

# Hyperspectral Image Segmentation by Spatialized Gaussian Mixtures and Model Selection

E. Le Pennec

(SELECT - Inria Saclay / Université Paris Sud)

and

S. Cohen (IPANEMA - CNRS / Soleil)

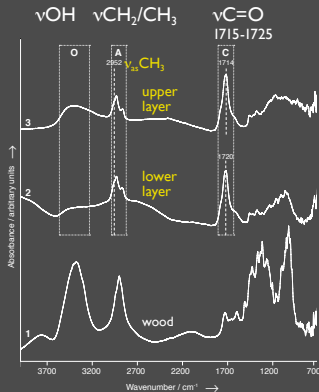
SMAI 2013

# A. Stradivari (1644 - 1737)

Provigny (1716)



A. Giordan © Cité de la Musique



SOLEIL  
SYNCHROTRON

4 / 8 cm<sup>-1</sup> resolution  
64 / 128 scans  
typ. 1 min/sp, 400sp

very simple process  
no protein (amide I, amide II)  
no gums, nor waxes  
@SOLEIL: SMIS



J.-P. Echard, L. Bertrand, A. von Bohlen, A.-S. Le Hô, C. Paris, L. Bellot-Gurlet, B. Soulier, A. Lattuati-Derieux, S. Thao, L. Robinet, B. Lavédrine, and S. Vaiedelich. *Angew. Chem. Int. Ed.*, 49(1), 197-201, 2010.

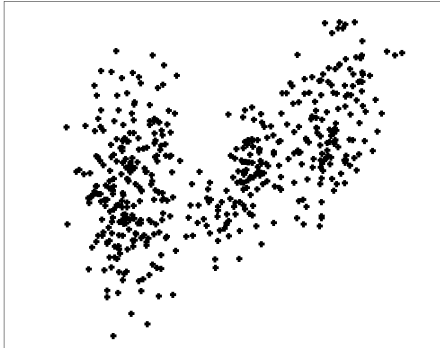


# Hyperspectral Image Segmentation

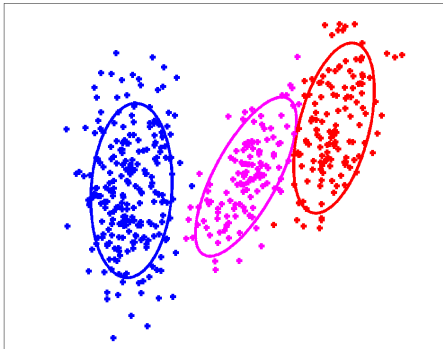
- Data :
  - image of size  $N$  between  $\sim 1000$  and  $\sim 100000$  pixels,
  - spectrums  $\mathcal{S}$  of  $\sim 1024$  points,
  - very good spatial resolution,
  - ability to measure a lot of spectrums per minute,
- Immediate goal :
  - automatic image segmentation,
  - without human intervention,
  - help to data analysis.
- Advanced goal :
  - automatic classification,
  - interpretation...

# A “Toy” Problem

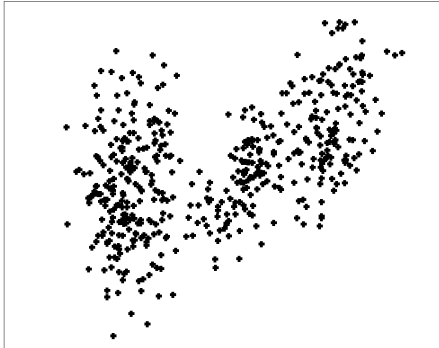
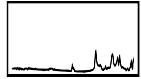
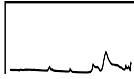
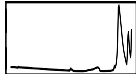
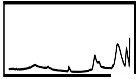
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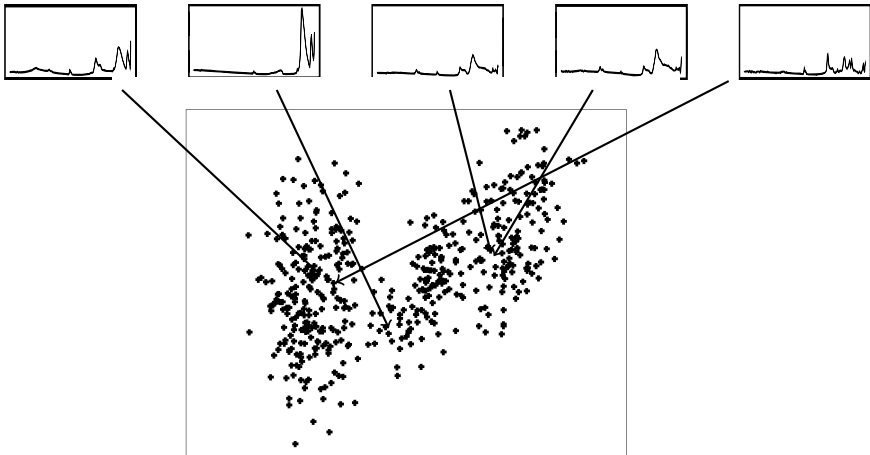
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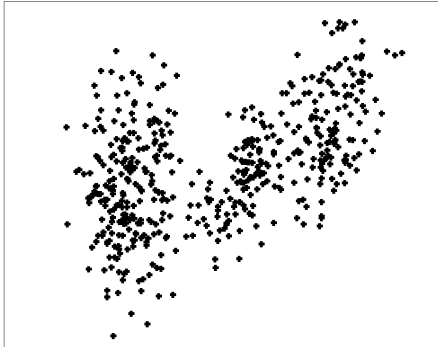
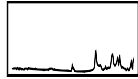
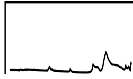
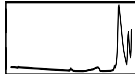
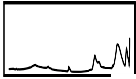


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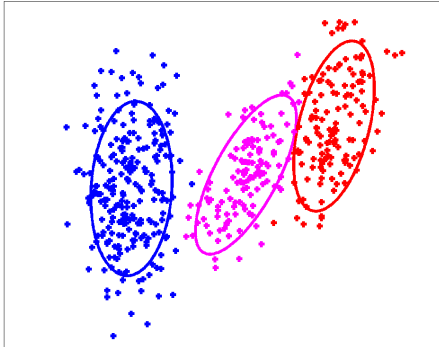
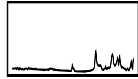
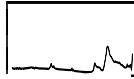
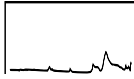
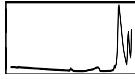
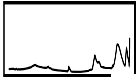




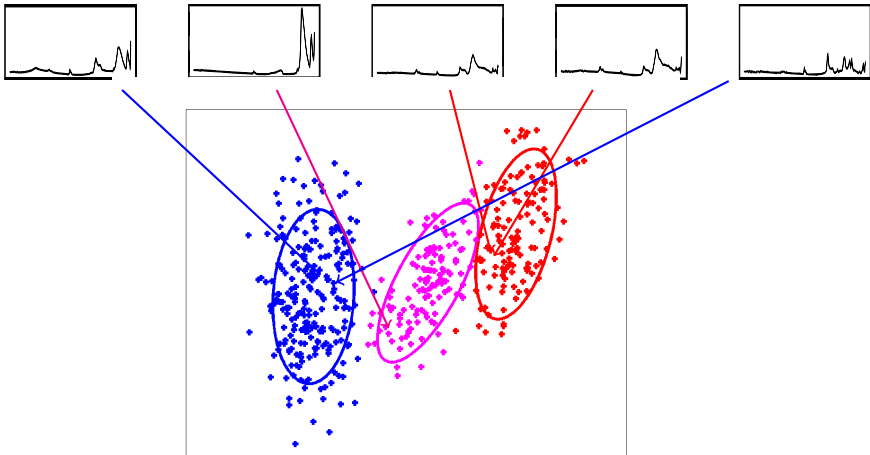
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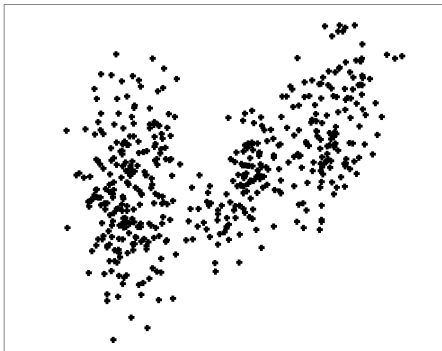
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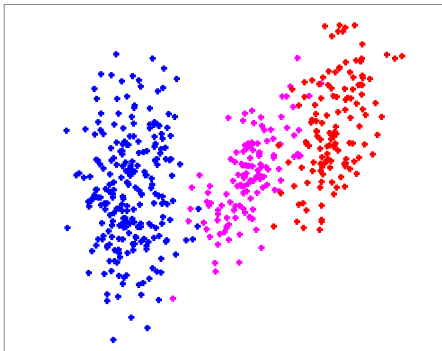
- Representation : mapping between spectrums and points in a large dimension space.
- Spectral method.

# “Stochastic” Modeling

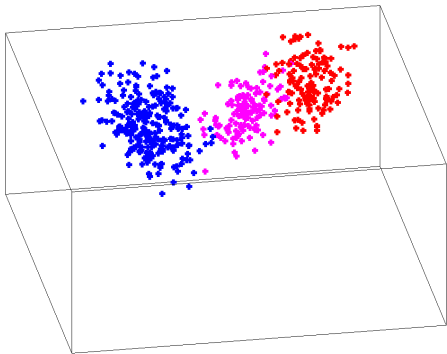
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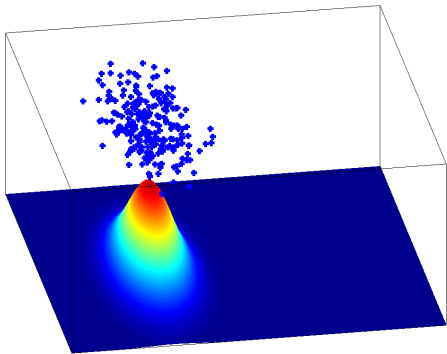
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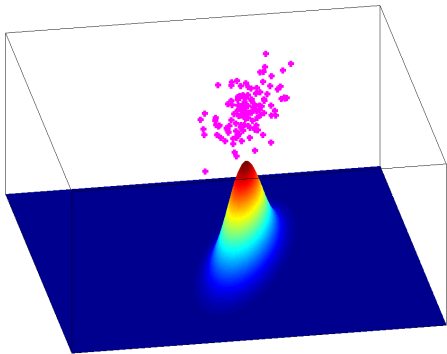


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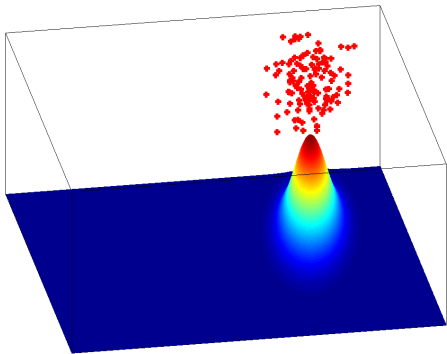




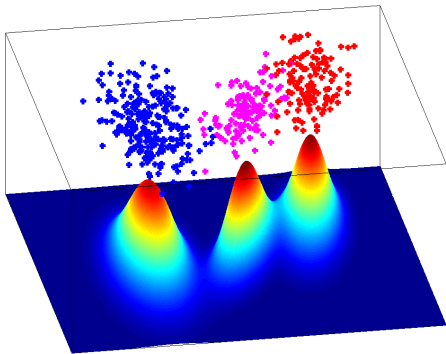
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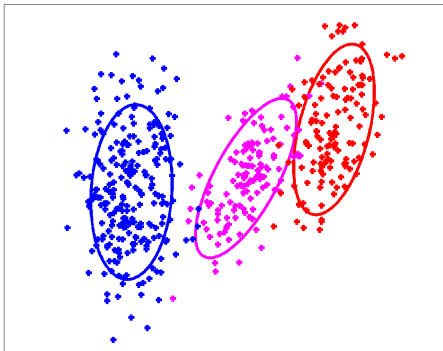
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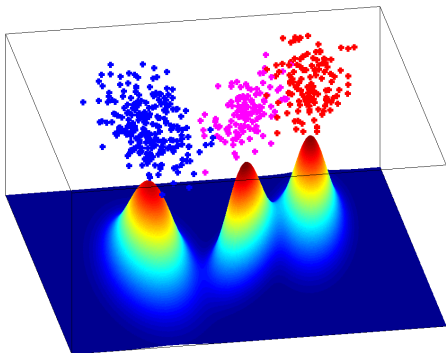
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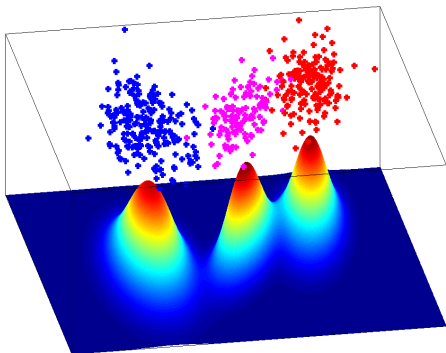
# “Stochastic” Modeling



- Model : Gaussian Mixture with  $K$  classes.
- Mixture density :

$$\begin{aligned} s_{K,\pi,\mu,\Sigma}(\mathcal{S}) &= \sum_{k=1}^K \pi_k \frac{1}{\sqrt{(2\pi)^d |\Sigma_k|}} e^{-\frac{1}{2}(\mathcal{S}-\mu_k)^t \Sigma_k^{-1} (\mathcal{S}-\mu_k)} \\ &= \sum_{k=1}^K \pi_k \mathcal{N}_{\mu_k, \Sigma_k}(\mathcal{S}) \end{aligned}$$

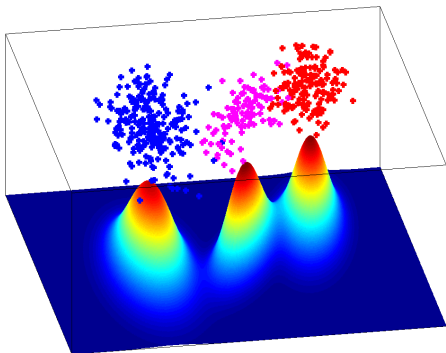
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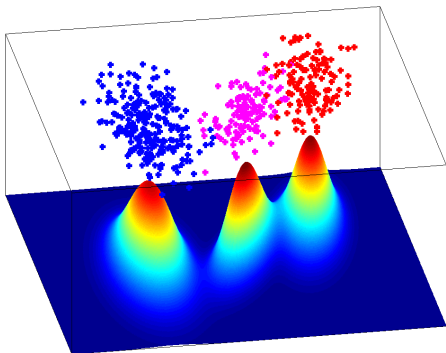
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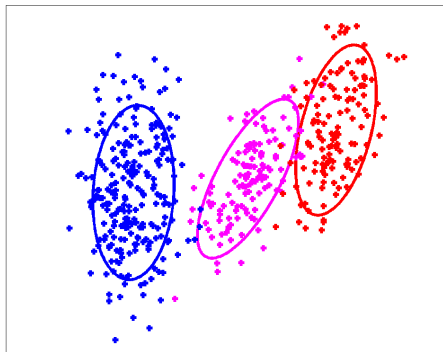
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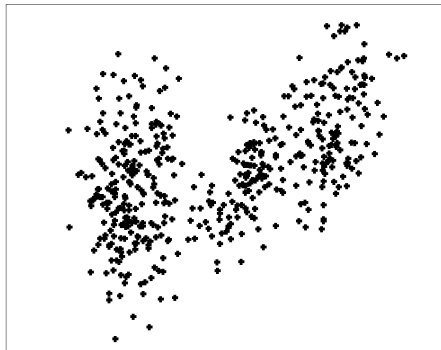


# “Statistical” Estimation

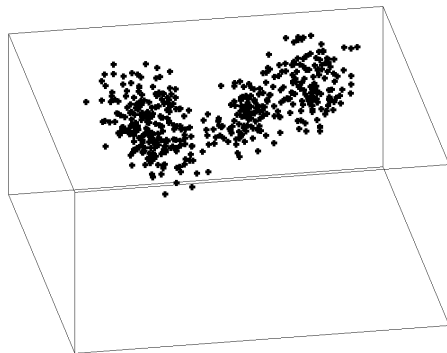
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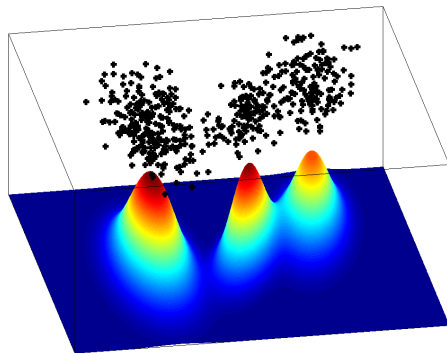
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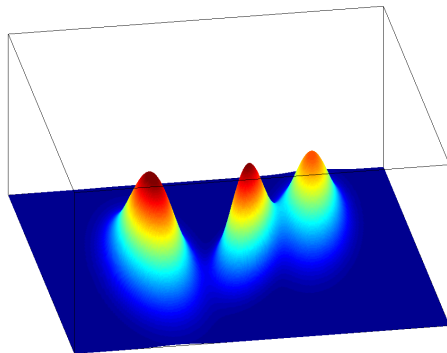
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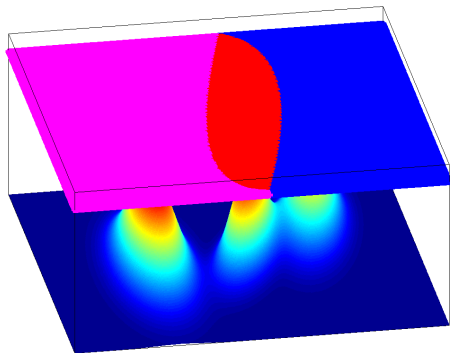
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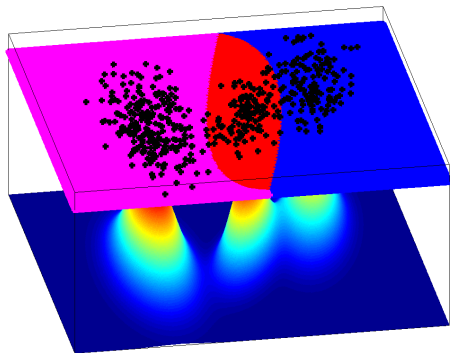
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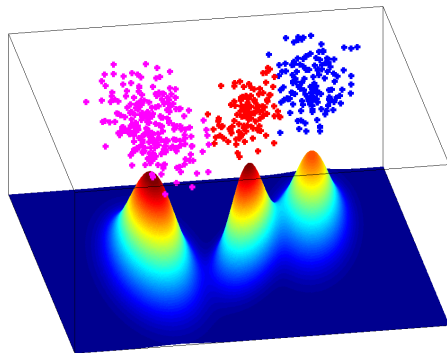


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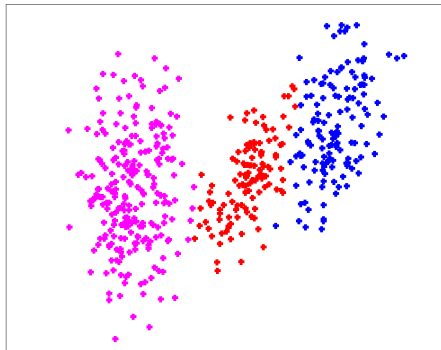




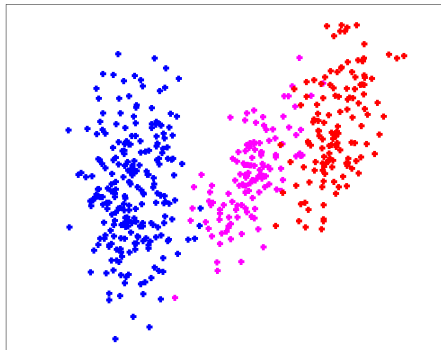
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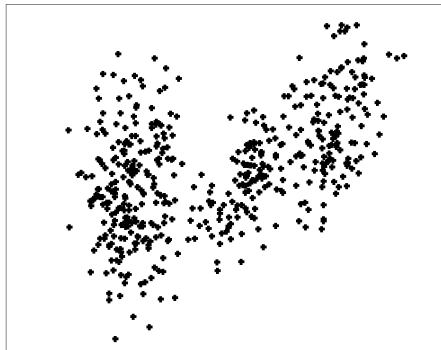
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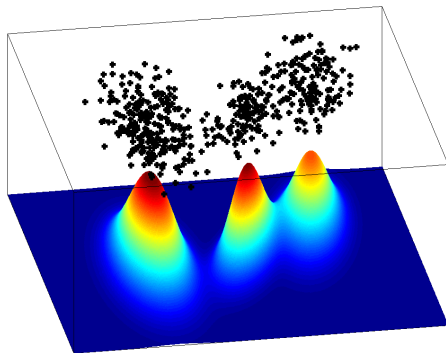
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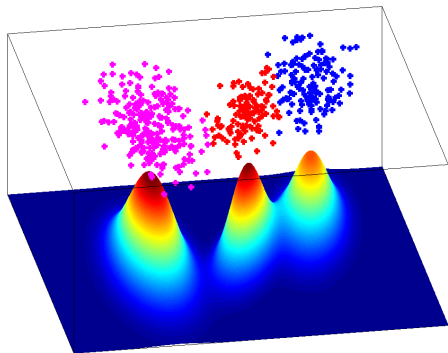
# “Statistical” Estimation



- Estimation of  $\pi_k$ ,  $\widehat{\mu}_k$  and  $\widehat{\Sigma}_k$  by maximum likelihood :

$$(\widehat{\pi}_k, \widehat{\mu}_k, \widehat{\Sigma}_k) = \operatorname{argmax} \sum_{i=1}^N \log s_{K, (\pi_k, \mu_k, \Sigma_k)}(\mathcal{S}_i)$$

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- Estimation of  $\widehat{k}(\mathcal{S})$  by maximum a posteriori (MAP) :

$$\widehat{k}(\mathcal{S}) = \operatorname{argmax}_{\mu_k, \Sigma_k} \widehat{\pi}_k \mathcal{N}_{\widehat{\mu}_k, \widehat{\Sigma}_k}(\mathcal{S})$$

# Hyperspectral image segmentation with GMM

- Classical stochastic model of spectrum  $\mathcal{S}$  :
  - $K$  spectrum classes,
  - with proportion  $\pi_k$  for each class ( $\sum_{k=1}^K \pi_k = 1$ ),
  - Gaussian law  $\mathcal{N}_{\mu_k, \Sigma_k}$  within each class (strong assumption !)
- Heuristic : true density  $s_0$  of  $\mathcal{S}$  close from

$$s(\mathcal{S}) = \sum_{k=1}^K \pi_k \mathcal{N}_{\mu_k, \Sigma_k}(\mathcal{S}).$$

- Goal : estimate all parameters ( $K$ ,  $\pi_k$ ,  $\mu_k$  and  $\Sigma_k$ ) from the data.
- Why : yields a classification/segmentation by a maximum likelihood principle

$$\hat{k}(\mathcal{S}) = \operatorname{argmax}_{\mu_k, \Sigma_k} \hat{\pi}_k \mathcal{N}_{\hat{\mu}_k, \hat{\Sigma}_k}(\mathcal{S})$$

- Typical result in term of density estimation and not classification...

# Gaussian Mixture Model

- True density  $s_0$  of  $\mathcal{S}$  close from

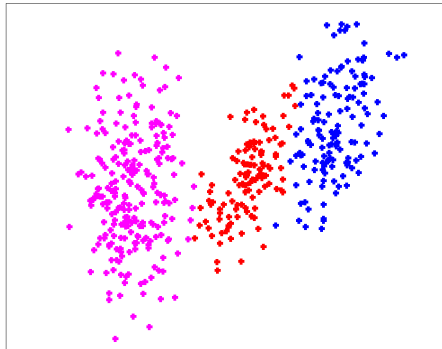
$$s(\mathcal{S}) = \sum_{k=1}^K \pi_k \mathcal{N}_{\mu_k, \Sigma_k}(\mathcal{S}).$$

- Gaussian Mixture Model  $S_m = \{s_m\}$  specified by
  - a number of classes  $K$ ,
  - a structure for the means  $\mu_k$  and the covariance matrices  $\Sigma_k = L_k D_k A_k D_k'$  (Volume  $L_k$ , basis  $D_k$  and rescaled eigenvalues  $A_k$ )
- Structure  $[\mu \ L \ D \ A]^K$  for the  $K$ -tuples of Gaussian parameters :
  - know, common or free values for each parameter
  - plus compactness and condition number assumptions.
- GMM  $S_m$  : parametric model of dimension  $(K - 1) + \dim([\mu \ L \ D \ A]^K)$ .
- Maximum likelihood estimation by EM algorithm of :
  - the mean  $\mu_k$  and the covariance matrix  $\Sigma_k = L_k D_k A_k D_k'$  for each class
  - and the mixing proportions  $\pi_k$

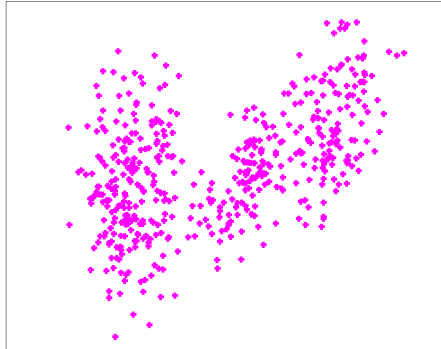


How many classes ?

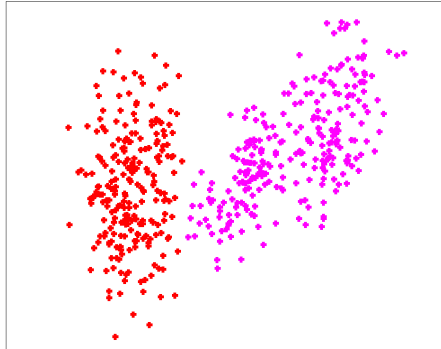
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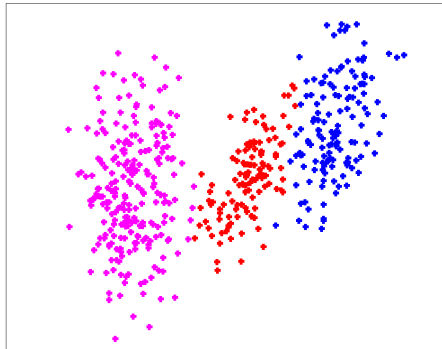
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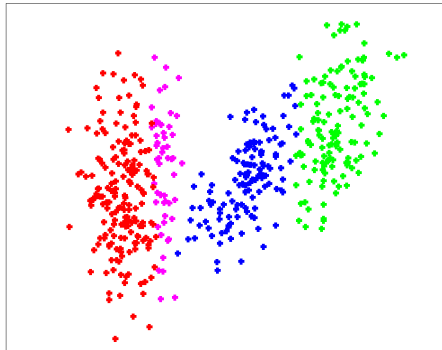
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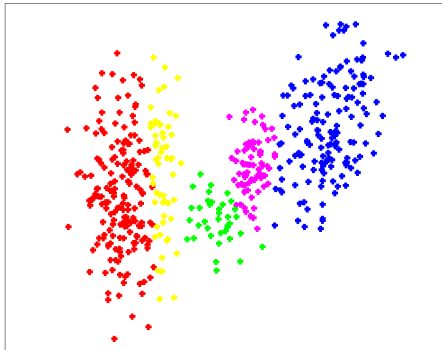
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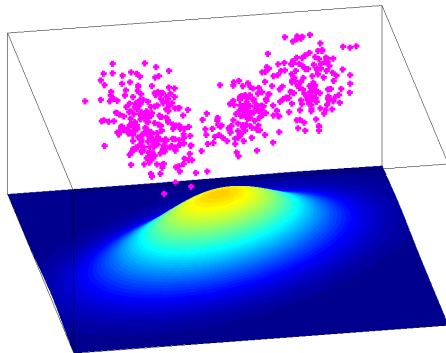
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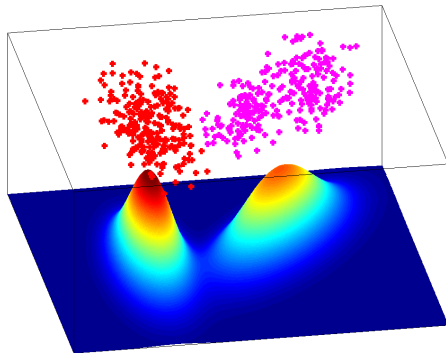


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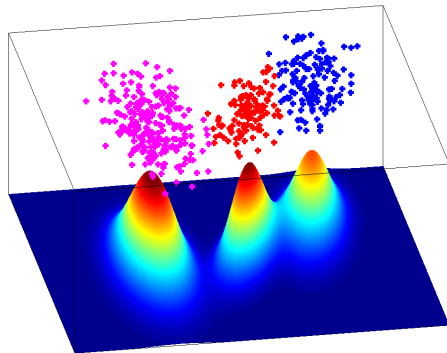




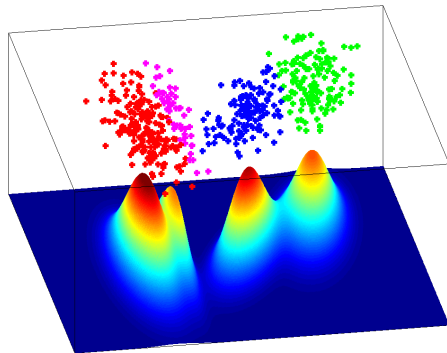
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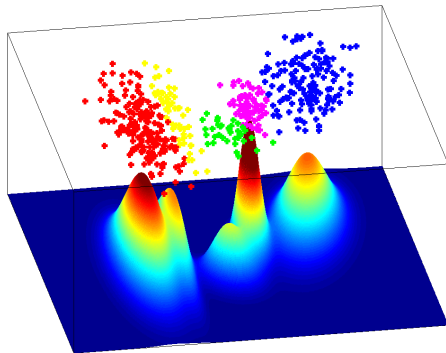
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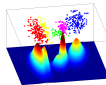
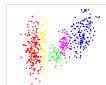
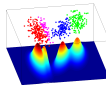
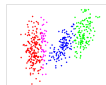
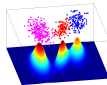
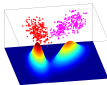
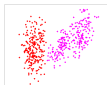
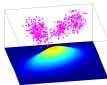
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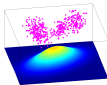


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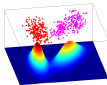
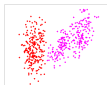


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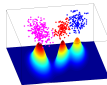
Fidelity



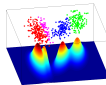
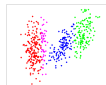
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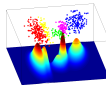
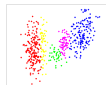
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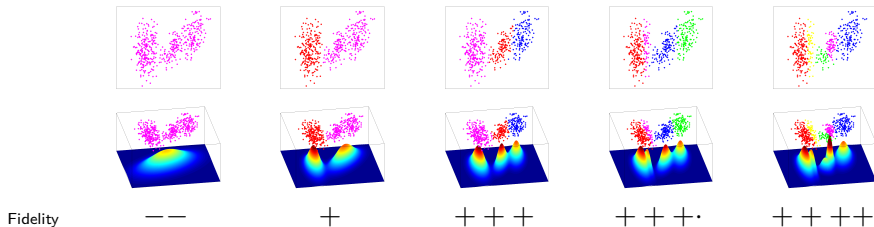


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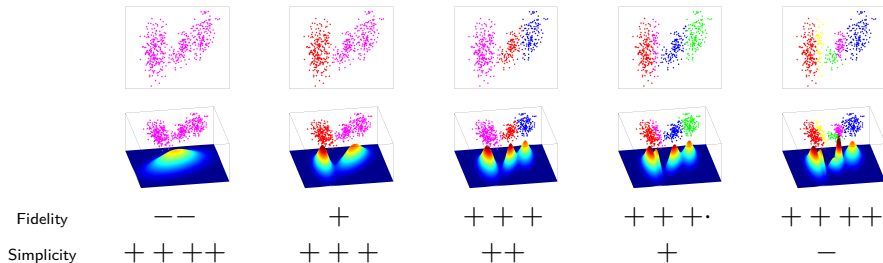
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# How many classes?



- Tough question for which the likelihood (the fidelity) is not sufficient!

# How many classes?



- Tough question for which the likelihood (the fidelity) is not sufficient!
- How to take into account the model complexity?



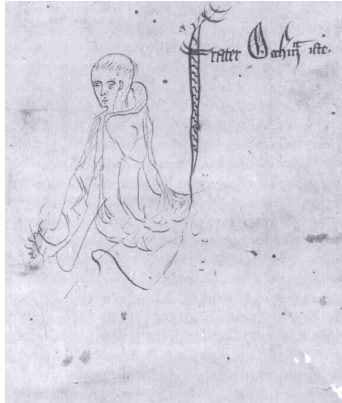
# Ockham's Razor

# Ockham's Razor



*entities must not be multiplied beyond necessity*  
William of Ockham (~ 1285 - 1347)

# Ockham's Razor

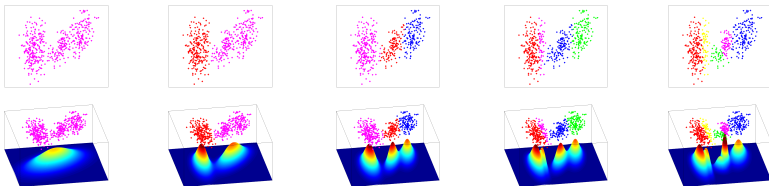


*entities must not be multiplied beyond necessity*  
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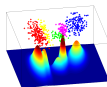
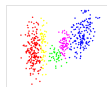
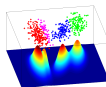
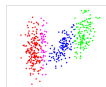
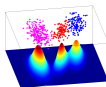
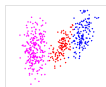
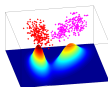
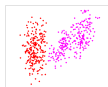
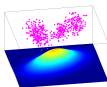
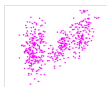
- Ockham's Razor (simplicity principle) : one should not add hypotheses, if the current ones are already sufficient !
- Balance between observation explanation power and simplicity.

# Selection by Penalization

# Selection by Penalization



# Selection by Penalization



Likelihood

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+++ .

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Simplicity

++++

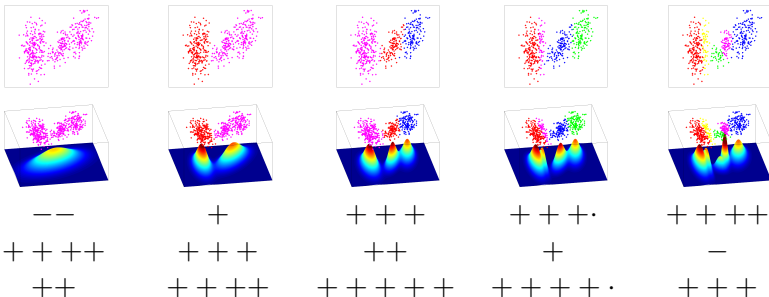
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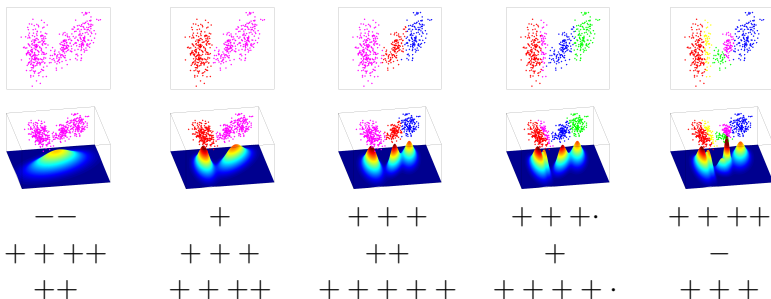
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# Selection by Penalization



# Selection by Penalization



● Likelihood :  $\sum_{i=1}^N \log \hat{s}_K(X_i)$ .

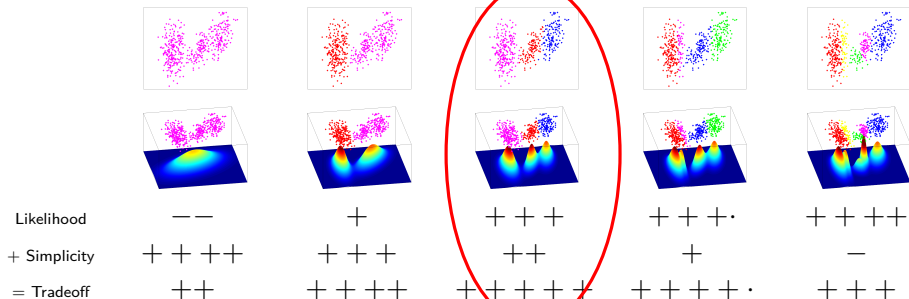
● Simplicity :  $-\lambda \text{Dim}(S_K)$ .

● Penalized estimator :

$$\underset{K}{\operatorname{argmin}} \underbrace{- \sum_{i=1}^N \log \hat{s}_K(X_i)}_{\text{Likelihood}} + \underbrace{\lambda \text{Dim}(S_K)}_{\text{Penalty}}$$



# Selection by Penalization



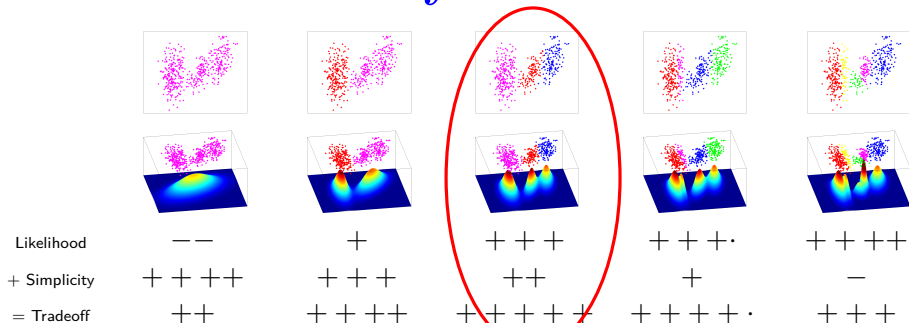
● Likelihood :  $\sum_{i=1}^N \log \hat{s}_K(X_i).$

● Simplicity :  $-\lambda \text{Dim}(S_K).$

● Penalized estimator :

$$\underset{K}{\operatorname{argmin}} - \underbrace{\sum_{i=1}^N \log \hat{s}_K(X_i)}_{\text{Likelihood}} + \underbrace{\lambda \text{Dim}(S_K)}_{\text{Penalty}}$$

# Selection by Penalization



● Likelihood :  $\sum_{i=1}^N \log \hat{s}_K(X_i)$ .

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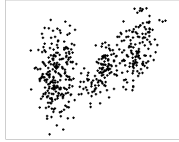
● Penalized estimator :

$$\underset{K}{\operatorname{argmin}} \underbrace{- \sum_{i=1}^N \log \hat{s}_K(X_i)}_{\text{Likelihood}} + \underbrace{\lambda \text{Dim}(S_K)}_{\text{Penalty}}$$

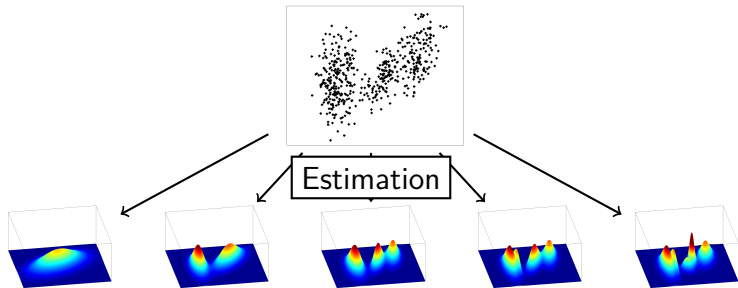
● Optimization in  $K$  by exhaustive exploration !

# Methodology

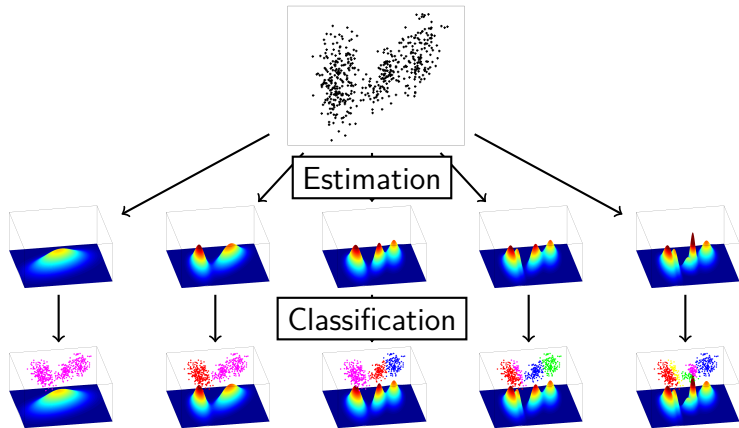
# Methodology



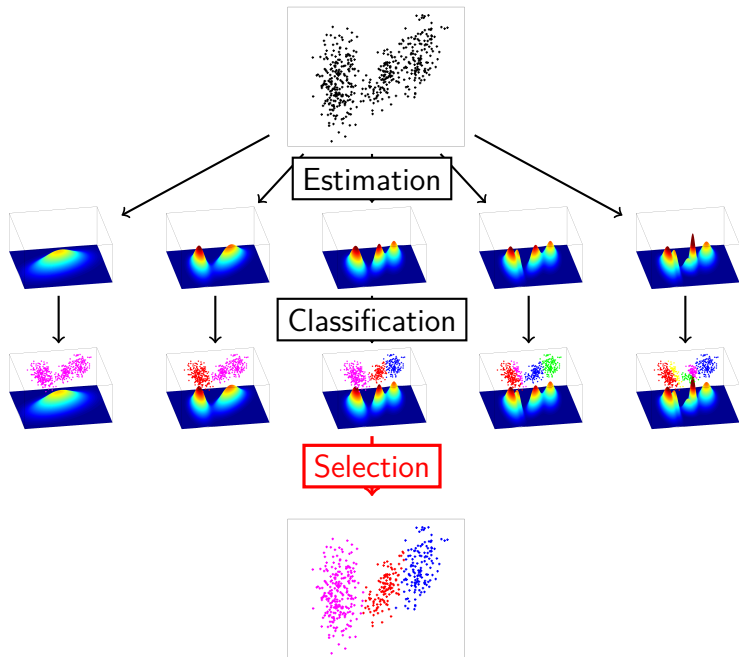
# Methodology



# Methodology



# Methodology



# Model selection

- How to choose the *good* model  $S_m$  :
  - the number of classes  $K$ ,
  - the structure model  $[\mu L D A]^K$  ?
- Penalized model selection principle :
  - Choice of a collection of models  $S_m = \{s_m\}$  with  $m \in \mathcal{S}$ ,
  - Maximum likelihood estimation of a density  $\hat{s}_m$  for each model  $S_m$ ,
  - Selection of a model  $\hat{m}$  by

$$\hat{m} = \operatorname{argmin} -\ln(\hat{s}_m) + \operatorname{pen}(m).$$

with  $\operatorname{pen}(m) = \kappa(\ln(n)) \dim(S_m)$  (parametric dimension of  $S_m$ ),

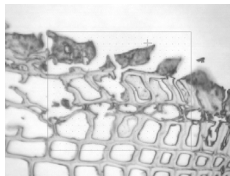
- Results (Birgé, Massart, Celeux, Maugis, Michel...) :
  - Density estimation : for  $\kappa$  large enough,

$$\mathbb{E} [d^2(s_0, \hat{s}_m)] \leq C \inf_{m \in \mathcal{S}} \left( \inf_{s_m \in S_m} KL(s_0, s_m) + \frac{\operatorname{pen}(m)}{n} \right) + \frac{C'}{n}.$$

- Clustering or unsupervised classification : numerical results.
- Consistency of the classification as soon as  $\ln \ln(n)$  in the penalty...



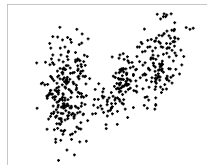
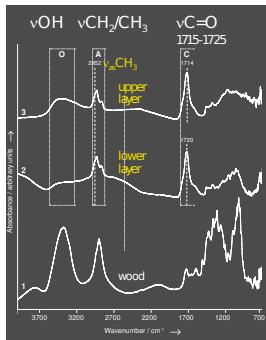
# Back to our violins



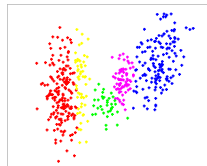
Segmentation



Representation



Classification



Spatial Info.

# Segmentation and Spatialized GMM

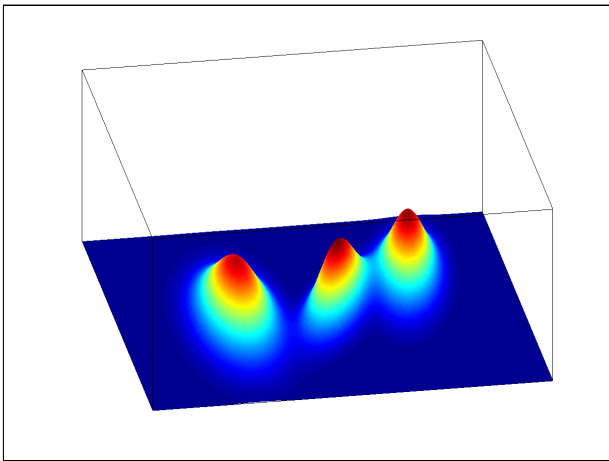
- Initial goal : segmentation  $\neq$  clustering.
- Idea of Kolaczyk et al (cf Bigot) : take into account the spatial position  $x$  of the spectrum in the mixing proportions.
- Conditional density model :

$$s(\mathcal{S}|x) = \sum_{k=1}^K \pi_k(x) \mathcal{N}_{\mu_k, \Sigma_k}(\mathcal{S}).$$

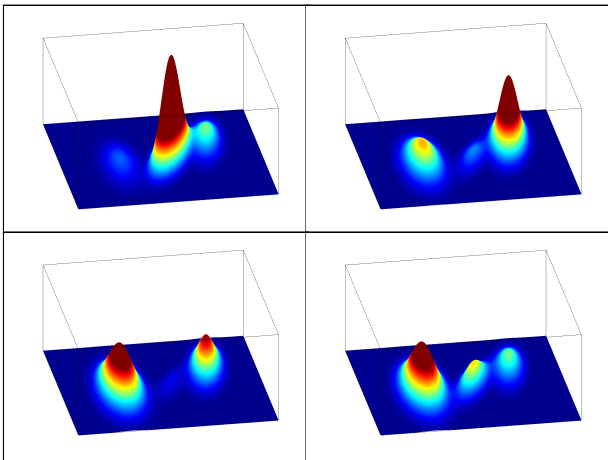
- Estimation from the data :
  - the mean  $\mu_k$  and the covariance matrix  $\Sigma_k = L_k D_k A_k D_k'$  for each class
  - and the mixing proportion functions  $\pi_k(x)$ .
- Segmentation by MAP principle :

$$\hat{k}(\mathcal{S}|x) = \arg \max_k \hat{\pi}_k(x) \mathcal{N}_{\hat{\mu}_k, \hat{\Sigma}_k}(\mathcal{S})$$

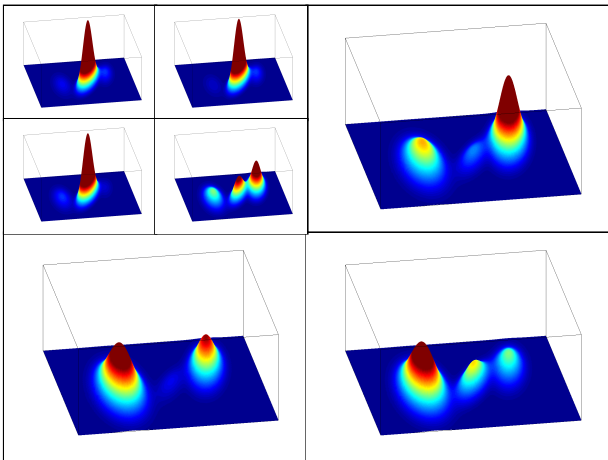
# Segmentation and Spatialized GMM



# Segmentation and Spatialized GMM

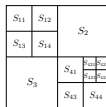
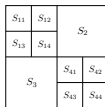


# Segmentation and Spatialized GMM



# Spat. GMM and hierarchical partition

- How to choose the *right* model  $S_m$  ? :
  - the number of classes  $K$ ,
  - the structure model  $[\mu L D A]^K$ ,
  - the structure of the mixing proportion functions  $\pi_k(x)$ .
- Simple structure for  $\pi_k(x)$  :  $\pi_k(x) = \sum_{\mathcal{R} \in \mathcal{P}} \pi_k[\mathcal{R}] \chi_{\{x \in \mathcal{R}\}} = \pi_k[\mathcal{R}(x)]$ 
  - piecewise constant on a *hierarchical* partition,
  - efficient optimization algorithm,
  - good approximation properties.
- $\dim(S_m) = |\mathcal{P}|(K - 1) + \dim([\mu L D A]^K)$ .
- Penalty  $\text{pen}(m) = \kappa \ln(n) \dim(S_m)$  allows
  - a numerical optimization scheme (EM + dynamic programming)
  - a theoretical control : for  $\kappa$  large enough



$$\mathbb{E} [d^2(s_0, \hat{s}_m)] \leq C \inf_{m \in \mathcal{S}} \left( \inf_{s_m \in S_m} KL(s_0, s_m) + \frac{\text{pen}(m)}{n} \right) + \frac{C'}{n}.$$

# Conditional density and selection

- General framework : observation of  $(X_i, Y_i)$  with  $X_i$  independent and  $Y_i$  cond. independent of law of density  $s_0(y|x)$ .
- Goal : estimation of  $s_0(y|x)$ .
- Penalized model selection principle :
  - choice of a collection of cond. dens. models  $S_m = \{s_m(y|x)\}$  with  $m \in \mathcal{S}$ ,
  - Maximum likelihood estimation of a cond. density  $\hat{s}_m$  for each model  $S_m$  :

$$\hat{s}_m = \operatorname{argmin}_{s_m \in S_m} - \sum_{i=1}^n \ln s_m(Y_i|X_i)$$

- Selection of a model  $\hat{m}$  by
$$\hat{m} = \operatorname{argmin}_{m \in \mathcal{S}} - \sum_{i=1}^n \ln \hat{s}_m(Y_i|X_i) + \operatorname{pen}(m).$$

with  $\operatorname{pen}(m)$  well chosen.

- Conditional density estimation result of type :

$$\mathbb{E} \left[ d^2(s_0, \hat{s}_{\hat{m}}) \right] \leq C \inf_{m \in \mathcal{S}} \left( \inf_{s_m \in S_m} KL(s_0, s_m) + \frac{\operatorname{pen}(m)}{n} \right) + \frac{C'}{n}.$$

- Short biblio : Rosenblatt, Fan et al., de Gooijer and Zerom, Efromovitch, Brunel, Comte, Lacour... / Plugin, direct estimation,  $L^2$ , minimax, censure...

# Theorem

**Assumption (H)** : For every model  $S_m$  in the collection  $\mathcal{S}$ , there is a non-decreasing function  $\phi_m(\delta)$  such that  $\delta \mapsto \frac{1}{\delta}\phi_m(\delta)$  is non-increasing on  $(0, +\infty)$  and for every  $\sigma \in \mathbb{R}^+$  and every  $s_m \in S_m$

$$\int_0^\sigma \sqrt{H_{[1, d^{\otimes n}]}(\epsilon, S_m(s_m, \sigma))} d\epsilon \leq \phi_m(\sigma).$$

**Assumption (K)** : There is a family  $(x_m)_{m \in \mathcal{M}}$  of non-negative number such that

$$\sum_{m \in \mathcal{M}} e^{-x_m} \leq \Sigma < +\infty$$

## Theorem

Assume we observe  $(X_i, Y_i)$  with unknown conditional  $s_0$ . Let  $\mathcal{S} = (S_m)_{m \in \mathcal{M}}$  a at most countable collection of conditional density sets. Assume Assumptions (H), (K) and (S) hold.

Let  $\hat{s}_m$  be a  $\delta$  -log-likelihood minimizer in  $S_m$  :

$$\sum_{i=1}^n -\ln(\hat{s}_m(Y_i|X_i)) \leq \inf_{s_m \in S_m} \left( \sum_{i=1}^n -\ln(s_m(Y_i|X_i)) \right) + \delta$$

Then for any  $\rho \in (0, 1)$  and any  $C_1 > 1$ , there is a constant  $\kappa_0$  depending only on  $\rho$  and  $C_1$  such that, as soon as for every index  $m \in \mathcal{M}$   $\text{pen}(m) \geq \kappa(\mathfrak{D}_m + x_m)$  with  $\kappa > \kappa_0$

where  $\mathfrak{D}_m = n\sigma_m^2$  with  $\sigma_m$  the unique root of  $\frac{1}{\sigma}\phi_m(\sigma) = \sqrt{n}\sigma$ ,  
the penalized likelihood estimate  $\hat{s}_{\hat{m}}$  with  $\hat{m}$  defined by

$$\hat{m} = \underset{m \in \mathcal{M}}{\text{argmin}} \sum_{i=1}^n -\ln(\hat{s}_m(Y_i|X_i)) + \text{pen}(m)$$

satisfies  $\mathbb{E} \left[ JKL_{\rho}^{\otimes n}(s_0, \hat{s}_{\hat{m}}) \right] \leq C_1 \left( \inf_{S_m \in \mathcal{S}} \left( \inf_{s_m \in S_m} KL^{\otimes n}(s_0, s_m) + \frac{\text{pen}(m)}{n} \right) + \frac{\kappa_0 \Sigma + \delta}{n} \right).$



# Simplified Theorem...

- Oracle inequality :

$$\mathbb{E} \left[ JKL_{\rho}^{\otimes n}(s_0, \widehat{s}_m) \right] \leq C_1 \left( \inf_{S_m \in \mathcal{S}} \left( \inf_{s_m \in S_m} KL^{\otimes n}(s_0, s_m) + \frac{\text{pen } m}{n} \right) + \frac{\kappa_0 \Sigma + \delta}{n} \right)$$

as soon as

$$\text{pen}(m) \geq \kappa (\mathfrak{D}_m + x_m) \quad \text{with } \kappa > \kappa_0,$$

where  $\mathfrak{D}_m$  measure the complexity of the model  $S_m$  (entropy term) and  $x_m$  the coding cost within the collection.

- Distances used  $KL^{\otimes n}$  and  $JKL_{\rho}^{\otimes n}$  : *tensorized* Kullback divergence and *Jensen-Kullback* divergence.
- $\mathfrak{D}_m$  linked to the *bracketing entropy* of  $S_m$  with respect to the tensorized Hellinger distance  $d^{2 \otimes n}$ .
- Often  $\mathfrak{D}_m \propto (\log n) \dim(S_m) \dots$

# Spatialized Gaussian Mixture Case

- Computation of an upper bound of the bracketing entropy possible (cf Maugis et Michel) implying :

$$\mathfrak{D}_m \leq \kappa' \left( C' + \frac{1}{2} \left( \ln \left( \frac{N}{C' \dim(S_m)} \right) \right)_+ \right) \dim(S_m).$$

- Collection coding with  $x_m \leq \kappa'' |\mathcal{P}| \leq \frac{\kappa''}{K-1} \dim(S_m)$ .
- Constraint on the penalty :

$$\begin{aligned} \text{pen}(m) &\geq \left( \kappa' \left( C' + \frac{1}{2} \left( \ln \left( \frac{N}{C' \dim(S_m)} \right) \right)_+ \right) + \frac{\kappa''}{K-1} \right) \dim(S_m) \\ &\geq \lambda_{0,N} |\mathcal{P}| (K-1) + \lambda_{1,N} \dim([\mu L D A]^K) \end{aligned}$$

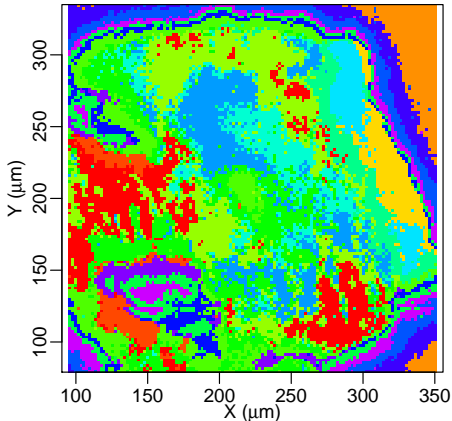




# Unsupervised Segmentation

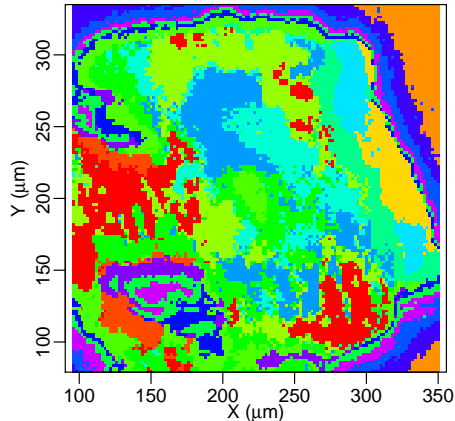
- Numerical result taking into account the spatial modeling :

Without



1 scan / 2min acquisition –simple EM–

With



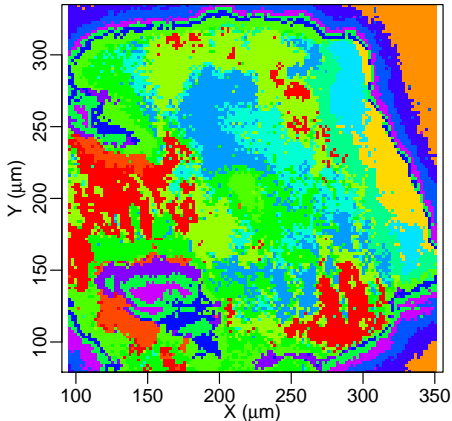
1 scan / 2min acquisition –spatial EM–

- Automatic choice of  $K$ ,  $[L_k D A]^K$  and partition.

# Unsupervised Segmentation

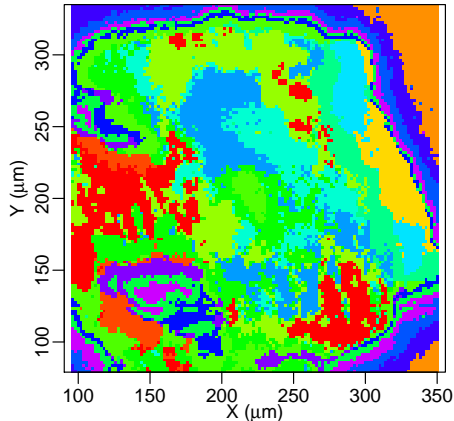
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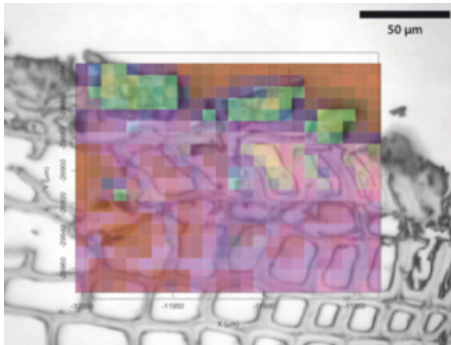
With



1 scan / 2min acquisition –spatial EM–

- Automatic choice of  $K$ ,  $[L_k D A]^K$  and partition.
- Penalty calibration by slope heuristic.
- Dimension reduction by random projection.

# Stradivari's Secret



- Two fine layers of varnish :
  - a first simple oil layer, similar to the painter's one, penetrating mildly the wood,
  - a second layer made from a mixture of oil, pine resin and red pigments.
- Classical technique up to the specific color choice (and a very good varnishing skill).
- Stradivari's secret was not his varnish !

# Conclusion

- Framework :
  - Unsupervised segmentation problem.
  - Proposed tool : Spatialized Gaussian Mixture Model
  - Penalized maximum likelihood conditional density estimation.
- Results :
  - Theoretical guaranty for the conditional density estimation problem.
  - Direct application to the unsupervised segmentation problem.
  - Efficient minimization algorithm.
  - Unsupervised segmentation algorithm in between *spectral* methods and *spatial* ones.
- Perspectives :
  - Formal link between conditional density estimation and unsupervised segmentation.
  - Penalty calibration by slope heuristic.
  - Dimension reduction adapted to unsupervised segmentation/classification.
  - Enhanced Spatialized Gaussian Mixture Model with piecewise logistic weights (L. Montuelle).