# Exact posterior distributions over the segmentation space and model selection for multiple change-point detection problems

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#### Abstract

In segmentation problems, inference on change-point position and model selection are two difficult issues due to the discrete nature of change-points. In a Bayesian context, we derive exact, nonasymptotic, explicit and tractable formulae for the posterior distribution of variables such as the number of change-points or their positions. We also derive a new selection criterion that accounts for the reliability of the results. All these results are based on an efficient strategy to explore the whole segmentation space, which is very large. We illustrate our methodology on both simulated data and a comparative genomic hybridisation profile.

Keywords: BIC, change-point detection, ICL, model selection, posterior distribution of change-points

Short title: Posterior distribution over the segmentation space

# 1 Introduction

Segmentation and change-point detection problems arise in many scientific domains such as econometrics, climatology, agronomy or molecular biology. The general problem can be written as follows. It is assumed that the observed data  $\{y_t\}_{t=1,...,n}$  is a realization of an independent random process  $Y = \{Y_t\}_{t=1,...,n}$ . This process is drawn from a probability distribution G, which depends on a set of parameters denoted by  $\theta$ . These parameters are assumed to be affected by K - 1 abrupt changes, called change-points, at some unknown positions  $\tau_2, \ldots, \tau_K$  (with the convention  $\tau_1 = 1$  and  $\tau_{K+1} = n + 1$ ). Thus, the change-points delimit a partition m of  $\{1, \ldots, n\}$ , called here a segmentation, into K segments  $r^{(k)}$  such that  $r^{(k)} = [\![\tau_k, \tau_{k+1}]\![= \{\tau_k, \tau_k + 1, \ldots, \tau_{k+1} - 1\}$  and

$$m = \{r^{(k)}\}_{k=1,\dots,K}$$

The segmentation model has the following general form for a given m:

$$Y_t \sim G(\theta_r)$$
 if  $t \in r$  and  $r \in m$ 

where  $\theta_r$  stands for the parameters of segment r. In this study, all the change-points are detected simultaneously, a strategy called off-line detection (as opposed to on-line detection). With this strategy, the question of finding the best segmentation in a given number of segments has already been largely studied (see for example Lavielle (2005), Braun and Müller (2000), Bai and Perron (2003)). But two important issues remain: assessing the quality of the proposed segmentation and selecting the number of segments (also called dimension). In both cases, the main problem is the discrete nature of the change-points, which prevents the use of routine statistical inference. On the one hand, the quality of a given segmentation can be assessed by studying the uncertainty of the change-point positions. From a non-asymptotic and non-parametric point of view, the standard likelihood-based inference is very intricate, since the required regularity conditions for the change-point parameters are not satisfied (Feder (1975)). Different methods to obtain change-point confidence intervals have been proposed. Most of them are based on the limit distribution of the change-point estimators (Feder (1975), Bai and Perron (2003)) or the asymptotic use of a likelihood-ratio statistic (Muggeo (2003)). Others proposed confidence intervals are based on bootstrap techniques (Husková and Kirch (2008) and references therein). A practical comparison of these methods can be found in Toms and Lesperance (2003).

On the other hand, choosing the number of segments is also a critical issue. This is usually done by minimising a penalised contrast function and the problem is to find a good penalty. General penalized criteria have been developed, such as AIC (Akaike (1973)) and BIC (Schwarz (1978)). In the segmentation framework, these criteria are not adapted since an exponential model collection is considered (Birgé and Massart (2007), Baraud *et al.* (2009)) and these criteria tend to overestimate the number of segments (see for example Lavielle (2005)). Recently, some penalised criteria have been proposed specially for the segmentation framework. Some depend on constants to be calibrated (Lavielle (2005) and Lebarbier (2005)), but others do not (Zhang and Siegmund (2007)). More precisely, Zhang and Siegmund (2007) discussed the fact that the classical BIC was not theoretically justified in the segmentation context. Indeed, the BIC criterion is derived from an asymptotic approximation of the posterior model probabilities and requires the likelihood function to be three times differentiable with respect to the parameters of the model (Kass and Raftery (1995), Lebarbier and Mary-Huard (2006)). As the change-points are discrete parameters, the previous condition is not satisfied. A modified BIC criterion has thus been developed by Zhang and Siegmund (2007) by considering a continuous-time version of the problem.

The purpose of our work is to provide exact, non-asymptotic, explicit and tractable formulae for both the posterior probability of a segmentation and that of a change-point occurring at a given position. More specifically, we consider the segmentation problem in a Bayesian framework so that the posterior probability of a segmentation is well defined. To tackle the discrete nature of change-points, we work at the segment level, where statistical inference is straightforward. From these segments, the issue is to get back to the segmentation or dimension level. Provided that the segments are independent, it will be necessary to calculate quantities such as:

$$\sum_{m \in \mathcal{M}^{\star}} P(Y|m)P(m) = \sum_{m \in \mathcal{M}^{\star}} P(m) \prod_{r \in m} P(Y^{r}|r)$$
(1)

where  $Y^r$  stands for all observations in segment r and  $\mathcal{M}^*$  is usually a very large set of segmentations. We propose a close-form (in terms of matrix products) and tractable formulation of such quantities. Some similar quantities were computed by Guédon (2008) in a non-Bayesian context, using a forwardbackward-like algorithm. However, this author computes all these quantities for fixed values of the segment parameters, which are the maximum likelihood estimators. From our formula, we derive key quantities to assess the quality of a segmentation and select the number of segments.

On the one hand, we obtain the exact formulae for both the posterior probability of a segmentation and that of a change-point occurring at a given position. This enables the construction of credibility intervals for change-points. Moreover, we retrieve the exact posterior probability of a segment within a given dimension, the exact entropy of the posterior distribution of the segmentations within a given dimension and the exact posterior mean of the signal.

On the other hand, we derive a so-called 'exact' BIC criterion for choosing the number of segments K, taking  $\mathcal{M}^{\star} = \mathcal{M}_{K}$  which is the set of all possible segmentations with K segments. In the same way, we derive the ICL criterion of Biernacki *et al.* (2000) in the segmentation framework. This last criterion takes into account the reliability of the results.

In Section 2, we give some exact formulae to explore the segmentation space and assess the quality of a segmentation. In Section 3, we focus on the model selection problem: we derive an exact BIC criterion and propose a new ICL criterion. In the last section, we illustrate our results first on Poisson simulated data and second on comparative genomic hybridization (CGH) data in a Gaussian framework.

# 2 Exploring the segmentation space

A naive computation of (1) is impossible when  $\mathcal{M}^*$  is large, which is usually the case. For example, if  $\mathcal{M}^* = \mathcal{M}_K$ , there are  $\binom{n-1}{K-1}$  segmentations of n data into K segments. In this section we propose a tractable and close-form formula of (1). The following assumption enables us to derive an exact matrix product formulation of (1) enabling its straightforward computation in  $O(Kn^2)$  time.

Factorability assumption: A model satisfies the factorability assumption if

$$(\mathbf{H}): P(Y,m) = C \prod_{r \in m} a_r P(Y^r | r)$$
(2)

where  $P(Y^r|r) = \int P(Y^r|\theta_r)P(\theta_r)d\theta_r$ . In the following, for the sake of clarity, we will simply denote  $P(Y^r)$ . This is true when all segment parameters are different but this is false, for example, for the normal homoscedastic model  $G(\theta_r) = \mathcal{N}(\mu_r, 1/\tau)$  with unknown precision  $\tau$ .

We denote by  $\mathcal{M}_K(\llbracket i, j \rrbracket)$  the set of all possible segmentations of  $\llbracket i, j \rrbracket$  into K segments. The simplified notation  $\mathcal{M}_K$  refers to  $\mathcal{M}_K(\llbracket 1, n+1 \rrbracket)$ .

**Theorem 2.1** Consider a function F such that, for all  $k \in [\![1,K]\!]$  and for all segmentation  $m \in \mathcal{M}_k([\![1,j]\!])$  (for  $1 \leq j \leq n+1$ ), there exists a function f such that:  $F(m) = \prod_{r \in m} f(r)$ . Let  $\mathbf{A}$  be a square matrix with n+1 columns such that

$$\begin{aligned} \mathbf{A}_{ij} &= f(\llbracket i, j \rrbracket) & \quad if \ 1 \leq i < j \leq n+1 \\ &= 0 & \quad otherwise. \end{aligned}$$

Then,

$$\sum_{m \in \mathcal{M}_k(\llbracket 1, j \rrbracket)} F(m) = (\mathbf{A}^k)_{1,j}$$

and the  $K \times (n+1)$  elements of

$$\left\{\sum_{m \in \mathcal{M}_k(\llbracket 1, j \rrbracket)} F(m)\right\}_{k \in \llbracket 1, K \rrbracket \cap j \in \llbracket 1, n+1 \rrbracket}$$

can all be computed in  $O(Kn^2)$ 

The proof is given in Appendix A.1. It is based on a linear algebra lemma. The lower triangular part of matrix **A** is set to 0 to fit the segmentation context. Note that, similarly, we have  $\sum_{m \in \mathcal{M}_k([i,j])} F(m) = (\mathbf{A}^k)_{i,j}$  for all  $1 \leq i \leq j \leq n+1$ . Theorem 2.1 will be used many times in the following sections, using a specific function f(r) for each quantity of interest.

#### 2.1 Joint distribution of the data and the segmentation or the dimension

P(Y,m) and P(Y,K) are key ingredients to calculate various quantities of interest, such as (1). To calculate P(Y,m) and

$$P(Y,K) = \sum_{m \in \mathcal{M}_K} P(Y,m), \tag{3}$$

we first need to define priors for the segmentation m. We consider here two typical priors.

Uniform conditional on the dimension: For any prior on the dimension P(K), we define a uniform prior distribution for m given its dimension K:

$$P(m|K(m)) = {\binom{n-1}{K(m)-1}}^{-1} \qquad \Rightarrow \qquad P(m) = P(K(m)) \left/ {\binom{n-1}{K(m)-1}} \right. \tag{4}$$

that is  $a_r = 1$  in (2), denoting K(m) the number of segments (i.. the dimension) of the segmentation m.

Homogeneous segment lengths: Segmentation with balanced segment lengths are sometimes desirable. They are favoured by the following prior:

$$P(m) = C \prod_{r \in m} n_r^{-1}, \quad \text{where } C \text{ ensures that} \sum_{m \in \mathcal{M}} P(m) = 1.$$
(5)

that is  $a_r = n_r^{-1}$  in (2), where  $n_r$  denotes the length of segment r and  $\mathcal{M}$  the set of all considered segmentations. In this case, the prior distribution of m is directly defined and the prior distribution of the dimension P(K) is not explicit. Determining the constant C requires summing over all possible segmentations. This sum can be handled using the properties given below.

**Proposition 2.2** Under assumption (**H**), for prior distributions (4) and (5), P(Y,K) can be computed in  $O(Kn^2)$  as  $P(Y,K) = C(\mathbf{A}^k)_{1,n+1}$  with  $\mathbf{A}_{i,j} = 0$  for  $j \leq i$  and, for j > i, for prior distribution (4):

$$\mathbf{A}_{i,j} = P(Y^{\llbracket i,j \rrbracket}) \quad and \quad C^{-1} = \binom{n-1}{K-1};$$

and for prior distribution (5):

$$\mathbf{A}_{i,j} = n_{[\![i,j]\![}^{-1} P(Y^{[\![i,j]\!]}) \quad and \quad C^{-1} = \sum_{m \in \mathcal{M}_K} \prod_{r \in m} n_r^{-1}.$$

**Proof.** For prior distribution (4), we use Theorem 2.1 with  $f(r) = P(Y^r)$ , implying  $\mathbf{A}_{i,j} = f(\llbracket i, j \rrbracket) = P(Y^{\llbracket i, j} \rrbracket)$ .

For prior distribution (5), we first retrieve C using Theorem 2.1 with  $f(r) = n_r$ . The result follows, using Theorem 2.1 again, taking  $f(r) = n_r^{-1} P(Y^r)$ .

The preceding results require the calculation of  $P(Y^r)$ . Hence, n(n-1)/2 integrals need to be evaluated, corresponding to each possible segment. For general priors, they can be evaluated numerically or via any stochastic algorithm. A close form can be obtained if conjugate priors are used.

**Poisson and Gaussian models.** We recall classical results for two models that will be used later. First is the segmentation problem of a piecewise constant Poisson rate model:

$$\{\mu_r\} \text{ i.i.d.}, \quad \mu_r \quad \sim \quad \mathcal{G}am(\alpha_r, \beta_r);$$
  
$$\{Y_t\} \text{ independent}, \quad Y_t \quad \sim \quad \mathcal{P}(\mu_r) \quad \text{if } t \in r.$$
(6)

Second is the segmentation of a Gaussian signal where both the mean and the variance are affected by the change-points:

$$\{\tau_r\} \text{ i.i.d.,} \quad \tau_r \sim \mathcal{G}am(\nu_0/2, 2/s_0);$$
  
$$\{\mu_r\} \text{ independent,} \quad \mu_r | \tau_r \sim \mathcal{N}(\mu_0, (n_0\tau_r)^{-1});$$
  
$$\{Y_t\} \text{ independent,} \quad Y_t \sim \mathcal{N}(\mu_r, 1/\tau_r) \quad \text{if } t \in r.$$
(7)

For the Poisson model, we get

$$P(Y^r) = \frac{\Gamma(\alpha + \sum_{t \in r} Y_t^r) \ \beta_r^{\alpha_r}}{(\beta_r + n_r)^{\alpha_r + \sum_{t \in r} Y_t^r} \ \Gamma(\alpha_r) \prod_{t \in r} (Y_t^r!)}.$$

For the Gaussian heteroscedastic model, we get

$$P(Y^{r}) = \frac{n_{0}^{1/2} (s_{0}/2)^{\nu_{0}/2} \Gamma((\nu_{0} + n_{r})/2)}{(2\pi)^{n_{r}/2} \Gamma(\nu_{0}/2) \sqrt{n_{r} + n_{0}}} \theta^{(\nu_{0} + n_{r})/2}$$
(8)

where  $\theta = 2(n_r S_r^2 + s_0 + \frac{n_r n_0 (\bar{y}_r - \mu_0)^2}{n_r + n_0})^{-1}$ ,  $S_r^2 = \sum_{t \in r} (Y_t - \bar{y}_r)^2 / n_r$  and  $\bar{y}_r$  is the empirical mean of the signal within segment r.

## 2.2 Posterior distribution of the change-points and segments

We now give explicit formulae for the posterior distribution of change-points and segments. We first define the corresponding segmentation subsets:

 $\mathcal{B}_{K,k}(t)$  is the subset of segmentations from  $\mathcal{M}_K$  such that the k-th segment starts at position t, i.e. that the (k-1)-th change-point is at t:

$$\mathcal{B}_{K,k}(t) = \{ m \in \mathcal{M}_K : \tau_k = t \};$$

 $\mathcal{B}_K(t)$  is the subset of segmentations having a change-point at position t:

$$\mathcal{B}_K(t) = \bigcup_k \mathcal{B}_{K,k}(t);$$

 $\mathcal{S}_{K,k}(\llbracket t_1, t_2 \rrbracket)$  is the subset of segmentations having segment  $r = \llbracket t_1, t_2 \rrbracket$  as their k-th segment:

$$\mathcal{S}_{K,k}(\llbracket t_1, t_2 \llbracket) = \{ m \in \mathcal{M}_K(\llbracket 1, n+1 \llbracket) : \tau_k = t_1, \tau_{k+1} = t_2 \};$$

 $\mathcal{S}_K(\llbracket t_1, t_2 \rrbracket)$  is the subset of segmentations including segment  $\llbracket t_1, t_2 \rrbracket$ :

$$\mathcal{S}_{K}(\llbracket t_{1}, t_{2} \llbracket) = \bigcup_{k} \mathcal{S}_{K,k}(\llbracket t_{1}, t_{2} \llbracket)$$

We denote the conditional probability given the data Y and the dimension K of each of these subsets by the corresponding capital letters with same indices, e.g.

$$B_{K,k}(t) = \Pr\{m \in \mathcal{B}_{K,k}(t) | Y, K\}.$$

 $B_K(t)$ ,  $S_{K,k}(t)$  and  $S_K(t)$  are defined similarly. The following proposition gives explicit formulae for these probabilities.

**Proposition 2.3** For all  $\llbracket t_1, t_2 \llbracket$  such that  $t_1 < t_2$ , we define, for  $K \ge 1$ ,

$$F_{t_1,t_2}(K) = \sum_{m \in \mathcal{M}_K(\llbracket t_1,t_2 \rrbracket)} P(Y^{\llbracket t_1,t_2 \rrbracket}|m) P(m|K),$$

and we set  $F_{t_1,t_2}(K) = 0$  if  $t_1 \ge t_2$ . Under assumption (**H**), the probabilities  $B_{K,k}(t)$ ,  $B_K(t)$ ,  $S_{K,k}(t)$ and  $S_K(t)$  are

$$B_{K,k}(t) = \frac{F_{1,t}(k-1)F_{t,n+1}(K-k+1)}{P(Y|K)},$$
  

$$S_{K,k}(t_1, t_2) = \frac{F_{1,t_1}(k-1)F_{t_1,t_2}(1)F_{t_2,n+1}(K-k)}{P(Y|K)}$$

 $B_K(t) = \sum_{k=1}^K B_{K,k}(t)$  and  $S_K(t_1, t_2) = \sum_k S_{K,k}(t_1, t_2).$ 

The proof is given in Appendix A.2. It is mainly based on set decompositions, such as

$$\mathcal{B}_{K,k}(t) = \mathcal{M}_{k-1}(\llbracket 1, t \rrbracket) \times \mathcal{M}_{K-k+1}(\llbracket t, n+1 \rrbracket)$$
(9)

and all sums over  $\mathcal{M}_{k-1}(\llbracket 1,t \llbracket)$  and  $\mathcal{M}_{K-k+1}(\llbracket t,n+1 \rrbracket)$  can be obtained with Theorem 2.1.

 $\{B_{K,k}(t)\}_t$  provides the exact posterior distribution of the starting point of the k-th segment, given dimension K. From that, we get the exact credibility of interval  $[t_1, t_2]$  for change-point  $\tau_k$ :

$$C_{K,k}(\llbracket t_1, t_2 \rrbracket) = \Pr\{\tau_k \in \llbracket t_1, t_2 \rrbracket | Y, K\} = \sum_{t=t_1}^{t_2} B_{K,k}(t).$$

## 2.3 Retrieving the mean signal

In many applications, the mean value  $\mu_t$  of the signal at a given position can also provide some insight about the phenomenon under study. This mean signal can be retrieved via model averaging over the segmentation space. The posterior mean of the signal is

$$\bar{s}_K(t) = \sum_{m \in \mathcal{M}_K} P(m|Y, K) \hat{s}_m(t), \tag{10}$$

where  $\widehat{s}_m(t) = \mathbb{E}[\mu_t | m, Y].$ 

**Proposition 2.4** The posterior mean of the signal given the dimension is

$$\bar{s}_K(t) = \sum_{r \ni t} S_K(r) \widehat{\mu}_r$$

where  $\hat{\mu}_r = \mathbb{E}[\mu_r | Y^r]$ . Under assumption (**H**), it can be computed with a quadratic complexity.

**Proof.** If a segment r belongs to a segmentation m and if position t lies in segment r then  $\hat{s}_m(t) = \hat{\mu}_r$ . The rest of the formula is straightforward. Assumption (**H**) ensures that the  $S_K(r)$  can be computed in  $O(Kn^2)$ .

# 2.4 Posterior entropy

Segmentation problems are often reduced to choosing  $\hat{m}_K$ , the best segmentation (i.e. the one with maximal posterior probability) with dimension K. The other segmentations with dimension K are rarely considered. The entropy of the distribution P(m|Y, K)

$$\mathcal{H}(K) = -\sum_{m \in \mathcal{M}_K} P(m|Y, K) \log P(m|Y, K)$$

measures how the posterior distribution is concentrated around the best segmentation. Intuitively, a small entropy  $\mathcal{H}(K)$  means that the best segmentation is a much better fit to the data than any other segmentation. We use this information in Section 3 for model selection.

**Proposition 2.5** Under assumption (**H**), the posterior entropy  $\mathcal{H}(K)$  is

$$\mathcal{H}(K) = -\sum_{r} S_{K}(r) \log f(r) + \log A_{K}$$

where  $f(r) = a_r P(Y^r)$  and  $A_K = \sum_{m \in \mathcal{M}_K} \prod_{r \in m} f(r)$ , which can be computed using Proposition 2.2.

**Proof.** Since all distributions can be factorized, we have

$$\mathcal{H}(K) = -\sum_{m \in \mathcal{M}_K} \sum_{r \in m} P(m|Y, K) \log f(r) + \sum_{m \in \mathcal{M}_K} P(m|Y, K) \log A_K$$
$$= -\sum_r \log f(r) \sum_{m \in \mathcal{M}_K, m \ni r} P(m|Y, K) + \log A_K \sum_{m \in \mathcal{M}_K} P(m|Y, K)$$

and the result follows.  $\blacksquare$ 

# 3 Model selection

In a Bayesian framework, the BIC criterion aims to choose the model which maximises P(M|Y), where M is the model. To calculate the BIC criterion, one needs to know  $P(Y|M) = \int P(Y|\theta_M, M)P(\theta_M|M)d\theta_M$ , where  $\theta_M$  is the set of parameters of the model M. Similar quantities are involved in the Bayes factor for model comparison (Kass and Raftery (1995)).

In our case, the word 'model' is too broad and we have to distinguish between the selection of the dimension K and the selection of the segmentation m. When considering the choice of K, a direct application of the Laplace approximation is not theoretically justified to calculate the previous integral because the required differentiability condition is not satisfied for change-points (Zhang and Siegmund (2007)). However, we can bypass the problem by working at the segment level and then going back at the dimension level using Proposition 2.2. Thus, the derivation of BIC criteria only requires the calculation of  $P(Y^r) = \int P(Y^r | \theta_r) P(\theta_r) d\theta_r$ , which can be obtained in a close form for the Poisson model and the heteroscedastic Gaussian model as shown in Section 2.1. Moreover, we derive an adaptation of the ICL criterion, first proposed for mixture models, to the segmentation context (Biernacki *et al.* (2000)).

# 3.1 Exact BIC criterion for dimension and segmentation selection

**Choice of the dimension.** In segmentation problems, the selection of the 'best' number of segments K can be addressed per se, or as a first step toward the selection of the 'best' segmentation. The Bayesian framework suggests to choose

$$\widehat{K} = \underset{K}{\operatorname{arg\,min}} \operatorname{BIC}(K), \quad \text{where} \quad \operatorname{BIC}(K) = -\log P(Y, K).$$
(11)

BIC(K) can be computed in a quadratic time, using Proposition 2.2.

**Choice of the segmentation.** The best segmentation can be chosen in two ways.

Two-step strategy: The 'best' segmentation m can be chosen, conditionally to the pre-selected dimension  $\hat{K}$  as

$$\widehat{m}(\widehat{K}) = \underset{m \in \mathcal{M}_{\widehat{K}}}{\operatorname{arg\,min}} \operatorname{BIC}(m|\widehat{K}), \quad \text{where} \quad \operatorname{BIC}(m|\widehat{K}) = -\log P(Y, m|\widehat{K}).$$
(12)

One-step strategy: The 'best' segmentation m can also be directly chosen among a larger collection  $\mathcal{M} = \bigcup_{k=1}^{K} \mathcal{M}_k$  as

$$\widehat{m} = \underset{m \in \mathcal{M}}{\operatorname{arg\,min}} \operatorname{BIC}(m), \quad \text{where} \quad \operatorname{BIC}(m) = -\log P(Y, m).$$
(13)

Both BIC(m|K) and BIC(m) can be computed efficiently thanks to Proposition 2.2.

## 3.2 ICL criterion for dimension selection

In the framework of incomplete data models (e.g. mixture models), Biernacki *et al.* (2000) suggest to use the criterion ICL(M), which is an estimate of  $\mathbb{E}[\log P(Y, Z, M)|Y]$  where Z stands for the unobserved variables. Based on the equation

$$\mathbb{E}[\log P(Y, Z|M)|Y] = \log P(Y|M) + \mathbb{E}[\log P(Z|Y, M)|Y],$$

they argue that the entropy  $H(Z|Y, M) = -\mathbb{E}[\log P(Z|Y, M)|Y]$  is an intrinsic penalty term. The ICL criterion will tend to select models that provide a reliable prediction of Z, i.e. with a small entropy. This may be desirable, for example in the classification context.

In the segmentation context, the segmentation m can be considered as an unobserved variable. The dimension K can then be chosen according to the ICL as

$$K = \arg\min_{K} \operatorname{ICL}(K) \quad \text{where} \quad \operatorname{ICL}(K) = -\log P(Y, K) + H(m|Y, K).$$

Biernacki *et al.* (2000) We expect ICL to favour the dimension K where the best segmentation  $\widehat{m}(K)$  clearly outperforms the other segmentations in K segments, so that  $\widehat{m}(K)$  is more reliable.

## 3.3 Comparison with other penalized criteria

Many model selection criteria have the following form:

$$\log P(Y|\widehat{\theta}, m) - \operatorname{pen}(m)$$

and use a two-step strategy. Interestingly, since the penalty generally depends only on the dimension (Lebarbier (2005), Lavielle (2005)), the best segmentation  $\hat{m}(K)$  does not actually depend on the penalty.

The calculation of the exact BIC does not provide any explicit penalty enabling a direct comparison with such criteria. For such comparison, we derive two approximations of  $\log P(Y^r) = \log \int P(Y^r | \theta_r) P(\theta_r) d\theta_r$  in the heteroscedastic Gaussian case. The first one is based on a Laplace approximation:

$$\log P(Y^r) \approx \log P(Y^r|\hat{\theta}_r) - \frac{D}{2}\log n_r$$

where D stands for the number of parameters involved in each segment (here, D = 2). This approximation is valid only for large segments, i.e. where  $P(Y^r|\theta_r)$  satisfies regularity conditions. For the second approximation, we let the hyperparameters  $n_0, \nu_0$  and  $S_0$  go to 0 in (8) and we obtain

$$\log P(Y^r) \approx -\frac{n_r}{2} \log S_r^2 - \frac{D}{2} \log n_r \approx \log P(Y^r | \hat{\theta}_r) - \frac{D}{2} \log n_r$$

We emphasize that these approximations are both questionable since the asymptotic framework of the Laplace approximation is not correct for small segments and because the priors are improper for null hyperparameters. Our purpose is only to show that they both provide the same penalty form:

$$\log P(m|Y) \approx \log P(m) + \log P(Y|\widehat{\theta}, m) - \frac{D}{2} \sum_{r \in m} \log n_r$$

Using uniform prior (4), we get

$$pen(m) = \log P(K(m)) - \log \binom{n-1}{K(m)-1} - \frac{D}{2} \sum_{r \in m} \log n_r.$$

A similar form is obtained in the Poisson case. The complexity term,  $\log {\binom{n-1}{K-1}}$ , is similar to the one of Lebarbier (2005). The regularity term,  $\sum_{r \in m} \log n_r$ , favours segments with equal lengths and is similar to the one of Zhang and Siegmund (2007). Using the alternative prior (5) reinforces the regularity term. Due to this term, the best segmentation  $\widehat{m}(K)$  within  $\mathcal{M}_K$  does depend on the penalty.

# 4 Applications

In this section, we first present a simulation study to assess the ability of the exact BIC and ICL criteria to select the dimension and the ability of model averaging to retrieve the mean signal. We then analyse a real CGH profile and use our formulae to assess the quality of the segmentation.

# 4.1 Simulations

**Simulation design.** We performed the simulation study in the Poisson model (6) so that only one parameter had to be chosen. We simulated a sequence of 150 observations affected by six change-points at the following positions: 21, 29, 68, 82, 115, 135. Odd segments had a mean of 1, while even segments had a mean of  $1 + \lambda$ , where lambda varies from 0 to 10. The higher  $\lambda$  is, the easier it should be to recover the true number of change-points. The hyperparameters  $\alpha$  and  $\beta$  were set to be equal and we considered three values for them: 0.01, 0.1 and 1. For each configuration, we simulated 300 sequences.



Figure 1: Percentage of true dimension recoveries as a function of  $\lambda$ . Left panel: for the three criteria. BIC $(\hat{m}_K)$  :  $\blacksquare$ -, BIC(K) :  $\bullet$ -- and ICL(K) :  $\bullet$ ... Right panel: for the BIC criteria;  $\bullet$ : uniform prior over all segmentations,  $\blacksquare$ : uniform prior over all segmentations of a dimension,  $-: \alpha = \beta = 1$ ,  $--: \alpha = \beta = 0.1, \dots : \alpha = \beta = 0.01$ .

## 4.2 Recovering the number of change-points

#### 4.2.1 The ICL criterion performed better than the BIC criterion

**Model selection.** The BIC criterion for dimension selection, BIC(K), almost never returned the true dimension, even for high values of  $\lambda$  (Figure 1, where  $\alpha$  and  $\beta$  were set to 1). On the other hand, both the BIC criterion for model selection, BIC(m), and the ICL criterion, ICL(K), tend to recover the true dimension more often when  $\lambda$  became larger. ICL(K) even increased to a maximum of 99% true recoveries compared to a maximum of 91% for the BIC(m) criterion for model selection.

Influence of the priors. The ability of BIC(m) to retrieve the true dimension was greatly affected by the prior distribution of the segmentation (Figure 1). To illustrate this effect, we considered a prior that gave equal probability to all segmentations, whatever their dimension: P(m) = cst. This led to a 90% decrease in the ability to return the true dimension compared to a conditional uniform prior given the dimension (4) (with P(K(m)) = cst whatever m). The impact of the two hyperparameters  $\alpha$  and  $\beta$  seemed relatively limited in comparison: less than 10% difference in the ability to return the true dimension (Figure 1).

**Estimation of the mean signal.** We then compared the ability of the maximum likelihood estimators (MLE) and that of the posterior mean signal to recover the true signal in terms of the Kullback-Leibler distance. For each simulation, we computed the following:

$$d(\widehat{\mu}, \mu) = \sum_{t} KL[\mathcal{P}(\widehat{\mu}_{t}); \mathcal{P}(\mu_{t})]$$

for both the MLE estimate  $\hat{\mu} = \hat{\mu}_{\text{MLE}}$  and the posterior mean  $\hat{\mu} = \bar{s}_K(t)$  (see equation (10)).

When K was lower than the true dimension (7 segments), the two estimates were almost equivalent (Figure 2). However, for larger dimensions, the distance of the MLE to the true signal increased whereas the distance of the posterior mean did not (Figure 2). The posterior mean seemed less prone to over-fitting. Moreover, for a very small signal-to-noise ratio ( $\lambda = 1$ ), the distance between the posterior mean of the signal and the true signal still decreased when K was higher than the true dimension. Therefore, when the signal was of poor quality and led to a poor assessment of the true dimension, the posterior mean of the signal led to better results. Moreover, the standard deviation of d for the posterior mean is almost always smaller than the one of the MLE (not shown).



Figure 2: Kullblack-Leibler-based distance d to the true signal as a function of the dimension.  $\blacksquare$ :  $d(\widehat{\mu}_{\text{MLE}}, \mu)$ ,  $\blacktriangle$ :  $d(\overline{\mu}, \mu)$  for three value of  $\lambda$  1: -, 2: -- and 6: .... The true number of segments was 7.



Figure 3: Left panel: Chromosome 10 profile of cell line BT474. The DNA copy number logratio is represented as a function of its position along the chromosome. Right panel: (Left axis) BIC(m):  $\blacktriangle$ , BIC(K):  $\bullet$  and ICL(K):  $\blacksquare$  as a function of the dimension. (Right axis)  $\mathcal{H}(K) - \mathcal{H}(K-1)$ :  $\circ$  as a function of the dimension.

# 4.3 Analysis of a CGH profile

In the following subsection, we used a comparative genomic hybridation (CGH) profile to illustrate our methodology. CGH enables the study of DNA copy number gains and losses along the genome (Pinkel *et al.* (1998)). We used the Gaussian segmentation model defined in (7) that is often used for this type of data (Picard *et al.* (2005)). The profile shown in Figure 3 represents the copy number logratio of cell line BT474 to a normal reference sample, along chromosome 10.

**Model selection.** Since the true dimension was unknown, the first issue was to choose one. The ICL(K) criterion selected 4 segments whereas BIC(m) selected a segmentation with 3 segments (Figure 3). The additional penalty term involved in ICL does not necessarily penalise larger dimensions. In our example, ICL selected a segmentation with a larger dimension because it was more reliable. The choice of ICL was motivated by the relatively small gain of entropy between dimensions 3 and 4. This choice was also supported by the posterior distributions of the change-points and that of the segments shown below. The best segmentations for 3 and 4 segments are shown on Figure 4 (i).

**Posterior probability of the change-point positions.** The distribution of the successive changepoints for dimensions 3 and 4 are shown on Figure 4 (*ii*). For dimension 3, the exact intervals with credibility 95% were [[64, 78]] and [[92, 97]] for  $\tau_2$  and  $\tau_3$ , respectively. For dimension 4, the intervals were [[66, 78]], [[78, 97]] and [[91, 112]] for  $\tau_2$ ,  $\tau_3$  and  $\tau_4$ , respectively.

The existence of a change-point at a given position t is assessed by posterior probability  $B_K(t)$ . Note that, contrarily to  $B_{K,k}(t)$ ,  $B_K(t)$  is not a probability distribution over the positions, because its sum is the number of change-points: K - 1. In our example, the posterior probabilities  $B_4(t)$  presented sharper peaks than  $B_3(t)$  (see Figure 4 (*iii*)), which was consistent with the choice of the ICL criterion that favours reliable segmentations.

**Posterior probability of a segment.** Similar conclusions were drawn from the posterior probability of the segments. In Figure 4 (*iv*) each point corresponds to a segment. A reliable dimension should display K sharp peaks. The position of the first two segments are very uncertain for K = 3, due to the uncertainty of  $\tau_2$ . Their position were much more certain with K = 4. In particular, the smallest segment from K = 4 at positions [78, 79] had a relatively high probability of 0.34.

**Posterior mean of the signal.** Similarly, the posterior mean for 3 segments was different from the one for 4 segments (Figure 5); the former failed to capture the small deletion at [78, 79]. As soon as K exceeded 4, the posterior mean of the signal was very stable, see the example for K = 5 segments in Figure 5.

All presented results show that, the segmentation in 4 segments selected by the ICL(K) is more reliable than the segmentation in 3 segments selected by the BIC(m).

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# A Lemma and Proofs

# A.1 Proof of Theorem 2.1

The proof of the theorem relies on the following lemma.

**Lemma A.1** Let A be a square matrix with n columns. For all  $k \in \mathbb{N}$ , we define the function  $f_{\mathbf{A},k}$  as:

$$\forall (i,j) \in [\![1,n]\!]^2 \qquad f_{\mathbf{A},k}(i,j) = \sum_{(t_2 \cdots t_k) \in [\![1,n]\!]^{k-1}}^{t_1 = i, \ t_{k+1} = j} \prod_{i=1}^k \mathbf{A}_{t_i,t_{i+1}}$$

The *n* elements of  $\{f_{\mathbf{A},k}(i,j)\}_{\{i \in [1,n]\}}$  for  $1 \leq k \leq K$  can all be computed in  $O(Kn^2)$  as

$$f_{\mathbf{A},k}(i,j) = (\mathbf{A}^k)_{i,j}$$

**Proof of the Lemma.**  $f_{\mathbf{A},k}(i,j) = \mathbf{A}_{i,j}^1$  holds for k = 1. Suppose that  $f_{\mathbf{A}}(k,i,j) = \mathbf{A}_{i,j}^k$  holds for a given  $k \in \mathbb{N}$ . For k + 1, we have:

$$f_{\mathbf{A},k+1}(i,j) = \sum_{(t_2 \cdots t_{k+1}) \in [\![1,n]\!]^k}^{t_1 = i,t_{k+2} = j} \prod_{i=1}^{k+1} \mathbf{A}_{t_i,t_{i+1}} = \sum_{t=1}^n \sum_{(t_2 \cdots t_k) \in [\![1,n]\!]^{k-1}}^{t_1 = i,t_{k+1} = t} \prod_{i=1}^k \mathbf{A}_{t_i,t_{i+1}}. \quad \mathbf{A}_{t,j} = \sum_{t=1}^n f_{\mathbf{A},k}(i,t). \quad \mathbf{A}_{t,j} = \sum_{t=1}^n f_{\mathbf{A},k}(i,t).$$

Using our induction hypothesis and by definition of the matrix product, we obtain:

$$f_{\mathbf{A},k+1}(i,j) = \sum_{t=1}^{n} \mathbf{A}_{i,t}^{k} \mathbf{A}_{t,j} = \mathbf{A}_{i,j}^{k+1}$$

Thus, the  $K \times n$  elements of the form

 $\{f_{\mathbf{A},k}(t_1,t_{k+1})\}_{\{k \in [[1,K]] \cap t_{k+1} \in [[1,n]]\}}$ 

can be computed in  $O(Kn^2)$  as the  $t_1$ -th line of matrices  $\mathbf{A}, \mathbf{A}^2 \cdots, \mathbf{A}^K$  respectively.

**Proof of the Theorem.** For any  $(t_1, ..., t_{k+1})$  in  $[\![1, n+1]\!]^{k+1}$  such that we do not have  $t_1 < t_2 \cdots < t_{k+1}$ ,  $\prod_{i=1}^k \mathbf{A}_{t_i, t_{i+1}} = 0$ . Therefore, for all  $k \in [\![1, K]\!]$  and for all j in  $[\![1, n]\!]$ :

$$\sum_{m \in \mathcal{M}_k(\llbracket 1, j \llbracket)} F(m) = \sum_{t_1 < t_2 \dots < t_{k+1}}^{t_1 = 1, t_{k+1} = j} \prod_{i=1}^k \mathbf{A}_{t_i, t_{i+1}} = \sum_{(t_2, \dots, t_k) \in \llbracket 1, n+1 \rrbracket^{k-1}}^{t_1 = 1, t_{k+1} = j} \prod_{i=1}^k \mathbf{A}_{t_i, t_{i+1}}$$

Using Lemma A.1 on matrix **A** and integer K, we see that the  $K \times (n+1)$  terms of the form

$$\left\{\sum_{m\in\mathcal{M}_{k}(\llbracket 1,j\llbracket)}F(m)\right\}_{k\in\llbracket 1,K\rrbracket\cap j\in\llbracket 1,n+1\rrbracket}$$

can be computed as  $\sum_{m \in \mathcal{M}_k([\![1,j]\!])} F(m) = (\mathbf{A}^k)_{1,j}$  and that therefore they can all be computed in  $O(Kn^2)$  as the first line of the successive powers of matrix  $\mathbf{A}$ .

## A.2 Proof of Proposition 2.3

**Proof.** We first consider the posterior distribution of the change-points. With Equation (9), we obtain

$$B_{K,k}(t) = \frac{\sum_{m \in \mathcal{B}_{K,k}(t)} P(Y|m) P(m|K)}{P(Y|K)} = \frac{F_{1,t}(k-1)F_{t,n+1}(K-k+1)}{P(Y|K)}.$$

Using Theorem 2.1, we see that all the F functions can be computed in  $O(Kn^2)$ .  $O(K^2n)$  products and divisions remain to be done to compute all  $B_{K,k}(t)$ , so the overall complexity is in  $O(Kn^2)$ . The probability  $B_K(t)$  follows straightforwardly.

We now consider the posterior distribution of the segments. We first quote that if  $t_1 = 1$ , then  $S_{K,1}(1,t_2) = B_{K,2}(t_2)$ . Similarly, when  $t_2 = n + 1$ , we have  $S_{K,K}(t_1,t_2) = B_{K,K}(t_1)$ . So we only have to consider the case where  $1 < t_1 \le t_2 < n + 1$ . Since  $\mathcal{S}_{K,k}([t_1,t_2[t_1]))$  can be decomposed as

$$\mathcal{S}_{K,k}(\llbracket t_1, t_2 \rrbracket) = \mathcal{M}_{k-1}(\llbracket 1, t_1 \rrbracket) \times \{\llbracket t_1, t_2 \rrbracket\} \times \mathcal{M}_{K-k}(\llbracket t_2, n+1 \rrbracket),$$

we have

$$S_{K,k}(t_1, t_2) = \frac{\sum_{m \in \mathcal{S}_{K,k}(\llbracket t_1, t_2 \rrbracket)} P(Y|m) P(m|k)}{P(Y|K)} = \frac{F_{1,t_1}(k-1)F_{t_1,t_2}(1)F_{t_2,n+1}(K-k)}{P(Y|K)}$$

Again using Theorem 2.1, we see that all the F functions can be computed in  $O(Kn^2)$ . We then need to compute  $O(n^2)$  products and divisions to get the  $S_{K,k}(t_1, t_2)$ , thus the overall complexity is in  $O(Kn^2)$ . The last probability comes from the definition of  $S_K(t_1, t_2)$ .  $O(Kn^2)$  additions remain to be done the overall complexity is therefore in  $O(Kn^2)$ .



Figure 4: (i): Best segmentation of the profile in 3 (left) and 4 (right) segments. • represent the logratio as a function of the position along the chromosome. -: averaged signal of the segment. · · · : change-point positions. (ii): Posterior probability that the k-th change-point is at position t knowing that there is either 3 (left) or 4 (right) segments. Probability of the first change-point: -, probability of the second change-point: -- and probability of the third change-point: · · · . (iii): Posterior probability that there is a change-point at position t knowing that there is 3 (right) or 4 (left) segments. (iv) : 3D plot of the probability of all segments. Left panel: K = 3 segments; right panel: K = 4 segments. x-axis:  $t_1$ , y-axis:  $t_2$ , z-axis:  $S(\llbracket t_1, t_2 \rrbracket)$ .



Figure 5: Posterior mean of the signal; Left: K = 3 segments; Center: K = 4 segments; Right: K = 5 segments. •: logratio as a function of the position along the chromosome. -: posterior mean of the signal. ···: change-point positions of the best segmentation.