

# Mixture of multivariate multiple-scaled Student distributions : application to the characterization of brain tumors.

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1<sup>st</sup> year-PhD

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# Outline

- 1 Motivation : brain tumor characterization
- 2 Clustering of MRI data
- 3 Mixture of multivariate multiple-scaled Student distributions
- 4 Estimation of a MMSD mixture
- 5 Tumor characterization from multiparametric MRI
- 6 Bayesian extension
- 7 Work in progress

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## How to characterize brain tumor ?

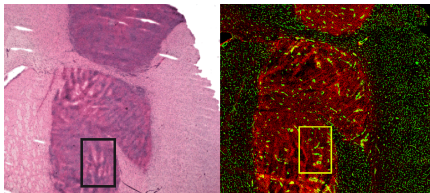
Healthy ?



Not healthy ?

# How to characterize brain tumor ?

## Histology vs multiparametric MRI

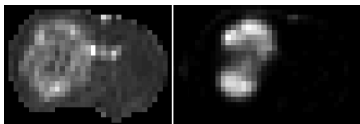


Histology section

- + gold standard : provides the ground truth
- + precise information
- local information : only parts of the tumor may be sampled
- invasive operation (biopsy), not always feasible

# How to characterize brain tumor ?

## Histology vs multiparametric MRI



2 MRI maps

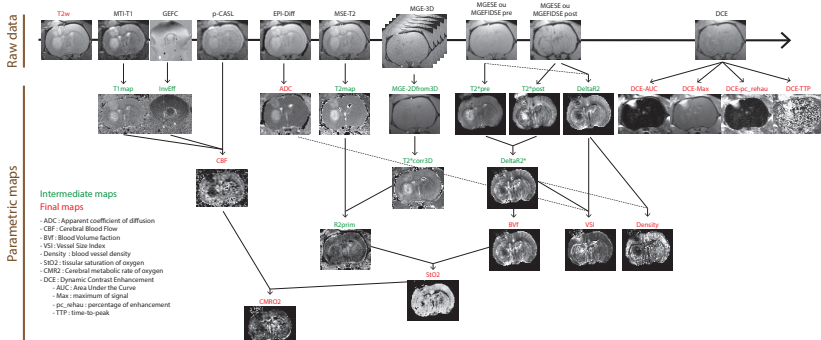
- under development method
- + global information : whole tumor visible
- + non-invasive operation

**Goal** : find the voxels inside the MRI maps which belong to the tumor, in order to characterize a tumor, to avoid invasive biopsies.

# How to characterize brain tumor ?

## Problem of multiparametric MRI

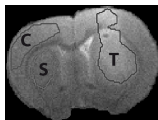
### How to extract information from all of the parametric maps ?



► **Approach** : multivariate clustering with mixture models.

# How to characterize brain tumor ?

Previous study (Coquery *et al.* 2014)

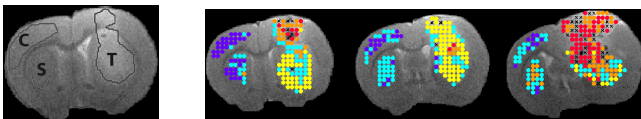


- 3 Regions of interest were manually delimited on each MRI map :
- 2 healthy regions on the left (Cortex and Striatum)
  - 1 tumor region on the right (Tumor)



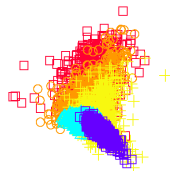
# How to characterize brain tumor ?

Previous study (Coquery *et al.* 2014)



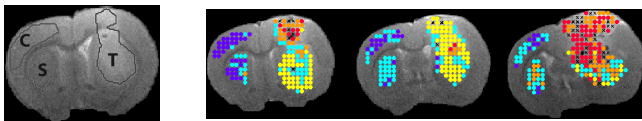
Voxels were partitioned using a Gaussian mixture into a number of classes :

- + link between classes and tissue types
- tissue values may not have Gaussian shapes



# How to characterize brain tumor ?

Previous study (Coquery *et al.* 2014)

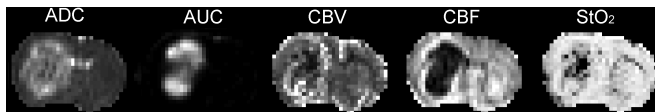


- ▶ Proposed approach : classification of voxels using a mixture of heavy-tailed distributions, the multivariate multiple-scaled Student distributions (MMSD).

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## Multiparametric MRI data



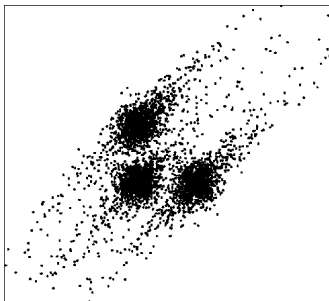
- 5 physiological parameters :
  - **ADC** : apparent diffusion coefficient
  - **CBV** : cerebral blood volume
  - **CBF** : cerebral blood flow
  - **AUC** : blood vessel permeability
  - **StO<sub>2</sub>** : oxygen saturation

- 5 dimensional data set :

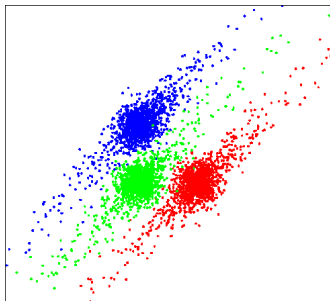
$\mathbf{Y} = \{\mathbf{Y}_1, \dots, \mathbf{Y}_N\}$  the set of all voxels, of size  $N$   
with  $\mathbf{Y}_n = \{\mathbf{Y}_{n,ADC}, \dots, \mathbf{Y}_{n,StO_2}\}$  the mesures on the nth voxel

## Clustering of MRI data

We suppose that data arise from  $K$  different classes (for  $K$  different tissues), and we want to recover those classes.



Simulated data



Latent classification

## Clustering of MRI data via mixture modeling

Let  $\mathbf{Z}$  be the latent variable which links one observation to one class :

$$\begin{cases} (\mathbf{Y}_n | \mathbf{Z}_n = k) & \sim f_k(\boldsymbol{\theta}_k) \\ \mathbf{Z}_n & \sim \mathcal{M}(\pi_1, \dots, \pi_K) \end{cases} \quad (1)$$

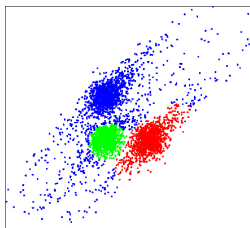
$\Leftrightarrow$

$$\Pr(\mathbf{y}_n; \boldsymbol{\theta}) = \sum_{k=1}^K \pi_k f_k(\mathbf{y}_n; \boldsymbol{\theta}_k) \quad (2)$$

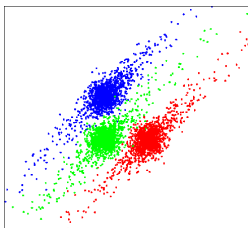
## Clustering of MRI data via mixture modeling

In the previous study,  $f_k(\theta_k) = \mathcal{N}_5(\mu_k, \Sigma_k)$  with  $\mu_k \in \mathbb{R}^5$  and  $\Sigma_k \in \mathcal{S}_{5 \times 5}^+(\mathbb{R})$  : lack of flexibility in cluster shape modeling (Coquery *et al.* - 2014).

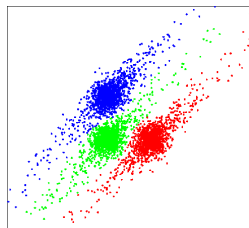
In this study,  $f_k(\theta_k)$  is a heavy-tailed distribution : a multivariate multiple-scaled Student distribution (MMSD).



Gaussian



Simulation



MMSD

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# Clustering

## Gaussian mixture

- Mixture model :

$$\Pr(\mathbf{y}_n; \boldsymbol{\theta}) = \sum_{k=1}^K \pi_k f_k(\mathbf{y}_n; \boldsymbol{\theta}_k) \quad (3)$$

$$f_k(\boldsymbol{\theta}_k) \sim \mathcal{N}_M(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \quad (4)$$

With :  $\boldsymbol{\mu}_k \in \mathbb{R}^M$ ,  $\boldsymbol{\Sigma}_k \in \mathcal{S}_{M \times M}^+(\mathbb{R})$

- Decomposition of the covariance matrix for a better flexibility :

$$\boldsymbol{\Sigma}_k = \mathbf{U}_k \mathbf{D}_k \mathbf{U}_k^t \quad (5)$$

with :

$\mathbf{U}_k \in \mathcal{O}(M)$  the orthogonal matrix of eigenvectors

$\mathbf{D}_k \in \mathcal{D}(M)$  the diagonal matrix of eigenvalues

# Clustering

## Gaussian mixture

- Decomposition of the covariance matrix :

$$\Pr(\mathbf{y}_n ; \boldsymbol{\theta}) = \sum_{k=1}^K \pi_k f_k(\mathbf{y}_n ; \boldsymbol{\theta}_k) \quad (3)$$

$$f_k(\boldsymbol{\theta}_k) \sim \mathcal{N}_M(\boldsymbol{\mu}_k, \mathbf{U}_k, \mathbf{D}_k) \quad (4)$$

With :  $\boldsymbol{\mu}_k \in \mathbb{R}^M, \mathbf{U}_k \in \mathcal{O}(M), \mathbf{D}_k \in \mathcal{D}(M)$

- Tractable estimation using an Expectation-Maximization (EM) algorithm and a minimization algorithm of type Flury and Gautschi for the orthogonal matrices.
- The Gaussian tail is very short and sensitive to atypical observations (outliers).

# Clustering

## Student mixture

Mixture model with one-dimensional Student distributions :

$$\begin{aligned}
 \Pr(y_n ; \boldsymbol{\theta}) &= \sum_{k=1}^K \pi_k f_k(y_n ; \boldsymbol{\theta}_k) \\
 f_k(\boldsymbol{\theta}_k) &\sim t_1(\mu_k, \sigma_k^2, \nu_k) \\
 t_1(y_n ; \mu_k, \sigma_k^2, \nu_k) &= \frac{\Gamma\left(\frac{\nu_k+1}{2}\right)}{\sigma_k \Gamma\left(\frac{\nu_k}{2}\right) (\pi \nu_k)^{\frac{1}{2}}} \left[ 1 + \frac{(y_n - \mu_k)^2}{\nu_k \sigma_k^2} \right]^{-\frac{\nu_k+1}{2}} \quad (5)
 \end{aligned}$$

- How to get a multidimensional Student distribution ?

## Standard multivariate Student distribution

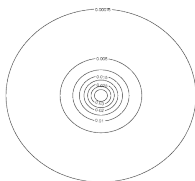
One possible generalization to a  $M$ -dimensional distribution

$$p_{\text{MS}}(\mathbf{y}; \boldsymbol{\mu}, \boldsymbol{\Sigma}, \nu) = \frac{\Gamma\left(\frac{\nu+M}{2}\right)}{|\boldsymbol{\Sigma}|^{\frac{1}{2}} \Gamma\left(\frac{\nu}{2}\right) (\pi\nu)^{\frac{M}{2}}} \left[ 1 + \frac{\delta^2(\mathbf{y}, \boldsymbol{\mu}, \boldsymbol{\Sigma})}{\nu} \right]^{-\frac{\nu+M}{2}}$$

with :  $\delta^2(\mathbf{y}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = (\mathbf{y} - \boldsymbol{\mu})^t \boldsymbol{\Sigma}^{-1} (\mathbf{y} - \boldsymbol{\mu})$

the Mahalanobis distance

- But the degree of freedom remains scalar.



$\nu = 5$



$\nu = 10$

## Standard multivariate Student distribution

Useful representation : infinite mixture of scaled Gaussians

$$\begin{aligned} p_{\text{MS}}(\mathbf{y}; \boldsymbol{\mu}, \boldsymbol{\Sigma}, \nu) &= \frac{\Gamma\left(\frac{\nu+M}{2}\right)}{|\boldsymbol{\Sigma}|^{\frac{1}{2}} \Gamma\left(\frac{\nu}{2}\right) (\pi\nu)^{\frac{M}{2}}} \left[1 + \frac{\delta^2(\mathbf{y}, \boldsymbol{\mu}, \boldsymbol{\Sigma})}{\nu}\right]^{-\frac{\nu+M}{2}} \\ &= \int_0^{\infty} \mathcal{N}_M\left(\mathbf{y}; \boldsymbol{\mu}, \frac{1}{w} \boldsymbol{\Sigma}\right) \mathcal{G}\left(w; \frac{\nu}{2}, \frac{\nu}{2}\right) dw \end{aligned}$$

with :

$\mathcal{N}_M$  the M-multivariate Gaussian distribution

$\mathcal{G}$  the Gamma distribution

the real latent variable  $w$  is called the weight

# Multivariate multiple-scaled Student distribution

Use of the eigenvalue decomposition to get a multidimensional degree of freedom  
(Forbes and Wraith - 2014)

Let  $U$  and  $D$  the eigenvalue decomposition of the symmetric positive definite  $T = \Sigma^{-1}$  :  $T = UDU^t$  .

$$\rho_{MS}(\mathbf{y} ; \boldsymbol{\mu}, U, D, \nu) = \int_{\mathbb{R}_+^*} \mathcal{N}_M \left( \mathbf{y} ; \boldsymbol{\mu}, \frac{1}{w} U D^{-1} U^t \right) \mathcal{G} \left( w ; \frac{\nu}{2}, \frac{\nu}{2} \right) dw$$

## Multivariate multiple-scaled Student distribution

Use of the eigenvalue decomposition to get a multidimensional degree of freedom  
(Forbes and Wraith - 2014)

Let  $U$  and  $D$  the eigenvalue decomposition of the symmetric positive definite  $T = \Sigma^{-1}$  :  $T = UDU^t$ .

Let  $\mathbf{W} \in \mathbb{R}_{+*}^M$  a  $M$ -dimensional weight (one scalar weight for each dimension) :

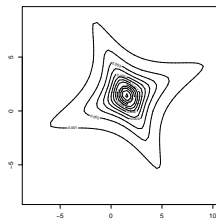
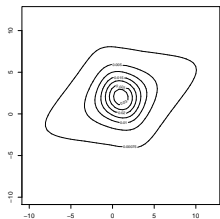
$$p_{\text{MMS}}(\mathbf{y}; \boldsymbol{\mu}, U, D, \boldsymbol{\nu}) = \int_{\mathbb{R}_{+*}^M} \mathcal{N}_M(\mathbf{y}; \boldsymbol{\mu}, U \text{diag}(\mathbf{w})^{-1} D^{-1} U^t) \prod_{m=1}^M \mathcal{G}\left(w_m; \frac{\nu_m}{2}, \frac{\nu_m}{2}\right) d\mathbf{w}$$

# Multivariate multiple-scaled Student distribution

Use of the eigenvalue decomposition to get a multidimensional degree of freedom  
(Forbes and Wraith - 2014)

$$p_{\text{MMS}}(\mathbf{y}; \boldsymbol{\mu}, \mathbf{U}, \mathbf{D}, \boldsymbol{\nu}) =$$

$$\int_{\mathbb{R}_{+*}^M} \mathcal{N}_M(\mathbf{y}; \boldsymbol{\mu}, \mathbf{U} \text{diag}(\mathbf{w})^{-1} \mathbf{D}^{-1} \mathbf{U}^t) \prod_{m=1}^M \mathcal{G}(w_m; \frac{\nu_m}{2}, \frac{\nu_m}{2}) dw$$





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# Estimation of a MMSD mixture

## Mixture of MMSD

- density of the model :

$$p(\mathbf{y}_n; \boldsymbol{\theta}) = \sum_{k=1}^K \pi_k p_{\text{MMSD}}(\mathbf{y}_n; \boldsymbol{\mu}_k, \mathbf{U}_k, \mathbf{D}_k, \boldsymbol{\nu}_k)$$

$$\text{with : } \boldsymbol{\theta} = \{\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_K\}$$

$$\boldsymbol{\theta}_k = (\pi_k, \boldsymbol{\mu}_k, \mathbf{U}_k, \mathbf{D}_k, \boldsymbol{\nu}_k)$$

- estimation of parameters :
  - a simple EM algorithm
  - with a Flury and Gautschi algorithm for the orthogonal matrices

# Estimation of a MMSD mixture

## EM algorithm

For  $k \in \{1, \dots, K\}$ , and  $n = \{1, \dots, N\}$  :

- $Z_n$  is the unknown class variable :  $\Pr(Z_n = k) = \pi_k$
- $W_n$  is the unknown weight
- $\Delta_n = \text{diag}(W_n) = \text{diag}(W_{n1}, \dots, W_{nM}) \in \mathbb{R}_{+*}^M$

$$Y_n | Z_n = k, W_n = w_n ; \mu_k, U_k, D_k \sim \mathcal{N}_M(\mu_k, U_k \Delta_n^{-1} D_k^{-1} U_k^t)$$

$$W_n | Z_n = k ; \nu_k \sim \bigotimes_{m=1}^M \mathcal{G}\left(\frac{\nu_{km}}{2}, \frac{\nu_{km}}{2}\right)$$

$$Z_n ; \pi \sim \mathcal{M}(1, \pi_1, \dots, \pi_K)$$

# Estimation of a MMSD mixture

## Outliers accommodation

At the E-step of the iteration  $r$ , the conditional density use :

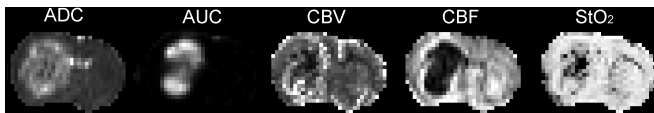
$$\begin{aligned}
 \mathbf{w}_{nk}^{(r)} &= \left( w_{nk1}^{(r)}, \dots, w_{nkM}^{(r)} \right) \\
 \text{with : } w_{nkm}^{(r)} &= \mathbb{E} \left[ W_{nm} \mid Z_n = k, \mathbf{y}_n ; \boldsymbol{\theta}^{(r)} \right] \\
 &= \frac{\nu_{km}^{(r)} + 1}{\nu_{km}^{(r)} + \left[ \mathbf{D}_k^{(r)} \right]_m \left[ \mathbf{U}_k^{(r)\top} \left( \mathbf{y}_n - \boldsymbol{\mu}_k^{(r)} \right) \right]_m^2} \quad (6)
 \end{aligned}$$

The higher  $\left[ \mathbf{D}_k^{(r)} \right]_m \left[ \mathbf{U}_k^{(r)\top} \left( \mathbf{y}_n - \boldsymbol{\mu}_k^{(r)} \right) \right]_m^2$ , the more the observation is atypical.

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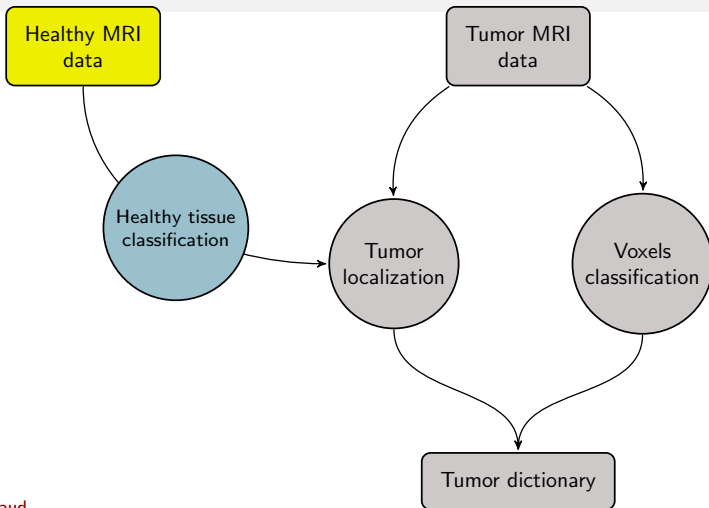
## Multiparametric MRI data



- data in **dimension 5**
- **26 parameters per class**
- estimation by **EM** and **Flury & Gautschi** or **Stiefel manifold optimization** algorithms
- choice of the number of classes according with **BIC** and **ICL** criterions
- **8 healthy rats** (49 000 voxels)
- **37 rats with tumors** (290 000 voxels)
- 4 tumor models : **9L, C6, F98, RG2**

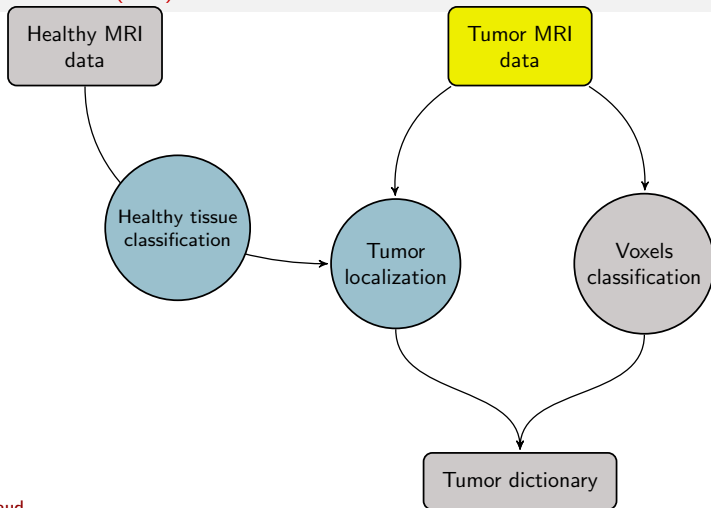
# Processing pipeline

## Healthy voxels classification



# Processing pipeline

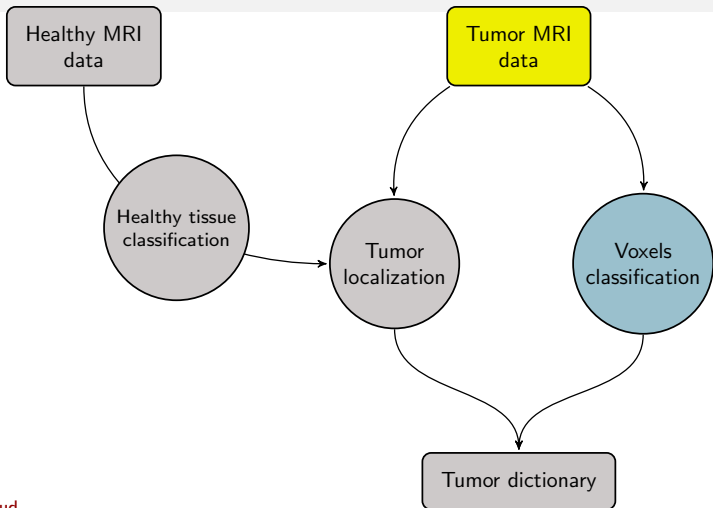
## Tumor localization (ROI)





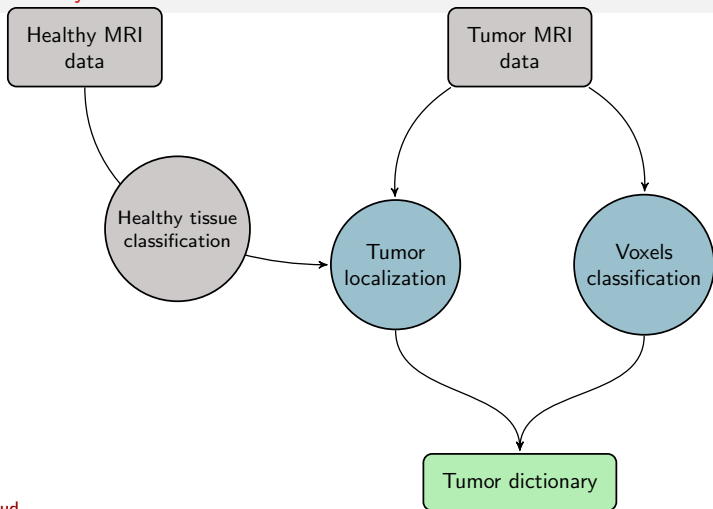
# Processing pipeline

## Voxels classification



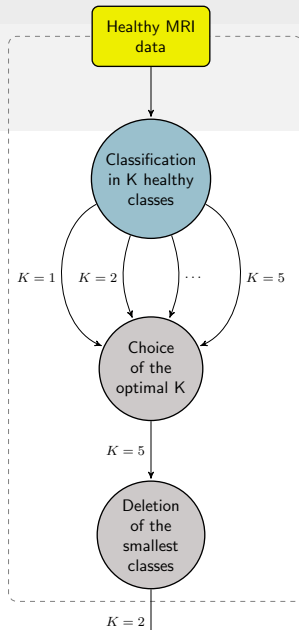
# Processing pipeline

## Tumor dictionary



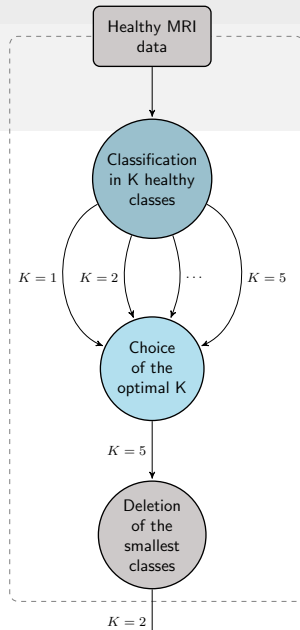
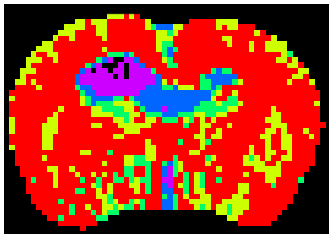
# Healthy MRI voxels classification

Classification in  $K$  healthy classes



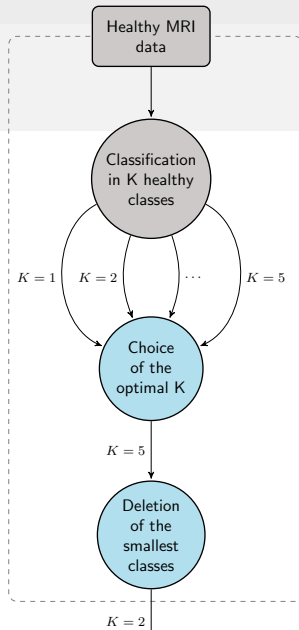
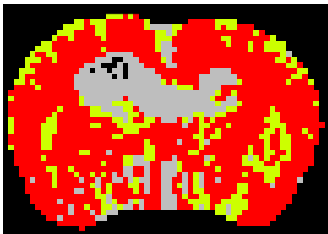
# Healthy MRI voxels classification

Choice of the optimal  $K$  ( $K = 5$ )



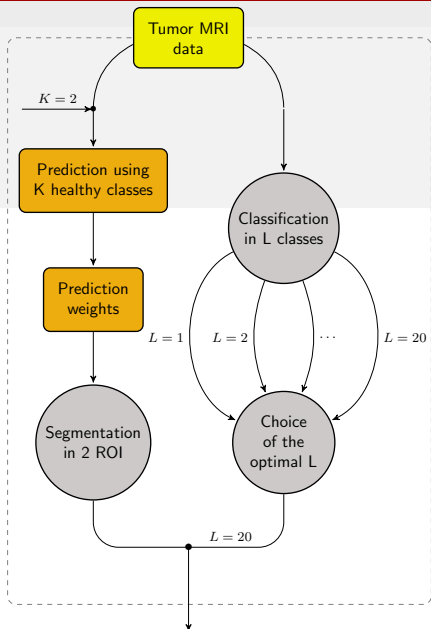
# Healthy MRI voxels classification

Deletion of the smallest classes ( $K = 2$ )



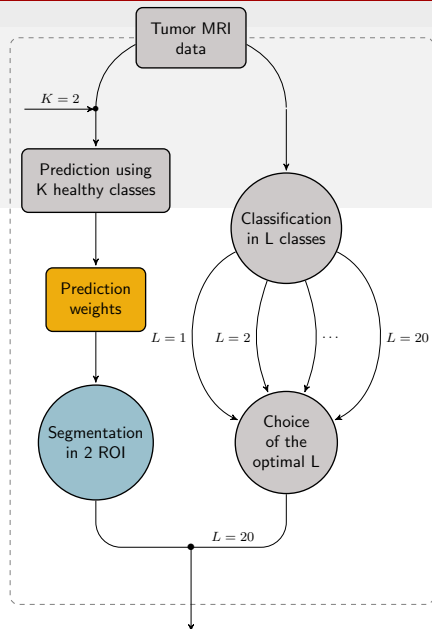
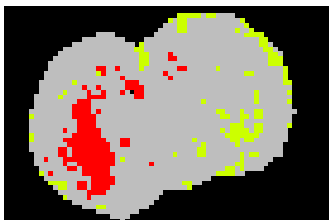
# Tumor localization & voxels classification

Prediction using  $K$  healthy classes  
to get weights



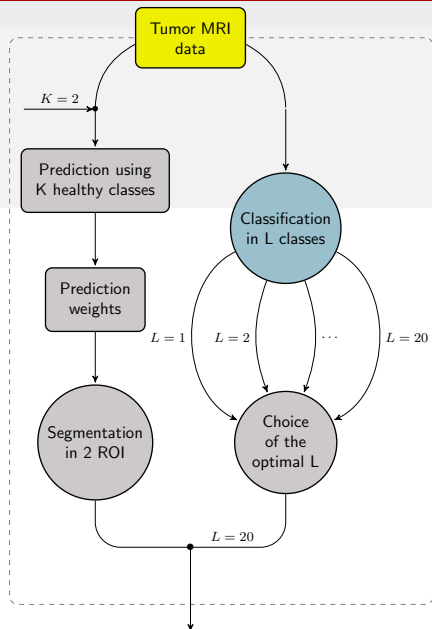
# Tumor localization & voxels classification

Detection of atypical weight  
(segmentation in 2 ROI)



# Tumor localization & voxels classification

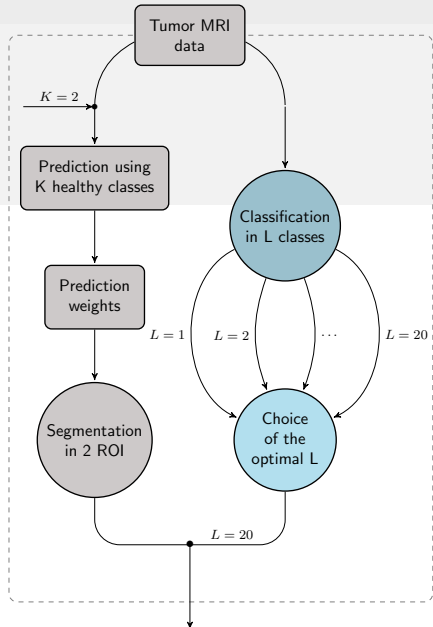
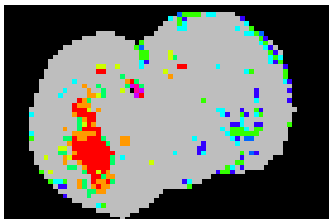
Classification in  $L$  tumoral classes





# Tumor localization & voxels classification

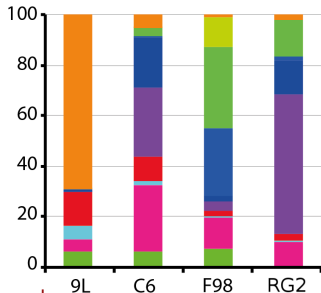
Choice of the optimal  $L$  ( $L = 20$ )



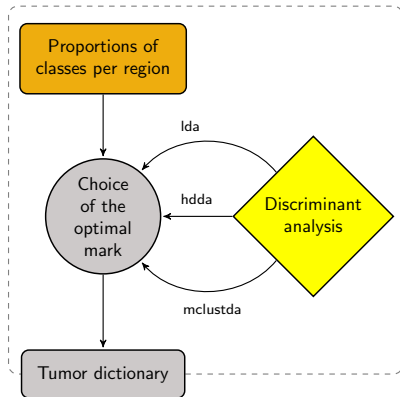
# Tumor dictionary

## Compute different features

- Characteristic of the MRI clustering : proportions of classes inside each ROI.
- Discriminant analysis used : lda, hdda, mclustda.



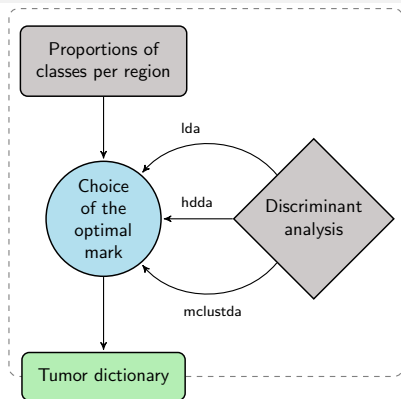
Alexis Arnaud



# Tumor dictionary

## Choice of the optimal mark

- Cross-validation of type : leave-one-out.
- Average classification rate : 70% .



## Tumor dictionary

Classification rate <i>Truth</i>	<i>Prediction</i>							
	9L		C6		F98		RG2	
<b>9L</b> outliers (12)	<b>50</b>	8.3	.	8.3	.	33	.	.
<b>9L</b> inliers (12)	.	<b>50</b>	8.3	.	33	.	8.3	.
<b>C6</b> outliers (8)	.	25	<b>62.5</b>	12.5	.	.	.	.
<b>C6</b> inliers (8)	.	.	.	<b>75</b>	12.5	12.5	.	.
<b>F98</b> outliers (8)	12.5	12.5	.	.	<b>75</b>	.	.	.
<b>F98</b> inliers (8)	.	.	.	.	.	<b>100</b>	.	.
<b>RG2</b> outliers (7)	.	14.3	.	.	.	.	<b>85.7</b>	.
<b>RG2</b> inliers (7)	14.3	.	.	.	.	.	.	<b>85.7</b>

Except for the 9L rats, the classification of tumors is as good as the previous study but with more tumor types and automatic tumor localisation.

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# Bayesian extension

## Motivations

- more general and flexible model (use of a priori)
- model selection (automatic choice of the class number)

# Bayesian extension

## Hierarchical view of the current mixture model

$$\begin{aligned} Y_n | Z_n = k, \mathbf{W}_n = \mathbf{w}_n; \mu_k, \mathbf{U}_k, \mathbf{D}_k &\sim \mathcal{N}_M(\mu_k, \mathbf{U}_k \mathbf{\Delta}_n^{-1} \mathbf{D}_k^{-1} \mathbf{U}_k^t) \\ \mathbf{W}_n = (\mathbf{W}_{n1}, \dots, \mathbf{W}_{nM}) | Z_n = k; \nu &\sim \bigotimes_{m=1}^M \mathcal{G}\left(\frac{\nu_{km}}{2}, \frac{\nu_{km}}{2}\right) \\ Z_n; \pi &\sim \mathcal{M}(1, \pi_1, \dots, \pi_K) \end{aligned}$$

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## Hierarchical view of the current mixture model

$$\begin{aligned}
 Y_n | Z_n = k, \mathbf{W}_n = \mathbf{w}_n; \boldsymbol{\mu}_k, \mathbf{U}_k, \mathbf{D}_k &\sim \mathcal{N}_M(\boldsymbol{\mu}_k, \mathbf{U}_k \boldsymbol{\Delta}_n^{-1} \mathbf{D}_k^{-1} \mathbf{U}_k^t) \\
 \mathbf{W}_n = (\mathbf{W}_{n1}, \dots, \mathbf{W}_{nM}) | Z_n = k; \boldsymbol{\nu} &\sim \bigotimes_{m=1}^M \mathcal{G}\left(\frac{\nu_{km}}{2}, \frac{\nu_{km}}{2}\right) \\
 Z_n; \boldsymbol{\pi} &\sim \mathcal{M}(1, \pi_1, \dots, \pi_K)
 \end{aligned}$$

Bayesian extension : a standard prior for  $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k = \mathbf{U}_k \mathbf{D}_k^{-1} \mathbf{U}_k^t$  is :

$$\begin{aligned}
 \boldsymbol{\mu}_k | \boldsymbol{\Sigma}_k &\sim \mathcal{N}_M \\
 \boldsymbol{\Sigma}_k &\sim \mathcal{IW}_M
 \end{aligned}$$



# Bayesian extension

## Hierarchical view of the current mixture model

$$\mathbf{Y}_n | Z_n = k, \mathbf{W}_n = \mathbf{w}_n ; \boldsymbol{\mu}_k, \mathbf{U}_k, \mathbf{D}_k \sim \mathcal{N}_M(\boldsymbol{\mu}_k, \mathbf{U}_k \boldsymbol{\Delta}_n^{-1} \mathbf{D}_k^{-1} \mathbf{U}_k^t)$$

$$\mathbf{W}_n = (\mathbf{W}_{n1}, \dots, \mathbf{W}_{nM}) | Z_n = k ; \boldsymbol{\nu} \sim \bigotimes_{m=1}^M \mathcal{G}\left(\frac{\nu_{km}}{2}, \frac{\nu_{km}}{2}\right)$$

$$Z_n ; \boldsymbol{\pi} \sim \mathcal{M}(1, \pi_1, \dots, \pi_K)$$

Bayesian extension : a standard prior for  $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k = \mathbf{U}_k \mathbf{D}_k^{-1} \mathbf{U}_k^t$  is :

$$\begin{aligned} \boldsymbol{\mu}_k | \boldsymbol{\Sigma}_k &\sim \mathcal{N}_M \\ \boldsymbol{\Sigma}_k &\sim \mathcal{IW}_M \end{aligned}$$

- ▷ How to get priors on  $\mathbf{U}_k, \mathbf{D}_k$  ?

# Bayesian extension

## Hierarchical Bayesian mixture model

$$\begin{aligned}
 \mathbf{Y}_n | Z_n = k, \mathbf{W}_n = \mathbf{w}_n, \mathbf{M}_k = \boldsymbol{\mu}_k, \mathbf{D}_k = \mathbf{d}_k ; \mathbf{U}_k &\sim \mathcal{N}_M(\boldsymbol{\mu}_k, \mathbf{U}_k \boldsymbol{\Delta}_n^{-1} \mathbf{d}_k^{-1} \mathbf{U}_k^t) \\
 \mathbf{W}_n = (\mathbf{W}_{n1}, \dots, \mathbf{W}_{nM}) | Z_n = k ; \mathbf{a}, \mathbf{b} &\sim \bigotimes_{m=1}^M \mathcal{G}(a_{km}, b_{km}) \\
 Z_n ; \boldsymbol{\pi} &\sim \mathcal{M}(1, \pi_1, \dots, \pi_K) \\
 \mathbf{M}_k | \mathbf{D}_k = \mathbf{d}_k ; \mathbf{U}_k &\sim \mathcal{N}_M(\mathbf{m}_k, \eta_k^{-1} \mathbf{U}_k \mathbf{d}_k^{-1} \mathbf{U}_k^t) \\
 \mathbf{D}_k = (\mathbf{D}_{k1}, \dots, \mathbf{D}_{kM}) &\sim \bigotimes_{m=1}^M \mathcal{G}(\boldsymbol{\alpha}_{km}, \boldsymbol{\beta}_{km})
 \end{aligned}$$

# Outline

- 1 Motivation : brain tumor characterization
- 2 Clustering of MRI data
- 3 Mixture of multivariate multiple-scaled Student distributions
- 4 Estimation of a MMSD mixture
- 5 Tumor characterization from multiparametric MRI
- 6 Bayesian extension
- 7 Work in progress**

## Work in progress

- Validation of the protocol.
- Taking into account spatial dependences using a hidden Markov field.
- Parameters sensitivity analysis.
- Automatic selection of the number of classes.
- Link between histology and automatic tissue characterization.

## Bibliography

- **Coquery N, Francois O, Lemasson B, Debacker C, Farion R, Rémy C, et Barbier E (2014)**, *Microvascular MRI and unsupervised clustering yields histology-resembling images in two rat models of glioma*, *Journal of Cerebral Blood Flow & Metabolism*, volume 34, number 8, 1354–62.
- **Forbes F, et Wraith D (2014)**, *A new family of multivariate heavy-tailed distributions with variable marginal amounts of tailweights: Application to robust clustering*, *Statistics and Computing*, volume 24, number 6, 971–984.

# The end

## Thank you !



Image credit : [dianepotos.deviantart.com](http://dianepotos.deviantart.com)

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