Clusterwise multiblock PLS

N'Dèye Niang⁽¹⁾, Stéphanie Bougeard⁽²⁾, Gilbert Saporta⁽¹⁾ & Hervé Abdi⁽³⁾





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Context of clusterwise regression



FIGURE 2. Utility functions and price.

From DeSarbo et al. (1989), Psychometrika

- "For one group of consumers, higher utility corresponds to lower prices ...
- ... while the opposite is true for the other group."



Extension of clusterwise regression to clusterwise multiblock regression



Clusterwise multiblock data features

- Large number of explanatory variables organized in meaningful blocks
 [X¹,...,X^K] (known block structure),
- Several variables Y to explain and predict,
- Unknown cluster structure of the N individuals (in G clusters).

- Clustering: Get the optimal clustering of individuals (cluster number defined in advance) ...,
- Multiblock regression: ... and compute the cluster multiblock regression coefficients within each cluster in order to improve the Y explanation and prediction.



Extension of clusterwise regression to clusterwise multiblock regression



Example of individual clustering in G=2 clusters

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Available clusterwise regression methods: finite mixture models

Mixture model field (clusterwise methods)

- Earliest works: DeSarbo & Cron, 1988; Hennig, 2000
- Minimize ∑_{g=1}^G ||Y_g X_gB_g||² by means of an EM algorithm,
 Y = [y₁,..., y_Q] are mixtures of conditional normal densities of *G* underlying clusters.

Advantages and limits

- Fast algorithm, available programs (commercial softwares, Flexmix R package)
- Necessary conditions
 - Multivariate normal distributions of dependent variables Y,
 - N_g (nb of individuals within the gth cluster) > P (nb of explanatory variables)... but recent extension for high-dimensional data (Lasso estimator, PhD of E. Devijver),
- Oriented towards modelling and not towards prediction.

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Available clusterwise regression methods: geometrical approach

Distance-based model field (typological methods)

- Earliest works: Diday, 1974 (typological factorial analysis); Charles, 1977; Späth, 1979
- Minimize $\sum_{g=1}^{G} \|\mathbf{Y}_g \mathbf{X}_g \mathbf{B}_g\|^2$ by means of a K-means algorithm,
- Interesting extensions to high-dimensional data: typological PCR (Charles, 1977), typological PLS (Vinzi, 2005; Preda, 2005).

Advantages and limits

- No available programs,
- Problem of non-monotonicity decrease of the criterion (batch versus stochastic algorithm),
- Oriented towards both modelling and prediction.



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Proposition: Extend this approach to multiblock regression with high-dimensional data (+ improve monotonicity, prediction and program availability).

Aims & criterion
 Stochastic algorith

33. Prediction

34. Parameter selection

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Clusterwise multiblock PLS: aims

Context: clusterwise multiblock regression.

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Clusterwise multiblock PLS: criterion

Get the optimal clusters on components which summarize **X** Min. the sum of the residuals $\sum_{g=1}^{G} \|\mathbf{Y}_g - \sum_k \mathbf{T}_g^{k(H)} (\mathbf{a}_g^{k(H)} \mathbf{C}_g^{(H)'})\|^2$ where: $\mathbf{T}_g^{k(H)}$ are the matrices of block components with *H* (given) dimensions obtained

from the
$$G$$
 mbPLS, such as $\mathsf{T}_g^{k(H)} = [t_g^{k(1)}| \ldots |t_g^{k(H)}]$

a $a_g^{k(H)}$ are the normalized covariances between components from \mathbf{X}_g^k and \mathbf{Y}_g **(C**₁^{(H)'},..., **C**_G^{(H)'}) are the regression coefficients of \mathbf{Y}_g on ($\sum_k a_g^{k(H)} \mathbf{T}_g^{k(H)}$)



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Clusterwise multiblock PLS: stochastic algorithm

Algorithm

For each individual n

- Compute mbPLS where n belongs alternatively to each of the G clusters
- For each of the G solutions, compute the residual sums
 - $\sum_{g=1}^{G} \|\mathbf{Y}_{g} \sum_{k} \mathbf{T}_{g}^{k(H)} (a_{g}^{k(H)} \mathbf{C}_{g}^{(H)'})\|^{2}$

 Assign n to the cluster which minimize the latter residual sums.

- 2 Select the best initialization to get the optimal individual clusters.
- 3 Compute the *G* mbPLS within each optimal cluster.
- 4 Several initializations (random clusters of the *N* individuals to *G* clusters)

Comments

1 Decreasing monotonicity of the criterion $\sum_{g=1}^{G} \|\mathbf{Y}_{g} - \sum_{k} \mathbf{T}_{g}^{k(H)} (a_{g}^{k(H)} \mathbf{C}_{g}^{(H)'})\|^{2}$ according to *n*

2 Get the G clusters.

- 3 Get the G regression coefficients matrices.
- 4 Avoid local optimum

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Clusterwise multiblock PLS: prediction of new individuals

Problem: Assign a new individual to its optimal cluster and predict its dependent variable values.

Bayesian affectation to clusters

- Project the new individual into each of the G component spaces from the cw.mbpls model (X_{new} → T^{k(H)}_{g,new}),
- Process the Bayesian Mahalanobis distances between the new individual and the G cluster gravity centres; transform them into probabilities,
- Maximize the G probabilities $(proba_g) \rightarrow cluster$ membership of the new individual.

Averaging prediction

$$\hat{\mathbf{Y}}_{new} = \sum_{g=1}^{G} proba_g \times [\sum_k \mathbf{T}_{g,new}^k (a_g^k \mathbf{C}_g')]$$

This prediction takes into account the predictions to the G clusters.



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Clusterwise multiblock PLS: parameter selection (10-fold cross-validation)

Aims

■ Parameter selection: minimize the RMSE_{G,H} processed for several model dimensions H and several cluster numbers G → get H_{opt} and G_{opt},

Algorithm: 10-fold cross-validation

- Split the data into ten folds,
- Apply clusterwise multiblock PLS on the train data (9/10 folds),
- Get the assignation to clusters and the predictions of the test data (1/10 fold),
- Compare the observed and the predicted dependent values \rightarrow RMSE.



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Simulation study
 Real example

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Simulation: multiblock data

Several Y variables, limited number of observations compared to the number of explanatory variables, multiblock case



Simulated data features

- G=2 clusters with the same size, volume, orientation and shape,
- Limited number of N=32 individuals compared to P=20 explanatory variables X (max. of 16 individuals within each cluster),
- X variables organized in K=2 blocks
 - $X^1 X^{10}$ are correlated (cor=0.8) and not correlated with $X^{11} - X^{20}$ (cor=0.1)
 - $X^{11} X^{20}$ are correlated (cor=0.8) and not correlated with $X^1 - X^{10}$ (cor=0.1)
- Q=2 dependent variables Y, positively linked with X for the cluster 1 and negatively for the cluster 2.



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Simulation: clusterwise multiblock PLS performance

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Selection of the optimal number of components (10-fold cross-validation)



 \rightarrow Optimal number of components selected: 2

Cluster 1 (model with 2 components)

Cluster 2 (model with 2 components)

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Cluster 1 (model with 2 components)

Expected regression coefficients: 0.1 (for all explanatory and dependent variables)



100% of corresponding results (10 random initializations)

Cluster 2 (model with 2 components)

Expected regression coefficients: -0.1 (for all explanatory and dependent variables)



100% of corresponding results (10 random initializations)

Simulation study
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Indoor air quality data: multiblock data & aims



Data features [Kirchner et al., 2007]

- Y: 2 pollutants
- X: 14 potential risk factors of pollution organized into 3 blocks: household characteristics (5 var.), dwelling structure (4 var.), living habits (5 var.)
- Individuals: 199 main residences
- Pre-processing: Variables are centred and scaled; block are weighted to have the same weight.

- Clustering: Get the optimal clustering of residences ...,
- **Regression:** ... and compute the multiblock regression coefficients within each residence cluster to improve the pollutant prediction.



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Indoor air quality data: comparison to the global model & parameter selection



- Comparison to the global model: (small) RMSE improvement in comparison with "no cluster"
- Selection of the optimal number of clusters: 3 ($N_g = [90, 58, 51]$)
- Selection of the optimal number of model dimensions: 1



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Indoor air quality data: cluster regression coefficients

Dependent variable: acroleine, significant regression coefficients by means of bootstrap simulations



- Cluster 1: significantly linked to the number and the age of children,
- Cluster 2: significantly linked to housing age, rate of laminate ground, number of solvent use and ground cleaning,
- Cluster 3: significantly linked to housing age, number of persons and of more than 10y-children and number of barbecues.



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Indoor air quality data: cluster block importance

Significant block importance by means of bootstrap simulations



- Household characteristics: average effect for all clusters,
- **Dwelling structure**: significantly less important for cluster 2,
- Living habits: significantly more important for cluster 2.



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 - Aim: improve the prediction,
 - Meaningful criterion to minimize,
 - Parameters (number of dimensions and clusters) obtained through cross-validation,
 - Prediction of new individuals (clusters, predicted Y values).
- Useful tools to deal with real data especially in biology (*e.g.*, different risk factors of a disease according to sub-populations).

Perspectives

- Any other supervised multiblock methods can be included in the algorithm,
- Next step: allow specific clusters (and dimensions) for each block (Y,X¹,...,X^K),
- Programs will be transformed into a R package.



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