Bayesian Model Based Clustering Procedures

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Abstract

This paper establishes a general framework for Bayesian model-based clustering, in which subset labels are exchangeable, and items are also exchangeable, possibly up to covariate effects. It is rich enough to encompass a variety of existing procedures, including some recently discussed methodologies involving stochastic search or hierarchical clustering, but more importantly allows the formulation of clustering procedures that are optimal with respect to a specified loss function. Our focus is on loss functions based on pairwise coincidences, that is, whether pairs of items are clustered into the same subset or not.

Optimisation of the posterior expected loss function can be formulated as a binary integer programming problem, which can be readily solved, for example by the simplex method, when clustering a modest number of items, but quickly becomes impractical as problem scale increases. To combat this, a new heuristic item-swapping algorithm is introduced. This performs well in our numerical experiments, on both simulated and real data examples. The paper includes a comparison of the statistical performance of the (approximate) optimal clustering with earlier methods that are model-based but ad hoc in their detailed definition.

Some key words: Dirichlet process, Hierarchical clustering, Loss functions, Stochastic search.

1 Introduction

Clustering methods aim to separate a heterogeneous collection of items into homogeneous subsets, and are an important tool in scientific investigations in many different domains. There is a particular focus of activity in recent years, as biologists have become interested in clustering high-dimensional data generated by modern high-throughput assay techniques: for example, in order to cluster genes on the basis of gene expression measurements from microarrays. With the rapid growth in availability of computer power, Bayesian statisticians have become able to implement principled computer-intensive inferential methods for clustering, based for example on mixture models [see Fraley and

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Raftery (2002), Medvedovic and Sivaganesan (2002), Medvedovic et al. (2004), Yeung et al. (2001), etc.].

In a Bayesian formulation of a clustering procedure, the partition of items into subsets becomes a parameter of a probability model for the data, subject to prior assumptions, and inference about the clustering derives from properties of the posterior distribution. There are the usual opportunities for simultaneous inference about the partition and other parameters, characterising the cluster locations and spreads, for example, but our principal focus in this paper is the partition itself. In contrast to most other unknowns in a Bayesian model, where the posterior mean provides an often adequate default choice of point estimator, there is no simple natural choice for an estimator of a partition. Unlike the case of classical approaches, such as hierarchical clustering and K-means clustering procedures, Bayesian alternatives seem not to be fully developed. Medvedovic and Sivaganesan (2002) and Medvedovic et al. (2004) generate a sample of partitions based on the kernel mixture of Dirichlet process model and employ classical traditional procedures [see Gordon (1999)] to define a 'best' partition.

A loss function approach allows us to remove this arbitrariness, and deliver an objective procedure. Binder (1978, 1981) has discussed loss functions for Bayesian clustering, although many of his choices are not appropriate for our setting, as we wish to respect exchangeability *a priori* in the labelling of clusters and of items. We therefore concentrate on loss functions defined on pairwise *coincidences*. We penalise pairs of items that are assigned to different clusters when they should be in the same one, and vice versa; the total loss is obtained by summing over all pairs. The resulting posterior expected loss is a simple linear function of posterior marginal coincidence probabilities (that is, for each pair the posterior probability they are clustered together), which are readily estimated from a Markov chain Monte Carlo (MCMC) simulation from the posterior.

We show in Section 4 that optimisation of this expected loss is a binary integer programming problem. Standard techniques such as the simplex method are far too slow for practical use for large numbers n of items (say of the order of 1000), since the size of the integer program grows rapidly (the numbers of constraints as n^3, and of variables as n^2), and so approximations are required.

Our methods are illustrated on both simulated and real data sets. The simulated data are generated from bivariate normal mixtures with from one to four components. The real data used are the galaxy data from Roeder (1990), and gene expression data from a leukaemia study reported in Golub et al. (1999).

2 Bayesian Clustering Models

A partition $\mathbf{p}$ separates n items with observed responses $\mathbf{y} = \{\mathbf{y}_1, \ldots, \mathbf{y}_n\}$ into subsets. Such a partition is represented as $\{C_1, \ldots, C_{n(\mathbf{p})}\}$ where C_j denotes the jth subset or cluster, for $j = 1, \ldots, n(\mathbf{p})$. Each C_j contains indices of the items in that cluster, and the positive integer $n(\mathbf{p})$ denotes the number of clusters, which depends of course on the partition. There is a positive number

e_j of items in each cluster j. Given the partition $\mathbf{p}$ of items, a model for the data is defined as

$$\pi\left(\mathbf{y}\,|\mathbf{p}\,\right) = \prod_{j=1}^{n(\mathbf{p})} m\left(\{\mathbf{y}_i, i \in C_j\}\right) = \prod_{j=1}^{n(\mathbf{p})} m(\mathbf{y}_{C_j}), \tag{1}$$

say, where $m(\mathbf{y}_{C_j})$ is the joint distribution of the responses for items in cluster C_j. We preserve exchangeability across cluster labels and item indexing by requiring this function to not depend on j, and, typically, to be an exchangeable function of its arguments $\{\mathbf{y}_i, i \in C_j\}$. Since we also wish to perform clustering in the presence of covariate information $\{\mathbf{x}_i, i = 1, 2, \ldots, n\}$ on the items, we allow $m(\mathbf{y}_{C_j})$ to depend tacitly on $\{\mathbf{x}_i, i \in C_j\}$, and exchangeability over items then relates to permuting $(\mathbf{y}_i, \mathbf{x}_i)$ pairs jointly.

Typically, we suppose

$$m\left(\mathbf{y}_{C_j}\right) = \int_{\mathcal{U}} \prod_{i \in C_j} k\left(\mathbf{y}_i \mid u_j\right) G_0\left(du_j\right) \quad \text{or} \quad \int_{\mathcal{U}} \prod_{i \in C_j} k\left(\mathbf{y}_i \mid u_j; \mathbf{x}_i\right) G_0\left(du_j\right) \tag{2}$$

and $k\left(\mathbf{y}_i\,|u_j\,\right)$ is a density for $\mathbf{y}_i$s with parameters/latent variables u_j and G_0 is a distribution function of u_j on the space $\mathcal{U}$.

Equation (2), which guarantees the required exchangeability properties, may be viewed either as a formal representation [de Finetti (1930, 1974), Hewitt and Savage (1955) and Diaconis and Freedman (1984, 1987)], or as an ingredient in the specification of a Bayesian hierarchical model, in which clusters are assigned characterising parameters u_j, i.i.d. from distribution G_0, and item responses within clusters drawn independently from distribution $k\left(\mathbf{y}_i \mid u_j\right)$ or $k\left(\mathbf{y}_i \mid u_j; \mathbf{x}_i\right)$.

In the full Bayesian formulation, a prior probability would be assigned to each partition $\mathbf{p}$, leading to a posterior of the form

$$\pi\left(\mathbf{p} \mid \mathbf{y}\right) \propto \phi\left(\mathbf{p}\right) = \pi\left(\mathbf{p}\right) \prod_{j=1}^{n(\mathbf{p})} m\left(\mathbf{y}_{C_j}\right) \tag{3}$$

[References include Hartigan(1990), Barry and Hartigan (1992), and Quintana and Iglesias (2003), they call it as a product partition model ($\mathcal{PPM}$). See also Brunner and Lo (1999) and Lo (2005)]

Of key importance to practical inference in this model setting is the question whether $m(\mathbf{y}_{C_j})$ is explicitly known or not. When it is, MCMC procedures are greatly simplified, since cluster-specific parameters u_j can be integrated out, and the posterior distribution of $\mathbf{p}$ alone (or possibly $\mathbf{p}$ together with a few hyperparameters) can be the target of an MCMC sampler. For the remainder of this paper, we will suppose that $m(\mathbf{y}_{C_j})$ is explicitly available: in the context of (2) this amounts to assuming that G_0 is conjugate for the density $k(\mathbf{y}_i \mid \cdot)$.

2.1 The prior part of the clustering model

In the absence of real prior information about the items, we will assign positive prior probability to every possible partition. In the interests of computational convenience, we might be attracted to prior models for which posterior simulation methods are fully developed, and this leads us to models based on random probability measures. The Ferguson (1973) Dirichlet process [see also Antoniak (1974)] is a popular choice, suggested by Lo (1984). Recently, Ishwaran and James (2001, 2003a, 2003b) employ stick breaking random probability measures, including Kingman–Pitman–Yor Poisson–Dirichlet process, as a prior for the kernel mixture model. Another familiar example is the finite mixture model with κ components, and a symmetric Dirichlet distribution with parameters $(\delta, \delta, \ldots, \delta)$ on the component weights; this yields an explicit prior on the partition when the weights are integrated out. For these models, the corresponding $\pi(\mathbf{p})$s are

Random Probability Measures	Parameters	$\pi(\mathbf{p}) \propto$
Dirichlet Process	$\theta > 0$	$\theta^{n(\mathbf{p})} \prod_{j=1}^{n(\mathbf{p})} \Gamma(e_j)$
Finite mixture model, Dirichlet weights	κ,$\delta > 0$	$\frac{\kappa!}{(\kappa - n(\mathbf{p}))!} \prod_{j=1}^{n(\mathbf{p})} \frac{\Gamma(\delta + e_j)}{\Gamma(\delta)}$
Poisson–Dirichlet Process	$\theta > -\alpha, 0 \leq \alpha < 1$	$\prod_{j=1}^{n(\mathbf{p})} \left[(\theta + \alpha(j-1)) \frac{\Gamma(e_j - \alpha)}{\Gamma(1-\alpha)} \right]$

James (2002, 2005) considers more general construction of kernel mixture of some classes of random probability measures. James et al. (2005) and Lijoi et al. (2005) discuss kernel mixture of normalized random measures. For more random probability measures, we can consult Kingman (1975, 1993), Pitman (1995, 1996, 2003) as well as Pitman and Yor (1997).

In fact, however, in the conjugate setting, posterior simulation is equally straightforward for much wider classes of prior, and all that is needed for implementation is the ratio of prior probabilities $\pi(\mathbf{p}')/\pi(\mathbf{p})$ when $\mathbf{p}'$ is obtained from $\mathbf{p}$ by re-assigning a single item. Thus, given prior information, we are free to assign prior probabilities $\pi(\mathbf{p})$ to suit the situation; the procedures discussed in this paper will still work for most choices.

2.2 The data part of the clustering model

We discuss two kinds of model (2). One of them follows standard Bayesian modelling lines, taking the density k of (2) to be normal with unknown mean and unknown variance/precision, and G_0 as the (Normal–Gamma) parameter prior. Then $m(\mathbf{y}_{C_j})$ will be a t-density. For the other kind of model, we directly assign $m(\mathbf{y}_{C_j})$ to be an exchangeable density of $\mathbf{y}_{C_j}$. This can be a convenient way to proceed, and also allows us to make connections with the classical theory of clustering.

Normal–Gamma set up. Motivated by application to clustering gene expression profiles, we discuss a regression type model that expresses a vector response in terms of a linear combination of known covariates. We take $\mathbf{y}_i$ as a vector, written as $\mathbf{y}_i = [y_{i1} \cdots y_{iS}]'$ for $i = 1, \ldots, n$. Given the covariates $\mathbf{x}_s = [x_{s1} \cdots x_{sK}]'$ and the cluster j, the parameters/latent variables are $\boldsymbol{\beta}_j = [\beta_{j1} \cdots \beta_{jK}]'$

and τ_j. The regression part of the model can be written as

$$\mathbf{y}_i = \begin{bmatrix} y_{i1} \\ \vdots \\ y_{iS} \end{bmatrix} = \sum_{k=1}^{K} \beta_{jk} \begin{bmatrix} x_{1k} \\ \vdots \\ x_{Sk} \end{bmatrix} + \begin{bmatrix} \epsilon_{j1} \\ \vdots \\ \epsilon_{jS} \end{bmatrix} = [\mathbf{x}_1 \cdots \mathbf{x}_S]' \boldsymbol{\beta}_j + \boldsymbol{\epsilon}_j \tag{4}$$

where $\boldsymbol{\epsilon}_j \sim N\left(\mathbf{0}_{S\times 1}, \tau_j^{-1}\mathbf{I}_{S\times S}\right)$. where $\mathbf{0}_{S\times 1}$ is the S-dimensional zero vector and $\mathbf{I}_{S\times S}$ is the $S \times S$ identity matrix. The covariates $[\mathbf{x}_1 \cdots \mathbf{x}_S]'$ are fixed and observed, and may as usual include dummy covariates for factor levels. It could be an identity matrix (when $K = S$). From (4), $\mathbf{y}_i$ follows a multivariate Normal density with mean $\boldsymbol{\beta}_j$ and variance $\tau_j^{-1}\mathbf{I}_{S\times S}$. Writing $u_j = \left(\boldsymbol{\beta}_j, \tau_j\right)$, the kernel is represented as $k\left(\mathbf{y}_i \left|\boldsymbol{\beta}_j, \tau_j\right.\right)$, a multivariate normal density, $N\left([\mathbf{x}_1 \cdots \mathbf{x}_S]' \boldsymbol{\beta}_j, \tau_j^{-1}\mathbf{I}_{S\times S}\right)$. To complete the normal set up, given τ_j, $\boldsymbol{\beta}_j$ follows the K-dimensional multivariate normal with mean $\mathbf{m}_0$ and variance $\left(\tau_j \mathbf{t}_0\right)^{-1}$, and τ_j follows the univariate Gamma with shape a_0 and scale b_0. We denote the joint distribution $G_0(d\boldsymbol{\beta}_j, d\tau_j)$ as a joint Gamma–Normal distribution, Gamma–Normal $(a_0, b_0, \mathbf{m}_0, \mathbf{t}_0)$. Based on the set up, we have

$$m\left(\mathbf{y}_{C_j}\right) = \frac{\Gamma\left(\dfrac{2a_0 + e_j S}{2}\right)}{\Gamma\left(\dfrac{2a_0}{2}\right)} \frac{\left|\dfrac{b_0}{a_0}\left(\mathbf{X}_{C_j}\mathbf{t}_0^{-1}\mathbf{X}_{C_j}' + \mathbf{I}_{e_jS\times e_jS}\right)\right|^{-1/2}}{\left(2a_0\pi\right)^{e_jS/2}} \tag{5}$$
$$\times \left(1 + \frac{1}{2a_0}\left(\mathbf{y}_{C_j} - \mathbf{X}_{C_j}\mathbf{m}_0\right)' \left(\frac{b_0}{a_0}\left(\mathbf{X}_{C_j}\mathbf{t}_0^{-1}\mathbf{X}_{C_j}' + \mathbf{I}_{e_jS\times e_jS}\right)\right)^{-1} \left(\mathbf{y}_{C_j} - \mathbf{X}_{C_j}\mathbf{m}_0\right)\right)^{-(2a_0+e_jS)/2}$$

where $\mathbf{y}_{C_j} = \left[\mathbf{y}_{i_1}' \cdots \mathbf{y}_{i_{e_j}}'\right]'$ and $\mathbf{X}_{C_j} = [[\mathbf{x}_1 \cdots \mathbf{x}_S] \cdots [\mathbf{x}_1 \cdots \mathbf{x}_S]]'$ for $C_j = \left\{i_1, \ldots, i_{e_j}\right\}$. Note that $\mathbf{y}_{C_j}$ is a e_jS vector and $\mathbf{X}_{C_j}$ is a $e_jS \times K$ matrix. Moreover, $m\left(\{\mathbf{y}_i, i \in C_j\}\right)$ is a multivariate t density with mean $\mathbf{X}_{C_j}\mathbf{m}_0$, scale $\dfrac{b_0}{a_0}\left(\mathbf{X}_{C_j}\mathbf{t}_0^{-1}\mathbf{X}_{C_j}' + \mathbf{I}_{e_jS\times e_jS}\right)$ and degree of freedom $2a_0$.

Directly assigned marginals approach. Alternatively, we can directly assign $m\left(\mathbf{y}_{C_j}\right)$ to be some exchangeable (symmetric) function, that is non-negative and integrable. One interesting construction is

$$m\left(\mathbf{y}_{C_j}\right) = e^{-\psi\left(\mathbf{y}_{C_j}\right)} \tag{6}$$

where the function ψ is non-negative and exchangeable. A popular choice of function ψ is

$$\psi\left(\mathbf{y}_{C_j}\right) = w_j \times \sum_{i\in C_j} \left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_j}\right)' \left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_j}\right) \tag{7}$$

where

$$\bar{\mathbf{y}}_{C_j} = \frac{1}{e_j} \sum_{i\in C_j} \mathbf{y}_i$$

Usually, we would like to choose $w_j = 1$ and the ψ is related to the sum of squared errors within each cluster. This gives a stochastic version of Ward (1963) clustering model. Moreover, $w_j = e_j$ gives us an interesting case, that is

$$\psi\left(\mathbf{y}_{C_j}\right) = e_j \times \sum_{i \in C_j} \left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_j}\right)' \left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_j}\right) = \sum_{i_1 < i_2, i_1, i_2 \in C_j} d_{i_1,i_2} \tag{8}$$

where

$$d_{i_1,i_2} = \left(\mathbf{y}_{i_1} - \mathbf{y}_{i_2}\right)' \left(\mathbf{y}_{i_1} - \mathbf{y}_{i_2}\right)$$

These models focus on the sum of the pairwise distances of all pairs in each cluster. We can also consult Banfield and Raftery (1993) to relate our models and some existing models. To have an analogous version of (5), we could take

$$\psi\left(\mathbf{y}_{C_j}\right) = \sum_{i \in C_j} \left(\mathbf{y}_i - [\mathbf{x}_1 \cdots \mathbf{x}_S]' \hat{\boldsymbol{\beta}}_{C_j}\right)' \left(\mathbf{y}_i - [\mathbf{x}_1 \cdots \mathbf{x}_S]' \hat{\boldsymbol{\beta}}_{C_j}\right) \tag{9}$$

where

$$\hat{\boldsymbol{\beta}}_{C_j} = \left(\mathbf{X}'_{C_j} \mathbf{X}_{C_j}\right)^{-1} \mathbf{X}'_{C_j} \mathbf{y}_{C_j} \tag{10}$$

This is an extension from the random sample case (7) to the regression case. It is also the contour part of a normal density which is a limiting case of (5), in which we take $b_0 = a_0, \mathbf{t}_0 = \mathbf{0}, \mathbf{m}_0 = \mathbf{0}$ and $2a_0 \to \infty$. Note that (10) is valid for any size of cluster if and only if $S \geq K$; otherwise estimators other than least squares could be used.

3 Clustering procedures

MCMC procedures deliver an approximation to the posterior of the partition $\mathbf{p}$, but for many purposes a single point estimate $\widehat{\mathbf{p}}$ will be sought. In the following section, we consider optimal point estimates based on loss functions, but using the posterior alone, perhaps the only natural estimate is the posterior mode, maximising (3). Two main kinds of approach have been considered recently, and will be discussed in the section.

First, stochastic search methods simply run a MCMC sampler in equilibrium for the posterior distribution, and record the $\mathbf{p}$ with highest posterior probability encountered during the run. For example, Brunner and Lo (1999) do this for a Dirichlet process model, using the usual Gibbs sampler for the partition allocation variables (the "weighted Chinese restaurant process" procedure). Recently, Nobile and Fearnside (2005) proposed an allocation sampler which seems to be an efficient alternative sampler for such models, although their setting is the finite mixture model with Multinomial–Dirichlet prior. The chief weakness of such stochastic search schemes is that, since the number of possible partitions is huge (refer to the Bell number), it is impossible to visit all possible partitions to obtain the $\hat{\mathbf{p}}$. Moreover, it seems intractable to produce proper summary statistics, say frequency counts, of the visited partitions as the set of visited partitions may be very irregular.

Yet, we might be lucky to encounter a partition close to $\hat{\mathbf{p}}$.

An approach to approximating that posterior mode in a Bayesian clustering model that avoids MCMC sampling has been taken by Heard et al. (2005), who propose a deterministic hierarchical agglomerative model based clustering procedure. The idea is simple: two clusters are combined iteratively to maximise the posterior probability (3). A sequence of partitions is built up from initial n clusters to the end of a single cluster. A slight difference from us is that the finite mixture models over the Multinomial–Dirichlet prior are considered in the article. With reduction of the number of clusters $n(\mathbf{p})$, the values of the posterior probability (3) are increasing up to a $n(\mathbf{p})$ and decreasing afterward. A best partition over the sequence of partitions can be obtained though comparisons.

3.1 Stochastic search by posterior sampling of partitions

We briefly discuss the Gibbs sampler, or weighted Chinese restaurant process procedure. The objective is to sample $\mathbf{p}$ from the stationary distribution $\pi(\mathbf{p}\,|\mathbf{y})$ [see Escobar and West (1995, 1998), Ishwaran and James (2001, 2003a, 2003b), Lo et al. (1996), MacEachern (1994), MacEachern and Müller (1998, 2000), Neal (2000), West et al. (1994), etc.]. Here we simply introduce the procedures. Given a partition $\mathbf{p}$, one item, say k, is taken out from the partition, leaving a partiton of $n-1$ items which we denote as $\mathbf{p}_{-k} = \left\{C_{1,-k}, \ldots, C_{n(\mathbf{p}_{-k}),-k}\right\}$. The size of each cluster is $e_{j,-k}$ for $j = 1, \ldots, n(\mathbf{p}_{-k})$ and the number of clusters is $n(\mathbf{p}_{-k})$. The item will be assigned to a new cluster with probability proportional to

$$m\left(\mathbf{y}_{\{k\}}\right) \times \begin{cases} \theta & \text{for the Dirichlet Process} \\ (\kappa - n(\mathbf{p}_{-k}))\delta & \text{for the finite mixture model} \\ \theta + \alpha n(\mathbf{p}_{-k}) & \text{for the Poisson–Dirichlet Process} \\ 1 & \text{for the Uniform Prior} \end{cases}$$

and the item will be assigned to the cluster j with probability proportional to

$$\frac{m\left(\mathbf{y}_{\{k\}\cup C_{j,-k}}\right)}{m\left(\mathbf{y}_{C_{j,-k}}\right)} \times \begin{cases} e_{j,-k} & \text{for the Dirichlet Process} \\ e_{j,-k} + \delta & \text{for the finite mixture model} \\ e_{j,-k} - \alpha & \text{for the Poisson–Dirichlet Process} \\ 1 & \text{for the Uniform Prior} \end{cases}$$

for $j = 1, \ldots, n(\mathbf{p}_{-k})$. In general, the sampler can be described as follows. The item will be assigned to a new cluster with probability proportional to

$$m\left(\mathbf{y}_{\{k\}}\right) \times \frac{\pi\left(C_{1,-k}, \ldots, C_{n(\mathbf{p}_{-k}),-k}, \{k\}\right)}{\pi\left(C_{1,-k}, \ldots, C_{n(\mathbf{p}_{-k}),-k}\right)}$$

and the item will be assigned to the cluster j with probability proportional to

$$\frac{m\left(\mathbf{y}_{\{k\}\cup C_{j,-k}}\right)}{m\left(\mathbf{y}_{C_{j,-k}}\right)} \times \frac{\pi\left(C_{1,-k},\ldots,C_{j,-k}\cup\{k\},\ldots,C_{n(\mathbf{p}_{-k}),-k}\right)}{\pi\left(C_{1,-k},\ldots,C_{j,-k},\ldots,C_{n(\mathbf{p}_{-k}),-k}\right)}$$

for $j = 1,\ldots,n\left(\mathbf{p}_{-k}\right)$.

As an alternative to the weighted Chinese restaurant process procedure, Nobile and Fearnside (2005) propose a series of procedures to sample from a partition model generated by a finite mixture models with a Multinomial–Dirichlet prior in order to enhance the mixing of the sampler. Inspired by the reversible jump sampling idea, it is an efficient Metropolis–Hastings sampler for re-allocating items among partitions. Here we describe two related moves. The *Absorption/Merge Move* proposes combining two randomly chosen clusters into one; the *Ejection/Split Move* is the reverse move. If the two clusters concerned are C_{j_1} and C_{j_2}, the acceptance probabilities for these moves are $\min\{1, R\}$ and $\min\{1, R^{-1}\}$, where in general,

$$R = \frac{m\left(\mathbf{y}_{C_{j_1}\cup C_{j_2}}\right)}{m\left(\mathbf{y}_{C_{j_1}}\right)m\left(\mathbf{y}_{C_{j_2}}\right)} \frac{\pi\left(C_1,\ldots,C_{j_1}\cup C_{j_2},\ldots,C_{n(\mathbf{p})}\right)}{\pi\left(C_1,\ldots,C_{n(\mathbf{p})}\right)}$$

Other moves are available by systematically transferring items between partition subsets.

3.2 Bayesian hierarchical clustering procedures

Heard et al. (2005) propose a deterministic hierarchical agglomerative model based clustering procedure. We will use our model (3) to present the idea. There are some interesting features that only appear in partition models generated by the class of random probability measures, e.g, Dirichlet process and Poisson–Dirichlet process. We initiate the procedure with all singleton clusters, and step-by-step, combine pairs of clusters until all items are clustered together.

The iterative step is at each stage to combine the two clusters C_{j_1} and C_{j_2} that maximise

$$\frac{m\left(\mathbf{y}_{C_{j_1}\cup C_{j_2}}\right)}{m\left(\mathbf{y}_{C_{j_1}}\right)m\left(\mathbf{y}_{C_{j_2}}\right)} \times \eta\left(e_{j_1}, e_{j_2}\right)$$

where

$$\eta\left(e_{j_1}, e_{j_2}\right) = \begin{cases} \dfrac{\Gamma\left(e_{j_1}+e_{j_2}\right)}{\Gamma\left(e_{j_1}\right)\Gamma\left(e_{j_2}\right)} & \text{for the Dirichlet Process} \\ \dfrac{\Gamma\left(e_{j_1}+e_{j_2}+\delta\right)}{\Gamma\left(e_{j_1}+\delta\right)\Gamma\left(e_{j_2}+\delta\right)} & \text{for the finite mixture model} \\ \dfrac{\Gamma\left(e_{j_1}+e_{j_2}-\alpha\right)}{\Gamma\left(e_{j_1}-\alpha\right)\Gamma\left(e_{j_2}-\alpha\right)} & \text{for the Poisson–Dirichlet Process} \\ 1 & \text{for the Uniform Prior} \end{cases}$$

This choice of clusters to combine maximises the posterior quantity (3) among all partitions that can be obtained from the present one by merging a pair of clusters. To show this, consider the Dirichlet process case; the other cases are similar. Suppose we move $\mathbf{p} = \left\{C_1,\ldots,C_{n(\mathbf{p})}\right\}$ to $\mathbf{p}^* =$

$\left\{C_1^*, \ldots, C_{n(\mathbf{p}^*)}^*\right\}$ where e_j for $j = 1, \ldots, n(\mathbf{p})$ and e_j^* for $j = 1, \ldots, n(\mathbf{p}^*)$ are the size of clusters respectively. Then, from (3), we find:

$$\begin{aligned}
\phi(\mathbf{p}^*) &= \theta^{n(\mathbf{p}^*)} \prod_{j=1}^{n(\mathbf{p}^*)} \Gamma\left(e_j^*\right) m\left(\mathbf{y}_{C_j^*}\right) \\
&= \left(\theta^{n(\mathbf{p})} \prod_{j=1}^{n(\mathbf{p})} \Gamma\left(e_j\right) m\left(\mathbf{y}_{C_j}\right)\right) \times \left(\frac{\theta\Gamma\left(e_{j_1}+e_{j_2}\right) m\left(\mathbf{y}_{C_{j_1}\cup C_{j_2}}\right)}{\theta\Gamma\left(e_{j_1}\right) m\left(\mathbf{y}_{C_{j_1}}\right) \theta\Gamma\left(e_{j_2}\right) m\left(\mathbf{y}_{C_{j_2}}\right)}\right) \\
&= \phi(\mathbf{p}) \times \left(\frac{1}{\theta} \frac{\Gamma\left(e_{j_1}+e_{j_2}\right)}{\Gamma\left(e_{j_1}\right)\Gamma\left(e_{j_2}\right)} \frac{m\left(\mathbf{y}_{C_{j_1}\cup C_{j_2}}\right)}{m\left(\mathbf{y}_{C_{j_1}}\right) m\left(\mathbf{y}_{C_{j_2}}\right)}\right)
\end{aligned}$$

For the other cases, we have

$$\phi(\mathbf{p}^*) = \phi(\mathbf{p}) \times \left(\frac{1}{\xi} \eta\left(e_{j_1}, e_{j_2}\right) \frac{m\left(\mathbf{y}_{C_{j_1}\cup C_{j_2}}\right)}{m\left(\mathbf{y}_{C_{j_1}}\right) m\left(\mathbf{y}_{C_{j_2}}\right)}\right)$$

where

$$\xi = \begin{cases} \theta & \text{for the Dirichlet Process} \\ \dfrac{(\kappa - (n(\mathbf{p}) - 1))\,\delta}{\Gamma(\delta+1)} & \text{for the finite mixture model} \\ \dfrac{\theta + \alpha\,(n(\mathbf{p}) - 1)}{\Gamma(1-\alpha)} & \text{for the Poisson–Dirichlet Process} \\ 1 & \text{for the Uniform Prior} \end{cases}$$

In practice, Heard et al. (2005) construct a sequence of partitions from the all-singletons partition to a single cluster partition, and then determine the best partition by comparisons though (3). Note that the maximizing process does not depend on the quantity ξ.

We now consider particular cases of this procedure for specific directly assigned choices of $m(\mathbf{y}_{C_j})$. If we choose $m\left(\mathbf{y}_{C_j}\right)$, (2), to be (7) and tailor-make $\pi(\mathbf{p}) \propto \theta^{n(\mathbf{p})}$, the procedure works as follows. Iteratively, we combine two clusters C_{j_1} and C_{j_2} if

$$\frac{e_{j_1}e_{j_2}}{e_{j_1}+e_{j_2}}\left(\bar{\mathbf{y}}_{C_{j_1}} - \bar{\mathbf{y}}_{C_{j_2}}\right)'\left(\bar{\mathbf{y}}_{C_{j_1}} - \bar{\mathbf{y}}_{C_{j_2}}\right) \le \min_{j_2, j_1 \in \{1,\ldots,n(\mathbf{p})\}, j_1 \neq j_2} \left\{\frac{e_{j_1}e_{j_2}}{e_{j_1}+e_{j_2}}\left(\bar{\mathbf{y}}_{C_{j_1}} - \bar{\mathbf{y}}_{C_{j_2}}\right)'\left(\bar{\mathbf{y}}_{C_{j_1}} - \bar{\mathbf{y}}_{C_{j_2}}\right)\right\} \tag{11}$$

see appendix for the proof. To determine the number of clusters and the best partition, we take the presumed number θ and calculate (3) for all partitions via the maximizing process. Thus we can interpret the procedure as an instance of the hierarchical clustering algorithm of Ward (1963), as one may see that the parameter θ is an analogy of presumed number of clusters in the classical Ward (1963) procedure. The quantity θ is taken to determine the target partition (the approximation of the point estimates). With the number θ, we know the prior information we assigned to partitions, say expected number of clusters, through simulation.

Next we take $m\left(\mathbf{y}_{C_j}\right)$ to be (8). The procedure works as follows. Iteratively, we combine two clusters C_{j_1} and C_{j_2} if

$$\sum_{i_1 \in C_{j_1}} \sum_{i_2 \in C_{j_2}} d_{i_1,i_2} \leq \min_{j_2,j_1 \in \{1,\ldots,n(\mathbf{p})\}, j_1 \neq j_2} \left\{ \sum_{i_1 \in C_{j_1}} \sum_{i_2 \in C_{j_2}} d_{i_1,i_2} \right\}. \tag{12}$$

For the regression case, we take $m\left(\mathbf{y}_{C_j}\right)$ to be (9), and the procedure then works as follows.

$$\begin{aligned} &\left(\hat{\boldsymbol{\beta}}_{C_{j_1}} - \hat{\boldsymbol{\beta}}_{C_{j_2}}\right)' \mathbf{W}_{C_{j_1},C_{j_2}} \left(\hat{\boldsymbol{\beta}}_{C_{j_1}} - \hat{\boldsymbol{\beta}}_{C_{j_2}}\right) \\ &\quad \leq \min_{j_2,j_1 \in \{1,\ldots,n(\mathbf{p})\}, j_1 \neq j_2} \left\{ \left(\hat{\boldsymbol{\beta}}_{C_{j_1}} - \hat{\boldsymbol{\beta}}_{C_{j_2}}\right)' \mathbf{W}_{C_{j_1},C_{j_2}} \left(\hat{\boldsymbol{\beta}}_{C_{j_1}} - \hat{\boldsymbol{\beta}}_{C_{j_2}}\right) \right\} \end{aligned} \tag{13}$$

where

$$\mathbf{W}_{C_{j_1},C_{j_2}} = \left[\left(\mathbf{X}'_{C_{j_1}} \mathbf{X}_{C_{j_1}}\right)^{-1} + \left(\mathbf{X}'_{C_{j_2}} \mathbf{X}_{C_{j_2}}\right)^{-1} \right]^{-1}$$

3.3 Real and simulated data sets

In order to make comparisons with different procedures, we employ 4 sets of artificial data and 2 sets of real data to illustrate our methodology.

3.3.1 Simulated mixtures

We generate 4 sets of data. We first consider a 4 component mixture of bivariate Normal densities,

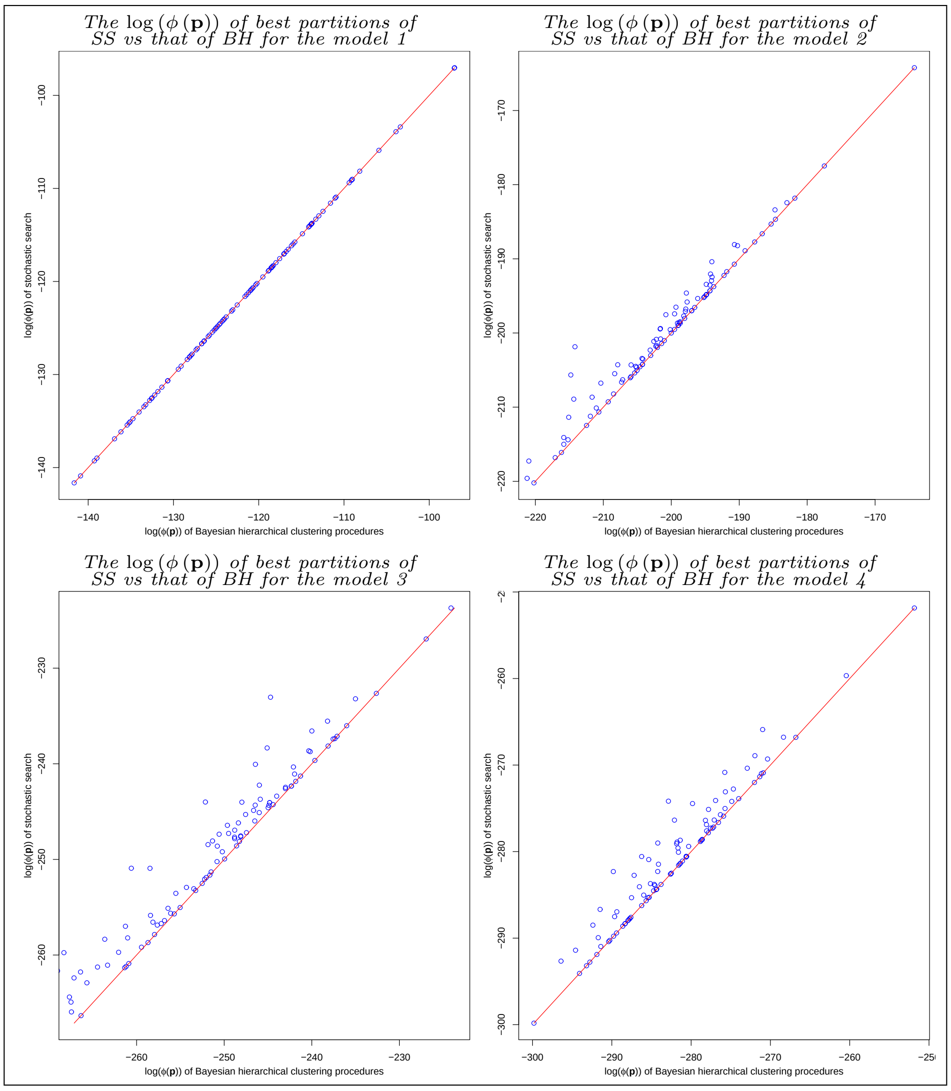
$$\sum_{i=1}^{4} w_i N\left(\mu_i, \Sigma_i\right) \text{ with parameters } \begin{array}{cccc} \mu_1 = (2,2)' & \mu_2 = (2,-2)' & \mu_3 = (-2,2)' & \mu_4 = (-2,-2)' \\ \Sigma_1 = \mathbf{I}_{2\times 2} & \Sigma_2 = \mathbf{I}_{2\times 2} & \Sigma_3 = \mathbf{I}_{2\times 2} & \Sigma_4 = \mathbf{I}_{2\times 2} \end{array}$$

where $\mathbf{I}_{2\times 2}$ represent the identity matrix of order 2. We generate an artificial data set with the following settings,

	w_1	w_2	w_3	w_4
Model 1	1	0	0	0
Model 2	1/2	1/2	0	0
Model 3	1/3	1/3	1/3	0
Model 4	1/4	1/4	1/4	1/4

We take the covariate $[\mathbf{x}_1 \cdots \mathbf{x}_S]' = \mathbf{I}_{2\times 2}$ for $S = 2$ and $K = 2$. A comparison between the stochastic search procedures and hierarchical clustering procedures is performed. We take 100 sets of data from each of the models 1–4, each with $n = 100$ data points. We fit the data to the model (5) with the Dirichlet Process prior. The parameters are assigned to be $\theta = 1, a_0 = 1, b_0 = 0.01, \mathbf{m}_0 = [0 \cdots 0]', \mathbf{t}_0 = 0.01\mathbf{I}$. We employ both SS and BH procedures. For the stochastic search method, we run the Gibbs version of WCR for 20000 cycles. We record the partition of greatest posterior probability among all 20000 cycles. Here we plot the $\log\left(\phi\left(\mathbf{p}\right)\right)$ of the stochastic search (SS) versus that of Bayesian hierarchical clustering procedures (BH). Figure 1 seems to suggest that

Figure 1: **Comparisons between SS and BH under Model 1–4 based on** $\log(\phi(\mathbf{p}))$

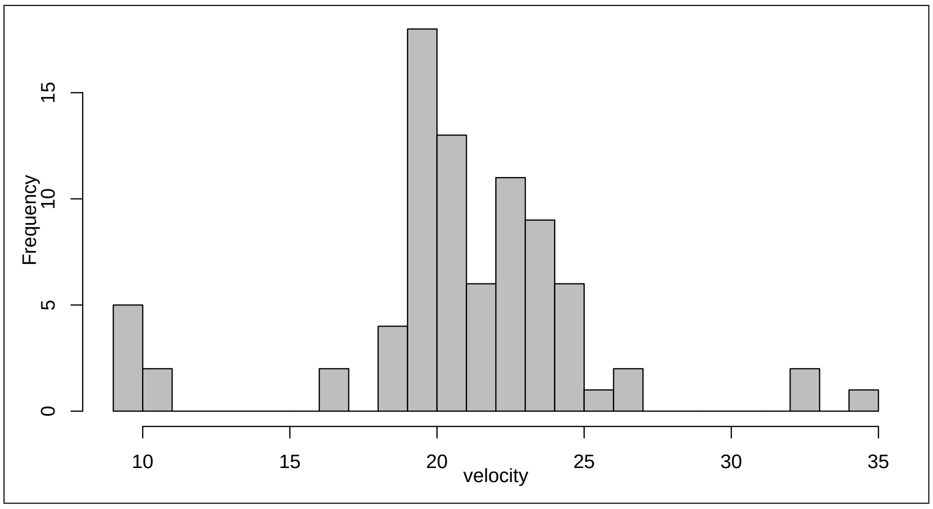


the "hidden" number of components has an effect on the performance of both procedures. The stochastic search (SS) attains higher posterior probability partitions than the Bayesian hierarchical clustering procedure (BH) when the "hidden" number of components increases.

3.3.2 Galaxy data

The famous Roeder (1990) galaxy data consists measurements of velocities in km/sec of 82 galaxies from 6 well-separated conic sections of an unfilled survey of the Corona Borealis region. The data set is available in the paper, as well as in both the ELEMSTATLEARN and VR packages of the statistical

Figure 2: **Histogram of the galaxy data**



software R. We take the covariate $[\mathbf{x}_1 \cdots \mathbf{x}_S]' = 1$ for $S = 1$ and $K = 1$. We fit our models to these data. Here we plot the log posterior probability $\log(\phi(\mathbf{p}))$ against the number of clusters of the Bayesian hierarchical clustering procedures (BH) (Figure 3) and against iteration number for the first 200 iterations of the stochastic search (SS) (Figure 4) . Interestingly, both procedures attain the same highest-posterior-probability $\mathbf{p}$, suggesting that the optimal number of clusters is 3. Moreover, stochastic search (SS) first attains the best $\mathbf{p}$ at the 181^{th} iteration of the 20000 iterations used for comparison. Of course, we may want more iterations to get better performance. In this case, the Bayesian hierarchical clustering procedure (BH) performs much better than stochastic search (SS) in term of time as it makes many fewer comparisons. In addition to the histogram, we add the observations on the histogram and the corresponding clusters. Note that the clusters are in no particular order.

3.3.3 Leukaemia data

The leukemia data of Golub et al. (1999) consists of 7129 gene expression levels of 72 patients with either acute myeloid leukaemia (AML) or acute lymphoblastic leukaemia (ALL). Golub et al. (1999) splits the data into two, training and test sets. The training set consists of 38 patients, of which 27 have acute lymphoblastic (ALL) and 11 have acute myeloid leukaemia (AML) cases. The test set consists of 34 patients, 20 have acute lymphoblastic (ALL) and 14 have acute myeloid leukaemia (AML) cases. Acute lymphoblastic (ALL) actually arises from two different types of lymphocytes (T-cell and B-cell). Among all acute lymphoblastic (ALL), there are 38 B-cell and 9 T-cell. The data set is available at the website `http://www-genome.wi.mit.edu/mpr/data_set_ALL_AML.html` and GOLUBESETS package of the statistical software R, part of the data is available in MULTTEST and PLSGENOMICS packages as well. Following Dudoit et al. (2002), to transform the data we employ: (a)

Figure 3: **The** $\log(\phi(\mathbf{p}))$ **vs the number of clusters via BH**

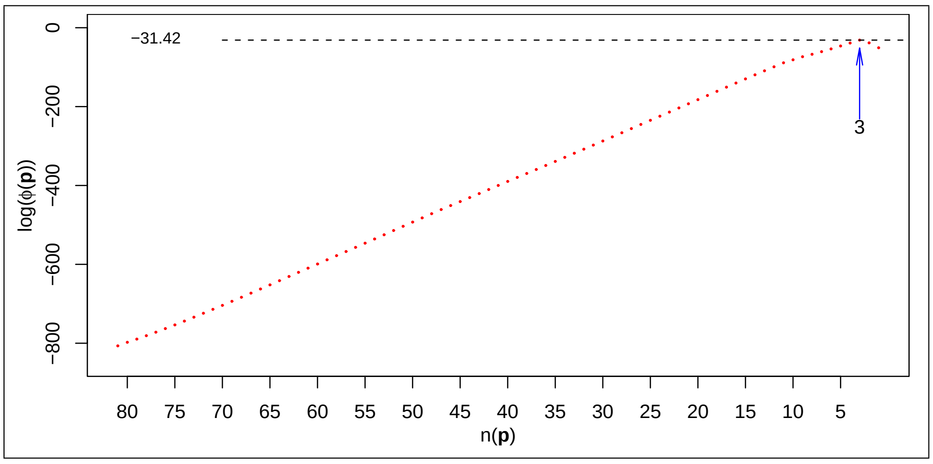


Figure 4: **The** $\log(\phi(\mathbf{p}))$ **vs the first 200 iterations via SS**

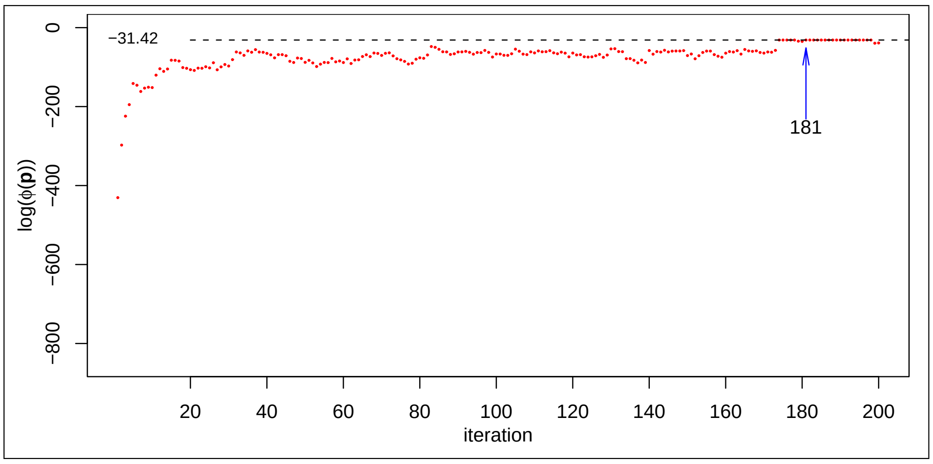
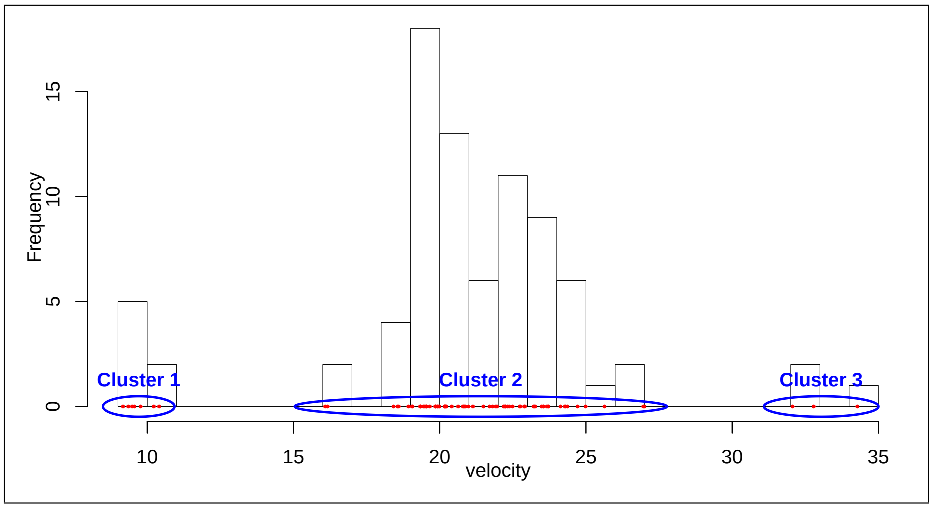


Figure 5: **The best partition produced by SS and BH**



thresholding, floor of 100 and ceiling of 16,000; (b) filtering, exclusion of genes with max/min$\leq$5 or max$-$min$\leq$1600, where max and min refer to the maximum and minimum intensities for a particular gene across the 72 mRNA samples; and (c) base 10 logarithmic transformation. There are 1656 genes left. The analyzed data set is a normalized version of the selected gene expressions. Each gene is normalized by subtracted by its means across patients/samples and divided by its standard deviation across patients/samples. The design matrix/covariates $[\mathbf{x}_1 \cdots \mathbf{x}_S]'$ is taken to be

$$[\mathbf{x}_1 \cdots \mathbf{x}_S]' = \underbrace{\begin{bmatrix} 1\cdots1 & 1\cdots1 & 1\cdots1 \\ 1\cdots1 & 0\cdots0 & 0\cdots0 \\ 0\cdots0 & 1\cdots1 & 0\cdots0 \end{bmatrix}'}_{\text{ALL (B-CELL)} \quad \text{ALL (T-CELL)} \quad \text{AML}}$$

for $S = 72$ and $K = 3$.

We fit cluster models to the leukemia data. Here we plot the log posterior probability $\log(\phi(\mathbf{p}))$ against the number of clusters of the Bayesian hierarchical clustering procedures (BH) (Figure 7) and against iteration number for 20000 iterations of the stochastic search (SS) (Figure 8). In the plots, we also indicate where the best partitions are. In this case, stochastic search (SS) perform much better than Bayesian hierarchical clustering procedures(BH) both in terms of time and quality, in that it attains higher posterior probability partitions. A rough calculation shows why SS is faster than BH. Here BH needs $\sum_{i=2}^{1656} i \times (i-1)/2 = 1,513,768,920$ comparisons, while since the posterior average number of clusters is about 13, SS requires only $1656 \times (13+1) \times 20000 = 463,680,000$ comparisons.

Figure 6: **profile plot of the leukaemia data**

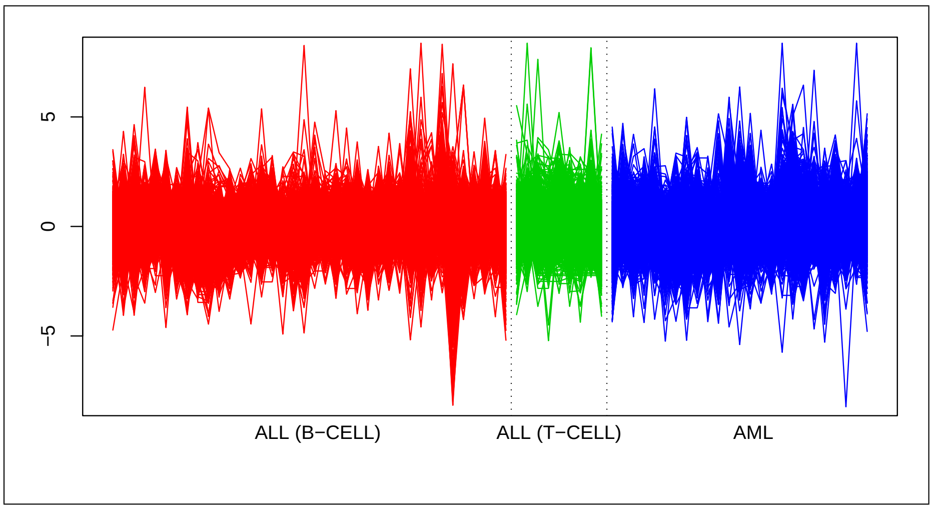


Figure 7: **The $\log(\phi(\mathbf{p}))$ vs the number of clusters via BH**

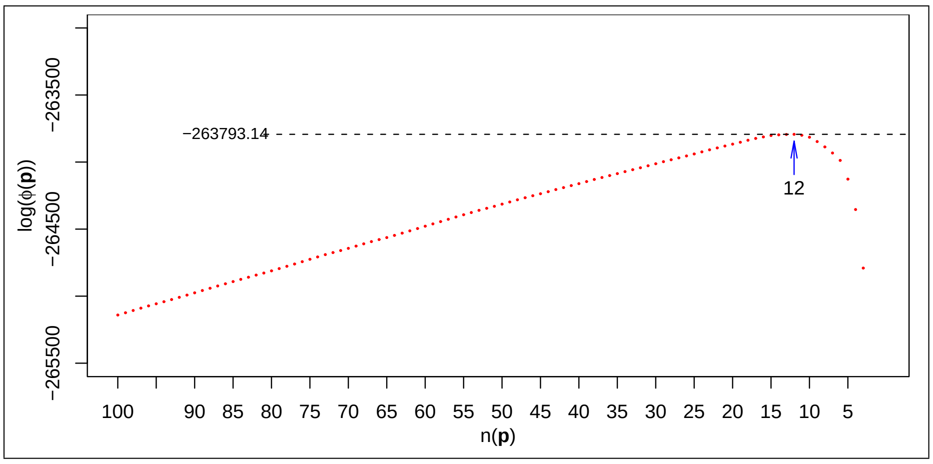
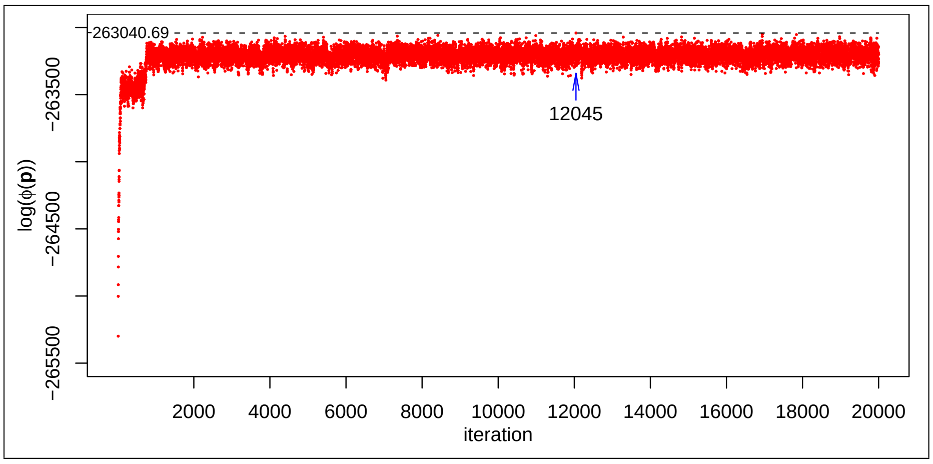


Figure 8: **The $\log(\phi(\mathbf{p}))$ vs all 20000 iterations via SS**



4 Optimal Bayesian clustering using a pairwise coincidence loss function

As previously commented, the maximum a posteriori partition has no objective status as a best estimate of the clustering of the data. Posterior modes can be increasingly unrepresentative measures of the 'centre' of a posterior distribution as the dimensionality of the unknown parameter increases. In normative Bayesian theory, point estimation can only be accomplished after specifying a loss function: the optimal estimate is that parameter value minimising the posterior expected loss. That is, if the focus is on the partition $\mathbf{p}$, we have to define a loss function $L(\mathbf{p}, \widehat{\mathbf{p}})$, the cost incurred in declaring that the true partition is $\widehat{\mathbf{p}}$ when it is really $\mathbf{p}$, and choose as our optimal partition that $\widehat{\mathbf{p}}$ which minimises $E(L(\mathbf{p}, \widehat{\mathbf{p}})|\mathbf{y})$.

The requirements of exchangeability of subset labels and items imposes strong constraints on the form of $L(\cdot, \cdot)$, and the interests of tractability are even more demanding. We choose to use one of the loss functions discussed by Binder (1978, 1981), which considers pairs of items and incurs a penalty for each pair that are clustered together when they should not be, and vice versa. That is, if c_i denotes the allocation variable: $c_i = k$ if and only if $i \in C_k$, we define

$$L(\mathbf{p}, \widehat{\mathbf{p}}) = \sum_{(i,j)\in\mathcal{M}} \left(a\mathbb{I}[c_i = c_j, \widehat{c}_i \neq \widehat{c}_j] + b\mathbb{I}[c_i \neq c_j, \widehat{c}_i = \widehat{c}_j]\right).$$

Here $\mathcal{M} = \{(i, j) : i < j; i, j \in \{1, \ldots, n\}\}$, and a and b are given non-negative constants, the unit costs for each kind of pairwise misclassification.

The posterior expected loss is evidently

$$E(L(\mathbf{p},\widehat{\mathbf{p}})|\mathbf{y}) = \sum_{(i,j)\in\mathcal{M}} (a\mathbb{I}[\widehat{c}_i \neq \widehat{c}_j]P\{c_i = c_j|\mathbf{y}\} + b\mathbb{I}[\widehat{c}_i = \widehat{c}_j]P\{c_i \neq c_j|\mathbf{y}\})$$

Let us abbreviate the *posterior coincidence probabilities* $P\{c_i = c_j|\mathbf{y}\} = \rho_{ij}$, then we can write

$$E(L(\mathbf{p},\widehat{\mathbf{p}})|\mathbf{y}) = a \sum_{(i,j)\in\mathcal{M}} \rho_{ij} - (a+b) \sum_{(i,j)\in\mathcal{M}} \mathbb{I}[\widehat{c}_i = \widehat{c}_j](\rho_{ij} - K)$$

where $K = b/(a+b) \in [0,1]$. Minimising the posterior expected loss is thus equivalent to maximising

$$\ell(\widehat{\mathbf{p}},K) = \sum_{(i,j)\in\mathcal{M}} \mathbb{I}[\widehat{c}_i = \widehat{c}_j](\rho_{ij} - K) \tag{14}$$

over choice of $\widehat{\mathbf{p}}$.

Curves of the objective function $\ell(\widehat{\mathbf{p}},K)$ regarded as a function of K are linear and have non-positive integer slopes and non-negative intercepts, for each $\widehat{\mathbf{p}}$. These functions of K characterise the quality of each possible $\widehat{\mathbf{p}}$, and the whole ensemble of such functions determines in particular for which K, if any, each partition is optimal, as well as defining the optimal $\widehat{\mathbf{p}}$ for each K. Our approach, therefore, is to consider all values of K simultaneously.

Example 1 *Suppose there are 5 items. The partitions of the 5 items have probabilities*

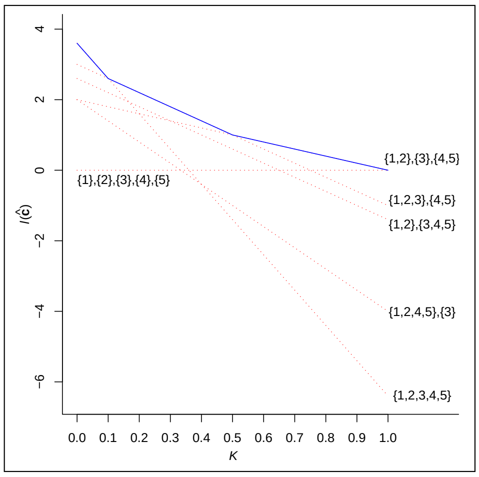
$$\begin{array}{ll}
\mathbf{p}_1 = \{\{1,2,3\},\{4,5\}\} & \mathbb{P}\{\mathbf{p} = \mathbf{p}_1\} = 0.5 \\
\mathbf{p}_2 = \{\{1,2\},\{3\},\{4,5\}\} & \mathbb{P}\{\mathbf{p} = \mathbf{p}_2\} = 0.2 \\
\mathbf{p}_3 = \{\{1,2\},\{3,4,5\}\} & \mathbb{P}\{\mathbf{p} = \mathbf{p}_3\} = 0.3
\end{array}$$

The ρ matrix can be calculated easily based on those probabilities.

	1	2	3	4	5
1	–	1	0.5	0	0
2	–	–	0.5	0	0
3	–	–	–	0.3	0.3
4	–	–	–	–	1
5	–	–	–	–	–

Figure 9 shows the objective function $\ell(\widehat{\mathbf{p}},K)$ and related partitions. The dotted lines represent the performance of various partitions. The solid curves represent the optimal performance for each value of K. It is easy to observe that the solid curve is formed from three straight line segments. Each of these segments corresponds to a partition that is optimal for certain K.

Figure 9: $\ell(\hat{\mathbf{p}}, K)$ **vs** K **for some partitions**



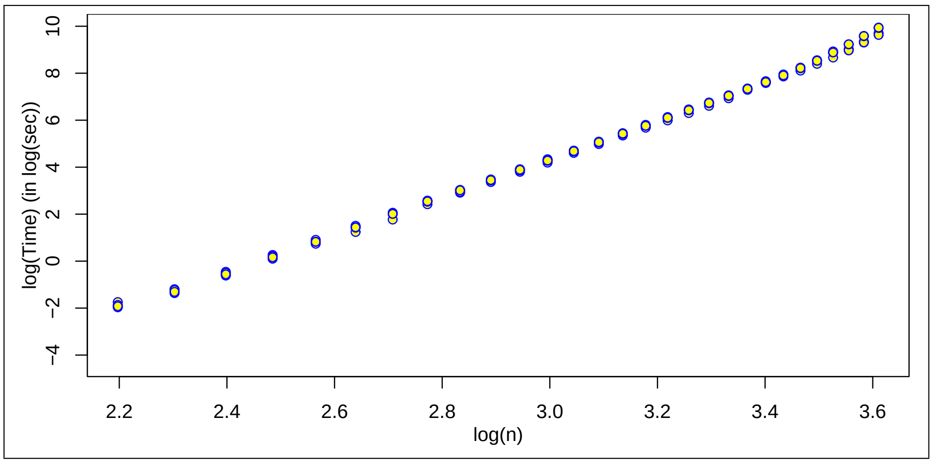
4.1 A binary integer programming formulation

We will represent the maximisation of (14) as a binary integer programming problem. Let us replace the indicator function $\mathbb{I}[\hat{c}_i = \hat{c}_j]$ by a binary (0/1) variable X_{ij}; the objective function is a linear combination of the X_{ij} with weights $(\rho_{ij} - K)$. Since $\hat{c}$ represents a proper partition of the items, the X_{ij} are subject to constraints. It is easy to see that what we require is that for all triples (i, j, k), if $X_{ij} = 1$ then $X_{ik} = X_{jk}$. These boolean constraints can be represented as algebraic inequalities, and we find that maximisation of (14) is equivalent to solving the optimisation problem:

$$\begin{aligned} \max_{\{X_{ij}: i,j \in \mathcal{M}\}} & \sum_{i,j \in \mathcal{M}} X_{ij} (\rho_{ij} - K) \\ \text{s.t. } & X_{ij} + X_{ik} - X_{jk} \leq 1 \text{ for } \{i \neq j \neq k \neq i : i, j, k \in \{1, \ldots, n\}\} \\ & X_{ij} \in \{0, 1\} \text{ for } i, j \in \mathcal{M} \end{aligned} \tag{15}$$

We conduct a modest experiment to study the feasability of solving this programming problem, although Bansal et al. (2004) have already shown that it is an NP hard problem. Here we simulate 10 sets of data sequences. Each data sequence has n data points for each model, they are from models 1–4. The regression marginal (5) is fitted to each data set, using a Dirichlet process prior with settings $\theta = 1.0, a_0 = 1.0, b_0 = 0.01, m_0 = \mathbf{0}, t_0 = 0.01\mathbf{I}$. The matrix $[\mathbf{x}_1 \cdots \mathbf{x}_S]'$ is chosen to be an identity matrix $\mathbf{I}_{S \times S}$. The MCMC sampler discussed in Section 3.1 was used to generate 10,000 partitions following 10,000 burn-in for each data sequence. We then estimated ρ_{ij} for each data sequence using the last 10,000 partitions. We use the LPSOLVE package of the statistical system R to solve the programming problem (15) given $K = \{0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9\}$. The times spent on solving the problem are recorded in seconds. We plot the $\log(\text{Time})$ against $\log(n)$ per

Figure 10: $\log(\textbf{Time})$ **vs** $\log(n)$



each data set and least square regression parameters are estimated. In our very rough prediction, we may spend 225.57 billion years to solve a programming program with $n = 1000$. This demonstrates the need for a faster algorithm to perform the optimisation, or at least to obtain an approximation to the optimum.

4.2 A novel algorithm

When $K = 1$ or $K = 0$, the optimal partitions are trivially obtained – they are those corresponding to $X_{ij} = 0$ and $X_{ij} = 1$ for all i, j in the set $\mathcal{M}$, respectively. For other K, as we have seen, the solution is not obvious and the problem NP hard. We propose an iterative procedure that gives a locally optimal solution for the problem. The main idea is to solve the problem partially in each iteration; see the following algorithm 1. We subsequently introduce a procedure that gives locally optimal solutions simultaneously for all $K \in [0, 1]$; see algorithm 2.

Algorithm 1 *Define* $\mathcal{M}_i = \{(1, i), \ldots, (i-1, i), (i, i+1), \ldots, (i, n)\}$*. Given a value* K *and a partition* $\mathbf{p}$*,*

Step 1 *For* $i = 1, \ldots, n$*, given* $\{X_{jk} : j, k \in \mathcal{M}\backslash\mathcal{M}_i\}$ *are fixed, solve a binary integer programming problem*

$$\max_{\{X_{jk}:j,k\in\mathcal{M}_i\}} \sum_{j,k\in\mathcal{M}_i} X_{jk}\left(\rho_{jk} - K\right)$$
$$\text{s.t. } X_{ij} + X_{ik} - X_{jk} \leq 1 \text{ for } \{i \neq j \neq k \neq i : i, j, k \in \{1, \ldots, n\}\}$$
$$X_{ij} \in \{0, 1\} \text{ for } i, j \in \mathcal{M}$$

Step 2 *Go to step 1 if the value of the objective function evaluated at the new partition exceeds* *that on the previous cycle.*

Algorithm 1 expresses the idea that we can seek to increase the objective function by cycling over items i, taking i out of the current partition and reallocating it in the optimal way: either by assigning it to an existing cluster or by creating a new one.

As we vary $K \in [0, 1]$, the relative costs of the two kinds of pairwise error in clustering, the optimal partition varies. If K is not pre-determined, we may repeat Algorithm 1 for several choices of K, but there are advantages of convenience and efficiency in considering all K simultaneously. This also helps to avoid converging to local optima.

As we see from (15), each partition $\mathbf{p}$ is characterised by a non-increasing linear function of K, with intercept and slope depending on $\mathbf{p}$. For any set of partitions $\mathcal{P}$, we can define

$$\ell(\mathcal{P}, K) = \max_{\mathbf{p}\in\mathcal{P}} \ell(\mathbf{p}, K)$$

and by basic properties of convexity, this is a non-increasing convex polygonal (piecewise linear) function of K for each $\mathcal{P}$, and is non-decreasing (with respect to set inclusion) in $\mathcal{P}$ for each K. Further, $\ell(\mathcal{P}, K)$ can be parameterised by a set of increasing values $0 = K_0 < K_1 < \cdots < K_r = 1$ and partitions $\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_r \in \mathcal{P}$, with

$$\ell(\mathcal{P}, K) = \ell(\mathbf{p}_s, K) \qquad \text{for all } K \in [K_{s-1}, K_s] \tag{16}$$

for $s = 1, 2, \ldots, r$. Note that $\mathbf{p}_s$ is optimal among $\mathbf{p} \in \mathcal{P}$ ($\ell(\mathbf{p}_s, K) \geq \ell(\mathbf{p}, K)$) for all $K \in [K_{s-1}, K_s]$.

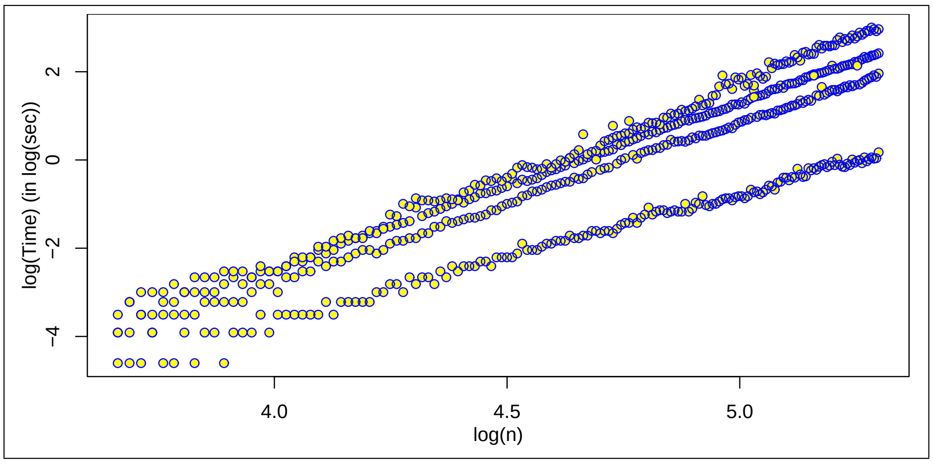
Our true objective is, for every K, to maximise $\ell(\mathbf{p}, K)$ over the set $\widetilde{\mathcal{P}}$ of *all* partitions; we could then use (16) with $\mathcal{P} = \widetilde{\mathcal{P}}$ to read off the optimal partition (which is evidently constant on intervals of K) for each K. For any subset $\mathcal{P} \subseteq \widetilde{\mathcal{P}}$, $\ell(\mathcal{P}, K)$ is a lower bound for $\ell(\widetilde{\mathcal{P}}, K)$. Algorithm 2 is a heuristic for iteratively increasing $\mathcal{P}$ and hence the lower bound $\ell(\mathcal{P}, K)$ to obtain successive approximations to the optimum.

Algorithm 2 *Initiate the algorithm by setting $\mathcal{P} = \{\mathbf{p}_a, \mathbf{p}_s\}$ where $\mathbf{p}_a$ is the partition that has all items in one cluster and $\mathbf{p}_s$ is the partition consisting of all singleton clusters.*

- *Step 1* *Take a pair of adjacent partitions, say $\mathbf{p}_s$ and $\mathbf{p}_{s+1}$, from the set representing $\ell(\mathcal{P}, K)$ defined in (16).*
- *Step 2* *Run Algorithm 1 twice using the value K_s, starting from partitions $\mathbf{p}_s$ and $\mathbf{p}_{s+1}$. The resulting partitions are $\mathbf{p}^*_s$ and $\mathbf{p}^*_{s+1}$.*
- *Step 3* *Insert $\mathbf{p}^*_s$ and $\mathbf{p}^*_{s+1}$ into the set $\mathcal{P}$.*
- *Step 4* *Recompute the representation (16) for the modified set of partitions $\mathcal{P}$.*
- *Step 5* *End if all pairs $(\mathbf{p}_s, \mathbf{p}_{s+1})$ have been visited and the representation of the set $\mathcal{P}$ is unchanged; go to step 1 otherwise.*

We perform an experiment based on the same settings as in the previous section, using Algorithm 2 on the interval $[0, 0.99]$. (We find that the optimal partition changes rapidly for K near 1, so that Algorithm 2 is computationally expensive applied to the full interval.) We plot the log (Time) against

Figure 11: $\log(\textbf{Time})$ **vs** $\log(n)$



$\log(n)$ for each data set, and estimate the least squares regression. Interestingly, the run time of the algorithm is an increasing function of the number of hidden components. We predict a run time of 3.51 hours to solve the optimisation for $n = 1000$ items under model 4.

4.3 Numerical experiments

4.3.1 Assessment of heuristic approximation

Our assessment of the performance of the algorithm uses models 1–4, but with small data sets, n varying from 3 to 15. 10000 replications are made of each case. We fit the regression marginal (5) to each data set, with the Dirichlet process prior. The matrix $[\mathbf{x}_1 \cdots \mathbf{x}_S]'$ is chosen to be the identity matrix $\mathbf{I}_{S\times S}$. The sampling uses the Gibbs version of the weighted Chinese restaurant process with parameters $\theta = 1.0, a_0 = 1.0, b_0 = 0.01, m_0 = \mathbf{0}, t_0 = 0.01\mathbf{I}$ and generates 10,000 partitions following 10,000 burn-in for each data set. We estimate ρ_{ij} for each data set based on the last 10,000 sweeps. We use the LPSOLVE package of the software system R to solve the programming problem given $K = \{0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9\}$. We also use our algorithm 2 to generate best partitions for $K \in [0, 0.99]$. A comparison between the true optimum and the best partition generated by the algorithm 2 is made. Table 1 − 4 show the proportions of runs in which the algorithm finds the true optimum for different K and n. Figure 5 − 8 show the mean of the ratios of the optimised $\ell(\mathbf{p}, K)$ for different K and n.

4.3.2 Optimal vs. maximum probability partitions

To get some appreciation of the difference between (approximate) MAP partitions and (approximate) optimal partitions according to our loss function, we make some comparisons of point estimates based on three different approaches, stochastic search (SS), Bayesian hierarchical clustering procedure

Table 1: **Proportion of getting the optimum of the algorithm 2 for model 1 over the 10,000 set of data sequences in different K and n**

	$K = 0.1$	$K = 0.2$	$K = 0.3$	$K = 0.4$	$K = 0.5$	$K = 0.6$	$K = 0.7$	$K = 0.8$	$K = 0.9$
$n = 3$	1	1	1	1	1	1	1	1	1
$n = 4$	1	1	1	1	1	1	1	1	1
$n = 5$	1	1	1	1	1	1	1	1	0.9999
$n = 6$	0.9990	0.9993	0.9994	0.9998	0.9996	0.9994	0.9996	0.9998	0.9998
$n = 7$	0.9985	0.9983	0.9984	0.9985	0.9984	0.9986	0.9993	0.9993	0.9995
$n = 8$	0.9971	0.9974	0.9982	0.9986	0.9982	0.9980	0.9982	0.9991	0.9991
$n = 9$	0.9966	0.9978	0.9978	0.9966	0.9977	0.9979	0.9981	0.9990	0.9988
$n = 10$	0.9986	0.9980	0.9983	0.9987	0.9983	0.9984	0.9985	0.9991	0.9984
$n = 11$	0.9983	0.9986	0.9987	0.9985	0.9987	0.9982	0.9979	0.9982	0.9982
$n = 12$	0.9987	0.9981	0.9983	0.9978	0.9987	0.9986	0.9993	0.9993	0.9984
$n = 13$	0.9989	0.9987	0.9987	0.9986	0.9990	0.9987	0.9986	0.9991	0.9982
$n = 14$	0.9985	0.9993	0.9996	0.9990	0.9986	0.9989	0.9991	0.9985	0.9987
$n = 15$	0.9992	0.9997	0.9997	0.9992	0.9994	0.9993	0.9997	0.9987	0.9984

Table 2: **Proportion of getting the optimum of the algorithm 2 for model 2 over the 10,000 set of data sequences in different K and n**

	$K = 0.1$	$K = 0.2$	$K = 0.3$	$K = 0.4$	$K = 0.5$	$K = 0.6$	$K = 0.7$	$K = 0.8$	$K = 0.9$
$n = 3$	1	1	1	1	1	1	1	1	1
$n = 4$	1	1	1	1	1	1	1	1	1
$n = 5$	1	1	1	1	1	1	1	1	1
$n = 6$	0.9978	0.9996	0.9999	0.9998	0.9998	0.9998	0.9996	0.9997	0.9995
$n = 7$	0.9871	0.9952	0.9983	0.9995	0.9998	0.9996	0.9997	0.9995	0.9993
$n = 8$	0.9748	0.9875	0.9945	0.9972	0.9989	0.9995	0.9995	0.9993	0.9988
$n = 9$	0.9648	0.9775	0.9904	0.9945	0.9965	0.9979	0.9988	0.9989	0.9980
$n = 10$	0.9564	0.9748	0.9875	0.9927	0.9969	0.9976	0.9983	0.9992	0.9987
$n = 11$	0.9529	0.9696	0.9852	0.9918	0.9955	0.9971	0.9967	0.9975	0.9986
$n = 12$	0.9493	0.9673	0.9829	0.9914	0.9943	0.9955	0.9970	0.9971	0.9983
$n = 13$	0.9478	0.9688	0.9838	0.9899	0.9922	0.9943	0.9950	0.9961	0.9973
$n = 14$	0.9517	0.9702	0.9825	0.9902	0.9926	0.9932	0.9951	0.9965	0.9962
$n = 15$	0.9475	0.9689	0.9836	0.9877	0.9928	0.9937	0.9959	0.9955	0.9968

Table 3: **Proportion of getting the optimum of the algorithm 2 for model 3 over the 10,000 set of data sequences in different K and n**

	$K = 0.1$	$K = 0.2$	$K = 0.3$	$K = 0.4$	$K = 0.5$	$K = 0.6$	$K = 0.7$	$K = 0.8$	$K = 0.9$
$n = 3$	1	1	1	1	1	1	1	1	1
$n = 4$	1	1	1	1	1	1	1	1	1
$n = 5$	1	1	1	1	1	1	1	1	1
$n = 6$	0.9970	0.9993	1	0.9999	0.9999	0.9999	0.9999	0.9997	0.9996
$n = 7$	0.9891	0.9961	0.9991	0.9999	0.9998	0.9998	0.9997	0.9996	0.9992
$n = 8$	0.9752	0.9904	0.9958	0.9978	0.9992	0.9995	0.9992	0.9987	0.9984
$n = 9$	0.9616	0.9817	0.9883	0.9961	0.9982	0.9987	0.9993	0.9989	0.9982
$n = 10$	0.9463	0.9690	0.9828	0.9884	0.9956	0.9975	0.9980	0.9989	0.9987
$n = 11$	0.9377	0.9620	0.9776	0.9862	0.9931	0.9962	0.9979	0.9986	0.9983
$n = 12$	0.9240	0.9582	0.9745	0.9854	0.9907	0.9943	0.9970	0.9986	0.9983
$n = 13$	0.9168	0.9537	0.9741	0.9844	0.9885	0.9919	0.9953	0.9974	0.9974
$n = 14$	0.9164	0.9522	0.9719	0.9828	0.9881	0.9897	0.9926	0.9961	0.9968
$n = 15$	0.9257	0.9517	0.9723	0.9806	0.9867	0.9897	0.9929	0.9945	0.9962

Table 4: **Proportion of getting the optimum of the algorithm 2 for model 4 over the 10,000 set of data sequences in different K and n**

	$K = 0.1$	$K = 0.2$	$K = 0.3$	$K = 0.4$	$K = 0.5$	$K = 0.6$	$K = 0.7$	$K = 0.8$	$K = 0.9$
$n = 3$	1	1	1	1	1	1	1	1	1
$n = 4$	1	1	1	1	1	1	1	1	1
$n = 5$	1	1	1	1	1	1	1	1	1
$n = 6$	0.9985	0.9999	0.9998	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999
$n = 7$	0.9925	0.9981	0.9991	0.9996	0.9997	0.9995	0.9994	0.9992	0.9987
$n = 8$	0.9773	0.9917	0.9959	0.9983	0.9991	0.9991	0.9987	0.9977	0.9968
$n = 9$	0.9626	0.9807	0.9894	0.9942	0.9962	0.9981	0.9984	0.9969	0.9955
$n = 10$	0.9581	0.9759	0.9831	0.9893	0.9938	0.9968	0.9978	0.9975	0.9957
$n = 11$	0.9519	0.9698	0.9790	0.9869	0.9905	0.9948	0.9958	0.9984	0.9973
$n = 12$	0.9522	0.9658	0.9755	0.9828	0.9909	0.9934	0.9954	0.9971	0.9961
$n = 13$	0.9527	0.9677	0.9780	0.9821	0.9870	0.9917	0.9939	0.9967	0.9961
$n = 14$	0.9539	0.9676	0.9804	0.9825	0.9860	0.9906	0.9921	0.9958	0.9969
$n = 15$	0.9584	0.9709	0.9782	0.9847	0.9865	0.9888	0.9945	0.9948	0.9953

Table 5: **Mean of the ratio,** $\dfrac{E[L\,(\textbf{Algorithm 2 optimum}, \mathbf{p}) \mid \mathbf{y}]}{E[L\,(\textbf{TRUE optimum}, \mathbf{p}) \mid \mathbf{y}]}$**, for model 1 over 10,000 set of data sequences in different** K **and** n

	$K = 0.1$	$K = 0.2$	$K = 0.3$	$K = 0.4$	$K = 0.5$	$K = 0.6$	$K = 0.7$	$K = 0.8$	$K = 0.9$
$n = 3$	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$n = 4$	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$n = 5$	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$n = 6$	1.00032	1.00019	1.00010	1.00000	1.00005	1.00005	1.00002	1.00000	1.00000
$n = 7$	1.00036	1.00032	1.00016	1.00013	1.00008	1.00004	1.00004	1.00001	1.00003
$n = 8$	1.00058	1.00042	1.00019	1.00012	1.00011	1.00008	1.00005	1.00002	1.00001
$n = 9$	1.00084	1.00030	1.00017	1.00017	1.00014	1.00008	1.00006	1.00002	1.00002
$n = 10$	1.00057	1.00032	1.00010	1.00006	1.00007	1.00004	1.00003	1.00002	1.00001
$n = 11$	1.00041	1.00022	1.00007	1.00005	1.00005	1.00006	1.00004	1.00002	1.00002
$n = 12$	1.00043	1.00019	1.00010	1.00007	1.00005	1.00005	1.00001	1.00001	1.00001
$n = 13$	1.00015	1.00014	1.00008	1.00007	1.00004	1.00004	1.00002	1.00001	1.00002
$n = 14$	1.00022	1.00004	1.00002	1.00005	1.00004	1.00004	1.00001	1.00001	1.00001
$n = 15$	1.00010	1.00002	1.00002	1.00003	1.00001	1.00002	1.00000	1.00001	1.00001

Table 6: **Mean of the ratio,** $\dfrac{E[L\,(\textbf{Algorithm 2 optimum}, \mathbf{p}) \mid \mathbf{y}]}{E[L\,(\textbf{TRUE optimum}, \mathbf{p}) \mid \mathbf{y}]}$**, for model 2 over 10,000 set of data sequences in different** K **and** n

	$K = 0.1$	$K = 0.2$	$K = 0.3$	$K = 0.4$	$K = 0.5$	$K = 0.6$	$K = 0.7$	$K = 0.8$	$K = 0.9$
$n = 3$	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$n = 4$	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$n = 5$	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$n = 6$	1.00063	1.00004	1.00001	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$n = 7$	1.00508	1.00064	1.00009	1.00003	1.00001	1.00002	1.00001	1.00004	1.00006
$n = 8$	1.01201	1.00305	1.00083	1.00023	1.00005	1.00001	1.00001	1.00002	1.00008
$n = 9$	1.01520	1.00436	1.00129	1.00052	1.00016	1.00006	1.00002	1.00005	1.00011
$n = 10$	1.01813	1.00441	1.00121	1.00036	1.00011	1.00003	1.00005	1.00003	1.00006
$n = 11$	1.01723	1.00408	1.00107	1.00037	1.00012	1.00009	1.00006	1.00005	1.00004
$n = 12$	1.01816	1.00469	1.00111	1.00038	1.00020	1.00010	1.00006	1.00005	1.00003
$n = 13$	1.01764	1.00432	1.00116	1.00047	1.00026	1.00012	1.00008	1.00005	1.00004
$n = 14$	1.01568	1.00391	1.00123	1.00048	1.00022	1.00011	1.00007	1.00004	1.00005
$n = 15$	1.01733	1.00420	1.00100	1.00044	1.00018	1.00012	1.00006	1.00004	1.00003

Table 7: **Mean of the ratio,** $\dfrac{E[L\,(\textbf{Algorithm 2 optimum}, \mathbf{p}) \mid \mathbf{y}]}{E[L\,(\textbf{TRUE optimum}, \mathbf{p}) \mid \mathbf{y}]}$**, for model 3 over 10,000 set of data sequences in different** K **and** n

	$K = 0.1$	$K = 0.2$	$K = 0.3$	$K = 0.4$	$K = 0.5$	$K = 0.6$	$K = 0.7$	$K = 0.8$	$K = 0.9$
$n = 3$	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$n = 4$	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$n = 5$	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$n = 6$	1.00101	1.00017	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$n = 7$	1.00308	1.00037	1.00006	1.00000	1.00000	1.00000	1.00001	1.00004	1.00009
$n = 8$	1.00966	1.00263	1.00069	1.00015	1.00003	1.00003	1.00009	1.00014	1.00019
$n = 9$	1.01412	1.00413	1.00130	1.00023	1.00005	1.00004	1.00003	1.00005	1.00010
$n = 10$	1.01809	1.00552	1.00191	1.00061	1.00011	1.00005	1.00002	1.00003	1.00003
$n = 11$	1.01780	1.00523	1.00177	1.00065	1.00015	1.00006	1.00003	1.00002	1.00002
$n = 12$	1.01822	1.00463	1.00160	1.00059	1.00023	1.00011	1.00008	1.00004	1.00004
$n = 13$	1.02111	1.00538	1.00169	1.00066	1.00024	1.00012	1.00006	1.00003	1.00003
$n = 14$	1.01828	1.00463	1.00144	1.00054	1.00024	1.00016	1.00013	1.00006	1.00004
$n = 15$	1.01742	1.00511	1.00149	1.00060	1.00028	1.00013	1.00008	1.00007	1.00005

Table 8: **Mean of the ratio,** $\frac{E[L\,(\textbf{Algorithm 2 optimum}, \mathbf{p}) \mid \mathbf{y}]}{E[L\,(\textbf{TRUE optimum}, \mathbf{p}) \mid \mathbf{y}]}$**, for model 4 over 10,000 set of data sequences in different K and n**

	$K = 0.1$	$K = 0.2$	$K = 0.3$	$K = 0.4$	$K = 0.5$	$K = 0.6$	$K = 0.7$	$K = 0.8$	$K = 0.9$
$n = 3$	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$n = 4$	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$n = 5$	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$n = 6$	1.00025	1.00000	1.00001	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$n = 7$	1.00104	1.00013	1.00003	1.00001	1.00000	1.00000	1.00000	1.00000	1.00007
$n = 8$	1.00455	1.00119	1.00037	1.00007	1.00002	1.00003	1.00011	1.00020	1.00015
$n = 9$	1.00786	1.00243	1.00088	1.00023	1.00006	1.00004	1.00006	1.00011	1.00014
$n = 10$	1.00914	1.00312	1.00112	1.00037	1.00013	1.00005	1.00005	1.00013	1.00016
$n = 11$	1.01060	1.00332	1.00128	1.00048	1.00020	1.00008	1.00005	1.00005	1.00008
$n = 12$	1.00960	1.00325	1.00132	1.00049	1.00018	1.00011	1.00008	1.00005	1.00008
$n = 13$	1.00849	1.00257	1.00092	1.00046	1.00026	1.00013	1.00005	1.00003	1.00006
$n = 14$	1.00767	1.00268	1.00095	1.00049	1.00024	1.00011	1.00008	1.00003	1.00002
$n = 15$	1.00708	1.00201	1.00084	1.00035	1.00019	1.00013	1.00004	1.00004	1.00004

(BH) and the loss function (Algorithm 2), using simulated data from models 1–4. Similarly to the simulation study in section 3.3.1, we take 100 sets of data from each of the models 1–4, each with $n = 100$ data points. We fit the model (5) with the Dirichlet Process prior. The parameters are assigned to be $\theta = 1, a_0 = 1, b_0 = 0.01, \mathbf{m}_0 = [0 \cdots 0]', \mathbf{t}_0 = 0.01\mathbf{I}$.

For the stochastic search method, we run the Gibbs version of WCR for 20000 cycles. We record the partition of greatest posterior probability among all 20000 cycles. We then use algorithm 2 based on the last 10,000 MCMC samples, following 10,000 burn-in to produce the ρ matrix. We run algorithm 2 and the ℓ functions (defined by equation (14)) to get the point estimates for $K \in \{0.1, 0.2, \ldots, 0.9\}$. Figure 12 compares log posterior probabilities $\log(\phi(\mathbf{p}))$ for the partitions produced by the three procedures, stochastic search (SS), Bayesian hierarchical clustering procedure (BH) and the loss function method (Algorithm 2). As expected, the results show that the approximate MAP methods tend to yield higher probability partitions, with SS outperforming BH on average. However, to an extent increasing with the number of components in the simulation of the data, the loss function approach nevertheless produces higher probability partitions for a substantial proportion of the data sets.

On the other hand, Figure 13 compares the quantity $\ell(\mathbf{p}, K)$ for the partitions produced by the three procedures. The results show that the loss function nethod (Algorithm 2) always yields partitions with lower posterior expected loss than the approximate MAP methods, particularly for larget values of K. Among the methods inferior by this criterion, SS is again slightly superior to BH, although for smaller values of K, all three methods perform very similarly.

4.3.3 Optimal partition of galaxy and leukaemia data sets

Now we consider the galaxy data. We calculate the ρ matrix based on the last 10000 partitions sampled. We run algorithm 2 and the ℓ functions (defined by equation (14)) for the partitions in $\mathcal{P}$ are plotted in Figure 14. Here we can see that we have the same best partition for all $K \in [0.1, 0.9]$. Moreover, this partition is the same as that found by SS and BH, and we conclude that for this data set, the optimal partition for such values of K coincides with the maximum a posteriori partition.

Finally we present the case of the Leukaemia data. Figure 15 shows $\ell(\mathcal{P}, K)$ over the interval

Figure 12: **Comparisons among SS, BH and Loss function approach under Model 1–4 based on** $\log(\phi(\mathbf{p}))$

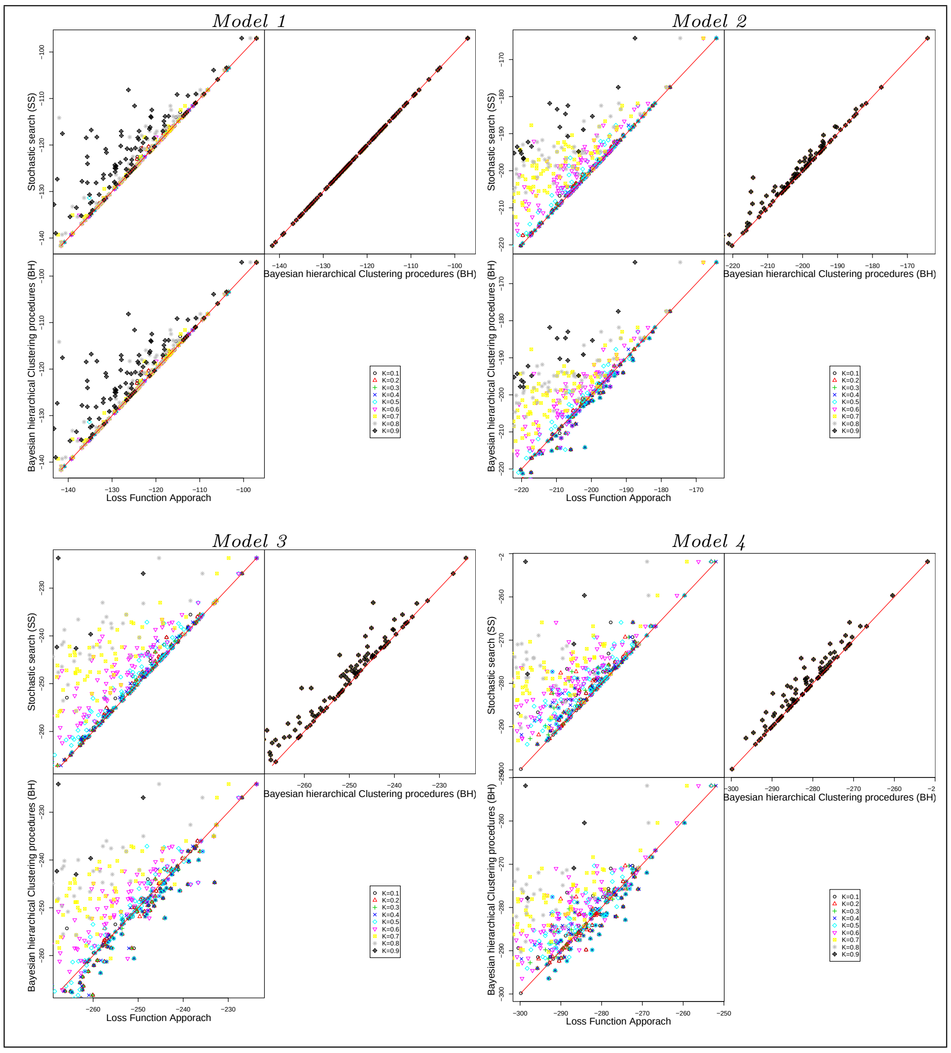


Figure 13: **Comparisons among SS, BH and Loss function approach under Model 1–4 based on $\ell(\mathbf{p}, K)$**

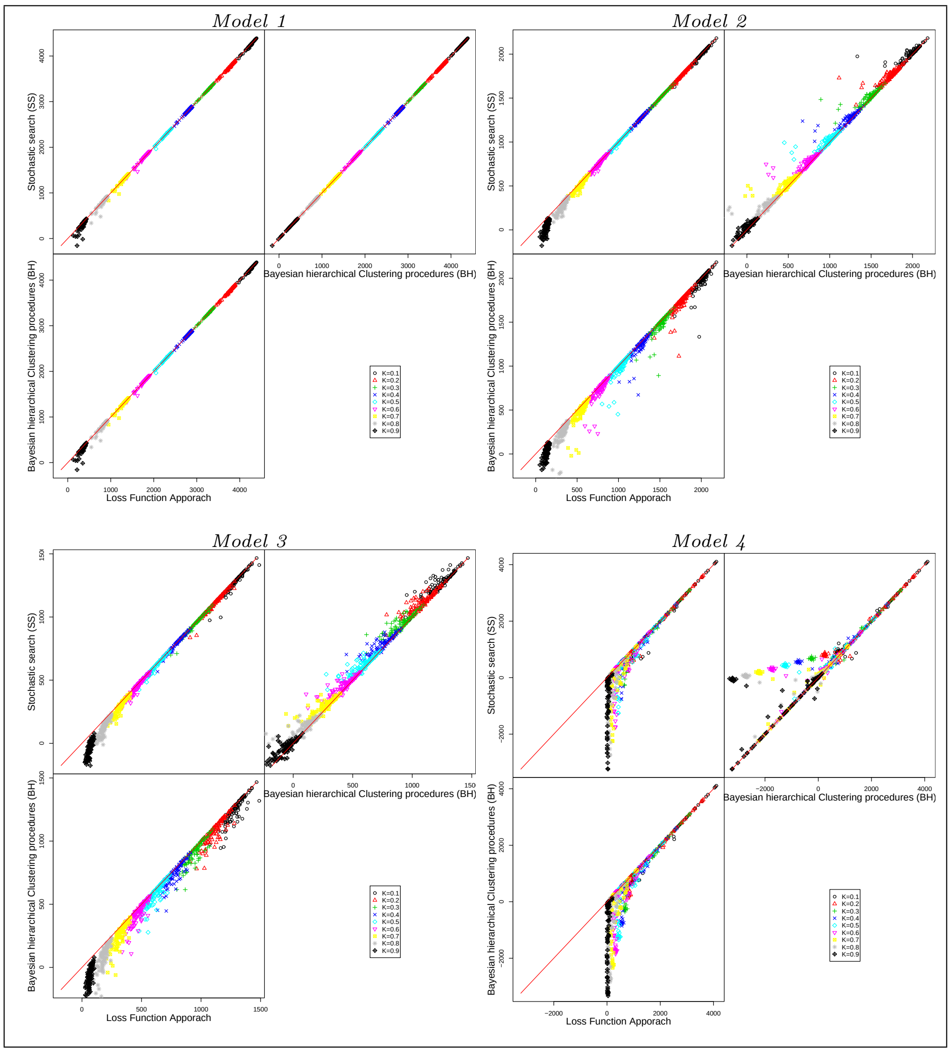


Figure 14: $\ell(\mathcal{P}, K)$ **vs** K **for the galaxy data**

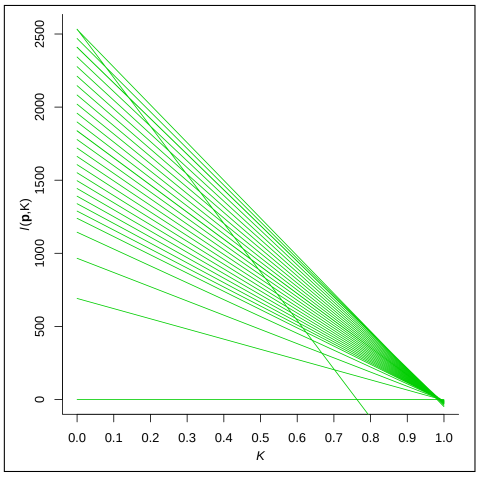
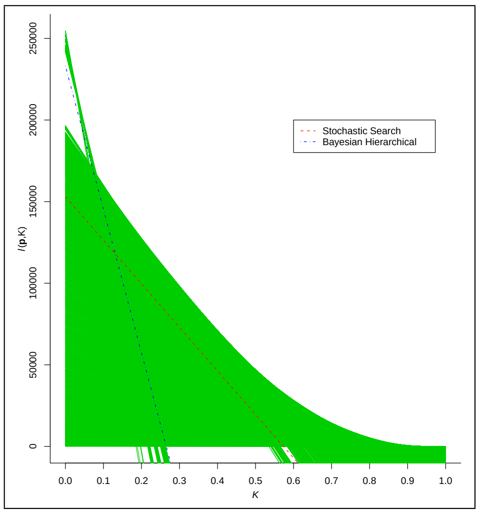


Figure 15: $\ell(\mathcal{P}, K)$ **vs** K **for the Leukaemia data**



[0,1]. We also plot the ℓ functions for the partitions produced by the SS and BH procedures. For this loss function, these approximate maximum a posteriori partitions are not optimal whatever the value of K, although the result from the BH procedure is close to optimal for $K \approx 0.08$. We calculate $\log(\phi(\mathbf{p}))$ for the partitions generated by the algorithm for different Ks, Table 9. Interestingly, for $K = 0.1, 0.2, 0.3$, the highest posterior probability partitions are produced by our algorithm! In this example, our algorithm produces the best partitions under both the MAP and loss function criteria.

Table 9: $\log(\phi(\mathbf{p}))$ **of partitions of SS, BH and algorithm 2**

K	$\log(\phi(\mathbf{p}))$
$K = .1$	-262774.69
$K = .2$	-262744.51
$K = .3$	-262753.13
$K = .4$	-263451.11
$K = .5$	-265768.95
$K = .6$	-270588.76
$K = .7$	-274760.07
$K = .8$	-279583.08
$K = .9$	-286715.36
SS	-263040.69
BH	-263793.14

5 Acknowledgements

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6 Appendix

6.1 Proof of equation (11)

We first consider the ratio used to combine two clusters, say C_{j_1} and C_{j_2},

$$\frac{m\left(\mathbf{y}_{C_{j_1}\cup C_{j_2}}\right)}{m\left(\mathbf{y}_{C_{j_1}}\right)m\left(\mathbf{y}_{C_{j_2}}\right)} = e^{-\left[\psi\left(\mathbf{y}_{C_{j_1}\cup C_{j_2}}\right)-\psi\left(\mathbf{y}_{C_{j_1}}\right)-\psi\left(\mathbf{y}_{C_{j_2}}\right)\right]}$$

and the exponent term is now,

$$\begin{aligned}
& \psi\left(\mathbf{y}_{C_{j_1}\cup C_{j_2}}\right) - \psi\left(\mathbf{y}_{C_{j_1}}\right) - \psi\left(\mathbf{y}_{C_{j_2}}\right) \\
= \quad & \sum_{i\in C_{j_1}\cup C_{j_2}}^{n} \left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_{j_1}\cup C_{j_2}}\right)'\left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_{j_1}\cup C_{j_2}}\right) - \sum_{i\in C_{j_1}}^{n} \left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_{j_1}}\right)'\left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_{j_1}}\right) - \sum_{i\in C_{j_2}}^{n} \left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_{j_2}}\right)'\left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_{j_2}}\right) \\
= \quad & \sum_{i\in C_{j_1}}^{n} \left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_{j_1}\cup C_{j_2}}\right)'\left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_{j_1}\cup C_{j_2}}\right) - \sum_{i\in C_{j_1}}^{n} \left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_{j_1}}\right)'\left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_{j_1}}\right) \\
& + \sum_{i\in C_{j_2}}^{n} \left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_{j_1}\cup C_{j_2}}\right)'\left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_{j_1}\cup C_{j_2}}\right) - \sum_{i\in C_{j_2}}^{n} \left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_{j_2}}\right)'\left(\mathbf{y}_i - \bar{\mathbf{y}}_{C_{j_2}}\right) \\
= \quad & e_{j_1}\left(\bar{\mathbf{y}}_{C_{j_1}} - \bar{\mathbf{y}}_{C_{j_1}\cup C_{j_2}}\right)'\left(\bar{\mathbf{y}}_{C_{j_1}} - \bar{\mathbf{y}}_{C_{j_1}\cup C_{j_2}}\right) + e_{j_2}\left(\bar{\mathbf{y}}_{C_{j_2}} - \bar{\mathbf{y}}_{C_{j_1}\cup C_{j_2}}\right)'\left(\bar{\mathbf{y}}_{C_{j_2}} - \bar{\mathbf{y}}_{C_{j_1}\cup C_{j_2}}\right) \\
= \quad & e_{j_1}\bar{\mathbf{y}}'_{C_{j_1}}\bar{\mathbf{y}}_{C_{j_1}} + e_{j_2}\bar{\mathbf{y}}'_{C_{j_2}}\bar{\mathbf{y}}_{C_{j_2}} - \left(e_{j_1} + e_{j_2}\right)\bar{\mathbf{y}}'_{C_{j_1}\cup C_{j_2}}\bar{\mathbf{y}}_{C_{j_1}\cup C_{j_2}} \\
= \quad & \frac{e_{j_1}e_{j_2}}{e_{j_1} + e_{j_2}}\left(\bar{\mathbf{y}}_{C_{j_1}} - \bar{\mathbf{y}}_{C_{j_2}}\right)'\left(\bar{\mathbf{y}}_{C_{j_1}} - \bar{\mathbf{y}}_{C_{j_2}}\right)
\end{aligned}$$

The equality will be useful,

$$\begin{aligned}
&\sum_{i\in C_{j_1}\cup C_{j_2}}^{n}\left(\mathbf{y}_i-\bar{\mathbf{y}}_{C_{j_1}\cup C_{j_2}}\right)'\left(\mathbf{y}_i-\bar{\mathbf{y}}_{C_{j_1}\cup C_{j_2}}\right)\\
&\quad-\sum_{i\in C_{j_1}}^{n}\left(\mathbf{y}_i-\bar{\mathbf{y}}_{C_{j_1}}\right)'\left(\mathbf{y}_i-\bar{\mathbf{y}}_{C_{j_1}}\right)-\sum_{i\in C_{j_2}}^{n}\left(\mathbf{y}_i-\bar{\mathbf{y}}_{C_{j_2}}\right)'\left(\mathbf{y}_i-\bar{\mathbf{y}}_{C_{j_2}}\right)\\
&\qquad=\frac{e_{j_1}e_{j_2}}{e_{j_1}+e_{j_2}}\left(\bar{\mathbf{y}}_{C_{j_1}}-\bar{\mathbf{y}}_{C_{j_2}}\right)'\left(\bar{\mathbf{y}}_{C_{j_1}}-\bar{\mathbf{y}}_{C_{j_2}}\right)
\end{aligned}\tag{17}$$

6.2 Proof of equation (12)

Similar to the proof of (11), we need only consider the exponent term. In this case we first prove an equality

$$\begin{aligned}
&\sum_{i_1\in C_{j_1}}\sum_{i_2\in C_{j_2}}\left(\mathbf{y}_{i_1}-\mathbf{y}_{i_2}\right)'\left(\mathbf{y}_{i_1}-\mathbf{y}_{i_2}\right)\\
=&\sum_{i_1\in C_{j_1}}\sum_{i_2\in C_{j_2}}\left(\mathbf{y}_{i_1}-\bar{\mathbf{y}}_{C_{j_1}}+\bar{\mathbf{y}}_{C_{j_1}}-\bar{\mathbf{y}}_{C_{j_2}}+\bar{\mathbf{y}}_{C_{j_2}}-\mathbf{y}_{i_2}\right)'\left(\mathbf{y}_{i_1}-\bar{\mathbf{y}}_{C_{j_1}}+\bar{\mathbf{y}}_{C_{j_1}}-\bar{\mathbf{y}}_{C_{j_2}}+\bar{\mathbf{y}}_{C_{j_2}}-\mathbf{y}_{i_2}\right)\\
=&\ e_{j_2}\sum_{i_1\in C_{j_1}}\left(\mathbf{y}_{i_1}-\bar{\mathbf{y}}_{C_{j_1}}\right)'\left(\mathbf{y}_{i_1}-\bar{\mathbf{y}}_{C_{j_1}}\right)+e_{j_1}e_{j_2}\left(\bar{\mathbf{y}}_{C_{j_1}}-\bar{\mathbf{y}}_{C_{j_2}}\right)'\left(\bar{\mathbf{y}}_{C_{j_1}}-\bar{\mathbf{y}}_{C_{j_2}}\right)\\
&+e_{j_1}\sum_{i_2\in C_{j_2}}\left(\bar{\mathbf{y}}_{C_{j_2}}-\mathbf{y}_{i_2}\right)'\left(\bar{\mathbf{y}}_{C_{j_2}}-\mathbf{y}_{i_2}\right)
\end{aligned}$$

This is combined with the equality (17),

$$\begin{aligned}
&\psi\left(\mathbf{y}_{C_{j_1}\cup C_{j_2}}\right)-\psi\left(\mathbf{y}_{C_{j_1}}\right)-\psi\left(\mathbf{y}_{C_{j_2}}\right)\\
=&\left(e_{j_1}+e_{j_2}\right)\sum_{i\in C_{j_1}\cup C_{j_2}}\left(\mathbf{y}_i-\bar{\mathbf{y}}_{C_{j_1}\cup C_{j_2}}\right)'\left(\mathbf{y}_i-\bar{\mathbf{y}}_{C_{j_1}\cup C_{j_2}}\right)\\
&\quad-e_{j_1}\sum_{i\in C_{j_1}}\left(\mathbf{y}_i-\bar{\mathbf{y}}_{C_{j_1}}\right)'\left(\mathbf{y}_i-\bar{\mathbf{y}}_{C_{j_1}}\right)-e_{j_2}\sum_{i\in C_{j_2}}\left(\mathbf{y}_i-\bar{\mathbf{y}}_{C_{j_2}}\right)'\left(\mathbf{y}_i-\bar{\mathbf{y}}_{C_{j_2}}\right)\\
=&\sum_{i_1\in C_{j_1}}\sum_{i_2\in C_{j_2}}\left(\mathbf{y}_{i_1}-\mathbf{y}_{i_2}\right)'\left(\mathbf{y}_{i_1}-\mathbf{y}_{i_2}\right)\\
=&\sum_{i_1\in C_{j_1}}\sum_{i_2\in C_{j_2}}d_{i_1,i_2}
\end{aligned}$$

6.3 Proof of equation (13)

Again we consider only the exponent term. We first prove

$$\begin{aligned}
& \psi\left(\mathbf{y}_{C_{j_1}\cup C_{j_2}}\right) - \psi\left(\mathbf{y}_{C_{j_1}}\right) - \psi\left(\mathbf{y}_{C_{j_2}}\right) \\
= & \sum_{i\in C_{j_1}\cup C_{j_2}} \left(\mathbf{y}_i - [\mathbf{x}_1\cdots\mathbf{x}_S]'\hat{\boldsymbol{\beta}}_{C_{j_1}\cup C_{j_2}}\right)'\left(\mathbf{y}_i - [\mathbf{x}_1\cdots\mathbf{x}_S]'\hat{\boldsymbol{\beta}}_{C_{j_1}\cup C_{j_2}}\right) \\
& \quad - \sum_{i\in C_{j_1}} \left(\mathbf{y}_i - [\mathbf{x}_1\cdots\mathbf{x}_S]'\hat{\boldsymbol{\beta}}_{C_{j_1}}\right)'\left(\mathbf{y}_i - [\mathbf{x}_1\cdots\mathbf{x}_S]'\hat{\boldsymbol{\beta}}_{C_{j_1}}\right) \\
& \quad - \sum_{i\in C_{j_2}} \left(\mathbf{y}_i - [\mathbf{x}_1\cdots\mathbf{x}_S]'\hat{\boldsymbol{\beta}}_{C_{j_2}}\right)'\left(\mathbf{y}_i - [\mathbf{x}_1\cdots\mathbf{x}_S]'\hat{\boldsymbol{\beta}}_{C_{j_2}}\right) \\
= & \sum_{i\in C_{j_1}} \left([\mathbf{x}_1\cdots\mathbf{x}_S]'\hat{\boldsymbol{\beta}}_{C_{j_1}} - [\mathbf{x}_1\cdots\mathbf{x}_S]'\hat{\boldsymbol{\beta}}_{C_{j_1}\cup C_{j_2}}\right)'\left([\mathbf{x}_1\cdots\mathbf{x}_S]'\hat{\boldsymbol{\beta}}_{C_{j_1}} - [\mathbf{x}_1\cdots\mathbf{x}_S]'\hat{\boldsymbol{\beta}}_{C_{j_1}\cup C_{j_2}}\right) \\
& \quad + \sum_{i\in C_{j_2}} \left([\mathbf{x}_1\cdots\mathbf{x}_S]'\hat{\boldsymbol{\beta}}_{C_{j_2}} - [\mathbf{x}_1\cdots\mathbf{x}_S]'\hat{\boldsymbol{\beta}}_{C_{j_1}\cup C_{j_2}}\right)'\left([\mathbf{x}_1\cdots\mathbf{x}_S]'\hat{\boldsymbol{\beta}}_{C_{j_2}} - [\mathbf{x}_1\cdots\mathbf{x}_S]'\hat{\boldsymbol{\beta}}_{C_{j_1}\cup C_{j_2}}\right) \\
= & \hat{\boldsymbol{\beta}}'_{C_{j_1}}\mathbf{X}'_{C_{j_1}}\mathbf{X}_{C_{j_1}}\hat{\boldsymbol{\beta}}_{C_{j_1}} + \hat{\boldsymbol{\beta}}'_{C_{j_2}}\mathbf{X}'_{C_{j_2}}\mathbf{X}_{C_{j_2}}\hat{\boldsymbol{\beta}}_{C_{j_2}} - \hat{\boldsymbol{\beta}}'_{C_{j_1}\cup C_{j_2}}\left(\mathbf{X}'_{C_{j_1}}\mathbf{X}_{C_{j_1}} + \mathbf{X}'_{C_{j_2}}\mathbf{X}_{C_{j_2}}\right)\hat{\boldsymbol{\beta}}_{C_{j_1}\cup C_{j_2}} \\
= & \left(\hat{\boldsymbol{\beta}}_{C_{j_1}} - \hat{\boldsymbol{\beta}}_{C_{j_2}}\right)'\left[\left(\mathbf{X}'_{C_{j_1}}\mathbf{X}_{C_{j_1}}\right)^{-1} + \left(\mathbf{X}'_{C_{j_2}}\mathbf{X}_{C_{j_2}}\right)^{-1}\right]^{-1}\left(\hat{\boldsymbol{\beta}}_{C_{j_1}} - \hat{\boldsymbol{\beta}}_{C_{j_2}}\right)
\end{aligned}$$

Note that

$$\mathbf{X}'_{C_{j_1}}\mathbf{X}_{C_{j_1}} = \sum_{i\in C_{j_1}} [\mathbf{x}_1\cdots\mathbf{x}_S][\mathbf{x}_1\cdots\mathbf{x}_S]' \text{ and } \mathbf{X}'_{C_{j_2}}\mathbf{X}_{C_{j_2}} = \sum_{i\in C_{j_2}} [\mathbf{x}_1\cdots\mathbf{x}_S][\mathbf{x}_1\cdots\mathbf{x}_S]'$$

7 References

Antoniak, C. E. (1974). Mixtures of Dirichlet processes with applications to Bayesian nonparametric problems. *The Annals of Statistics*, **2**, 1152–1174.

Banfield, J. D., and Raftery, A. E. (1993). Model-based Gaussian and mon-Gaussian clustering. *Biometrics*, **49**, 803–821

Bansal, N., Blum, A., and Chawla, S. (2004). Correlation clustering. *Machine Learning*, **56**, 89–113.

Barry, D., and Hartigan, J. A. (1992). Product partition models for change point problems. *The Annals of Statistics*, **20**, 260–279

Binder, D. A. (1978). Bayesian cluster analysis. *Biometrika*, **65**, 31–38

Binder, D. A. (1981). Approximations to Bayesian clustering rules. *Biometrika*, **68**, 275–285

Blackwell, D., and MacQueen, J. B. (1973). Ferguson distribution via Pólya Urn Scheme. *The Annals of Statistics*, **1**, 353–355.

Brunner, L. J., and Lo, A. Y. (1999). Bayesian classifications. *Preprint, University of Toronto, Canada.* Available at `http://www.erin.utoronto.ca/~jbrunner/papers/BayesClass.pdf`

de Finetti, B. (1930). Funzione caratteristica di un fenomeno aleatorio. *Atti Reale Accademia Nazionale dei Lincei, Mem.* **4**, 86–133.

de Finetti, B. (1974). *Theory of Probability 1.* Wiley.

Diaconis, P., and Freedman, D. (1984). Partial exchangeability and sufficiency. in *Statistics: Applications and New Directions, eds. J. K. Ghosh and J. Roy.* 205–236.

Diaconis, P., and Freedman, D. (1987). A dozen de Finetti-style results in search of a theory. *Annales de l'Institut Henri Poincaré (B) Probabilités et Statistiques*, **23**, 397–423.

Escobar, M. D., and West, M. (1995). Bayesian density estimation and inference using mixtures. *Journal of the American Statistical Association*, **90**, 577–588.

Escobar, M. D., and West, M. (1998). Computing monparametric hierarchical models. in *Practical Nonparametric and Semiparametric Bayesian Statistics, eds. D. Dey, P. Müller, and D. Sinha, New York: Springer*, 1–22.

Ferguson, T. S. (1973). A Bayesian analysis of some nonparametric problems. *The Annals of Statistics*, **1**, 209–230.

Fraley, C., and Raftery, A. E. (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association*, **97**, 611–631.

Golub, T. R., Slonim, D. K., Tamayo, P., Huard, C., Gaasenbeek, M., Mesirov, J. P., Coller, H., Loh, M. L., Downing, J. R., Caligiuri, M. A., Bloomfield, C. D., and Lander, E. S. (1999). Molecular classification of cancer: class discovery and class prediction by gene expression monitoring. *Science*, **286**, 531–537.

Gordon, A. D. (1999). *Classification*, 2nd edition. Chapman & Hall.

Green, P. J., and Richardson, S. (2001). Modelling heterogeneity with and without the Dirichlet process. *Scandinavian Journal of Statistics*, **28**, 355–375.

Hartigan, J. A. (1990). Partition models. *Communications in statistics – Simulation and computation*, **19**, 2745–2756.

Heard, N. A., Holmes, C. C., and Stephens, D. A. (2005). A quantitative study of gene regulation involved in the immune response of Anopheline mosquitoes: an application of Bayesian hierarchical clustering of curves. *Journal of the American Statistical Association*, to appear.

Hewitt, E., and Savage, L. J. (1955). Symmetric measures on Cartesian products. *Transactions of the American Mathematical Society*, **80**, 470–501

Hurn, M., Justel, A., and Robert, C. P. (2003). Estimating mixtures of regressions. *Journal of Computational and Graphical Statistics*, **12**, 55–79

Ishwaran, H., and James, L. F. (2001). Gibbs sampling methods for stick-breaking priors. *Journal of the American Statistical Association*, **96**, 161–173.

Ishwaran, H., and James, L. F. (2003a). Generalized weighted Chinese restaurant processes for species sampling mixture models, *Statistica Sinica* **13** 1211–1235.

Ishwaran, H., and James, L. F. (2003b). Some further developments for stick-breaking priors: finite and infinite clustering and classification. *Sankhya Series A*, **65**, 577–592.

James, L. F. (2002). Poisson process partition calculus with applications to exchangeable models and Bayesian Nonparametrics. Available at `http://arXiv.org/abs/math/0205093`

James, L. F. (2005). Bayesian Poisson process partition calculus with an application to Bayesian Levy moving averages. *The Annals of Statistics*, **33**, 1771–1799.

James, L. F., Lijoi, A. and Prüenster, I. (2005) Bayesian inference for classes of normalized random measures. Avaiable at `http://arxiv.org/abs/math.ST/0503394`

Kingman, J. F. C. (1975). Random discrete distributions. *Journal of the Royal Statistical Society: Series B*, **37**, 1–22

Kingman, J. F. C. (1993). *Poisson Processes*, Oxford University Press.

Lijoi, A., Mena, R. H., and Prünster, I. (2005). Hierarchical mixture modeling with normalized inverse-Gaussian priors. *Journal of the American Statistical Association*, **14**, 1278–1291.

Lo, A. Y. (1984). On a class of Bayesian nonparametric estimates. I. Density estimates. *The Annals of Statistics*, **12**, 351–357.

Lo, A. Y. (2005). Weighted Chinese restaurant processes. *COSMOS*, **1**, 59–63.

Lo, A. Y., Brunner, L. J. and Chan, A. T. (1996). Weighted Chinese restaurant processes and Bayesian mixture models. *Research Report, Hong Kong University of Science and Technology.* Available at `http://www.erin.utoronto.ca/~jbrunner/papers/wcr96.pdf`

MacEachern, S. N. (1994). Estimating normal means with a conjugate style Dirichlet process prior. *Communications in statistics – Simulation and computation*, **23**, 727–741.

MacEachern, S. N., and Müller, P. (1998). Estimating mixture of Dirichlet process models. *Journal of Computational and Graphical Statistics* , **7**, 223–238

MacEachern, S. N., and Müller, P. (2000). Efficient MCMC schemes for robust model extensions using encompassing Dirichlet process mixture models. *Robust Bayesian analysis*, 295–315.

Medvedovic, M., and Sivaganesan, S. (2002). Bayesian infinite mixture model based clustering of gene expression profiles. *Bioformatics*, **18**, 1194–1206.

Medvedovic, M., Yeung, K. Y., and Bumgarner, R. E. (2004). Bayesian mixture model based clustering of replicated microarray data. *Bioformatics*, **20**, 1222–1232.

Neal, R. M. (2000). Markov chain sampling methods for Dirichlet process mixture models. *Journal of Computational and Graphical Statistics*, **9**, 249–265.

Nobile, A., and Fearnside, A. (2005). Bayesian finite mixtures with an unknown number of components: the allocation sampler. *Technical Report 05-4, University of Glasgow.* Avaiable at: `http://www.stats.gla.ac.uk/~agostino/mixalloc.pdf`

Pitman, J. (1995). Exchangeable and partially exchangeable random partitions. *Probability Theory and Related Fields*, **102**, 145–158

Pitman, J. (1996). Some developments of the Blackwell–MacQueen urn scheme. *Statistics, Probability and Game Theory. Papers in honor of David Blackwell*, 245–267

Pitman, J. (2003). Poisson Kingman partitions. Available at `http://arxiv.org/abs/math/0210396`

Pitman, J., and Yor, M. (1997). The two-parameter Poisson–Dirichlet distribution derived from a stable subordinator. *The Annals of Probability*, **25**, 855–900.

Quintana F. A., and Iglesias P. L. (2003). Bayesian clustering and product partition models. *Journal of the Royal Statistical Society: Series B*, **65**, 557–574

Richardson, S., and Green, P. J. (1997). On Bayesian analysis of mixtures with an unknown number of components (with discussion). *Journal of the Royal Statistical Society: Series B*, **59**, 731–792.

Roeder, K. (1990). Density estimation with confidence sets exemplified by superclusters and voids in the galaxies. *Journal of the American Statistical Association*, **85**, 617–624.

West, M., Müller, P., and Escobar, M. D. (1994). Hierarchical priors and mixture models, with applications in regression and density estimation. in *A tribute to D. V. Lindley, eds. A. F. M Smith and P. R. Freeman, New York: Wiley.*

Ward, J. H. (1963). Hierarchical grouping to optimize an objective function. *Journal of the American Statistical Association*, **58**, 236–244.

Yeung, K. Y., Fraley, C., Murua, A., Raftery, A. E., and Ruzzo, W. L. (2001). Model-based clustering and data transformations for gene expression data. *Bioinformatics*, **17**, 977–987.