A mono/multi-block sparse PLS for heterogeneous data with missing samples

Hadrien Lorenzo[1], Jérôme Saracco[2], Rodolphe Thiébaut[1]

[1]SISTM (Inserm, U1219, Bordeaux Population Health and Inria, Talence, France) and Vaccine Research Institute, Creteil, France.
[2]CQFD (INRIA Bordeaux Sud-Ouest, France), CNRS (UMR5251)

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Context

rVSV-ZEBOV Ebola Vaccine phase I dose escalation trial

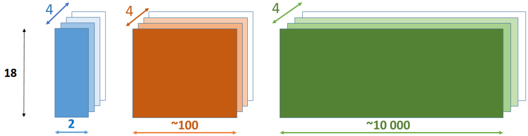
- First vaccine to show efficiency during the Ebola outbreak [Henao-Restrepo et al., *The Lancet*, 2017]

Hamburg vaccination dataset content

- 3 types of responses :
  Antibody response Cellular functionnality Genomic expression
- 18 participants divided in 2 vaccination groups :
  $3 \cdot 10^6 pfu$ $20 \cdot 10^6 pfu$

rVSV-ZEBOV Ebola Vaccine phase I datasets

3 families of blocks of longitudinal data



Data analysis : high dimensional problem

$n = 18,\ p \in \{129, 18301\},$ 8 blocks ($T = 8$)

T : number of blocks $\Longrightarrow$ **multi-block** approach,

Variety of technologies $\Longrightarrow$ **heterogeneous data**.

Objective

Predict the antibody response (after months) with the immune response (after days). Unfolded analysis : forget temporal structure.

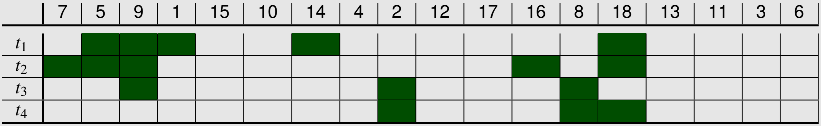
→ See [Rechtien et al., 2017]

Remaining big challenge : the missing values

Missing origins in the Genomic expression dataset

Poor sample qualities in case of :

- Low RNA integrity number (RIN)
- Insufficient library concentration
- Low sequencing depth



Preliminar observations

- 30% of missing samples/values,
- Missing structure, parallel to time structure

$\Longrightarrow$ Interest of a block structure

Existing solutions

Try many methods of imputations such as :

- **Mean** imputation per variable per block,
- **softImpute** [Hastie and Mazumder, 2015], no grouping structure
- **missMDA** [Josse and Husson, 2016], variable grouping structure

Main problems of those methods :

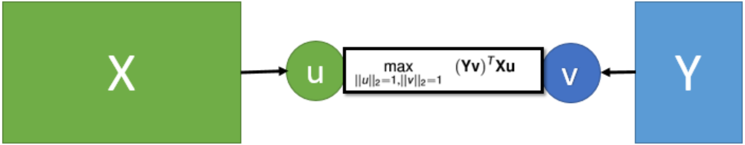
- No variable selection,
- Not supervised,
- Not converging,
- **Mean** is the best in that case.

Today : show you what we got!

A PLS-based method

- Do variable selection,
- Is supervised,
- Converges,
- Better than **Mean**

The PLS approaches, from [Wold father & son, 1983]



Equivalent to a eigen-space problem, or Singular Value Decomposition problem (**SVD**), with deflation. Under the common notations :

- **Weights** or **loadings** or "**poids**" u and v : power given to a variable from X, via u, and from Y, via v.
- **Scores** or **variates** of **(principal) components** Xu and Yv : projections of X and Y in the sub-spaces defined by u and v.

$\Longrightarrow$ Research, by projections, in X the information linked to Y.

Resolution of the PLS problem

Under the $\mathcal{L}$agrangian formalism :

$$\boxed{\max_{u,v,\alpha_x \geqslant 0,\alpha_y \geqslant 0} v^T \mathbf{Y}^T \mathbf{X} u - \alpha_x/2(||u||_2^2 - 1) - \alpha_y/2(||v||_2^2 - 1),}$$

$\mathbf{X}_{n\times p}$ and $\mathbf{Y}_{n\times q}$ the sample matrices, centered, of the covariates and of the response, then :

System $\partial_{\cdot} = 0$:

$$\begin{cases} \partial_{u\cdot} : & \alpha_x u = \mathbf{X}^T\mathbf{Y}v \\ \partial_{v\cdot} : & \alpha_y v = \mathbf{Y}^T\mathbf{X}u \\ \partial_{\alpha_x\cdot} : & ||u||_2^2 = 1 \\ \partial_{\alpha_y\cdot} : & ||v||_2^2 = 1 \end{cases}$$

Optimization (NIPALS) :

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Deflation :

$$\begin{aligned} \mathbf{X} &\leftarrow \mathbf{X} - \mathbf{X}uu^T \\ \mathbf{Y} &\leftarrow \mathbf{Y} - \mathbf{Y}vv^T \end{aligned}$$

Regression :

$\mathbf{Y} \approx \mathbf{X}\mathbf{B}$

$$\mathbf{B} = \frac{v^T\mathbf{Y}^T\mathbf{X}u}{||\mathbf{X}u||_2^2} uv^T$$

Classification (*PLS-DA*) :
LDA on $(\mathbf{X}u, \mathbf{Y})$, u is built on the R successive components.

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Variable selection in PLS → sparse PLS

Principle, interest and actual solutions

- Interest : Limit the number of biological measurements,
- Regularization shrinking $\mathcal{L}_1$-norm of the weights, see [Tibshirani, 1996].

$\Longrightarrow$ Selection & regularization.

Some sparse PLS

- [Lê Cao et al., 2008], 2 para./axis :
$$\min_{u,v} ||\mathbf{Y}^T\mathbf{X} - vu^T||_F^2 + \lambda_x||u||_1 + \lambda_y||v||_1$$
- [Chun and Keleş, 2010], $M = \mathbf{X}^T\mathbf{Y}\mathbf{Y}^T\mathbf{X}$, 3 para./axis :
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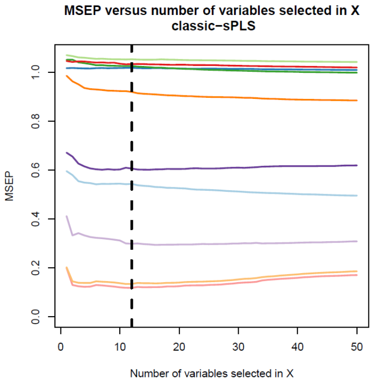
Application : Liver Toxicity Dataset via classical sPLS [Lê Cao et al., 2008]

From [Heinloth et al., 2004]. 64 drugged mice and their RNA expression, 10 response variables about liver : $\mathbf{X}_{64\times 3116}$, $\mathbf{Y}_{64\times 10}$.



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- Min of error : 12 select. var. in X. **PB** : How many Y var. in the model ? 2?...3?...5?...6?... $|keep_y = 2\}$
- **Good prediction** : Many errors minimized,
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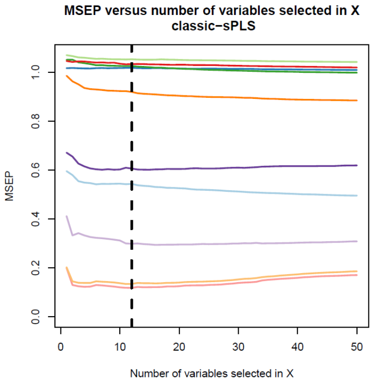

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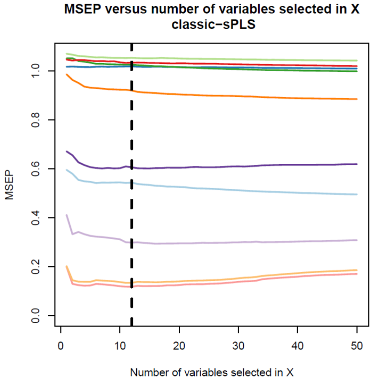

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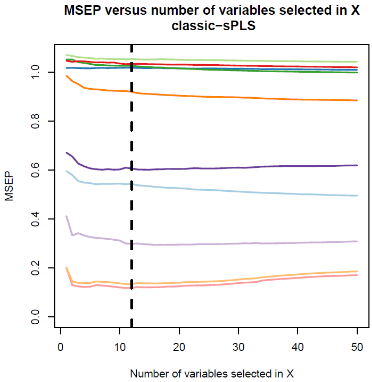

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Our idea

Flip S_λ, a non linear function, and $v \rightarrow \mathbf{X}^T\mathbf{Y}v$ and $u \rightarrow \mathbf{Y}^T\mathbf{X}u$, linear functions with a common λ.

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3. $v \leftarrow \mathbf{S}_{\beta_\mathbf{y}}(\mathbf{Y}^T\mathbf{X}u)$
4. $v \leftarrow v/||v||_2$

where $t \rightarrow S_\lambda(t)$ is the soft-thresholding function.

Our idea

Flip S_λ, a non linear function, and $v \rightarrow \mathbf{X}^T\mathbf{Y}v$ and $u \rightarrow \mathbf{Y}^T\mathbf{X}u$, linear functions with a common λ.

sparse PLS : Resolution of the data-driven problem

Optimization :

1. $u \leftarrow \mathbf{S}_\lambda(\mathbf{X}^T\mathbf{Y}/(n-1))v$
2. $u \leftarrow u/||u||_2$
3. $v \leftarrow \mathbf{S}_\lambda(\mathbf{X}^T\mathbf{Y}/(n-1))u$
4. $v \leftarrow v/||v||_2$

Interests

- Select on X and on Y with **1 parameter** : λ,
- Interpret λ : correlation threshold if $\mathbf{X}$ and $\mathbf{Y}$ standardized.

dd-sPLS : data driven sPLS on R components

$$\mathbf{u} = \underset{\substack{\mathbf{u}\in\mathbb{R}^{p\times R}\\ \mathbf{u}^T\mathbf{u}=\mathbb{I}_R}}{\arg\max} ||S_\lambda\left(\frac{\mathbf{Y}^T\mathbf{X}}{n-1}\right)\mathbf{u}||_F^2, \quad \mathbf{v} = \left(\frac{S_\lambda(\mathbf{N})^T u^{(r)}}{||S_\lambda(N)^T u^{(r)}||_2}\right)_{\text{r=1..R}} \tag{2}$$

Regression : PLS of $(t = \mathbf{Xu}, s = \mathbf{Yv}) \implies$ scores$(\mathfrak{u}, \mathfrak{v})$, $\mathfrak{a} = diag(\mathfrak{a}^{(\mathrm{r})})_{\mathrm{r=1..R}} | \mathfrak{a}^{(\mathrm{r})} =< s\mathfrak{v}^{(\mathrm{r})}, t\mathfrak{u}^{(\mathrm{r})} > /||t\mathfrak{u}^{(\mathrm{r})}||_2^2$ then

$$\mathbf{Y} \approx \mathbf{XB}, \quad \mathbf{B} = \mathbf{u}\mathfrak{u}\mathfrak{a}\mathfrak{v}^T\mathbf{v}^T$$

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dd-sPLS, a few theoretical results

Proposition 1, where $\mathbf{N} = \mathbf{Y}^T\mathbf{X}/(n-1)$:

$\mathcal{L} : \lambda \rightarrow \max\{||S_\lambda(\mathbf{N})u||_2^2 | u^T u = 1\}$, *is decreasing on* $[0,1]$ *and continuous on* $[0,1] - \{||\mathbf{N}||_\infty\}$.

Interpretation : $\lambda \in [0,1]$, permits to control the information in common to $\mathbf{X}$ and $\mathbf{Y}$ to put in the model $\rightarrow$ Regularization

Proposition 2, symmetric in u and v :

$\forall \lambda \in [0,1]$, *denoting* $C_i^{(\lambda)}$ *the* i^{th}*-column of* $S_\lambda(\mathbf{N})$, $u = (u_i)_{i=1..p}$ *sol. of* (2) *and* $v = S_\lambda(\mathbf{N})^T u/||S_\lambda(N)^T u||_2$ *then:*
$\forall i = 1..p : \quad u_i = 0 \iff < C_i^{(\lambda)}, v >= 0.$

Interpretation : The problem implies sparsity and admits **Upper bounds** on u and v cardinalities, decreasing with λ.

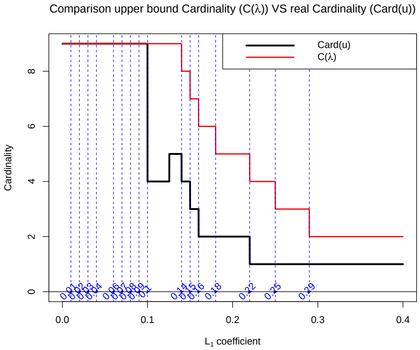
dd-sPLS, a question of monotonicity

Is the cardinality monotonically decreasing per component ?

No, a counter-example :

$\frac{\mathbf{Y}^T\mathbf{X}}{n-1} =$

	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9
Y_1	1.00	-0.06	-0.10	0.07	0.09	0.15	0.16	0.14	0.22
Y_2	-0.08	0.98	0.29	-0.18	0.25	0.02	0.04	-0.01	-0.03



2 components :

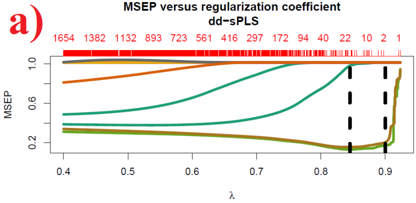
- Close in $\mathcal{L}_2$-norm,
- Different in $\mathcal{L}_0$-norm.

Reverse order in $\lambda \approx 0.13$.

Remark : Ordered through $\mathcal{L}_2$-norm while $\mathcal{L}_0$-norm is optimized in selection problems.

Application : Back to the Liver Toxicity Dataset

a)



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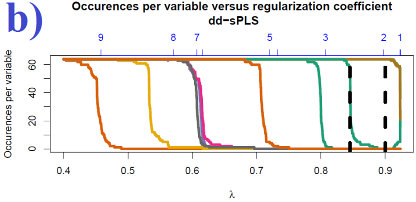

Results of the Cross-Validation

- **a)** : MSEP,
- **b)** : Selection per Y var.

Observations

- Via **a)** , $\lambda = 0.845$:

  ? 2 Y var. sel. **?**

- Via **b)** :
  - $\lambda = 0.845$:

    3^{rd} Y var. sel. **half times**
  - $\lambda \approx 0.9$:

    Exactly 2 Y var. sel.

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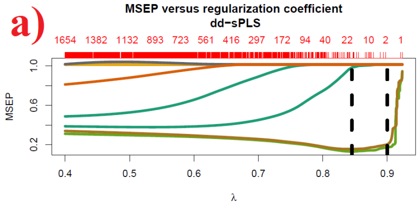

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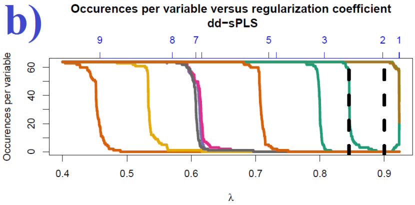

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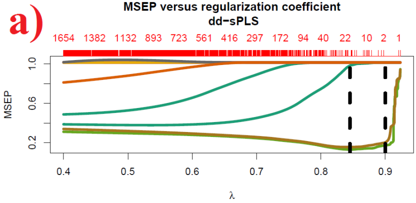

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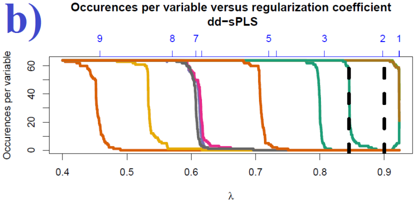

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Liver Toxicity Dataset : Comparison

Selection X variables comparison sPLS/dd-sPLS

Variable		A_43_P14131	A_42_P620915	A_43_P11724	A_42_P802628	A_43_P10606	A_42_P675890	A_43_P23376	A_42_P758454	A_42_P578246	A_43_P17415	A_42_P610788	A_42_P840776	A_42_P705413	A_43_P22616	Mean MSEP(LOO)	Min MSEP(LOO)
sPLS	$kx = 12$	-0.6	-0.52	0.17	-0.12	-0.14	-0.18	-0.21	-0.18	-0.14	-0.33	-0.07	-0.26			0.65	0.11
dd-sPLS	$\lambda = 0.845$	-0.6	-0.52	0.17	-0.12	-0.14	-0.18	-0.21	-0.18	-0.14	-0.33	-0.07	-0.26	-0.03	-0.01	0.84	0.13
	$\lambda = 0.9$	-0.86	-0.51													0.85	0.17

- 12 X var. sel. for classical sPLS. 15 in the case $\lambda = 0.845$ and 2 for $\lambda = 0.9$.
- Best **min** and **mean** errors for classical sPLS method.

Conslusion

dd-sPLS is better to select but worse to predict on that example.

Conclusion on the mono-block dd-sPLS

- Easy and well known problem (SVD),
- Selects X and Y variables with one parameter,
- Interpretable parameter : λ :

The minimum level of correlation between one X (or Y) variable and any of the Y (or X) variables to potentially get this variable in the model.

Multiblock PLS, called MBPLS

Formulation

Wold in 1984 [Wold, 1984] and Wangen & Kowalski [Wangen and Kowalski, 1989] consider T blocks indexed $\mathbf{X}_t$ of predictors that can be bound to a response matrix $\mathbf{Y}$. Recalled weights u_t and scores $t_t = \mathbf{X}_t u_t$ for block $\mathbf{X}_t$, weight v and score $s = \mathbf{Y}v$ for $\mathbf{Y}$ and finally super-weights $\mathbf{b} = (b_t)_{t=1..T}$ and super-score $\mathbf{t} = \sum_{t=1}^{T} \mathbf{X}_t u_t b_t$ such as the 1^{st} component of the classical **MBPLS** maximizes :

$$\boxed{cov^2(t,s) = (\sum_{t=1}^{T} v^T \mathbf{Y}^T \mathbf{X}_t u_t b_t)^2, \quad \text{subj. to } v^T v = u_t^T u_t = \mathbf{b}^T \mathbf{b} = 1 \qquad (3)}$$

Then deflation of $\mathbf{X}_t$'s and $\mathbf{Y}$ and solves (3) anew, loop R times, R fixed by the user.

MBPLS and mdd-sPLS

The deflation question

Component-wise method : solve sequential **MBPLS** with 2 cases of deflation in [Westerhuis and Smilde, 2001] :

- On each score : Poor prediction results,
- On the super-score : Better prediction results but mixing intra-block information.

→ Problem of variance restraining by outer axes. Thought shared with **François Husson** and **Arthur Tenenhaus**. **missMDA** [Josse and Husson, 2016] with no deflation and **RGCCA**, from [Tenenhaus and Tenenhaus, 2011], talk about a deflation-free solution.

$\Longrightarrow$ No use of a deflation-based method.

mdd-sPLS : model definition

An (inter/intra)-blocks separable problem with no global iteration!

$$\underset{(u_t^{(r)},\beta_t^{(r)})\in\mathbb{R}^{p_t}\times\mathbb{R}}{\arg\max} \sum_{r=1}^{R}\sum_{t=1}^{T}\beta_t^{(r)^2}||S_\lambda\left(\frac{\mathbf{Y}^T\mathbf{X}_t}{n-1}\right)u_t^{(r)}||_2^2 \quad \text{subj. to } \forall r,s|r\neq s \begin{array}{l} u_t^{(r)^T}u_t^{(r)}=1 \\ u_t^{(r)^T}u_t^{(s)}=0 \\ \sum_{t=1}^{T}\beta_t^{(r)^2}=1 \end{array}, \tag{4}$$

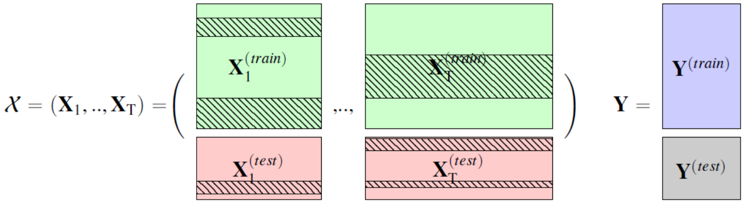
Inter-block : T independent dd-sPLS problems

$$\mathbf{u}_t = (u_t^{(1)},\cdots,u_t^{(R)}) = \underset{\mathbf{u}\in\mathbb{R}^{p_t\times r}}{\arg\max}\,||\mathbf{M}_t(\lambda)\mathbf{u}||_F^2, \text{ subj. to } \mathbf{u}^T\mathbf{u} = \mathbb{I}_R \tag{5}$$

Intra-block : R SVD problems

$$\beta^{(r)} = \underset{\beta\in\mathbb{R}^T}{\arg\max}\,||z^{(r)}(\lambda)\beta||_2^2, \text{ subj. to } \beta^T\beta = 1 \tag{6}$$

Missing data estimation : The *Koh-Lanta* algorithm



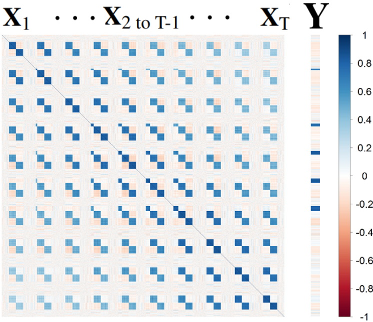
- **The Tribe Stage** : **train** dataset imputation using mdd-sPLS prediction on $\mathfrak{s}$ and λ. Using selected variables of global model : *Koh-Lanta* way of selection. Iterative process reestimating global model
- **The Reunification Stage** : **test** dataset imputation, using mdd-sPLS prediction on $\mathfrak{t}_{train}$ for non missing blocks and λ, on selected variables of main model. Non iterative process. Estimate $\mathbf{Y}_{test}$ reunifying all info.

Simulations

Build T-blocks data-set +$\mathbf{Y}$ matrix :

- Inter-block correlations : ρ_t,
- Intra-block correlations : ρ_i,
- Predictor/Response correlations : ρ_t.

In each case define groups of variables with different sizes. Half of the blocks not linked to the response.



Chosen parameters

$T = 10$ blocks, 3 groups of variables, 40 variables per group & variable number of variables correlated to Y.

Baseline methods & question

2 step methods :

- Imputation : **missMDA**, **softImpute**, **Mean**, **nipals** (mixOmics solution),
- Prediction : **mdd-sPLS**, **Lasso** classical **sPLS** (for **nipals** imputation).

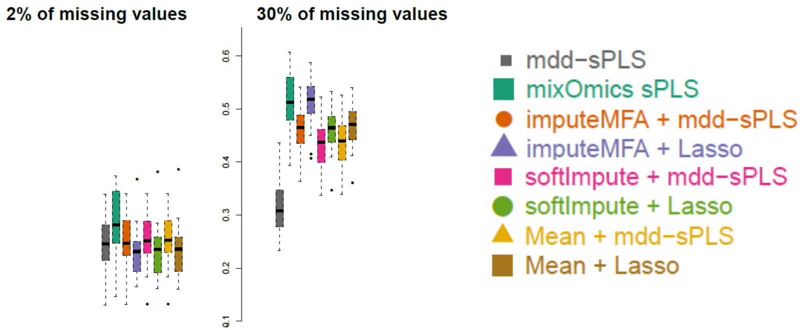
All-in-One method : [Che et al., *Scientific reports*, 2018], dealing with classification problems. Challenging recurrent neural networks. Huge n.

Simulation questions

- Robustness to increasing number of missing values ?
- Robustness to low n and $n << p$?
- Robustness to low inter-block correlations ?

Robustness to increasing number of missing values ?

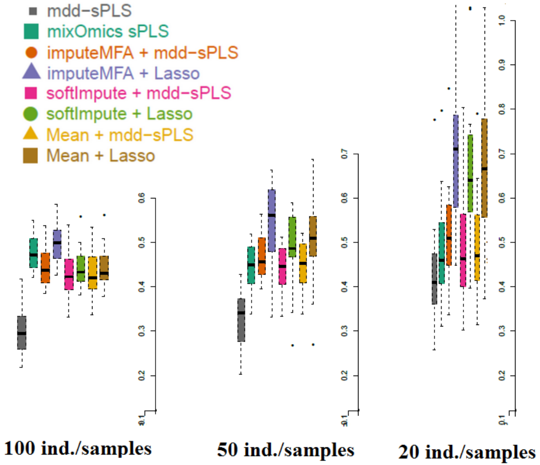
20 samples of **100 individuals** for **10 blocks** of **40 variables each** with **3 principal directions** where only **1** is correlated with the univariate response. $\rho_i = \rho_t = 0.9$. Mean Square Error (MSE).



The answer seems to be **Yes**.

Robustness to low n and $n << p$?

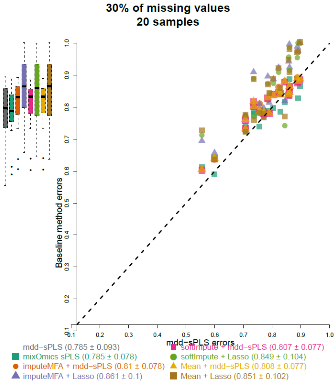
Change the number of individuals. MSE error



The answer seems to be **Yes**.

Robustness to Robustness to low inter-block correlations ?

$\rho_i = 0.9, \rho_t = 0.2$. MSE error



Hard for the all methods
Another type of simulations ?

Application to the real data-set

Comparaison Koh-Lanta/Mean imputation for dd-sPLS model

	Day 28		Day 56		Day 84		Day 180		Mean
	Error	#	Error	#	Error	#	Error	#	Error
Mean $\lambda \approx 0.863$	1.058	2	0.3985	18	1.084	6	1.059	0	0.8711
Koh-Lanta $\lambda \approx 0.865$	1.056	4	0.3796	18	0.9147	17	1.060	1	0.8318
Rel. gain ($\%$)	0.19		4.7		16		-0.094		4.5

Final model : dd-sPLS with Koh-Lanta for $\lambda = 0.8653761$

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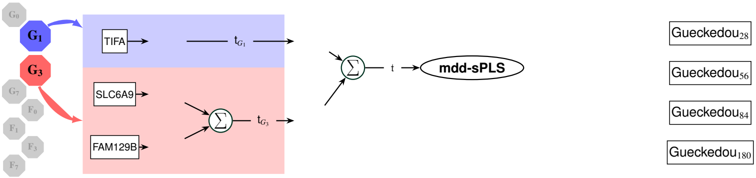

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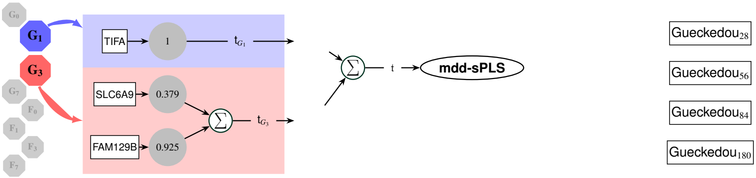

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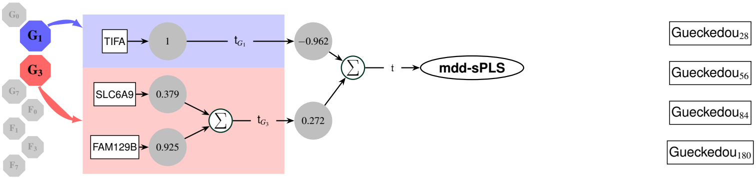

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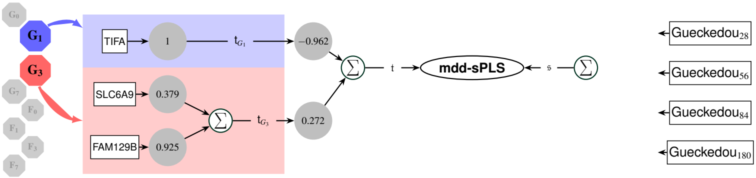

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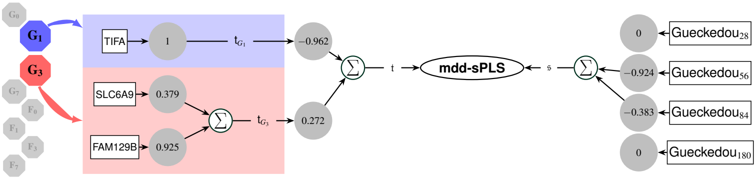

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  The minimum level of correlation between one X (or Y) variable and any of the Y (or X) variables to potentially get this variable in the model.

mdd-sPLS+Koh-Lanta :

- + dd-sPLS,
- Ok according to simulations,
- Works on real data,

Futur work :

- Test on new datasets,
- Publish + Finish package+vignette
- Create kernel dd-sPLS,

Thank you!

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mdd-sPLS : Regression model

Objective and problem

$$\hat{\mathbf{Y}} = \sum_{t=1}^{T} \mathbf{X}_t \mathbf{B}_t,$$

Only $(\mathbf{X}_t \leftrightarrow \mathbf{Y})$ relations used :
$\Longrightarrow$ No adequacy between block components.
$\Longrightarrow$ Re-order components taking all info.

Solution : classical PLS solution on the super-scores

Denoting $\mathbf{b}_t = diag(\beta_t^{(1)}, \cdots, \beta_t^{(R)})_{(R\times R)}$ the super-weights for each block, $\mathfrak{t} = (\sum_{t=1}^{T} \mathbf{X}_t u_t^{(r)} \beta_t^{(r)})_{r=1..R}$ and $\mathfrak{s} = (\mathbf{Y} v^{(r)})_{r=1..R}$:

$$\mathbf{B}_\mathfrak{t} = \mathbf{u}_\mathfrak{t} \mathbf{b}_\mathfrak{t} \mathfrak{u} \mathfrak{a} \mathfrak{v}^T \mathbf{v},^T \qquad \begin{cases} (\mathfrak{u}, \mathfrak{v}) & : \text{Weights of PLS}(\mathfrak{t}, \mathfrak{s}) \\ \mathfrak{a} & = \left(\dfrac{< \mathfrak{s}\mathfrak{v}^{(r)}, \mathfrak{t}\mathfrak{u}^{(r)} >}{||\mathfrak{t}\mathfrak{u}^{(r)}||_2^2}\right)_{r=1..R} \end{cases}$$

Regularization path for rVSV-ZEBOV on mdd-sPLS