Non-supervised hyperspectral image segmentation, a conditional density approach

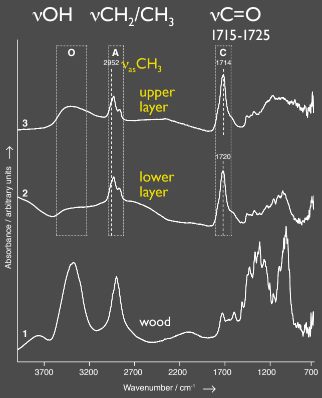
E. Le Pennec
(CMAP - École Polytechnique)
and
S. Cohen (IPANEMA - CNRS / Soleil)

Daspac
21 may 2014

A. Stradivari (1644 - 1737)

Provigny (1716)

A. Giordan © Cité de la Musique

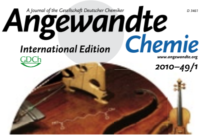


SOLEIL SYNCHROTRON

4 / 8 cm^{-1} resolution
64 / 128 scans
typ. 1 min/sp, 400sp

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

cité de la musique · SOLEIL SYNCHROTRON · CRCC · CENTRE DE RECHERCHE ET DE RESTAURATION DES MUSÉES DE FRANCE · Laboratoire de Dynamique, Interactions et Réactivité



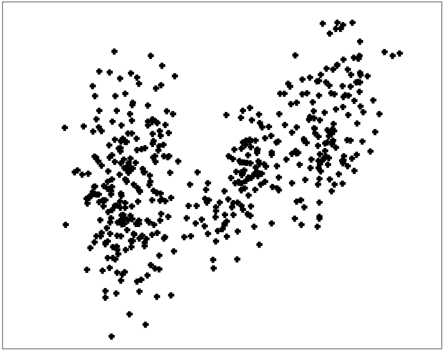
J.-P. Echard, L. Bertrand, A. von Bohlen, A.-S. Le Hô, C. Paris, L. Bellot-Gurlet, B. Soulier, A. Lattuati-Derieux, S. Thao, L. Robinet, B. Lavédrine, and S. Vaiedelich. *Angew. Chem. Int. Ed.*, 49(1), 197-201, 2010.

Hyperspectral Image Segmentation

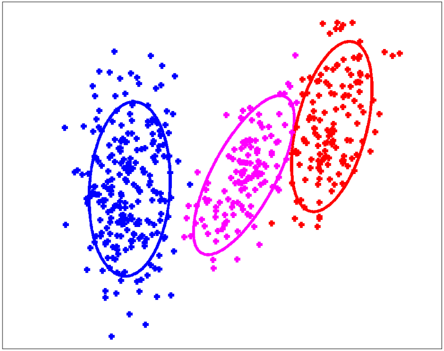
- Data :
  - image of size N between ~ 1000 and ~ 100000 pixels,
  - spectrums $\mathcal{S}$ of ~ 1024 points,
  - very good spatial resolution,
  - ability to measure a lot of spectrums per minute,
- Immediate goal :
  - automatic image segmentation,
  - without human intervention,
  - help to data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

A “Toy” Problem

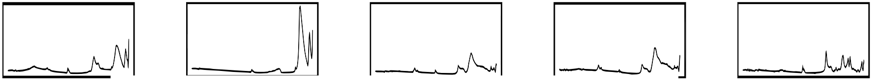
A "Toy" Problem

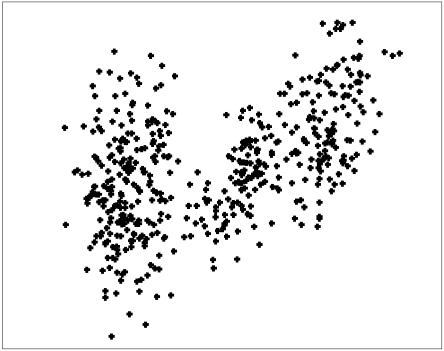


A “Toy” Problem

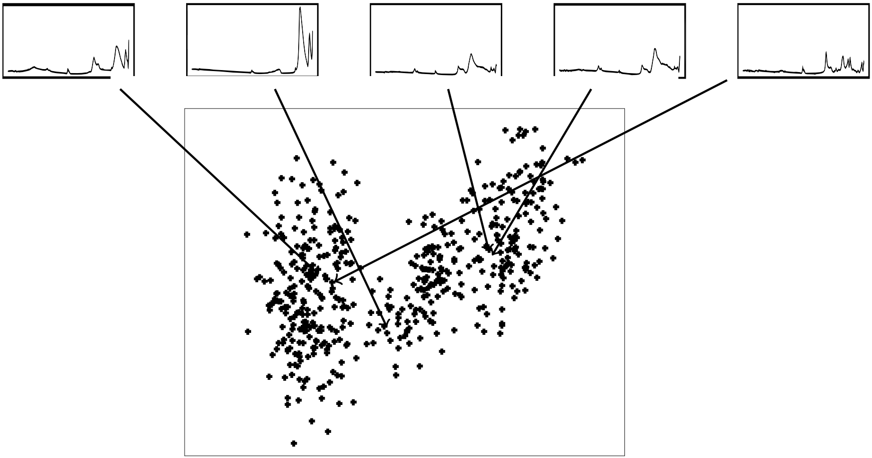


A “Toy” Problem

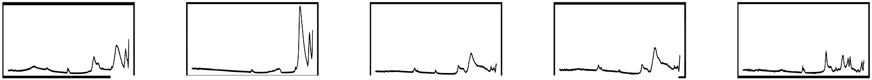


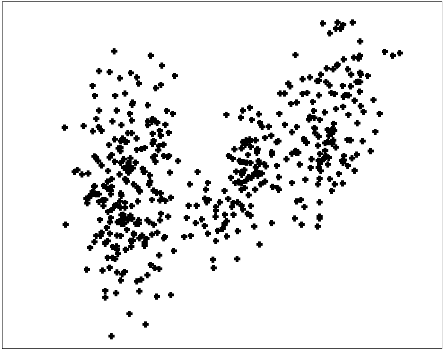


A "Toy" Problem

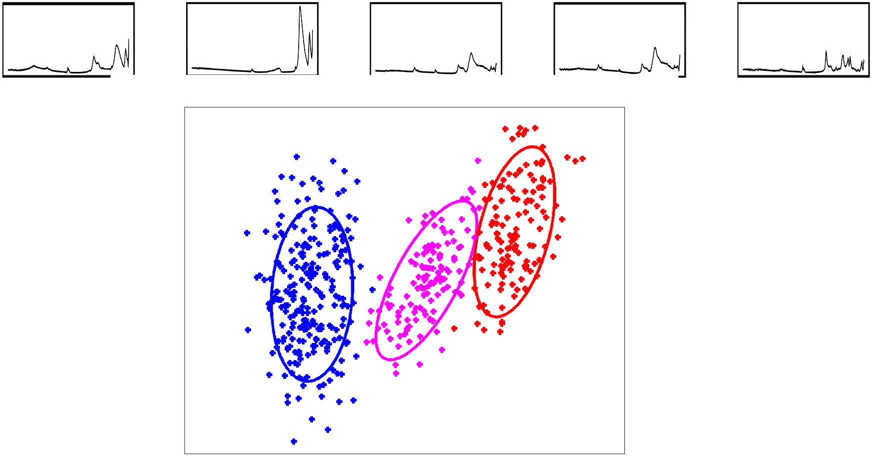


A “Toy” Problem

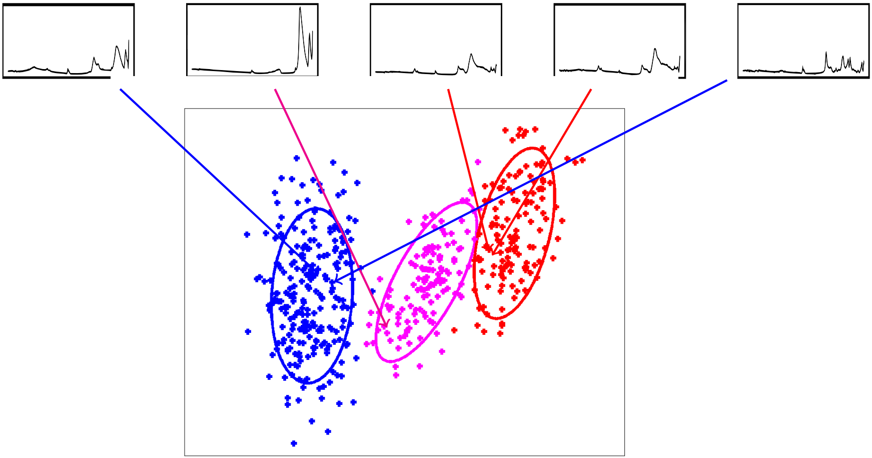




A “Toy” Problem



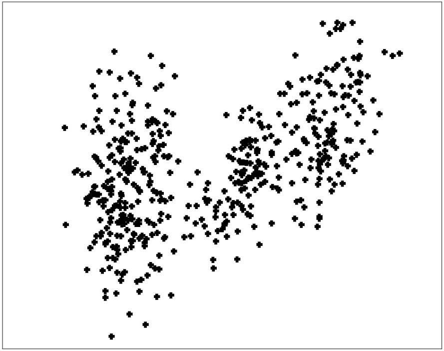
A "Toy" Problem



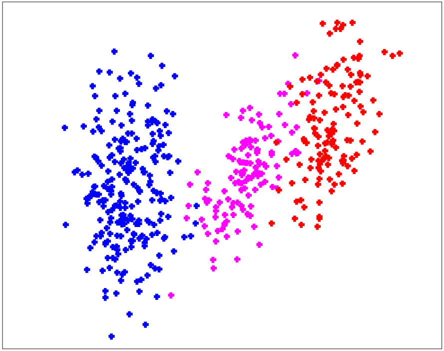
- Representation : mapping between spectrums and points in a large dimension space.
- Spectral method.

“Stochastic” Modeling

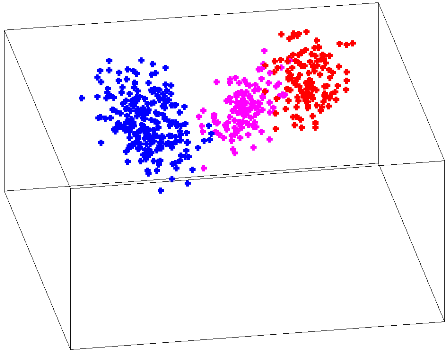
“Stochastic” Modeling



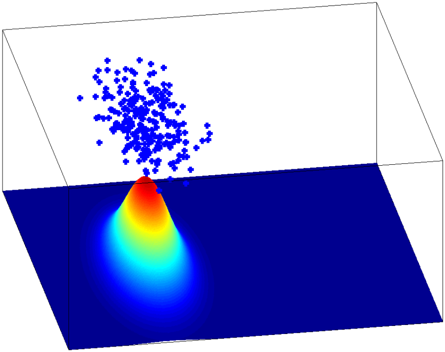
“Stochastic” Modeling



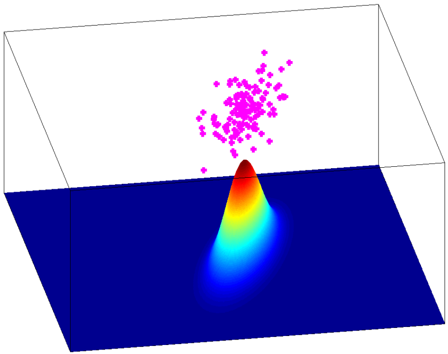
"Stochastic" Modeling



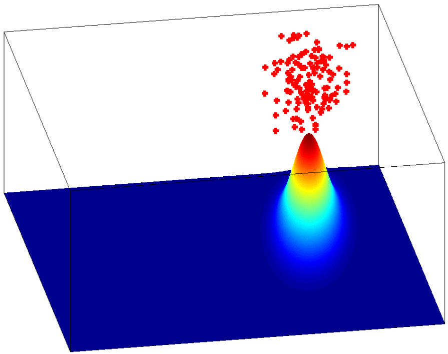
“Stochastic” Modeling



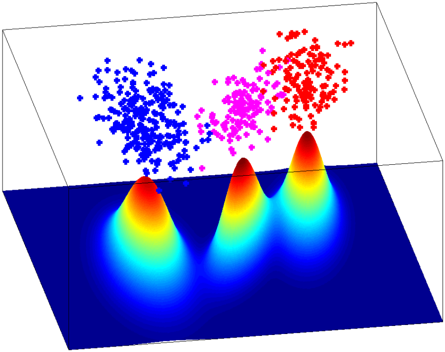
“Stochastic” Modeling



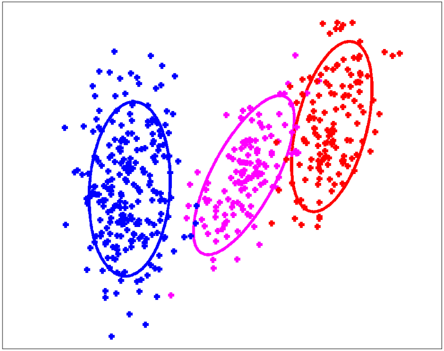
“Stochastic” Modeling



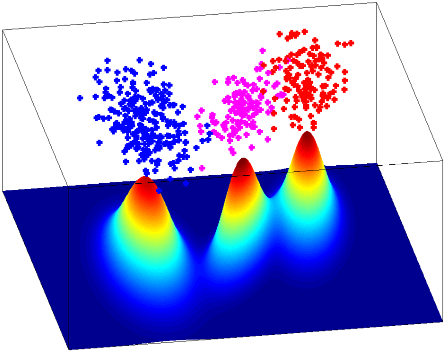
"Stochastic" Modeling



“Stochastic” Modeling



“Stochastic” Modeling

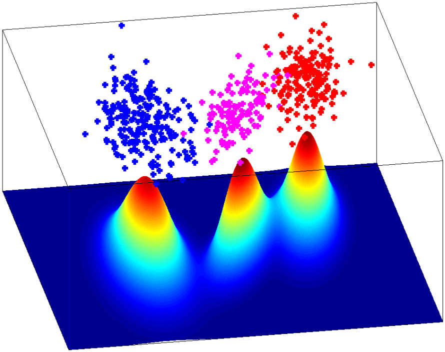


- Model : Gaussian Mixture with K classes.
- Mixture density :

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

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

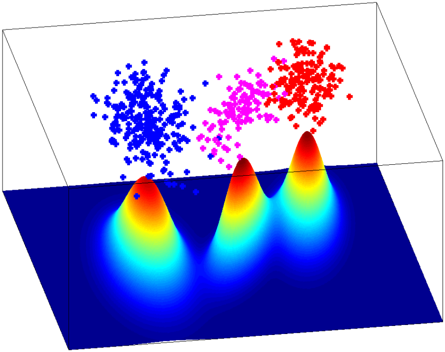
“Stochastic” Modeling



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

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

"Stochastic" Modeling

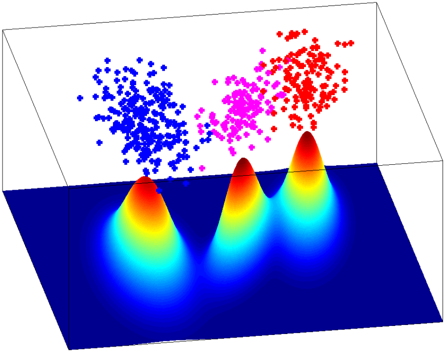


- Model : Gaussian Mixture with K classes.
- Mixture density :

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

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

“Stochastic” Modeling



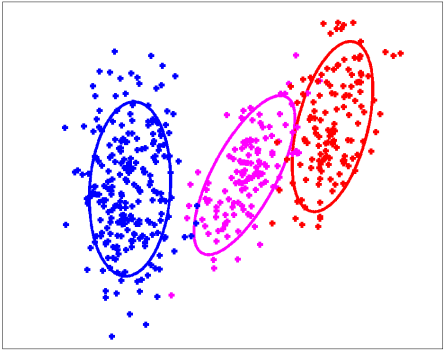
- Model : Gaussian Mixture with K classes.
- Mixture density :

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

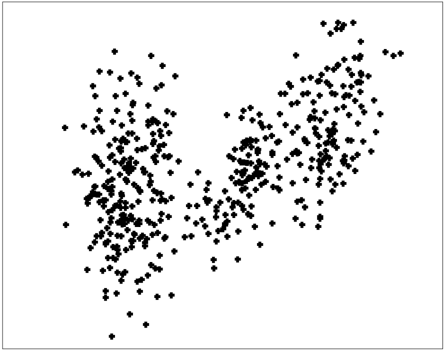
$$= \sum_{k=1}^{K} \pi_k \mathcal{N}_{\mu_k,\Sigma_k}(\mathcal{S})$$

“Statistical” Estimation

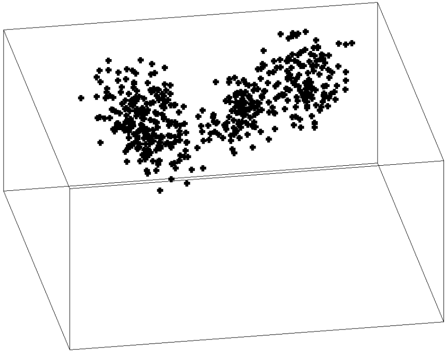
“Statistical” Estimation



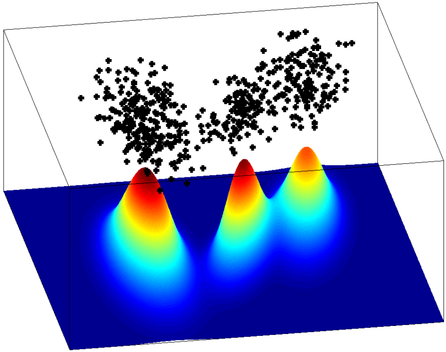
“Statistical” Estimation



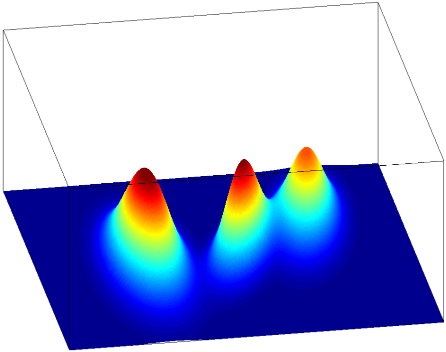
“Statistical” Estimation



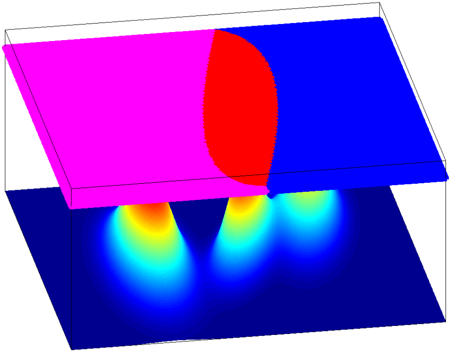
“Statistical” Estimation



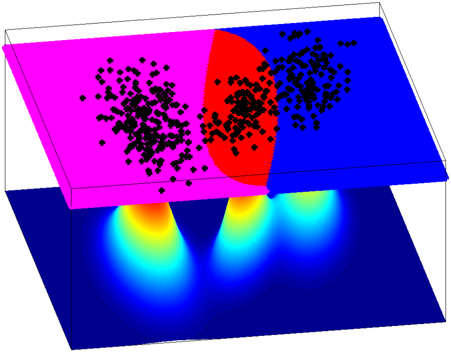
“Statistical” Estimation



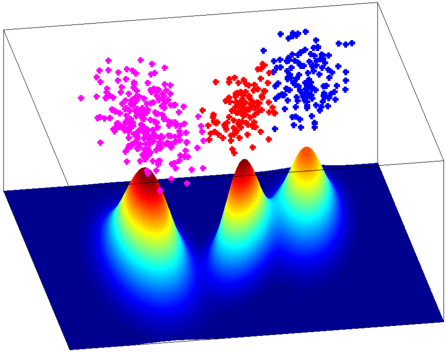
“Statistical” Estimation



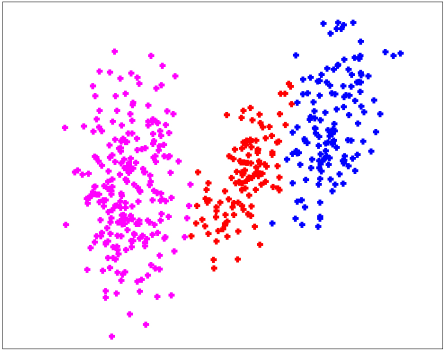
“Statistical” Estimation



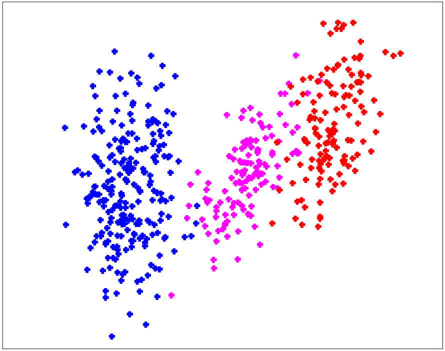
“Statistical” Estimation



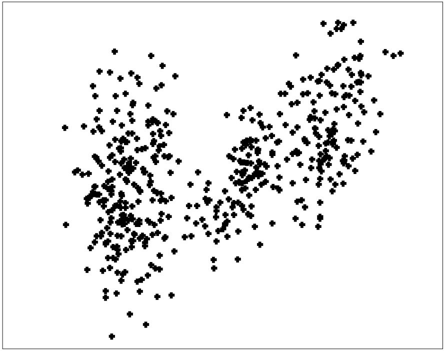
"Statistical" Estimation



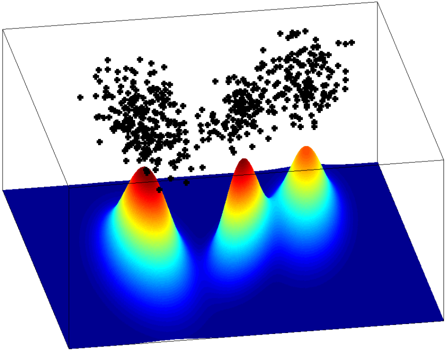
“Statistical” Estimation



"Statistical" Estimation



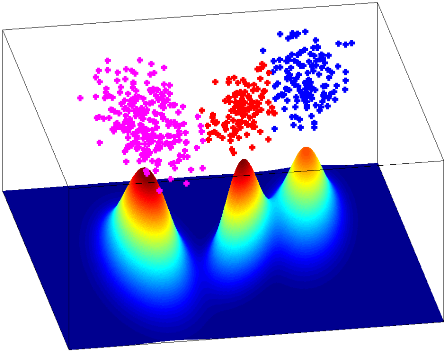
"Statistical" Estimation



- Estimation of π_k, $\widehat{\mu_k}$ and $\widehat{\Sigma_k}$ by maximum likelihood :

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

"Statistical" Estimation



- Estimation of π_k, $\widehat{\mu_k}$ and $\widehat{\Sigma_k}$ by maximum likelihood :

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

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

$$\widehat{k}(\mathcal{S}) = \operatorname{argmax} \widehat{\pi_k} \mathcal{N}_{\widehat{\mu_k},\widehat{\Sigma_k}}(\mathcal{S})$$

Hyperspectral image segmentation with GMM

- *Classical* stochastic model of spectrum $\mathcal{S}$:
  - K spectrum classes,
  - with proportion π_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, π_k, μ_k and Σ_k) from the data.
- Why : yields a classification/segmentation by a maximum likelihood principle

$$\widehat{k}(\mathcal{S}) = \operatorname{argmax} \widehat{\pi_k} \mathcal{N}_{\widehat{\mu_k},\widehat{\Sigma_k}}(\mathcal{S})$$

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

Gaussian Mixture Model

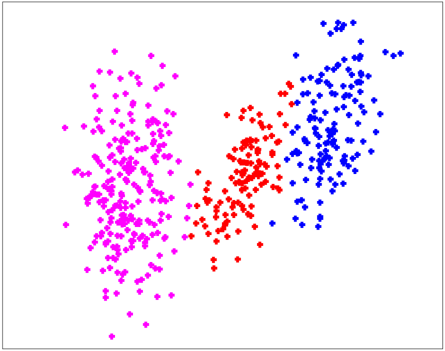
- True density s_0 of $\mathcal{S}$ close from

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

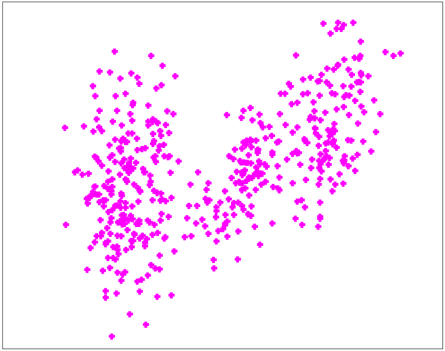
- Gaussian Mixture Model $S_m = \{s_m\}$ specified by
  - a number of classes K,
  - a structure for the means μ_k and the covariance matrices $\Sigma_k = L_k D_k A_k D_k'$ (Volume L_k, basis D_k and rescaled eigenvalues A_k)
- Structure $[\mu\, L\, D\, A]^K$ for the K-tuples of Gaussian parameters :
  - 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 μ_k and the covariance matrix $\Sigma_k = L_k D_k A_k D_k'$ for each class
  - and the mixing proportions π_k

How many classes ?

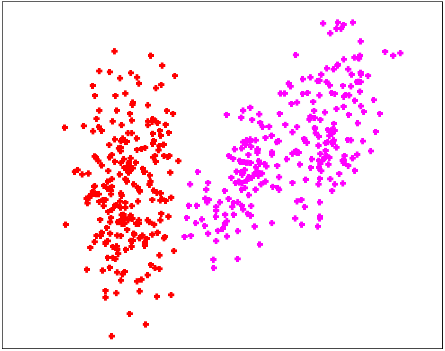
How many classes ?



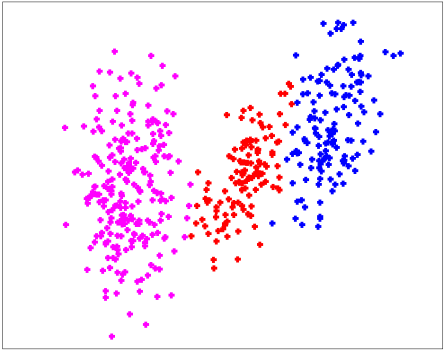
How many classes?



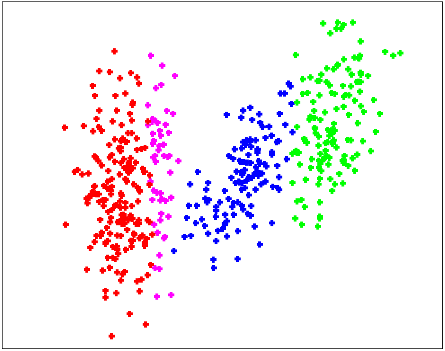
How many classes ?



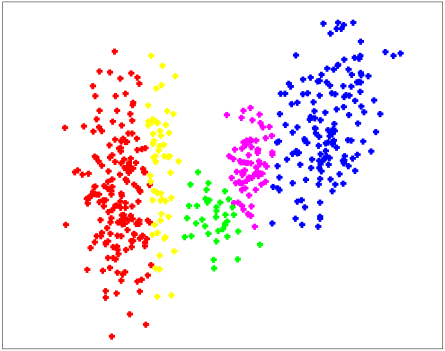
How many classes ?



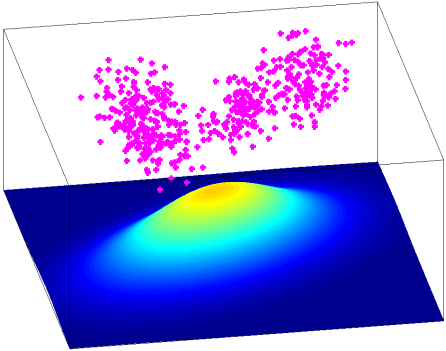
How many classes ?



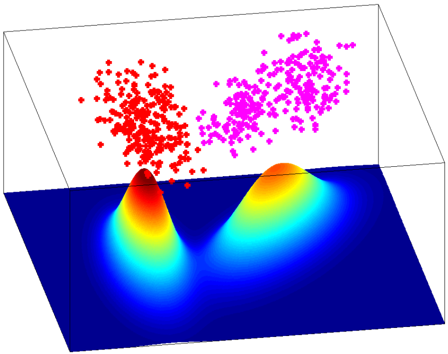
How many classes ?



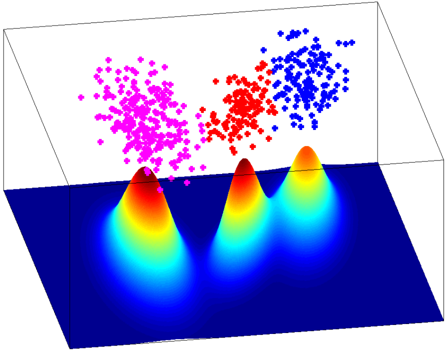
How many classes ?



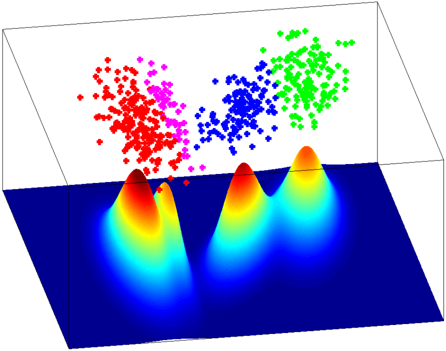
How many classes ?



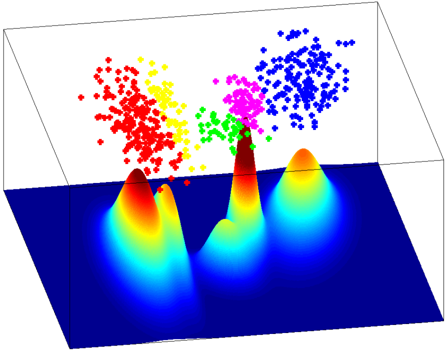
How many classes ?



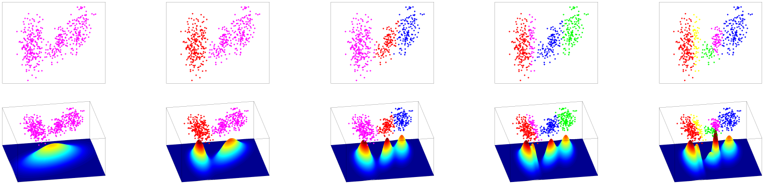
How many classes ?



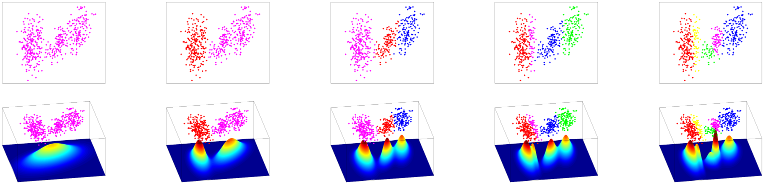
How many classes ?



How many classes ?

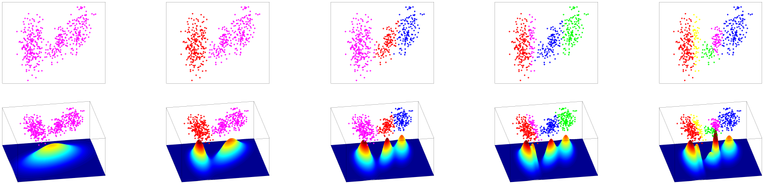


How many classes ?



Fidelity	−−	+	+ + +	+ + +·	+ + ++

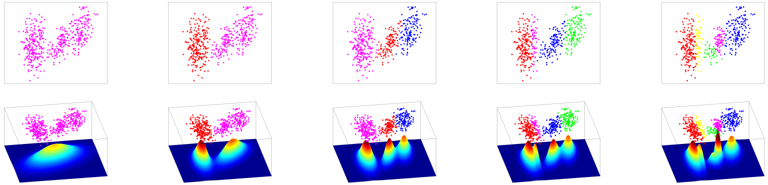
How many classes ?



Fidelity	$--$	$+$	$+++$	$+++\cdot$	$++++$

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

How many classes ?



Fidelity	− −	+	+ + +	+ + +·	+ + ++
Simplicity	+ + ++	+ + +	++	+	−

- 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 ($\sim$ 1285 - 1347)

Ockham's Razor

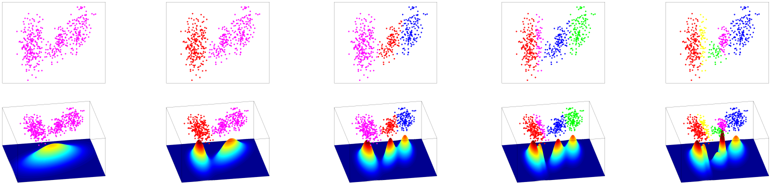
entities must not be multiplied beyond necessity

William of Ockham ($\sim$ 1285 - 1347)

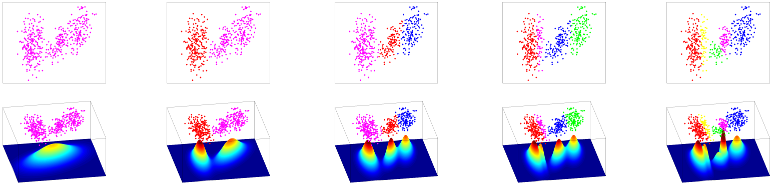
- Ockham's Razor (simplicity principle) : one should not add hypotheses, if the current ones are already sufficient !
- Balance between observation explanation power and simplicity.

Selection by Penalization

Selection by Penalization

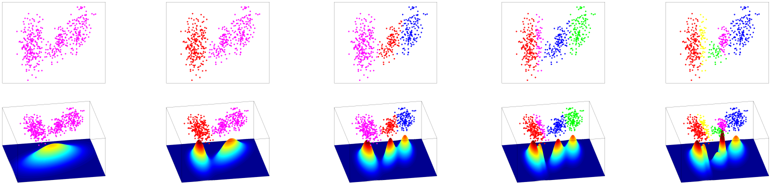


Selection by Penalization



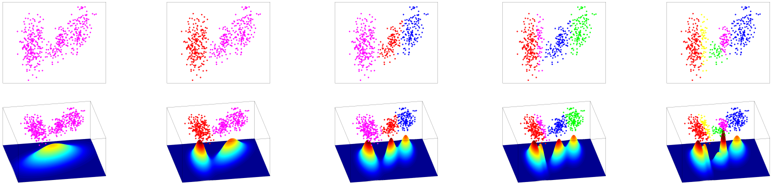
Likelihood	– –	+	+ + +	+ + +.	+ + ++
Simplicity	+ + ++	+ + +	++	+	–

Selection by Penalization



Likelihood	−−	+	+ + +	+ + +·	+ + ++
+ Simplicity	+ + ++	+ + +	++	+	−
= Tradeoff	++	+ + ++	+ + + + +	+ + + + ·	+ + +

Selection by Penalization

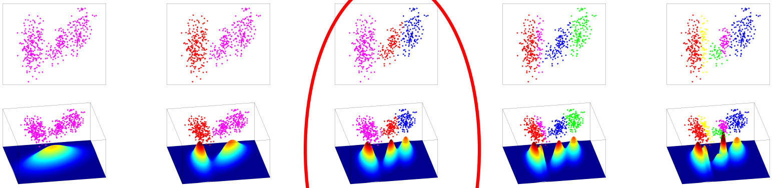


Likelihood	$--$	$+$	$+++$	$+++\cdot$	$++++$
$+$ Simplicity	$++++$	$+++$	$++$	$+$	$-$
$=$ Tradeoff	$++$	$++++$	$+++++$	$++++\cdot$	$+++$

- Likelihood : $\sum_{i=1}^{N} \log \hat{s}_K(X_i)$.
- Simplicity : $-\lambda \mathrm{Dim}(S_K)$.
- Penalized estimator :

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

Selection by Penalization

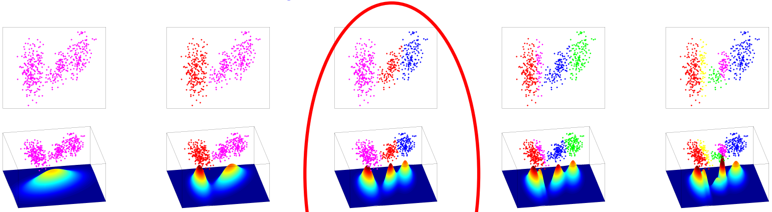


Likelihood	$--$	$+$	$+++$	$+++\cdot$	$++++$
$+$ Simplicity	$++++$	$+++$	$++$	$+$	$-$
$=$ Tradeoff	$++$	$++++$	$+++++$	$++++\cdot$	$+++$

- Likelihood : $\sum_{i=1}^{N} \log \hat{s}_K(X_i)$.
- Simplicity : $-\lambda \mathrm{Dim}(S_K)$.
- Penalized estimator :

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

Selection by Penalization



Likelihood	−−	+	+++	+++·	++++
+ Simplicity	++++	+++	++	+	−
= Tradeoff	++	++++	+++++	++++·	+++

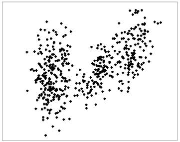
- Likelihood : $\sum_{i=1}^{N} \log \hat{s}_K(X_i)$.
- Simplicity : $-\lambda \mathrm{Dim}(S_K)$.
- Penalized estimator :

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

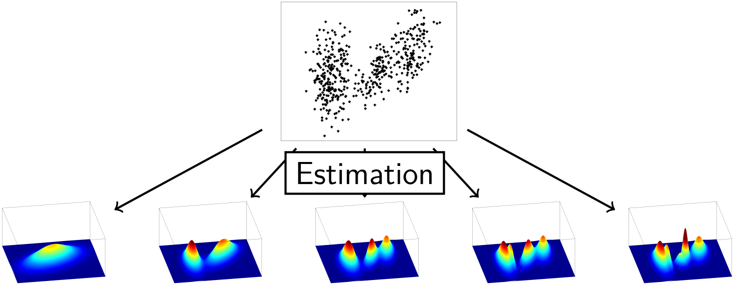
- Optimization in K by exhaustive exploration !

Methodology

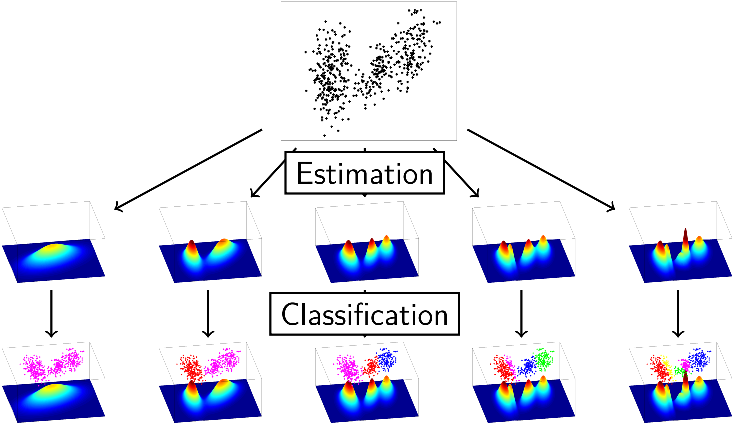
Methodology



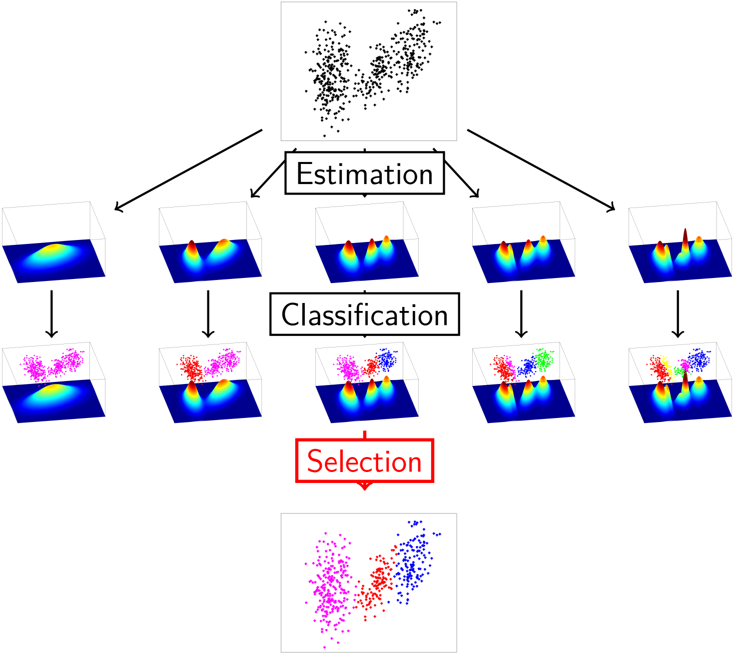
Methodology



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 $\widehat{m}$ by

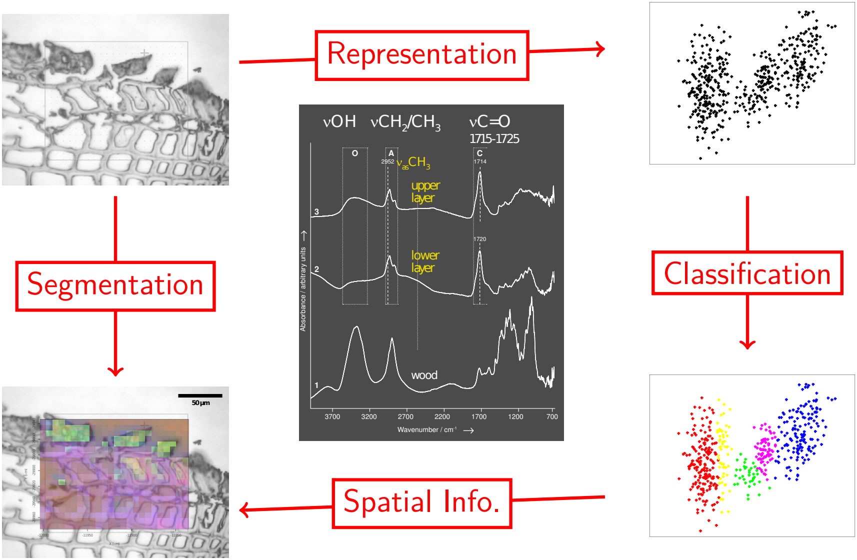
$$\widehat{m} = \mathrm{argmin} - \ln(\widehat{s}_m) + \mathrm{pen}(m).$$

  with $\mathrm{pen}(m) = \kappa(\ln(n))\,\dim(S_m)$ (parametric dimension of S_m),
- Results (Birgé, Massart, Celeux, Maugis, Michel...) :
  - Density estimation : for κ large enough,

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

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

Back to our violins



Segmentation and Spatialized GMM

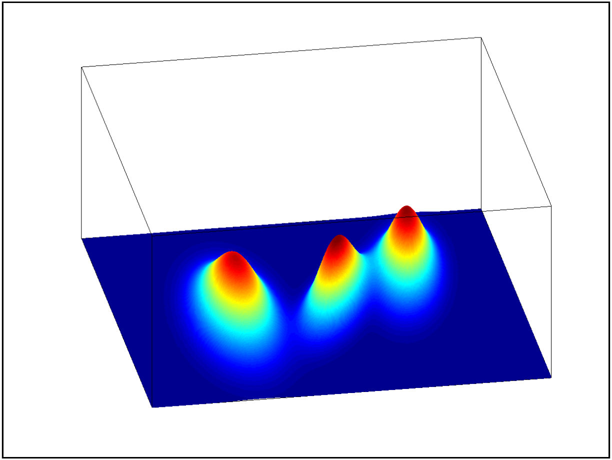
- Initial goal : segmentation $\neq$ clustering.
- Idea of Kolaczyk et al (cf Bigot) : take into account the spatial position x of the spectrum in the mixing proportions.
- Conditional density model :

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

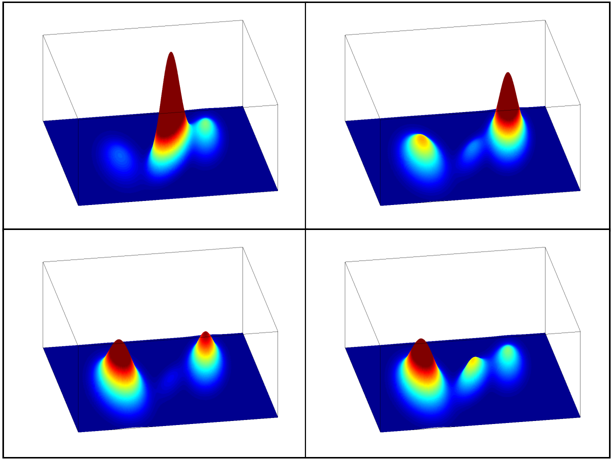
- Estimation from the data :
  - the mean μ_k and the covariance matrix $\Sigma_k = L_k D_k A_k D_k'$ for each class
  - and the mixing proportion functions $\pi_k(x)$.
- Segmentation by MAP principle :

$$\widehat{k}(\mathcal{S}|x) = \arg\max_k \widehat{\pi_k}(x) \mathcal{N}_{\widehat{\mu_k},\widehat{\Sigma_k}}(\mathcal{S})$$

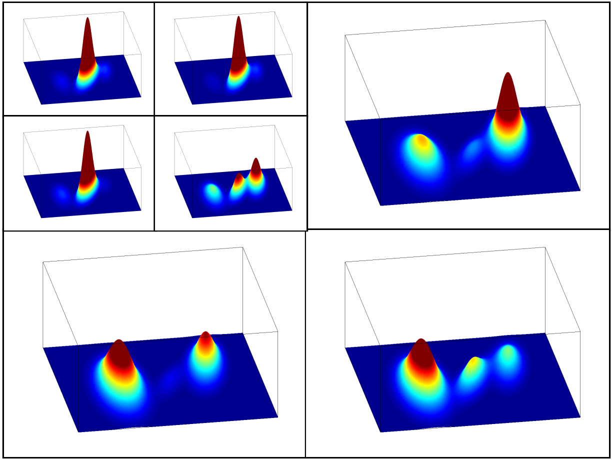
Segmentation and Spatialized GMM



Segmentation and Spatialized GMM

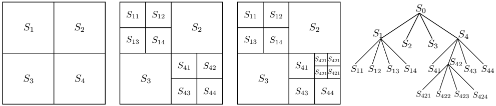


Segmentation and Spatialized GMM



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 $\mathrm{pen}(m) = \kappa \ln(n) \dim(S_m)$ allows
  - a numerical optimization scheme (EM + dynamic programing)
  - a theoretical control : for κ large enough

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

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 $s_0(y|X_i)$.
- 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 $\widehat{m}$ by

$$\widehat{m} = \operatorname*{argmin}_{m \in \mathcal{S}} - \sum_{i=1}^{n} \ln \widehat{s}_m(Y_i|X_i) + \mathrm{pen}(m).$$

  with $\mathrm{pen}(m)$ *well chosen*.
- Conditional density estimation result of type :

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

- 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 $s_m \in S_m$

$$\int_0^\sigma \sqrt{H_{[\cdot],d^{\otimes_n}}\left(\epsilon, S_m(s_m, \sigma)\right)}\, d\epsilon \leq \phi_m(\sigma).$$

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 $\widehat{s}_m$ be a δ -log-likelihood minimizer in S_m :

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

Then for any $\rho \in (0,1)$ and any $C_1 > 1$, there is a constant κ_0 depending only on ρ and C_1 such that, as soon as for every index $m \in \mathcal{M}$ $\mathrm{pen}(m) \geq \kappa\left(\mathfrak{D}_m + x_m\right)$ with $\kappa > \kappa_0$
where $\mathfrak{D}_m = n\sigma_m^2$ with σ_m the unique root of $\frac{1}{\sigma}\phi_m(\sigma) = \sqrt{n}\sigma$,
the penalized likelihood estimate $\widehat{s}_{\widehat{m}}$ with $\widehat{m}$ defined by

$$\widehat{m} = \operatorname*{argmin}_{m\in\mathcal{M}} \sum_{i=1}^{n} -\ln(\widehat{s}_m(Y_i|X_i)) + \mathrm{pen}(m)$$

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

Simplified Theorem...

- Oracle inequality :

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

  as soon as

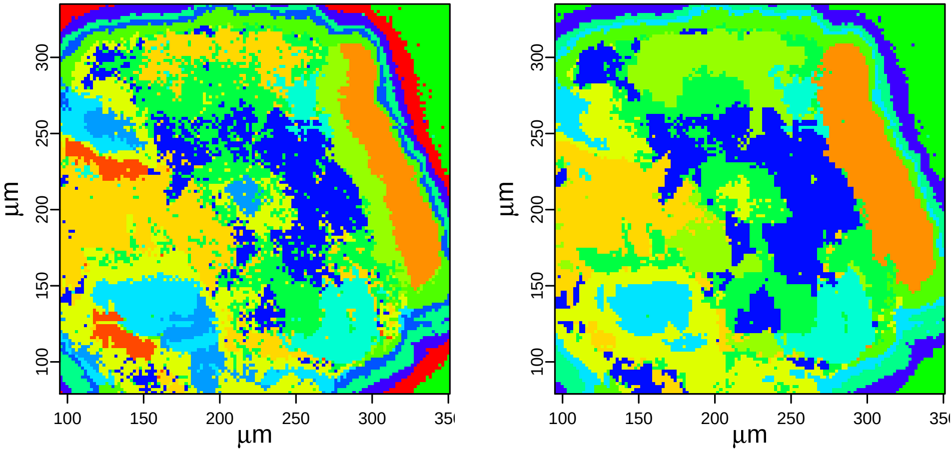
$$\mathrm{pen}(m) \geq \kappa\left(\mathfrak{D}_m + x_m\right) \quad \text{with } \kappa > \kappa_0,$$

  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 $\mathfrak{D}_m \propto (\log n)\dim(S_m)$...

Unsupervised Segmentation

- Numerical result taking into account the spatial modeling :

Without | With



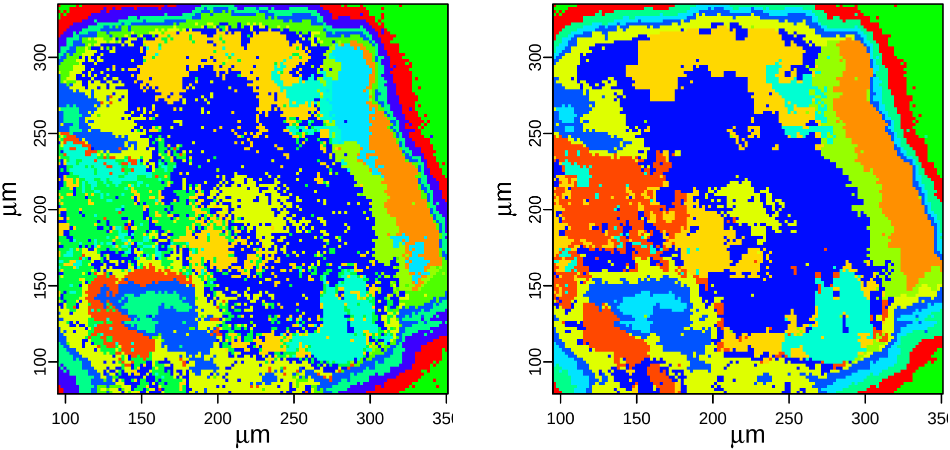
30 min.

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

Unsupervised Segmentation

- Numerical result taking into account the spatial modeling :

Without With

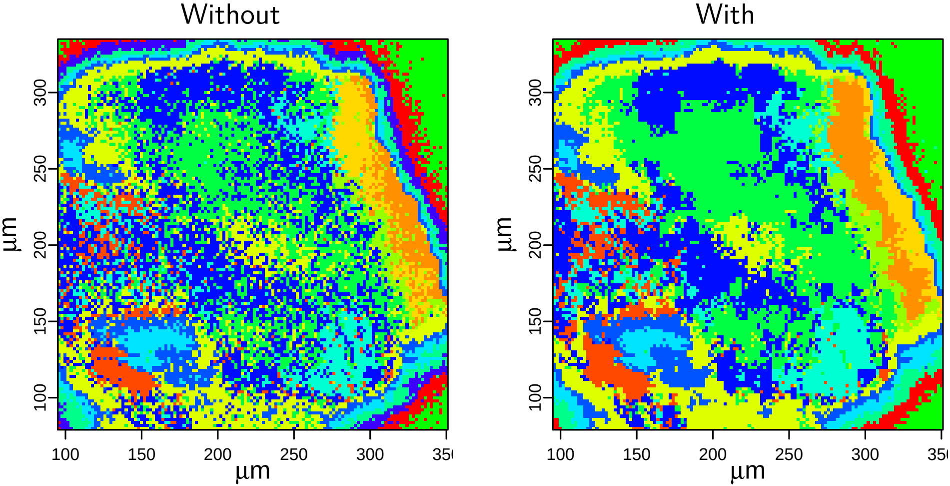


5 min.

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

Unsupervised Segmentation

- Numerical result taking into account the spatial modeling :



1 min.

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

Numerical optimization

- Penalized Model Selection :

$$\operatorname*{argmin}_{K,[\mu\, L\, D\, A]^K,\mu,\Sigma,\mathcal{P},\pi} -\sum_{i=1}^{N} \ln\left(\sum_{k=1}^{K} \pi_k[\mathcal{R}(x_i)]\,\mathcal{N}_{\mu_k,\Sigma_k}(\mathcal{S}_i)\right) + \lambda_{0,N}|\mathcal{P}|(K-1) + \lambda_{1,N}\dim([\mu\, L\, D\, A]^K)$$

- Optimization on the number of classes K and the mean and covariance structure by exhaustive exploration.
- Model selection for a given number of classes K and a given structure $[\mu\, L\, D\, A]^K$:

$$\operatorname*{argmin}_{\mu,\Sigma,\mathcal{P},\pi} -\sum_{i=1}^{N} \ln\left(\sum_{k=1}^{K} \pi_k[\mathcal{R}(x_i)]\,\mathcal{N}_{\mu_k,\Sigma_k}(\mathcal{S}_i)\right) + \lambda_{0,n}|\mathcal{P}|(K-1)$$

- Two tricks :
  - EM algorithm (a MM algorithm)
  - CART (dynamic programming)

Maximum likelidood estimation

- Model selection for a given number of classes K and a given structure $[\mu\, L\, D\, A]^K$:

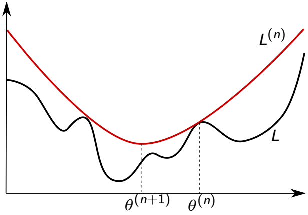
$$\underset{\mu,\Sigma,\mathcal{P},\pi}{\operatorname{argmin}} -\sum_{i=1}^{N} \ln\left(\sum_{k=1}^{K} \pi_k[\mathcal{R}(x_i)]\,\mathcal{N}_{\mu_k,\Sigma_k}(\mathcal{S}_i)\right) + \lambda_{0,n}|\mathcal{P}|(K-1)$$

- If one also fixes $\mathcal{P}$, back to maximum likelihood estimation :

$$\underset{\mu,\Sigma,\pi}{\operatorname{argmin}} -\sum_{i=1}^{N} \ln\left(\sum_{k=1}^{K} \pi_k[\mathcal{R}(x_i)]\,\mathcal{N}_{\mu_k,\Sigma_k}(\mathcal{S}_i)\right)$$

- Non convex minimization problem !
- Majorization/Minimization approach

MM approach



- Iterative approach to minimize $L(\theta)$ by minimizing a sequence of (convex) proxies of L.
- Majorization/Minimization :
  - Current estimate of the minimizer : $\theta^{(n)}$
  - Construction of a Majorization $L^{(n)}$ of L such that $L^{(n)}(\theta^{(n)}) = L(\theta^{(n)})$ with $L^{(n)}$ easy to minimize (convex for example).
  - Computation of a Minimizer

$$\theta^{(n+1)} = \operatorname{argmin} L^{(n)}(\theta)$$

- By construction, $L(\theta^{(n+1)}) \leq L(\theta^{(n)})$!
- Very generic methodology...
- Minimization can be replaced by a diminution...

Maximum Likelihood and EM

- Back to our maximum likelihood for a fixed partition :

$$L(\mu,\Sigma,\pi)=\sum_{i=1}^{N}-\ln\left(\sum_{k=1}^{K}\pi_k[\mathcal{R}(x_i)]\,\mathcal{N}_{\mu_k,\Sigma_k}(\mathcal{S}_i)\right)$$

- EM : specific case of MM for this type of mixture.
- (Conditional) Expectation : at step n, we let

$$P_k^{i,(n)}=P\left(k_i=k\middle|\mathcal{S}_i,\mu^{(n)},\Sigma^{(n},\pi^{(n)}\right)$$

and $$L^{(n)}(\mu,\Sigma,\pi)=-\sum_{i=1}^{N}\sum_{k=1}^{K}P_k^{i,(n)}\ln\left(\pi_k[\mathcal{R}(x_i)]\mathcal{N}_{\mu_k,\Sigma_k}(\mathcal{S}_i)\right).$$

- Majorization prop. : $L\leq L^{(n)}+\mathrm{Cst}^{(n)}$ with equ. at $(\mu^{(n)},\Sigma^{(n},\pi^{(n)})$.
- Bonus :
  - Separability in (μ,Σ) and π :

$$L^{(n)}(\mu,\Sigma,\pi)=-\sum_{i=1}^{N}\sum_{k=1}^{K}P_k^{i,(n)}\ln\left(\mathcal{N}_{\mu_k,\Sigma_k}(\mathcal{S}_i)\right)-\sum_{i=1}^{N}\sum_{k=1}^{K}P_k^{i,(n)}\ln\left(\pi_k[\mathcal{R}(x_i)]\right)$$

  - Close formulas for the Minimization of $L^{(n)}$ in (μ,Σ) and π !

Partition and EM Algorithm

- Maximum likelihood :

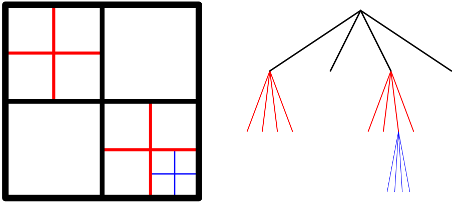
$$L(\mu, \Sigma, \mathcal{P}, \pi) = -\sum_{i=1}^{N} \ln\left(\sum_{k=1}^{K} \pi_k[\mathcal{R}(x_i)]\, \mathcal{N}_{\mu_k,\Sigma_k}(\mathcal{S}_i)\right) + \lambda_{0,n}|\mathcal{P}|(K-1)$$

- E Step : with $P_k^{i,(n)} = P(k_i = k | x_i, \mathcal{S}_i, \mu^{(n)}, \Sigma^{(n}, \mathcal{P}^{(n)}, \pi^{(n)})$

$$\begin{aligned} L(\mu, \Sigma, \mathcal{P}, \pi) & \\ \leq -\sum_{i=1}^{N}\sum_{k=1}^{K} P_k^{i,(n)} \ln\left(\mathcal{N}_{\mu_k,\Sigma_k}(\mathcal{S}_i)\right) & \\ -\sum_{i=1}^{N}\sum_{k=1}^{K} P_k^{i,(n)} \ln\left(\pi_k[\mathcal{R}(x_i)]\right) + \lambda_{0,N}|\mathcal{P}|(K-1) + \mathrm{Cst}^{(n)} & \end{aligned}$$

  with equality at $(\mu^{(n)}, \Sigma^{(n)}, \mathcal{P}^{(n)}, \pi^{(n)})$.
- M Step : Separate optimization in (μ, Σ) and $(\mathcal{P}, \pi)$ possible,
  - Optimization in (μ, Σ) : close formulas (classical...).
  - Optimization in $(\mathcal{P}, \pi)$ more interesting !

M Step and CART



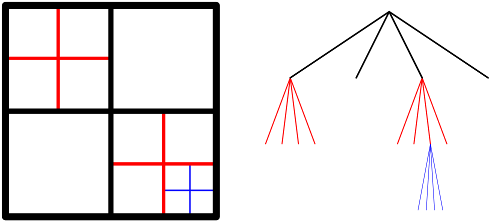
- Optimization in $(\mathcal{P}, \pi)$ of

$$-\sum_{i=1}^{N}\sum_{k=1}^{K} P_k^{i,(n)} \ln\left(\pi_k[\mathcal{R}(x_i)]\right) + \lambda_{0,n}|\mathcal{P}|(K-1)$$

$$= -\sum_{\mathcal{R}\in\mathcal{P}}\left(\sum_{i|x_i\in\mathcal{R}}\sum_{k=1}^{K} P_k^{i,(n)} \ln\left(\pi_k[\mathcal{R}(x_i)]\right) + \lambda_{0,N}(K-1)\right)$$

- Two key properties :
  - For each $\mathcal{R}$, simple (classical) optimization of $\pi_k[\mathcal{R}]$.
  - Additivity in $\mathcal{R}$ of the cost structure.
- $\Rightarrow$ Fast CART optimization algorithm (Dynamic programming on tree structure).

CART Optimization



- Aim : compute efficiently $\operatorname*{argmin}_{\mathcal{P}} \sum_{\mathcal{R}\in\mathcal{P}} C[\mathcal{R}]$ where $\mathcal{P}$ is a recursive dyadic partition (associated to quadtree) of limited depth.
- Key property : the optimal partition $\widehat{\mathcal{P}}[\mathcal{R}]$ of a dyadic square is
  - either this square, $\widehat{\mathcal{P}}[\mathcal{R}] = \{\mathcal{R}\}$
  - or the union of the opt. part. of its children, $\widehat{\mathcal{P}}[\mathcal{R}] = \cup_{\mathcal{R}'\in\mathsf{Child}[\mathcal{R})} \widehat{\mathcal{P}}[\mathcal{R}']$

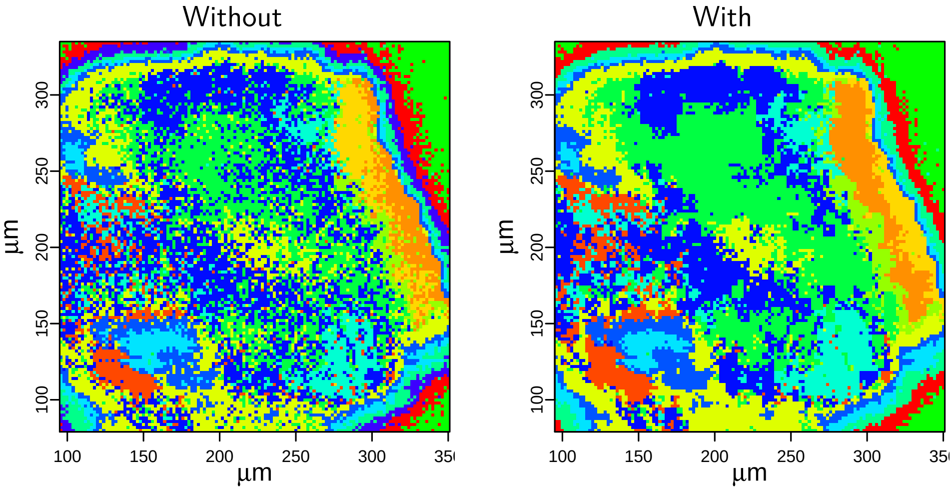
  with a decision based on

$$C[\mathcal{R}] \leq \sum_{\mathcal{R}'\in\mathsf{Child}(\mathcal{R})} \sum_{\mathcal{R}''\in\widehat{\mathcal{P}}[\mathcal{R}']} C[\mathcal{R}'']$$

- Fast bottom-up algorithm.

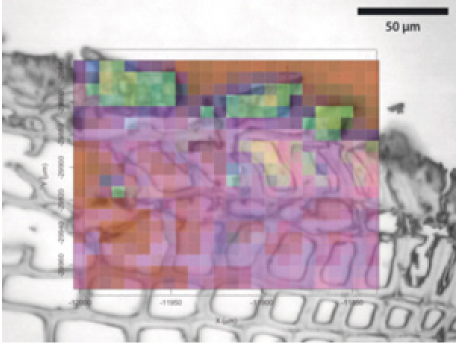
Unsupervised Segmentation

- Numerical result taking into account the spatial modeling :



- 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).