity with the constant term." In Marquardt's comment to the paper presented by Stewart (1987b), he stated: "I fully

*Professor, Department of Quantitative Methods for Economics and Business, Campus Universitario de la Cartuja 18071 Granada (Spain), University of Granada (e-mail: romansg@ugr.es).

†Professor, Department of Quantitative Methods for Economics and Business, Campus Universitario de la Cartuja 18071 Granada (Spain), University of Granada (e-mail: cbgarcia@ugr.es).

‡Professor, Department of Economic and Business, Carretera Sacramento, 04120, Almería (Spain), University of Almería, Spain (e-mail: jgarcia@ual.es).

agree with Stewart that when there is a constant term in the model, the model should be centered before the importance of the remaining variables is assessed and the centering simply shows the variable for what it is."

This discussion is extended to study how these transformations affect the traditionally applied measures to diagnose collinearity such as the variance inflator factor (VIF) and the condition number (CN) that are obtained from the following expressions, respectively:

$$VIF(\widehat{\beta}_i) = \frac{1}{1 - R^2_{X_i}}, \quad i = 2, \dots, m, \tag{2}$$

where $R^2_{X_i}$ is the coefficient of determination of the auxiliary regression

$$\mathbf{X}_i = \mathbf{X}_{-i} \cdot \boldsymbol{\alpha} + \boldsymbol{\nu}. \tag{3}$$

where $\mathbf{X}_i$ is explained as a function of the rest of the exogenous variables, $\mathbf{X}_{-i} = [\mathbf{1}\ \mathbf{X}_2 \dots \mathbf{X}_{i-1}\ \mathbf{X}_{i+1} \dots \mathbf{X}_m]$ (Theil (1971)), and

$$CN(\mathbf{X}) = \frac{\mu_{max}}{\mu_{min}}, \tag{4}$$

where μ_{max} and μ_{min} are the minimum and maximum singular values of matrix $\mathbf{X}$, respectively.

Recently, Velilla (2018a) studied the problem of centering for collinearity diagnostics and presented a new method for finding collinearity that combines an assessment of the role of the constant term. We agree with Christensen (2018) who, in a letter to editor, showed that the VIF calculation in Velilla's Equation (5) and its later extension to Equation (16) and (17) are problematic. Although, there was a reply in return Velilla (2018b), we consider the debate about an appropriate calculation for the variance inflation factor (VIF) to remain open. In our opinion, the following two questions should be considered:

1. García et al. (2016) showed that the VIF is invariant to origin and scale changes, which is the same as saying that the following two models present the same VIF:

$$\mathbf{Y} = \mathbf{X} \cdot \boldsymbol{\beta} + \boldsymbol{\varepsilon}, \quad \mathbf{Y} = \mathbf{x} \cdot \boldsymbol{\beta} + \boldsymbol{\varepsilon},$$

   where

$$\mathbf{x}_i = \frac{\mathbf{X}_i - a_i}{b_i} \tag{5}$$

   with $a_i \in \mathbb{R}$ and $b_i > 0$ for $i = 2, \dots, m$.

2. On the other hand, Salmerón et al. (2018) showed that “for $m = 2$, it is not possible to establish a relation between the variance inflation factors and the condition number due to the first always being equal to 1. This fact supports the claim that the VIF ignores relations between the exogenous variables and the constant term”. Thus, we conclude that VIF is not an appropriate measure to detect linear relations between the intercept and other explanatory variables (nonessential collinearity).

The expression of the VIF applied by Velilla (2018a) is based on the expression provided by Stewart (1987b) and does not verify the first question. For this reason, this paper analyzes the expression given by Stewart (1987b) finding that the indices of Stewart and the variance inflation factor only coincide when data present mean zero. Thus, the measure proposed by Velilla (2018a) will be appropriate to measure the relation between the intercept and the independent variables of the model. This paper contributes to clarifying the debate between Velilla (2018a) and Christensen (2018) by taking into consideration the two previous questions. After some preliminaries presented in Section 2, Section 3 analyzes the invariability of the VIF and Section 4 shows that the VIF is not able to detect the nonessential collinearity. Section 5 treats the indices of Stewart and, finally, Section 6 summarizes the main conclusions.

2 Preliminaries

Belsley (1984) suggests the establishment of a basic model where variables “are measured relative to an origin that affords structural interpretability”. Cook (1984) indicates that the collinearity should be measured in relation to a second model “to isolate the effects of collinearity or any other potential failing that may be of interest”. It is well known that the collinearity caused by the relation with the constant term is eliminated when centering the rest of the exogenous variables. This fact justifies the analysis of collinearity through the comparison of model (1) with the following model:

$$\mathbf{Y} = \tilde{\mathbf{X}} \cdot \boldsymbol{\beta} + \boldsymbol{\varepsilon}, \tag{6}$$

where $\tilde{\mathbf{X}} = [\mathbf{1} \ \tilde{\mathbf{X}}_2 \dots \tilde{\mathbf{X}}_m]$ with $\tilde{\mathbf{X}}_i = \mathbf{X}_i - \overline{\mathbf{X}}_i$ being $\overline{\mathbf{X}}_i$ the mean of variable $\mathbf{X}_i$ for $i = 2, \dots, m$. Note that this transformation is a particular case of those presented in expression 5, when $a_i = \overline{\mathbf{X}}_i$ and $b_i = 1$, that allows for the constant term to be orthogonal to the rest of the exogenous variables.

Finally, note that although the relation with the constant term is eliminated when centering the rest of the exogenous variables, it is possible that this transformation will not

Table 1: Estimation of models (1) and (6) presented by Belsley (1984) (estimation of the standard deviation in parenthesis)

Variable	Model (1)	Model (6)
Intercept	3.1918 (0.7844)	2.69915 (0.00124)
2	0.8095 (0.5545)	0.8095 (0.5545)
3	-1.3021 (0.5549)	-1.3021 (0.5549)
Condition Number	1341.692	1.000119

be interpretable. This question will not be addressed in this paper, but we only pretend to measure collinearity when comparing this model with the basic model (1).

Example 1 *Belsley (1984) presented an example to establish that "the centered estimates and their standards errors are unchanged. Clearly centering can in no way change, much less reduce, any inflated variances" and that "the centered-data estimates retain the same sensitivity and ill conditioning as the uncentered-data estimates despite the perfect conditioning of the centered data matrix".*

We consider that the conclusions obtained by Belsley (1984) are motivated by the fact that the two models that are compared are essentially the same. Thus, the basic model is compared to the same model but centered in relation to the mean, where the estimation of the constant term can be recovered from the means of the dependent and independent variables.

***In particular**, if we estimate models (1) and (6) for this same example (data can be found in Belsley (1984)), we obtain the results shown in Table 1. Note that the estimated coefficient of centered variables are unchanged and their estimated standard deviations or global characteristics such as the coefficient of determination, $R^2 = 0.31$, or the estimation of the variance of the random disturbance, $\widehat{\sigma} = 0.005546$, also remain constant. However, the estimation of the constant term changes, as does its estimated standard deviation that presents a relevant reduction.*

This example serves to highlight the relevance of selecting correctly a model as reference to measure the collinearity.

3 The invariability of the VIF

Considering the basic model (1) and expression (2) it is evident that:

$$R_{X_i}^2 = \frac{\sum\limits_{j=1}^{n} \left(\widehat{X}_{ji} - \overline{\mathbf{X}}_i \right)^2}{\sum\limits_{j=1}^{n} \left(X_{ji} - \overline{\mathbf{X}}_i \right)^2}. \tag{7}$$

On the other hand, in the case of model $\mathbf{Y} = \mathbf{x} \cdot \boldsymbol{\beta} + \boldsymbol{\varepsilon}$, where $\mathbf{x}_i = \frac{\mathbf{X}_i - a_i}{b_i}$ with $a_i \in \mathbb{R}$ and $b_i > 0$ for $i = 2, \dots, m$, VIF will be calculated from the following regression:

$$\mathbf{x}_i = \mathbf{x}_{-i} \cdot \boldsymbol{\alpha} + \boldsymbol{\nu}, \tag{8}$$

whose coefficient of determination is given by:

$$R_{x_i}^2 = \frac{\sum\limits_{j=1}^{n} \left(\widehat{x}_{ji} - \overline{\mathbf{x}}_i \right)^2}{\sum\limits_{j=1}^{n} \left(x_{ji} - \overline{\mathbf{x}}_i \right)^2} = \frac{\frac{1}{b_j^2} \cdot \sum\limits_{j=1}^{n} \left(\widehat{X}_{ji} - \overline{\mathbf{X}}_i \right)^2}{\frac{1}{b_j^2} \cdot \sum\limits_{j=1}^{n} \left(X_{ji} - \overline{\mathbf{X}}_i \right)^2} = R_{X_i}^2. \tag{9}$$

Since the coefficients of determination of regressions (3) and (8) coincide, the VIF values obtained from them are also the same. Thus, as centering is a particular case of the transformation proposed ($a_i = \overline{\mathbf{X}}_i$ and $b_i = 1$), the VIFs obtained from models (1) and (6) coincide.

4 The VIF does not detect the nonessential collinearity

Marquandt and Snee (1975), Marquandt (1980) and Snee and Marquardt (1984) refer to nonessential multicollinearity that is caused by the relation with the independent term. This section shows that the VIF is unable to detect this kind of collinearity.

Following Salmerón et al. (2018) when $m = 2$, the basic model (1) is given by:

$$\mathbf{Y} = \beta_1 \cdot \mathbf{1} + \beta_2 \cdot \mathbf{X}_2 + \boldsymbol{\varepsilon},$$

and the auxiliary regression to calculate the VIF is expressed as $\mathbf{X}_2 = \alpha \cdot \mathbf{1} + \boldsymbol{\nu}$, where it is verified that $\widehat{\alpha} = \overline{\mathbf{X}}_2$ and, consequently, in the auxiliary regression, the sum of squares of the residuals (SSR) and totals (SST) coincide:

$$SSR = \sum_{j=1}^{n} (X_{j2} - \overline{\mathbf{X}}_2)^2 = SST$$

.

In this case, it is always verified that, regardless of the dataset, the coefficient of determination of the auxiliary regression is equal to 0, and consequently, the corresponding VIF will be also equal to 1. In conclusion, the VIF is unable to detect the possible linear relation between $\mathbf{X}_2$ and the constant term. The extension to the general case ($m > 2$) is immediate.

5 Stewart index

Parting from the invariability of VIF (raised in question a) and developed in section 3), we agree with Christensen (2018) that expression (17) of Velilla (2018a) is problematic, since both VIFs should coincide, as shown in García et al. (2016). Indeed, the application of the VIF that Velilla (2018a) proposed to analyze the role of the constant term in a model with collinearity is not possible when taking into account question b) developed in section 4.

In order to clarify this question, the following subsections analyze the expression and properties of the VIF used in Velilla (2018a), concluding that it coincides with the VIF only if the variable $\mathbf{X}_i$ has a mean of zero.

5.1 Calculation and properties

Velilla (2018a)[Equation 5] presents the following expression to calculate the variance inflation factor:

$$VIF(\widehat{\beta}_i) = \frac{\mathbf{X}_i'\mathbf{X}_i}{\mathbf{X}_i' \cdot (\mathbf{I} - \mathbf{H}_{(i)}) \cdot \mathbf{X}_i}, \quad i = 1, \dots, m, \tag{10}$$

where $\mathbf{I}$ is the identity matrix, and $\mathbf{H}_{(i)}$ is the orthogonal projection matrix onto space spanned by the constant.

Comparing expressions (2) and (10), **only the second** can be calculated for $i = 1$. **Taking into account the well known formula for the inversion of a partitioned**

matrix, note that expression (10) comes from the index of collinearity defined by Stewart (1987a):

$$k_i = \left[\left(\mathbf{X}'\mathbf{X} \right)^{-1} \right]_{ii} \cdot \left(\mathbf{X}'\mathbf{X} \right)_{ii}, \quad i = 1, \dots, m, \tag{11}$$

where $\left[\left(\mathbf{X}'\mathbf{X} \right)^{-1} \right]_{ii}$ is the element i of the main diagonal of $\left(\mathbf{X}'\mathbf{X} \right)^{-1}$ and $\left(\mathbf{X}'\mathbf{X} \right)_{ii}$ is the element i of the main diagonal of $\mathbf{X}'\mathbf{X}$.

Note that $k_i = 1$ if $|\mathbf{X}'\mathbf{X}| = |\mathbf{X}'_{-i}\mathbf{X}_{-i}| \cdot \mathbf{X}'_i\mathbf{X}_i$, due to $\left[\left(\mathbf{X}'\mathbf{X} \right)^{-1} \right]_{ii} = \frac{|\mathbf{X}'_{-i}\mathbf{X}_{-i}|}{|\mathbf{X}'\mathbf{X}|}$ and $\left(\mathbf{X}'\mathbf{X} \right)_{ii} = \mathbf{X}'_i\mathbf{X}_i$, where $|\cdot|$ denotes the determinant of a matrix. **Moreover,** $|\mathbf{X}'\mathbf{X}| = |\mathbf{X}'_{-i}\mathbf{X}_{-i}| \cdot |\mathbf{X}'_i\mathbf{X}_i - \mathbf{X}'_i\mathbf{X}_{-i} \cdot \left(\mathbf{X}'_{-i}\mathbf{X}_{-i} \right)^{-1} \cdot \mathbf{X}'_{-i}\mathbf{X}_i|$, that is, $k_i = 1$ if $\mathbf{X}'_i\mathbf{X}_{-i} = \mathbf{0}$, where $\mathbf{0}$ is a vector of zeros.

Thus, with the index given by expression (11), it is possible to measure the orthogonality between $\mathbf{X}_i$ and $\mathbf{X}_{-i}$, but it does not imply that $\mathbf{X}_i$ is uncorrelated with variables in $\mathbf{X}_{-i}$ unless this last matrix has a column of ones. In our case, since the proposed basic model (1) contains a constant term, the value of $k_i = 1$ does imply that $\mathbf{X}_i$ is uncorrelated with the rest of the exogenous variables of the model.

5.2 Relation with the VIF

The index k_i is identified by Stewart as the VIF as follows: "Since our collinearity indices (or rather their squares) are already present in the statistics literature as variance inflation factors, the introduction of new nomenclature requires some justification"; additionally, in this same way, the index is reproduced in Velilla (2018a), "Stewart (1987) defined a set of collinearity indices of the form $(1 - R_j^2)^{-1/2}$, $j = 1, \dots, p$, that is related to the $VIF(\widehat{\alpha}_j)$ of (6)". The consideration of the Stewart indices as VIFs has been wrongly reproduced in the scientific literature since its initial presentation. We have only found a reference in Jensen and Ramírez (2013) that dedicated a remark to state that "the label Variance Inflation Factors is a misnomer", but they maintain the familiar notation without further consideration.

However, since expression (11) can be rewritten as:

$$k_i = \frac{\mathbf{X}_i^t\mathbf{X}_i}{\mathbf{X}_i^t\mathbf{X}_i - \mathbf{X}_i^t\mathbf{X}_{-i} \left(\mathbf{X}_{-i}^t\mathbf{X}_{-i} \right)^{-1} \mathbf{X}_{-i}^t\mathbf{X}_i}, \quad i = 1, \dots, m, \tag{12}$$

for $i = 2, \dots, m$, it is possible to conclude that:

- $\mathbf{X}_i^t \mathbf{X}_i = SST_i + n \cdot \overline{\mathbf{X}}_i^2$, where SST_i is the total sum of squares of regression (3), and
- $\mathbf{X}_i^t \mathbf{X}_i - \mathbf{X}_i^t \mathbf{X}_{-i} \left(\mathbf{X}_{-i}^t \mathbf{X}_{-i} \right)^{-1} \mathbf{X}_{-i}^t \mathbf{X}_i = SSR_i$ is the residual sum of squares of the same regression.

Then, taking into account the expression of the VIF given in (2), the expression (12) can be rewritten as:

$$k_i = \frac{SST_i}{SSR_i} + n \cdot \frac{\overline{\mathbf{X}}_i^2}{SSR_i} = VIF(\widehat{\beta}_i) + n \cdot \frac{\overline{\mathbf{X}}_i^2}{SSR_i}, \quad i = 2, \dots, m. \tag{13}$$

From expression (13), it is evident that Equation (5) given in Velilla (2018a) coincides with the VIF only if the variable $\mathbf{X}_i$ has a mean of zero. We consider that the problematic aspects of Velilla's Equations (16) and (17) appear to be due to the transformation proposed by Velilla's equation (9), which does not guarantee that the variables are transformed to have means of zero.

Finally, note that it is evident that expression (13) is not invariant to origin or scale changes. Thus, for example, in the model (6) where the constant term is orthogonal to the rest of exogenous variables, k_i coincides with the VIF.

Example 2 *Considering the dataset of Example 1 of Velilla (2018a) known as Cheddar Cheese taste data about the contribution of three chemicals (acetic, A, hydrogen sulfide, H, and lactic acid, L) to a response variable taste, T, the following models are estimated:*

Model 1 $: T = \beta_1 + \beta_2 \cdot A + \beta_3 \cdot H + \beta_4 \cdot L + u,$

Model 2 $: T = \beta_1 + \beta_2 \cdot \tilde{A} + \beta_3 \cdot H + \beta_4 \cdot L + u,$

Model 3 $: T = \beta_1 + \beta_2 \cdot \tilde{A} + \beta_3 \cdot \tilde{H} + \beta_4 \cdot L + u,$

Model 4 $: T = \beta_1 + \beta_2 \cdot \tilde{A} + \beta_3 \cdot \tilde{H} + \beta_4 \cdot \tilde{L} + u,$

where $\tilde{\cdot}$ denotes the corresponding centered variable.

From Table 2, it is possible to conclude the following:

- *In Model 1, the VIFs indicate that the collinearity is not worrying contrarily to the condition number. This apparent contradiction is a symptom that the existing collinearity resides in the relationship between the constant term and the rest of the exogenous variables because VIF is unable to detect the nonessential collinearity (section 4).*

Table 2: Analysis of models 1 to 4 (significantly nonzero coefficients in bold are highlighted. The standard deviation estimates are in parentheses.)

	Model 1			Model 2		
Variable	Estimation	k_i	$VIF(\widehat{\beta}_i)$	Estimation	k_i	$VIF(\widehat{\beta}_i)$
Intercept	-28.8768 (19.7354)	113.85039		**-27.0748** (11.5433)	38.949301	
Acetic	0.3277 (4.4598)	177.57494	1.831589	0.3277 (4.4598)	1.831589	1.831589
Hydrogen	**3.9118** (1.2484)	18.07648	1.9922	**3.9118** (1.2484)	18.07648	1.9922
Lactic	**19.6705** (8.6291)	47.1962758	1.937912	**19.6705** (8.6291)	47.1962758	1.937912
Condition Number		33.13441			15.22255	

	Model 3			Model 4		
Variable	Estimation	k_i	$VIF(\widehat{\beta}_i)$	Estimation	k_i	$VIF(\widehat{\beta}_i)$
Intercept	-3.8316 (12.5798)	46.258363		**24.533** (1.8496)	1	
Acetic	0.3277 (4.4598)	1.831589	1.831589	0.3277 (4.4598)	1.831589	1.831589
Hydrogen	**3.9118** (1.2484)	1.9922	1.9922	**3.9118** (1.2484)	1.9922	1.9922
Lactic	**19.6705** (8.6291)	47.1962758	1.937912	**19.6705** (8.6291)	1.937912	1.937912
Condition Number		13.74528			2.519039	

- *The values provided by Velilla (2018a)[Example 2] as the VIF associated to each variable are really the values of k_i for $i = 2, 3, 4$.*

- *The transformations proposed in the different **models** do not modify the estimation and inference of centered variables or the global characteristics of the model ($R^2 = 0.6518$, $\widehat{\sigma} = 10.13$). However, the estimation and inference of the constant term are modified. Note that the estimated standard deviation associated to the constant term decreases with the centering of the variables. This behavior was expected since the constant term is responsible for the approximate collinearity existing in the model.*

- *Note that the VIF is invariant to the transformations (as shown in section 3), while k_i, for $i = 2, 3, 4$, changes as the variables are centered becoming the VIF.*

- *In Model 4 (where the constant term is orthogonal to the rest of the exogenous variables), the index of Stewart associated to the constant term, k_1, is equal to 1. This fact shows that the linear relation between the constant term and the rest of the exogenous variables was eliminated.*

- *The conclusions obtained in Model 4 from the VIF and the condition number are similar.*

6 Conclusion

We consider that this contribution clarifies the debate between Christensen (2018) and Velilla (2018b) concerning the appropriate calculation for variance inflation factors (VIF). Thus, we conclude that the doubts raised by Christensen (2018) in relation to expressions (16) and (17) of Velilla (2018a) are due to the measure used by Velilla (2018a) as VIF is not really VIF because the transformation indicated in (9) by Velilla (2018a) does not imply that the exogenous variables present a zero mean.

In addition, we found the proposal of Velilla (2018a) appropriate to detect collinearity between the intercept and the independent variables by replacing the identification of the VIF with the notation of the index of collinearity given by Stewart, k_i.

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