THE UNIVERSITY *of* EDINBURGH
School of Mathematics

Bayesian Cluster Analysis

Sara Wade
University of Edinburgh

Joint work with Zoubin Ghahramani (University of Cambridge & Uber)

O'Bayes Conference, University of Warwick
28 June - 2 July, 2019

Outline

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Mixture models[1]

The data are conditionally iid with density

$$f(y|P) = \int K(y|\theta)dP(\theta),$$

for parametric density $K(y|\theta)$, $y \in \mathcal{Y}$, $\theta \in \Theta$, and P is a p.m. on Θ.

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In Bayesian setting: prior on P s.t.

$$P = \sum_{j=1}^{J} w_j \delta_{\theta_j} \text{ a.s.} \quad \rightarrow f(y|P) = \sum_{j=1}^{J} w_j K(y|\theta_j).$$

This induces a random partition: data points belong to the same cluster if they were generated from the same mixture component.

[1] Frühwirth-Schnatter, Celeux, Robert (2019)

How to choose J?

1. Bayes Factors/information criterion.
2. Mixtures of finite mixtures (MFM): prior on J.
3. Overfitted mixtures.
4. Infinite mixtures.

Mixtures of finite mixtures

Inference:

- Computational issue: dimension of the parameter space changes with J - 'one of the things we don't know is the number of things we don't know'.
- Addressed through, e.g. reversible-jump MCMC (Richardson and Green (1997); Miller and Harrison (2018)).

Positive asymptotics: e.g. Nobile (1994), Guha, Ho, and Nguyen (2019).

Overfitted (sparse) mixtures

- Set J to be larger than the 'true/expected' number of clusters.
- Define: k_N to be the number of clusters in the sample $(y_1, \ldots, y_N)$.

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Will extra components automatically be emptied? yes!

Rousseau and Mengersen (2011): Assume:

$$(w_1, \ldots, w_J) \sim \text{Dir}(\alpha_1, \ldots, \alpha_J),$$

overfitted mixture converges to the truth if $\alpha_j < d/2$, with d denoting the dimension of θ (in this called, called sparse mixtures).

Infinite mixtures

Set $J = \infty$ and define k_N to be the number of clusters in the sample $(y_1, \ldots, y_N)$.

Specify a prior on P s.t. $P = \sum_{j=1}^{\infty} w_j \delta_{\theta_j}$: e.g. Dirichlet process, Pitman-Yor (Lijoi and Prünster (2010))

Inference: collapsed Gibbs (Neal (2000)); slice sampling (Kalli, Griffin, and Walker (2011)); finite-dimensional approximations (Ishwaran and James (2001)).

Mixed asymptotics: e.g. Ghosal and van der Vaart (2007); Miller and Harrison (2013); Rajkowski (2019).

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Summarising the posterior of the partition

These approaches (MFM, overfitted, infinite) provide a model-based framework for Bayesian cluster analysis, returning a posterior over a large partition space, expressing belief and uncertainty in the clustering given the data.

How can we summarize this posterior?

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How can we summarize this posterior?

In typical Bayesian analysis, the posterior of a univariate parameter θ is summarized by a point estimate (ex. $\mathrm{E}[\theta|\mathcal{D}]$) with 95% credible interval. Can we extend these ideas to Bayesian cluster analysis?

Summarising the posterior of the partition

- Developing summary tools is complicated by the discrete and unordered nature and huge dimension of the partition space:

  Dimension of the entire partition space is $B_N = \sum_{k=1}^{N} S_{N,k}$, for example

$$B_{10} = 115975 \text{ and } B_{20} = 51724158235372.$$

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- MCMC is often used for posterior inference $\rightarrow$ How can we summarise the MCMC draws of clusterings?
- Summary measures such as mean and standard deviation are not applicable.
- Mode is unreliable due to huge dimension of space.

Summarising the posterior of the partition

Aim: develop summary tools for the posterior:

1. Point estimate of the clustering,
2. Representation of the uncertainty.

Point estimation

Point estimates used in practice:

- Last iteration of the MCMC- subject to high variability.
- Posterior mode - may be unrepresententive, computational drawbacks.
- Ad-hoc methods: posterior similarity matrix is used as input in hierarchical or partitioning algorithms.
- Decision theoretic approach: minimize the posterior expected loss.

Decision theoretic approach

Notation: clustering $\mathbf{c} = (c_1, \ldots, c_N)$ where $c_n = j$ if y_n is in cluster j.

- **Loss function:** $L(\mathbf{c}, \widehat{\mathbf{c}}) \geq 0$ is the loss of estimating the "true" $\mathbf{c}$ with $\widehat{\mathbf{c}}$.
- We seek $\mathbf{c}^*$ which minimizes

$$\mathsf{E}[L(\mathbf{c}, \widehat{\mathbf{c}})|\mathcal{D}].$$

- Note: $\mathbf{c}^*$ corresponds to the posterior mode under the $0-1$ loss
  - $0-1$ loss does not take into account similarity between two clusterings.
- Need an appropriate loss function.

Loss functions

Binder's loss: (Binder (1978)) [2]

$$\mathrm{B}(\mathbf{c}, \widehat{\mathbf{c}}) = \sum_{n<n'} a\mathbf{1}(c_n = c_{n'}, \widehat{c}_n \neq \widehat{c}_{n'}) + b\mathbf{1}(c_n \neq c_{n'}, \widehat{c}_n = \widehat{c}_{n'}),$$

If $a = b$, and the point estimate c^* is that which minimizes

$$\sum_{n<n'} \left| P(c_n = c_{n'} | \mathcal{D}) - \mathbf{1}(\widehat{c}_n = \widehat{c}_{n'}) \right| .$$

[2] used in Lau and Green (2007) and Dahl (2006).

Loss functions

N-**invariant Binder's loss:**

$$\tilde{\mathsf{B}}(\mathbf{c}, \widehat{\mathbf{c}}) = \frac{2}{N^2}\mathsf{B}(\mathbf{c}, \widehat{\mathbf{c}})$$
$$= \sum_{i=1}^{k_N}\left(\frac{n_{i+}}{N}\right)^2 + \sum_{j=1}^{\widehat{k}_N}\left(\frac{n_{+j}}{N}\right)^2 - 2\sum_{i=1}^{k_N}\sum_{j=1}^{\widehat{k}_N}\left(\frac{n_{ij}}{N}\right)^2,$$

where $n_{ij} = \sum_n \mathbf{1}(c_n = i, \hat{c}_n = j)$; $n_{i+} = \sum_j n_{ij}$; $n_{+j} = \sum_i n_{ij}$.

Loss functions

Variation of information: (Meilă (2007)) constructed from information theory

$$\mathsf{VI}(\mathbf{c}, \widehat{\mathbf{c}}) = \mathsf{H}(\mathbf{c}) + \mathsf{H}(\widehat{\mathbf{c}}) - 2\mathsf{I}(\mathbf{c}, \widehat{\mathbf{c}})$$

$$= -\sum_{i=1}^{k_N} \frac{n_{i+}}{N} \log\left(\frac{n_{i+}}{N}\right) - \sum_{j=1}^{\widehat{k}_N} \frac{n_{+j}}{N} \log\left(\frac{n_{+j}}{N}\right) - 2\sum_{i=1}^{k_N}\sum_{j=1}^{\widehat{k}_N} \frac{n_{ij}}{N} \log\left(\frac{n_{ij}N}{n_{i+}n_{+j}}\right)$$

$$= \sum_{i=1}^{k_N} \frac{n_{i+}}{N} \log\left(\frac{n_{i+}}{N}\right) + \sum_{j=1}^{\widehat{k}_N} \frac{n_{+j}}{N} \log\left(\frac{n_{+j}}{N}\right) - 2\sum_{i=1}^{k_N}\sum_{j=1}^{\widehat{k}_N} \frac{n_{ij}}{N} \log\left(\frac{n_{ij}}{N}\right).$$

Properties of $\tilde{\mathrm{B}}$ and VI

Both $\tilde{\mathrm{B}}$ and VI are metrics and "aligned" with the lattice of partitions.

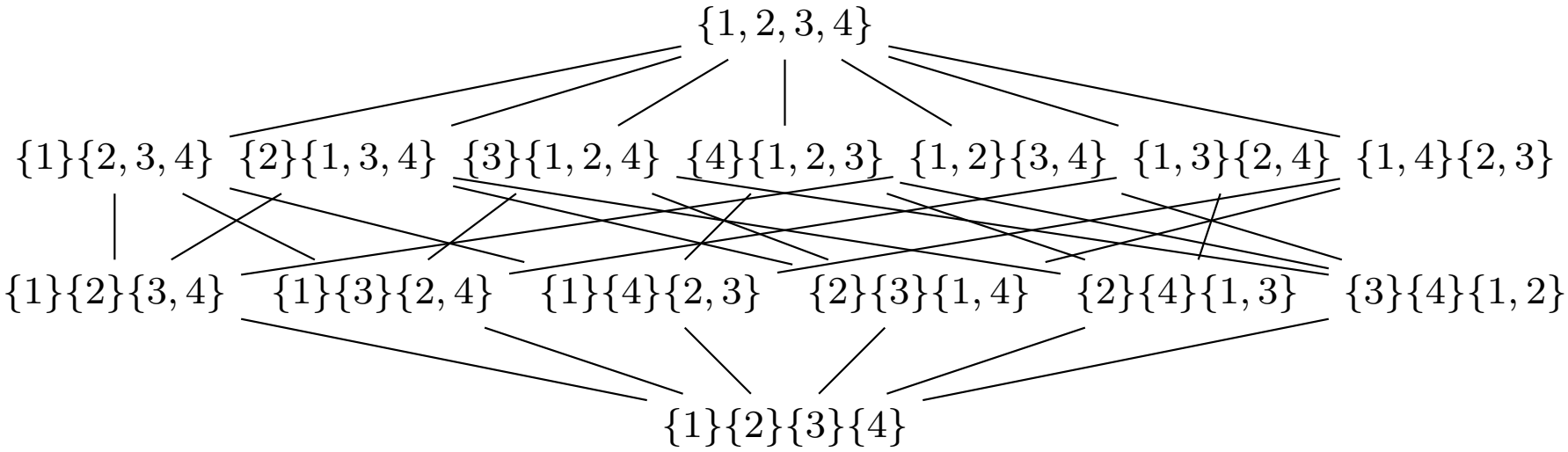


Figure: Hasse diagram for the lattice of partitions with a sample of size $N = 4$.

Properties of $\tilde{B}$ and VI

Property (Meilă (2007))

Both VI and $\tilde{B}$ are metrics on the space of partitions that satisfy,

i) *if* $\mathbf{c} \geq \widehat{\mathbf{c}} \geq \widehat{\widehat{\mathbf{c}}}$, *then*

$$d(\mathbf{c}, \widehat{\widehat{\mathbf{c}}}) = d(\mathbf{c}, \widehat{\mathbf{c}}) + d(\widehat{\mathbf{c}}, \widehat{\widehat{\mathbf{c}}}).$$

ii) *for any* $\mathbf{c}, \widehat{\mathbf{c}}$,

$$d(\mathbf{c}, \widehat{\mathbf{c}}) = d(\mathbf{c}, \widehat{\mathbf{c}} \wedge \mathbf{c}) + d(\widehat{\mathbf{c}}, \widehat{\mathbf{c}} \wedge \mathbf{c}).$$

Comparison of $\tilde{\mathrm{B}}$ and VI

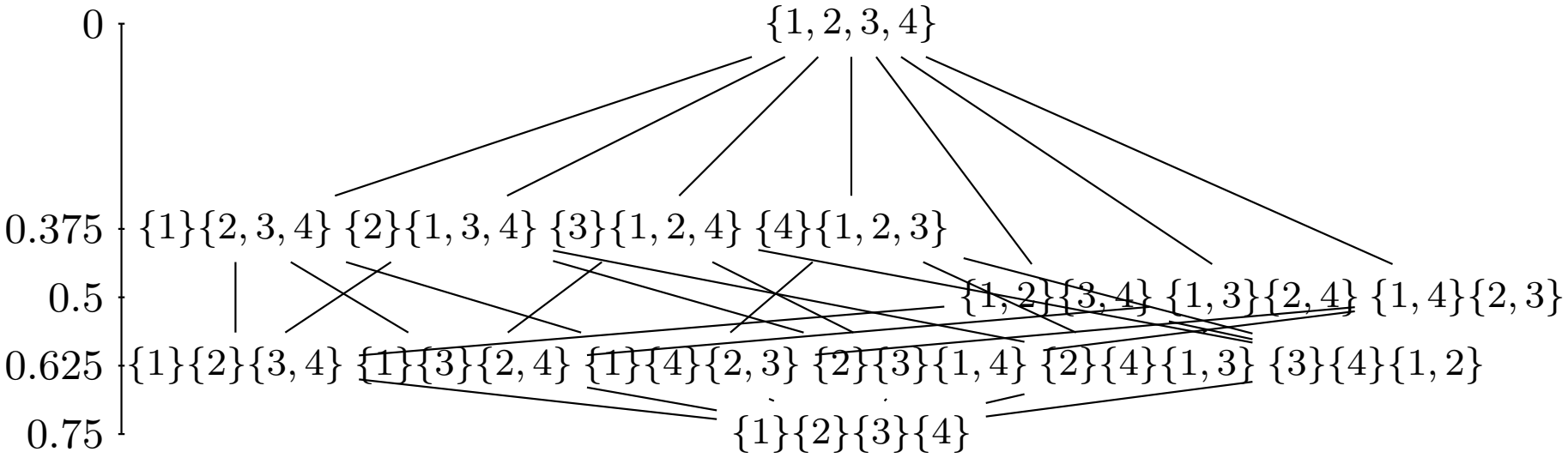


Figure: Hasse diagram stretched by $\tilde{\mathrm{B}}$ with a sample of size $N = 4$.

Comparison of $\tilde{\mathrm{B}}$ and VI

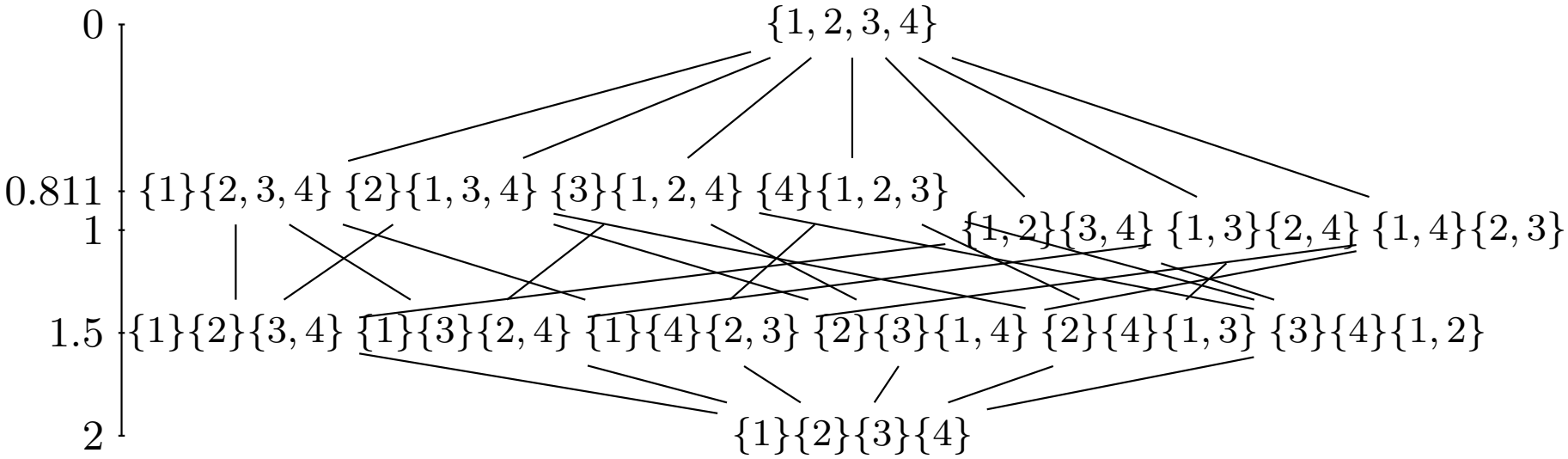


Figure: Hasse diagram stretched by VI with a sample of size $N = 4$. Note $2 - \frac{3}{4}\log(3) \approx 0.811$

Comparison of $\tilde{B}$ and VI

Property

Suppose N is divisible by k, and let $\mathbf{c}_k$ denote a partition with k clusters of equal size N/k.

$$\tilde{B}(\mathbf{1}, \mathbf{c}_k) = 1 - \frac{1}{k} > \frac{1}{k} - \frac{1}{N} = \tilde{B}(\mathbf{0}, \mathbf{c}_k).$$

$$VI(\mathbf{1}, \mathbf{c}_k) = \log(k) \leq \log(N) - \log(k) = VI(\mathbf{0}, \mathbf{c}_k), \quad \text{for } k \leq \sqrt{N},$$

and

$$VI(\mathbf{1}, \mathbf{c}_k) = \log(k) \geq \log(N) - \log(k) = VI(\mathbf{0}, \mathbf{c}_k), \quad \text{for } k \geq \sqrt{N}.$$

Comparison of $\tilde{B}$ and VI

Property

Suppose N is an even and square integer. Then, the partitions with two clusters of sizes $n = \frac{1}{2}(N - \sqrt{N})$ and $N - n$ are equally distance from $\mathbf{1}$ and $\mathbf{0}$ under $\tilde{B}$.

Point estimate under VI

Under the VI, the optimal partition $\mathbf{c}^*$ is

$$\begin{aligned}\underset{\widehat{\mathbf{c}}}{\operatorname{argmin}} \sum_{n=1}^{N} \log(1 + \sum_{n' \neq n} \mathbf{1}(\widehat{c}_{n'} = \widehat{c}_n)) \\ - 2 \sum_{n=1}^{N} \mathsf{E}[\log(1 + \sum_{n' \neq n} \mathbf{1}(c_{n'} = c_n)\mathbf{1}(\widehat{c}_{n'} = \widehat{c}_n)) | \mathcal{D}],\end{aligned} \tag{1}$$

To reduce computations, we can swap the log and expectation:

$$\begin{aligned}\underset{\widehat{\mathbf{c}}}{\operatorname{argmin}} \sum_{n=1}^{N} \log(1 + \sum_{n' \neq n} \mathbf{1}(\widehat{c}_{n'} = \widehat{c}_n)) \\ - 2 \sum_{n=1}^{N} \log(1 + \sum_{n' \neq n} P(c_{n'} = c_n | \mathcal{D})\mathbf{1}(\widehat{c}_{n'} = \widehat{c}_n)).\end{aligned} \tag{2}$$

Note: from Jensen's inequality, (2) provides a lower bound to (1).

Greedy search algorithm

Greedy search algorithm based on the Hasse diagram:

- For $i = 1, \ldots I$
  - Find the L closest partitions that cover $\widehat{\mathbf{c}}$ and the L closest partitions that $\widehat{\mathbf{c}}$ covers.
  - Compute $\mathsf{E}[L(\mathbf{c}, \widehat{\widehat{\mathbf{c}}})|\mathcal{D}]$ for all $2L$ partitions and select the partition $\mathbf{c}'$ with minimal $\mathsf{E}[L(\mathbf{c}, \mathbf{c}')|\mathcal{D}]$.
  - If $\mathsf{E}[L(\mathbf{c}, \mathbf{c}')|\mathcal{D}] < \mathsf{E}[L(\mathbf{c}, \widehat{\mathbf{c}})|\mathcal{D}]$, set $\widehat{\mathbf{c}} = \mathbf{c}'$. Otherwise, STOP.
- end

Credible balls

Credible ball around $\mathbf{c}^*$ of level $1-\alpha$, $\alpha \in [0,1]$:

$$B_{\epsilon^*}(\mathbf{c}^*) = \{\mathbf{c} : d(\mathbf{c}^*, \mathbf{c}) \leq \epsilon^*\},$$

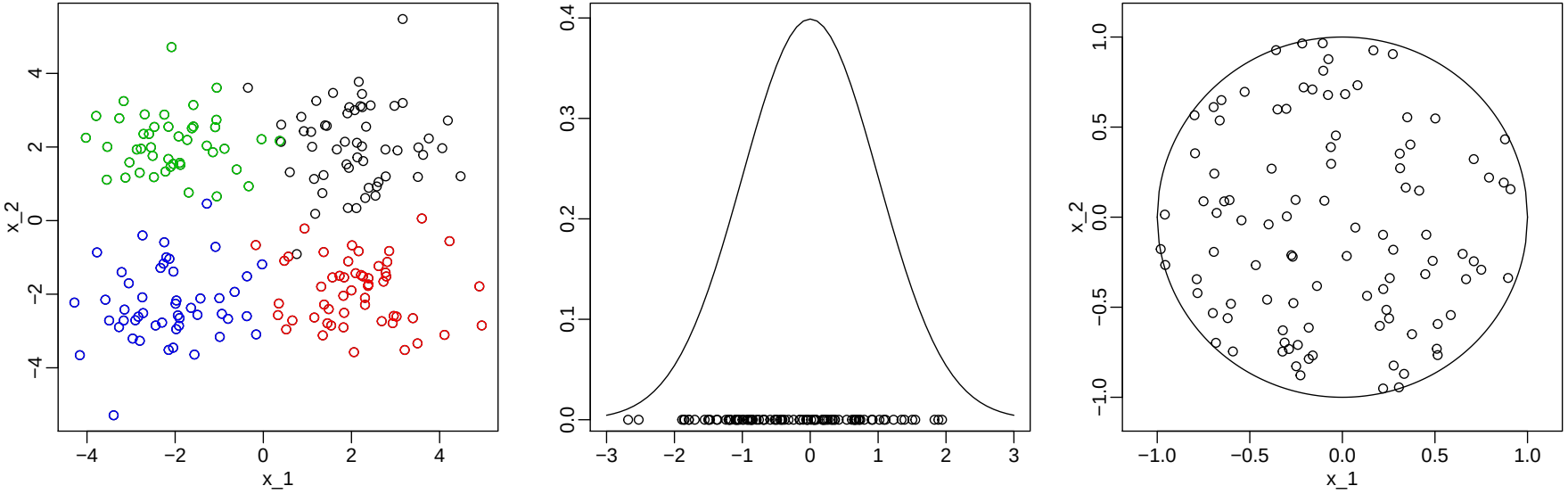
where ϵ^* is the smallest $\epsilon \geq 0$ such that

$$P(B_\epsilon(\mathbf{c}^*)|\mathcal{D}) \geq 1-\alpha.$$

- We can estimate ϵ^* from MCMC.
- To summarize the credible ball, we report the *vertical* and *horizontal bounds*:
  - **Vertical upper bounds:** partitions with the smallest number of clusters which are most distant from $\mathbf{c}^*$.
  - **Vertical lower bounds:** partitions with the largest number of clusters which are most distant from $\mathbf{c}^*$.
  - **Horizontal bounds:** partitions which are most distant from $\mathbf{c}^*$.

Outline

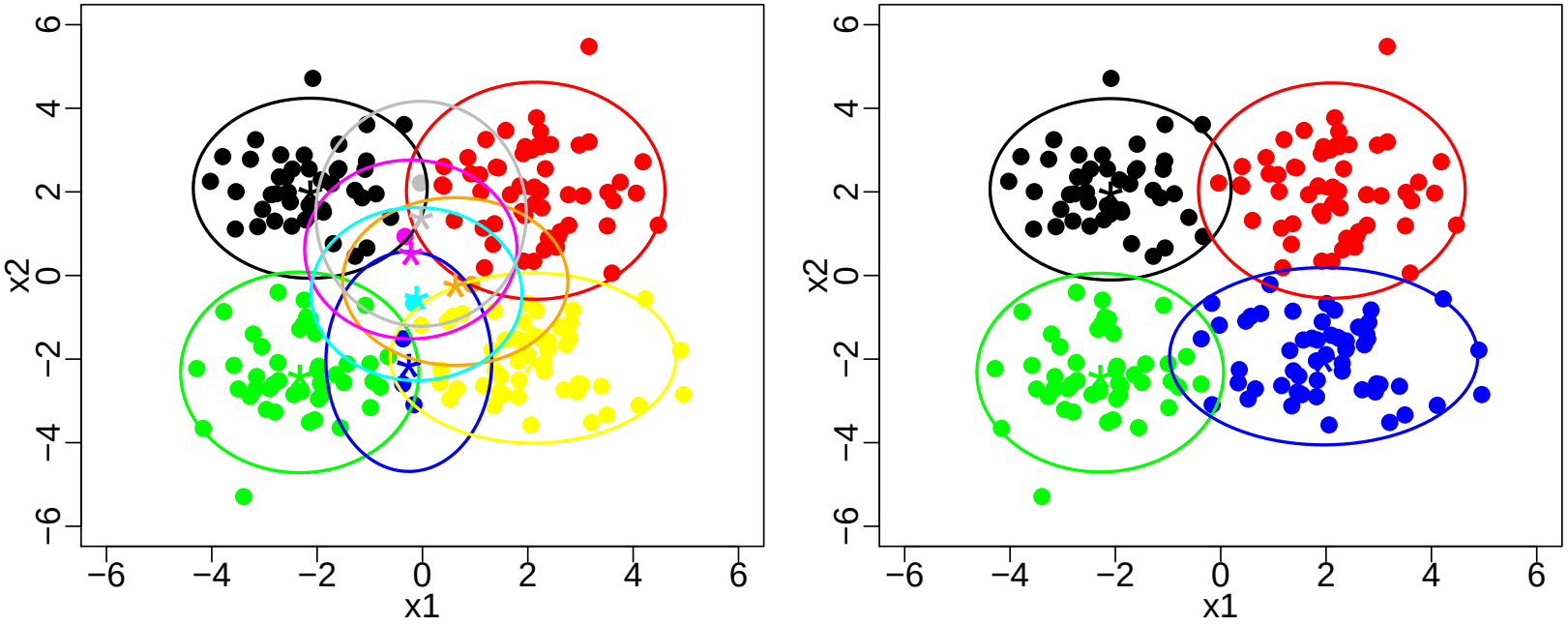
Simulated Examples



(a) Ex 1: 4 clusters (b) Ex Miller: 1 clusters (c) Ex Rajkowski: 1 clusters

Figure: Simulated scenarios: 1) mixture of 4 bivariate Gaussians (W. and Ghahramani (2018)); 2) standard normal (Miller and Harrison (2013)); 3) uniform within the unit circle (Rajkowski (2019)). Perform MCMC inference for a DPM.

Simulated Example: $N = 200$



(a) $\tilde{\mathrm{B}}$: 9 clusters

(b) VI: 4 clusters

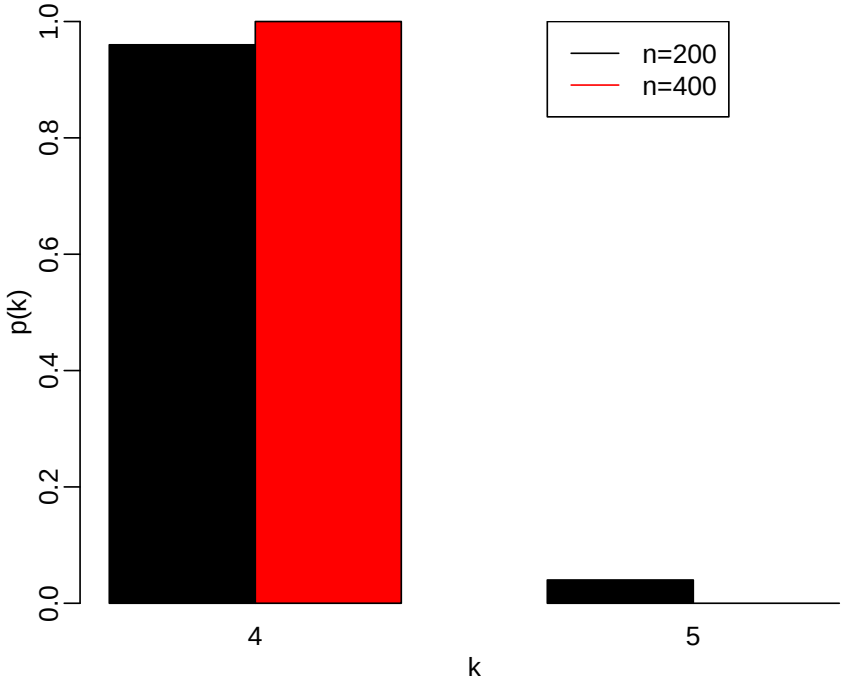
Figure: Point estimate of the clustering from a DPM.

Simulated Example: increasing N

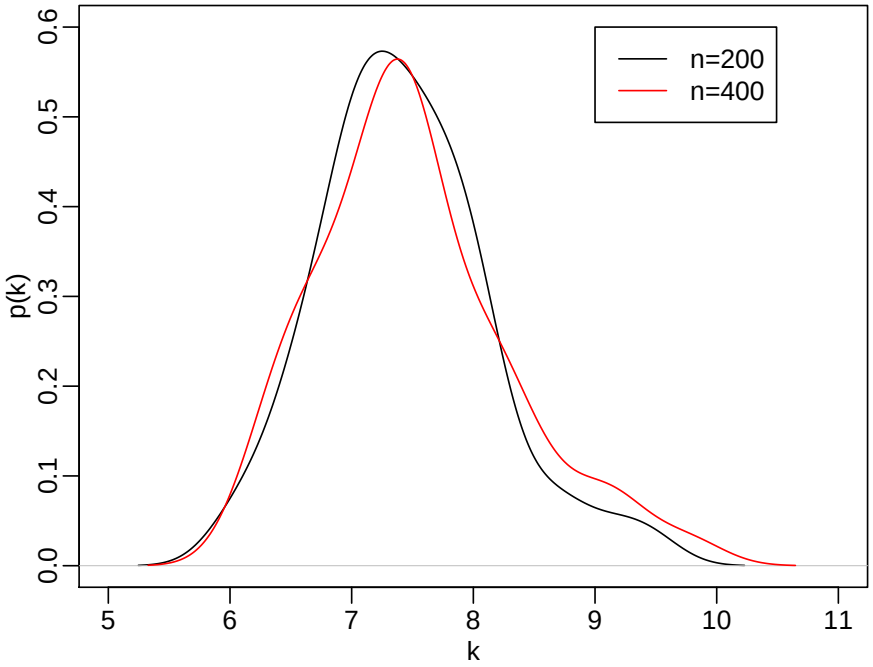
Ex 1	Loss	k_N^*	p_I	$\tilde{\mathrm{B}}(\mathbf{c}_t, \mathbf{c}^*)$	$\mathrm{VI}(\mathbf{c}_t, \mathbf{c}^*)$
$N = 200$:	$\tilde{\mathrm{B}}$	9	0.065	0.045	0.643
	VI	**4**	**0.045**	**0.044**	**0.569**
$N = 400$:	$\tilde{\mathrm{B}}$	17	0.0775	0.052	0.769
	VI	**4**	**0.045**	**0.044**	**0.54**
$N = 800$:	$\tilde{\mathrm{B}}$	24	0.0775	0.061	0.903
	VI	**4**	**0.0587**	**0.056**	**0.742**
$N = 1600$:	$\tilde{\mathrm{B}}$	41	0.0581	**0.044**	0.719
	VI	**4**	**0.0294**	0.045	**0.629**

Table: Comparison in terms of 1) number of clusters k_N^*; 2) proportion of data points incorrectly classified p_I; 3) $\tilde{\mathrm{B}}$ between the optimal and true clusterings; and 4) VI between the optimal and true clusterings.

Simulated Example: 100 repetitions



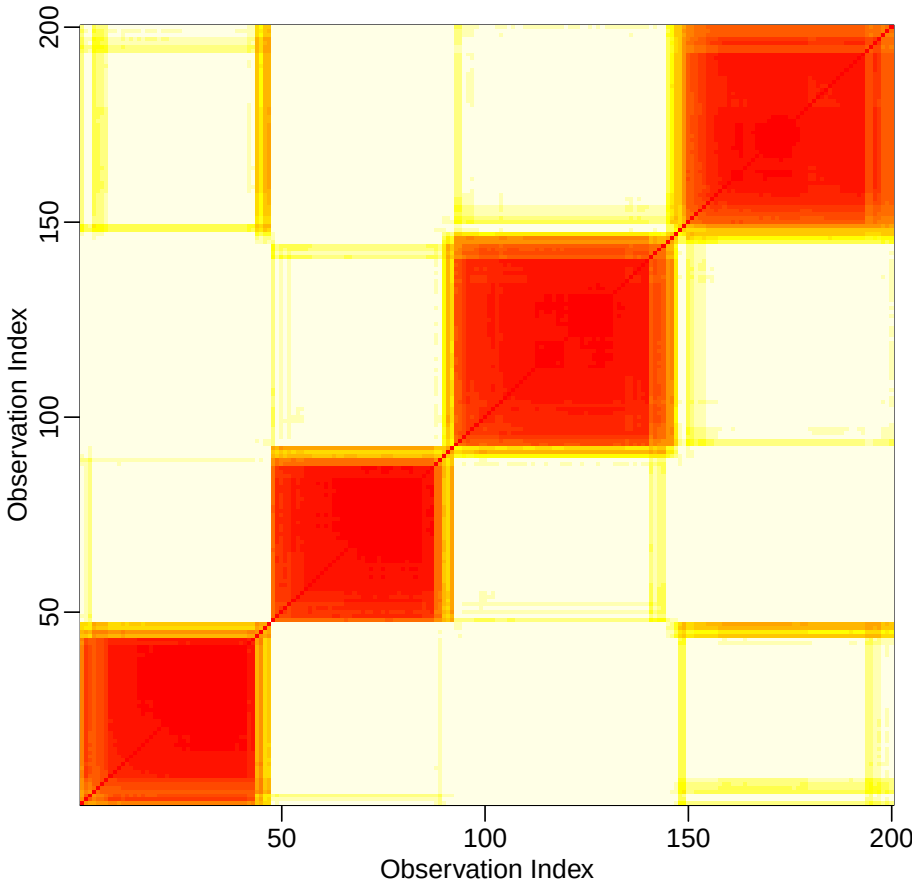
(a) VI estimate of k



(b) Posterior mean of k

Figure: (a) Distribution of $\widehat{k}$ from the VI clustering estimate and (b) (kernel) estimated density of the posterior mean k, across simulations.

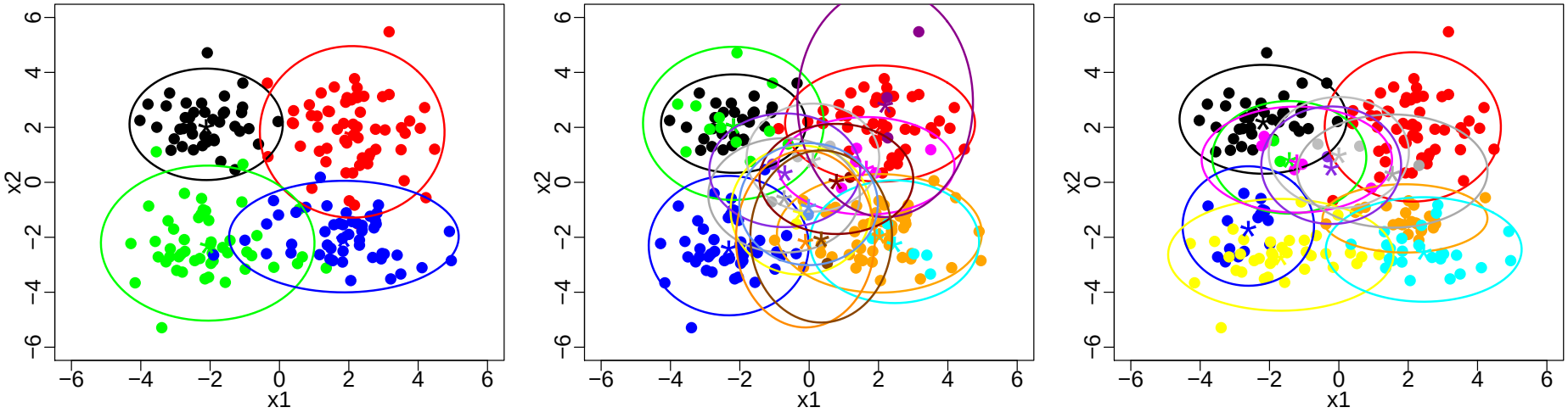
Simulated Example: $N = 200$



(a) Example 1

Figure: Posterior similarity matrix.

Simulated Example: $N = 200$



(a) VI upper vertical bound: 4 clusters

(b) VI lower vertical bound: 16 clusters

(c) VI horizontal bound: 7 clusters

Figure: 95% VI credible ball.

Simulated Example: 100 repetitions

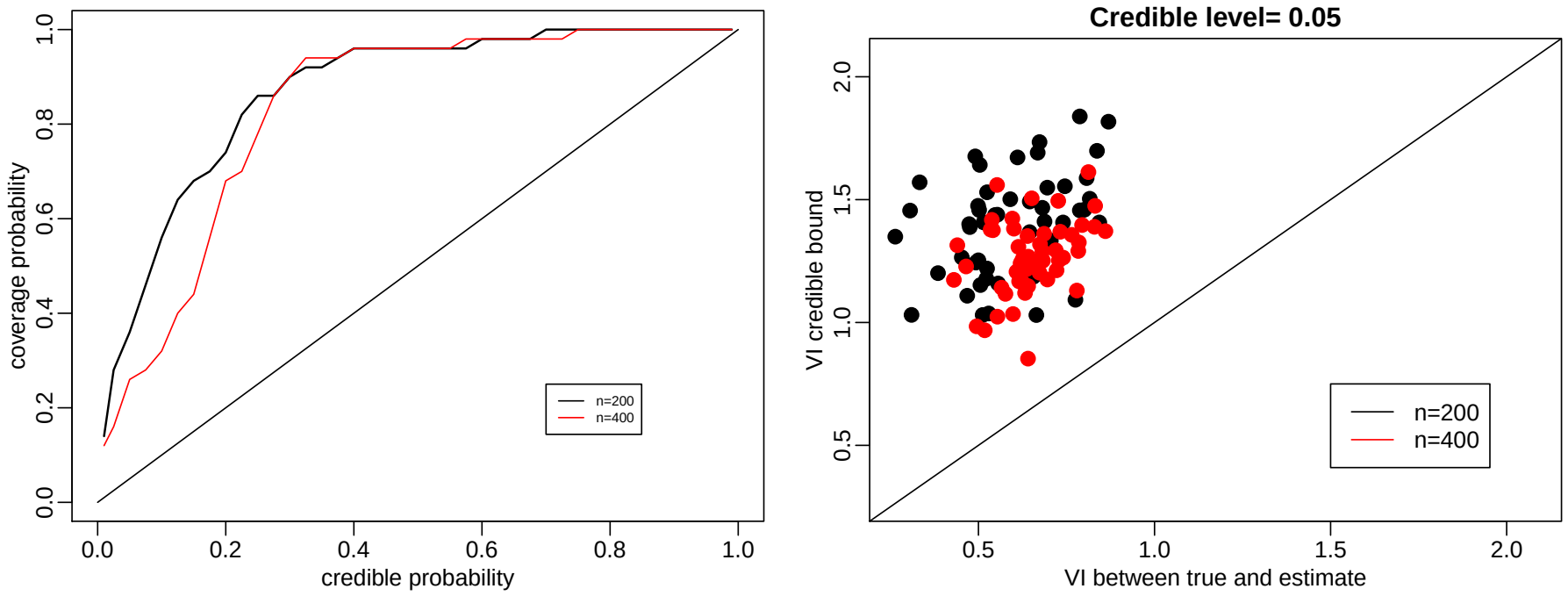
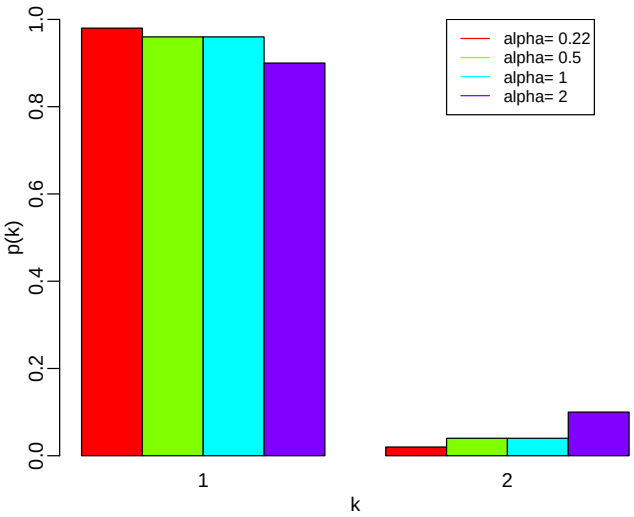
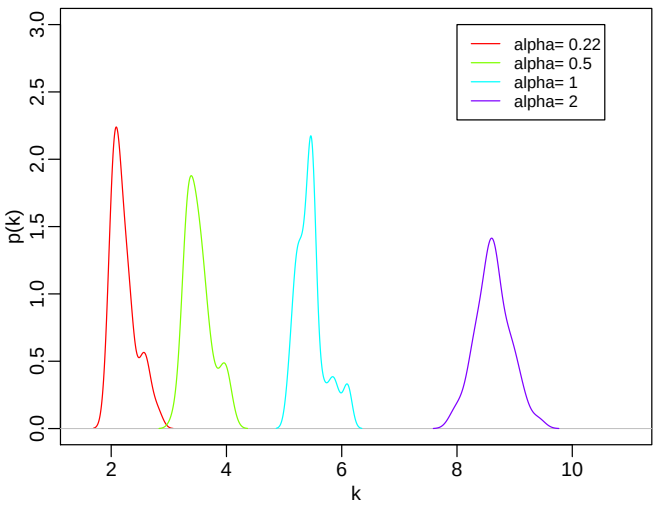


Figure: Coverage probability as a function of credible probability for the VI credible balls.

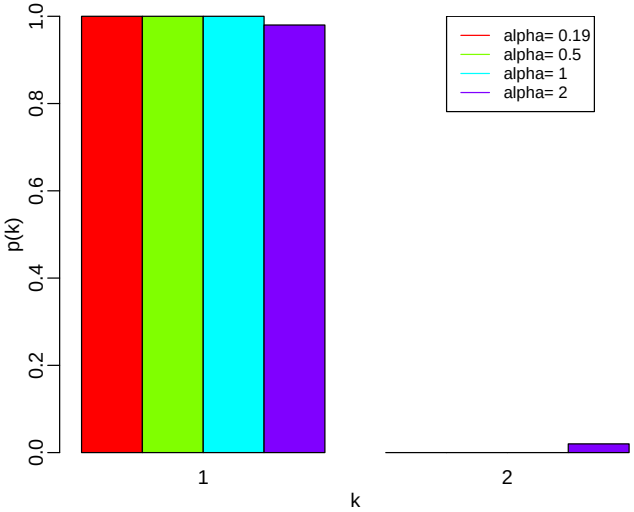
Miller & Harrison (2013) Example: 50 repetitions



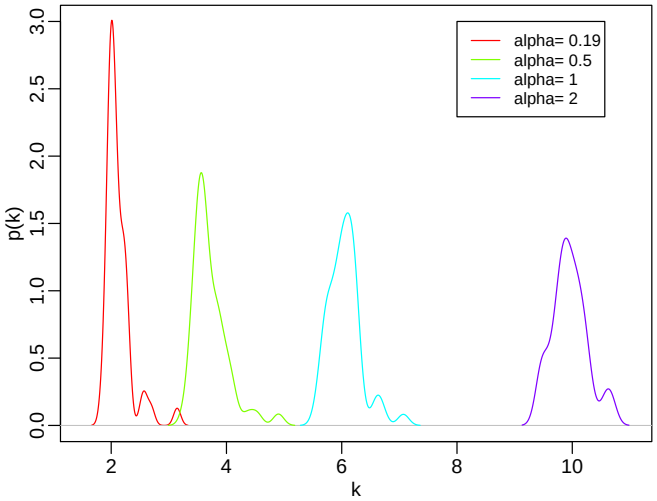
(a) VI partition: $N = 100$



(b) Post. mean of k: $N = 100$

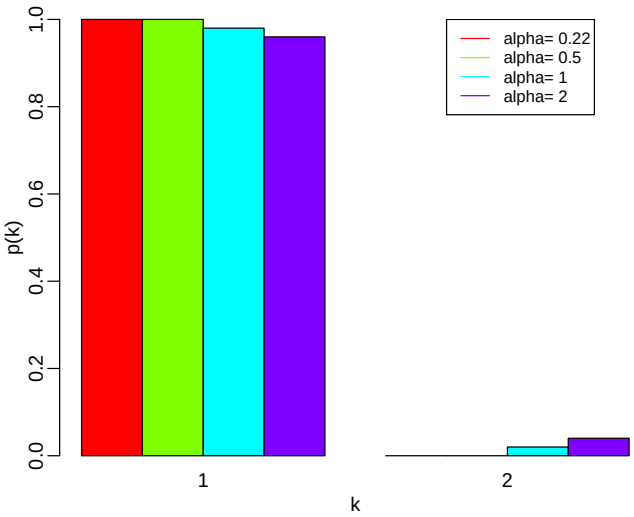


(c) VI partition: $N = 200$

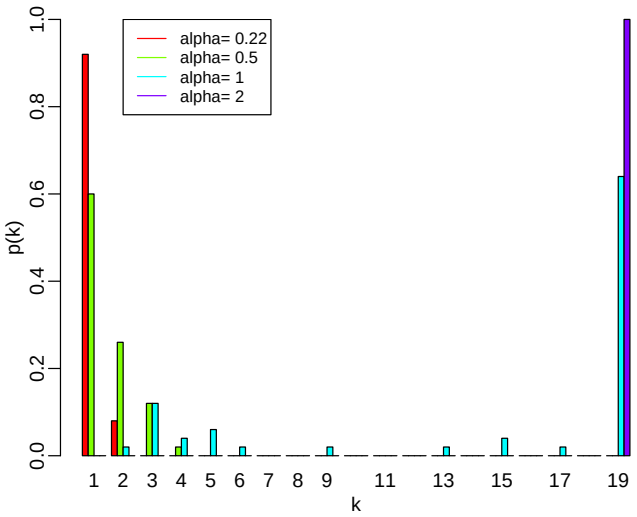


(d) Post. mean of k: $N = 200$

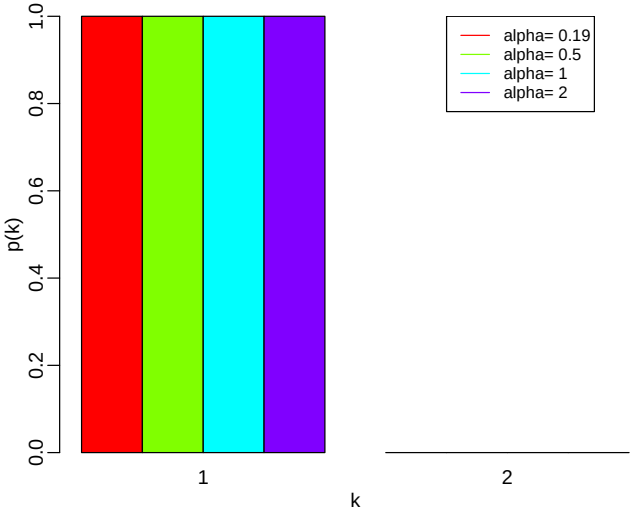
Miller & Harrison (2013) Example: 50 repetitions



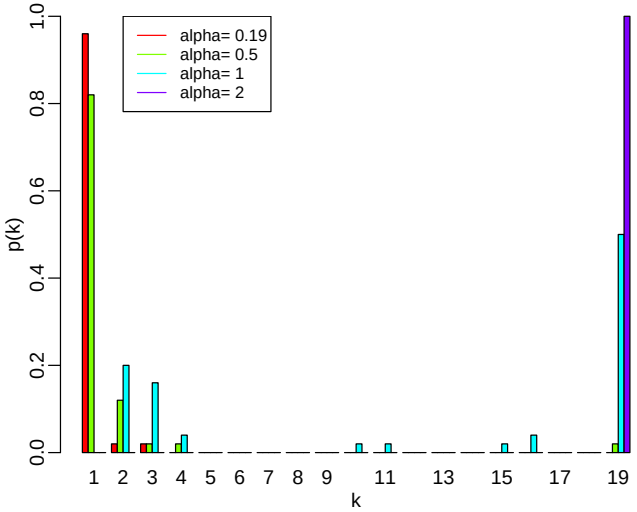
(e) MAP partition: $N = 100$



(f) Binder partition: $N = 100$

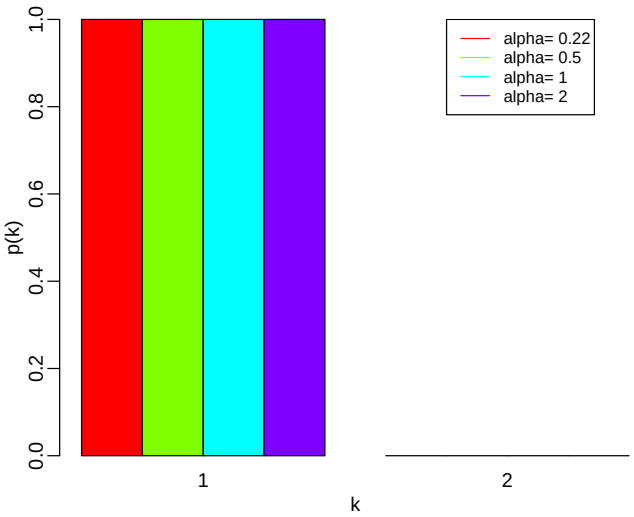


(g) MAP partition: $N = 200$

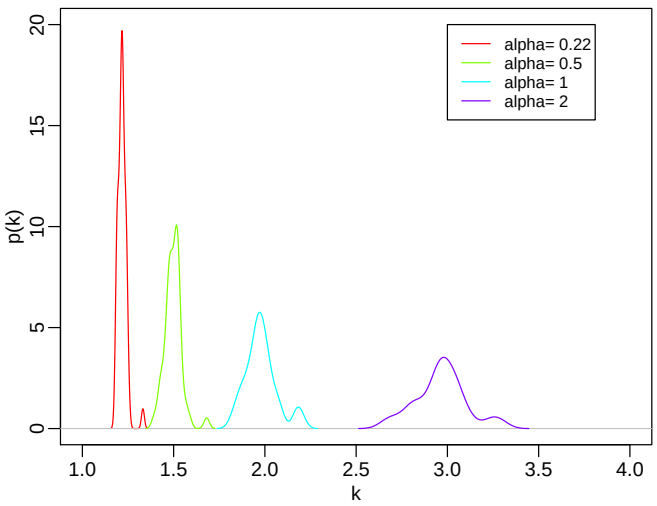


(h) Binder partition: $N = 200$

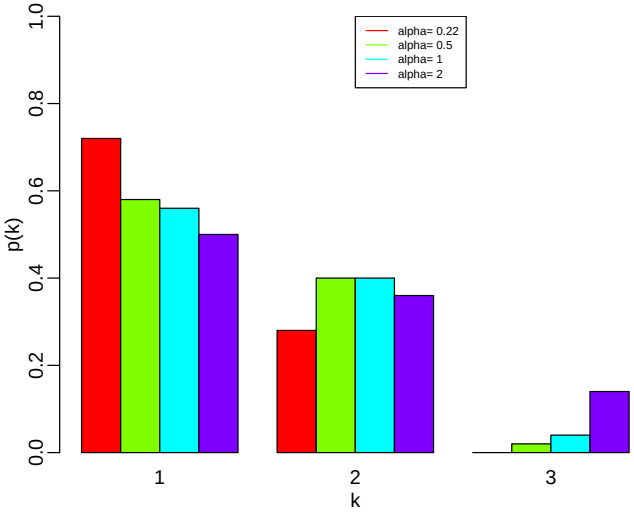
Rajkowski (2019) Example: 50 repetitions



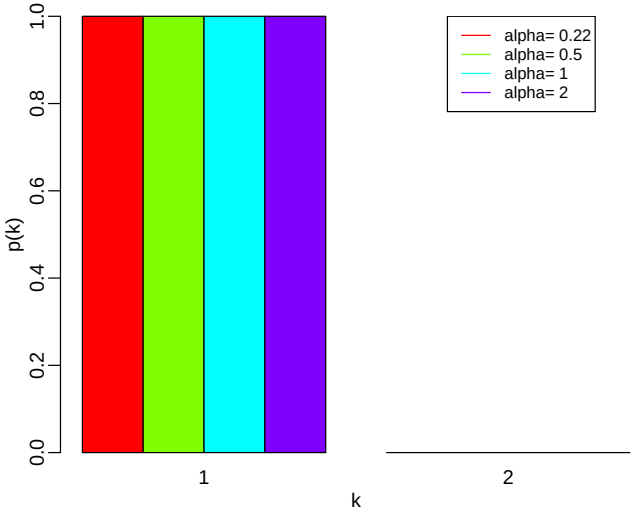
(i) VI partition: $N = 100$



(j) Post. mean of k: $N = 100$



(k) MAP partition: $N = 100$



(l) Binder partition: $N = 100$

Outline

Summary and Future Work

Summary:

- Developed summary tools for Bayesian cluster analysis:
  - point estimate through minimization of VI,
  - credible balls to describe uncertainty around estimate.
- Available in **R** package 'mcclust.ext' and **R** package 'sdols'. Alternative algorithms in Friel and Rastelli (2018) that are linear in N **R** package 'GreedyEPL'.
- Marginally focusing on the number of clusters may be misleading $\rightarrow$ estimate the clustering directly if it is the object of interest.

Future work:

- Extend to feature allocation analysis.
- Asymptotic study of the VI clustering estimate and coverage of the credible balls.
- Fast estimate of VI clustering estimate, avoiding MCMC.

Thanks!

https://projecteuclid.org/euclid.ba/1508378464
https://github.com/sarawade/mcclust.ext

We are grateful to all discussants for the their thoughtful comments and contributions.