MODEL BASED CO-CLUSTERING: HIGH DIMENSION & ESTIMATION CHALLENGES

Christophe Biernacki, Julien Jacques, Christine Keribin

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Outline

Clustering

Unsupervised ML framework

- data set $\boldsymbol{x} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n) \in \mathcal{X}^n$ with $dim(\mathcal{X}) = d$
- to partition into K clusters $G_1, \ldots, G_K$
- classification matrix $\mathbf{z} = (z_1, \ldots, z_n)$: $z_{ik} = \mathbb{1}_{i \in G_k}$

Model based clustering (MBC) reformulates cluster analysis in a well-posed estimation problem

- $\boldsymbol{x}_i$ are iid observations of a mixture pdf

$$f(.;\boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k \varphi(.;\boldsymbol{\alpha}_k); \quad \sum_{i=1}^{K} \pi_K = 1, \pi_k \geq 0; \quad \mathbb{P}(z_{ik} = k) = \pi_k$$

- estimation with EM algorithm, partition is deduced from the conditional probability $p(z_i|x_i;\widehat{\boldsymbol{\theta}})$, typically from the MAP principle, as soon as we have an estimate $\widehat{\boldsymbol{\theta}}$ of $\boldsymbol{\theta}$

High dimension (HD) settings: $d \sim n$, $d \gg n$

More and more variables (d) and not so much observations (n)

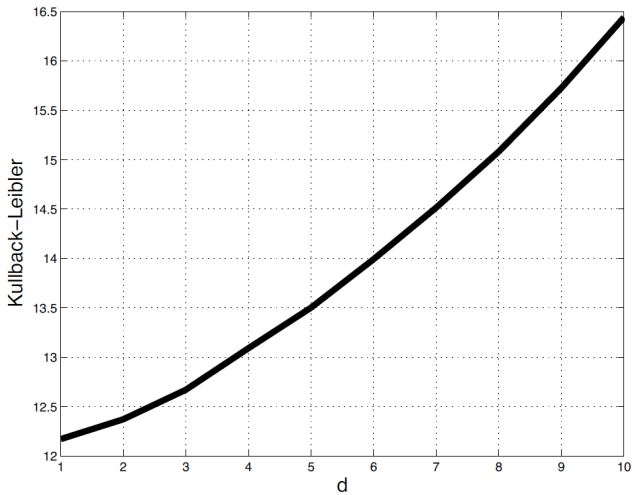
- marketing: $d \sim 10^2$ for $n = 10^4 - 10^6$
- microarray gene expression: $d \sim 10^2 - 10^4$ for $n = 20 - 50$ stress conditions
- fMRI images: $d \sim 10^4 - 10^5$ voxels for $n = 50 - 100$ patients
- text mining, curve, internet logs...

Moreover, variables can be of mixed types

- different modes: qualitative, quantitative, functional
- different semantic

Clustering in HD: curse (and blessing?)

- curse: density estimation quality decreases with d for a same n



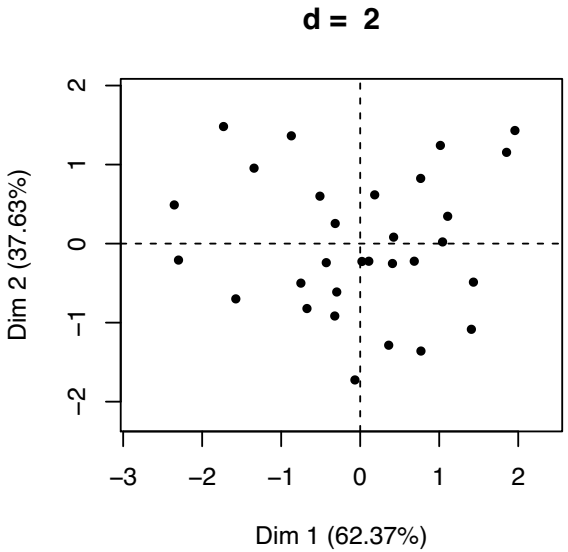
$Kullback(f, \widehat{f})$ for a two-component d-variate Gaussian mixture

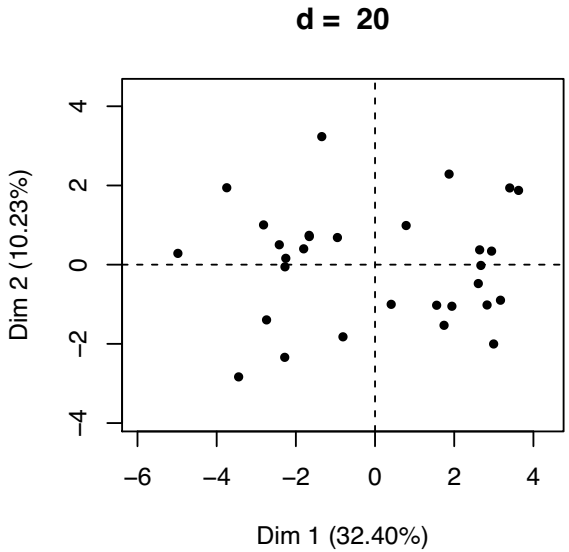
$$\boldsymbol{x}_i | z_i \sim \mathcal{N}_d(\mu_{z_i}, \Sigma); \pi_1 = \pi_2 = 0.5$$

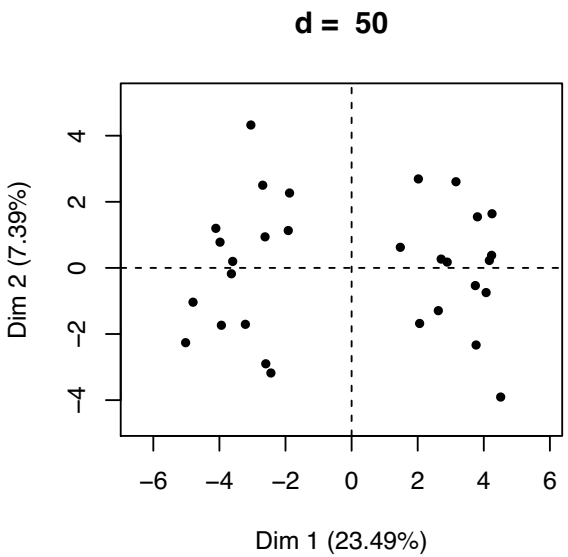
Basic case: $\mu_1 = 0_d; \mu_2 = 1_d; \Sigma = \mathbf{I}_d$

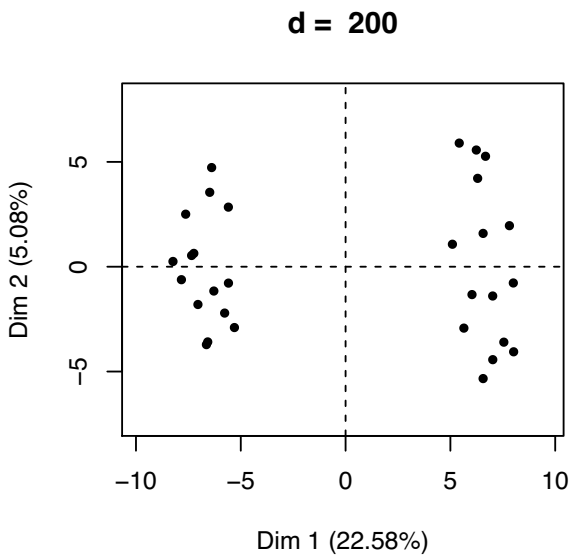
- blessing: but components are (in that case) more and more separated
- which impact on the misclassification error?
  - when the variables are correlated, redundant, non informative?
  - when $d \gg n$?

Basic case: HD is a blessing for clustering





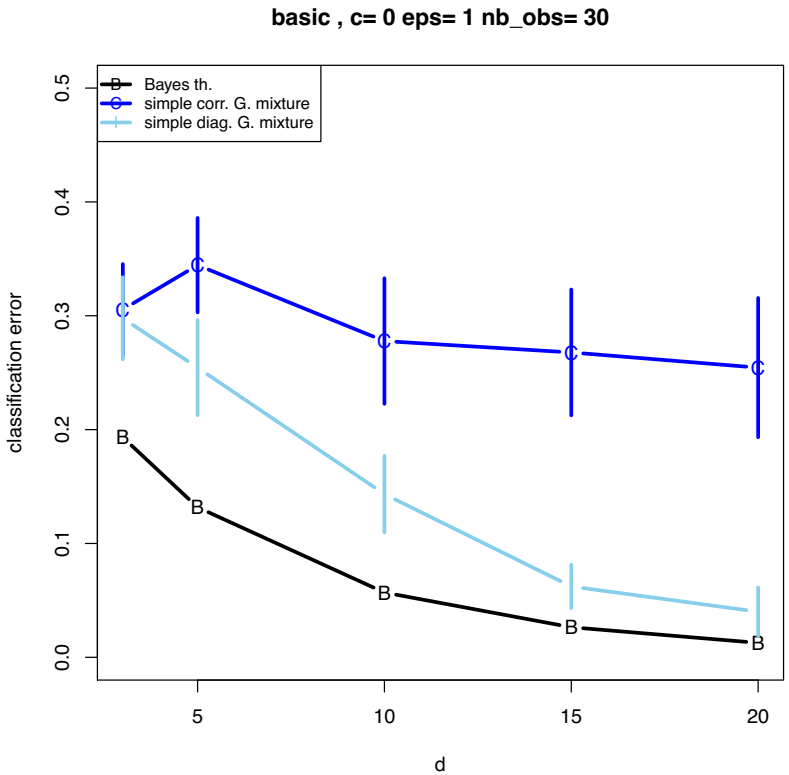




Basic case: HD is a blessing for clustering

Each new variable is informative, sufficiently large $n \sim d$

- theoretical classification error decreases when d grows: $err_{theo} = \Phi(-\sqrt{d}/2)$



A two-component d-variate Gaussian mixture

$$\boldsymbol{x}_i | z_i \sim \mathcal{N}_d(\mu_{z_i}, \Sigma); \quad \pi_1 = \pi_2 = 0.5$$

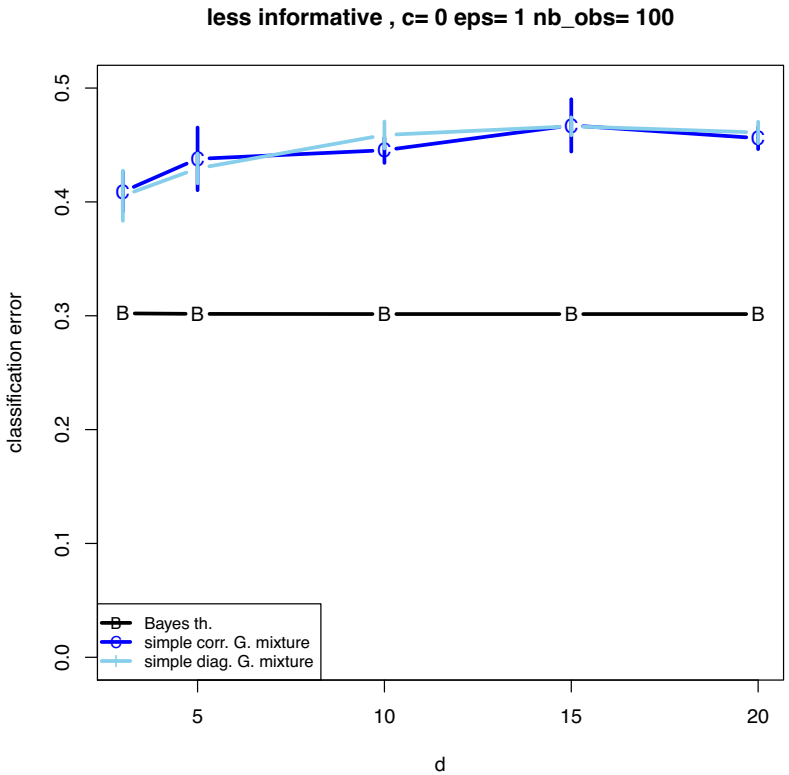
Basic case: $\Sigma = \mathbf{I}_d$; $\mu_1 = 0_d$; $\mu_2 = 1_d$

- and empirical error rate also decreases with d
- no model bias, classification ($\widehat{\mathbf{z}}$) variance decreases

But HD can be less favorable for clustering

(Many) less informative variables

- theoretical error slowly decreases when d grows: $err_{theo} = \Phi(-||\mu_1 - \mu_2||/2)$



A two-component d-variate Gaussian mixture

$$\boldsymbol{x}_i | z_i \sim \mathcal{N}_d(\mu_{z_i}, \Sigma); \;\; \pi_1 = \pi_2 = 0.5$$

Less informative: $\Sigma = \mathbf{I}_d$; $\mu_1 = 0_d$,

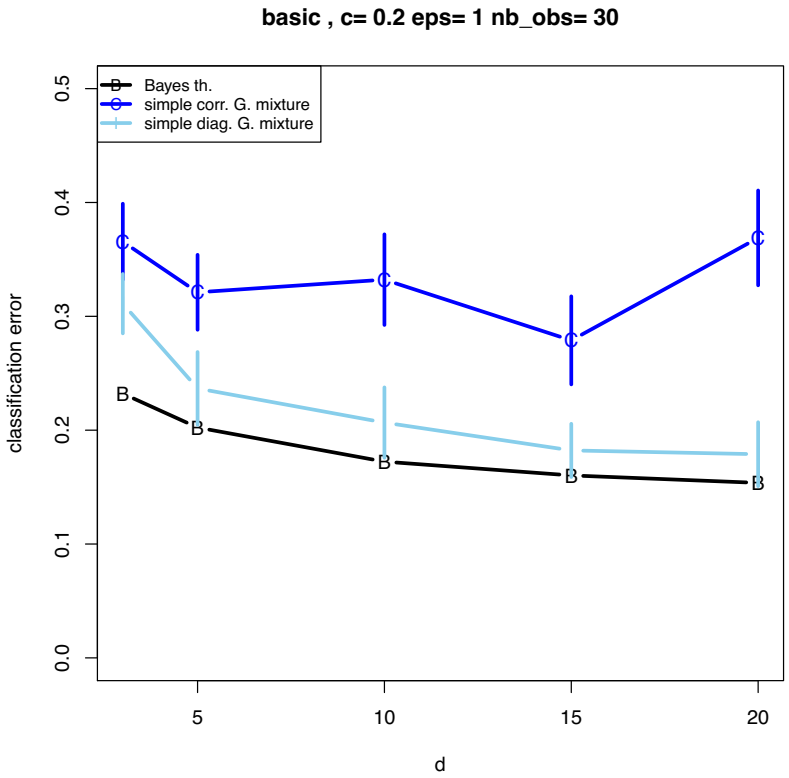
$$\mu_2 = \left(1, \frac{1}{2^2}, \ldots, \frac{1}{d^2}\right)$$

- but empirical error rate does not decrease any more...
- no model bias, classification ($\widehat{\mathbf{z}}$) variance increases

Bias/variance trade-off for clustering

Correlated variables

- theoretical error decreases $err_{theo} = \Phi\left(-||\mu_1 - \mu_2||_{\Sigma^{-1}}/2\right)$



A two-component d-variate Gaussian mixture

$$\boldsymbol{x}_i | z_i \sim \mathcal{N}_d(\mu_{z_i}, \Sigma); \ \pi_1 = \pi_2 = 0.5$$

Basic case+ correlated variables (correlation c):
$\Sigma = \Sigma(c); \ \mu_1 = 0_d; \ \mu_2 = 1_d$

- high error when clustered with the real (corr. G.) mixture model higher than with the biased (diag. G) mixture model, since corr. G. has too much variance
- error decreases with the biased model diag. G, which does not dammaged the separation

Some alternatives for reducing variance

- Dimension reduction in non canonical space (PCA-like typically)
- Dimension reduction in the canonical space (variable selection)
  - Gaussian mixture with 3 variable-clusters (informative, non informative, linearly dependent) [*Maugis et al (2009)*]
  - latent class analysis [*Fop et al (2018)*]
- Model parsimony in the initial HD space (constraints on model parameters)
  - parsimonious Gaussian mixture [*Celeux and Govaert, '95*]
  - mixture of factor analyzers [*[Ghahramani and Hinton, 97], [McLachlan et all], 03*]
  - HD Gaussian models [*[Bouveyron et al, 07]*]

↪ trade-off between "meaningful" modeling and what can be estimated in practice

An alternative for reducing the variance

Main message:

- clustering is a way for dealing with large n

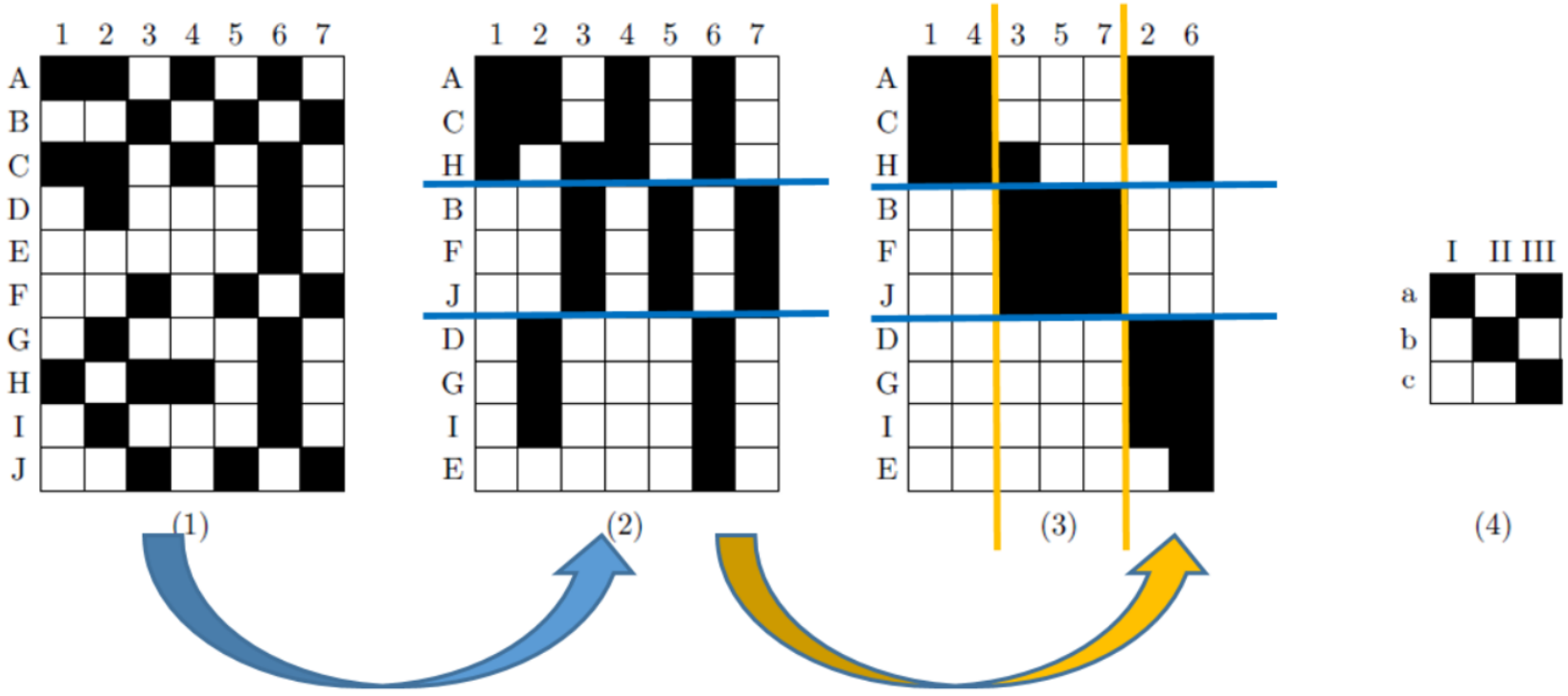
↪ why not also reusing this idea for large d?

Co-clustering (CC)

- simultaneously clusters rows and columns
- performs parsimony of row clustering through variable clustering

↪ parsimonious, model-based, independent of data type, available

From clustering to co-clustering



$(n = 10) \times (d = 7)$ $(K = 3) \times (d = 7)$ $(K = 3) \times (L = 3)$

[*Govaert (2008)*]

Interpreting LBM as an MBC dimension reduction method[1]

(See the Latent Block Model (LBM) definition in the next section...)

- PCA for the i-th data individual $\mathbf{x}_i$: acts as a dimension reduction method

$$\mathbf{x}_i = \sum_{j=1}^{d} x_i^j \mathbf{e}^j = \sum_{j=1}^{d} a_i^j \mathbf{u}^j \approx \sum_{j=1}^{J} a_i^j \mathbf{u}^j$$

- specific CC case reduced to $K = 1$: again, acts as a dim. reduction method

$$\mathbf{x}_i = \sum_{j=1}^{d} x_i^j \mathbf{e}^j = \sum_{j=1}^{d} (\mu_{\tilde{w}_j} + \varepsilon_i^j)\mathbf{e}^j = \sum_{\ell=1}^{L} \mu_\ell \mathbf{v}^\ell + \mathbf{r}_i \approx \sum_{\ell=1}^{L} \mu_\ell \mathbf{v}^\ell$$

with $\tilde{w}_j = \ell \Leftrightarrow w_{j\ell} = 1$, $\varepsilon_i^j \sim \mathcal{N}(0, \sigma^2_{\tilde{w}_j})$, $\mathbf{v}^\ell = \sum_{\{j:\tilde{w}_j=\ell\}} \mathbf{e}^j$ and $\mathbf{r}_i = \sum_{j=1}^{d} \varepsilon_i^j \mathbf{e}^j$

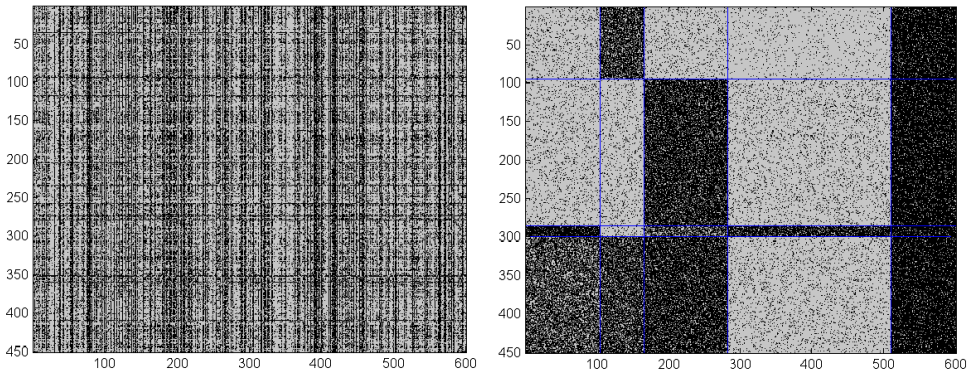
↪ return now to the clustering task:

- sequential clustering method: (1) PCA and then (2) MBC
- simultaneous clustering method: only CC, since dim. reduction is included

[1] [C. Biernacki, C. Keribin, J. Jacques, A survey on Model-Based Co-Clustering, JOC 2023]

Outline

Unsupervised block clustering framework



- co-clustering (CC): to find a block clustering structure simultaneously on rows and columns

H_1: blocks form a Cartesian product of a row-partition in K row-groups by a column-partition in L column-groups

$\mathbf{z} = (z_{ik})$ where $z_{ik} = 1$ if row i belongs to row-group k

$\mathbf{w} = (w_{j\ell})$ where $w_{j\ell} = 1$ if column j belongs to column-group ℓ

- traditional applications: huge data sets arising in recommendation systems (binary), genomic data analysis (Gaussian), text mining (Poisson),...
- our proposed application: dimension reduction for HD clustering

Latent Block Model (LBM): a mixture model[2]

H_2: row and column labels are independently assigned :

$$z_i \overset{i.i.d}{\sim} \mathcal{M}(1, \boldsymbol{\pi}) \perp w_j \overset{i.i.d}{\sim} \mathcal{M}(1, \boldsymbol{\rho})$$

H_3: the $n \times d$ blocks x_{ij} are conditionally independent given $\mathbf{z}$ and $\mathbf{w}$ and follow the same conditional distribution φ which parameter $\boldsymbol{\alpha}$ only depends on the block:

$$x_{ij}|z_{ik} = 1, w_{j\ell} = 1 \sim \varphi(x_{ij}; \boldsymbol{\alpha}_{k\ell})$$

Observed likelihood

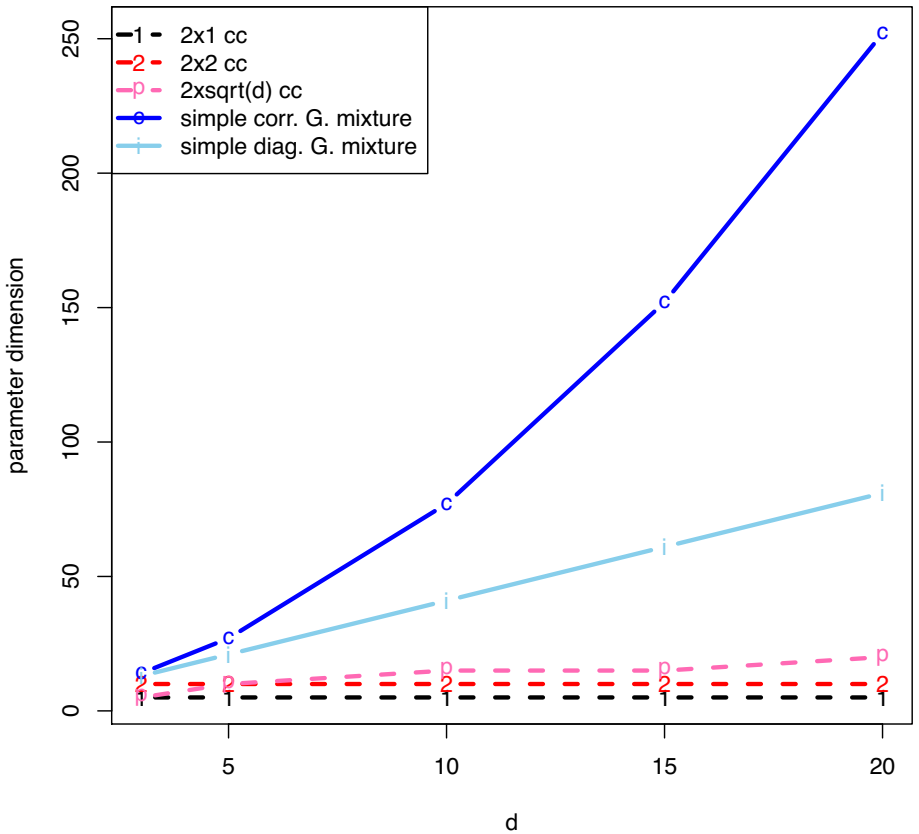
$$p(x;\boldsymbol{\theta}) = \sum_{(z,w)\in\mathcal{Z}\times\mathcal{W}} \underbrace{\prod_{i,k} \pi_k^{z_{ik}} \prod_{j,\ell} \rho_\ell^{w_{j\ell}}}_{p(z,w;\boldsymbol{\theta})=p(z;\boldsymbol{\theta})p(w;\boldsymbol{\theta})} \underbrace{\prod_{i,j,k,\ell} \varphi(x_{ij};\boldsymbol{\alpha}_{k\ell})^{z_{ik}w_{j\ell}}}_{p(x|z,w;\boldsymbol{\theta})}$$

with $\boldsymbol{\theta} = (\boldsymbol{\pi}, \boldsymbol{\rho}, \boldsymbol{\alpha}) \in \boldsymbol{\Theta}$

[2] [Govaert and Nadif (2008)]

Parametric model

- very parsimonious model, good candidate to deal with HD settings...



Model	Number of parameters
Binary	$\dim(\boldsymbol{\pi}) + \dim(\boldsymbol{\rho}) + KL$
Categorical	$\dim(\boldsymbol{\pi}) + \dim(\boldsymbol{\rho}) + KL(m-1)$
Contingency	$\dim(\boldsymbol{\pi}) + \dim(\boldsymbol{\rho}) + KL$
Continuous	$\dim(\boldsymbol{\pi}) + \dim(\boldsymbol{\rho}) + 2KL$

$$\text{nb. param.}_{\text{HD}} = \text{nb. param.}_{\text{classic}} \times \frac{L}{d}$$

Many appealing extensions

- variable type diversity: ordinal data [*Biernacki and Jacques, '18*], functional data [*Bouveyron et al, 18*], mixed-type data [*Selosse et al, '20*], textual interaction data [*Bergé et al, '19*]
- dynamic, e.g. [*Marchello, '23*] (zero inflated dLBM)

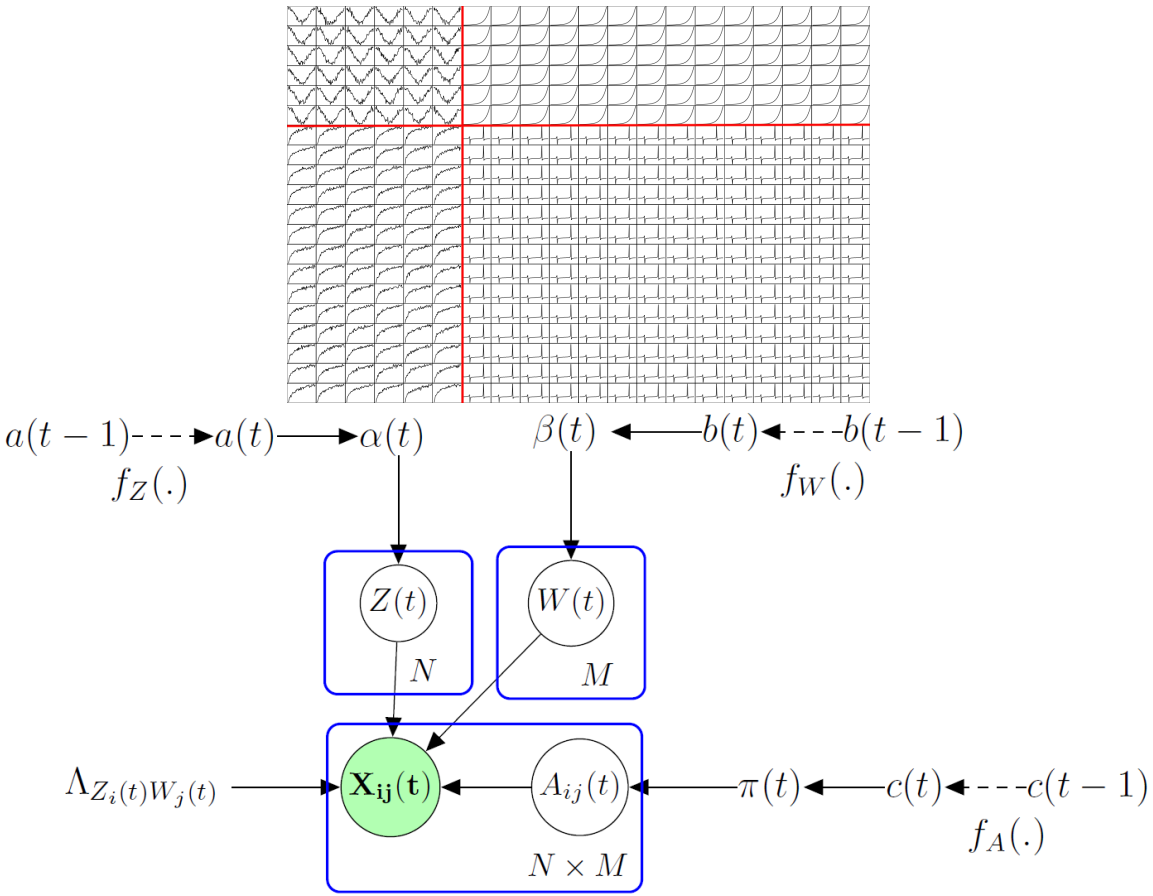
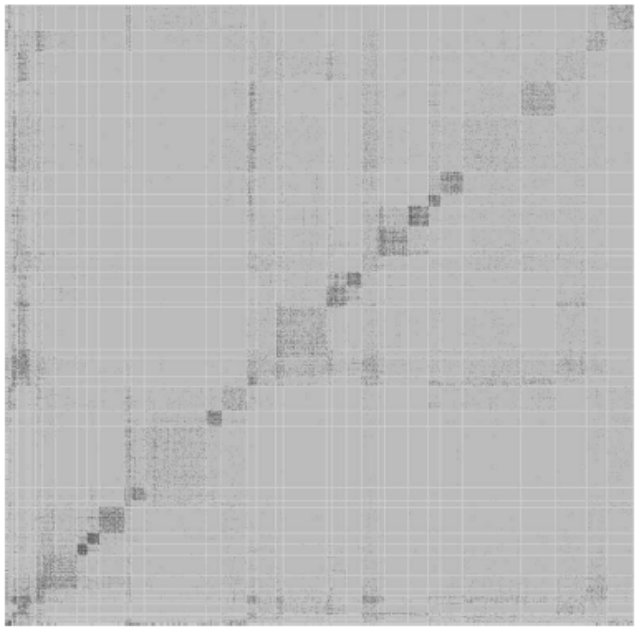


Figure 4.1: Graphical representation of the Zero-Inflated dLBM model.

Particular case: graph clustering

- Stochastic Block Model (SBM): $\boldsymbol{x}$ is the adjacency matrix of a graph
  $\hookrightarrow n = d$, $K = L$, $\mathbf{z} = \mathbf{w}$



Estimation

$$p(x;\theta) = \sum_{(z,w)\in\mathcal{Z}\times\mathcal{W}} \prod_{i,k} \pi_k^{z_{ik}} \prod_{j,\ell} \rho_\ell^{w_{j\ell}} \prod_{i,j,k,\ell} \varphi(x_{ij};\alpha_{k\ell})^{z_{ik}w_{j\ell}}$$

- generic identifiability [*Keribin et al., '15*]

- likelihood intractable: 2×2 blocks and 20×20 matrix: $\approx 2^{20} \times 2^{20} \approx 10^{12}$ terms
- E-step intractable
  ↪ approximation with Variational EM (VEM) [*Govaert and Nadif '08*]
  ↪ estimation with Stochastic EM (SEM) [*Keribin et al. '10*]
  ↪ stochastic gradient descent [*Baey et al. '23*]
  ↪ Bayesian versions: Gibbs and V-Bayes algorithms [*Keribin, Brault, Celeux, Govaert, '15*]

- consistency and asymptotic normality of ML- and V- estimators (when $\log(n)/d \to 0$ and $\log(d)/n \to 0$) [*Brault, Keribin, Mariadassou, '20*]
- model selection (ICL)

EM for LBM

$$\log p(\mathbf{x};\boldsymbol{\theta}) = \underbrace{\mathbb{E}[\log p(\mathbf{x},\mathbf{z},\mathbf{w};\boldsymbol{\theta})|\mathbf{x};\boldsymbol{\theta}^{(r)}]}_{Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(r)})} - \mathbb{E}[\log p(\mathbf{z},\mathbf{w}|\mathbf{x};\boldsymbol{\theta})|\mathbf{x};\boldsymbol{\theta}^{(r)}]$$

Expectation Maximization (iteration r)

- **E-step:** computing $Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(r)})$

$$Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(r)}) = \sum_{i,k} \underbrace{\mathbf{P}(z_{ik}=1|\mathbf{x};\boldsymbol{\theta}^{(r)})}_{s_{ik}^{(r)}} \log \pi_k + \sum_{j,\ell} \underbrace{\mathbf{P}(w_{j\ell}|\mathbf{x};\boldsymbol{\theta}^{(r)})}_{t_{j\ell}^{(r)}} \log \rho_\ell$$

$$+ \sum_{i,j,k,\ell} \underbrace{\mathbf{P}(z_{ik}w_{j\ell}=1|\mathbf{x};\boldsymbol{\theta}^{(r)})}_{e_{i,j,k,\ell}^{(r)}\text{ intractable}} \log \varphi(x_{ij};\boldsymbol{\alpha}_{k\ell})$$

- **M-step:** $\boldsymbol{\theta}^{(c+1)} = \arg\max_{\boldsymbol{\theta}} Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(r)})$, classical

VEM for LBM

$$\log p(\mathbf{x};\boldsymbol{\theta}) = \underbrace{\mathbb{E}_{q_z q_w}\left[\log \frac{p(\mathbf{x},\mathbf{z},\mathbf{w};\boldsymbol{\theta})}{q_z q_w}|\mathbf{x}\right]}_{\mathcal{F}(\boldsymbol{\theta};q_z,q_w)} + KL(q_z q_w, \log p(\mathbf{z},\mathbf{w}|\mathbf{x};\boldsymbol{\theta})]$$

VEM (iteration r)

- approximated **E-step:**

$$q_z^{(r)}, q_w^{(r)} = \arg\max_{q_z,q_w} \mathcal{F}(\boldsymbol{\theta}; q_z, q_w)$$

$$\hookrightarrow s_{ik}^{(r)} \approx q_{zik}^{(r)},\ t_{j\ell}^{(r)} \approx q_{wj\ell}^{(r)},\ e_{ijk\ell}^{(r)} \approx q_{zik}^{(r)} q_{wj\ell}^{(r)}$$

$$Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(r)}) \approx \sum_{i,k} q_{zik}^{(r)} \log \pi_k + \sum_{j,\ell} q_{wj\ell}^{(r)} \log \rho_\ell + \sum_{i,j,k,\ell} q_{zik}^{(r)} q_{wj\ell}^{(r)} \log \varphi(x_{ij};\boldsymbol{\alpha}_{k\ell})$$

- **M-step:** $\boldsymbol{\theta}^{(c+1)} = \arg\max_{\boldsymbol{\theta}} \mathcal{F}(\boldsymbol{\theta}; q_z^{(r)}, q_w^{(r)})$ in $\boldsymbol{\theta}$, classical

$$\max_{\boldsymbol{\theta}} \log p(\mathbf{x};\boldsymbol{\theta}) \geq \max_{\boldsymbol{\theta},q_z,q_w} \mathcal{F}(\boldsymbol{\theta}; q_z, q_w)$$

SEM for LBM

$$\log p(\mathbf{x};\theta) = \underbrace{\mathbb{E}[\log p(\mathbf{x},\mathbf{z},\mathbf{w};\theta)|\mathbf{x};\theta^{(r)}]}_{Q(\theta|\theta^{(r)})} - \mathbb{E}[\log p(\mathbf{z},\mathbf{w}|\mathbf{x};\theta)|\mathbf{x};\theta^{(r)}]$$

SEM-Gibbs (iteration r)

- **SE-step:** impute missing values $(\mathbf{z},\mathbf{w}) \sim p(\mathbf{z},\mathbf{w}|\mathbf{x};\theta^{(r)})$ [*Celeux and Diebolt (1986)*] with Gibbs-sampling
  - $\mathbf{z}^{(t+1)} \sim p(\mathbf{z}|\mathbf{w}^{(t)},\mathbf{x};\theta^{(r)})$
  - $\mathbf{w}^{(t+1)} \sim p(\mathbf{w}|\mathbf{z}^{(t+1)},\mathbf{x};\theta^{(r)})$

  $\hookrightarrow (\mathbf{z}^{(r)},\mathbf{w}^{(r)})$, after several Gibbs iterations
- **M-step:** maximize $\log p(\mathbf{x},\mathbf{z}^{(r)},\mathbf{w}^{(r)};\theta)$ in θ, classical

$\hookrightarrow$ stochastic, result fluctuates around the optimal value

Stochastic gradient descent for latent variables[3]

- Fisher Identity [*Cappé et al. '05*]: $\nabla_{\boldsymbol{\theta}} \log p(x;\boldsymbol{\theta}) = \mathbf{E}(\nabla_{\boldsymbol{\theta}} \log p(\mathbf{x},\mathbf{z}|\mathbf{x};\boldsymbol{\theta}))$

SGD-Gibbs for LBM (iteration r)

- **S-step:** Gibbs-sampling: $(\mathbf{z}^{(r)}, \mathbf{w}^{(r)}) \sim p(.,.|\mathbf{x};\boldsymbol{\theta}^{(r)})$
- gradient for observations $i = 1,\ldots,n; j = 1,\ldots,d$

$$J_{ij}^{(r),obs} = \nabla_{\boldsymbol{\theta} \log p(x_{ij}|z_i^{(r)},w_j^{(r)};\boldsymbol{\theta}^{(r)});\Delta_{ij}^{(r),obs} = (1-\gamma^{(r)})\Delta_{ij}^{(r),obs} + \gamma^{(r)} J_{ij}^{(r),obs}}$$

- gradient for latent variables $i = 1,\ldots,n; j = 1,\ldots,d$

$$J_i^{(r),z} = \nabla_{\boldsymbol{\theta} \log p(z_i^{(r)};\boldsymbol{\theta}^{(r)});\ \Delta_i^{(r),z} = (1-\gamma^{(r)})\Delta_i^{(c-1),z} + \gamma^{(r)} J_i^{(r),z}}$$

$$J_j^{(r),w} = \nabla_{\boldsymbol{\theta} \log p(w_j^{(r)};\boldsymbol{\theta}^{(r)});\ \Delta_j^{(r),w} = (1-\gamma^{(r)})\Delta_j^{(r-1),z} + \gamma^{(r)} J_j^{(r),w}}$$

- $\boldsymbol{\theta}^{(r+1)} = \boldsymbol{\theta}^{(r)} + \gamma^{(k)} P_k v_k$

[3] [*Baey, Delattre, Kuhn, Leger, Lemler '23*]

Outline

Estimation challenges

Challenges in the (classical) MBC context:

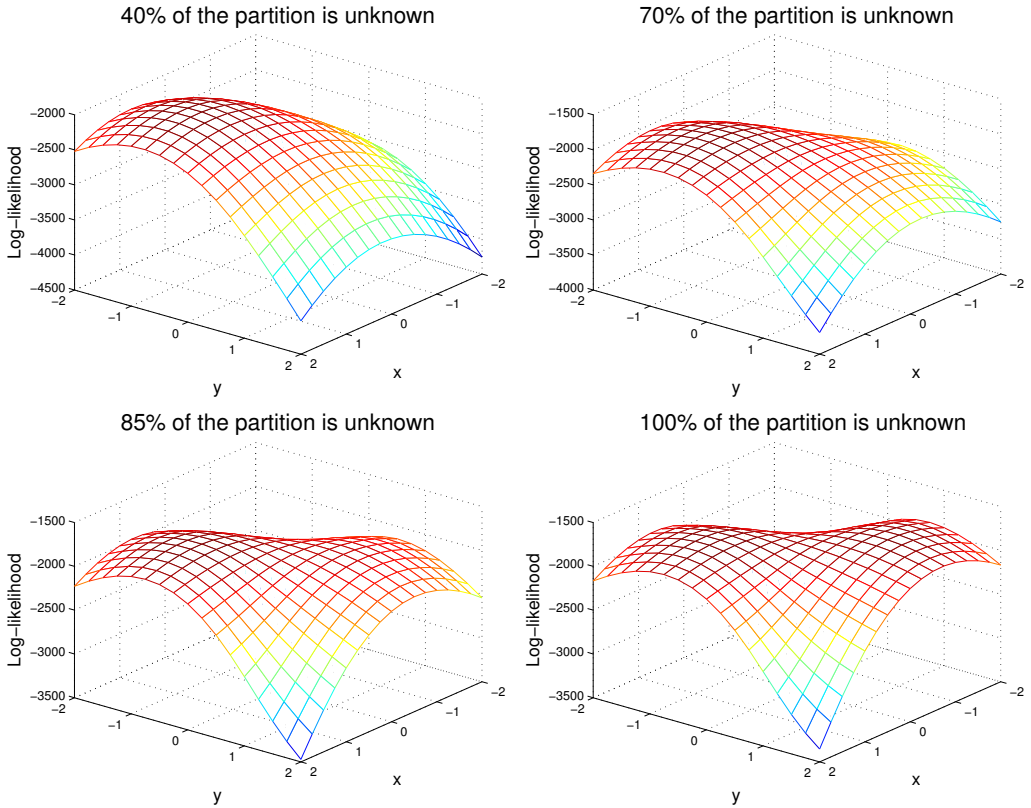
- local maxima solutions
- empty cluster solutions
- degenerate solutions

Question to be addressed here

What about LBM?

Local maxima

- not just linked to the number of parameters!
- linked to the number of latent variables (here a toy two-param. Gaussian mixture)



- additional order of magnitude: from K^n to $K^n L^d$ $\hookrightarrow$ pb for LBM?
  but no way to draw a likelihood map...

Empty clusters in LBM

Really frequent (and reported)!

- a component such that $\pi_k^{(r)} \simeq 0$
- number of empty clusters in MBC: $\#\mathcal{Z}^0$
- number of empty clusters in LBM: $\#(\mathcal{Z} \times \mathcal{W})^0$

$$\frac{\#(\mathcal{Z} \times \mathcal{W})^0}{\#\mathcal{Z}^0} = \frac{K^n L^d - S(n,K)S(d,L)K!L!}{K^n - S(n,K)K!} \to \infty \text{ when } n \to \infty \text{ or } d \to \infty$$

$S(n, K)$ is the Stirling number of second kind

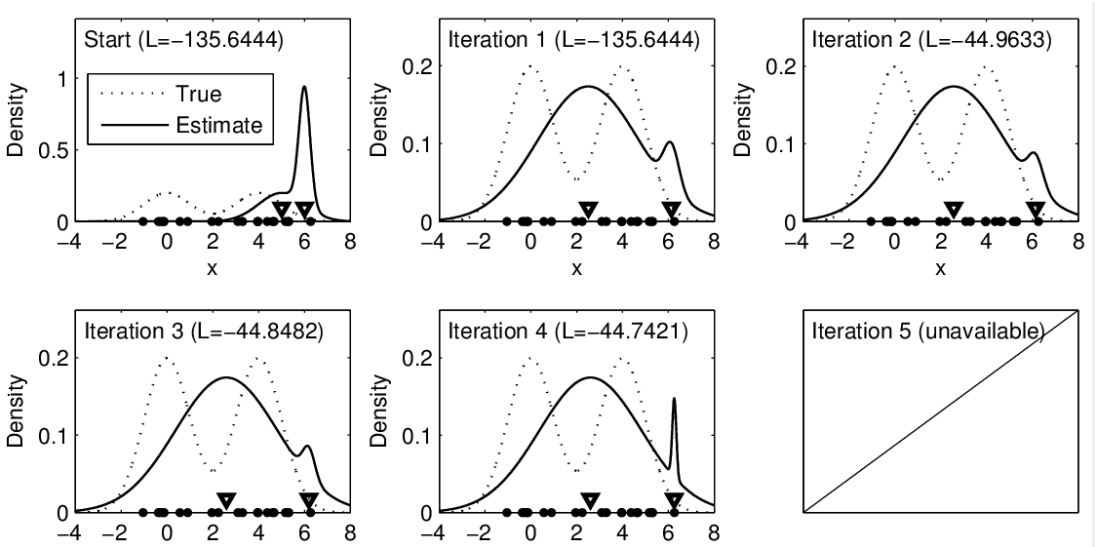
- exponential speed even with very small sample sizes

$$\frac{\#(\mathcal{Z} \times \mathcal{W})^0}{\#\mathcal{Z}^0} = \begin{cases} 62 & \text{when } n = d = 5 \text{ and } K = L = 2 \\ 710\,768 & \text{when } n = d = 9 \text{ and } K = L = 4 \end{cases}$$

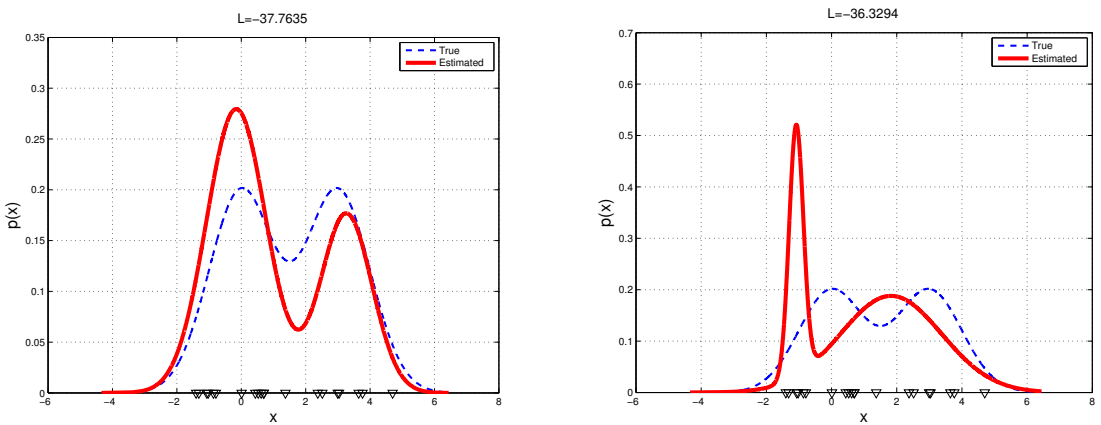
$\hookrightarrow$ initialization often achieved by performing independent clustering of the rows and columns but the best initialization strategy stays an open question

Degenerate and spurious solutions in MBC

- degenerate solutions lay on the border of the parameter space



- spurious local maximizers due to one or several relatively small (but not null) generalized variance



Degenerate and spurious solutions in LBM

No reported such problems?

- freq. of obtaining a cluster with a single element in the whole partition latent space

$$\frac{\#\mathcal{Z}_1^1}{\#\mathcal{Z}} = \left(\frac{K-1}{K}\right)^{n-1}$$

- freq. of obtaining a block with a single element in the whole partition latent space

$$\frac{\#(\mathcal{Z}\times\mathcal{W})_{1,1}^{1}}{\#(\mathcal{Z}\times\mathcal{W})} = \frac{\#\mathcal{Z}_1^1}{\#\mathcal{Z}}\left(\frac{L-1}{L}\right)^{d-1}$$

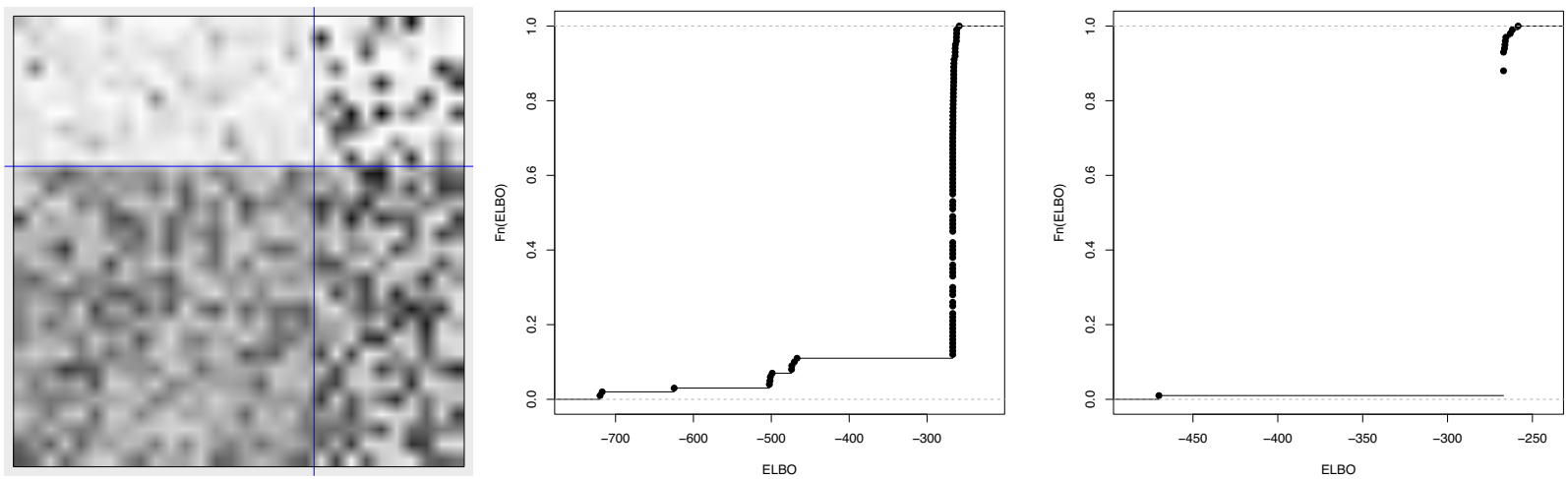
  $\hookrightarrow$ degeneracy situations are expected to be significantly less present in co-clustering than in clustering

  Ex with $L = 4$ and $d = 50$: $(1 - 1/L)^{d-1} = 7.5510^{-7}$

- spurious case: same combinatorial arguments (but more tedious computations)

Local maxima in Gaussian LBM: illustration[4]

Figure: Gaussian 2 $\times$ 2 LBM (*left*) ; e.c.d.f. of ELBO values obtained from $B = 100$ initializations, at both standard precision (*center*) and high precision (*right*)

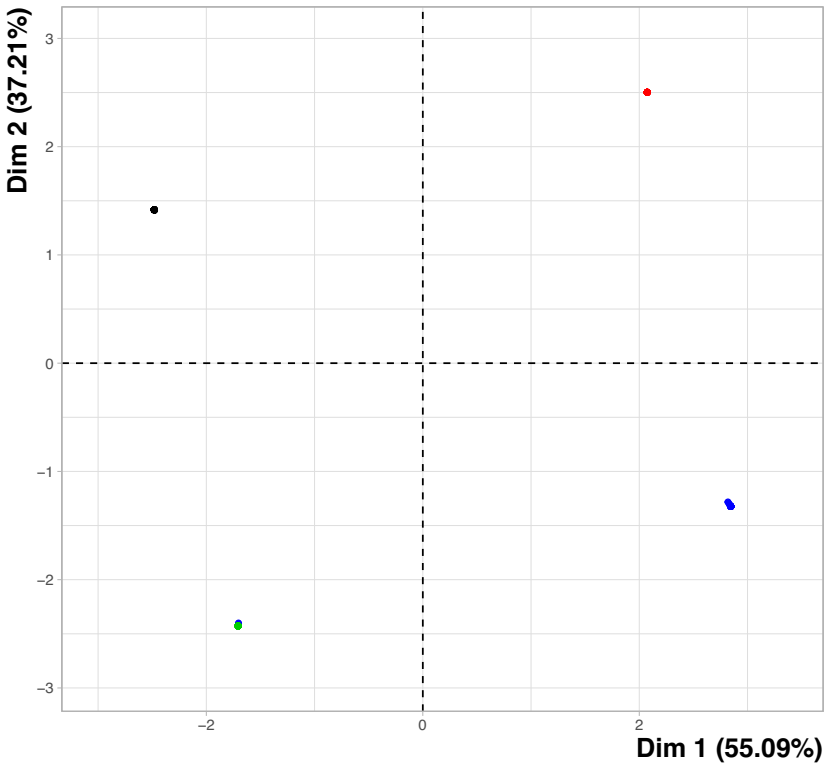


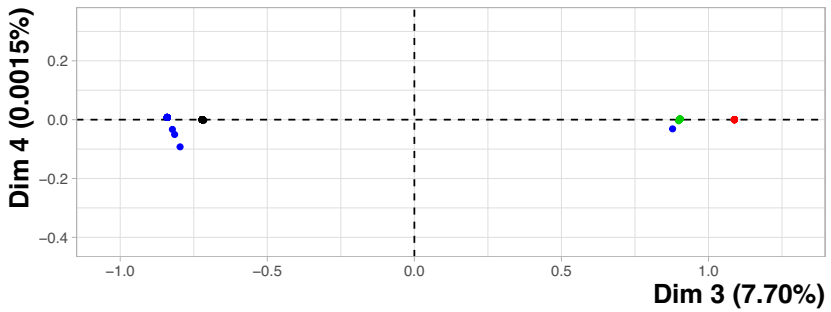
- some potential slow convergence effect
- different parameters but the same partition
  $\hookrightarrow$ clustering is easier than estimation, no need to estimate with too much precision

[4] R package `blockcluster`

Local maxima in Gaussian LBM: illustration (cont'd)

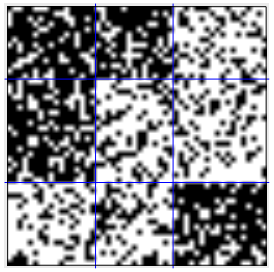
Projection of the solutions on the PCA planes



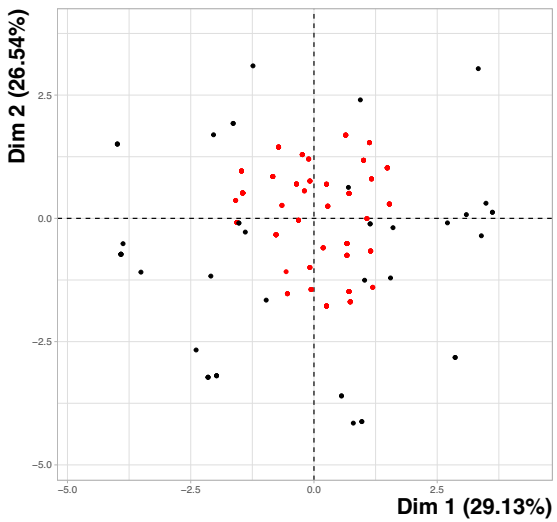


- `blockcluster` initialization performs several initial small VEM steps, that can explain these results

Local maxima in binary LBM: illustration[5]



ELBO	-1615.48	-1615.43	-1596.67
count	9	38	254
nb steps	$> 10^4$	$> 10^4$	< 100

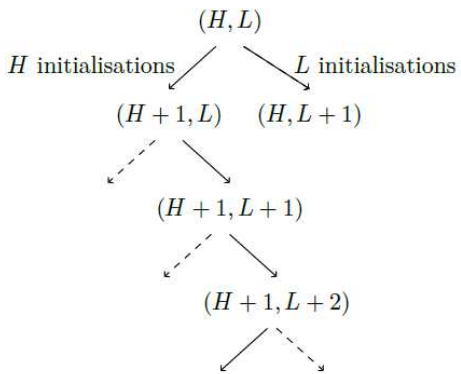


- high ELBO values (red): 36 relabelled configurations
- low ELBO values (black): 30 co-clustering configurations, all with an empty row or cluster
  ↪ very lazy convergence

[5] R package `bikm1`

Initialization strategies: crucial!

- two independent clustering (row / column)
- using several initializations with other algorithms (CEM, SEM, EM-VBayes) on few iterations
- resampling in order to avoid getting empty blocks during the first iterations
- `blockmodels` [*Leger, '16*] smart and robust initialization, combining spectral clustering adapted for LBM and a forward/backward reinitialization strategy:
  - forward exploration of the space of models (K, L) by splitting already existing clusters [*Robert '17*]
  - backward exploration by merging groups



Outline

Properties of LBM in view of HD clustering

- parsimonious model
- the true partition is recovered when there is a consistent estimator [*Mariadassou and Matias, '15*]

$$\hat{\theta} \overset{n,d\to\infty}{\longrightarrow} \theta^* \quad \Rightarrow \quad p(\hat{\mathbf{z}} = \mathbf{z}^*, \hat{\mathbf{w}} = \mathbf{w}^* | \mathbf{x}; \hat{\theta}) \overset{n,d\to\infty}{\longrightarrow} 1,$$

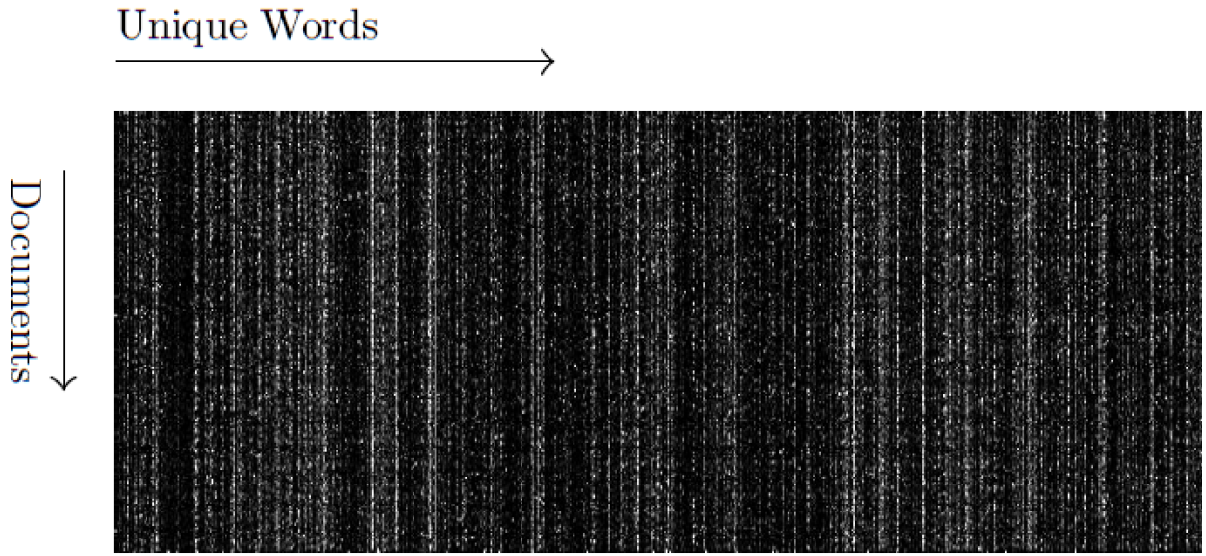
- non asymptotic properties (binary case) [*Brault, '14*]

$$\mathbb{P}(\hat{\mathbf{z}} \neq \mathbf{z}^*) \leq 2n \exp\left\{ -\frac{1}{8} d \Big[\underbrace{\min_{k \neq k'} |\tau_k - \tau_{k'}|}_{\text{overlap}} \Big] \right\} + K(1 - \min_k \pi_k)^n$$

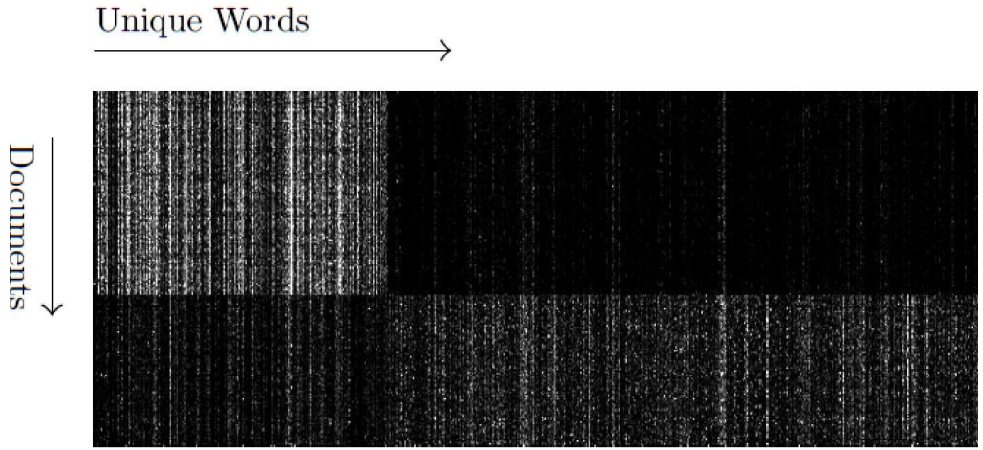
↪ LBM is a natural regularized candidate for HD clustering

Document clustering: exact recovery

- Mixture of 1033 medical summaries and 1398 aeronautics summaries
- Lines: 2431 documents
- Columns: present words (except stop), thus 9275 unique words
- Data matrix: cross counting document$\times$words
- Poisson model



Document clustering: exact recovery (cont'd)



Results with 2×2 blocks

	Medline	Cranfield
Medline	1033	0
Cranfield	0	1398

Experiment illustrates previous theory: HD clustering is blessing

Numerical illustrations: experimental design

Generating models, with two balanced ($\pi_1 = \pi_2$) row clusters in $\mathbb{R}^d$

	$\mathbf{I}_d$	$\mathbf{\Sigma}(c)$
$\boldsymbol{\mu}_1 = \mathbf{0}_d, \boldsymbol{\mu}_2 = \mathbf{1}_d$	(M_1)	(M_2)
$\boldsymbol{\mu}_1 = \mathbf{0}_d, \boldsymbol{\mu}_2 = (1, 2^{-2}, \ldots, d^{-2})$	(M_3)	(M_6)
(M_1) of size $n \times d/2$ duplicated twice	(M_4)	
$\boldsymbol{\mu}_1 \sim \mathcal{N}_d(\mathbf{0}, \mathbf{I}_d)$, $\boldsymbol{\mu}_2 \sim \mathcal{N}_d((\underbrace{1, \ldots, 1}_{\sqrt{d}}, 0, \ldots, 0), \mathbf{I}_d)$	(M_5)	

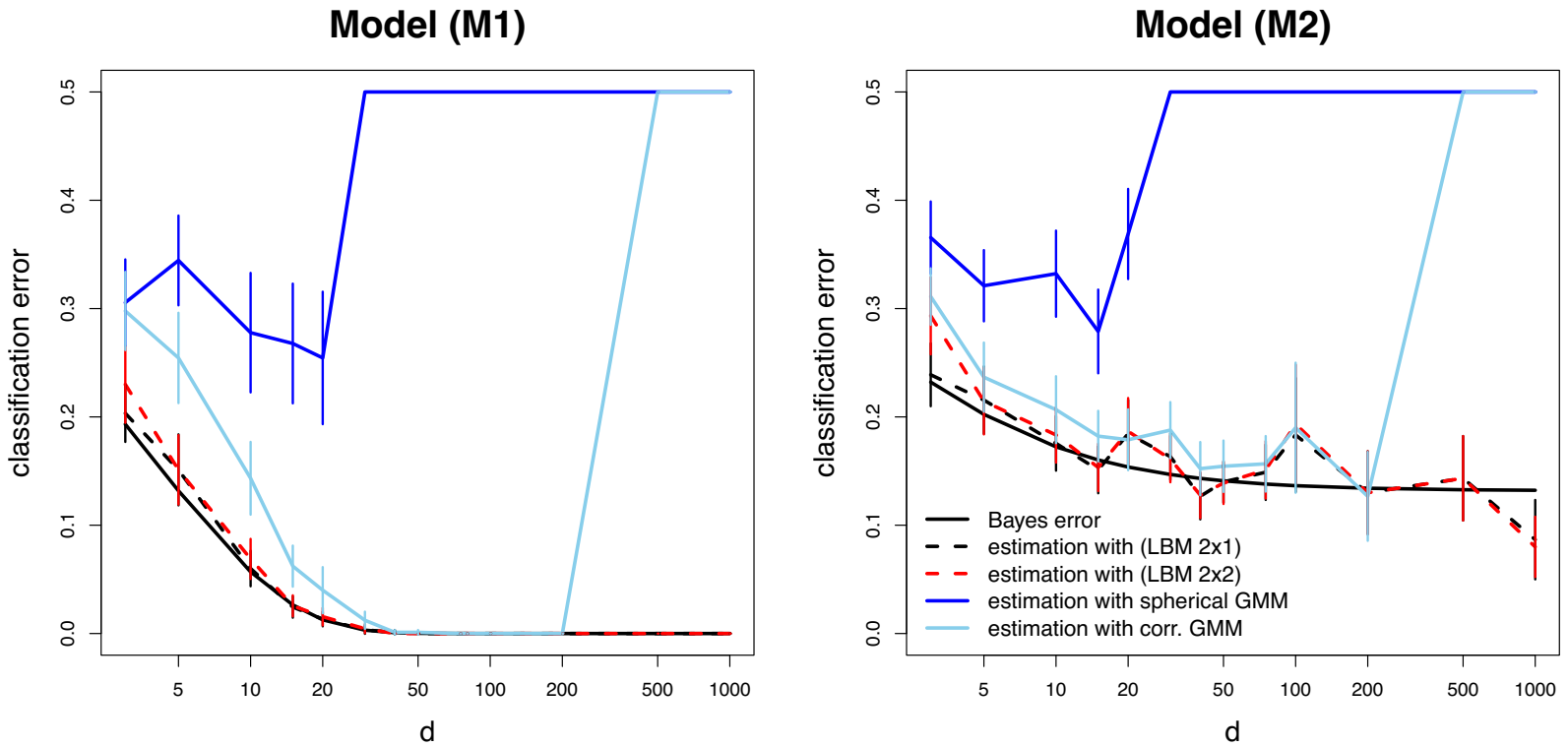
$\hookrightarrow$ only (M_1) is a nomimal LBM (2x1)

Row clustering is performed using four different methods

- clustering with a mixture of two spherical d-dim. Gaussian distributions
- clustering with a mixture of two full-covariance d-dim. Gaussian distr.
- co-clustering with a Gaussian (2×1) LBM
- co-clustering with a Gaussian (2×2) LBM

Classification error averaged over 30 samples of size $n = 30$

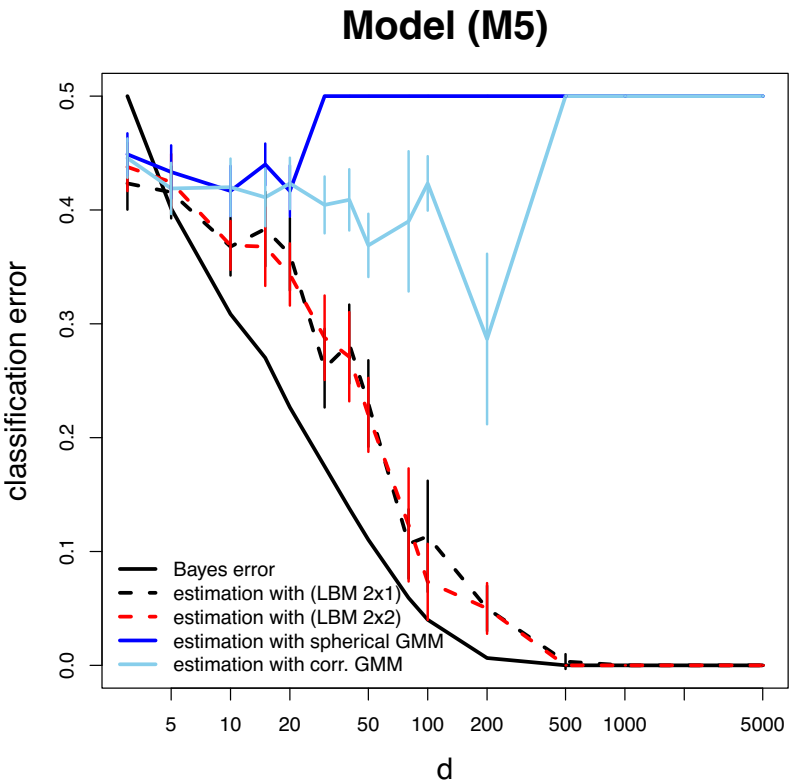
Numerical illustrations: results

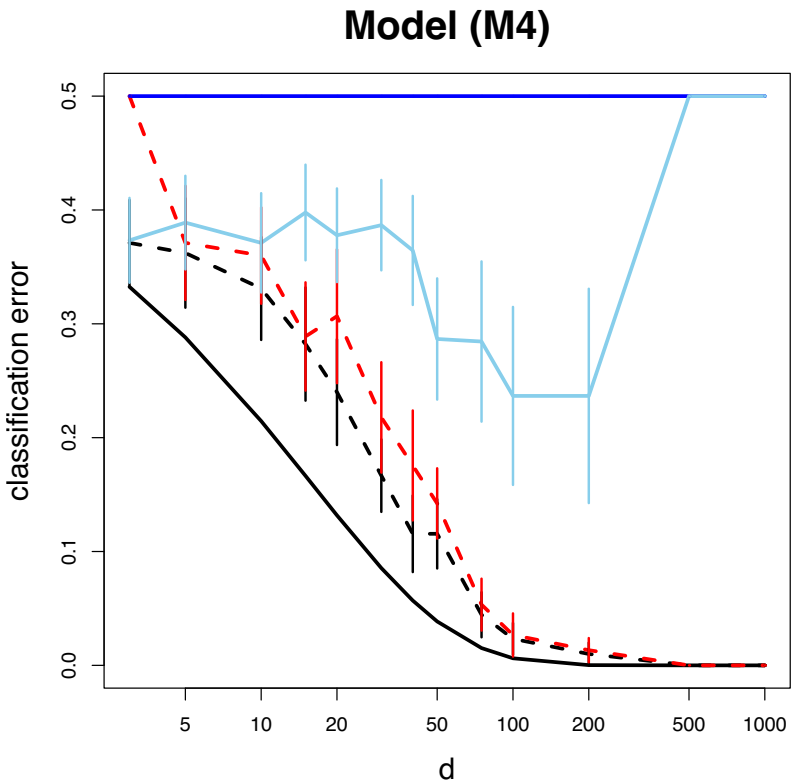


LBM resists to HD

LBM performs better than simple mixture, although the underlying model overrides the co-clustering conditional independence assumptions

Numerical illustrations: results (cont'd)



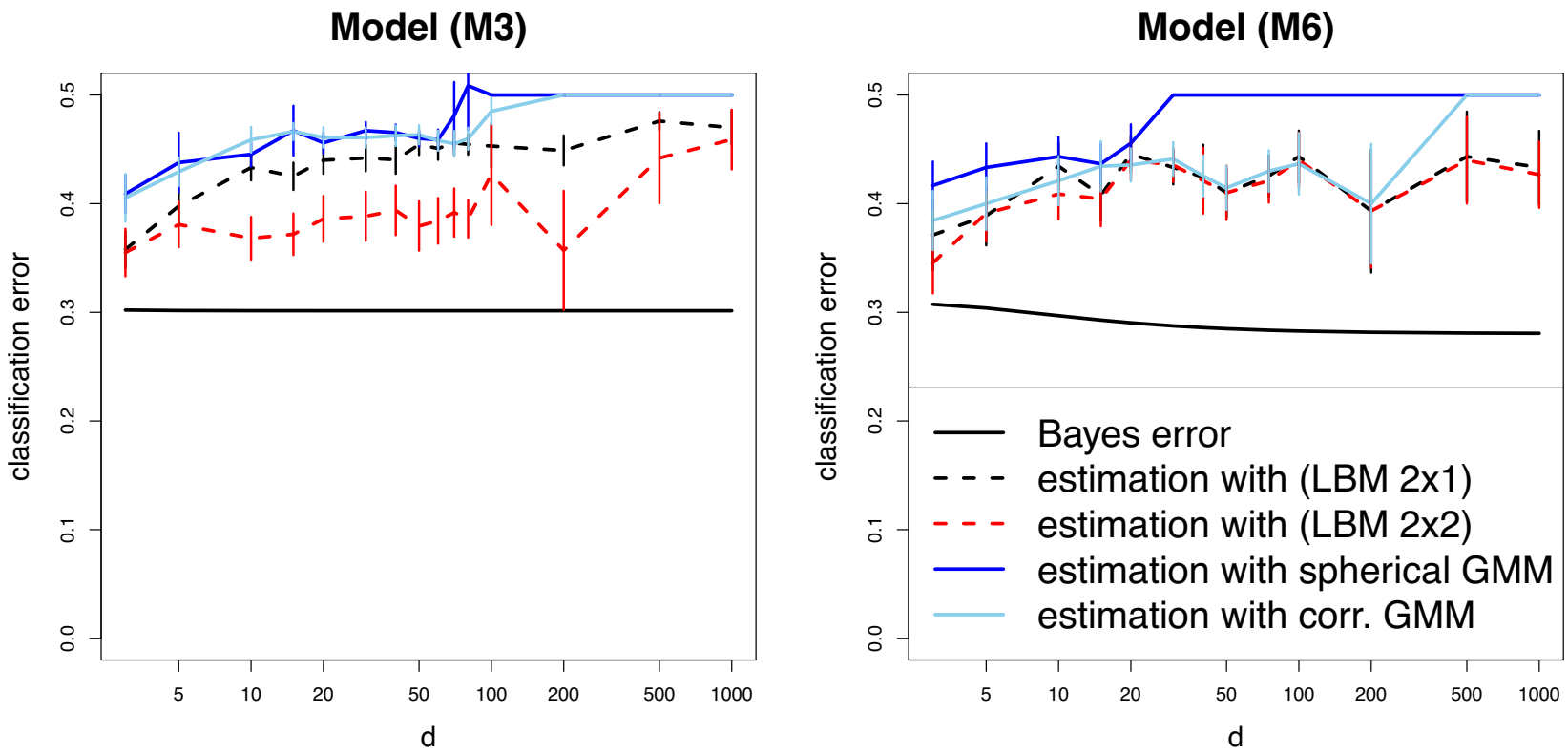


non informative variables

redundancy: duplicated variables

Same conclusion for LBM, which resists to such HD scenarios

Numerical illustrations: results (cont'd)



too many noninformative variables

- too much bias, classification error with CC no longer lines up with Bayes risk
- but CC methods still perform better than simple mixture

Take home message

- in HD clustering, accept model bias to reduce variance on the classification
- CC acts as a regularized tool to perform clustering
  ↪ very parsimonious model, with model bias but often offers better classification error
- LBM also offers a level of flexibility despite its parsimony
  ↪ using LBM for HD clustering should be more emphasized
  ↪ estimation is challenging, but there are solutions
  ↪ less cases of spurious / degenerate solutions than in simple mixture models

For further research...

- interpret the groups of variables in co-clustering
- extend the empirical results by theoretical guidelines
- robust estimation
- model selection: to be fixed by theoretical results

Merci / Thank you!

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INVITED ARTICLE

A Survey on Model-Based Co-Clustering: High Dimension and Estimation Challenges

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