Johnson indices in the context of linear regression with high-dimensional dependent inputs

24/04/2025 - SAMO Conference

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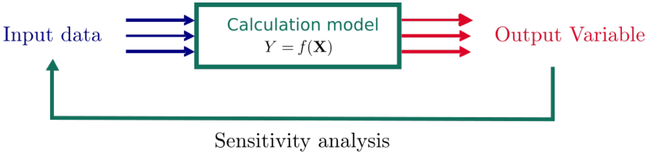
EDF R&D

Uncertainty quantification context in neutronic



Calculation model :

$$\vec{\Omega}.\vec{\nabla}\psi(\vec{r},E,\vec{\Omega}) + \mathbf{\Sigma_t}(\vec{r},E)\psi(\vec{r},E,\vec{\Omega}) = \int_0^\infty dE' \int_{4\pi} d^2\vec{\Omega}'\mathbf{\Sigma_S}(\vec{r},E' \to E,\vec{\Omega}.\vec{\Omega}')\psi(\vec{r},E',\vec{\Omega}') + \mathbf{Q}(\vec{r},E,\vec{\Omega})$$

Interest variable :

- ψ the neutron flux.

Input variables :

- $\sim$ 2000 variables : **large size and correlations**.

Approached model :

- **Linear regression model**

Basics of multivariate linear regression

Framework and notations

Experimental design

- n observations ($\mathbb{R}$-valued) of an **explained** random variable Y and of d **explanatory** random variables $\boldsymbol{X} = (X_1, \ldots, X_d)$:

$$(\mathbf{X}^n, \mathbf{y}^n) = \left(x_1^{(i)}, \ldots, x_d^{(i)}, y^{(i)}\right)_{i=1,\ldots,n}$$

> **Assumption.** *without any loss of generality*
>
> $$\mathbb{E}[X_j] = 0 \text{ for } j = 1, ..., d \text{ and } \mathbb{E}[Y] = 0$$

Basics of multivariate linear regression

Framework and notations

Multivariate linear regression model

$$Y = \boldsymbol{X}\beta + \varepsilon$$

- where $\beta = (\beta_1, \ldots, \beta_d)^\top \in \mathbb{R}^d$ is the vector of coefficients,
- ε is a centered and gaussion random error.

Assumption. $\varepsilon \sim \mathcal{N}(0, \sigma_\varepsilon^2)$ and $\mathbb{E}\left[\varepsilon | \boldsymbol{X}\right] = 0$.

- For each observation $i = 1, ..., n$, $y^{(i)} = \mathbf{x}^{(i)}\beta + \varepsilon^{(i)}$ where for all $i = 1, \ldots, n$, the $\varepsilon^{(i)}$s are independent and identically distributed with the same law as ε. Therefore, determine :

$$\mathbb{E}\left[Y | \boldsymbol{X} = \left(x_1^{(i)}, \ldots, x_d^{(i)}\right)\right] = \mathbf{x}^{(i)}\beta$$

Estimating model coefficients β

Hypothesis. The sample size is large enough ($n \gg d$), and the matrix $\mathbf{X}^{n\top}\mathbf{X}^n$ is positive-definite.

- The unbiased maximum likelihood estimator (Ordinary Least Squares [**chr90**]) :

$$\widehat{\boldsymbol{\beta}} = (\mathbf{X}^{n\top}\mathbf{X}^n)^{-1}\mathbf{X}^{n\top}\mathbf{y}^n$$

Coefficient of determination

- Quantify the **output variability captured** by the linear regression model :

$$R^2 = R^2_{Y(X)} := 1 - \frac{\mathbb{E}\left[\mathbb{V}(Y|X)\right]}{\mathbb{V}(Y)} = \frac{\mathbb{V}(\mathbb{E}[Y|\boldsymbol{X}])}{\mathbb{V}(Y)}$$

The R^2 for constructing importance measures

Variance-based importance measures (VIM) [**kurcoo06**]

- describe the impact of input data on **output dispersion**,
- equivalent to partition R^2 among the d inputs.

Variance decomposition

$$\mathbb{V}(Y) = \overbrace{\mathbb{V}(\mathbb{E}[Y|\boldsymbol{X}])}^{\text{explained variance}} + \overbrace{\mathbb{E}[\mathbb{V}(Y|\boldsymbol{X})]}^{\text{residual variance}}$$

The R^2 decomposition

Variance-based importance measures

Criteria for R^2 decomposition

Four basic desirability criteria can be sought after for a VIM (according to [**gro07**]) :

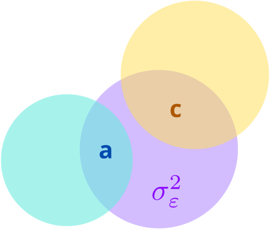
- ($\mathcal{C}_1$) ***Proper decomposition*** : the sum of all values should be equal to 1 ;
- ($\mathcal{C}_2$) ***Non-negativity*** : all values should be nonnegative ;
- ($\mathcal{C}_3$) ~~*Exclusion*~~ : if $\beta_j = 0$, then the share of X_j should be zero ;
- ($\mathcal{C}_4$) ***Inclusion*** : if $\beta_j \neq 0$, then the share of X_j should be nonzero.

An additional criterion that is sometimes mentioned in the literature, but more related to regularization-based techniques [**zouhas05** ; **wal19**] :

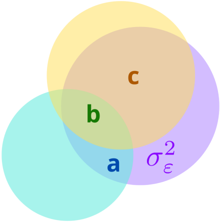
- ($\mathcal{C}_5$) ***Grouping*** : shares tend to equate for highly correlated inputs.

Multicolinearity illustration with Venn diagrams

When the variable tend to be correlated it becomes difficult to **isolate the contribution** of the variables.



(a) $r = 0, b = 0$



(b) $r \neq 0, b \neq 0$

- Three circles :
  - the variance of Y ; the variance of X_1 ; the variance of X_2 .
- Two overlapping area - the **additional explanatory power** :
  - of X_1 on the regression model $Y(X)$: $a = b_1^2(1 - r^2)$, with $b_1 = \beta_1\sigma_1$,
  - of X_2 on the regression model $Y(X)$: $c = b_2^2(1 - r^2)$, with $b_2 = \beta_2\sigma_2$.
- The area b : $b = b_1^2 r^2 + 2b_1 b_2 r + b_2^2 r^2$.

Shapley Values in regression model

Variance-based Importance Measures

Inspired from the cooperative game [**sha53**], they measure the **average marginal contribution** of each variable X_j to all possible combinations of variables in a regression model :

$$\psi_j = \frac{1}{d!} \sum_{\pi \in \mathcal{S}_D} \Delta_\pi(X_j)$$

where :

- $\mathcal{S}_D$ is the set of all permutations of $D = \{1, \ldots, d\}$,
- $\Delta_\pi(X_j) = c(v \cup j) - c(v)$ the **marginal performance difference** of the model between the permutation π with and without X_j,
- v the list of indices preceding j in the order π.

Owen[**owe14**] proposes to set the function c such as :

$$c(v) = \frac{\mathbb{V}(\mathbb{E}[Y|\boldsymbol{X}_v])}{\mathbb{V}(Y)}$$

Lindeman-Merenda-Gold indices

In the linear regression context **[linmer80]** :

- LMG_j average the additional explanatory power of X_j in each subset $\boldsymbol{X}_{u\cup\{j\}}$ defined for all the permutations of $D = \{1, \ldots, d\}$:

$$\mathrm{LMG}_j = \frac{1}{d!} \sum_{\pi \in \mathcal{S}_D} r^2_{Y,(X_j|\boldsymbol{x}_\pi)}$$

where

- the squared **semi-partial correlation coefficient**

$$r^2_{Y,(X_j|\boldsymbol{x}_\pi)} = R^2_{Y(\boldsymbol{x}_{u\cup\{j\}})} - R^2_{Y(\boldsymbol{x}_u)}$$

gives the **additional explanatory power** of X_j dans le modèle $Y(\boldsymbol{X}_{u\cup\{j\}})$.

Variance-based Importance Measures

Johnson indices

Drawback of LMG :

- its **exponential complexity** : one needs to perform $2^d - 1$ different linear regressions.

The Johnson indices

- equal to the LMG indices in the case of a two-input model.

$$\mathrm{J}_i = \mathrm{LMG}_i = \frac{{b_i}^2 + b_i b_j r + \frac{r^2}{2}({b_j}^2 - {b_i}^2)}{{b_i}^2 + 2 b_i b_j r + {b_j}^2 + \sigma_\varepsilon^2} \text{ with } b_i = \beta_i \sigma_i .$$

- give empirically similar results for a higher-dimensional input data ($d \geq 3$).

Johnson indices

The Johnson indices [**johnson66** ; **joh00**] :

- $\mathbf{X}^n \in \mathbb{R}^{n \times d}$ is **transformed in an orthogonal matrix** $\mathbf{Z}^n \in \mathbb{R}^{n \times d}$ in the least square sense. It consists in finding $\mathbf{Z}^n$ and $\mathrm{W} \in \mathbb{R}^{d \times d}$ such as :

$$\left\{ \begin{array}{rcl} \mathbf{X}^n & = & \mathbf{Z}^n \mathrm{W} \\ (\mathbf{Z}^n)^\top \mathbf{Z}^n & = & \mathrm{I} \\ \mathbf{Z}^n & = & \underset{\mathbf{\Pi}^n}{\arg\min} \operatorname{Tr} (\mathbf{X}^n - \mathbf{\Pi}^n)^\top (\mathbf{X}^n - \mathbf{\Pi}^n) \end{array} \right.$$

- Solution defined thanks to the **singular value decomposition** of $\mathbf{X}^n$:

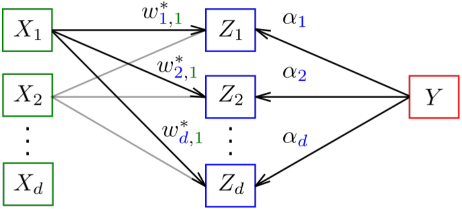
$$\mathbf{X}^n = \mathbf{P}^n \mathbf{\Delta} \mathrm{Q}^\top$$

$$\mathbf{Z}^n = \mathbf{P}^n \mathrm{Q}^\top \text{ and } \mathrm{W} = \mathrm{Q} \mathbf{\Delta} \mathrm{Q}^\top$$

Johnson indices

The **Johnson index** associated with the input X_j is finally expressed as :

$$J_j = \sum_{i=1}^{d} \alpha_i^{*^2} w_{ij}^{*^2}.$$



- A first least square regression of $\mathbf{y}^n$ on $\mathbf{Z}^n$ gives the vector of the standardized regression coefficient $\boldsymbol{\alpha}^*$ of the model $Y(Z)$.
- The d linear combinations between $\mathbf{X}^n$ and $\mathbf{Z}^n$ gives the *weights* W^* allowing to come back to the initial observations $\mathbf{X}^n$.

Alternative LMG inspired by Johnson's method

1st step : Expression of the **residu of the projection** of X_j onto $\boldsymbol{X_u}$

- as $X_j^{\perp \boldsymbol{u}}$, the component of X_j orthogonal to Xu,

$$\begin{aligned} X_j &= \mathbb{E}[X_j|\boldsymbol{X_u}] + X_j^{\perp \boldsymbol{u}} \\ &= \underbrace{\boldsymbol{X_u}(\boldsymbol{X_u}^t\boldsymbol{X_u})^{-1}\boldsymbol{X_u}^t X_j}_{\text{projection of } X_j \text{ onto } \boldsymbol{X_u}} + \underbrace{\varepsilon_{X_j|\boldsymbol{X_u}}}_{\text{orthogonal component of } X_j} \end{aligned}$$

2nd step : Expression of $r_{Y(X_j|\boldsymbol{X_u})}$ as a correlation between Y and $X_j^{\perp \boldsymbol{u}}$

$$\boxed{r^2_{Y(X_j|\boldsymbol{X_u})} = \mathrm{COR}^2(Y, X_j^{\perp \boldsymbol{u}})}$$

Alternative LMG inspired by Johnson's method

(Proof.)

- Expression of three **linear models** :

$$(1): \quad Y = \boldsymbol{X_u}\boldsymbol{\rho_u} + \epsilon_{Y|\boldsymbol{X_u}} \qquad \boldsymbol{\rho_u} = (\boldsymbol{X_u^t}\boldsymbol{X_u})^{-1}\boldsymbol{X_u^t}Y$$

$$(2): \quad Y = \boldsymbol{X_u}\boldsymbol{e_u} + X_j e_j + \epsilon_{Y|\boldsymbol{X_u}\cup X_j} \qquad \boldsymbol{e_{u\cup j}} = (\boldsymbol{X^t_{u\cup j}}\boldsymbol{X_{u\cup j}})^{-1}\boldsymbol{X^t_{u\cup j}}Y$$

$$(3): \quad Y = \boldsymbol{X_u}\boldsymbol{\rho_u} + X_j^{\perp \boldsymbol{u}}\rho_j^{\perp \boldsymbol{u}} + \epsilon_{Y|\boldsymbol{X_u}\cup X_j^{\perp \boldsymbol{u}}} \qquad \rho_j^{\perp \boldsymbol{u}} = ({X_j^{\perp \boldsymbol{u}}}^t X_j^{\perp \boldsymbol{u}})^{-1}{X_j^{\perp \boldsymbol{u}}}^t Y$$

- (2) and (3) : same **regression space** :

$$\boxed{\epsilon_{Y|\boldsymbol{X_u}\cup X_j^{\perp \boldsymbol{u}}} = \epsilon_{Y|\boldsymbol{X_u}\cup X_j}}$$

- using the **variance decomposition**

$$r^2_{Y(X_j|\boldsymbol{X_u})} = \frac{\mathbb{E}[\mathbb{V}(Y|\boldsymbol{X_u})] - \mathbb{E}[\mathbb{V}(Y|\boldsymbol{X_u}\cup X_j)]}{\mathbb{V}(Y)}$$

Alternative LMG inspired by Johnson's method

3rd step : Translate projection operations in $\boldsymbol{X}$ into operations in $\boldsymbol{Z}$.

$$\boxed{r^2_{Y(X_j|\boldsymbol{X_u})} = \frac{\left(\boldsymbol{\alpha}^{*t}\boldsymbol{w}_{.j}^{\perp \boldsymbol{u}}\right)^2}{\boldsymbol{w}_{.j}^{\perp \boldsymbol{u}\,t}\boldsymbol{w}_{.j}^{\perp \boldsymbol{u}}}}$$

- using $\boldsymbol{\alpha} = \boldsymbol{Z}^t Y$
- and $\boldsymbol{X} = \boldsymbol{Z}\mathrm{W}$:

$$X_j^{\perp \boldsymbol{u}} = \boldsymbol{Z}\boldsymbol{w}_{.j}^{\perp \boldsymbol{u}}$$

  · with $\boldsymbol{w}_{.j}^{\perp \boldsymbol{u}}$, the **residual part** that cannot be explained by $\boldsymbol{X_u}$,

$$\boldsymbol{w}_{.j}^{\perp \boldsymbol{u}} = (\mathrm{I} - \mathbf{P}_u)\,\boldsymbol{w}_{.j}$$

  · and $\mathbf{P}_u$, the **projector** on the vector space generated by the variables $\boldsymbol{u}$,

$$\mathbf{P}_u = \mathrm{W}_{.u}(\mathrm{W}_{.u}^t\mathrm{W}_{.u})^{-1}\mathrm{W}_{.u}^t.$$

Alternative LMG inspired by Johnson's Method

How to approach the link between LMG and Johnson ?

- Using the **Sherman-Morrison-Woodbury formula**, we can express $\mathbf{P}_u$ by iteration in function of all the projectors associated with the indices $u' = k, \ldots, l$:

$$\mathbf{P}_{u'} = \mathbf{P}_k + \sum_{i=k+1}^{l} \frac{(\mathbf{I} - \mathbf{P}_{i-1})\boldsymbol{w}_{.i}\boldsymbol{w}_{.i}^t(\mathbf{I} - \mathbf{P}_{i-1})}{\boldsymbol{w}_{.i}^t(\mathbf{I} - \mathbf{P}_{i-1})\boldsymbol{w}_{.i}}$$

.

- $(\mathbf{I} - \mathbf{P}_{i-1})\boldsymbol{w}_{.i}$ is the part of $\boldsymbol{w}_{.i}$ orthogonal to the space already projected by $\mathbf{P}_{i-1}$.
- The global projector $\mathbf{P}_u$ can thus be **constructed by successive accumulations**, where we progressively add the **contribution of $\boldsymbol{w}_{.i}$ to the projected space**.

Alternative LMG inspired by Johnson's Method

(Proof.)

- Considérant $u' = u \cup \{i\}$, le nouveau projecteur devient :

$$\mathbf{P}_{u'} = \mathrm{W}_{.u'} \Sigma_{\boldsymbol{u'}}^{-1} \mathrm{W}_{.u'}^{t}$$

avec

$$\mathrm{W}_{.u'} = [\mathrm{W}_{.u} \boldsymbol{w}_{.i}]\,,$$

et :

$$\Sigma_{\boldsymbol{u'}} = \mathrm{W}_{.u'}^{t} \mathrm{W}_{.u'} = \begin{bmatrix} \Sigma_{\boldsymbol{u}} \mathrm{W}_{.u}^{t} & \mathrm{W}_{.u}^{t} \boldsymbol{w}_{.i} \\ \boldsymbol{w}_{.i}^{t} \mathrm{W}_{.u} & \boldsymbol{w}_{.i}^{t} \boldsymbol{w}_{.i} \end{bmatrix}$$

- la formule de Sherman-Morrison-Woodbury permet d'exprimer :

$$\mathbf{P}_{u'} = \mathbf{P}_{u} + \frac{(\mathrm{I} - \mathbf{P}_{u}) \boldsymbol{w}_{.i} \boldsymbol{w}_{.i}^{t} (\mathrm{I} - \mathbf{P}_{u})}{\boldsymbol{w}_{.i}^{t} (I - \mathbf{P}_{u}) \boldsymbol{w}_{.i}}$$

- Par itération, si on classe par ordre croissant les indices dans u' tel que $u' = k, \ldots, l$:

$$\mathbf{P}_{u'} = \mathbf{P}_{k} + \sum_{i=k+1}^{l} \frac{(\mathrm{I} - \mathbf{P}_{i-1}) \boldsymbol{w}_{.i} \boldsymbol{w}_{.i}^{t} (\mathrm{I} - \mathbf{P}_{i-1})}{\boldsymbol{w}_{.i}^{t} (\mathrm{I} - \mathbf{P}_{i-1}) \boldsymbol{w}_{.i}}.$$

Alternative LMG inspired by Johnson's Method

How to approach the link between LMG and Johnson ?

$$\boxed{r^2_{Y(X_j|\boldsymbol{X_u})} = \frac{\left(\alpha^{*t}\boldsymbol{w}^*_{.j} - \alpha^{*t}\boldsymbol{w}^*_{.k} - \alpha^{*t}\mathbf{A}_{cc}\boldsymbol{w}^*_{.j}\right)^2}{1 - \boldsymbol{w}^{*t}_{.j}\mathbf{P}_k\boldsymbol{w}^*_{.j} - \boldsymbol{w}^{*t}_{.j}\mathbf{A}_{cc}\boldsymbol{w}^*_{.j}}}$$

with $\mathbf{A}_{cc} = \sum_{i=k+1}^{l} \frac{(\mathrm{I} - \mathbf{P}_{i-1})\boldsymbol{w}_{.i}\boldsymbol{w}^t_{.i}(\mathrm{I} - \mathbf{P}_{i-1})}{\boldsymbol{w}^t_{.i}(\mathrm{I} - \mathbf{P}_{i-1})\boldsymbol{w}_{.i}}$.

Numerical Application

Two-input regression model : $Y = \beta_1 X_1 + \beta_2 X_2 + \varepsilon$

R^2	$\mathrm{COR}(X_1, X_2)$	$b_1 = \beta_1\sigma_1$	$b_2 = \beta_2\sigma_2$	$\mathbb{V}(Y)$
0.35	0.80	23.0	15.0	798.0

Numerical equality :

Results	LMG_{R^2}	LMG_{P_u}	Rel. error	*Johnson*	Rel. error
X_1	**0.24**	0.24	1.4E-15	0.24	1.8E-15
X_2	**0.11**	0.11	2.5E-15	0.11	2.7E-15

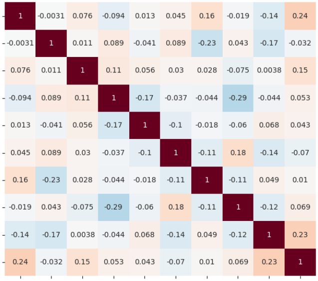
Numerical Application

Input regression model :

$d = 10$

$Y = \sum_{i=1}^{d} \beta_i X_i + \varepsilon$

R^2
0.35



Results	X_1	X_2	X_3	X_5	X_7	X_9
$b = \beta\sigma$	-8.8	-243.5	-112.9	-96.7	-89.45	-154.8
LMG_{R^2}	**0.0032**	**0.030**	**0.023**	**0.12**	**0.028**	**0.061**
LMG_{P_u}	**0.0032**	**0.030**	**0.022**	**0.12**	**0.028**	**0.061**
Abs. error			E-15			
Johnson	0.0035	0.029	0.023	0.12	0.028	0.062
Abs. error			E-4 - E-5			

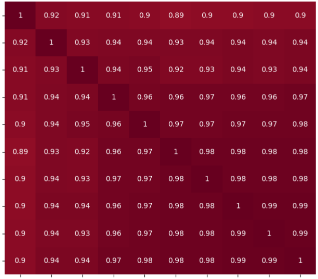
Numerical Application

Input regression model :

$d = 10$

$Y = \sum_{i=1}^{d} \beta_i X_i + \varepsilon$

R^2
0.34



Results	X_1	X_2	X_3	X_5	X_7	X_9
$b = \beta\sigma$	-9.7	-241.0	-125.4	-97.4	-99.2	-176.2
LMG_{R^2}	**0.030**	**0.042**	**0.041**	**0.036**	**0.035**	**0.035**
LMG_{P_u}	**0.030**	**0.042**	**0.041**	**0.036**	**0.035**	**0.035**
Abs. error			E-16 - E-18			
Johnson	0.028	0.043	0.042	0.038	0.037	0.036
Abs. error			E-3 - E-4			

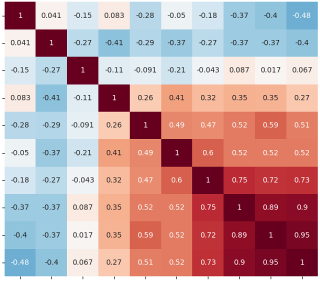
Numerical Application

Input regression model :

$d = 10$

$Y = \sum_{i=1}^{d} \beta_i X_i + \varepsilon$

R^2
0.29



Results	X_1	X_2	X_3	X_5	X_7	X_9
$b = \beta\sigma$	-27.7	-262.6	-129.8	-95.2	-90.6	-175.1
LMG_{R^2}	**0.011**	**0.103**	**0.019**	**0.071**	**0.014**	**0.010**
LMG_{P_u}	0.011	0.103	0.019	0.071	0.014	0.010
Abs. error			E-15			
Johnson	0.0093	0.100	0.018	0.072	0.015	0.012
Abs. error			E-3			

Conclusion & Perspectives

Conclusion :

- LMG offer a principled way to **attribute variance** in **multivariate linear regression** with correlated inputs.
- It provides a decomposition of R^2 that satisfies the **grouping property**.
- Because LMG is **computationally expensive**, Johnson's approximation offers an **efficient alternative** when the objective is to define a hierarchy between variables.

Article in SESMO Journal [**cloioo25**] : L. Clouvel, B. Iooss, V. Chabridon, M. Il Idrissi, F. Robin, *An overview of variance-based importance measures in the linear regression context : comparative analyses and numerical tests*.

Software : `R` package `sensitivity` : LMG/Johnson.

Future work :

- quantify the difference between LMG and Johnson,
- extend to PMVD indices which satisfy the **exclusion property**,
- imgaine how to extend to non-linear models.

Bibliography

Thank you for your attention !

Article in the journal SESMO [cloioo25]

Socio-Environmental Systems Modelling

SESMO

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

Laura Clouvel[1], Bertrand Iooss[2], Vincent Chabridon[2], Marouane Il Idrissi[2], and Frédérique Robin[1]

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[2]EDF R&D, PRISME Department, Chatou, France & SINCLAIR AI Lab., Saclay, France

Multicolinearity illustration

Two-input regression model

An illustrative example :

Two-input regression model

Consider the linear regression model (for $d = 2$) of the output Y with X_1 and X_2.

$$b_1 := \beta_1 \sigma_1, \quad b_2 := \beta_2 \sigma_2, \quad \text{and } r := r_{X_1, X_2}.$$

The **coefficient of determination is** :

$$R^2 = \frac{{b_1}^2 + 2 b_1 b_2 r + {b_2}^2}{{b_1}^2 + 2 b_1 b_2 r + \beta_2 {\sigma_2}^2 + \sigma_\varepsilon^2}.$$

Metrics to deal with multicollinearity

The full correlation coefficient (Pearson) :

- measures the degree of linear association between two variables :

$$r_{Y,X_j} = \frac{\mathrm{COV}(Y, X_j)}{\sigma_Y \sigma_j}$$

With independent inputs : $r = 0$

- r_{Y,X_j} is equal to β_j^* the **Standardized regression coefficients** (SRC) [**gro06** ; **antlam21**] :

$$\beta_j^* = \beta_j \frac{\sigma_j}{\sigma_Y} = r_{Y,X_j}$$

$$r^2_{Y,X_1} = \frac{{b_1}^2}{{b_1}^2 + {b_2}^2 + \sigma_\varepsilon^2} \quad \text{and} \quad r^2_{Y,X_2} = \frac{{b_2}^2}{{b_1}^2 + {b_2}^2 + \sigma_\varepsilon^2} \,.$$

$\mathcal{C}_1$	Proper decomposition	$\sum_j \mathrm{IM}_j = R^2$	YES
$\mathcal{C}_2$	Non-negativity	for all $j, \mathrm{IM}_j \geq 0$	YES
$\mathcal{C}_3$	Exclusion	*if* $\beta_j = 0, \mathrm{IM}_j = 0$	YES
$\mathcal{C}_4$	Inclusion	*if* $\beta_j \neq 0, \mathrm{IM}_j \neq 0$	YES

Metrics to deal with multicollinearity

The full correlation coefficient (Pearson) :

- measures the degree of linear association between two variables :

$$r_{Y,X_j} = \frac{\mathrm{COV}(Y, X_j)}{\sigma_Y \sigma_j}$$

With correlated inputs : $r \neq 0$

$$r^2_{Y,X_1} = \frac{(b_1 + r b_2)^2}{{b_1}^2 + 2 b_1 b_2 r + {b_2}^2 + \sigma^2_\varepsilon} \quad \text{and} \quad r^2_{Y,X_2} = \frac{(b_2 + r b_1)^2}{{b_1}^2 + 2 b_1 b_2 r + {b_2}^2 + \sigma^2_\varepsilon}\,.$$

$\mathcal{C}_1$	Proper decomposition	$\sum_j \mathrm{IM}_j = R^2$	NO
$\mathcal{C}_2$	Non-negativity	for all $j, \mathrm{IM}_j \geq 0$	YES
$\mathcal{C}_3$	Exclusion	*if* $\beta_j = 0, \mathrm{IM}_j = 0$	NO *ex* : if $r = 1$
$\mathcal{C}_4$	Inclusion	*if* $\beta_j \neq 0, \mathrm{IM}_j \neq 0$	YES

Metrics to deal with multicollinearity

The semi-partial correlation coefficient :

- quantify the additional explanatory power of a variable X_j on the variance of Y **[johleb04]**.

$$r^2_{Y,(X_j|\boldsymbol{x}_{-j})} = R^2_{Y(\boldsymbol{x})} - R^2_{Y(\boldsymbol{x}_{-j})} \ .$$

With independent inputs : $r = 0$

- $r^2_{Y,(X_j|X_i)}$ is equal to the correlation coefficient and the SRC^2 $\beta^*_j = r^2_{Y,X_j}$.

$$r^2_{Y,(X_1|X_2)} = \frac{{b_1}^2}{{b_1}^2 + {b_2}^2 + \sigma^2_\varepsilon} \quad \text{and} \quad r^2_{Y,(X_2|X_1)} = \frac{{b_2}^2}{{b_1}^2 + {b_2}^2 + \sigma^2_\varepsilon} \ .$$

$\mathcal{C}_1$	Proper decomposition	$\sum_j \mathrm{IM}_j = R^2$	YES
$\mathcal{C}_2$	Non-negativity	for all $j, \mathrm{IM}_j \geq 0$	YES
$\mathcal{C}_3$	Exclusion	*if* $\beta_j = 0, \mathrm{IM}_j = 0$	YES
$\mathcal{C}_4$	Inclusion	*if* $\beta_j \neq 0, \mathrm{IM}_j \neq 0$	YES

Metrics to deal with multicollinearity

The semi-partial correlation coefficient :

- quantify the additional explanatory power of a variable X_j on the variance of Y **[johleb04]**.

$$r^2_{Y,(X_j|\boldsymbol{x}_{-j})} = R^2_{Y(\boldsymbol{x})} - R^2_{Y(\boldsymbol{x}_{-j})} \ .$$

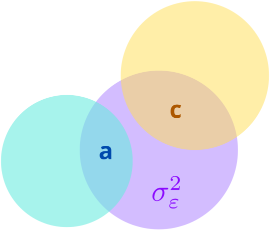
With correlated inputs : $r \neq 0$

$$r^2_{Y,(X_1|X_2)} = \frac{{b_1}^2(1-r^2)}{{b_1}^2 + 2b_1b_2r + {b_2}^2 + \sigma^2_\varepsilon} \quad \text{and} \quad r^2_{Y,(X_2|X_1)} = \frac{{b_2}^2(1-r^2)}{{b_1}^2 + 2b_1b_2r + {b_2}^2 + \sigma^2_\varepsilon}.$$

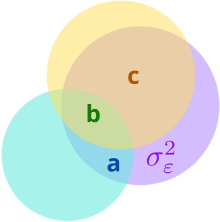
$\mathcal{C}_1$	Proper decomposition	$\sum_j \mathrm{IM}_j = R^2$	NO
$\mathcal{C}_2$	Non-negativity	for all $j, \mathrm{IM}_j \geq 0$	YES
$\mathcal{C}_3$	Exclusion	*if* $\beta_j = 0, \mathrm{IM}_j = 0$	YES
$\mathcal{C}_4$	Inclusion	*if* $\beta_j \neq 0, \mathrm{IM}_j \neq 0$	NO when $r = 1$

Metrics to deal with multicollinearity

Venn diagrams illustrating the challenges of the multicollinearity framework :



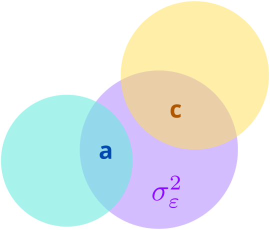
(a) $r = 0, b = 0$



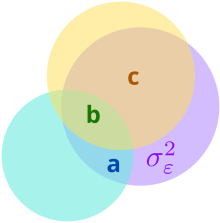
(b) $r \neq 0, b \neq 0$

- Three circles :
  - the variance of Y ; the variance of X_1 ; the variance of X_2.
- Two overlapping area - the **additional explanatory power** :
  - of X_1 on the regression model $Y(X)$: $a = \beta_1^2 \sigma_1^2 (1 - r^2)$,
  - of X_2 on the regression model $Y(X)$: $c = \beta_2^2 \sigma_2^2 (1 - r^2)$.
- The area b : $b = \beta_1^2 \sigma_1^2 r^2 + 2\beta_1 \beta_2 \sigma_1 \sigma_2 r + \beta_2^2 \sigma_2^2 r^2.$

Metrics to deal with multicollinearity



(a) $r = 0, b = 0$



(b) $r \neq 0, b \neq 0$

$\frac{a}{a+c+\sigma_\varepsilon^2}$	CC r^2_{Y,X_1}	$\frac{a+b}{a+b+c+\sigma_\varepsilon^2}$
$\frac{a}{a+c+\sigma_\varepsilon^2}$	semi-partial CC $r^2_{Y,(X_1\|X_2)}$	$\frac{a}{a+b+c+\sigma_\varepsilon^2}$
$\frac{a+c}{a+c+\sigma_\varepsilon^2}$	R^2	$\frac{a+b+c}{a+b+c+\sigma_\varepsilon^2}$

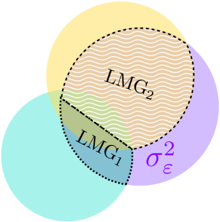
Importance measures : How to allocate a portion of zone b to the two variables X_1 and X_2 ?

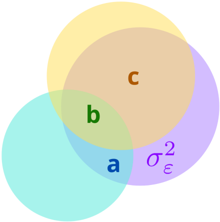
Lindeman-Merenda-Gold indices

Two-input regression model

$$\mathrm{LMG}_1 = \frac{{b_1}^2 + b_1 b_2 r + \frac{r^2}{2}({b_2}^2 - {b_1}^2)}{{b_1}^2 + 2b_1 b_2 r + {b_2}^2 + \sigma_\varepsilon^2} = \frac{a + b/2}{a + b + c + \sigma_\varepsilon^2}$$

$$\mathrm{LMG}_2 = \frac{{b_2}^2 + b_1 b_2 r + \frac{r^2}{2}({b_1}^2 - {b_2}^2)}{{b_2}^2 + 2b_1 b_2 r + {b_1}^2 + \sigma_\varepsilon^2} = \frac{c + b/2}{a + b + c + \sigma_\varepsilon^2}$$





LMG redistributes b equally between the portions attributed to X_1 and X_2.

Variance-based Importance Measures
LMG

With independent inputs : $r = 0$

- LMG is equal to the squared SPCC, the squared CC and the SRC^2.

$$\mathrm{LMG}_1 = \frac{{b_1}^2}{{b_1}^2 + {b_2}^2 + \sigma_\varepsilon^2} \quad \mathrm{LMG}_2 = \frac{{b_2}^2}{{b_2}^2 + {b_1}^2 + \sigma_\varepsilon^2}$$

$\mathcal{C}_1$	Proper decomposition	$\sum_j \mathrm{IM}_j = R^2$	YES
$\mathcal{C}_2$	Non-negativity	for all $j, \mathrm{IM}_j \geq 0$	YES
$\mathcal{C}_3$	Exclusion	*if* $\beta_j = 0, \mathrm{IM}_j = 0$	YES
$\mathcal{C}_4$	Inclusion	*if* $\beta_j \neq 0, \mathrm{IM}_j \neq 0$	YES

LMG as a R^2 decomposition
Appendix

With correlated inputs : $r \neq 0$

$$\mathrm{LMG}_1 = \frac{{b_1}^2 + b_1 b_2 r + \frac{r^2}{2}({b_2}^2 - {b_1}^2)}{{b_1}^2 + 2b_1 b_2 r + {b_2}^2 + \sigma_\varepsilon^2} \quad \mathrm{LMG}_2 = \frac{{b_2}^2 + b_1 b_2 r + \frac{r^2}{2}({b_1}^2 - {b_2}^2)}{{b_2}^2 + 2b_1 b_2 r + {b_1}^2 + \sigma_\varepsilon^2}$$

$\mathcal{C}_1$	Proper decomposition	$\sum_j \mathrm{IM}_j = R^2$	YES
$\mathcal{C}_2$	Non-negativity	for all $j, \mathrm{IM}_j \geq 0$	YES
$\mathcal{C}_3$	Exclusion	*if* $\beta_j = 0, \mathrm{IM}_j = 0$	NO if $r \neq 0$
$\mathcal{C}_4$	Inclusion	*if* $\beta_j \neq 0, \mathrm{IM}_j \neq 0$	YES
$\mathcal{C}_5$	Grouping	shares equate for high correlations	YES
			$\mathrm{LMG}_1 = \mathrm{LMG}_2,\ \text{if } r = 1$

Variance-based Importance Measures

Johnson indices

With a linear relation hypothesis between Y and $\boldsymbol{X}$:

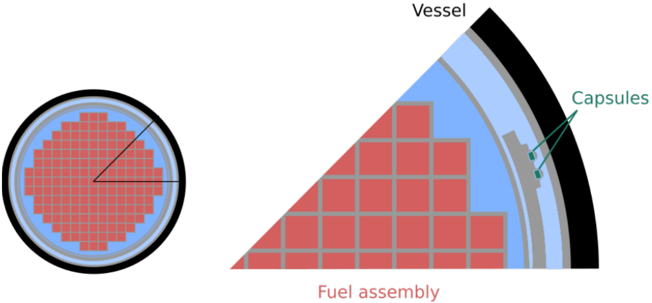
- The Johnson indices are equal to the LMG indices in the case of a two-input model.

$$\mathrm{J}_1 = \mathrm{LMG}_1 = \frac{{b_1}^2 + b_1 b_2 r + \frac{r^2}{2}({b_2}^2 - {b_1}^2)}{{b_1}^2 + 2 b_1 b_2 r + {b_2}^2 + \sigma_\varepsilon^2} \quad \mathrm{J}_2 = \mathrm{LMG}_2 = \frac{{b_2}^2 + b_1 b_2 r + \frac{r^2}{2}({b_1}^2 - b}{{b_2}^2 + 2 b_1 b_2 r + {b_1}^2 + \sigma}$$

- They give empirically similar results for a higher-dimensional input data ($d \geq 3$).

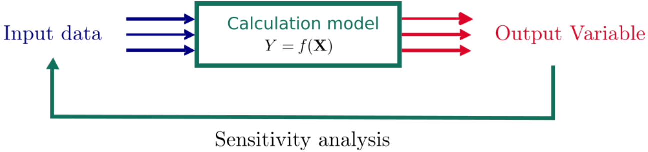
Sensitivity analysis in a neutronic study

Assessment of the neutron irradiation contributing to the aging of the reactor vessel [clo19]



- The neutron flux is calculated to be compared with the measured flux.
- The calculation gives a prediction of the neutron flux received by the vessel, which is not measured.

Sensitivity analysis in a neutronic study



Calculation model :

$$\vec{\Omega}.\vec{\nabla}\psi(\vec{r},E,\vec{\Omega}) + \mathbf{\Sigma_t}(\vec{r},E)\psi(\vec{r},E,\vec{\Omega}) = \int_0^\infty dE' \int_{4\pi} d^2\vec{\Omega}' \mathbf{\Sigma_S}(\vec{r},E' \to E,\vec{\Omega}.\vec{\Omega}')\psi(\vec{r},E',\vec{\Omega}') + \mathbf{Q}(\vec{r},E,\vec{\Omega})$$

Interest variable :

- ψ the neutron flux.

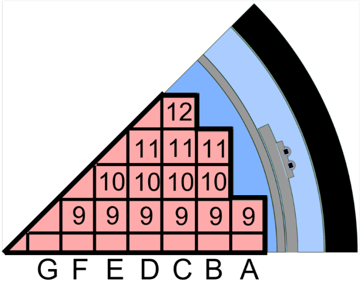
Input variables :

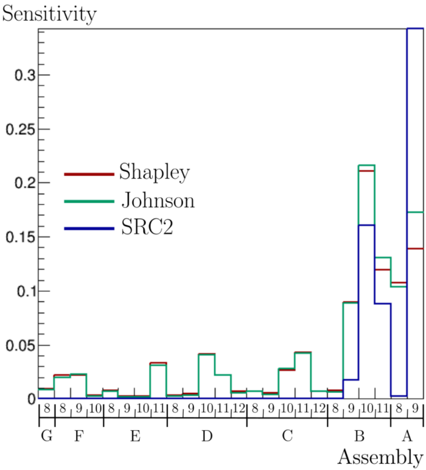
- the **power of 25 assemblies**

Approached model :

- Linear regression model

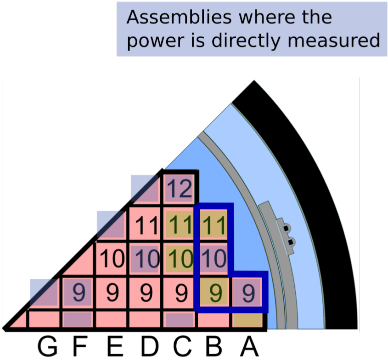
Sensitivity analysis in a neutronic study

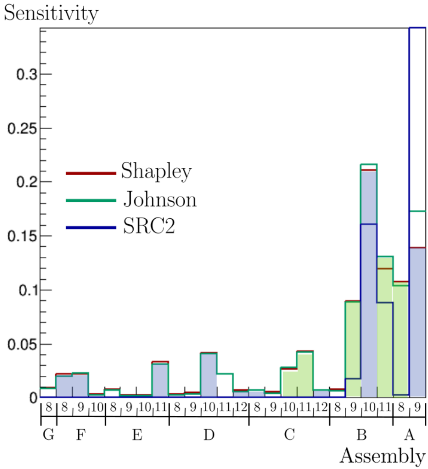




- The SRC² indices (blue) of the assemblies **A9**, **B10**, **B11** are the highest.
- The SRC² indices only explain 75% of the output variance.

Sensitivity analysis in a neutronic study

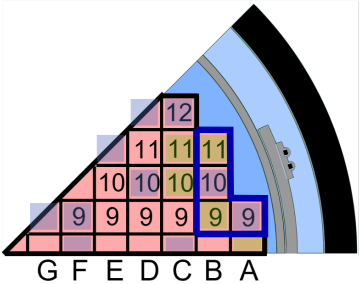


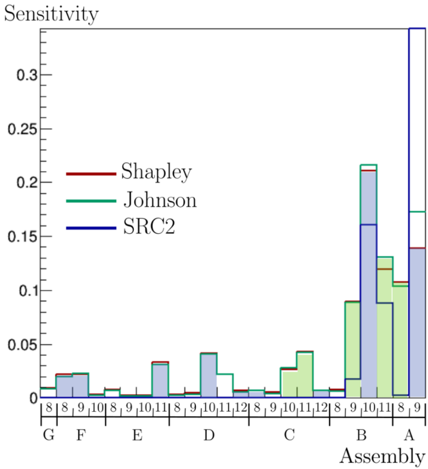


- The variables with a **stronger correlation** with A9, B10, B11 have a **higher Johnson/Shapley index** than the associated SRC^2 index.

Sensitivity analysis in a neutronic study

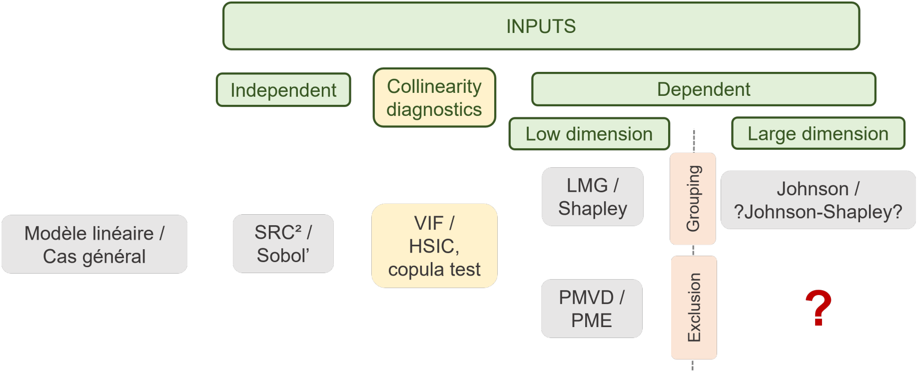
Assemblies where the power is directly measured





- The power map is based on calculation and measures. Some powers are measured and the value of the other variables are **reconstructed thanks to measured assemblies**.
- The variables positioned next to a **measured and influential power** in the model have a higher Johnson/Shapley index than that of SRC^2.

Conclusion


INPUTS
Independent
Collinearity diagnostics
Dependent
Low dimension
Large dimension
Modèle linéaire / Cas général
SRC² / Sobol'
VIF / HSIC, copula test
LMG / Shapley
PMVD / PME
Grouping
Exclusion
Johnson / ?Johnson-Shapley?
?