Going further in cluster analysis and classification: Bi-clustering and co-clustering

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Going further in cluster analysis and classification: **Bi-clustering and co-clustering**

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Outline

Motivation

High dimensional (HD) data sets are now frequent:

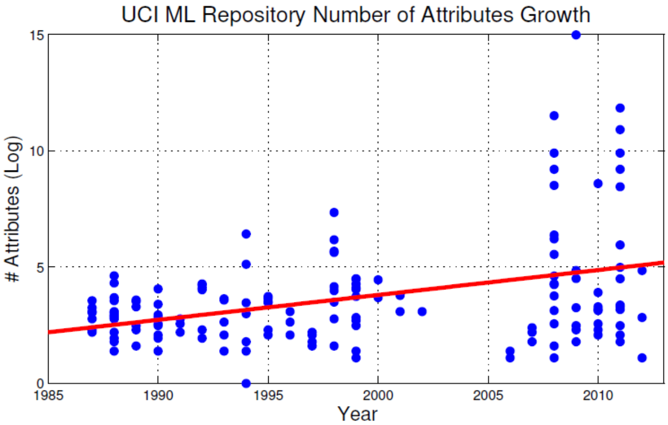
- Marketing: $d \sim 10^2$
- microarray gene expression: $d \sim 10^2$–10^4
- SNP data: $d \sim 10^6$
- Curves: depends on discretization but can be very high
- Text mining
- ...

Clustering has to be applied for HD datasets for the same reasons as the lower dimensional datasets:

- Data summary
- Data exploratory
- Preprocessing for more flexibility of a forthcoming prediction step

But clustering is even more important since visualization in the HD setting can be hazardous...

Today': exponential growing of dimension[1]



[1] S. Alelyani, J. Tang and H. Liu (2013). Feature Selection for Clustering: A Review. *Data Clustering: Algorithms and Applications*, **29**

HD data: definition (1/2)

An attempt in the non-parametric case

Dataset $\mathbf{x} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$, $\mathbf{x}_j$ described by d variables, where $n = o\left(e^d\right)$

Justifications:

- To approximate within error ϵ a (Lipschitz) function of d variables, about $(1/\epsilon)^d$ evaluations on a grid are required [Bellman, 61]
- Approximate a Gaussian distribution with fixed Gaussian kernels and with approximate error of about 10% [Silverman, 86]

$$\log_{10} n(d) \approx 0.6(d - 0.25)$$

For instance, $n(10) \approx 7.10^5$

HD data: definition (2/2)

An attempt in the parametric case

Dataset $\mathbf{x} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$, $\mathbf{x}_j$ described by d variables and a model $\mathbf{m}$ with ν parameters, where $n = o(g(\nu))$, with g a given function

Justification:

- We consider the heteroscedastic Gaussian mixture with of true parameter $\boldsymbol{\theta}^*$ with K^* components. We note $\hat{\boldsymbol{\theta}}$ the Gaussian MLE with K^* components. We have g linear from the following result [Michel, 08]: it exists constants κ, A and C such that

$$\mathrm{E}_{\mathbf{x}}[\mathrm{Hellinger}^2(\mathrm{p}_{\boldsymbol{\theta}^*}, \mathrm{p}_{\hat{\boldsymbol{\theta}}_{\hat{K}}})] \leq C \left[\kappa \frac{\nu}{n} \left\{ 2A \ln d + 1 - \ln \left(1 \wedge \left[\frac{\nu}{n} A \ln d \right] \right) \right\} + \frac{1}{n} \right].$$

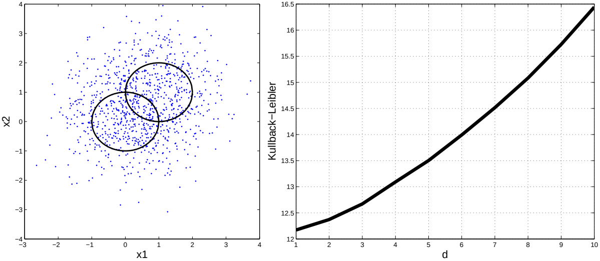
But ν can be high since $\nu \sim d^2/2$, combined with potentially large constants.

HD density estimation: curse

A two-component d-variate Gaussian mixture:

$$\pi_1 = \pi_2 = \frac{1}{2}, \quad \mathbf{X}_1 | z_{11} = 1 \sim \mathrm{N}_d(\mathbf{0}, \mathbf{I}), \quad \mathbf{X}_1 | z_{12} = 1 \sim \mathrm{N}_d(\mathbf{1}, \mathbf{I})$$

Components are more and more separated when d grows: $\|\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1\|_{\mathbf{I}} = \sqrt{d}$...



...but density estimation quality decreases with d

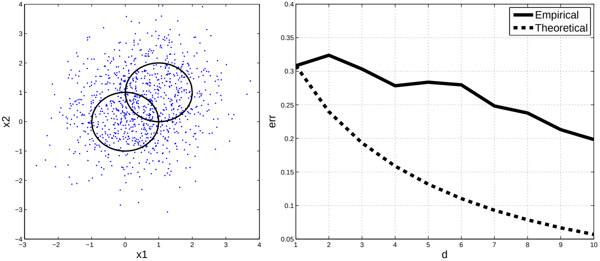
HD clustering: blessing (1/2)

A two-component d-variate Gaussian mixture:

$$\pi_1 = \pi_2 = \frac{1}{2}, \quad \mathbf{X}_1 | z_{11} = 1 \sim \mathrm{N}_d(\mathbf{0}, \mathbf{I}), \quad \mathbf{X}_1 | z_{12} = 1 \sim \mathrm{N}_d(\mathbf{1}, \mathbf{I})$$

Each variable provides equal and own separation information

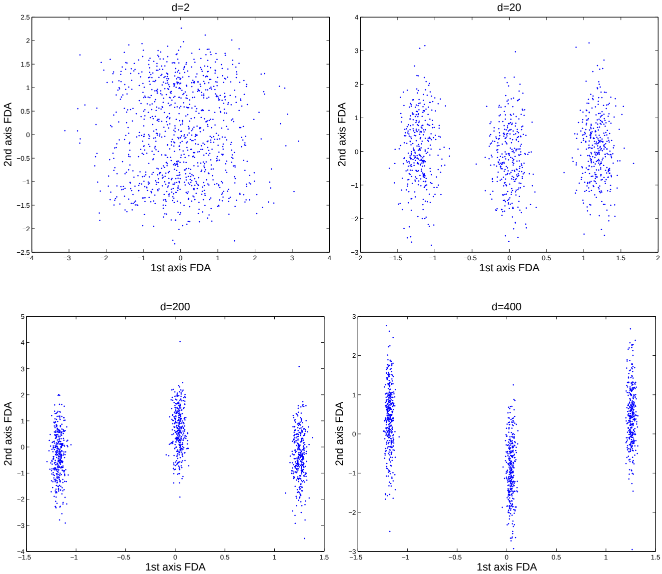
Theoretical error decreases when d grows: $\mathrm{err}_{theo} = \Phi(-\sqrt{d}/2)\ldots$



. . . and empirical error rate decreases also with d!

HD clustering: blessing (2/2)

FDA



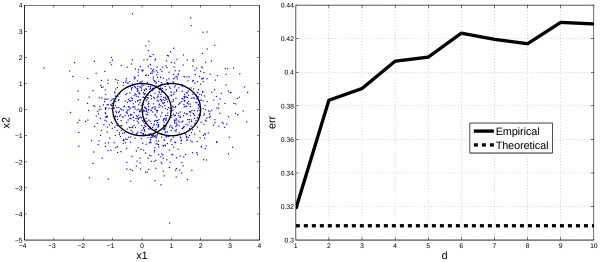
HD clustering: curse (1/2)

Many variables provide no separation information

Same parameter setting except:

$$\mathbf{X}_1|z_{12} = 1 \sim \mathrm{N}_d((1\ 0\ \ldots\ 0)', \mathbf{I})$$

Groups are not separated more when d grows: $\|\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1\|_{\mathbf{I}} = 1\ldots$



…thus theoretical error is constant $(= \Phi(-\frac{1}{2}))$ and empirical error increases with d

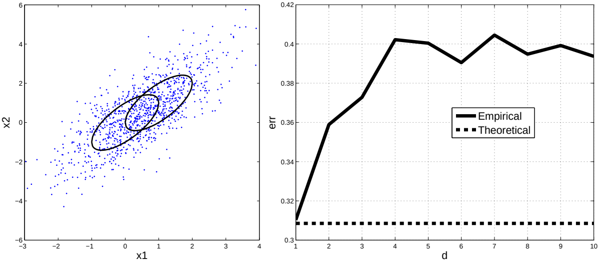
HD clustering: curse (2/2)

Many variables provide redundant separation information

Same parameter setting except:

$$\mathbf{X}_1^j = \mathbf{X}_1^1 + \mathrm{N}_1(0,1) \quad (j = 2, \ldots, d)$$

Groups are not separated more when d grows: $\|\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1\|_{\boldsymbol{\Sigma}} = 1\ldots$



...thus err_{theo} is constant $(= \Phi(-\frac{1}{2}))$ and empirical error increases (less) with d

The trade-off bias/variance

The fundamental statistical principle

Always minimize an error err between truth ($\mathbf{z}$) and estimate ($\hat{\mathbf{z}}$)

- Gap between true ($\mathbf{z}$) and model-based ($\mathcal{Z}_\mathrm{p}$) partitions: $\mathbf{z}^* = \arg\min_{\tilde{z} \in \mathcal{Z}_\mathrm{p}} \Delta(\mathbf{z}, \tilde{\mathbf{z}})$
- Estimation $\hat{\mathbf{z}}$ of $\mathbf{z}^*$ in $\mathcal{Z}_\mathrm{p}$: any relevant method (bias, consistency, efficiency. . .)
- Fundamental decomposition of the observed error $\mathrm{err}(\mathbf{z}, \hat{\mathbf{z}})$:

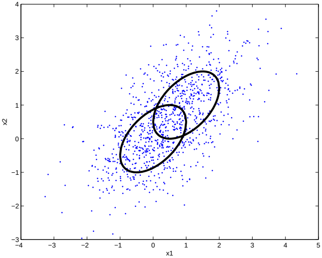
$$\begin{aligned}
\mathrm{err}(\mathbf{z}, \hat{\mathbf{z}}) &= \Big\{\mathrm{err}(\mathbf{z}, \mathbf{z}^*) - \mathrm{err}(\mathbf{z}, \mathbf{z})\Big\} + \Big\{\mathrm{err}(\mathbf{z}, \hat{\mathbf{z}}) - \mathrm{err}(\mathbf{z}, \mathbf{z}^*)\Big\} \\
&= \Big\{\text{bias}\Big\} + \Big\{\text{variance}\Big\} \\
&= \Big\{\text{error of approximation}\Big\} + \Big\{\text{error of estimation}\Big\}
\end{aligned}$$

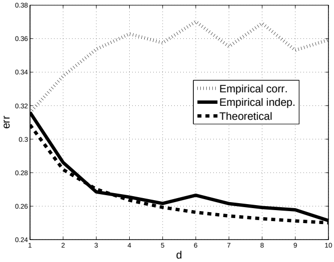
Bias/variance in HD: reduce variance, accept bias

A two-component d-variate Gaussian mixture with intra-dependency:

$$\pi_1 = \pi_2 = \frac{1}{2}, \quad \mathbf{X}_1 | z_{11} = 1 \sim \mathrm{N}_d(\mathbf{0}, \mathbf{\Sigma}), \quad \mathbf{X}_1 | z_{12} = 1 \sim \mathrm{N}_d(\mathbf{1}, \mathbf{\Sigma})$$

- Each variable provides equal and own separation information
- Theoretical error decreases when d grows: $\mathrm{err}_{theo} = \Phi(-\|\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1\|_{\mathbf{\Sigma}^{-1}}/2)$
- Empirical error rate with the (true) intra-correlated model worse with d
- Empirical error rate with the (false) intra-independent model better with d!





Some alternatives for reducing variance

- Dimension reduction in non-canonical space (PCA-like typically)
- Dimension reduction in the canonical space (variable selection)
- Model parsimony in the initial HD space (constraints on model parameters)

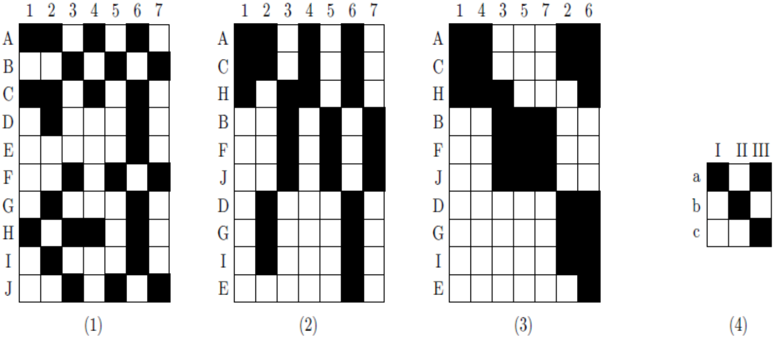
But which kind of parsimony?

- Remember that clustering is a way for dealing with large n
- Why not reusing this idea for large d?

Co-clustering

It performs parsimony of row clustering through variable clustering

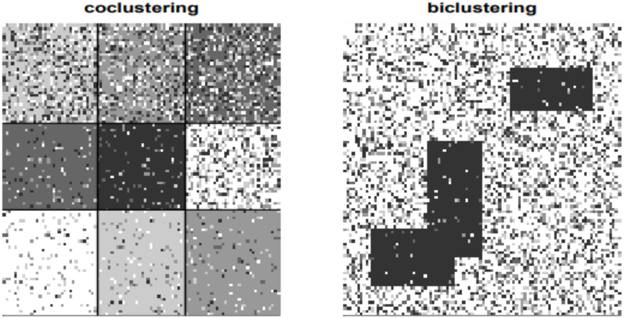
From clustering to co-clustering



[Govaert, 2011]

Bi-clustering

- A generalization of co-clustering
- Look for submatrices of $\boldsymbol{x}$ which are homogeneous
- We do not consider bi-clustering here



Outline

Notations

- $\boldsymbol{z}_i$: the cluster of the row i
- $\boldsymbol{w}_j$: the cluster of the column j
- $(\boldsymbol{z}_i, \mathbf{w}_j)$: the block of the element $\boldsymbol{x}_{ij}$ (row i, column j)

- $\mathbf{z} = (\boldsymbol{z}_1, \ldots, \boldsymbol{z}_n)$: partition of individuals in K custers of rows
- $\mathbf{w} = (\boldsymbol{w}_1, \ldots, \boldsymbol{w}_d)$: partition of variables in L clusters of columns
- $(\boldsymbol{z}, \mathbf{w})$: bi-partition of the whole data set $\boldsymbol{x}$
- Both space partitions are respectively denoted by $\mathcal{Z}$ and $\mathcal{W}$

Restriction

All variables are of the same kind (see discussion at the end)

A geometric approach

- Example in the continuous case: $\boldsymbol{x} \in \mathbb{R}^{n \times d}$
- It could be possible to define a within-block inertia criterion

$$W(\boldsymbol{z}, \boldsymbol{w}) = \underbrace{\sum_{k=1}^{K} \sum_{l=1}^{L} \sum_{i=1}^{n} \sum_{j=1}^{d}}_{\sum_{i,j,k,l}} z_{ik} w_{jl} \|x_{ij} - \mu_{kl}\|^2$$

with μ_{kl} the center of the block (k, l)

$$\mu_{kl} = \frac{1}{n_{kl}} \sum_{i,j} z_{ik} w_{jl} x_{ij}$$

where $n_{kl} = \sum_{ij} z_{ik} w_{jl}$ is the sample size of the block (k, l)

But we know now that it hides some model-based assumptions. . .

The latent block model (LBM)

- Generalization of some existing non-probabilistic methods
- Extend the latent class principle of local (or conditional) independence
- Thus x_{ij} is assumed to be independent once z_i and w_j are fixed ($\boldsymbol{\alpha} = (\boldsymbol{\alpha}_{kl})$):

$$\mathrm{p}(\mathbf{x}|\mathbf{z},\mathbf{w};\boldsymbol{\alpha}) = \prod_{i,j} \mathrm{p}(x_{ij};\boldsymbol{\alpha}_{z_i w_j})$$

- $\boldsymbol{\pi} = (\pi_k)$: vectors of proba. π_k that a row belongs to the kth row cluster
- $\boldsymbol{\rho} = (\rho_k)$: vectors of proba. ρ_k that a row belongs to the lth column cluster
- Independence between all z_i and w_j
- Extension of the traditional mixture model-based clustering ($\boldsymbol{\alpha} = (\boldsymbol{\alpha}_{kl})$):

$$\mathrm{p}(\mathbf{x};\boldsymbol{\theta}) = \sum_{(\mathbf{z},\mathbf{w})\in\mathcal{Z}\times\mathcal{W}} \prod_{i,j} \pi_{z_i}\rho_{w_j}\mathrm{p}(x_{ij};\boldsymbol{\alpha}_{z_i w_j})$$

Distribution for different kinds of data

[Govaert and Nadif, 2014] The pdf $p(\cdot;\boldsymbol{\alpha}_{z_i w_j})$ depends on the kind of data x_{ij}:

- Binary data: $x_{ij} \in \{0,1\}$, $p(\cdot;\boldsymbol{\alpha}_{kl}) = \mathcal{B}(\alpha_{kl})$
- Categorical data with m levels:
  $\mathbf{x}_{ij} = \{x_{ijh}\} \in \{0,1\}^m$ with $\sum_{h=1}^m x_{ijh} = 1$ and $p(\cdot;\boldsymbol{\alpha}_{kl}) = \mathcal{M}(\boldsymbol{\alpha}_{kl})$ with $\boldsymbol{\alpha}_{kl} = \{\alpha_{kjh}\}$
- Count data: $x_i^j \in \mathbb{N}$, $p(\cdot;\boldsymbol{\alpha}_{kl}) = \mathcal{P}(\mu_k \nu_l \gamma_{kl})$[2]
- Continuous data: $x_i^j \in \mathbb{R}$, $p(\cdot;\boldsymbol{\alpha}_{kl}) = \mathcal{N}(\mu_{kl}, \sigma^2_{kl})$

[2] The Poisson parameter is here split into μ_k and ν_l the effects of the row k and the column l respectively and γ_{kl} the effect of the block kl. Unfortunately, this parameterization is not identifiable. It is therefore not possible to estimate simultaneously μ_k, ν_l and γ_{kl} without imposing further constraints. Constraints $\sum_k \pi_k \gamma_{kl} = \sum_l \rho_l \gamma_{kl} = 1$ and $\sum_k \mu_k = 1, \sum_l \nu_l = 1$ are a possibility.

Extreme parsimony ability

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	$\dim(\boldsymbol{\pi}) + \dim(\boldsymbol{\rho}) + 2KL$

Very parsimonious so well suitable for the (ultra) HD setting

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

Other advantage: stay in the canonical space thus meaningful for the end-user

Binary illustration: easy interpretation

[Govaert, 2011]

	abcdefghij
y_1	1010001101
y_2	0101110011
y_3	1000001100
y_4	1010001100
y_5	0111001100
y_6	0101110101
y_7	0111110111
y_8	1100111011
y_9	0100110000
y_{10}	1010101101
y_{11}	1010001100
y_{12}	1010000100
y_{13}	1010001101
y_{14}	0010011100
y_{15}	0010010100
y_{16}	1111001100
y_{17}	0101110011
y_{18}	1010011101
y_{19}	1010001000
y_{20}	1100101100

Raw data

	a c g h	b d e f i j
y_2	0 0 0 0	1 1 1 1 1 1
y_6	0 0 0 1	1 1 1 1 0 1
y_7	0 1 0 1	1 1 1 1 1 1
y_8	1 0 1 0	1 0 1 1 1 1
y_9	0 0 0 0	1 0 1 1 0 0
y_{17}	0 0 0 0	1 1 1 1 1 1
y_1	1 1 1 1	0 0 0 0 0 1
y_3	1 0 1 1	0 0 0 0 0 0
y_4	1 1 1 1	0 0 0 0 0 0
y_5	0 1 1 1	1 1 0 0 0 0
y_{10}	1 1 1 1	0 0 1 0 0 1
y_{11}	1 1 1 1	0 0 0 0 0 0
y_{12}	1 1 0 1	0 0 0 0 0 0
y_{13}	1 1 1 1	0 0 0 0 0 1
y_{14}	0 1 1 1	0 0 0 1 0 0
y_{15}	0 1 0 1	0 0 0 1 0 0
y_{16}	1 1 1 1	1 1 0 0 0 0
y_{18}	1 1 1 1	0 0 0 1 0 1
y_{19}	1 1 1 0	0 0 0 0 0 0
y_{20}	1 0 1 1	1 0 1 0 0 0

Permuted data (rows/columns)

iid Bin(0.83)

mode

0	1
1	0

Summary

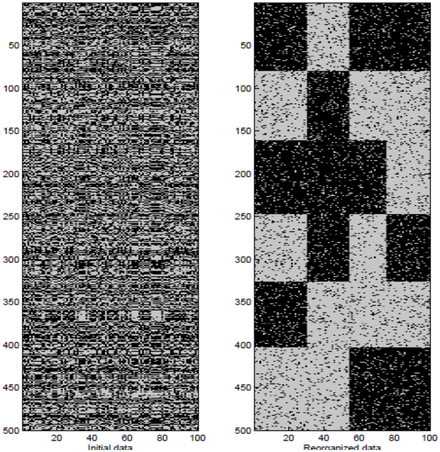
0.86	0.79
0.83	0.86

Homogeneity

proba=mode

Binary illustration: user-friendly visualization

[Govaert, 2011]



$$n = 500, \ d = 10, \ K = 6, \ L = 4$$

Other kind of data: ordinal

[Jacques and Biernacki, 2018]

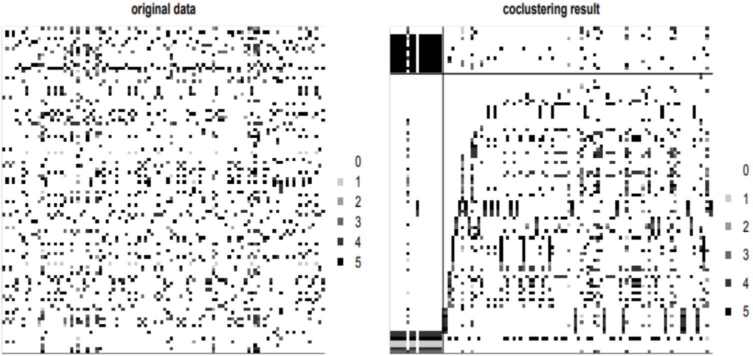
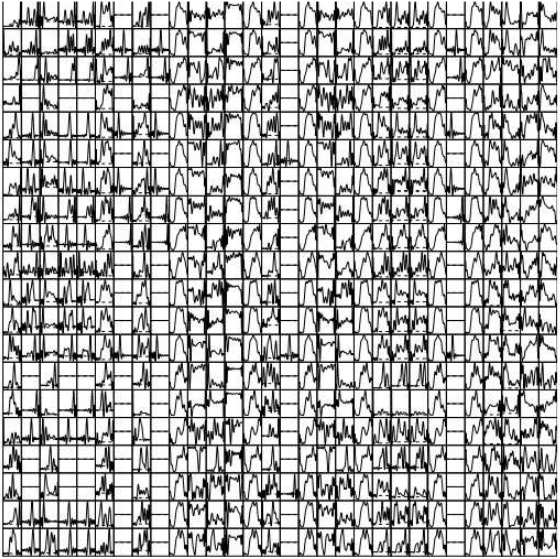


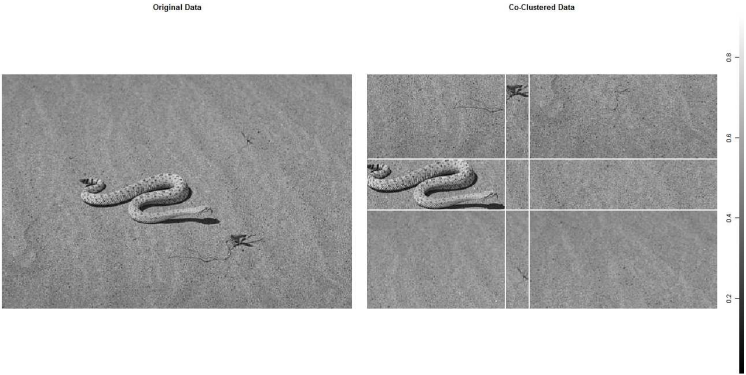
Figure 11: Top 100 Amazone Fine Food Review data (left) and co-clustering result (right).

Other kind of data: functional

[Jacques, 2016]

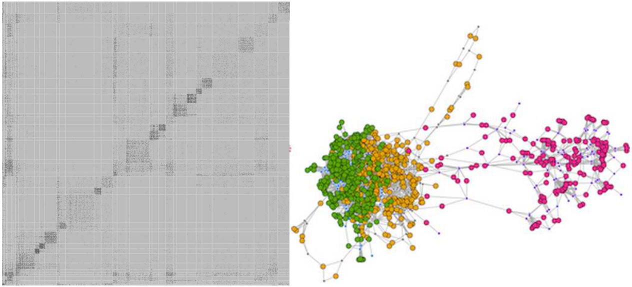


Other kind of data: image



Particular case: graph clustering

Stochastic Block Model (SBM): adjacency matrix with $n = d$ and $K = L$



Outline

MLE estimation: log-likelihood(s)

- Remember Lesson 3: first estimate $\boldsymbol{\theta}$, then deduce estimate of $(\boldsymbol{z}, \boldsymbol{w})$
- Observed log-likelihood: $\ell(\boldsymbol{\theta}; \boldsymbol{x}) = \ln \mathrm{p}(\boldsymbol{x}; \boldsymbol{\theta})$
- MLE:

$$\hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}; \boldsymbol{x})$$

- Complete log-likelihood:

$$\begin{aligned} \ell_c(\boldsymbol{\theta}; \mathbf{x}, \mathbf{z}, \mathbf{w}) &= \ln \mathrm{p}(\boldsymbol{x}, \boldsymbol{z}, \boldsymbol{w}; \boldsymbol{\theta}) \\ &= \sum_{i,k} z_{ik} \log \pi_k + \sum_{k,l} w_{jl} \log \rho_l + \sum_{i,j,k,l} z_{ik} w_{jl} \log \mathrm{p}(x_i^j; \boldsymbol{\alpha}_{kl}) \end{aligned}$$

Be careful with asymptotics...

If $\ln(d)/n \to 0$, $\ln(n)/d \to 0$ when $n \to \infty$ and $d \to \infty$, then the MLE is consistent [Brault *et al.*, 2017]

MLE estimation: EM algorithm

- E-step of EM (iteration q):

$$
\begin{aligned}
Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{(q)}) &= E[\ell_c(\boldsymbol{\theta}; \mathbf{x}, \mathbf{z}, \mathbf{w}) | \boldsymbol{x}; \boldsymbol{\theta}^{(q)}] \\
&= \sum_{i,k} \underbrace{p(z_i = k | \mathbf{x}; \boldsymbol{\theta}^{(q)})}_{t_{ik}^{(q)}} \ln \pi_k + \sum_{j,l} \underbrace{p(w_i = l | \mathbf{x}; \boldsymbol{\theta}^{(q)})}_{s_{jl}^{(q)}} \ln \rho_l \\
&\quad + \sum_{i,j,k,l} \underbrace{p(z_i = k, w_j = l | \mathbf{x}; \boldsymbol{\theta}^{(q)})}_{e_{ijkl}^{(q)}} \ln \mathrm{p}(x_{ij}; \boldsymbol{\alpha}_{kl})
\end{aligned}
$$

- M-step of EM (iteration q): classical. For instance, for the Bernoulli case, it gives

$$
\pi_k^{(q+1)} = \frac{\sum_i t_{ik}^{(q)}}{n}, \quad \rho_l^{(q+1)} = \frac{\sum_j s_{jl}^{(q)}}{d}, \quad \alpha_{kl}^{(q+1)} = \frac{\sum_{i,j} e_{ijkl}^{(q)} x_{ij}}{\sum_{i,j} e_{ijkl}^{(q)}}
$$

MLE: intractable E step

$e_{ijkl}^{(q)}$ is usually intractable. . .

- Consequence of dependency between $\boldsymbol{x}_{ij}$s (link between rows and columns)
- Involve $K^n L^d$ calculus (number of possible blocks)
- Example: if $n = d = 20$ and $K = L = 2$ then 10^{12} blocks
- Example (cont'd): 33 years with a computer calculating 100,000 blocks/second

Alternatives to EM

- Variational EM (numerical approx.): conditional independence assumption

$$\mathrm{p}(\mathbf{z}, \mathbf{w}|\mathbf{x}; \boldsymbol{\theta}) \approx \mathrm{p}(\mathbf{z}|\mathbf{x}; \boldsymbol{\theta})\mathrm{p}(\mathbf{w}|\mathbf{x}; \boldsymbol{\theta})$$

- SEM-Gibbs (stochastic approx.): replace E-step by a S-step approx. by Gibbs

$$\mathbf{z}|\mathbf{x}, \mathbf{w}; \boldsymbol{\theta} \quad \text{and} \quad \mathbf{w}|\mathbf{x}, \mathbf{z}; \boldsymbol{\theta}$$

MLE: variational EM (1/2)

- Use a general variational result from [Hathaway, 1985]
- Maximizing $\ell(\boldsymbol{\theta}; \boldsymbol{x})$ on $\boldsymbol{\theta}$ is equivalent to maximize $\tilde{\ell}_c(\boldsymbol{\theta}; \boldsymbol{x}, \mathbf{e})$ on $(\boldsymbol{\theta}, \mathbf{e})$

$$\tilde{\ell}_c(\boldsymbol{\theta}; \boldsymbol{x}, \mathbf{e}) = \sum_{i,k} t_{ik} \ln \pi_k + \sum_{j,l} s_{jl} \ln \rho_l + \sum_{i,j,k,l} e_{ijkl} \ln \mathrm{p}(x_{ij}; \boldsymbol{\alpha}_{kl})$$

where $\mathbf{e} = (e_{ijkl})$, $e_{ijkl} \in \{0,1\}$, $\sum_{k,l} e_{ijkl} = 1$, $t_{ik} = \sum_{j,l} e_{ijkl}$, $s_{jl} = \sum_{i,k} e_{ijkl}$

- Of course maximizing $\ell(\boldsymbol{\theta}; \boldsymbol{x})$ or $\tilde{\ell}_c(\boldsymbol{\theta}; \boldsymbol{x}, \mathbf{e})$ are both intractable
- Idea: restriction on $\mathbf{e}$ to obtain tractability $\mathbf{e}_{ijkl} = t_{ik} s_{jl}$
- New variables are thus now $\mathbf{t} = (t_{ik})$ and $\mathbf{s} = (s_{jl})$
- As a consequence, it is a maximization of a lower bound of the max. likelihood

$$\max_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}; \boldsymbol{x}) \geq \max_{\boldsymbol{\theta}, \mathbf{t}, \mathbf{s}} \tilde{\ell}_c(\boldsymbol{\theta}; \boldsymbol{x}, \mathbf{e})$$

MLE: variational EM (2/2)

Approximated E-step

$$Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{(q)}) \approx \sum_{i,k} t_{ik}^{(q)} \ln \pi_k + \sum_{j,l} s_{jl}^{(q)} \ln \rho_l + \sum_{i,j,k,l} t_{ik}^{(q)} s_{jl}^{(q)} \ln \mathrm{p}(x_{ij}; \boldsymbol{\alpha}_{kl})$$

- We called it now VEM
- Also known as mean field approximation
- Consistency of the variational estimate [Brault *et al.*, 2017]

MLE: local maxima

- More local maxima than in classical mixture models
- It is a consequence of many more latent variables (blocks)
- Thus: either many VEM runs, or use the SEM-Gibbs algorithm

MLE: SEM-Gibbs

- We have already seen the SEM algorithm in Lesson 3 (thus we do not detail more)
- It limits dependency to starting point, so it limits local maxima
- The S-step: a draw $(\boldsymbol{z}^{(q)}, \boldsymbol{w}^{(q)}) \sim \mathrm{p}(\boldsymbol{z}, \boldsymbol{w}|\boldsymbol{x}; \boldsymbol{\theta}^{(q)})$ instead an expectation
- But it is still intractable, thus use a Gibbs algorithm to approx. this draw

Approximated S-step

Two easy draws

$$\boldsymbol{z}^{(q)} \sim \mathrm{p}(\boldsymbol{z}|\boldsymbol{w}^{(q-1)}, \boldsymbol{x}; \boldsymbol{\theta}^{(q)})$$

and

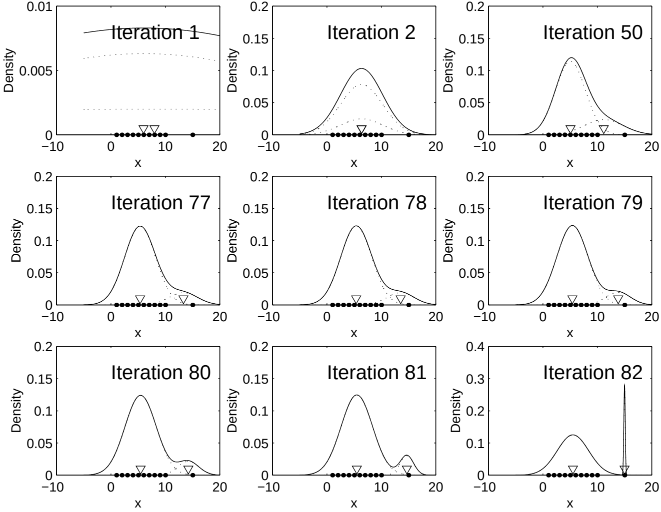
$$\boldsymbol{w}^{(q)} \sim \mathrm{p}(\boldsymbol{w}|\boldsymbol{z}^{(q)}, \boldsymbol{x}; \boldsymbol{\theta}^{(q)})$$

- Rigorously speaking, many draws within the S-step should be performed
- Indeed, Gibbs has to reach a stochastic convergence
- In practice it works well while saving computation time

MLE: degeneracy

- More degenerate situations than in classical mixture models
- It is again a consequence of many more latent variables (blocks)
- The Bayesian regularization (instead MLE) can be an answer

Illustration of a degenerate situation



Bayesian estimation: pitch

- Everything passes by the posterior distribution of $\boldsymbol{\theta}$

$$\mathrm{p}(\boldsymbol{\theta}|\boldsymbol{x}) \propto \underbrace{\mathrm{p}(\boldsymbol{x}|\boldsymbol{\theta})}_{\text{log-likelihood}} \underbrace{\mathrm{p}(\boldsymbol{\theta})}_{\text{prior}}$$

- Then, take (for instance) the MAP as a $\boldsymbol{\theta}$ estimate (use a VEM like algo. . .)

$$\hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} \mathrm{p}(\boldsymbol{\theta}|\boldsymbol{x})$$

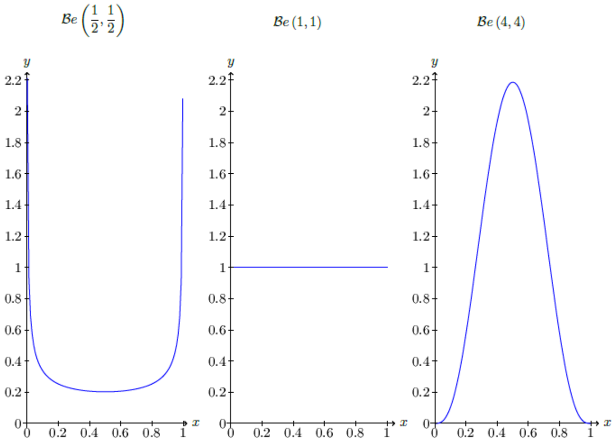
Bayesian estimation: limiting degeneracy

- Interest for avoiding degeneracy is the prior: it acts as a penalization term
- Typical choices are Dirichlet for $\boldsymbol{\pi}$ and $\boldsymbol{\rho}$ (with independence between $\boldsymbol{\pi}$, $\boldsymbol{\rho}$, $\boldsymbol{\alpha}$)

$$\mathrm{p}(\boldsymbol{\theta}) = \underbrace{\mathrm{p}(\boldsymbol{\pi})}_{D_K(a,\ldots,a)} \times \underbrace{\mathrm{p}(\boldsymbol{\rho})}_{D_L(a,\ldots,a)} \times \underbrace{\mathrm{p}(\boldsymbol{\alpha})}_{\text{model dependent}}$$

- The Dirichlet distribution is conjugate, thus easy calculus
- Control degeneracy frequency with the a value:
  - $a = 1$: uniform prior, so $\hat{\boldsymbol{\theta}}$ is strictly the MLE (no regularisation)
  - $a = 1/2$: Jeffreys prior, classical (no informative prior) but may favor degeneracy
  - $a = 4$: a rule of thumb working well for limiting degeneracy frequency

Bayesian estimation: prior overview



Block estimation: estimate

- Once we have a parameter estimate $\hat{\boldsymbol{\theta}}$, we need to have an block estimate $(\hat{\boldsymbol{z}}, \hat{\boldsymbol{w}})$
- But MAP not directly available because of the following maximization difficulty

$$(\hat{\boldsymbol{z}}, \hat{\boldsymbol{w}}) = \arg\max_{(\boldsymbol{z},\boldsymbol{w})} \underbrace{\mathrm{p}(\boldsymbol{z}, \boldsymbol{w} | \boldsymbol{x}; \hat{\boldsymbol{\theta}})}_{\text{intractable}}$$

- Instead the following (easily, as classical mixtures) estimates are usually retained

$$\hat{\boldsymbol{z}} = \arg\max_{\boldsymbol{z}} \mathrm{p}(\boldsymbol{z} | \boldsymbol{x}; \hat{\boldsymbol{\theta}}) \quad \text{and} \quad \hat{\boldsymbol{w}} = \arg\max_{\boldsymbol{w}} \mathrm{p}(\boldsymbol{w} | \boldsymbol{x}; \hat{\boldsymbol{\theta}})$$

Block estimation: evaluation

- Empirical error rate between blocks:

$$\mathrm{err}_{\mathrm{blocks}}(\underbrace{(\boldsymbol{z},\boldsymbol{w})}_{\text{“True” blocks}},\underbrace{(\hat{\boldsymbol{z}},\hat{\boldsymbol{w}})}_{\text{Estimated blocks}}) = \mathrm{err}(\boldsymbol{z},\hat{\boldsymbol{z}}) + \mathrm{err}(\boldsymbol{w},\hat{\boldsymbol{w}}) - \mathrm{err}(\boldsymbol{z},\hat{\boldsymbol{z}}) \times \mathrm{err}(\boldsymbol{w},\hat{\boldsymbol{w}})$$

- Rand index between blocks: it exists also a recent definition...

Block estimation: consistency

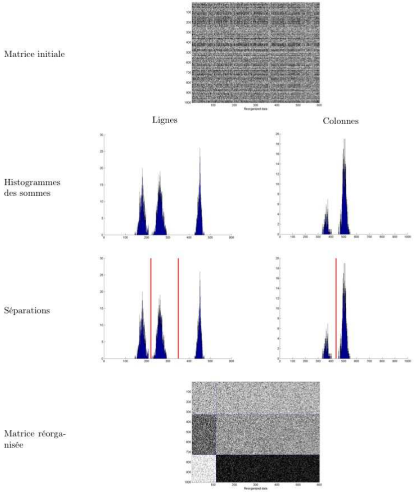
[Mariadassou and Matias, 12]

$$\underbrace{\hat{\boldsymbol{\theta}} \stackrel{n,d\to\infty}{\longrightarrow} \boldsymbol{\theta}^*}_{\text{we have seen that...}} \quad \Rightarrow \quad \underbrace{\mathrm{p}(\hat{\mathbf{z}} = \mathbf{z}^*, \hat{\mathbf{w}} = \mathbf{w}^* | \mathbf{x}; \hat{\boldsymbol{\theta}}) \stackrel{n,d\to\infty}{\longrightarrow} 1}_{\text{exact bi-partition retrieval!}}$$

Thus we retrieve the HD clustering blessing...

Block estimation: non asymptotic properties (1/2)

Binary case: marginals seems so simple mixtures! [Brault, 14]



Block estimation: non asymptotic properties (2/2)

[Brault, 14]

- Probability of x_{ij} with no regard to the column membership is Bernoulli

$$\mathrm{p}(x_{ij} = 1 | z_{ik} = 1) = \tau_k = \sum_{l=1}^{L} \alpha_{kl} \rho_l$$

- Thus marginal distribution of x_{ij} is a mixture (indep. of x_{ij} cond. $z_{ik} = 1$)

$$\left(\sum_j x_{ij} \right) | z_{ik} = 1 \sim \mathrm{B}(d, \tau_k)$$

- Control of error on this partition mixture estimate $\hat{\mathbf{z}}^{mix}$ of binomial distributions

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

- We retrieve also consistency for very high dimension with constraint

$$\ln(n) = o(d)$$

Illustration: document clustering (1/2)

- 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×words
- Poisson model

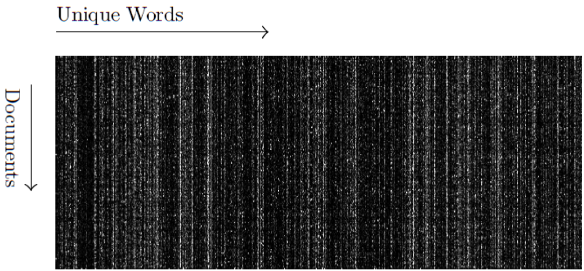
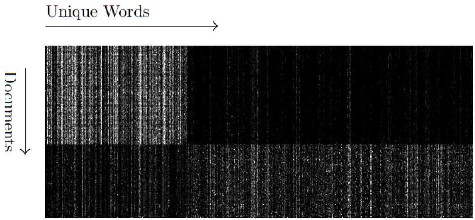


Illustration: document clustering (2/2)



Results with 2×2 blocks

	Medline	Cranfield
Medline	1033	0
Cranfield	0	1398

Experiment illustrates previous theory: HD clustering is blessing

Outline

Models in competition

$\mathbf{m} = (K, L)$ typically, but not restricted to

BIC criterion: two difficulties

- Difficult 1: which BIC definition because of the double asymptotic on n and d?
- Difficult 2: the observed log-likelihood value is intractable

$$\ell(\boldsymbol{\theta}; \mathbf{x}) = \sum_{(\mathbf{z},\mathbf{w}) \in \mathcal{Z} \times \mathcal{W}} \mathrm{p}(\mathbf{x}, \mathbf{z}, \mathbf{w}; \boldsymbol{\theta})$$

Could be estimated by harmonic mean but time consuming and high variance

ICL criterion: overcome both difficulties

- ICL uses complete likelihood thus no intractability

$$\text{ICL} = \ln \text{p}(x, \hat{\mathbf{z}}, \hat{\mathbf{w}}) = \ln \text{p}(\mathbf{x}|\hat{\mathbf{z}}, \hat{\mathbf{w}}) + \ln \text{p}(\hat{\mathbf{z}}) + \ln \text{p}(\hat{\mathbf{w}})$$

- Multinomial case (r levels): [Keribin *et al., 2014*]
  - Derive an exact (non-asymptotic) ICL version
  - Deduce an asymptotic approximation of ICL

$$\text{ICLbic} = \ell_c(\hat{\boldsymbol{\theta}}; \mathbf{x}, \hat{\mathbf{z}}, \hat{\mathbf{w}}) - \frac{K-1}{2}\ln(n) - \frac{L-1}{2}\ln(d) - \frac{KL(r-1)}{2}\ln(nd)$$

- We can make a conjecture for the general case

$$\text{ICLbic} = \ell_c(\hat{\boldsymbol{\theta}}; \mathbf{x}, \hat{\mathbf{z}}, \hat{\mathbf{w}}) - \frac{K-1}{2}\ln(n) - \frac{L-1}{2}\ln(d) - \frac{KL\nu_{\boldsymbol{\alpha}_{kl}}}{2}\ln(nd)$$

ICL criterion: consistency

- We can obtain a BIC expression from ICLbic

$$\begin{aligned} \text{BIC} &= \text{ICLbic} - \ln \text{p}(\hat{\mathbf{z}}, \hat{\mathbf{w}} | \mathbf{x}; \hat{\boldsymbol{\theta}}) \\ &= \underbrace{\ell(\hat{\boldsymbol{\theta}}; \mathbf{x})}_{\text{difficult}} - \frac{K-1}{2} \ln(n) - \frac{L-1}{2} \ln(d) - \frac{KL(m-1)}{2} \ln(nd) \end{aligned}$$

- [Brault *et al.*, 2017] establish that asymptotically on n and d

$$\text{“}\ell(\hat{\boldsymbol{\theta}}; \mathbf{x}) = \ell_c(\hat{\boldsymbol{\theta}}; \mathbf{x}, \hat{\boldsymbol{z}}, \hat{\boldsymbol{w}})\text{”}$$

- Thus, since BIC is consistent, ICL is also consistent

Again the HD clustering blessing is here!

Strategy to smart browsing of (K, L)

[Robert, 2017] Algorithm Bi-KM1

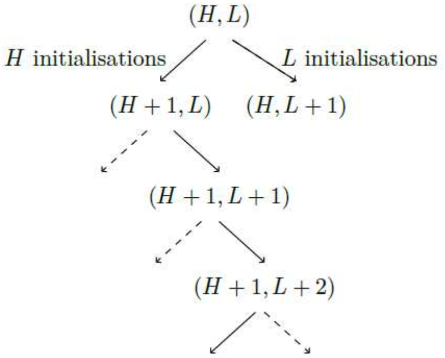


Illustration: discuss the dimension (1/2)

- SPAM E-mail Database[3]
- $n = 4601$ e-mails composed by 1813 "spams" and 2788 "good e-mails"
- $d = 48 + 6 = 54$ continuous descriptors[4]
  - 48 percentages that a given word appears in an e-mail ("make", "you'...)
  - 6 percentages that a given char appears in an e-mail (";", "$"...)
- Transformation of continuous descriptors into binary descriptors

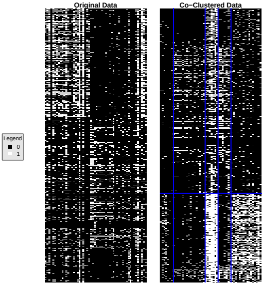
$$x_{ij} = \begin{cases} 1 & \text{if word/char } j \text{ appears in e-mail } i \\ 0 & \text{otherwise} \end{cases}$$

[3] https://archive.ics.uci.edu/ml/machine-learning-databases/spambase/

[4] There are 3 other continuous descriptors we do not use

Illustration: discuss the dimension (2/2)

- Perform co-clustering with $K = 2$ and $L = 5$: ICL=-92,682, err=0.1984



- Perform clustering[5] with $K = 2$: ICL=-89,433, err=0.1837

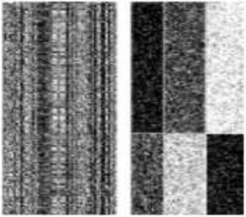
Thus use preferably co-clustering in the HD setting

[5] Equivalent to co-clustering with $L = 54$

Outline

MASSICCC platform for the BLOCKCLUSTER software

https://massiccc.lille.inria.fr/

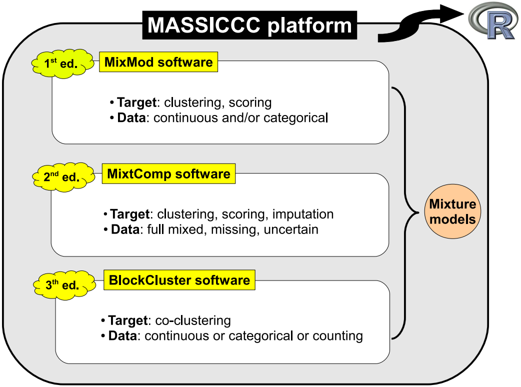


BlockCluster

BlockCluster can estimate the parameters of co-clustering models for binary, contingency and continuous data. Simply put, when considering a set of data as rows and columns, BlockCluster will make simultaneous permutations of rows and columns in order to organise the data into homogenous blocks.

Read more about BlockCluster

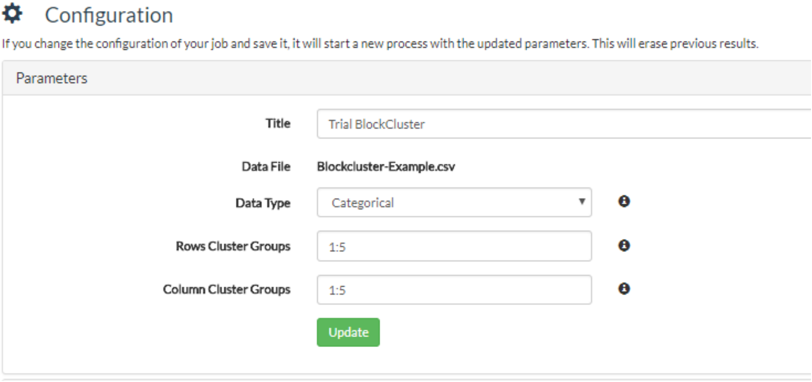
MASSICCC?



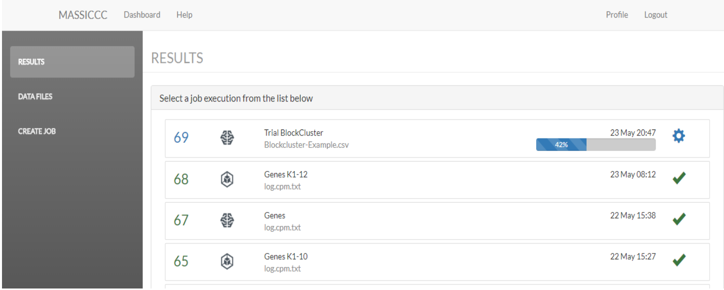
A high quality and easy to use web platform
where are transfered mature research clustering (and more) software
towards (non academic) professionals

Here is the computer you need!

Running BlockCluster



Running BlockCluster



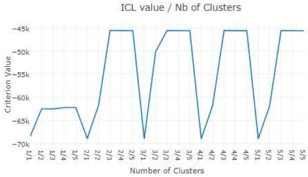
Running BlockCluster

Model	Criterion	Nb Clusters	Error
pik_rhol_multi	ICL (-45557.1)	[2,3]	No error
pik_rhol_multi	ICL (-45563.3)	[3,3]	No error
pik_rhol_multi	ICL (-45566.6)	[2,4]	No error
pik_rhol_multi	ICL (-45573.9)	[4,3]	No error
pik_rhol_multi	ICL (-45574.6)	[5,3]	No error
pik_rhol_multi	ICL (-45577.7)	[3,4]	No error
pik_rhol_multi	ICL (-45578.8)	[2,5]	No error

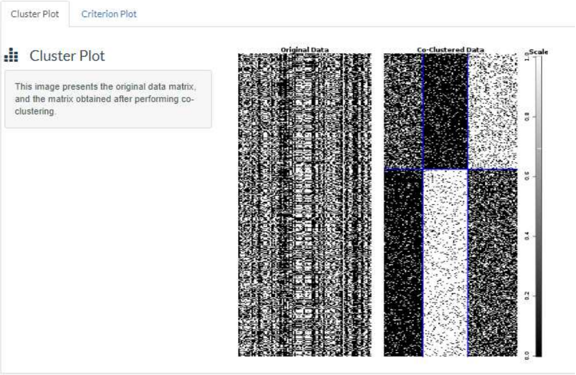
Cluster Plot | Criterion Plot

Model Criterion

This chart represents the criterion value for each model that was built. The higher the value (close to 0) the better the model.



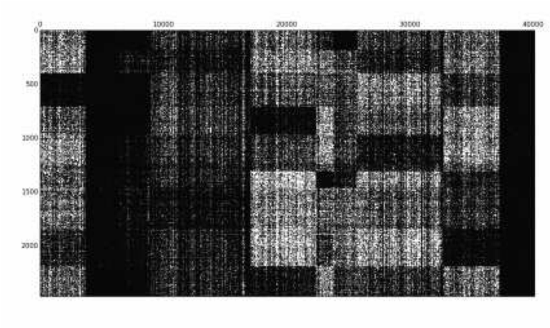
Running BlockCluster



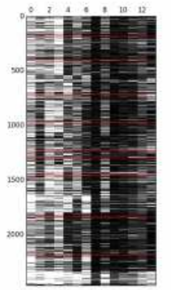
Outline

Co-clustering of mixed data

- Same partitions in lines, disjoint partitions in columns
- Example: data set TED talks, with talks $\times$ (terms,scores)



Poisson



Gaussian