Tensor multiblock logistic regression

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Tensor data

Measuring the same variables across several modalities (position, time, etc...) $\rightarrow$ features with tensor structure.

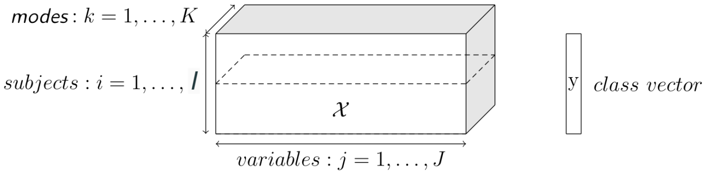

Figure 1: Type of data: tensorial

Warning: Often strong correlation between features of the same variable across different modalities $\rightarrow$ adapt the model to this structure.

Multiblock data

Each block is a tensor with its own structure.

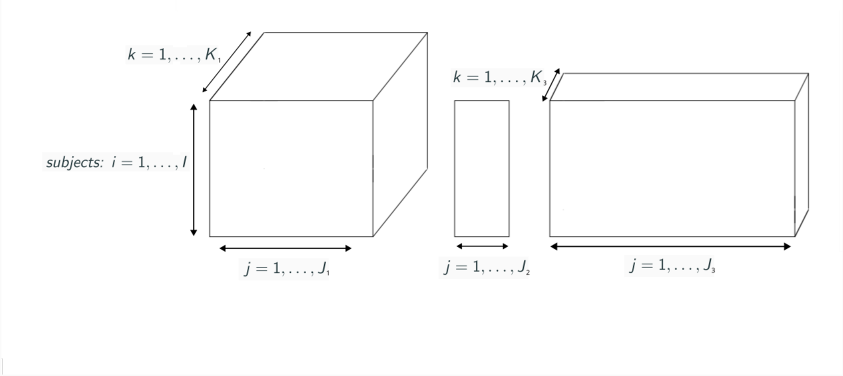

Figure 2: Type of data: multiblock

Application example of real multiblock tensor data

classification of liver tumors through MRI:

Same variables extracted from each MRI image at 3 times (arterial, portal, late) $\rightarrow$ **tensor structure**

• MRI images in 3D of liver tumors. Information about grey levels, shape and correlations $\rightarrow$ **multiblock structure**

• Also include univariate features: gender and age

Conclusion: **Multiblock tensor data** $\rightarrow$ train a tensor multiblock logistic regression model.

Some MRI images

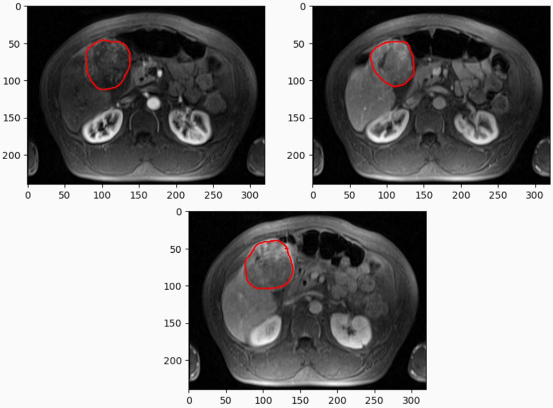

Figure 3: Example of MRI images of a liver tumor (arterial, portal, late) from From Henri Mondor hospital: the 3 images look quite similar

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New model for logistic regression

Logistic regression

Generalized linear regression model for classification:

$$x : \text{ features vector} \tag{1}$$

$$Y : \text{ binary response (explained variable)} \tag{2}$$

$$P(Y = 1|x) = \frac{\exp(\beta_0 + \boldsymbol{x}^T\boldsymbol{\beta})}{1 + \exp(\beta_0 + \boldsymbol{x}^T\boldsymbol{\beta})}$$

Defines a likelihood function $\mathcal{L}(\boldsymbol{\beta}) = \prod_{i=1}^{I} P(Y_i = y_i|x_i)$.

penalization

To many features (vs I) $\rightarrow$ need to limit variance of prediction.

Search for sparse easily interpretable model $\rightarrow$ choice of lasso:

$$\text{penalization} = \lambda \|\boldsymbol{\beta}\|_1 \qquad (\lambda > 0)$$

Function to minimize :

$$-\log(\mathcal{L}(\boldsymbol{\beta})) + \lambda \|\boldsymbol{\beta}\|_1$$

Convex optimization problem.

Naive approach: unfolding

$\boldsymbol{\beta} = (\beta_{j,k})_{j \in [\![1,J]\!], k \in [\![1,K]\!]}$ so JK parameters to determine.

$$x^T \boldsymbol{\beta} \rightsquigarrow \sum_k \sum_j \beta_{j,k} x_{j,k} \quad \text{and} \quad \|\boldsymbol{\beta}\|_1 = \sum_k \sum_j |\beta_{j,k}|$$

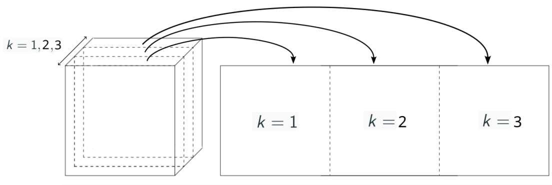

Figure 4: Unfolding a tensor

Limitation of lasso: Elimination of features without specific consideration for the same feature at other times/ other features at the same time.

Group lasso

Common solution: grouping regression coefficients together in the penalization.

$$\sum_{j,k} |\beta_{j,k}| \rightsquigarrow \sum_{g=1}^{G} \|\beta^g\|_2$$

Tendency to set regression coefficients to zero by entire blocks.

Downsides:

- grouping either by mode or by variable, not both.
- no tensor structure (or at least grouping of variables) in the likelihood term.

Tensor regression models

Idea: each variable and mode has its own influence on the prediction (i.e. on $\boldsymbol{\beta}$) [2].

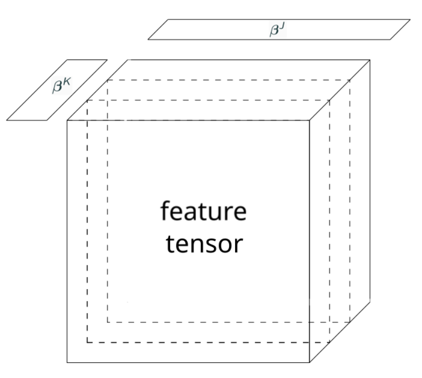

Figure 5: Tensor structure of $\boldsymbol{\beta}$

Tensor regression models

Idea: each variable and mode has its own influence on the prediction (i.e. on $\boldsymbol{\beta}$) [2].

For J variables observed on K modalities (e.g. times)

$$\beta_{j,k} = \beta_j^J \beta_k^K$$

β_j : impact of variable j

β_k : impact of modality k

Only $J + K$ parameters to determine (instead of JK).

Limits of rank 1

$\beta_{j,k} = \beta_j^J \beta_k^K$ implies that $\boldsymbol{\beta}$ looks like:

Figure 6: Example of rank 1 pictogram (only 0 and 1)

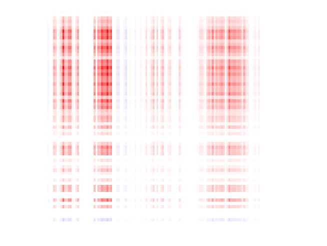

Figure 7: Example of rank 1 matrix (all values allowed)

This can be too simplistic.

Rank R tensor logistic regression [1]

$$\text{Summing rank 1 together : } \beta_{j,k} = \sum_{r=1}^{R} \beta^J_{j,r}\beta^K_{k,r}$$

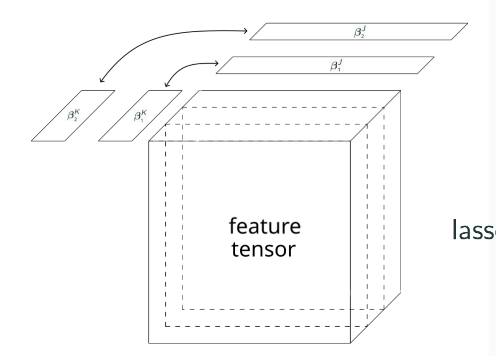

Figure 8: Tensor structure of $\boldsymbol{\beta}$

$$\text{lasso} \rightsquigarrow \lambda \sum_{r=1}^{R} \left(\|\boldsymbol{\beta}^J_r\|_1 \|\boldsymbol{\beta}^K_r\|_1 \right)$$

Blocks of variables

Problem: Several groups of variables of different natures (first order, shape, texture). But β_r^K and β_r^J common to all groups. $K_1 = K_2 = K_3$ needed or else:

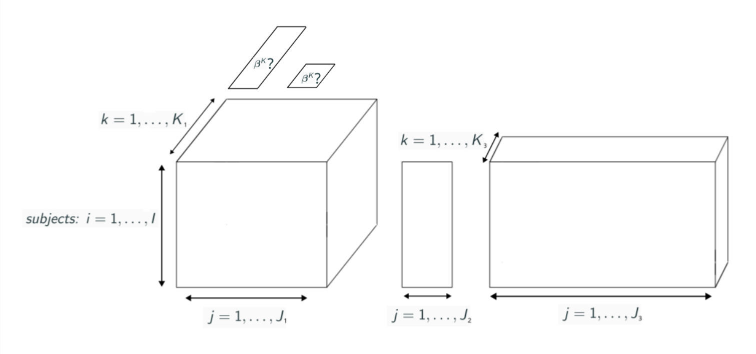

Figure 9: Problem if blocks have different orders or dimensions

Tensor multiblock logistic regression

Solution: giving each block its own β^J and β^K.

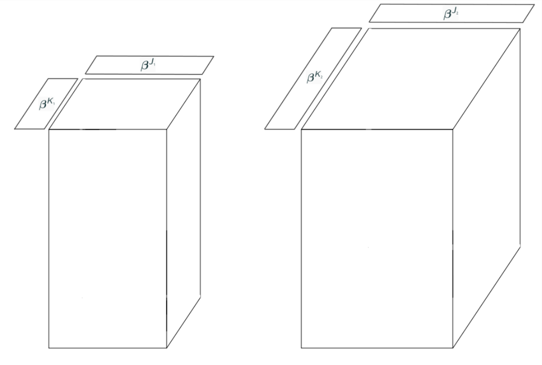

Figure 10: Tensor multiblock model for rank 1

Tensor multiblock logistic regression

Mathematically, this gives (for L blocks):

$$\mathbf{x}^T \boldsymbol{\beta} \rightsquigarrow \sum_{\ell=1}^{L} \sum_{j,k} x^{\ell}_{j,k} (\beta_\ell)_{j,k}$$

With, for rank 1: $(\beta_\ell)_{j,k} = (\beta^J_\ell)_j (\beta^K_\ell)_k$

But each $\boldsymbol{\beta}_\ell$ can have a different rank R_ℓ, which gives:

$$(\beta_\ell)_{j,k} = \sum_{r=1}^{R_\ell} (\beta^J_{\ell,r})_j \, (\beta^K_{\ell,r})_k$$

Lasso penalty $\rightsquigarrow \lambda \sum_{\ell,r} \left(\|\boldsymbol{\beta}^K_{\ell,r}\|_1 \|\boldsymbol{\beta}^J_{\ell,r}\|_1 \right)$

Fitting algorithm

likelihood term

Likelihood term of the loss determined by

$$\mathbf{x}^T \boldsymbol{\beta} = \sum_{\ell,r,j} \left(\sum_k x^{\ell}_{j,k} (\beta^K_{\ell,r})_k \right) (\beta^J_{\ell,r})_j \tag{3}$$

$$= \sum_{\ell,r,k} \left(\sum_j x^{\ell}_{j,k} (\beta^J_{\ell,r})_j \right) (\beta^K_{\ell,r})_k \tag{4}$$

Strategy: alternating logistic regressions (to optimize respectively $\boldsymbol{\beta}^J$ and $\boldsymbol{\beta}^K$).

If a mode is inexistent in a block, renumber the modes of that block to perform the optimization on another (existing) mode of this block.

Lasso penalty in fitting algorithm

$$\text{penalty} \propto \sum_{\ell,r} \left(\|\boldsymbol{\beta}^K_{\ell,r}\|_1 \|\boldsymbol{\beta}^J_{\ell,r}\|_1 \right) \tag{5}$$

$$= \sum_{\ell,r} \left(\left\| \|\boldsymbol{\beta}^K_{\ell,r}\|_1 \boldsymbol{\beta}^J_{\ell,r} \right\|_1 \right) = \sum_{\ell,r} \left(\left\| \|\boldsymbol{\beta}^J_{\ell,r}\|_1 \boldsymbol{\beta}^K_{\ell,r} \right\|_1 \right) \tag{6}$$

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Strategy: dilate $\beta^J_{\ell,r}$ by $\|\boldsymbol{\beta}^K_{\ell,r}\|_1$ and $x^\ell_{j,k}$ by $\|\boldsymbol{\beta}^K_{\ell,r}\|_1^{-1}$, so

$$\mathbf{x}^T \boldsymbol{\beta} = \sum_{j,\ell,r} \left(\sum_k x^\ell_{j,k} (\beta^K_{\ell,r})_k \right) (\beta^J_{\ell,r})_j$$

does not change but

$$\|\boldsymbol{\beta}^J\|_1 \rightsquigarrow \sum_{\ell,r} \left(\|\boldsymbol{\beta}^K_{\ell,r}\|_1 \|\boldsymbol{\beta}^J_{\ell,r}\|_1 \right)$$

Lasso penalty in fitting algorithm

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does not change but

$$\|\boldsymbol{\beta}^J\|_1 \rightsquigarrow \sum_{\ell,r} \left(\|\boldsymbol{\beta}^K_{\ell,r}\|_1 \|\boldsymbol{\beta}^J_{\ell,r}\|_1 \right)$$

Then, do logistic lasso regression with $\mathbf{x} = (x^l_{ijk} \|\boldsymbol{\beta}^K_{\ell,r}\|_1^{-1})$ and λ penalty coefficient to find $\left((\beta^J_{\ell,r})_j \|\boldsymbol{\beta}^K_{\ell,r}\|_1 \right)$.

Stopping criterion

Before each optimization cycle, calculate the loss:

$$C = -\log(\mathcal{L}(\beta)) + \text{penalty}$$

Before the t-th optimization cycle, its value is C^t and after this cycle it becomes C^{t+1}.

End the optimization when:

$$|C^{t+1} - C^t| < \epsilon |C^t|$$

(typically $\epsilon = 10^{-4}$)

Simulations and results

Aim of the simulations

Allow to choose

- Difficulty of the classification (overlap between classes, distance between means of classes etc ...)
- Balance between classes
- Structure of the regression parameter $\boldsymbol{\beta}$ (several blocks)

Allow to evaluate

- Quality of the classification (Area Under the ROC Curve : AUC)
- Quality of the reconstruction of $\boldsymbol{\beta}$

Illustration in 2D

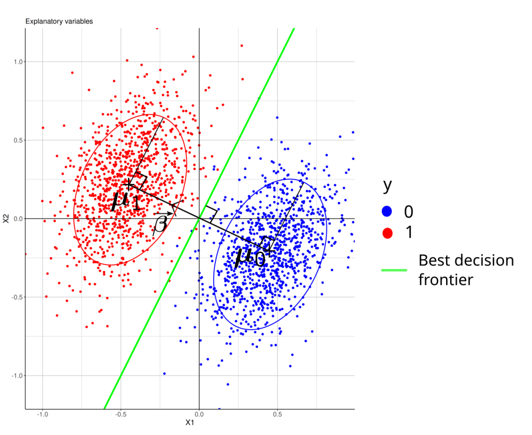


Figure 11: Example of explanatory variables for $\beta = (-2, 1)$

Data generation

Choose the $\boldsymbol{\beta}$ to be reconstructed (pictograms).

Generate the $(\mathbf{x}_i)_{i \in [\![1,I]\!]}$ with 2 multivariate normal laws of means $\boldsymbol{\mu}_0$ and $\boldsymbol{\mu}_1$ and common covariance matrix $\boldsymbol{\Sigma}$ such that:

- $\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0$ colinear to $\boldsymbol{\beta}$
- One of the principal axis of $\boldsymbol{\Sigma}$ colinear to $\boldsymbol{\beta}$

Separation of classes linked with eigenvalues of $\boldsymbol{\Sigma}$ (to be compared with $\|\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0\|$).

AUC simulated data

Table 1: Cross validated AUC for each model on simulated data for 3000 individuals

$(\sigma_{\boldsymbol{\beta}}, \sigma_{\text{noise}})$	lasso	g.l. (blocks)	g.l. (mode)	g.l. (var)	tensor	tensor blocks
(0.1,0.5)	0.83	0.86	0.94	0.94	0.99	0.99
(0.1,0.8)	0.63	0.64	0.68	0.68	0.93	0.99

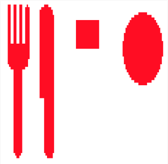
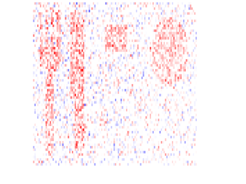
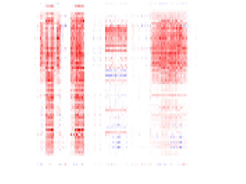


Figure 12: Pictogram of shape 66×117

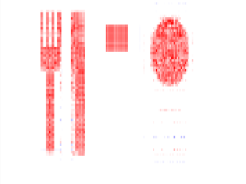
Reconstructed β



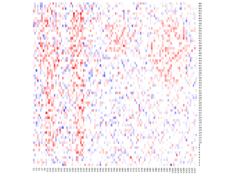
(a) lasso
$(\sigma_{\beta}, \sigma_{\text{noise}}) = (0.1, 0.5)$



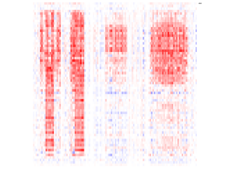
(b) tensor $R : 10$
$(\sigma_{\beta}, \sigma_{\text{noise}}) = (0.1, 0.5)$



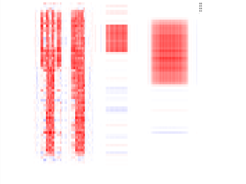
(c) T.M. $R : (12, 1, 10)$
$(\sigma_{\beta}, \sigma_{\text{noise}}) = (0.1, 0.5)$



(d) lasso
$(\sigma_{\beta}, \sigma_{\text{noise}}) = (0.1, 0.8)$



(e) tensor $R : 10$
$(\sigma_{\beta}, \sigma_{\text{noise}}) = (0.1, 0.8)$



(f) T.M. $R : (6, 1, 1)$
$(\sigma_{\beta}, \sigma_{\text{noise}}) = (0.1, 0.8)$

Interpretation of the results

Better reconstruction by tensor multiblock logistic model.

Performance (AUC) in adequation with quality of reconstruction (because small changes in $\boldsymbol{\beta} \rightsquigarrow$ big changes in the classification, when σ_{noise} increases).

Efficient sparse (low rank) approximation of pictograms by tensor multiblock logistic model in contrast with simple tensor model.

Tendency to choose rank 1 for both tensor model when too few data (or too high noise).

Application of proposed logistic regression to liver tumor classification

Feature extraction with pyradiomics [4]

Extraction of $\simeq 100$ features (about intensities, shape, texture) for each 2D or 3D image.

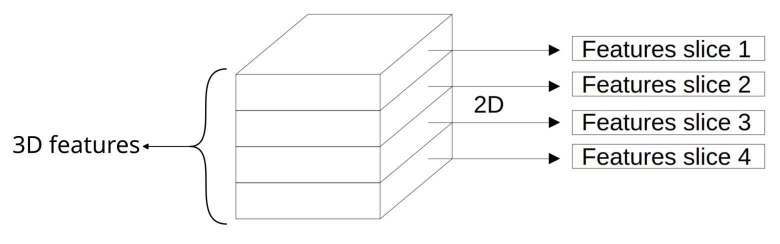


Figure 14: Feature extraction with pyradiomics for an MRI image composed of 4 slices

Results

Type of data	lasso	g.l. (block)	g.l. (time)	g.l. (var)	tensor	tensor blocks
3D	0.74 ± 0.04	0.78 ± 0.03	0.76 ± 0.03	0.73 ± 0.03	0.77 ± 0.03	0.77 ± 0.03

Cross validated AUC on 3D real data

Type of data	lasso	g.l. (block)	g.l. (slice)	g.l. (time)	g.l. (var)	tensor	tensor blocks
2D	0.73± 0.03	0.71± 0.03	0.70± 0.04	0.71± 0.03	0.71± 0.03	0.66± 0.04	0.71± 0.03

Cross validated AUC on 2D real data

Conclusion

State of the art performances.

Better than state of the art in simulated data when few overlapping between classes.

Scales better than regular logistic regression for high order tensors.

Lowers the complexity of the regression model an therefore reduces overfitting.

Good interpretability (sparse + displays importance of each block, mode and variable in $\boldsymbol{\beta}$).

Further work

Testing on other real datasets wether the performances on the simulated dataset can be replicated.

Testing other penalizations (group lasso, elastic net).

Extending the multiblock approach to other classical machine learning algorithms (other GLMs, SVM etc...). Comparing it to CNN.

Improving the optimization, by using coordinate descent (as done in glmnet [3] in R).

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