

## Supplementary Material

# An overview of variance-based importance measures in the linear regression context: comparative analyses and numerical tests

## Supplementary Material A: Equivalence between the LMG measures and the standardized Johnson indices for the case of two variables

The equivalence between the LMG and the standardized Johnson indices in dimension two is proved with a different demonstration from the one of Thomas et al. (2014) which relies on geometrical arguments.

**Proposition 1.** *If  $d=2$ , the LMG and the standardized Johnson indices are equal:*

$$J_j^{*2} = \text{LMG}_j \text{ for } j = 1, 2.$$

*Proof.* The correlation matrix  $\mathbf{R}_{X,X}$  is given by:

$$\mathbf{R}_{X,X} = \mathbf{W}^{*2} = \begin{pmatrix} w_{11}^{*2} + w_{12}^{*2} = 1 & w_{12}^{*2}(w_{11}^{*2} + w_{22}^{*2}) \\ w_{12}^{*2}(w_{11}^{*2} + w_{22}^{*2}) & w_{12}^{*2} + w_{22}^{*2} = 1 \end{pmatrix}$$

The standardized Johnson index associated with the input  $X_1$  (resp.  $X_2$ ) is given according to the Eq. (32) by:

$$J_j^{*2} = [\alpha_1^{*2} w_{11}^{*2} + \alpha_2^{*2} w_{21}^{*2}]$$

With  $\alpha_i^* = \beta_1^* w_{i1}^* + \beta_2^* w_{i2}^*$  for  $i \in \{1, 2\}$ . We then have:

$$J_1^{*2} = [(\beta_1^* w_{11}^* + \beta_2^* w_{12}^*)^2 w_{11}^{*2} + (\beta_1^* w_{21}^* + \beta_2^* w_{22}^*)^2 w_{21}^{*2}] \quad (33)$$

Because the singular values involved in Eq. (21) are positive, the diagonal elements of  $\mathbf{W}$  and  $\mathbf{W}^*$  are also positive. Using Eq. (26), we thus have  $w_{11}^* = w_{22}^* = \sqrt{1 - w_{12}^{*2}}$  and after several simplifications, Eq. (33) becomes:

$$J_1 = [\beta_1^{*2} + 2\beta_1^* \beta_2^* w_{12}^* w_{11}^* + 2w_{11}^{*2} w_{12}^{*2} (\beta_2^{*2} - \beta_1^{*2})]$$

Knowing that, with standardized variables:

$$\begin{aligned} b_1 &= \beta_1 \sigma_1 = \beta_1^* \sigma_Y, \\ b_2 &= \beta_2 \sigma_2 = \beta_2^* \sigma_Y, \\ r &= 2w_{12}^* w_{11}^*, \end{aligned}$$

We find that:

$$J_1^* = \sigma_Y^{-2} \left[ b_1^2 + b_1 b_2 r + \frac{r^2}{2} (b_2^2 - b_1^2) \right].$$

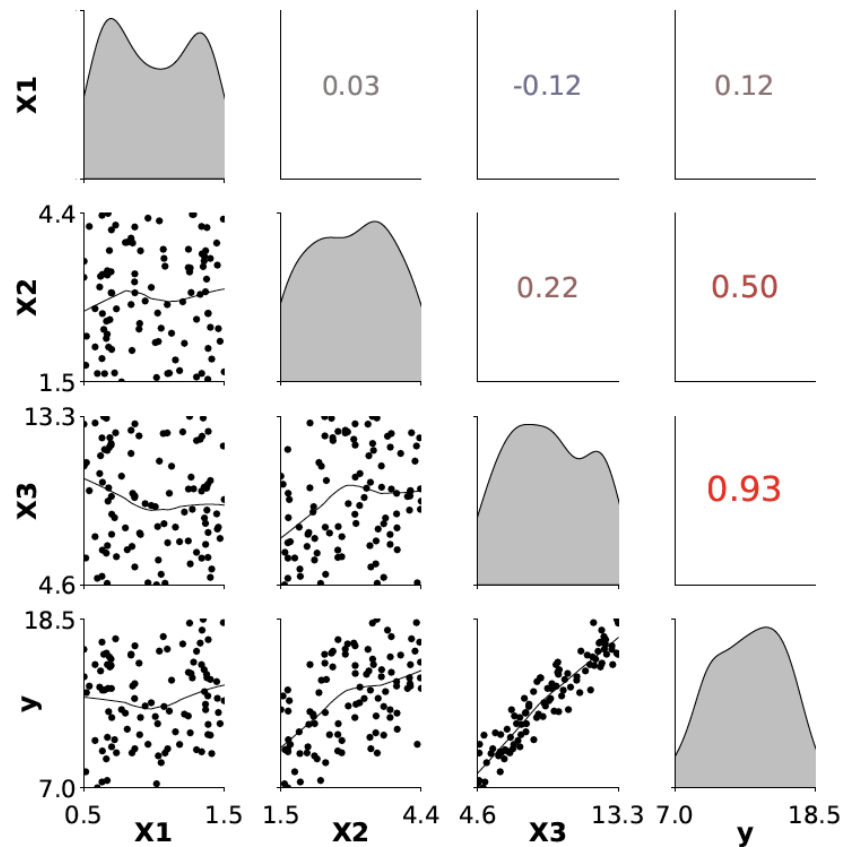
And finally with Eqs. (17):

$$J_1^* = \text{LMG}_1 \text{ (and similarly, } J_2^* = \text{LMG}_2).$$

## Supplementary Material B: Pair plots and results tables on the public datasets

This appendix gives results tables and pair plots on the previous public datasets presented in Section 7. The pair plots provide in the upper panel the CC of each variables' pair, in the diagonal panel the kernel density estimation (or the histogram) of each variable marginal and in the lower panel the scatter plots and fitted smoothers of each variables' pair.

### B.1. Independent inputs' case

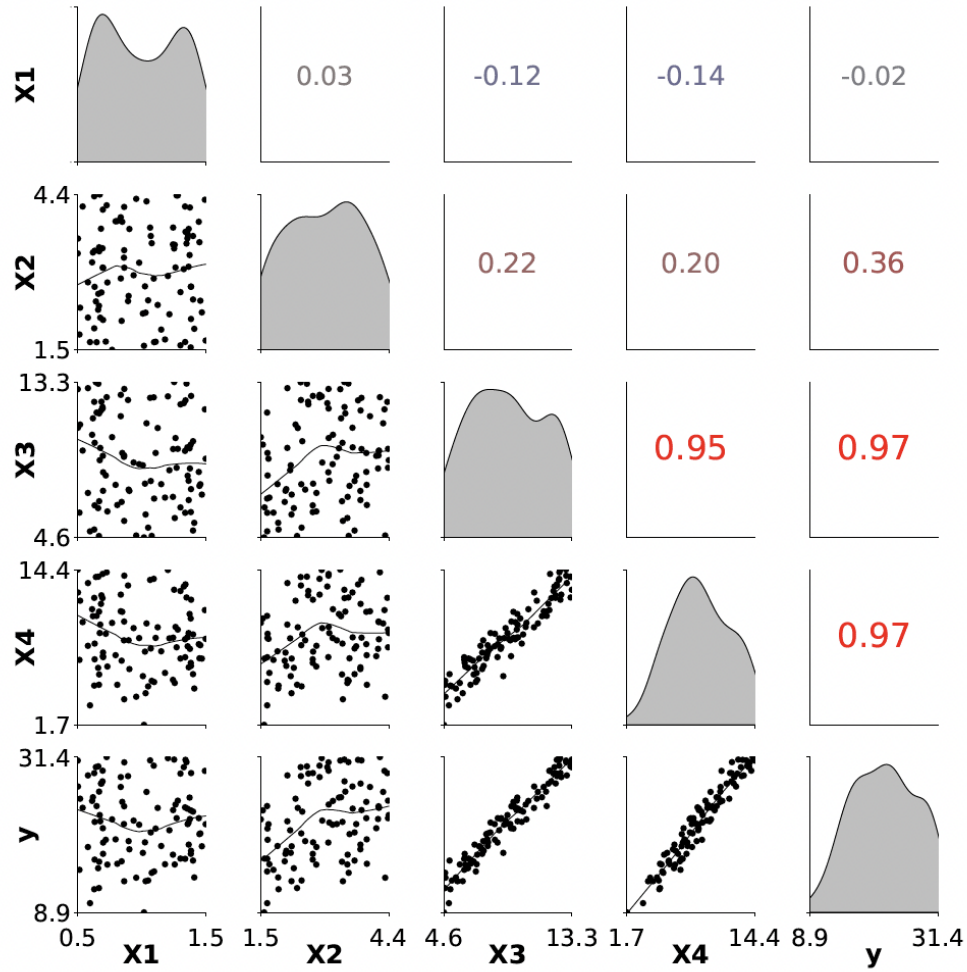


**Figure S1:** Data pairs plot for the independent inputs' case providing: the variable histograms (diagonal), and for each variable pair, the CC (upper panel), as well as scatter plots and fitted smoothers (lower panel).

**Table S1: Metrics and VIMs for the independent inputs' case. All indices are in %.**

Input	PCC <sup>2</sup>	SPCC <sup>2</sup>	SRC <sup>2</sup>	LMG	Johnson	PMVD
$X_1$	98.7	4.49	4.57	3.0	3.01	4.56
$X_2$	99.3	8.20	8.66	16.7	16.61	10.47
$X_3$	99.9	73.94	79.16	80.3	80.32	84.91
Sum	298.0	86.62	92.39	99.9	99.94	99.94

## B.2. Collinear case

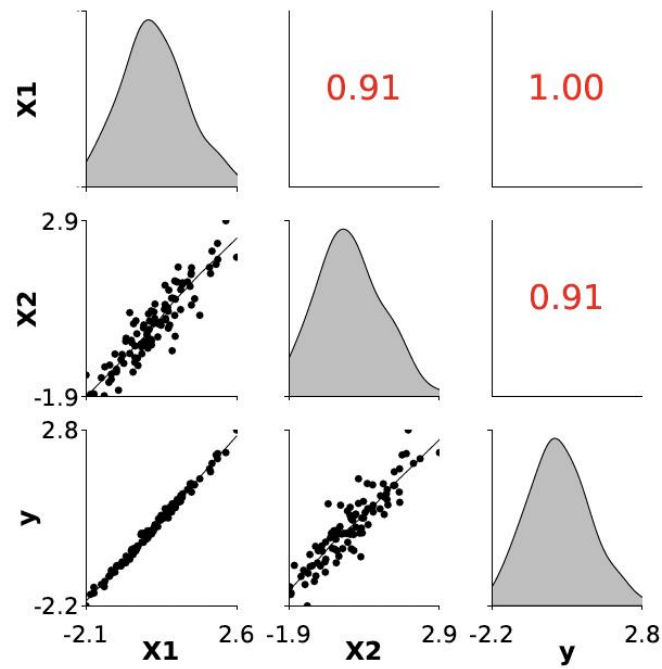


**Figure S2:** Data pairs plot providing: the variable histograms (diagonal), and for each variable pair, the CC (upper panel), as well as scatter plots and fitted smoothers (lower panel).

**Table S2:** Metrics and VIMs for the collinear case data. All indices are in %.

Input	PCC <sup>2</sup>	SPCC <sup>2</sup>	SRC <sup>2</sup>	LMG	Johnson	PMVD
X <sub>1</sub>	98.8	1.16	1.19	0.81	0.62	1.19
X <sub>2</sub>	99.3	2.12	2.24	5.81	6.28	2.63
X <sub>3</sub>	99.3	2.09	19.85	46.52	46.16	45.92
X <sub>4</sub>	99.5	3.00	28.39	46.85	46.92	50.24
Sum	396.9	8.36	51.67	99.99	99.99	99.99

## B.2.1 Model with a dummy (not included in the model) correlated input

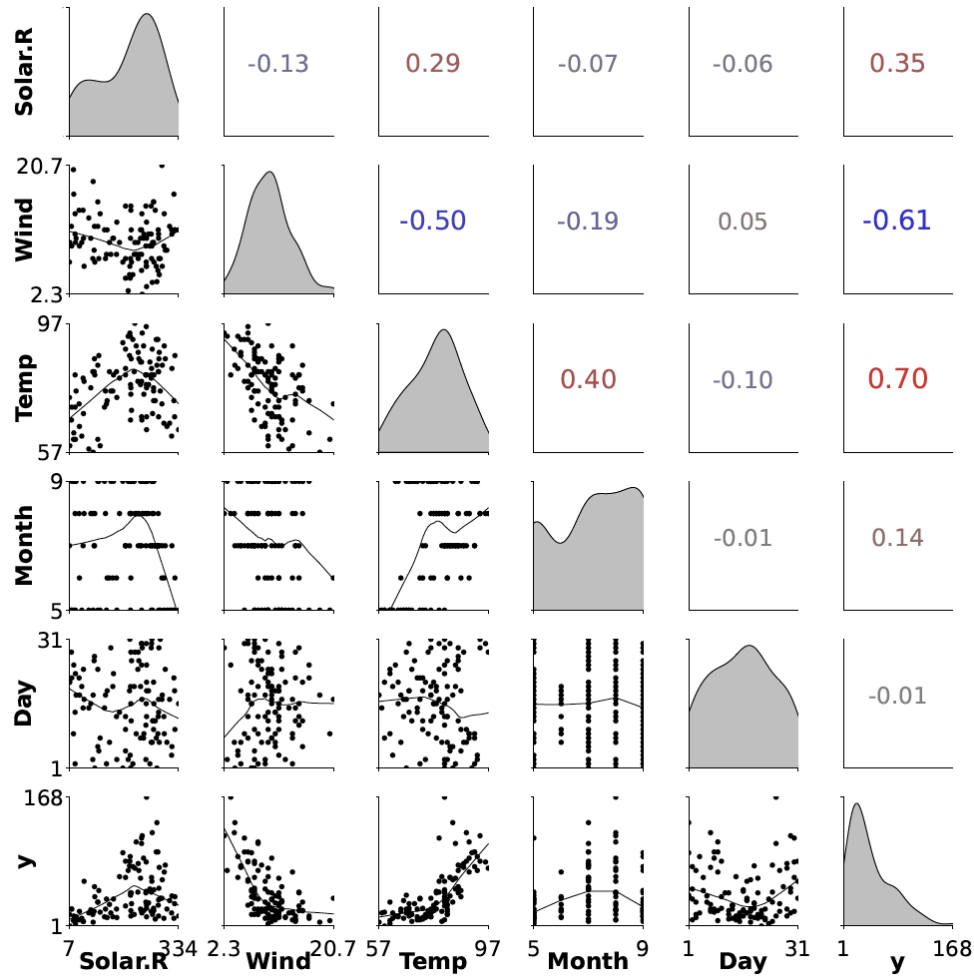


**Figure S3:** Data pairs plot providing: the variable histograms (diagonal), and for each variable pair, the CC (upper panel), as well as scatter plots and fitted smoothers (lower panel).

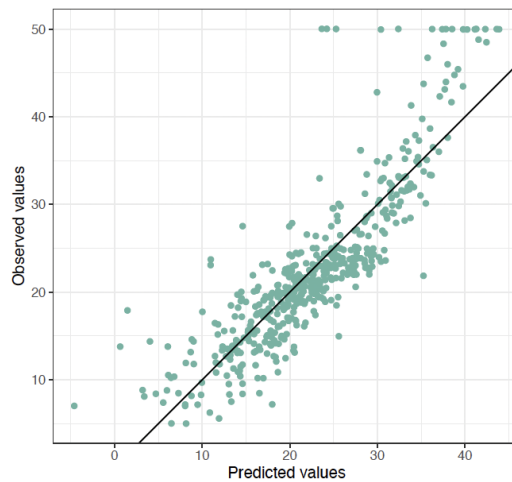
**Table S3:** Metrics and VIMs for the non-included correlated input model toy data. All indices are in %.

Input	PCC <sup>2</sup>	SPCC <sup>2</sup>	SRC <sup>2</sup>	LMG	Johnson	PMVD
$X_1$	95.67	17.01	102.86	58.1	58.1	99.19
$X_2$	0.84	0.01	0.04	41.1	41.1	0.04
Sum	96.50	17.01	102.90	99.2	99.2	99.2

### B.3. Public dataset on air quality



**Figure S4:** Data pairs plot for the air quality dataset providing: the variable histograms (diagonal), and for each variable pair, the CC (upper panel), as well as scatter plots and fitted smoothers (lower panel).

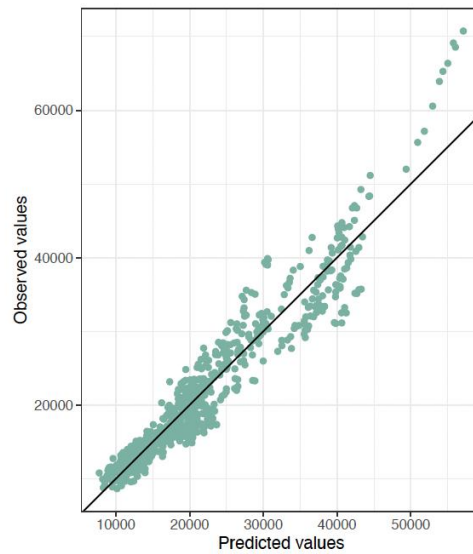


**Figure S5:** Linear model prediction vs. observation data for the air quality data:  $R^2 = 0.625$  and  $Q^2 = 0.582$ .

**Table S4: Metrics and VIMs for the air quality data. All indices are in %.**

Input	n°	PCC <sup>2</sup>	SPCC <sup>2</sup>	SRC <sup>2</sup>	LMG	Johnson	PMVD
Solar.R	1	4.20	1.65	1.90	6.30	6.49	2.65
Wind	2	20.16	9.47	12.59	22.33	22.91	18.25
Temp	3	31.33	17.11	29.48	31.96	31.28	39.37
Month	4	3.70	1.44	1.81	1.65	1.60	1.75
Day	5	1.34	0.51	0.51	0.26	0.22	0.48
Sum	6.47	60.73	30.18	46.29	62.49	62.49	62.49

#### B.4. Public dataset on cars prices data

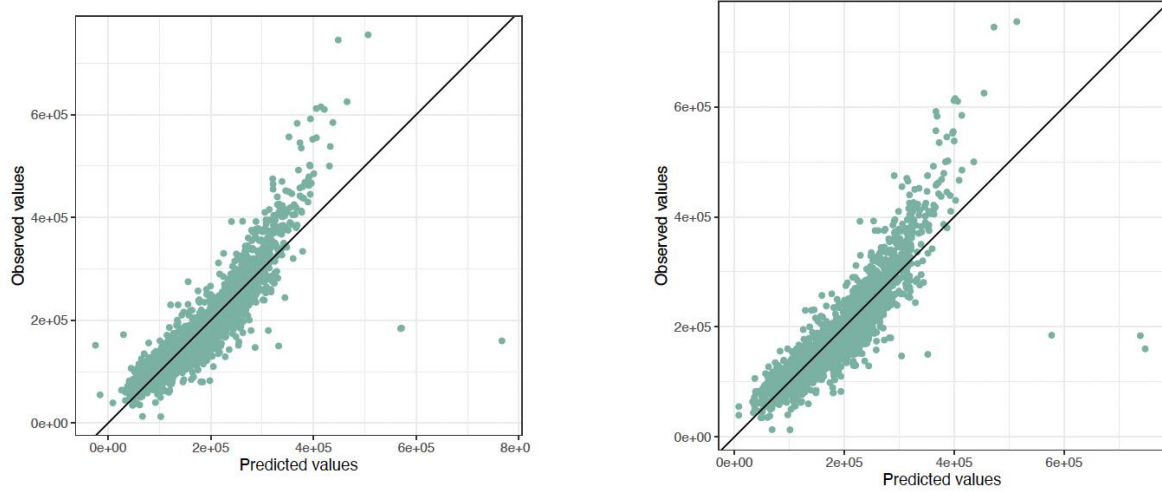
**Figure S6:** Linear model prediction vs. observation data for the cars data:  $R^2 = 0.915$  and  $Q^2 = 0.911$ .**Table S5: Metrics and VIMs for the cars data. All indices are in %. The last column gives the sense of variation of inputs with significantly influence (LMG > 1).**

Input	n°	PCC <sup>2</sup>	SPCC <sup>2</sup>	SRC <sup>2</sup>	LMG	Johnson	PMVD	Cor. sign
Mileage	1	21.42	2.31	2.33	2.25	2.24	2.15	-
Cylinder	2	56.92	11.22	26.39	21.20	21.96	25.65	+
Doors	-	4.43	0.39	1.82	1.22	1.07	0.37	+
Cruise	3	0.17	0.01	0.02	6.10	5.54	0.03	+
Sound	-	0.45	0.04	0.04	0.42	0.37	0.04	
Leather	-	1.26	0.11	0.13	1.35	1.41	0.11	+
Buick	-	0.37	0.03	0.08	0.84	0.86	0.18	+
Cadillac	4	36.70	4.92	16.39	22.40	22.58	29.57	+
Chevy	5	0.20	0.02	0.07	6.97	5.68	0.04	-
Pontiac	6	1.04	0.09	0.30	2.51	2.39	0.12	+
Saab	7	38.32	5.28	18.80	10.32	11.23	19.68	+
Convertible	8	34.40	4.45	7.26	13.16	12.95	12.16	+
Hatchback	-	12.10	1.17	2.86	1.70	1.93	0.76	-
Sedan	-	11.19	1.07	4.83	1.08	1.30	0.65	-
Sum		218.95	31.12	81.34	91.51	91.51	91.51	

## B.5. Ames housing dataset



**Figure S7:** Data pairs plot for the Ames housing dataset providing: the variable histograms (diagonal), and for each variable pair the CC (upper panel), as well as scatter plots and fitted smoothers (lower panel).



(a) With 34 inputs:  $R^2 = 0.799$  and  $Q^2 = 0.770$

(b) With 10 inputs:  $R^2 = 0.777$  and  $Q^2 = 0.769$

**Figure S8:** Linear model prediction vs. observation data for the Ames housing data.

**Table S6:** Metrics and VIMs for the Ames housing data considering 10 variables. All indices are in %.

Input	PCC <sup>2</sup>	SPCC <sup>2</sup>	SRC <sup>2</sup>	LMG	Johnson	PMVD
SecondFlrSF	16.58	4.43	13.46	6.84	6.31	11.54
FirstFlrSF	12.79	3.27	14.12	13.89	13.34	24.51
TotalBsmtSF	4.85	1.14	3.53	12.52	12.28	10.49
YearBuilt	4.12	0.96	1.97	8.56	8.60	8.38
YearRemodAdd	3.82	0.88	1.56	8.21	8.09	5.82
BedroomAbvGr	3.53	0.82	1.68	1.17	1.34	1.08
KitchenAbvGr	4.40	1.03	1.24	.161	1.60	1.45
MasVnrArea	3.15	0.72	0.98	7.12	6.73	2.49
TotRmsAbvGrd	0.69	0.16	0.64	6.42	7.65	0.54
GarageCars	5.18	1.22	2.22	11.37	11.76	11.41
Sum	59.10	14.62	41.40	77.70	77.70	77.70



**Table S7: Metrics and VIMs for the Ames housing data considering 34 variables. All indices are in %.**

Input	PCC <sup>2</sup>	SPCC <sup>2</sup>	SRC <sup>2</sup>	Johnson
LotFrontage	0.59	0.12	0.13	0.96
LotArea	0.39	0.08	0.10	1.42
YearBuilt	3.22	0.66	2.12	5.31
YearRemodAdd	4.53	0.94	1.79	6.05
MasVnrArea	2.51	0.51	0.72	5.23
BsmtFinSF1	0.02	0.00	0.01	0.45
BsmtFinSF2	0.35	0.07	0.08	0.09
BsmtUnfSF	0.86	0.17	0.54	0.97
TotalBsmtSF	4.30	0.89	4.31	8.18
FirstFlrSF	8.06	1.74	9.73	8.67
SecondFlrSF	10.08	2.22	11.50	4.20
LowQualFinSF	0.06	0.01	0.01	0.06
BsmtFullBath	0.42	0.08	0.18	1.93
BsmtHalfBath	0.01	0.00	0.00	0.06
FullBath	0.03	0.01	0.02	4.50
HalfBath	0.11	0.02	0.05	1.71
BedroomAbvGr	2.54	0.52	1.15	0.85
KitchenAbvGr	2.89	0.59	0.81	1.25
TotRmsAbvGrd	0.73	0.15	0.64	4.27
Fireplaces	1.07	0.21	0.33	4.42
GarageCars	0.47	0.09	0.54	6.07
WoodDeckSF	0.61	0.12	0.15	1.95
OpenPorchSF	0.00	0.00	0.00	1.40
EnclosedPorch	0.23	0.05	0.06	0.29
Threeseasonporch	0.00	0.00	0.00	0.03
ScreenPorch	0.88	0.17	0.19	0.52
PoolArea	0.38	0.08	0.08	0.07
MiscVal	2.14	0.43	0.45	0.26
MoSold	0.00	0.00	0.00	0.02
YearSold	0.11	0.02	0.02	0.05
Longitude	0.01	0.00	0.00	1.00
Latitude	1.34	0.27	0.32	1.77
<b>Sum</b>	<b>49.27</b>	<b>10.29</b>	<b>36.37</b>	<b>80.20</b>

## Supplementary Material C: Classification case

### Introduction

Several metrics and variance-based importance measures (VIMs) have been defined in the main paper in the classical linear regression context where the response (output) one tries to fit is a quantitative (often continuous) variable, while the predictors (inputs) can be either continuous quantitative variables or qualitative ones (but still, numerically valued). However, many practical applications deal with classification data, where the output is a categorical variable. In this supplementary material, by the way of the generalized linear model (GLM), we give extensions of metrics and VIMs to the linear logistic regression model. We deal with the case of a binary output, namely in the context of the linear logistic regression.

The structure of this supplementary material is as follows. Section C.1 reminds some basics about logistic regression model. Section C.2 develops the correlation ratio that is the correlation coefficient between an input and the binary output. Then, Section C.3 develops the Johnson indices in the logistic regression context. Finally, Section C.4 applies all the studied metrics on several simulated or public datasets. In this paper, the same acronyms and mathematical notations as those of the main paper are used.

#### C.1. The logistic regression model

In a classification problem, the output  $Y$  is no longer continuous (nor quantitative) but binary (e.g.  $Y \in \{0, 1\}$ ). The GLM (McCullagh & Nelder, 1989) allows considering a binomial distribution for  $Y$  and to perform a linear regression on a transformed output (by a so-called *link function*). For example, if  $p = p(X) = \mathbb{P}(Y = 1 | X)$ , the logistic regression model writes:

$$g(p) = \log\left(\frac{p}{1-p}\right) = X\beta. \quad (1)$$

It is usually called the “regression model on the link scale” and the link function  $g(p)$  is known as the “logit” transform. Other transforms such as the “probit” one can be used (McCullagh & Nelder, 1989).

Via the “inverse logit” transform  $p = [1 + \exp(-g(p))]^{-1}$ , the model in Eq. (1) returns probability values as predictions. In practice, to predict a binary value for the output, a threshold  $s \in ]0, 1]$  has to be defined and the following predictor is used:

$$\hat{Y}(x^*) = \mathbb{I}_{\{\hat{p}(x^*) \geq s\}}(x^*) \quad (2a)$$

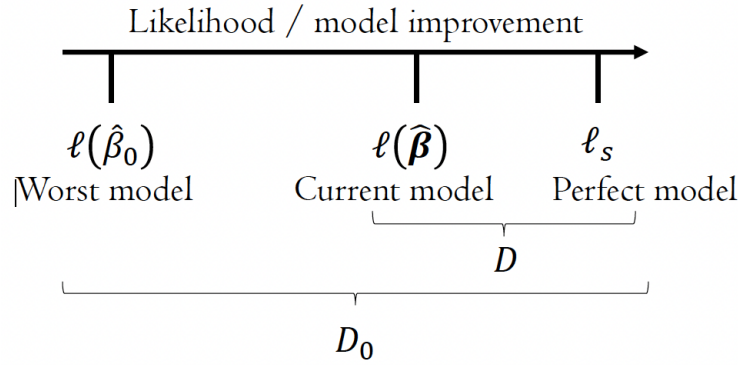
$$\text{with } \hat{p}(x^*) = [1 + \exp(x^* \hat{\beta})]^{-1}. \quad (2b)$$

**Remark 1.** The logistic regression parameters (i.e.  $\beta_i$ ,  $i = 0, \dots, d$  in Eq. (1)) are intrinsically interpretable, through an exponential transformation, as odds ratios. The quantity  $\exp(\beta_i)$  quantifies the marginal effect of  $X_i$  on the modeled probability  $p$ . The set of odds ratios, while providing an interpretable tool to quantify input importance in the sense of the marginal effect of a variable on the conditional probability, does not fall under the definition of an importance measure (IM) for linear models, and are thus out of the scope of this report. In the following, the focus is put on IM with respect to the linear link between the inputs and the quantity  $g(p)$ . These IMs are not directly interpretable with respect to the output of interest. IM on non-linear links between an output of interest and the inputs (see, e.g. Raguet & Marrel (2018); Marrel & Chabridon (2021)) are beyond the scope this report and will be described in other works. Here, we limit ourselves to the interpretation of  $g(p)$ , being aware that IMs are not directly linked to the classes of the output (but still highly correlated).

In order to validate the model in Eq. (1),  $R^2$  and  $Q^2$  have to be computed. Considering GLM, several metrics can be used (see, e.g., Zheng & Agresti (2000) for a review). A popular one is the following (Guisan & Zimmerman, 2000):

$$R^2 = 1 - \frac{D}{D_0}, \quad (3)$$

where  $D$  and  $D_0$  are, respectively, the *deviance* and the *null deviance*. Deviance can be seen as a generalization of the variance when the error distribution is non-Gaussian (as provided by the GLM). More precisely, the deviance is twice the difference in log-likelihood between the current model and a saturated model (i.e. a model that fits the data perfectly). As for the null deviance, it is a generalization of the total sum of squares of the linear model. Figure S9 provides an illustrative summary of how these two quantities are connected. Again, other coefficients of determination have been proposed for the logistic regression model (Tonidandel & LeBreton, 2010) but their study is beyond the scope of this report.



**Figure S9:** Illustration of deviance and null deviance for GLM validation (inspired from García-Portugués, 2021).

The  $Q^2$  estimation is usually computed from cross-validation residuals. As this formula also involves the variance of the observations on the link scale, we compute it by dividing the variance of the linear fits (on the link scale) by  $R^2$ .

In order to validate the model in Eq. (2a), several criteria are useful:

- If one considers that the important class to be predicted (e.g. typically the one which is critical regarding safety purposes) is “TRUE” ( $Y = 1$ ) and the other class is “FALSE” ( $Y = 0$ ), the confusion matrix distinguishes:
  - the number of true positive (TP):  $Y = 1$  and  $\hat{Y} = 1$ ;
  - the number of true negative (TN):  $Y = 0$  and  $\hat{Y} = 0$ ;
  - the number of false positive (FP):  $Y = 0$  and  $\hat{Y} = 1$ ;
  - the number of false negative (FN):  $Y = 1$  and  $\hat{Y} = 0$ .
- The error rate is the number of errors (false positive and false negative) divided by the number of observations:

$$\varepsilon = \frac{FP+FN}{n} \quad (4)$$

- The sensitivity is related to the important class to be predicted. It is the number of good predictions in this class divided by the number of observations in this class:

$$\tau = \frac{TP}{TP+FN}. \quad (5)$$

## C.2. Correlation coefficient with the binary output

In the classification context,  $Y$  is a binary variable which can be treated as a qualitative one. The analogue of CC when dealing with a qualitative  $Y$  (of any modalities) and one quantitative  $X_j$  (instead of two quantitative) variables is called the correlation ratio (CR). It writes (Saporta, 1990):

$$CR_j = \eta_{X_j|Y}^2 = \frac{\text{VAR}(\mathbb{E}[X_j|Y])}{\text{VAR}(X_j)} \quad (6)$$

where one can recognize a first-order Sobol' index (Sobol', 1993) formula. CR is also equivalent to the coefficient of determination ( $R^2$ ) of the linear regression explaining the quantitative variable by the qualitative one (Saporta, 1990).

Returning to the binary case for  $Y$ , from the sample  $(X_n, Y_n)$ , it can be easily estimated by:

$$\hat{\eta}_{X_j|Y}^2 = \frac{n_0 n_1}{n} \frac{(\bar{X}_{j,0} - \bar{X}_{j,1})^2}{\sum_{i=1}^n (X_j^{(i)} - \bar{X}_j)^2} \quad (7)$$

where  $n_0$  and  $\bar{X}_{j,0}$  (resp.  $n_1$  and  $\bar{X}_{j,1}$ ) are the sample size and the empirical mean of  $X_{j,0}$  (resp.  $X_{j,1}$ ) which is the restriction of  $X_j$  to the case  $\{Y = 0\}$  (resp.  $\{Y = 1\}$ ). Let us remark that CR can also be used in a regression context (case of a quantitative variable  $Y$ ) when  $X_j$  is a qualitative variable (by exchanging the role of  $X_j$  and  $Y$  in Eqs. (6) and (7)).

### C.3. Johnson indices in the logistic regression context

Following the calculation methodology of the standardized logistic regression coefficient proposed by Menard (2004), Tonidandel & LeBreton (2010) suggests extending the definition of the Johnson indices to the logistic regression context. By considering the logistic regression model described by Eq. (1), the standardized logistic regression coefficient associated with the variable  $X_i$  is defined as

$$\beta_i^* = \frac{\sigma_{X_i}}{\sigma_{\text{logit}(g(p))}} \beta_i. \quad (8)$$

To define the standard deviation  $\sigma_{\text{logit}(g(p))}$ , one can use the alternative definition of  $R = (\sigma_{\text{logit}(\hat{g}(\hat{p}))}) / (\sigma_{\text{logit}(g(p))})$  and thus calculate the  $\beta_i$  such as:

$$\beta_i^* = \frac{\sigma_{X_i}}{\sigma_{\text{logit}(\hat{g}(\hat{p}))}} \beta_i R. \quad (9)$$

The idea is then to apply this definition to the methodology previously defined for a classical linear regression. The matrices  $Z^n$  (associated to a  $n$ -sample) and  $W$  (see Section 6.1 of the main paper), as well the matrix  $A_{\text{logit}}$  are estimated in function of the variables  $X^n$  and  $g^n(p)$  ( $n$ -sample of  $g(p)$ ) standardized beforehand. In particular, we have

$$\hat{A}_{\text{logit}} = (Z^{n\top} Z^n)^{-1} Z^{n\top} g^n(p) = Z^{n\top} g^n(p) = (\hat{\alpha}_{\text{logit},j})_{1 \leq j \leq d}. \quad (10)$$

The Johnson index associated with the variable  $X_i$  in the logistic regression context is thus given by:

$$J_{\text{logit},i} = R^2 \sum_{j=1}^d \alpha_{\text{logit},j}^{*2} w_{ij}^{*2} \quad (11)$$

A natural plug-in estimator of the Johnson index can then be obtained.

### C.4. Application cases

Classification problems deal with binary  $Y$  and Section C.1 has developed the linear logistic regression model which allows modelling  $g(p) = \log \frac{p}{1-p}$  (with  $p = \mathbb{P}(Y = 1)$ ). Metrics of such models, fitted on the link scale, are then associated to the quantity  $g(p)$  and do not give a direct interpretation of the output on which we focus.

Table S8 provides a summary of the various datasets used in this section and their corresponding characteristics: the name and corresponding subsection, the input dimension  $d$ , the number of observations  $n$ , information about the presence of quantitative vs. qualitative inputs (qt/ql), and the source of the dataset. The first five rows correspond to toy cases with simulated data while the remaining ones correspond to public datasets. Note that the +1 sometimes mentioned in the input dimension column refers to the fact that a dummy correlated variable is introduced (but without being explicitly part of the model).

**Table S8:** Summary of the toy and public use cases.

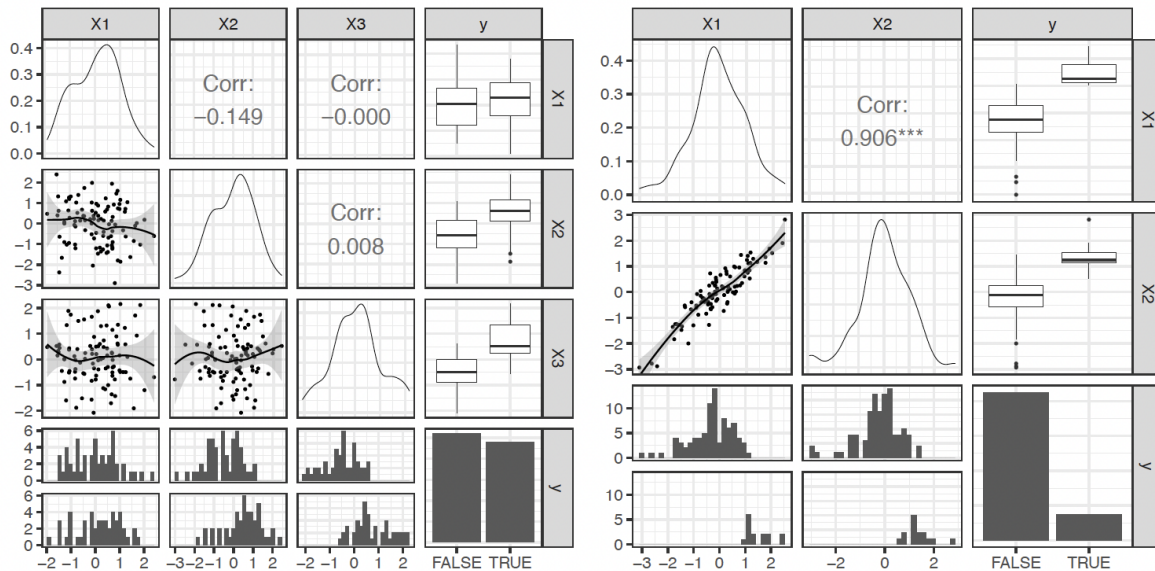
Name	$s$	$d$	$n$	qt/ql	Source
Classif #1	4.1	3	100	qt	-
Classif #2 (dummy)	4.1	2+1	100	qt	-
Car prices	4.2	15	804	qt/ql	cars dataframe (caret package)

#### C.4.1 Illustration on simulation data from toy cases

We first study the three-dimensional ( $d = 3$ ) linear classification model:

$$Y = \mathbb{I}_{\{\sum_{i=1}^d \alpha_i X_i \geq k\}} \quad (12)$$

with  $k \in \mathbb{R}$  and  $X_i \sim \mathcal{N}(0, 1)$   $i = 1, \dots, d$ . In our case, we take  $k = 0$ ,  $\alpha = (1, 2, 3)$  and we simulate a 100-size sample of  $X$ . The matrix plot is given in Figure S10 (left).



**Figure S10:** Data pairs plot for the linear classification case (left) and the dummy-correlated-variable classification case (right). The upper panel provides the CC of each variable pair; the diagonal panel gives the kernel density estimation of the marginals; the lower panel gives scatter plots and fitted GLM with CI. As the output variable is not continuous but binary, other representations are given in the right column and bottom line.

On the link scale, the linear regression between the output and the inputs gives  $R^2 = 1.000$  and  $Q^2 = 0.921$ . By taking the threshold  $s$  (see Eq. (2a)) at the mid-value and classical value 0.5 to distinguish the two classes, the classification error rate (Eq. (4)) is  $\varepsilon = 0$  and the classification sensitivity (Eq. (5)) is  $\tau = 1$ , which mean a perfect fit (as expected). The metrics and the VIMs, from the regression on the link scale, are given in Table S9 and Figure S11 (left). It shows that LMG, Johnson and PMVD provide similar results that  $\text{SRC}^2$  (which is only based on the regression coefficients that give a higher weight to  $X_2$  than to  $X_1$ ). The output corresponds to a threshold exceedance that is mainly explained by  $X_3$ .  $X_1$  and  $X_2$  compete  $X_3$  only via their interaction effects (concomitant large values). Therefore, this interaction effect is shared between these inputs in the LMG/Johnson/PMVD approach, and their effect is equalized.

**Table S9:** Metrics and VIMs (in %) for the linear classification data.

Input	VIF	CR	SRC <sup>2</sup>	PCC <sup>2</sup>	SPCC <sup>2</sup>	LMG	Johnson	PMVD
X <sub>1</sub>	8.86	0.723	8.65	6.86	2.58	5.36	6.27	10.2
X <sub>2</sub>	14.83	24.977	37.78	40.54	26.28	35.91	35.19	35.9
X <sub>3</sub>	28.63	44.577	58.20	62.22	44.01	58.73	58.55	53.8
Sum	52.31	70.277	104.62	109.62	72.88	100.00	100.00	100.00

We now study a model with  $d = 2$  correlated inputs with one dummy variable (i.e. non-included in the model):

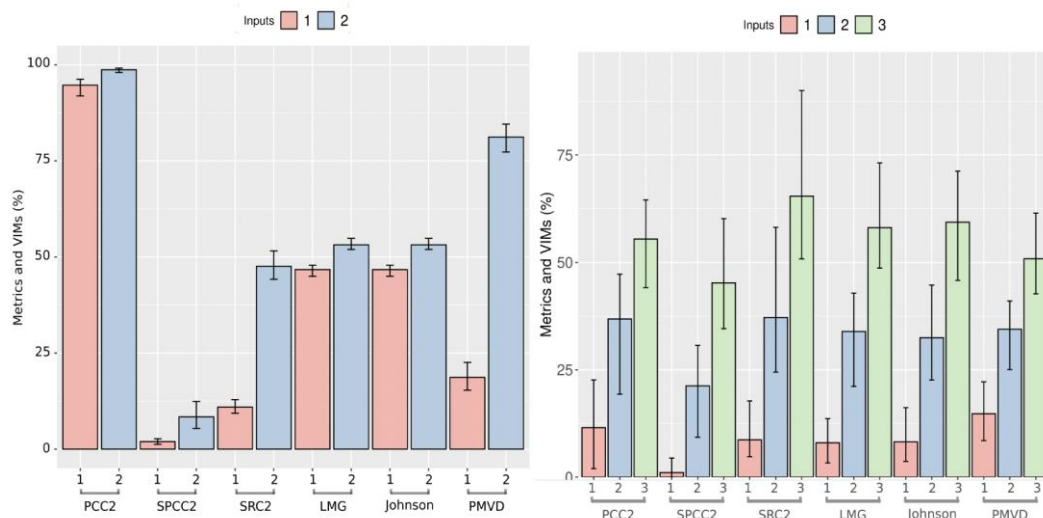
$$Y = \mathbb{I}_{\{X_i + \eta \geq 1\}} \quad (13)$$

with  $\eta \sim \mathcal{N}(0, 0.01)$  and  $X \sim \mathcal{N}_2\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix}\right)$ . We simulate a 100-size sample of  $X$ . The matrix plot is given in Figure S10 (right).

On the link scale, the linear regression between the output and the inputs gives  $R^2 = 0.951$  and  $Q^2 = 0.841$ . By taking the threshold  $s = 0.5$ , we have  $\varepsilon = 0.02$  and  $\tau = 0.93$ . The metrics and the VIMs, from the regression on the link scale, are given in Table S10 and Figure S11 (right). PMVD allows drastically decreasing the importance measure of  $X_2$  which is only due to its correlation with  $X_1$ . One also observes the closeness between LMG and the (logistic regression-based) Johnson indices.

**Table S10:** Metrics and VIMs (in %) for the non-included-input classification model toy data.

Input	VIF	CR	PCC <sup>2</sup>	SPCC <sup>2</sup>	SRC <sup>2</sup>	LMG	Johnson	PMVD
X <sub>1</sub>	12.3	41.1	11.994	9.176	111.51	64.1	57.9	91.27
X <sub>2</sub>	12.3	32.1	0.323	0.126	1.36	31.0	37.3	3.87
Sum	24.6	73.2	12.317	9.301	112.87	95.1	95.1	95.14

**Figure S11:** Estimates (with bootstrap) of the metrics and VIMs in the linear classification case (left) and in the dummy-correlated-variable classification case (right).

#### C.4.2 Application to a public dataset: car prices data

We use the car data for a classification exercise ( $Y$  is binary) by distinguishing the cars prices above and below a given price (\$40, 000). The important class to be predicted ( $Y = 1$ ) is for the high prices. On the link scale, the linear logistic regression between the output and the inputs gives  $R^2 = 0.757$  and  $Q^2 = 0.601$ . By taking the threshold  $s = 0.2$  to distinguish the two classes, the classification error rate (Eq. (4)) is  $\varepsilon = 0.037\%$  and the

classification sensitivity (Eq. (5)) is  $\tau = 1$ . The metrics and VIMs, from the regression on the link scale, are given in Table S11. The difference with the regression case is that some variables (as Saab) have no more influence. The influence of the three main influential inputs (Cylinder, Cadillac and convertible) are still present.

**Table S11:** Metrics and VIMs (in %) for the cars classification data. The last column gives the sense of variation of inputs with significantly influence (LMG> 1).

Input	n°	VIF	CR	SRC <sup>2</sup>	PCC <sup>2</sup>	SPCC <sup>2</sup>	LMG	Johnson	PMVD	Cor. sign
Mileage	1	1.01	1.40	0.79	2.26	1.03	4.67	1.42	5.13	-
Cylinder	2	2.35	18.85	1.94	1.09	1.61	21.68	14.20	27.9	+
Doors	3	4.61	0.56	1.49	0.00	0.59	1.45	0.81	0.00	+
Cruise	4	1.55	1.72	0.21	0.00	0.04	2.30	1.06	0.00	-
Sound	5	1.14	0.26	0.00	0.00	0.02	0.31	0.13	0.02	
Leather	6	1.19	2.00	0.01	0.00	0.03	3.01	0.57	0.00	+
Buick	7	2.60	0.58	0.05	0.00	0.17	1.20	0.66	0.00	-
Cadillac	8	3.33	35.14	16.99	0.10	5.25	20.90	27.05	31.3	+
Chevy	9	4.41	1.63	0.32	0.00	0.03	3.11	1.91	0.00	-
Pontiac	10	3.42	1.20	0.44	0.00	0.30	3.34	1.15	0.00	-
Saab	11	3.56	0.87	18.91	0.00	0.42	3.10	15.44	0.15	-
convertible	12	1.63	8.78	13.47	1.69	5.10	8.90	10.56	11.2	+
hatchback	13	2.45	0.42	0.53	0.00	0.53	0.51	0.16	0.00	
sedan	14	4.51	0.01	1.79	0.00	0.63	1.27	0.62	0.00	-
Sum		37.77	73.42	56.93	5.14	15.75	75.74	75.74	75.7	

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