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Label switching in mixtures



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The label switching problem

Mixture of g distributions

$$p(\cdot|\theta) = \sum_{k=1}^g \alpha_k p(\cdot|\beta_k)$$

- α_k : mixtures weights ($\alpha_k > 0$ and $\sum_k \alpha_k = 1$)
- β_k : parameters of each component distribution
- $\theta_k = (\alpha_k, \beta_k)$
- $\theta = (\theta_1, \dots, \theta_g) \in \Theta$

Generative interpretation

$x = (x_1, \dots, x_n)$ an n i.i.d. sample from $p(\cdot|\theta)$
 $z = (z_1, \dots, z_n) \in \mathcal{Z}$ is the *latent partition* which as been used to generate x

- $z_i \sim \mathcal{M}(1; \alpha_1, \dots, \alpha_g)$
- $x_i \sim p(\cdot|\beta_{z_i})$

Bayesian framework

- $p(\theta)$ a prior distribution on θ
- Bayesian inference is based on the posterior distribution $p(\theta|x) \propto p(x|\theta)p(\theta)$

The problem

If $p(x|\theta)$ and $p(\theta)$ are invariant up to a mixture component renumbering then so does $p(\theta|x)$

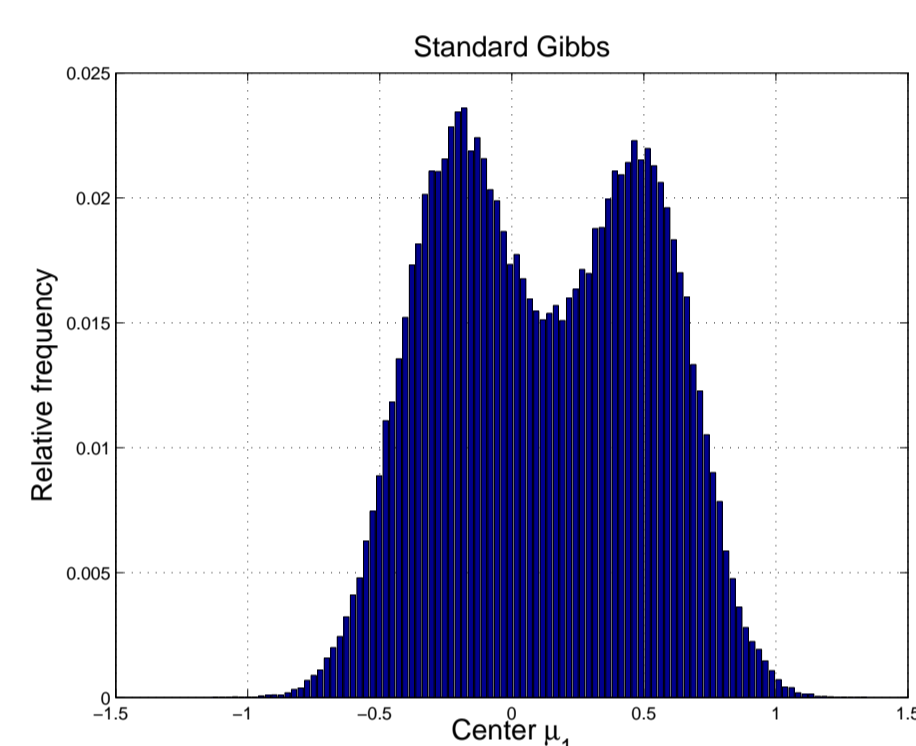
- \mathcal{P}_g is the set of $\{1, \dots, g\}$ permutations
- $\sigma(\theta) = (\theta_{\sigma(1)}, \dots, \theta_{\sigma(g)})$ is the parameter θ permuted in index with $\sigma \in \mathcal{P}_g$

$$p(\theta|x) = p(\sigma(\theta)|x)$$

This exact symmetry is called *label switching*. It then makes meaningless direct computation of many usual punctual estimators as the posterior mean. The aim of many approaches is to remove this symmetry.

Illustration of the problem

- Two univariate components ($g = 2$)
- $p(\cdot|\beta_k) = \mathcal{N}(\beta_k, 1)$
- $\alpha_1 = \alpha_2 = 0.5$
- Proportions and variances known and fixed
- Mean $\theta_1 = \beta_1$ et $\theta_2 = \beta_2$ unknown
- Prior distributions on $\theta_k \sim \mathcal{N}(0, 1)$ with $\theta_1 \perp \theta_2$
- Posterior distributions
 - ▶ $\theta_k|z, x \sim \mathcal{N}(n_k \bar{x}_k / (n_k + 1), 1 / (n_k + 1))$
 - ▶ $z_i|\theta, x \sim \mathcal{M}_2(1, t_{i1}(\theta), t_{i2}(\theta))$
 - ▶ $n_k = \sum_{i=1}^n \mathbb{1}_{z_i=k}$
 - ▶ $\bar{x}_k = \sum_{i=1}^n \mathbb{1}_{z_i=k} x_i / n_k$
 - ▶ $t_{ik}(\theta) = p(z_i = k|x, \theta)$
- $\theta_1 = 0$ and $\theta_2 = 0.25$



Posterior distribution $p(\theta_1|x)$.

Two modes can be seen on the posterior distribution of θ_1 when only one would be expected in absence of label switching. It is then impossible to make relevant analysis of the posterior distributions component-wise.

Standard solutions

Modified prior distribution

- Artificial identifiability constraints on the parameters (Diebolt et Robert, 1994)
- Ordering constraints : $\theta_1 < \theta_2$
- Modification of the prior distribution which becomes proportional to $p(\theta)\mathbb{1}_{\theta_1 < \theta_2}$
- Not enough to solve the label switching problem (Celeux et al., 2000 ; Jasra et al., 2005)

k - means algorithm on the parameters space

- Relabeling algorithm of the generated parameters (Stephens, 1997 ; Celeux, 1998)
- Find the permutation for the fixed parameter which minimizes a loss function
- k - means type algorithm on the parameters space
- Underestimation of the dispersion of the posterior distribution

Invariant loss function

- Loss function invariant up to the parameters permutation (Celeux et al., 2000)
- Choice of a loss function adapted to the inferential problem
- Optimization of this last

Probabilistic relabeling

- Probabilistic approach (Jasra et al., 2005) to take into account the uncertainty of the attribution of the permutation to the parameters
- Model on the deswitched posterior distribution learned from an unswitched sequence
- Probability for each permutation of the parameter get by the Gibbs sampler
- Computation of quantities of interest such as the posterior mean

Bibliographic overview

- Methods allowing to partially solve the problem
- Problem when posterior distributions are poorly separated, tuning parameters to set
- The latent partition is not taken into account

The *latent partition* is now used to solve the label-switching problem

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Idea: using the numbering information

$\tilde{\mathcal{Z}} = \{\mathcal{Z}_1, \dots, \mathcal{Z}_g\}$ a partition of the set of partitions \mathcal{Z} . It sets a particular numbering for each partition z of the dataset x

$$\forall h, h' \in \{1, \dots, g\}, \exists! \sigma \in \mathcal{P}_g \text{ tq } z \in \mathcal{Z}_h \Leftrightarrow \sigma(z) \in \mathcal{Z}_{h'}$$

with $\sigma(z) = (\sigma(z_1), \dots, \sigma(z_n))$ indicating that z is permuted in indexes for $\sigma \in \mathcal{P}_g$.
 Decomposition of the usual posterior distribution as a mixture of $g!$ posterior distributions conditioned by any particular numbering $\tilde{\mathcal{Z}}$ of the partitions.

$$p(\theta|x) = \sum_{h=1}^{g!} p(\theta|x, \mathcal{Z}_h) p(\mathcal{Z}_h|x) = \frac{1}{g!} \sum_{h=1}^{g!} p(\theta|x, \mathcal{Z}_h).$$

- $\tilde{\mathcal{Z}}$ is unknown but it corresponds to a latent numbering information
- $p(\theta|x, \mathcal{Z}_h)$ not strictly invariant up to a renumbering of z
- The asymmetry depends on the choice of $\tilde{\mathcal{Z}}$
- Choose the cutting $\tilde{\mathcal{Z}}$ which separates the best the distributions $p(\theta|x, \mathcal{Z}_h)$
- Keep as new definition of the posterior distribution any of these $g!$ distributions

Choosing a $g!$ fraction $\tilde{\mathcal{Z}}$ of \mathcal{Z}

Choice 1: $\tilde{\mathcal{Z}}^{KL}$

$\tilde{\mathcal{Z}}^{KL}$ maximizes the Kullback-Leibler divergence between the mixture components on \mathcal{Z}_h which is written

$$\tilde{\mathcal{Z}}^{KL} = \arg \max_{\tilde{\mathcal{Z}}} \min_{h=2, \dots, g!} \int_{\Theta} p(\theta|x, \mathcal{Z}_1) \ln \frac{p(\theta|x, \mathcal{Z}_1)}{p(\theta|x, \mathcal{Z}_h)} d\theta.$$

Intractable even for very small sample sizes.

Choice 2: $\tilde{\mathcal{Z}}^{MAP}$

$$\tilde{\mathcal{Z}}^{MAP} = \arg \max_{\tilde{\mathcal{Z}}} \min_{h=2, \dots, g!} \frac{p(\theta^{MAP}|x, \mathcal{Z}_1)}{p(\theta^{MAP}|x, \mathcal{Z}_h)}.$$

It is equivalent to find the most probable numbering unit by unit computed in θ^{MAP} :

$$\mathcal{Z}_1^{MAP} = \left\{ z \in \mathcal{Z} / Id = \arg \max_{\sigma \in \mathcal{P}_g} p(\sigma(z)|x, \theta^{MAP}) \right\},$$

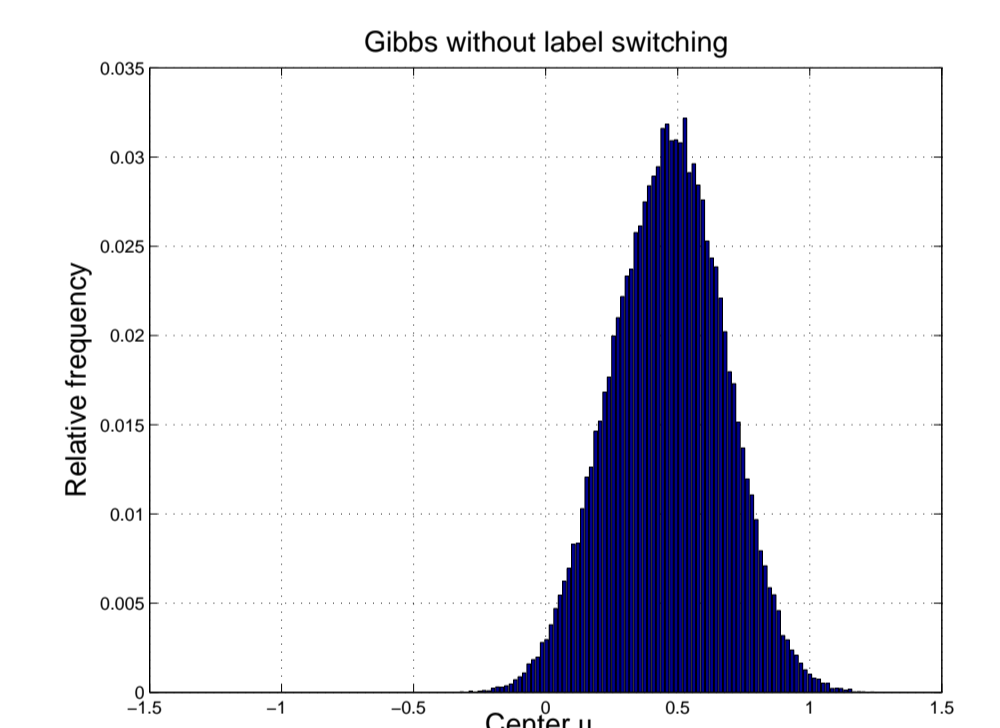
Id is the identity permutation. θ^{MAP} is the reference parameter for the numbering of the latent partition.

Proposed Gibbs algorithm

The classical Gibbs algorithm is slightly modified

- $z \sim p(\cdot|x, \theta)$,
- z permuted in order to $\sigma(z) \in \mathcal{Z}_1^{KL}$ or $\sigma(z) \in \mathcal{Z}_1^{MAP}$
- $\theta \sim p(\cdot|x, \sigma(z))$

Additional algorithmic complexity negligible for \mathcal{Z}_1^{MAP} .



New posterior distribution $p(\theta_1|x, \mathcal{Z}_1^{MAP})$.

Numerical experiments

Experiments in the Gaussian setting (running example continued)

| Strategy | $n = 3$ | $n = 10$ | $n = 100$ |
|--|-------------------------------------|-------------------|-------------------|
| • 100 samples x of size $n \in \{3, 10, 100\}$ | Gibbs/ k -means 0.18648 (0.10316) | 0.09613 (0.09677) | 0.02594 (0.04200) |
| • Burning sequence of 100 iterations | KL 0.03358 (0.04357) | NA | NA |
| • 2,000 iterations of Gibbs | MAP 0.03372 (0.04679) | 0.06135 (0.08815) | 0.02364 (0.04157) |

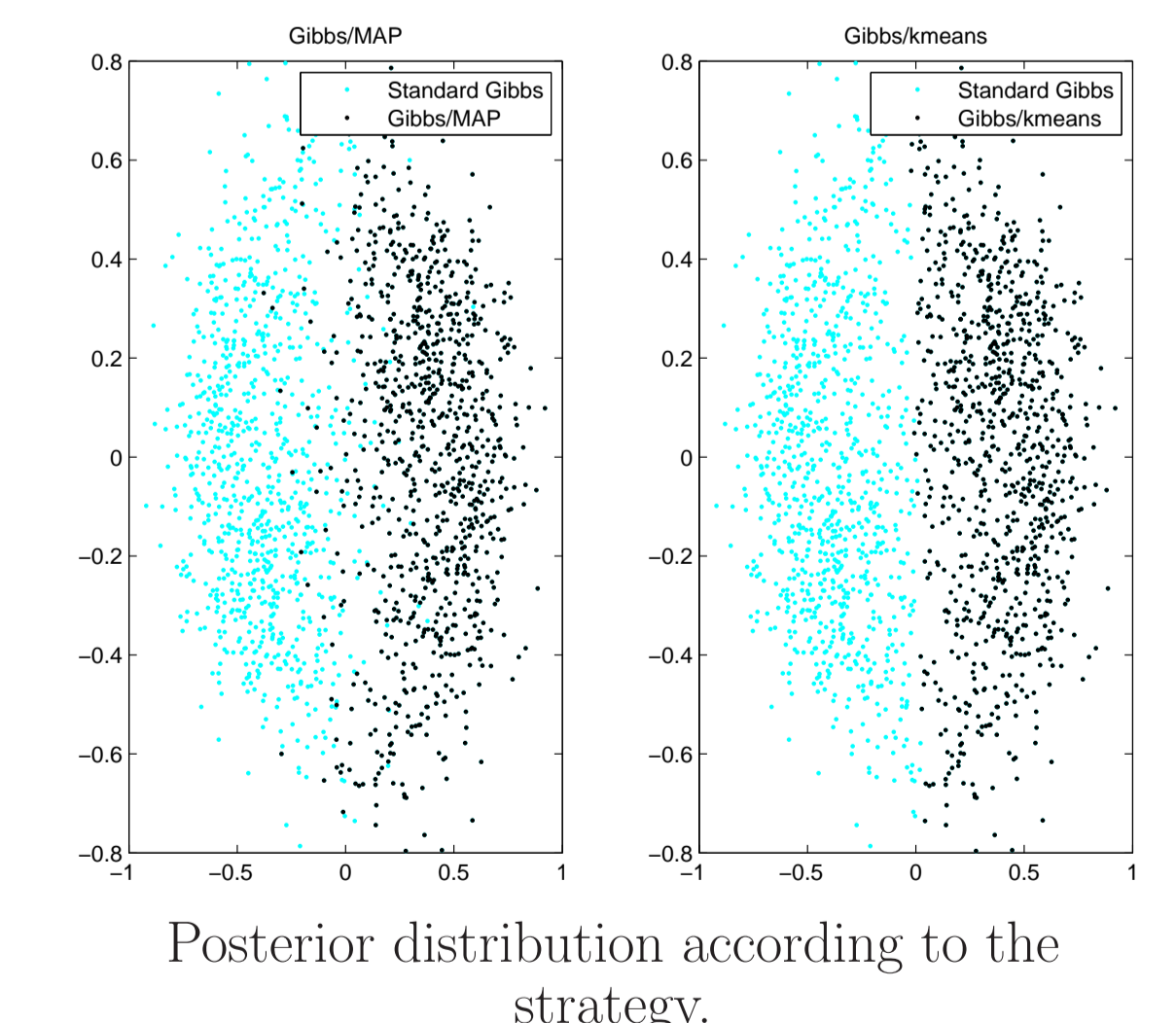
Mean (and standard deviation) of the posterior mean square error.

Experiments in the multinomial product mixture setting

- Qualitative simulated data with $g = 2$ poorly separated classes in equal proportions
- 6 variables: 4 with 3 modalities and 2 with 4 modalities
- Estimated model: mixture of $g = 2$ products of multinomial distributions, all parameters free
- 100 samples of sizes $n = 50$
- Burning sequence of 1,000 iterations
- 10,000 iterations of Gibbs

| Strategy | $n = 50$ |
|-------------------|-------------------|
| Gibbs/ k -means | 0.10949 (0.04588) |
| MAP | 0.10627 (0.04549) |

Mean (and standard deviation) of the Kullback divergence to the true distribution.



Posterior distribution according to the strategy.

Conclusion and perspectives

Conclusion

- Separation of the posterior modes without break
- Assumption free on the unswitched distribution
- Computational cost similar to standard solutions

Perspectives

- Monitor the convergence of the Gibbs algorithm
- Many application areas: hidden Markov models, Potts model, ...