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A Bayesian changepoint analysis
on spatio-temporal point processes

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Abstract

Change point analysis is a well-established area of statistical research, but in the context of spatio-temporal point processes it appears to be as yet relatively unexplored. Some substantial differences with regard to the standard change point analysis in time or in space have to be taken into account: firstly, at every time point the datum is not a single point but an irregular pattern of points distributed over a possibly irregular observation window; secondly, in many real situations spatial dependence between points and temporal dependence within time segments (*i.e.* time intervals delimited by two consecutive change points) have to be taken into account, and issues are raised in analytically obtaining mathematical quantities of interest, such as likelihood values and posterior distributions.

Our motivating example consists of data concerning the monitoring and recovery of radioactive particles from Sandside beach in Dounreay, in the North of Scotland; over recent years, there have been two major changes in the equipment used to detect the particles in the study area, representing known potential change points. In addition, offshore particle retrieval campaigns are believed may reduce the particle intensity onshore with an unknown temporal lag, potentially generating multiple unknown change points in the intensity function of the particle distribution.

In this work, we propose a Bayesian approach for detecting multiple change points in the intensity function of a spatio-temporal point process, allowing for spatial and temporal dependence within time segments. We restrict the study to Log-Gaussian Cox Processes, a very flexible class of point

process models suitable for environmental applications that can be extended to the spatio-temporal case. Log-Gaussian Cox models can be implemented using Integrated Nested Laplace Approximation (INLA), a computationally efficient alternative to Monte Carlo Markov Chain methods for approximating the posterior distribution of the parameters of interest. The use of INLA allows the posterior distribution of number and positions of multiple change-points to be accurately approximated even for complex models, without becoming computationally prohibitive.

Once the posterior distribution is obtained, we propose a few methods for detecting significant change-points. We present a simulation study assessing the validity and properties of the methods, which consists in generating spatio-temporal point pattern series with zero, one or multiple change-points, with or without spatial and temporal dependence; the proposed models are fitted on all data series, and the performance of the methods is assessed in terms of type I and II errors, detected changepoint locations and accuracy of the segment intensity estimates. We show that our methods have a good overall performance in detecting change-points over such complex data series, and we highlight good and bad aspects of all methods. For instance, one method based on a modified version of the Bayes Factor obtained using backward-type recursions performs well on simple models but is too conservative when used on more complex models including spatial dependence. Another method, based on fixing a threshold for the posterior distribution, suffers from the issues deriving from the arbitrariness of the threshold choice but is more flexible and holds better over all models. We also show that, when change-points are detected, they are located in the correct position by all methods. Finally, we show that INLA is a tool of great help: it returns tractable posterior distributions in all cases, it is computationally fast and it produces accurate estimates of the intensity function for every time segment.

We finally apply the above methods to the motivating real dataset, extend the models by including extra information and find good and sensible results concerning the presence and quality of changes in the process.

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Chapter 1

Introduction

In this Chapter, a brief overview of the work is presented, giving the analysis context together with the main research questions and aims to meet. Afterwards, the thesis structure is outlined.

1.1 Motivation for the work

Changepoint analysis consists in looking for significant changes in the parameters of a model from a subset of a data series to the following one; it is an interesting area of statistics, potentially able to answer many open research questions; it is frequently applied in a temporal context, less frequently over space and very rarely on spatio-temporal data. Nevertheless, as more and more data become available that show both a spatial and a temporal dimension (*e.g.* spatio-temporal lattice or point process data) there is a need to extend existing methods that currently apply to spatial data or temporal series separately.

We now introduce some theoretical and practical issues that are current challenges in changepoint analysis.

1.1.1 Theoretical issues

Some of the existing changepoint methods can potentially be extended to the general spatio-temporal context; however, for spatio-temporal point

processes this branch of analysis appears to be relatively unexplored. When dealing with point processes, some differences and difficulties with regard to a standard changepoint analysis in time have to be accounted for. Firstly, at every time point the datum is not a single point but an irregular pattern of points, distributed over a possibly irregular observation window. Secondly, frequently, point process data are collected over space, and it is not usual to have repeated measurements on the same observation window over time, in a sequence large enough to allow changepoint analysis. Furthermore, the response variable is the point location; further information, called *mark*, can be collected for every point but is not an essential component of a changepoint analysis. In addition, in many real situations spatial dependence among points and temporal dependence within time segments have to be taken into account, and analytically obtaining mathematical quantities of interest, such as likelihood values and posterior distributions, is not trivial. Modelling dependence within data segments in the context of unknown multiple changepoints is currently a challenge even for simple temporal series. Despite these complications, most of the studies on point processes aim at describing the behaviour of the intensity function, therefore its changes over time are certainly of interest, and the provision of tools for changepoint analysis on spatio-temporal processes would enlarge the number of questions that can be answered.

We do not have knowledge of a changepoint analysis carried over a spatio-temporal point process with recently developed techniques. For all the mentioned reasons, we believe a statistical analysis of changepoint detection methods in the context of spatio-temporal point processes is a challenging and interesting study area.

1.1.2 Motivating dataset

Our study was originally motivated by questions on the monitoring and recovery of radioactive particles from Sandside beach, North of Scotland, resulting from the presence of a former nuclear reactor and fuel processing facility (Tyler et al., 2010); the distribution of particles and their behaviour over time in the offshore and foreshore areas are of interest for a retrieval

campaign that has taken place over recent years with environment cleaning purposes. Questions on this dataset cover both the case of potential change-points in a known position and the most general case of unknown changes. Known potential changepoints are represented by two major changes in the equipment used to detect the particles. The interest lies in verifying if they significantly increased the ability to detect particles in the area. As for unknown changes, offshore particle retrieval campaigns might have reduced the particle intensity onshore with an unknown temporal lag; we want to check if the offshore campaigns have been effective in decreasing the point process intensity on the beach.

Questions on how to build a method able to detect changepoints in such a complex dataset are raised; the proposed method has to deal with the issues of spatial inhomogeneity, spatial dependence among points and temporal dependence of the process. The dataset motivates very interesting questions but is not big enough for relying on the performance of an untested method: the time series is quite short ($T = 15$) and some yearly patterns only contain very few data. Since we propose a new approach, we carry out a simulation study in order to evaluate the proposed methods before applying them to real data.

1.2 Background and tools

For understanding this work, the reader is required to have some knowledge of Bayesian statistics (in particular, the computational tool INLA), changepoint analysis techniques and spatio-temporal point processes. A general introduction of these main fields is given here, and a more detailed review of the recent literature can be found in Chapter 2.

Bayesian changepoint analysis

The basic assumption in a changepoint analysis is that data are ordered and split into segments, which generally follow the same model but under different parameter specifications (Wyse et al., 2011). The other common assumption is that observations are *i.i.d.* within a segment of time between

two changes. Modelling dependence within data segments in the context of unknown multiple changepoints is currently a challenge. Fearnhead (2006) proposed a method for simulating from the posterior distribution of multiple changepoints using a recursive technique; this is an important step forward in multiple changepoint analysis. When dependence is allowed, though, the segment marginal likelihood required by Fearnhead’s method usually becomes intractable: including any type of dependence increases the computational complexity of the problem, and there is a need for fast methods providing an accurate and tractable approximation of the likelihood. Recent work by Wyse et al. (2011) extended the method to allow for dependence within segments, using Integrated Nested Laplace Approximation (INLA) (Rue et al., 2009), an alternative, computationally efficient approach to MCMC methods for fitting a class of Bayesian hierarchical models to face the well known difficulty with analytically obtaining the posterior distribution of the parameters. The authors combined recursive methods with INLA to produce estimates for the segment marginal likelihoods and approximations for the posterior of both the number of changepoints and their position. The computational speed and flexibility of INLA has not been exploited for a spatio-temporal changepoint analysis yet.

Point process models

Our work extends these new techniques to the context of spatio-temporal point processes, in particular Log-Gaussian Cox point processes (LGCPs). Cox processes assume the point distribution over space (and potential aggregation) is due to stochastic environmental heterogeneity modelled as a random intensity function $\Lambda(s)$ (Illian et al., 2008); given $\Lambda(s)$, the distribution of points follows an inhomogeneous Poisson process. In LGCPs, the logarithm of the intensity surface over an observation window W is assumed to be a Gaussian (latent) field $\eta(s)$, *i.e.* $\Lambda(s) = \int_W \lambda(s) ds = \exp(\eta(s))$, and conditional on $\eta(s)$ the number of points $N \sim Poi(\Lambda(s))$. LGCPs constitute a very flexible class of models that can potentially be extended to spatio-temporal data; tractability issues that have impeded the use of these models up to very recent years can now be overcome using Integrated Nested Laplace

Approximation (INLA, Rue et al. (2009)).

Integrated Nested Laplace Approximation

INLA is an effective computational tool for implementing complex models. It is simulation free, which is the key to its fastness, and it exploits two approximations. Firstly, a Laplace approximation is employed to represent the posterior distributions with a Gaussian shape; secondly, the Gaussian Field is substituted by a Gaussian Markov Random Field with a sparse precision matrix, which makes calculations very efficient.

Thanks to its computational efficiency it allows extension from the temporal to the spatio-temporal context even for large datasets. Moreover, likelihood values resulting from different changepoint positions can be evaluated, and the posterior probability of every time point of being a changepoint is returned, allowing the changepoint position to be inferred *a posteriori*. We present a simulation study of a Bayesian approach to changepoint analysis using INLA by extending it to the spatio-temporal point process context, without reducing the problem to a one dimensional, simply temporal series.

1.3 Research objectives

Our work aims at finding a method for detecting multiple unknown changepoints over time in the spatially inhomogeneous intensity function of a spatio-temporal point process, when both spatial dependence among points and temporal dependence within time segments are allowed. We want to understand what happens when the usual assumptions of a changepoint analysis (simply temporal *i.i.d.* data) do not hold, which raises a few challenging issues especially when applied to the context of point processes.

When the point process under study is assumed spatially homogeneous, the intensity is constant over the window and can therefore be represented by a single number for each time point; this means we may achieve good and sensible results with a traditional changepoint analysis on a temporal series made by the number of points at each instant, since the observation window is fixed and the spatial distribution is of no interest as it is assumed constant

and completely random. In a more general inhomogeneous process, which is likely to be the case in many real situations, though, a changepoint analysis of the behaviour of the intensity function over time can concern different aspects:

- a change in scale, when the overall number of points increases or decreases significantly after a certain time point
- a change in spatial structure, when the expected number of points remains constant, but their distribution over space changes after a certain time point
- a change in both scale and spatial distribution.

We are interested in a method that is able to detect any of these changes over time, and that can therefore provide answers to a much wider variety of cases and carry much more information than a traditional changepoint analysis that ignores spatial structure. Focusing in changes over time on spatio-temporal data means that in this work there is no focus on analysing changes over space (*i.e.* describing the spatial inhomogeneity) at a fixed time point.

In this study, we take a Bayesian approach to changepoint analysis for two main reasons, that will be further discussed in Chapter 6. First of all, Bayesian inference allows knowledge brought by data (the likelihood) to be enriched by including extra information in the prior distributions of the parameters. This is very useful as in many real situations for contextual reasons some changepoints might be considered more likely than others. Secondly, a Bayesian approach allows dependence to be dealt with, while there are currently no satisfactory frequentist solutions to the problem.

Moreover, we aim at including the use of INLA in our approach as it brings several fundamental advantages when it comes to detecting multiple changepoints in a spatio-temporal point process context: first of all, the flexibility of LGCPs allows an extension of changepoint methods from the temporal to the spatio-temporal context, and very complex models can be accurately fitted using INLA. The extension to spatio-temporal models is not trivial and requires a higher computational effort, but, due to INLA's efficiency, it

is still feasible even for large datasets. Secondly, thanks to INLA's computational efficiency again, we can explore all the time series and compare the likelihood values resulting from different changepoint positions to choose the best position a posteriori. This is more efficient than traditional changepoint algorithms (Eckley et al., 2011), that often encounter computational issues. Such a complex exploration in such a complex dataset would not be possible in reasonable time without INLA. Moreover, we want to produce accurate and tractable approximations of the segment marginal likelihoods and with INLA we can fit general models including both spatial and temporal dependence within segments in our data so as to face all the real situations where assuming *i.i.d.* data is unrealistic. Besides, when the time series is very long and computations become too demanding (which may easily be the case with spatio-temporal data), the Reduced Filtering Recursion technique (Wyse et al., 2011), carefully applied and combined with INLA, overcomes computational issues.

In conclusion, with our approach we can provide a case study with new changepoint detection techniques, in the very general and complex framework of unknown multiple changepoints with dependence within segments; we can bring innovation by extending recent approaches such as Wyse et al. (2011) to the spatio-temporal context and to point process data, adapting the methods and solving computational issues. Furthermore, we move one step forward with respect to the traditional changepoint detection algorithms, that require data to be reduced to a temporal series: with this method, the 3 dimensions of the problem (two spatial and one temporal) are maintained. These theoretical issues have been motivated by the work on radioactive particle data; they are addressed in order to provide a method which is able to answer new questions and in particular to analyse our motivating dataset. We can therefore summarize our aims as follows: define some methods for the detection of multiple changepoints in the intensity of a spatio-temporal point process; allow decisions on whether, and how many, temporal changepoints are present; assess the methods' performance via simulation; finally, apply them to real data.

1.4 Thesis outline

This first introductory Chapter is aimed at giving an idea of the context and the objectives of our work. The next Chapter consists of a literature review on the topics of interest, presenting the state of art and the most recent developments in the field of Log-Gaussian Cox point processes, Integrated Nested Laplace Approximation and the Bayesian approach to changepoint analysis. In Chapter 3, the novelty in the methodology of the work is presented, explaining what models we use and what innovation they bring to the existing literature, and presenting and motivating the chosen detection methods. Chapter 4 illustrates the simulation study structure, and the performance of all methods is assessed and discussed. Chapter 5 shows the application to real data and how our method can answer the practical research questions. Lastly, Chapter 6 summarises what has been done, adds some general concluding remarks and gives some directions for further work.

Chapter 2

Literature Review

In this Chapter, we present the necessary background for understanding our work: firstly, an introduction to spatial and spatio-temporal point processes, with special focus on the class of point process models we fit to our data, *i.e.* Log-Gaussian Cox Processes; then, a presentation of the recently developed Integrated Nested Laplace Approximation (INLA) approach for obtaining the posterior distributions in case of computationally complex models with dependence between data. Lastly, we give an overview of the most recent Bayesian changepoint analysis techniques and of the current challenges in this field.

As the reader will understand, the presented topics are extremely broad and much more can be said about them. We choose to give some basic information in order to make the analysis context understandable, then we rapidly move on to the specific tools for our work.

2.1 Spatio-temporal Log-Gaussian Cox Processes

Spatial statistics is divided into three main branches: geostatistics, areal processes and point processes. The latter is the less studied, mainly because it is mathematically intense: analyses are often complicated in this field as the datum is the pattern of points altogether, therefore variables describing

such a structure and its distribution are likely to be complex, and the mathematical background is often heavy (Illian et al., 2013). Moreover, in most cases only a single spatial point pattern, *i.e.* a single realisation of the process, is available, which makes temporal analyses infeasible. Nevertheless, interest in this field has been recently raising, and new questions arise on how to adapt general methods to the context of point processes.

2.1.1 Introduction to spatial point processes

Points are defined as «reference locations for non overlapping objects of finite size» (Gelfand et al., 2010), and are sometimes called *events*, in order to distinguish them from arbitrary spatial locations in the considered space that do not belong to the process. A *spatial point pattern* is a set of random locations, irregularly distributed within a finite designated (usually bi-dimensional) region, where it is assumed that all points are observed and that points can potentially occur anywhere. In a spatial point pattern, randomness and questions concern the number of points and their locations. The pattern is generated by a stochastic mechanism called *spatial point process*, therefore the pattern itself is the observation or 'response' of interest. A realization of a point process is an unordered set of points, *i.e.* the points do not have a serial order in space, unless they are marked.

Point processes can in general also be temporal or spatio-temporal, but if the occurrence time is ignored and a picture of a situation is taken, spatial point processes are considered (Baddeley and Turner, 2006). Usually, point processes are assumed stationary and isotropic (*i.e.* invariant to the rigid motions of translation and rotation), even if in practice it is sufficient that these properties are acceptable for the planar region of interest (Diggle, 2014).

Point processes have numerous application areas, as forestry, ecology, geology, geography, astronomy and epidemiology (Diggle, 2014). A few simple examples of possible questions that can be addressed via point process analysis are: are two patterns independent? How much spatial segregation is present? Is it constant over time? Does it depend on any spatial covariate? For a complete introduction to spatial point processes, we refer to Diggle

(2014) and Illian et al. (2008). We follow the notation in Illian et al. (2008) and define

- $N(W)$: random number of points of the process in the observation window W ;
- X : point process defined on a measurable space and observed inside the window W ;
- $x_i, i = 1, \dots, N$: generic point/event of the process;
- $P(N(W) = n)$: (univariate) number distribution;
- $E(N(W)) = \Lambda(W)$: expected number of points in W .

The intensity function

Interest lies in the distribution of X , which is unknown and depends on the behaviour of an intensity function. The *intensity* of a process is defined as the abundance/frequency of events in an area (Baddeley and Turner, 2006), *i.e.* as the expected density of points per unit area; it is also defined as a measure of the potential for an event to appear at any location in the window (Cressie and Collins, 2001). Given a small spatial region ds with area $|ds|$ around a random location s , the first order intensity function $\lambda(s)$ of the point process X is

$$\lambda(s) = \lim_{|ds| \rightarrow 0} \frac{E(N(ds))}{|ds|}$$

i.e. the expected number of points in an extremely small region. The intensity may be constant, and the process is called *uniform/homogeneous*, or inconstant, and the process is *non-uniform/inhomogeneous*.

The intensity is homogeneous when the number of points in a region is

$$N(W) \sim Poi(\lambda|W|)$$

therefore

$$P(N(W) = n) = \exp(-\lambda|W|) \frac{(\lambda|W|)^n}{n!}.$$

This implies $\lambda(s) = \lambda$, *i.e.* the mean number of events per unit area does not depend on the location s .

The intensity of the process is inhomogeneous if

$$N(W) \sim Poi(\Lambda(W))$$

where

$$\Lambda(W) = E(N(W)) = \int_W \lambda(s) ds$$

and $\lambda(s)$ is the first order intensity at location s .

Point process models

Depending on the type of inhomogeneity and its cause, different processes can be defined. A general *inhomogeneous Poisson process* is characterized by independence of the process X for non-overlapping sets, but allows the intensity $\lambda(s)$ to vary over the window W (Cressie and Wikle, 2011). The class of *Poisson cluster processes* was introduced by Neyman and Scott with the idea that aggregated spatial point patterns can be generated by the clustering of groups of related events, as the case of parents producing offsprings. *Gibbs processes* are an extension of Poisson processes where interpoint interaction is considered, under the assumption that this is the direct cause of the pattern distribution and any clustering or repulsive behaviour (Baddeley et al., 2013): an example can be the competition for soil of food. Another broad class of point processes is given by *Cox processes*, that are of special interest for our work. One special case of Cox processes which is often used in point process analysis is the Thomas process, that also belongs to the class of Poisson cluster processes and that we briefly introduce as it is one of the models that will be fitted to our data in Chapter 5. First of all, a Poisson process of parent points takes place, then at each parent location clusters are generated, where each cluster consists of a Poisson number of random points with an isotropic Gaussian dispersion around its parent (Møller and Waagepetersen, 2004). The intensity of a stationary Thomas process is $\lambda = k\mu$ where k is the intensity of the homogeneous Poisson process for the parent points, and μ is the mean of the Poisson random variable 'number of offspring per parent'.

A wider and more flexible class of Cox processes consists of Log-Gaussian Cox Processes, that will be presented in detail in Section 2.1.4.

2.1.2 Preliminary tests on point processes

When dealing with spatial point processes, usually preliminary questions are performed that aim at understanding the general behaviour of the process. In particular, it is of interest to know if the pattern can be considered as randomly scattered, clustered or regular. The answer to this question gives hints on what class of models is most suitable for the data. The tests presented in this Section answer this question and are therefore part of a preliminary analysis to understand the kind of process under study. We now present them briefly as we will use these tests as an exploratory step on our real data (see Section 5.2). All tests are meant for checking the null hypothesis of Complete Spatial Randomness (CSR). CSR is defined as the absence of any type of interaction among points, *i.e.* the absence of any clustering or repulsive behaviour; the points occur in the observation area in a completely random fashion. The homogeneous spatial Poisson process is a model of CSR, *i.e.* it implies that the number of events follows a Poisson distribution with constant intensity λ and that the number of events in disjoint regions are independent. In a more formal definition, CSR occurs when

- the process is characterized by a single intensity parameter λ
- $P(N(W) = n) = \exp(-\lambda|W|) \frac{(\lambda|W|)^n}{n!}$
- the numbers of occurrences counted in disjoint sub-areas are independent of each other
- the probability distribution of the number of occurrences counted in any sub-area only depends on the area size.

Distance-based methods

One class of methods for testing CSR is based on measuring interpoint distances; these methods have the advantage of being independent from the window shape. They look for *interpoint interaction* (Baddeley, 2010), the

conventional term for stochastic dependence between points in a point pattern. These methods are Monte Carlo Markov Chain (MCMC) methods as they are based on simulations under the null hypothesis of CSR and comparison with the observed data: a summary characteristic is estimated for the data and is compared to the one estimated from simulated point patterns. We now introduce some well known distance-based methods.

- **Pairwise distance** (or interevent distance): it is defined as

$d_{ij} = \|x_i - x_j\|$ and it has to be computed between all distinct pairs of points x_i and x_j ($i \neq j$) in the pattern.

If the number of events is n , there are $\frac{1}{2}n(n-1)$ pairwise distances; the distribution function of the distances depends on the region shape and size (even if the test result does not). A simple visual test for CSR is given by the empirical distribution function of interevent distances: the function represents the observed proportion of distances which are at most equal to d :

$$\bar{H}_1(d) = \left(\frac{1}{2}n(n-1)\right) \sum I(d_{ij} \leq d) - 1.$$

If the true H is known and plotted against the empirical distribution function, the plot should be linear under CSR. To assess the significance of departures from CSR the following steps are needed:

1. estimate $\bar{H}_1(d)$
2. calculate $\nu - 1$ empirical distributions from $\nu - 1$ independent simulations on n events independently and uniformly distributed over the region: $\bar{H}_2(d), \bar{H}_3(d), \dots, \bar{H}_\nu(d)$ (*e.g.*: $\nu - 1 = 99$)
3. define the upper and lower 'simulation envelopes'
 $U(d) = \max_u \{\bar{H}_u(d)\}$ and $L(d) = \min_u \{\bar{H}_u(d)\}$, with $u = 2, \dots, \nu$
4. plot the envelopes together with the estimated $\bar{H}_1(d)$
5. if $\bar{H}_1(d)$ lies between the envelopes all over its range, the null hypothesis of CSR is not rejected, otherwise:
 - if $\bar{H}_1(d) > U(d)$ in small values, there is tendency to clustering (many small distances);

– if $\bar{H}_1(d) < L(d)$ in small values, there is tendency to a regular pattern.

- **Nearest neighbour distance:** the nearest neighbour distance between two events $G(d)$ is defined as the probability that the nearest event is within distance d from another event, and d_i is the distance from event x_i to the nearest event of the pattern (duplicate measurements occur between reciprocal nearest neighbours pairs). This distance measure is useful because often interaction between events only exists if the distance is 'small'.

The empirical distribution function is

$$\bar{G}(d) = (n - 1) \sum I(d_i \leq d).$$

A MCMC test for CSR proceeds analogously as for interevent distances, with similar conclusions.

- **Empty space distance** (or point to nearest event distance): it is measured as $d(s) = \min \|s - x_i\|$ and represents the distance from a reference location s in the window (not necessarily belonging to the pattern) to the nearest data event. The F function is defined as the nearest neighbour distance between an arbitrary point and an event, and $F(d)$ is the probability that the nearest event is within distance d from a point in the window.

After choosing m arbitrary sample points in the window, we can define the empirical distribution function:

$$\bar{F}(d) = (m - 1) \sum I(d_i \leq d).$$

Again, a MCMC test for CSR proceeds analogously as for interevent and nearest neighbour distances, with similar conclusions.

If the process is only observed inside a window, the observed empty space distance between a location near the border could be larger than the actual one, because the nearest event lies outside the window and is not considered (Baddeley and Turner, 2006). In this situation, the empirical \bar{F} is negatively biased, and an edge correction giving weights

to the observations is necessary.

For a homogeneous Poisson process, both the true empty space function and the true nearest neighbour functions are known (Diggle, 2014):

$$F(d) = G(d) = 1 - \exp(-\lambda\pi d^2)$$

where λ is the mean intensity per unit area and πd^2 is the circle area of radius d . Thus, $\lambda\pi d^2$ is the number of expected events within distance d from an arbitrary origin (and this number is constant all over the pattern because of CSR). This is a reference value to which we compare the estimated functions: higher values suggest that empty space distances in the point pattern are shorter than for a Poisson process and hint for a regularly spaced pattern, while smaller values suggest a clustered pattern. Analogously, if the empirical \bar{G} is negatively biased, a weight correction is needed.

The estimated curves can be compared with the true ones with a theoretical QQ plot (Duan et al., 2010), where shorter tails give a hint for clustering, and longer tails for repulsion.

Other non parametric tests against CSR

Other tests exist that are not based on distances and depend on the window size and shape.

1. Pearson chi-square test

The window W is divided into p sub-regions of equal area (usually, but not necessarily, quadrats), and the events in each region are counted. Then, the usual Pearson chi-square test is used (its distribution under CSR is $\chi^2_{(p-1)}$). The null hypothesis may be rejected either because the distribution of events in W is not uniform or because there are dependencies (interactions) among the events. Significantly large values indicate aggregation, while small values indicate regularity. The main critique to the quadrat test approach is the lack of information (Baddeley and Turner, 2006). This is a goodness-of-fit test in which the alternative hypothesis H_1 is simply the negation of H_0 , *i.e.* the

alternative is that 'the process is not a homogeneous Poisson process', but there are many types of departure from H_0 .

2. Variance-to-mean ratio

This is a well known index of dispersion. It can be computed for each quadrat and then for further aggregations of $k \times k$ adjacent quadrats (blocks); afterwards, the index is plotted against block size. If peaks or troughs in the graph are found, there is evidence of scales of patterns (aggregation or regularity, respectively). This is only a visual test.

3. Kolmogorov-Smirnov test

This is a more powerful test than the Pearson chi-square test (Baddeley and Turner, 2006) in which the observed and expected distributions of the values of some real-valued function $T(s)$, defined at every location s in the window, are compared. This function is evaluated at each of the data points; then, the empirical distribution of T is compared with the predicted distribution of T under CSR, using the classical Kolmogorov-Smirnov test.

The Kolmogorov-Smirnov test is usually preferred if a covariate Z is available, with continuously varying numerical values (Baddeley, 2010). If the covariate is a factor or discrete variable, then the Kolmogorov-Smirnov test is ineffective because of tied values, and the χ^2 test based on quadrat counts would be used.

If the preliminary tests reject the null hypothesis of CSR and give hint for clustering, one of the most general and suitable class of models to fit to many data is given by Cox processes.

2.1.3 Spatial Cox Processes

A spatial point pattern can have aggregation for various reasons; one of them is spatial heterogeneity (Møller et al., 1998). Cox processes model aggregation as due to stochastic environmental heterogeneity represented by an underlying latent field. They are a generalization of inhomogeneous Poisson processes where $\lambda(s)$ is random (Illian et al., 2008), indeed they are

also called *doubly stochastic Poisson processes*, as they are built by a 2 stage random mechanism:

1. generation of an intensity function $\lambda(s)$ from a distribution
2. conditioning on $\lambda(s)$ (*i.e.* knowing the value it takes at each location), construction of an inhomogeneous Poisson process with intensity $\lambda(s)$.

Given $\lambda(s)$, the distribution of points is random and there is no direct interaction among points. For a general introduction to Cox processes, we refer to Møller and Waagepetersen (2004).

Cox processes are particularly suitable for phenomena where it is plausible to consider an environmental driver as the main cause for clustering or repulsion; for this reason, they are widely used in environmental and ecological statistics. However, Cox processes often encounter the issue of having an analytically intractable likelihood; this traditionally leads to computationally expensive MCMC-type approaches, but complex Cox processes can also be fitted with Integrated Nested Laplace Approximation (INLA, see Section 2.2) by exploiting the latent random field.

2.1.4 Spatial Log-Gaussian Cox Processes

Log-Gaussian Cox Processes (LGCPs) are Cox point processes where the logarithm of the intensity surface is assumed to be Gaussian. They are an extremely flexible class of point process models, and provide excellent models, *e.g.*, for what is usually referred to in ecological studies as 'presence only' data, *i.e.* data where the presence is always recorded, but the absence can mean a true absence or a lack of recording. Inference for these models is historically very hard, but INLA (see Section 2.2) opens new possibilities.

Let $\{\eta(s)\}_{s \in W}$ be a random field; this is a Gaussian field if and only if, given s_1, \dots, s_n a finite set of locations and b_1, \dots, b_n a set of real numbers, $b_1\eta(s_1) + \dots + b_n\eta(s_n)$ is normally distributed; in other words, the vectors $\eta(s_1), \dots, \eta(s_n)$ follow a multivariate normal distribution for any location s . As a normal variable, $\eta(s)$ can take negative values, so the easiest transfor-

mation in order to define a non-negative intensity for a Cox process is

$$\Lambda(s) = \int_W \lambda(s) ds = \exp(\eta(s));$$

by construction $\{\Lambda(s)\}_{s \in W}$ is also a random field.

The distribution of a LGCP X is defined through the distribution of the Gaussian field $\{\eta(s)\}_{s \in W}$, which is specified by its mean, variance and correlation structure (positive semi-definite). If the process is stationary and isotropic, the joint distribution of (X, η) is invariant under rigid motions. Stationary LGCPs are particularly friendly to deal with (Møller et al., 1998) as their distribution is completely characterised by the intensity and the pair correlation function (1^{st} and 2^{nd} order quantities), so both interpretation and estimation are easy; moreover, there are no edge effect problems (Diggle, 2014), and they are flexible and easy to simulate. Under stationarity, $\mu = E(\Lambda(0)) = \lambda$ is the mean of the intensity field (the origin is chosen as a reference point here, but because of stationarity it could be any point). Let σ^2 be the variance and $C(r)$ the covariance function of the latent field at distance r (being stationary, it only depends on distance), *i.e.* $C(r) = \sigma^2 k(r) = Cov\{\eta(s), \eta(s-r)\}$. Then, for the moment properties of the log-Normal distribution (Diggle et al., 2013), the first order intensity of a LGCP is

$$\lambda = E(\Lambda(0)) = E(\exp(\eta(0))) = \exp\left(\mu + \frac{1}{2}\sigma^2\right)$$

and the covariance density is

$$g(r) = \lambda^2[\exp(\sigma^2 k(r)) - 1].$$

It is natural to extend the definition of LGCPs to multivariate LGCPs, by replacing the scalar-valued $\eta(s)$ with a vector-valued multivariate Gaussian process (Diggle et al., 2013), and to spatio-temporal processes (see Section 2.1.6) (Møller and Waagepetersen, 2004).

2.1.5 Estimation issues

Despite their flexibility and their suitability for many real situations, LGCPs have not been much used until very recent years. The problem with

LGCPs is that, except for very special cases, the density of X is analytically intractable (Waagepetersen, 2008), and has to be approximated. The general form of the Cox process likelihood involves integration over the distribution of Λ which has infinite dimensions (Diggle et al., 2013). The traditional approach for estimating LGCPs (Møller and Waagepetersen, 2004) consists in approximating its likelihood with a Poisson likelihood, by superimposing a grid over the window and counting the number of points N_i in each cell C_i . As this is a Cox process, $N_i \sim Poi(\Lambda_i)$, where $\Lambda_i = \int_{C_i} \lambda(s) ds$, but usually the integral in Λ_i is impossible to compute and approximation is needed: approximately, $N_i \sim Poi(|C_i| \exp(\eta_i))$, where η_i is a representative value of the (continuous) Gaussian random field inside the cell C_i . Under suitable regularity conditions and when the cell size $|C_i|$ tends to zero, the composite likelihood coincides with the likelihood function in the case of a Poisson process. The corresponding estimating function is given by the derivative of the likelihood, and by Campbell's theorem (Baddeley et al., 2013) an unbiased estimating equation is obtained, for which the estimate coincides with the MLE under a Poisson process with the same intensity function. The problem is that the vector $\boldsymbol{\eta} = (\eta_i)$ has a dense covariance matrix. In conclusion, the grid should be made of few cells to make computations easier, but this way a higher approximation error is obtained. It is then intuitive to understand that, even if an advantage of Cox processes is that they can potentially reach high levels of complexity, this method is not suitable for complex models (Illian, 2012): high dimensionality can become a huge obstacle. That is why recent developments have proposed INLA as an approximate estimation approach (see Section 2.2.4).

2.1.6 Extension to the spatio-temporal case

Much of the theory of spatio-temporal point processes comes from that of spatial point processes. However, the temporal aspect enables an ordering of the points, or of some of them, that does not generally exist for spatial processes. Generic methods for the analysis of spatio-temporal point processes are not well established yet (Cressie and Wikle, 2011).

A temporal point process is defined as $\{X(t) : t \in T\}$ where t is a time index

and $T \subset \mathbb{R}$ can be continuous or discrete and is a random set of randomly occurring points (Cressie and Wikle, 2011); a spatio-temporal point process (in two dimensions) is defined in a subset $W(s, t) \subset \mathbb{R}^d \times \mathbb{R}$ and has first order intensity $\lambda(s, t)$ (Cressie and Wikle, 2011). This means we take repeated 'pictures' of a spatial phenomenon at different time points.

A spatio-temporal LGCP can be defined as a spatio-temporal inhomogeneous Poisson process conditional on a stochastic intensity function that varies both in space and time:

$$\Lambda(s, t) = \exp(\eta(s, t))$$

where $\eta(s, t)$ is a Gaussian process. The spatio-temporal LGCP is extremely flexible as it enables the presence of both fixed and random effects (Taylor et al., 2013).

In a spatio-temporal LGCP, as given in Diggle et al. (2013) for disease mapping data, the number of cases occurring at a certain time $X(s, t)$, or at a certain time interval $X(s, [t_1, t_2])$, is then inhomogeneous Poisson with intensity parameter

$$X(s, [t_1, t_2]) \sim Poi\left(\int_W \int_{t_1}^{t_2} \lambda(s, t) dt ds\right).$$

The intensity, in separable models, is decomposable as

$$\lambda(s, t) = \lambda_0(s, t)R(s, t) = \lambda_0(s)\mu_0(t)\exp(\eta(s, t))$$

where $\lambda_0(s, t) = \lambda_0(s)\mu_0(t)$ is the predictable deterministic baseline part, often a product of a purely spatial and a purely temporal component. The spatial baseline $\lambda_0(s)$ can be estimated via adaptive kernel smoothing, using for example the first available data of the series and integrates to 1 over the window W ; the temporal baseline $\mu_0(t)$ is found fitting a Poisson log-linear regression to the point counts over time. The second term $R(s, t) = \exp(\eta(s, t))$ is the stochastic part, describing the spatio-temporal variation, where $\eta(s, t)$ is a Gaussian process continuous over both space and time; the available data have to be used to build the predictive distribution of this 'risk' surface R using the LGCP and moment-based methods (Brix and Diggle, 2001) with a separable correlation structure: the spatio-temporal correlation $k(r, v) = k_s(r)k_t(v)$ can be divided into two components, one simply spatial and one simply temporal.

2.2 Integrated Nested Laplace Approximation

In a nutshell, INLA (Integrated Nested Laplace Approximation) (Rue et al., 2009) is an alternative approach to MCMC methods for estimating Bayesian hierarchical models; it is a method not based on sampling (which is the key to its fastness), and it is only valid for latent Gaussian models with a small number of hyperparameters.

The INLA approach is mathematically intense; Section 2.2.1 and 2.2.2 aim at giving an intuitive idea of how INLA works.

2.2.1 Latent Gaussian Models

Latent Gaussian models are a very general class of hierarchical Bayesian models where the response variable is assumed to belong to an exponential family and to be conditionally independent given a latent field (normally distributed) and some hyperparameters.

The hierarchical model can be written as:

1. observation level

$$\mathbf{y}|\boldsymbol{\eta}, \boldsymbol{\theta} \sim \pi(\mathbf{y}|\boldsymbol{\eta}, \boldsymbol{\theta}) = \prod_i \pi(y_i|\eta_i, \boldsymbol{\theta})$$

2. latent field level

$$\boldsymbol{\eta}|\boldsymbol{\theta} \sim N(\boldsymbol{\mu}_\theta, \mathbf{Q}_\theta^{-1})$$

3. hyperparameter level:

$$\boldsymbol{\theta} \sim \pi(\boldsymbol{\theta}).$$

The marginal distribution of each parameter is:

$$(\eta_i|\boldsymbol{\eta}_{-i}, \boldsymbol{\theta}) \sim N\left(\mu_i - \frac{1}{Q_{ii}} \sum_{j \neq i} Q_{ij}(\eta_j - \mu_j), Q_{ii}^{-1}\right).$$

Combining the three levels the joint posterior gives (Illian et al., 2013):

$$\pi(\boldsymbol{\eta}, \boldsymbol{\theta}|\mathbf{y}) \propto \pi(\boldsymbol{\theta})N(\boldsymbol{\mu}_\theta, \mathbf{Q}_\theta^{-1}) \prod_i \pi(y_i|\eta_i, \boldsymbol{\theta})$$

and the analysis is aimed at finding the marginal posteriors for all the elements of the latent field, to make inference on the relationship between the response variable and all the covariates and spatial structures (Simpson et al., 2012).

Sparse dependence

In Gaussian Random Fields (GRFs), observations are jointly normally distributed with covariance matrix Σ . This matrix is generally dense, but the matrices for the analysis have to be sparse, as this solves computational efficiency and storage memory problems. A solution is to build a sparse precision matrix $\mathbf{Q} = \Sigma^{-1}$, which implies sparse conditional dependence; sparse conditional dependence intuitively means an event depends on a close neighbourhood in such a way that, given that neighbourhood, it is independent of all other events. Defining the idea of neighbourhood on continuous space is not trivial; an approximation can be given by a discrete grid structure as the one we will use in our work. When working with spatial data on a grid, neighbour cells are defined as the ones within a fixed distance from a reference cell: this way, first order neighbours are defined as the adjacent ones in the cardinal directions, second order neighbours as the adjacent ones on the diagonals, third order neighbours as the further four ones in the cardinal directions and so on. Working with discrete space allows to choose a neighbourhood structure and build as sparse a precision matrix as it is needed. That is why GRFs are often approximated by their discrete version, Gaussian Markov Random Fields (GMRFs), and marginal distributions are substituted by conditional distributions. A Markov Random Field can be defined as a set of random variables having the Markov property (Rue and Held, 2005), and when all variables are normally distributed, we have a GMRF. GMRFs are defined on a discrete space (often, a grid) where the single cell value is chosen as a representative value of the continuous GRF inside the cell. Building the precision matrix $\mathbf{Q} = \Sigma^{-1}$ as a sparse matrix implies full conditional independence (but not marginal independence) between variables belonging to the latent field: $\eta_i \perp \eta_j | \eta_{-\{ij\}} \Leftrightarrow Q_{ij} = 0$. We can build processes such that Σ is dense but \mathbf{Q} is sparse. If \mathbf{Q} is sparse, calculations can be made very

efficient.

As we are interested in the conditional distributions, we can define a GMRF by its conditional mean and precision; the conditional mean is a weighted sum of the neighbours, with weights corresponding to the values in \mathbf{Q}

$$E[\eta_i|\eta_{-i}] = \mu_i - \frac{1}{Q_{ii}} \sum_{j \sim i} Q_{ij}(\eta_j - \mu_j)$$

where $j \sim i$ means that η_j belongs to the neighbourhood of η_i .

The precision is

$$Prec[\eta_i|\eta_{-i}] = Q_{ii}.$$

Intrinsic GMRFs

Different types of random fields may be used to model the spatial effect on a lattice; one of them is the intrinsic GMRF (IGMRF) (Illian, 2012). IGMRFs are often called intrinsic CAR models, or Random Walks in two dimensions (RW2d), and are characterized by a precision matrix which is not of full rank (has at least one zero eigenvalue), *i.e.* they are *improper*; the Besag model belongs to this class. Following an IGMRF, the conditional expected value in a cell $E[\eta_i|\eta_{-i}]$ is a weighted average of its 12 neighbours $\eta_j, j \sim i$, with higher weights for closer neighbours: the four nearest neighbours have weight $Q_{ij} = 8$, the 4 second order neighbours in the cardinal directions have weight $Q_{ij} = -1$ and the 4 nearest neighbours on the diagonal are weighted $Q_{ij} = -2$ (Illian, 2012).

As for the precision hyperparameter, values have to be carefully chosen as a high variance might produce a function too smooth to explain spatial correlation, while too high a precision might lead to overfitting and miss the spatial trend.

A sum-to-zero constraint is needed for all IGMRFs to ensure identifiability of the model.

2.2.2 Obtaining posterior estimates with INLA

The Laplace approximation (Rue and Held, 2005) is a method for using a Gaussian distribution to represent a given probability density function (in

Bayesian analysis, the posterior distribution). This is obviously more effective for a single-mode distribution, as many popular distributions could be roughly represented with a Gaussian shape. The idea is that often the actual distribution $p(\boldsymbol{\eta}|\mathbf{y}, \boldsymbol{\theta})$ cannot be easily sampled, and an alternative way to draw samples from $p(\boldsymbol{\eta}|\mathbf{y}, \boldsymbol{\theta})$ is needed; one solution is to draw samples from another, 'nicer' distribution. It is preferable to use something simple and computable because, as the dimension of the problem increases, the required computational memory increases very quickly. This is why approximations are used.

The Laplace approximation exploits the Gaussian distribution and Taylor's series expansion to obtain a tractable and computationally fast approximation of the original distribution (Blangiardo et al., 2013). The aim of INLA is to provide accurate and fast deterministic approximations to all, or at least some of, the k posterior marginals for η_i s, the components of the latent Gaussian vector $\boldsymbol{\eta}$, plus possibly the posterior marginals for $\boldsymbol{\theta}$ (or some of its components θ_j s). For this purpose, INLA exploits two approximations:

- the latent Gaussian field is approximated by a discrete GMRF, *i.e.* the space is discretized and it is assumed that each value in the grid only depends on some neighbourhood structure, so that the precision matrix is sparse. The neighbourhood structure can be different for the different components of the field
- the latent field is Gaussian, so a Laplace approximation can be used for its posterior distribution.

The approximation applied by INLA is aimed at finding the marginal posterior distribution, *i.e.* the conditional distribution of the latent field $\boldsymbol{\eta}$ given the data $\pi(\eta_i|\mathbf{y})$ and of $\boldsymbol{\theta}$, $\pi(\theta_i|\mathbf{y})$ without integrating over $\boldsymbol{\eta}$: the problem is that usually these integrals are extremely high dimensional (they could involve billions of values). Here follow the main steps:

1. Laplace approximation $\tilde{\pi}$ of the joint posterior of the hyperparameters:

$$\pi(\boldsymbol{\theta}|\mathbf{y}) = \frac{\pi(\boldsymbol{\eta}, \boldsymbol{\theta}, \mathbf{y})}{\pi(\boldsymbol{\eta}|\boldsymbol{\theta}, \mathbf{y})\pi(\mathbf{y})} = \frac{\pi(\boldsymbol{\eta}, \boldsymbol{\theta}|\mathbf{y})}{\pi(\boldsymbol{\eta}|\boldsymbol{\theta}, \mathbf{y})} \propto \frac{\pi(\boldsymbol{\eta}, \boldsymbol{\theta}|\mathbf{y})}{\pi_G(\boldsymbol{\eta}|\boldsymbol{\theta}, \mathbf{y})} \Big|_{\boldsymbol{\eta}=\boldsymbol{\eta}^*} = \tilde{\pi}(\boldsymbol{\theta}|\mathbf{y})$$

where π_G is a Gaussian (Laplace) approximation of $\pi(\boldsymbol{\eta}|\boldsymbol{\theta}, \mathbf{y})$ with the characteristic of matching the true posterior at the mode: in fact, the full conditional of a GMRF can often be well approximated by a Gaussian distribution by matching the value and the curvature at the mode. This means the true full conditional of the latent field is approximated by a Gaussian distribution evaluated at the mode $\boldsymbol{\eta}_\theta^*$.

This approximation is very accurate in most cases (Rue et al., 2009) as $\pi(\boldsymbol{\eta}|\boldsymbol{\theta}, \mathbf{y})$ looks almost Gaussian, due to the assumption that the prior $\pi(\boldsymbol{\eta}|\boldsymbol{\theta})$ is Gaussian (Illian, 2012);

2. numerical integration to find the (approximate) posterior marginals $\tilde{\pi}(\theta_i|\mathbf{y})$, which is possible because we assume $\boldsymbol{\theta}$ is made of few hyperparameters;
3. Laplace approximation of the posterior marginals (that can be many): $\tilde{\pi}(\eta_i|\boldsymbol{\theta}, \mathbf{y})$. The most efficient (fast) algorithm is the 'Simplified Laplace approximation', which is based on a Taylor's series expansion of the Laplace approximation. This is usually corrected by including a mixing term (*e.g.* splines), to increase the fit to the required distribution;
4. integration out of θ to find the posterior marginals $\pi(\eta_i|\mathbf{y})$. In numerical integration, the Laplace approximation of $\pi(\boldsymbol{\theta}|\mathbf{y})$ (already obtained) is explored numerically in order to find support points θ_p for the numerical integration. These points are given area weights Δ_p that are plugged into the sum that approximates the integral:

$$\tilde{\pi}(\eta_i|\mathbf{y}) = \int \tilde{\pi}(\eta_i|\boldsymbol{\theta}, \mathbf{y})\tilde{\pi}(\boldsymbol{\theta}|\mathbf{y})d\boldsymbol{\theta} \approx \sum_p \pi_G(\eta_i|\theta_p, \mathbf{y})\tilde{\pi}(\theta_p|\mathbf{y})\Delta_p.$$

INLA first explores the marginal joint posterior of the hyperparameters $\boldsymbol{\theta}$ in order to locate the mode, which will become the mean of the approximate Gaussian posterior (Blangiardo et al., 2013). A grid search is then performed and produces a set of 'relevant' points $\boldsymbol{\theta}^* = \{\theta_p, p = 1, \dots, P\}$ together with a corresponding set of weights $\boldsymbol{\Delta}^* = \{\Delta_p, p = 1, \dots, P\}$ to give the approximation to this distribution. Each marginal posterior for the relevant points $\pi(\theta_p|\mathbf{y})$ can be obtained using interpolation based on the computed

values and correcting for (probable) skewness, *e.g.* by using log-splines. For each θ_p , the conditional posteriors $\pi(\eta_i|\theta_p, \mathbf{y})$ are then evaluated on a grid of selected values for η_i and the marginal posteriors $\pi(\eta_i|\mathbf{y})$ are obtained out by numerical integration.

2.2.3 Estimating models with INLA

As already said, the objectives of Bayesian inference are the marginal posterior distributions for each element of $\boldsymbol{\eta}$ and $\boldsymbol{\theta}$. Typically, the interest lies in estimating the effect of a set of relevant covariates on some function (usually the mean) of the observed data, while accounting for the spatial or spatio-temporal correlation implied in the model.

Latent Gaussian models are a subclass of structured additive regression models, *i.e.* a subset of all Bayesian additive models with a structured additive predictor.

A structured additive model can be written as

$$y_i = \mu_i + \epsilon_i$$

with

$$g(\mu_i) = \beta_0 + \sum \beta_k z_{ki} + \sum w_{ji} f_j(z_{ji}) + u_i$$

where the latent field is $\boldsymbol{\eta} = \{\beta_0, \beta_k (k = 1 \dots K), f_j (j = 1 \dots J), u_i (i = 1 \dots N)\}$, *i.e.* a collection of all random parameters, and specifically

- β_0 is a common intercept; it can be fixed, i -varying or have both components
- β_k are linear fixed effects of covariates
- $f_j(z_{ji})$ are smooth (large or small scale) spatial effects
- u_i is an unstructured error term that might be included.

With the INLA approach for latent Gaussian models:

- $\boldsymbol{\eta} \sim N(\mathbf{0}, \mathbf{Q}^{-1})$, *i.e.* all effects are assumed normal with zero mean

- the latent field can have any size, but \mathbf{Q} must be ruled by ≤ 7 different hyperparameters
- $\boldsymbol{\beta} \sim N(\mathbf{0}, \tau_\beta^{-1} \mathbf{I})$ *i.e.* all linear effects are assumed independent and depending on the same hyperparameter
- neighbourhood structures must be fixed for the f_j s, in order to define the non-zero values in \mathbf{Q} ; by fixing different neighbourhood structures, both small and large scale variation can be taken into account. Non-linear effects can also be unstructured, like error terms, and in this case they are uncorrelated. This way, the general precision matrix \mathbf{Q} has non-zero off-diagonal values only corresponding to the non-linear structured effects
- $\mathbf{u} \sim N(\mathbf{0}, \tau_u^{-1} \mathbf{I})$, *i.e.* the linear error terms u_i are *i.i.d.* and $\tau_u \sim Ga(\alpha, \beta)$. Note that $E(\tau_u) = \frac{\alpha}{\beta}$ and $\sigma_u^2 = \frac{1}{\tau_u} \sim InvGa(\alpha, \beta)$. This means that $E(\sigma_u^2) = \frac{\beta}{\alpha-1}$ and $V(\sigma_u^2) = \frac{\beta^2}{(\alpha-1)^2(\alpha-2)}$, which gives indications on how to choose the hyperparameters and is valid in all cases where the precision is modelled as a *Gamma*: $V(\sigma^2) < \infty \Leftrightarrow \alpha > 2$; if $\alpha \leq 2$ the prior is vague (infinite variance).

Note that a zero-mean for all latent field components is not a loss of generality, as this can be obtained by shifting data (under stationarity) or by considering residuals.

2.2.4 Estimating LGCPs with INLA

In the particular case of LGCPs, the log-intensity of the Poisson process can be described by a linear predictor (Illian et al., 2012) as

$$y_i = \lambda_i + \epsilon_i \sim Poi(\lambda_i)$$

where $y_i = N(C_i)$. The approximation of the point process X by a discrete Poisson process Y is good when cells are small enough, with

$$\log(\lambda_i) = \beta_0 + \beta_t + \sum_{k=1}^K \beta_k z_{ki} + \sum_{j=1}^J w_{ji} f_j(z_{ji})$$

where β_0 is a common intercept and β_t are time-specific intercepts and account for variation in the intensity across time/space. The Gaussian latent field is $\boldsymbol{\eta} = \{\beta_0, \beta_k(k = 1 \dots K), f_j(j = 1 \dots J)\}$ and the distribution of all the parameters of the field is approximated by a GMRF; a neighbourhood structure for all the parameters is fixed, which can be different (*e.g.* small-scale effects have first-order neighbours, large scale effects account for a wider neighbourhood, ...): practically, only neighbourhood structures for f functions must be set, while the linear effects are assumed independent.

With the INLA discretization to cell counts, the response variable is Poisson distributed; data usually look like zero-inflated Poisson data, as most cells (especially with a fine grid) have zero values; however, it would be wrong to model them as zero-inflated, as what they actually are is spatially correlated Poisson data.

2.2.5 Discussion on INLA performance

Experience (Rue et al., 2009) says practically exact results are obtained over a wide range of commonly used latent Gaussian models. Moreover, tools for assessing the approximation error are provided. The approach produces precise estimates in seconds and minutes, even for models involving thousands of variables, in situations where any MCMC computation typically takes hours or even days (Rue et al., 2009). This also means different models can be run and compared, usually by Deviance Information Criterion (DIC), within reasonable time, which is of great help.

Some disadvantages are encountered when using INLA:

- its computational cost is exponential with respect to the number of hyperparameters m (but in most applications m is small)
- it requires some analytic computation or/and some black box numerical differentiation, being based on a standard second-order Taylor approximation to the log-density
- it misses a clean evaluation of the associated error

- the calibration of the Laplace approximations seems to require a high level of expertise.

In a few words, INLA has two main disadvantages with regard to MCMC: it does not work for all possible models, and it has a harder mathematical background. As for the first aspect, INLA authors argue that in order to find a better performing method than MCMC they had to restrict the class of models that can be solved by a single method. Nevertheless, the class of Latent Gaussian Models is still very broad and flexible and provides a good solution in many real situations. As for the mathematical complexity, this mainly implies that using INLA can be prohibitive for non-statisticians or mathematicians. Despite this, when it is possible to use it results are extremely accurate, and the fastness of INLA in providing a solution is certainly its greatest advantage. Obtaining fast results is a key point in many analyses, especially when prediction is concerned; as for our work, it allows many models to be fitted and different methods to be tested in a very reasonable time despite the complexity of the dataset, as we show in Chapters 4 and 5. In addition, the R package `R-INLA` (see Section 2.2.6) now allows an easy implementation of the approach.

As for the choice of the grid size, this is in general an issue in practical work. As usual, the finer the grid, the more accurate the results, but the longer the computational time. However, there are a few nice aspects to point out. First, the grid need not be so fine as to contain maximum one point per cell, as is desirable in other situations (*e.g.* Waagepetersen (2008)): INLA models the resulting counts as a Poisson, therefore values higher than 1 are considered for what they are, there is no approximation to binary values. Moreover, the use of a GMRF keeps a small neighbourhood structure, so the covariance matrix will still be very sparse even if the grid is very fine, which will keep computations feasible. Furthermore, the computational efficiency of INLA allows the statistician to try different grid sizes in an acceptable time before choosing the best trade off between being accurate and being fast for the specific analysis. In most cases the conclusion will be that the grid can be as fine as the statistician wishes, and we found that after a certain fine resolution results are not substantially affected by the cell size.

If being as fast as it is possible is the main concern of an analysis, there are other approaches than the grid that further increase the computational efficiency. They are discussed in Chapter 6.

2.2.6 Notes on INLA software

The reference software for working with INLA is R (Rue et al., 2009): the R-INLA package can be used for many GMRF hierarchical models and aims at being user friendly and fairly easy to approach. The package is constantly under construction, and can be downloaded from the website www.r-inla.org, where examples and tutorials are also displayed, or by typing `source('http://www.math.ntnu.no/inla/givemeINLA.R')` in R.

The package implements many exponential models, and dependence, which is the main interest in our work, can be modelled using many random effects models, such as first order auto-regressive models, random walks of first and second order and in two dimensions. It is also possible to build user-defined dependence structures.

The R-INLA package is used for all the computations in this work.

2.3 Bayesian changepoint analysis

In this Section, we give a brief overview of what is meant by a temporal changepoint and give some examples of changepoint analysis questions. We show some likelihood based methods, as they have been widely used for detecting changepoints in time series up to recent years, and we highlight the issues that cannot be answered with these methods (*i.e.* dependence between data). We then introduce some recent Bayesian techniques for overcoming the problem and widen the range of real situations that can be dealt with.

2.3.1 Introduction to changepoint analysis

A changepoint is defined as a place or time point τ in a data series Y such that the observations follow one distribution, say F_0 , up to that point and another one, say F_1 , after that point (Chen and Gupta, 2012). The assumption

is that data are ordered from 1 to T (it usually is time order, but it may be some other natural order) and that the model describing them presents some abrupt changes; data are then split into segments, which generally follow the same model but under different parameter specifications (Wyse et al., 2011). Note that we only consider abrupt changes here; for a discussion on the differences with regard to gradual change we remind to Section 3.5.

The usual assumption in standard changepoint analysis is that observations are *i.i.d.* between every pair of changepoints, therefore the distribution of the sequence can be written as:

$$Y_i \sim F_0 \text{ for } i \leq \tau_1$$

$$Y_i \sim F_1 \text{ for } \tau_1 < i \leq \tau_2$$

$$Y_i \sim F_2 \text{ for } \tau_2 < i \leq \tau_3$$

...

where τ_1, τ_2, \dots are the changepoint locations, defined in our work as the last time point of every segment.

Changepoint problems can be developed on different complexity levels, a list of which follows.

1. **One changepoint, known location in τ_0 ;**

the underlying assumptions are:

- data follow a distribution $Y_i \sim F_i$ with one potential change in the parameters after τ_0
- $H_0: F_1 = \dots = F_T$
 $H_1: F_1 = \dots = F_{\tau_0} \neq G_{\tau_0+1} = \dots = G_T$
- rejection of H_0 means that there is a changepoint at location τ_0 , otherwise there is no distributional change.

2. **One changepoint, unknown location in τ , $\tau \in \{1, \dots, T\}$;**

the underlying assumptions are:

- data follow a distribution $Y_i \sim F_i$ with one potential change in the parameters which can occur at any time point
- $H_0: F_1 = \dots = F_T$
 $H_1: F_1 = \dots = F_\tau \neq G_{\tau+1} = \dots = G_T, \tau \in \{1, \dots, T\}$

- rejection of H_0 means that there is a changepoint at an unknown location τ that needs to be detected.

3. **Known number of changepoints M , unknown locations τ_1, \dots, τ_M ;** the underlying assumptions are:

- data follow a distribution $Y_i \sim F_i$ with M potential changes in the parameters which can occur at any time point
- $H_0: F_1 = \dots = F_T$
 $H_1: F_1 = \dots = F_{\tau_1} \neq G_{\tau_1+1} = \dots = G_{\tau_2} \neq \dots \neq H_{\tau_M+1} = \dots = H_T$
- rejection of H_0 means that there are M changepoints that need to be detected.

It is not possible to test all the possible combinations, as computations quickly become infeasible as M increases. There is a need for some dynamic algorithm. Note that in general the rejection of H_0 only means that there is at least one change at some location, and does not imply a specific number of changepoints. In this special case, thanks to some prior knowledge we know that, if H_0 is rejected, there are M changepoints.

4. **Unknown number of changepoints $m = 1, \dots, M$, unknown locations τ_1, \dots, τ_m ;**

the underlying assumptions are:

- data follow a distribution $Y_i \sim F_i$ with m potential changes in the parameters, m unknown, which can occur at any time point
- $H_0: F_1 = \dots = F_T$
 $H_1: F_1 = \dots = F_{\tau_1} \neq \dots \neq H_{\tau_m+1} = \dots = H_T, m = 1, \dots, M$
- rejection of H_0 means that there is at least one changepoint. Number and locations need to be detected.

The approach to concurrent estimation becomes infeasible with the currently available tools, therefore sequential methods such as binary

segmentation (or bisection) methods and model selection procedures are used. In Chapter 3, further details on sequential algorithms are given.

All the previous cases assume *i.i.d.* observations, therefore analyses get even more complex if we want to introduce any type of dependence between points. In the usual case of temporal series, temporal dependence within each time segment may be considered; in the unusual case of a changepoint analysis on spatio-temporal data, dependence can be over both space and time.

The most common methods for changepoint detection include parametric techniques (likelihood ratio), non parametric tests, Bayesian tests, stochastic processes. Most parametric works cover the case of a single changepoint in *i.i.d.* continuous variables (Chen and Gupta, 2012). Bayesian methods can be useful for our analysis, as they potentially allow for the presence and estimation of multiple changepoints at unknown locations in a wide range of models. The Bayesian approach offers an alternative to likelihood-based methods: frequentist procedures for changepoint analysis estimate specific locations of changepoints, while a Bayesian changepoint search produces a probability distribution, *i.e.* the probability of a changepoint at each location in a sequence of data (Erdman and Emerson, 2007). When running a Bayesian analysis, what has to be specified in addition to the likelihood is a prior distribution on the number of changepoints, on their positions and on the segment parameters.

We now briefly review the most important likelihood-based methods for changepoint analysis, and then illustrate the most recent developments in Bayesian changepoint analysis.

2.3.2 A partial solution: likelihood-based methods

Let $y_{1:T} = (y_1, \dots, y_T)$ be the time series data, indexed by $t = 1, \dots, T$. Let M be the (unknown) number of changepoints, whose positions are listed in $\tau = (\tau_1, \dots, \tau_m, \dots, \tau_M)$ (we focus on the fourth and last case in the above list of changepoint scenarios); by definition, $\tau_0 = 0$, $\tau_{M+1} = T$ and we assume the changepoints are ordered, *i.e.* $\tau_i < \tau_j \iff i < j$. The sequence of data with a constant value for the (vector of) parameter(s) θ is called a *segment*

or *block*; segments can be identified as $y_{a:b}$, where a identifies the first observation of the block and b the last one. A number M of changepoints splits data into $M + 1$ segments, and we indicate segment $j = 1, \dots, (M + 1)$ with $y_{\tau_{j-1}+1:\tau_j}$ where every τ_m marks the last point of a segment.

For a parametric family of distributions and under the assumption of *i.i.d.* data within segments, the null hypothesis coincides with $H_0 : \theta_1 = \dots = \theta_T$. To assess the hypothesis, the likelihood ratio between the overall likelihood L_0 (a product of T equal functions) and the likelihood under H_1 , L_1 (a product of $M + 1$ blocks of equal functions), is used.

For a single changepoint detection,

$$H_0 : M = 0$$

$$H_1 : M = 1.$$

Under H_0 , the maximum log-likelihood is

$$l_0 = \log p(y_{1:T}|\hat{\theta})$$

where $\hat{\theta}$ is the Maximum Likelihood Estimate for the whole dataset.

Under H_1 , the maximum log-likelihood for a given changepoint in τ_0 is

$$l_1(\tau_0) = \log p(y_{1:\tau_0}|\hat{\theta}_1) + \log p(y_{\tau_0+1:T}|\hat{\theta}_2).$$

In the case of discrete changepoints, the maximum is taken over all possible locations, so the maximum log-likelihood under H_1 is

$$l_1 = \max_{\tau} l_1(\tau).$$

A suitable test statistic is:

$$\gamma = 2[l_1 - l_0].$$

The statistician has to choose a threshold c and reject the null hypothesis if $\gamma > c$; once H_0 is rejected, the chosen changepoint position is the value $\hat{\tau}$ that maximises $l_1(\tau)$. The appropriate value for the threshold is still an open research question; in most cases, it is based on p-values and Information Criteria. Remember all this holds under the assumption of *i.i.d.* observations. The problem of multiple changepoints is not often considered, being computationally much more challenging: as datasets increase in length, the number

of possible solutions to the multiple changepoint problem increases combinatorially with M (Killick and Eckley, 2011); typically, it is tested how many segments are needed to represent the data, *i.e.* how many changepoints are present, and then the values of the parameters associated with each segment are estimated.

In the general case of M points, the most common approach is to minimise

$$\sum_{j=1}^{M+1} \mathcal{C}(y_{\tau_{j-1}+1:\tau_j}) + \beta f(M)$$

where

- \mathcal{C} is a cost function for each segment (*e.g.* $\mathcal{C} = -\log Lik$)
- $\beta f(M)$ is a penalty against over fitting. As for the choice of $f()$, usually $f(M) = M$, while the choice of β is different for different Information Criteria, for instance
 - AIC: $\beta = 2p$
 - BIC/SIC: $\beta = p \log T$

where p is the number of additional parameters to estimate when adding a changepoint.

AIC is a popular choice, but it is proved to asymptotically overestimate the number of changepoints (Killick et al., 2012); BIC asymptotically estimates the correct M .

For an overview of the most common sequential algorithms for multiple changepoint detection we refer to Eckley et al. (2011).

Likelihood-based methods have been widely used for detecting changepoints. Their common limit is that they heavily rely on the assumption of *i.i.d.* data within segments, as this makes all computations easier because segment likelihoods are simply products of data likelihoods. When dependence needs to be included, no solution has been provided with likelihood-based methods so far, as the segment likelihoods often become intractable. Some progress has been recently done using Bayesian methods, as we illustrate in Section 2.3.3.

2.3.3 The issue of dependence within segments

From now on, unless differently specified we will deal with the most general changepoint scenario of multiple changes at unknown locations.

As previously introduced, an usual assumption is that each observation y_t in the sequence y_1, \dots, y_T is independent, with a density parameter θ_t whose changes are of interest. The other usual assumption is that $y_t \sim N(\mu_t, \sigma^2)$, *i.e.* observations are normally distributed.

With a Bayesian approach, both assumptions can be weakened: normality can be replaced by any other parametric family, and as for independence it is enough that observations in different blocks are mutually independent (Barry and Hartigan, 1993). The difficulty in performing Bayesian changepoint analysis is that the segment marginal likelihood is required to be computable in order to find the posterior; this is not always possible, especially when independence assumptions are relaxed, and this is why approximate methods have to be employed.

The most complicated step in a changepoint analysis concerns situations where the number and locations of changepoints is not known. Further issues arise when any kind of dependence within data is included.

An important step toward the detection of multiple unknown changepoints in a temporal series is introduced by Fearnhead (2006). A Bayesian method is developed using recursive techniques for a number M of changepoints. Fearnhead aims at showing that, under some conditions, calculating the Bayes Factor for models with many changepoints is feasible. The use of the recursions is introduced to calculate posterior probabilities of different numbers of changepoints and posterior means of the segment parameters; besides, inference conditional on a number of changepoints is allowed.

The limit of this method is that it requires the segment marginal likelihoods to be analytically or numerically computable. This implies, again, that observations within a segment have to be independent, given the parameters, or that the number of parameters must be very small. In the case of independence the segment marginal likelihood is simply the product of each time point's likelihood; when dependence is allowed, segment likelihoods usually become intractable. This is the case in many real situations, where some

type of dependence must be included. Wyse et al. (2011) extend Fearnhead's method to the case of dependence within segments by substituting analytical computation of the segment likelihoods with a fast and (under some conditions) accurate approximation given by INLA (introduced in Section 2.2). Dependence within, but not between, segments implies that the data general likelihood conditional on the M changepoints and on the latent field can be still written as a product of $M + 1$ segment marginal likelihoods; thus, the approximation is only needed within time segments.

In this Section, we introduce the idea of recursions under the setting of the works by Fearnhead and Wyse et al..

2.3.4 Prior distributions

As Fearnhead (2006) illustrates, there are two possible classes of prior settings.

The first one is structured into two levels: firstly, a prior $\pi(m)$, $m = 0, \dots, M$ on the number of changepoints is defined and then, conditional on m , a set of priors for the changepoint positions is built, where every changepoint's prior depends on the following changepoint position

$$\begin{aligned} 1) \quad & \pi(m) \\ 2) \quad & \pi_m(\tau_1, \dots, \tau_m) = \pi_m(\tau_m)\pi_m(\tau_{m-1}|\tau_m) \dots \pi_m(\tau_1|\tau_2). \end{aligned} \tag{2.3.1}$$

By definition, we have $\tau_0 = 0$ and $\tau_{m+1} = T$.

The second prior setting consists of a joint prior on number and position of the changepoints, built by modelling the occurrence of changepoints by a discrete point process in $\mathbb{Z} \cap [1, T - 1]$. This might be particularly interesting in the context of our work, as we would have a point process on two levels: a temporal process at the prior level and a spatio-temporal process at the data level. The point process prior is built by looking at the mass density function $g(v)$ of the time v between two successive changepoints. Since the distribution is discrete, its cumulative distribution function (CDF) $G(v) = \sum_{u=1}^v g(u)$ will be stepwise.

$$\pi_m(\tau_1, \dots, \tau_m) = g_0(\tau_1) \left(\prod_{j=2}^m g(\tau_j - \tau_{j-1}) \right) (1 - G(\tau_{m+1} - \tau_m)).$$

where $g_0(\tau_1)$ is the mass function at the first changepoint, as initial value for the series of products.

A natural choice for the distribution of v is the Negative Binomial distribution:

$$v \sim NB(k, p)$$

$$g_0(v) = \sum_{i=1}^k \binom{v-i}{i-1} \frac{p^i (1-p)^{v-i}}{k}$$

$$g(v) = \binom{v-k}{k-1} p^k (1-p)^{v-k}$$

where k is the number of changepoints until the sequence is stopped, and p is the probability of each *i.i.d.* Bernoulli trial.

2.3.5 Likelihood: recursive methods

We now show how to derive the filtering recursions under either prior setting. A changepoint τ_j is the last point of segment j , therefore if a segment begins at time t it means the last changepoint occurred at $t - 1$: a general segment j defines the interval $[\tau_{j-1} + 1, \tau_j]$. Then, given $y_{a:b}$ as the set of data from time point a to time point b , we define the quantity

$$P(a, b) = Pr(y_{a:b} | a, b \text{ are in the same segment}).$$

This is the likelihood of a set of data within a segment, and, if a and b are the extreme values of a segment, this defines a segment's marginal likelihood. This is the quantity that becomes intractable in complex models and needs to be approximated using INLA.

Point process prior setting

Fearnhead's approach derives recursions under the point process prior, and assumes data are independent given the parameters. This would require conjugate priors on the parameters, or a small parameter vector to allow for numerical solutions.

Let

$$Q(a) = Pr(y_{a:T} | \text{there is a changepoint in } a-1)$$

be the probability of a segment or a union of segments; there are two differences with respect to $P(a, b)$: first, a must now be the start of a new segment, and second, a and T need not be within the same segment. As a consequence

$$Q(1) = Pr(y_{1:T})$$

is the likelihood of the whole dataset, which coincides with $P(1, T)$ iff there are no changepoints.

Fearnhead writes $Q(a)$ recursively as

$$Q(a) = \sum_{b=a}^{T-1} P(a, b)Q(b+1)g(b+1-a) + P(a, T)(1 - G(T-a)). \quad (2.3.2)$$

This can be intuitively proved: since $Q(a) = Pr(y_{a:T} | \text{changepoint in } a-1)$, where a further changepoint can occur at any time, this is a sum of many different cases

$$\begin{aligned} Q(a) = & \sum_{b=a}^{T-1} Pr(a, T, \text{ next changepoint is in } b) \\ & + Pr(a, T, \text{ no further changepoints}). \end{aligned} \quad (2.3.3)$$

The first term on the right hand side is a product of

- a prior probability that, given the changepoint in $a-1$, the next changepoint will be in b : $g(b - (a - 1)) = g(b + 1 - a)$
- a conditional probability $Pr(y_{a:T} | \text{next changepoint is in } b)$ where b is somewhere between a and T . This, in turn, can be split into
 - a single segment from a to the following changepoint b :
 $Pr(y_{a:b} | a, b \text{ are in the same segment}) = P(a, b)$
 - the union of segments from $b+1$ to T :
 $Pr(y_{b+1:T} | \text{there is a changepoint in } b) = Q(b+1)$

Therefore, as for the first term we obtain

$$\sum_{b=a}^{T-1} Pr(a, T, \text{ next changepoint is in } b) = \sum_{b=a}^{T-1} P(a, b)Q(b+1)g(b+1-a).$$

As for the second term on the right hand side of Formula(2.3.3), it is a product of

- a prior probability on the last time interval, given that the last changepoint is in $a - 1$: $g(T - a) = 1 - G(T - a)$
- a segment likelihood, as there are no further changepoints
 $Pr(y_{a:T}|a, T \text{ are in the same segment}) = P(a, T)$

and we obtain

$$Pr(a, T, \text{ no further changepoints}) = P(a, T)(1 - G(T - a)).$$

The sum of the two terms returns Formula(2.3.2).

Recursive equations are computed backwards from $a = T - 1$ to $a = 1$. $Q(1)$ is the likelihood of the data under the model with changepoints, and gives evidence for the model. It can be compared to the likelihood under the null model $P(1, T)$; if $Q(1) > P(1, T)$ then changepoints occur in the series. The joint posterior distribution of number and positions of changepoints will depend on the prior mass probability function and the results of the recursions.

Two level prior setting

The novelty of Wyse et al. (2011) is to relax the assumption of exchangeability of data within segments. The focus of the work is on inferring the changepoint positions after estimating the most likely number of changepoints a posteriori; this method is shown for a prior on two levels as in (2.3.1): a prior distribution on the number of changepoints and then, conditional on that, a prior distribution on their positions. However, the method also applies when there is a joint prior on the number and position of changepoints. If a two level prior is used, first of all the posterior distribution for each number of changepoints $m = 0, \dots, M$ can be found, using the usual Bayesian formula

$$\pi(m|y) \propto \pi(y|m)\pi(m)$$

where the likelihood is recursively computed. By doing this for many ms it is possible to compare the posterior distributions and estimate the most likely number of changepoints a posteriori. Once the best number of changepoints is found, their positions are inferred.

Having a different prior setting, recursions are built in a different way to Fearnhead's approach: the point process prior does not fix a number of changepoints, while, if we work on a two level prior, recursions are computed conditional on a number of changepoints. This means, for example, that if we look at $Q(a)$ where $a - 1$ is the j th changepoint, then there must be $m - j$ changepoints from a to T . Thus, we do not have both right hand side terms as in Formula(2.3.3): we only have either the first one if $a - 1$ is the j th changepoint, $j < m$, or the second one if $a - 1$ is the m th changepoint. Since recursions are not built the same way as in Fearnhead (2006), instead of labelling them with Q we use L , that depends on both m and j :

$$L_j^{(m)}(a) = Pr(y_{a:T} | \text{the } j\text{th changepoint is in } a-1, \text{ there are } m \text{ changepoints})$$

and, using the corresponding prior setting

$$L_j^{(m)}(a) = \sum_{b=a}^{T-m+j} P(a, b) L_{j+1}^{(m)}(b+1) \pi_m(\tau_j = a-1 | \tau_{j+1} = b) \quad (2.3.4)$$

where $j = (m - 1), \dots, 0$ and, for every j , $a = (T - m + j - 1), \dots, (j + 1)$. Formula(2.3.4) can be proved analogously to (2.3.3) for $j = 0, \dots, m$; in particular it is easy to derive that for $j = m$

$$L_m^{(m)}(a) = P(a, T)$$

since there are no further changepoints after $a - 1$.

The data marginal likelihood under m changepoints becomes

$$L(Y|m) = L_0^{(m)}(1) = \sum_{b=1}^{T-m} P(1, b) L_1^{(m)}(b+1) \pi_m(\tau_0 = 0 | \tau_1 = b)$$

where $Y = y_{1:T}$.

Case $m = 1$: relation to the Bayes Factor

If we assume there is a single changepoint, we have two segments $j = 0, 1$ and $a = (T - 1), \dots, 1$. Then

$$L_0^{(1)}(a) = \sum_{b=a}^{T-1} P(a, b) L_1^{(1)}(b+1) \pi_1(\tau_0 = a-1 | \tau_1 = b).$$

Note that, since by definition $\tau_0 = 0$, $\pi_1(\tau_0 = a - 1 | \tau_1 = b) \neq 0 \iff a = 1$, therefore

$$L_0^{(1)}(1) = \sum_{b=1}^{T-1} P(1, b) L_1^{(1)}(b+1) \pi_1(\tau_0 = 0 | \tau_1 = b).$$

If we have a single changepoint in b , for every b $L_1^{(1)}(b+1) = P(b+1, T)$, as what follows b is a single segment. We then find an important equality:

$$L_0^{(1)}(1) = \sum_{b=1}^{T-1} P(1, b) P(b+1, T) \pi_1(\tau_0 = 0 | \tau_1 = b) = \text{Bayes Factor} \times P(1, T). \quad (2.3.5)$$

Indeed, we have the segment likelihood before the changepoint $P(1, \tau_1)$, the segment likelihood after the changepoint $P(\tau_1 + 1, T)$ and the prior on the changepoint position τ_1 ; being a discrete distribution, we sum over all possible values for τ_1 , and this is exactly how the numerator of the Bayes Factor is built. The denominator of the Bayes Factor is the likelihood under the null model $P(1, T)$. Note that this relationship only holds for a single changepoint. See Section 3.2.4 for further details.

Case $m = 2$

In order to see a slightly more complex example where we can effectively check how the recursions work, we now derive the case for two changepoints; $j = 0, 1, 2$ and, for every j , $a = (T - 3 + j), \dots, (j + 1)$.

As the equations are built backwards, we start from

$$L_1^{(2)}(a) = \sum_{b=a}^{T-1} P(a, b) P(b+1, T) \pi_2(\tau_1 = a - 1 | \tau_2 = b). \quad (2.3.6)$$

This equation only concerns the part of the data series after the first changepoint τ_1 : the union of segments $y_{\tau_1:T}$ is split in correspondence of different possible positions for τ_2 . Note that this means that for every a we have $T - a$ terms to compute.

The following step concerns the whole dataset

$$L_0^{(2)}(1) = \sum_{b=1}^{T-2} P(1, b) L_1^{(2)}(b+1) \pi_2(\tau_0 = 0 | \tau_1 = b). \quad (2.3.7)$$

The result of Formula(2.3.6) for every possible value of $b + 1$ is plugged in Formula(2.3.7). In Formula(2.3.7) there are $T - 2$ terms to compute.

INLA and filtering recursions

When working with models as hierarchical GMRFs, which can include dependence within segments, the segment marginal likelihoods will never be available in close form. The INLA methodology provides computationally efficient approximations to GMRFs posterior distributions; an important advantage for this work is that approximations can be used to estimate the marginal likelihoods of the data under a model, and overcome the issue of intractability. Indeed, with INLA we can replace the (often) intractable terms $P(t, s)$ with good approximations, given that the segment model is a GMRF; moreover, accurate approximations for the posterior distribution of both number of changepoints and their positions can be quickly obtained. Problems may arise if every segment has a very small amount of data, *i.e.* if we expect the changepoints to be very close to each other, or if the total amount of data is very large, because computing all the possible segment likelihoods for the recursions can be computationally demanding. To overcome both problems, Reduced Filtering Recursion (RFR) is proposed (see Section 3.3.4), which consists in looking for changepoints in an adequately sampled subset of the whole data series (see Wyse et al., 2011 and Chapter 6 for details).

Choice of the prior and computational cost

Running all the computations required by the filtering recursion approach can become computationally demanding. They require computational effort in $O(T^2M^2)$. As far as the prior on two levels is concerned, the computational cost can be reduced by choosing appropriate priors on the changepoint positions that are built in such a way as to simplify the recursive equation. Both Fearnhead and Wyse et al. choose the same prior that gives a reduction by a factor M in computational effort. There are no notes in either work on how much results are affected by the choice of this prior.

2.3.6 Posterior distribution

The example with $m = 2$ in Section 2.3.5 shows how the recursions work in a very simple case; in the end we do not consider the intermediate steps, which are iteratively plugged into the following equations, and only look at the final equation which returns the data marginal likelihoods under m changepoints

$$L(Y|m) = L_0^{(m)}(1) = Pr(y_{1:T}|m).$$

When we compute the likelihood for many different m s, in general the value $m = 0$ must also be included; for this value recursive equations simply reduce to

$$L_0^{(0)}(1) = P(1, T),$$

a single segment marginal likelihood approximated in one single step by INLA.

The segment marginal likelihoods incorporate a prior term for that particular segment's parameters. Parameters have been marginalized out, to give the evidence for a segment. This is a model with quite high structure, and the incorporation of the prior in the $P(a, b)$ terms introduces a natural penalization for overfitting. This is similar to the way in which Bayes Factors naturally incorporate penalization for model complexity, so there is no need for an extra penalization term as in Information Criteria. This means higher values for m will not necessarily be preferred.

In order to make inference on m , recursions must be computed for many different m s, *i.e.* for all the m s that have a non zero prior $\pi(m)$. For every m we then obtain a posterior distribution following the Bayes Rule and, using the approximate likelihood given a number m of changepoints $L_0^{(m)}(1)$, we obtain

$$\pi(m|Y) \propto \pi(Y|m)\pi(m) \approx L_0^{(m)}(1)\pi(m).$$

The posterior distribution of m allows the best number of changepoints given the data, say \hat{M} , to be chosen. If $\hat{M} \geq 1$ the following step is to choose the best changepoint positions *a posteriori*. The most likely positions are found using the (already computed) recursions for $m = \hat{M}$ via the conditional distribution. Indeed, this method also allows the conditional posterior distribution for each changepoint to be obtained, which makes simulation of

changepoints under the chosen model possible. For any m , in general the distribution can be written as

$$Pr(\tau_j | \tau_{j-1}, y_{1:T}, m) \propto \frac{P(\tau_{j-1} + 1, \tau_j) L_j^{(m)}(\tau_j + 1) \pi_m(\tau_{j-1} | \tau_j)}{L_{j-1}^{(m)}(\tau_{j-1} + 1)} \quad (2.3.8)$$

where the numerator is a single term out of the ones inside the recursive equations.

Let us see a simple example with $\hat{M} = 1$:

$$\begin{aligned} P(\tau_1 = t | \tau_0, y_{1:T}, \hat{M} = 1) &\propto \frac{P(1, t) P(t + 1, T) \pi_1(\tau_0 | \tau_1 = t)}{L_0^{(1)}(1)} \\ &\propto \frac{P(1, t) P(t + 1, T) \pi_1(\tau_0 | \tau_1 = t)}{\sum_{b=1}^{T-1} P(1, b) P(b + 1, T) \pi_1(\tau_0 | \tau_1 = b)}. \end{aligned}$$

It is easy to see that this equation is a ratio between a specific case $\tau_1 = t$ and all possible cases $\tau_1 = b$, $b = 1, \dots, T - 1$. Therefore, in the case of a single changepoint, irrespective of the value of t the denominator is constant, and in order to know the most likely changepoint position it is sufficient to compare the numerators. In conclusion, for a single changepoint search the best changepoint position a posteriori τ^* will be

$$\tau^* = \arg \max_t \{P(1, t) P(t + 1, T) \pi_1(\tau_0 | \tau_1 = t)\}. \quad (2.3.9)$$

This idea holds for any m : the most likely position for τ_1, \dots, τ_m can be chosen a posteriori by comparing, for every changepoint, the numerators of the posterior probabilities corresponding to different potential positions.

2.4 Discussion

In this Chapter, we presented the main fields of our analysis: spatio-temporal statistics, in particular spatio-temporal point processes, and change-point analysis, which is mainly run on temporal data. In addition to these two fields, INLA, an innovative tool for fitting complex spatio-temporal models, is introduced.

These are the main topics that will be connected to carry out our work: we

run a changepoint analysis for multiple unknown changepoints on spatio-temporal point process data, and use INLA for computations. With respect to the recent literature presented here, our work adds some new contributions: first, we look for changepoints on spatio-temporal, instead of simply temporal, point process data. Moreover, we use a very broad, flexible and complex class of Cox process models, covering many more cases than the commonly used Poisson processes; LGCPs are not widely used yet because of the estimation issues that have only recently been overcome by INLA. Therefore, we use INLA for fitting the models, which is computationally much more competitive than MCMC methods and allows the fitting of a much wider class of models than other analytical or numerical solutions. In conclusion, we believe our work can open new ways of answering interesting questions in many applied fields.

The next three Chapters will show how the three components of our work that have been presented are pulled together and how results are produced. Indeed, in Chapter 3 we present some increasingly complex Log-Gaussian Cox Processes that can be fitted to the data time segments in order to describe the spatial and temporal behaviour of the data points. We also present some algorithms for running single and multiple changepoint analyses on point process data, and propose a few Bayesian methods for detecting changes in the point process intensity. When presenting the developments in methodology in Chapter 3, we assume the reader has knowledge of what has been presented in the current Chapter, where a strong theoretical support is given to the choice of both models and methods for detecting changepoints on spatio-temporal point process data. In Chapter 4, we carry out a simulation study using the models and methods provided. All the segment likelihoods are approximated using INLA, which also provides estimates for the segment parameters. In Chapter 5, after the performance of our methods has been evaluated by the simulation results, we run the same analysis on the motivating dataset and add some extensions to the models. After the work is fully presented, a final and more detailed discussion on the novelty of our study can be found in Chapter 6.

Chapter 3

Developments in Methodology

In this Chapter, we illustrate the models and the new methods that will be evaluated with a simulation study in Chapter 4 and then applied to real data in Chapter 5.

Recently, different Bayesian techniques have been developed to determine whether a change (or more) occurs in a time series; as stated in Section 2.3, Bayesian methods have the advantage of allowing the probability of change at each data point within the series to be calculated. Once the posterior probabilities are obtained, different techniques can be used for taking decisions on the presence and number of changepoints. As we use a Bayesian approach, prior distributions, likelihood functions and posterior distributions have to be defined; in this work, we use non informative prior distributions on both number and position of changepoints, but our methods are not linked to a specific prior setting and may therefore be combined with any prior distribution.

We first show the methodology for a single changepoint detection at an unknown location; we then propose a few options for decision making on the presence of a changepoint. Afterwards, we move on to the detection of changepoints at unknown locations, the most general framework for a changepoint analysis that can answer any question regarding changepoints. The cases of a known number of changepoints or even of known position(s) to test can be derived as special cases of what we propose here.

3.1 Framework and notation

In general, we look for significant changepoints over time in an intensity function describing the behaviour of the point process realizations, where each realization is a point pattern over an observation window at a specific time point, and time points are equispaced. We build methods for data in continuous space and discrete time and we aim at covering a wide range of point process scenarios.

We now present four increasingly complex Log-Gaussian Cox Process models. As for the intensity function structure, in the first two models (Section 3.2.2) we assume the intensity function to be constant over space, *i.e.* we have a spatially homogeneous process; this means the intensity function at each time point can be represented by a single value. In the third and fourth model, the function is allowed to vary over space as well as over time. In all inhomogeneous processes, at each time segment the intensity function is a 2-dimensional image to estimate.

As for the number of changepoints, in Section 3.2 we deal with a single changepoint; in Section 3.3 we face the more general multiple changepoint analysis.

As in Chapter 2, we define T as the time series length, labelled by $t = 1, \dots, T$; let M be the number of changepoints, so that data are split into $M + 1$ time segments; the changepoint positions are τ_1, \dots, τ_M , indexed by $m = 1, \dots, M$. As for the spatial component, the observation window is discretized into S cells indexed by $s = 1, \dots, S$. Note that in Chapter 2 s is the general space index; here, as we discretize the space into cells, the cell itself becomes the basic space unit, since the intensity value inside the cell is assumed constant.

The response variable Y is the number of points observed in each grid cell, and the notation for a general value at time t in cell s is y_{ts} . For every time point t , the datum is a $S \times 1$ vector $Y_t = (y_{t1}, \dots, y_{tS})'$ counting the observations for each cell at that specific time point; there are T different data points, and the overall vector Y is of length $(T \times S) \times 1$, made of blocks: $Y = (Y_1, \dots, Y_T)'$. Being counts, the general distribution of the data is $y_{ts} \sim Poi(|C|\lambda(t, s))$ where $|C|$ is the cell area and, again, the intensity is

assumed constant inside the cell: we use a discretized version of the continuous latent field in order to make estimation feasible with the INLA approach, as explained in Section 2.2.4. For the special case of a spatially homogeneous process, the distribution parameter reduces to $y_t \sim Poi(|C|\lambda(t))$. Having Poisson distributed data, we focus on discrete models that are less developed than continuous models in the context of changepoint analysis. Given the nature of the algorithm used, though, it is straightforward to extend the method to different distributions.

3.2 Single changepoint detection

In this framework, in the general case of an unknown position, our hypotheses are

H_0 : no changepoint

H_1 : one changepoint.

The hypotheses only concern the number of changepoints, not their position. If H_0 is rejected, the position τ^* of the changepoint has to be detected within the set $1, \dots, T$ as the 'best' one for the data, according to some criterion that will be explained in detail in Section 3.2.4. The alternative hypothesis is therefore complex and can be divided into T sub-hypotheses, each one specifying a different position for τ^* .

3.2.1 Prior distribution

We choose a prior setting on two levels, therefore a prior distribution must be set on both number (0 or 1) of changepoints and, given the alternative hypothesis, on their position; for details on this prior setting see Section 2.3.4. In absence of prior knowledge, the same probability mass is given to both values:

$$\begin{aligned}\pi(M) &= 0.5 & M = 0, 1 \\ \pi(M) &= 0 & M > 1.\end{aligned}$$

Note that a uniform prior implies that the prior ratio $\frac{\pi(1)}{\pi(0)}$ is 1, therefore any computation involving the posterior ratio, which is product of prior and (weighted) likelihood ratios, can be simplified.

As for the best position of the changepoint τ^* under H_1 , we exclude the endpoints of the range, assuming each segment must have a minimum number of time points; this is aimed at avoiding 'wasting' computational time on options that are not of interest, moreover the INLA changepoint detection algorithms are shown to perform better when segments are not too short (Wyse et al., 2011); this assumption can be easily relaxed if needed.

Let t_1 and t_2 be the extremes of the considered range. Conditional on $M = 1$, we take a non-informative prior distribution over the considered subset of points between t_1 and t_2 , assumed to have length $T_{1:2} = t_2 - t_1 + 1$:

$$\begin{aligned}\pi(\tau^*) &= \frac{1}{T_{1:2}} & \tau^* \in \{t_1, t_1 + 1, \dots, t_2 - 1, t_2\} \\ \pi(\tau^*) &= 0 & \tau^* < t_1 \vee \tau^* > t_2.\end{aligned}$$

Being non informative also means that all the conditional priors of a specific changepoints given the following (or previous) one are uniform on the considered interval.

3.2.2 Segment likelihood

The model likelihood becomes gradually more complicated as we switch from one model to the following one; for each model, we include different effects to describe the behaviour of the logarithm of the intensity function. Note that in this work we do not include the effect of any covariate, but the models we show can be extended to a more general case by adding covariates as fixed or smooth effects in the equations (an example is given in Section 5.5).

All the models presented here are fitted using the INLA approach with the R-INLA package (www.r-inla.org) as explained in Section 2.2.3. If there are no changepoints in a data series, the model equation is fitted to the whole dataset; if there are changepoints, for every occurring change data are split into two time segments and the chosen model is fitted separately to each segment.

Model 1: model with fixed effect

We initially consider a model which assumes a spatially homogeneous intensity function and *i.i.d.* data (where we remind that every single datum is a point pattern): $\lambda(t, s) = \lambda(t)$. The general model equation is

$$\log \lambda = \mu + \epsilon$$

where μ is an offset term taking different values under either hypothesis and ϵ is an unstructured error term as in Section 2.2.3.

$$\begin{aligned} H_0 : \quad & \log \lambda(t) = \mu + \epsilon_t \quad \text{for } t = 1, \dots, T \\ H_1 : \quad & \log \lambda(t) = \mu_1 + \epsilon_t \quad \text{for } t \leq \tau^* \\ & \log \lambda(t) = \mu_2 + \epsilon_t \quad \text{for } t > \tau^*. \end{aligned} \tag{3.2.1}$$

Under H_0 all values over both space and time depend on a single value for μ that must be estimated and is a common intercept, while under H_1 μ_t is a time-specific intercept, constant over space but allowed to vary over time, where its variation occurs in correspondence of the changepoint, in a position in the interval $\{t_1, \dots, t_2\}$. For $M = 1$ we have two time segments, *i.e.* two values of μ_t to estimate.

Model 2: model with temporal effect

In this second scenario, we keep the spatial homogeneity assumption, but relax the *i.i.d.* assumption: data can show temporal dependence on the point pattern of the previous time point. Dependence is only allowed within time segments, not across segments; the temporal effect is called ϕ . The model equation changes as

$$\log \lambda = \mu + \phi + \epsilon$$

and specifically

$$\begin{aligned} H_0 : \quad & \log \lambda(t) = \mu + \phi + \epsilon_t \quad \text{for } t = 1, \dots, T \\ H_1 : \quad & \log \lambda(t) = \mu_1 + \phi_1 + \epsilon_t \quad \text{for } t \leq \tau^* \\ & \log \lambda(t) = \mu_2 + \phi_2 + \epsilon_t \quad \text{for } t > \tau^*. \end{aligned} \tag{3.2.2}$$

Within each time segment, ϕ is a random effect modelled as an autoregressive model of order 1 (AR(1)), *i.e.* the logarithm of the intensity function at every

time point is supposed to depend on its own value at the previous time:

$$\phi_t = \rho\phi_{t-1} + u_t$$

where as usual $|\rho| < 1$. Hyperparameters are needed for the precision $\nu_\phi \sim \text{Gamma}(\alpha_\phi, \beta_\phi)$. Note that in a homogeneous process AR(1) dependence means that the whole pattern at a specific time point depends on the whole pattern at the previous time point.

Model 3: model with spatial effect

In this model, we assume point patterns are *i.i.d.* replicates over time, but we substitute the offset term with a smooth random effect allowing for spatial inhomogeneity and dependence named ψ .

$$\log \lambda = \alpha + \psi + \epsilon$$

and specifically

$$\begin{aligned} H_0 : \log \lambda(t, s) &= \delta + \psi_s + \epsilon_{ts} && \text{for } t = 1, \dots, T \text{ and } s = 1, \dots, S \\ H_1 : \log \lambda(t, s) &= \delta + \psi_{1s} + \epsilon_{ts} && \text{for } t \leq \tau^* \text{ and } s = 1, \dots, S \\ &= \delta + \psi_{2s} + \epsilon_{ts} && \text{for } t > \tau^* \text{ and } s = 1, \dots, S \end{aligned} \tag{3.2.3}$$

where δ is a common intercept and ψ_s describes spatial dependence; it is indexed by s as it may take different values for every grid cell. Under H_1 , a single value defines the intensity for each cell over all the first time segment, and after the changepoint the value for each cell changes. The spatial effect is modelled as an intrinsic CAR, *i.e.* as a Random Walk in two dimensions on a lattice; the model is easily specified with INLA, with a neighbourhood structure that gives non-zero weights to the first 12 neighbours in the lattice (see Section 2.2.1). This produces a very smooth spatial structure which is suitable for LGCPs, where the hypothesis is that there is a smooth underlying driver determining the behaviour of the intensity function. Here too, the precision hyperparameter can be modelled as $\nu_\psi \sim \text{Gamma}(\alpha_\psi, \beta_\psi)$.

Model 4: general model

In the most complicated scenario we include both effects, so the assumptions are very weak: we allow for spatial inhomogeneity, for temporal depen-

dence within segments and for spatial dependence at every time point. The model can be written as

$$\log \lambda = \alpha + \phi + \psi + \epsilon$$

and for each hypothesis

$$\begin{aligned} H_0 : \log \lambda(t, s) &= \delta + \phi + \psi_s + \epsilon_{ts} && \text{for } t = 1, \dots, T \text{ and } s = 1, \dots, S \\ H_1 : \log \lambda(t, s) &= \delta + \phi_1 + \psi_{1s} + \epsilon_{ts} && \text{for } t \leq \tau^* \text{ and } s = 1, \dots, S \\ &= \delta + \phi_2 + \psi_{2s} + \epsilon_{ts} && \text{for } t > \tau^* \text{ and } s = 1, \dots, S. \end{aligned} \tag{3.2.4}$$

Again, in these models temporal dependence is only assumed to be within, not across, segments. In an inhomogeneous process, AR(1) dependence concerns cells: for every time t and cell s , $\lambda(t, s)$ depends on $\lambda(t-1, s)$, *i.e.* each cell's intensity depends on its previous value. The final estimated value for ϕ is a synthesis of the cell values over space. The precision parameter for both temporal and spatial effects has a *Gamma* prior that is by default set as non-informative but can be tuned according to a specific context.

When looking for a single changepoint, each model is run one time for every possible changepoint position, *i.e.* for every time point with a non-zero prior probability of being a changepoint. By fitting every model with INLA, a series of approximate likelihood values is then produced and normalised (in absence of prior knowledge) to obtain the posterior distribution of the changepoints. Once we have the posterior distribution, methods for identifying significant changepoints are proposed in Section 3.2.4. Since each model is run many times assuming different changepoint positions, there is a need for efficient computational tools in order to obtain results in a reasonable time, and that is one of the reasons why we fit the models using INLA.

3.2.3 Posterior distribution

In a single changepoint search, we do not obtain a posterior distribution for the number of changepoints and their position separately: the algorithm produces a posterior distribution assigning a probability to every potential changepoint position.

In the case of the prior distribution proposed at Section 3.2.1 on the changepoint position, for each model scenario we run the model $T_{1:2}$ times under the alternative hypothesis; at each run, we condition on the changepoint occurring at a different specific location $\tau \in \{t_1, \dots, t_2\}$ and return the model log-likelihood given the changepoint location. This means at each run we have the same overall dataset, but the series is split in two time segments at a different point. Every time we choose a τ in the set and fit one of the models, we obtain two approximate log-likelihoods, $q_1(\tau)$ for the first segment and $q_2(\tau)$ for the second one, and we sum them to obtain the log-likelihood value $l_1(\tau)$ given the alternative hypothesis and the specific potential changepoint position. The T -dimensional vector $l_1 = \{l_1(\tau), \tau \in \{t_1, \dots, t_2\}\}$ is then transformed following the usual Bayes Rule to obtain the posterior distribution: the curve resulting from the combination of all these likelihood values, and rescaled in order to integrate to one, is the posterior distribution of interest. It might show peaks in correspondence of the candidate changepoint positions.

For every model scenario in the context of a single changepoint analysis, we take as the most likely changepoint position a posteriori τ^* the one producing the maximum value for the likelihood from the $T_{1:2}$ runs:

$$l_1^* = l_1(\tau^*) = \max_{\tau} \{l_1(\tau), \tau \in \{t_1, \dots, t_2\}\}.$$

The decision on the significance of the detected potential changepoint with respect to the null hypothesis can be taken with different methods that we now examine in more details.

The computational efficiency of INLA and the ability to return the (approximate) likelihood value for any model makes this changepoint search algorithm feasible, even for complex dataset such as the one we work with.

3.2.4 Methods for changepoint detection

In this Section, we present some different Bayesian techniques for assessing the presence of a single changepoint. In next Chapter, we implement all methods on our simulated data and we evaluate their performance, before applying them to real data.

Again, it is to note that the alternative hypothesis here is simply H_1 : one

changepoint. It is not tied to any specific changepoint position. This is important when assessing the probability of committing errors of decision-making techniques: they only refer to the rejection of H_0 , irrespective of how many changepoints are found and where they are. This is particularly worth noting when applied to the context of unknown changepoints. In the special case of a potential changepoint in a known position, thanks to a *ad hoc* prior setting the changepoint detection only evaluates that specific position, and the alternative hypothesis can be modified in order to include the position.

Method 1: Bayes Factor method

As presented in Eckley et al. (2011), when running a Bayesian changepoint detection in absence of prior knowledge the likelihood ratio is used to decide if there is a changepoint or not:

$$\gamma = \frac{L_1}{L_0} = \frac{\sum_{\tau} \pi(\tau) Q_1(\tau) Q_2(\tau)}{L_0} \quad (3.2.5)$$

where $Q_1(\tau)$ and $Q_2(\tau)$ are the segment maximum likelihood values, *i.e.* the maximum likelihoods for the two segments resulting from a changepoint position in $\tau \in \{1, \dots, T\}$. Specifically, $Q_1(\tau)$ is the log-likelihood value for segment $y_{1:\tau}$ and $Q_2(\tau)$ is the log-likelihood value for segment $y_{\tau+1:T}$. It is immediately seen that this method requires the likelihood value under the null model to be computed as well. This means we also explore the possibility of $M = 0$, *i.e.* we run each model once under H_0 assuming data are made of a single segment and obtain a likelihood value L_0 .

This ratio is commonly known as the Bayes Factor (BF), expressing the evidence showed by data in support of the alternative model with regard to the null model. Since independence across segments is assumed, for every changepoint position the maximum likelihood value under the alternative hypothesis is $L_1(\tau) = Q_1(\tau)Q_2(\tau)$.

For the model with no changepoints, the maximum log-likelihood value under H_0 is greater than the maximum log-likelihood value under H_1 : differently from the frequentist likelihood ratio, when using the Bayes Factor we find that models with more parameters do not necessarily produce higher likelihood values (Section 3.2.4). Therefore, higher values for m will not always

necessarily be preferred, and we show in Chapter 4 that the BF method performs very similarly, though not identically, to the Schwartz Information Criterion (SIC) model selection (presented in Section 3.2.4).

Formula (3.2.5) can be extended to the case of a non-vague prior distribution by taking the posterior ratio, *i.e.* the product of likelihood and prior ratios:

$$\gamma = \frac{\pi(1)}{\pi(0)} \frac{\sum_{\tau} \pi(\tau) Q_1(\tau) Q_2(\tau)}{L_0}.$$

As we explain in Section 2.3.5, for the case of a single changepoint there is a relationship between the Bayes Factor and the filtering recursions: from Formula (2.3.5) we have

$$L_0^{(1)}(1) = \sum_{b=1}^{T-1} P(1, b) P(b+1, T) \pi_1(\tau_0 = 0 | \tau_1 = b) = \text{Bayes Factor} \times P(1, T).$$

where, in the usual notation, $L_0^{(1)}(1) = L_1 = \sum_{\tau} L_1(\tau) \pi(\tau)$ is the numerator of the Bayes Factor, *i.e.* the evidence for the model with one changepoint. The denominator is $P(1, T) = L_0$, and for every value b taken by τ we have $P(1, b) = Q_1(b)$ and $P(b+1, T) = Q_2(b)$. Therefore Formula (2.3.5) becomes

$$L_1 = \sum_{\tau=1}^{T-1} Q_1(\tau) Q_2(\tau) \pi(\tau) = \text{Bayes Factor} \times L_0. \quad (3.2.6)$$

In order to choose the correct changepoint position, if there is a significant changepoint, we start from the posterior distribution of every changepoint in the general case, as in Formula (2.3.8):

$$P(\tau_j | \tau_{j-1}, y_{1:T}, m) \propto \frac{P(\tau_{j-1} + 1, \tau_j) L_j^{(m)}(\tau_j + 1) \pi_m(\tau_{j-1} | \tau_j)}{L_{j-1}^{(m)}(\tau_{j-1} + 1)}$$

which, in the case of $m = 1$, becomes

$$P(\tau = t | y_{1:T}, m = 1) \propto \frac{Q_1(t) Q_2(t) \pi(t)}{L_1}.$$

The denominator L_1 , as in Formula (3.2.6), is a sum over all possible τ s, *i.e.* the denominator is the same irrespective of the value t taken by τ . Therefore, in the case of a single changepoint, the most likely changepoint position a posteriori τ^* will be chosen by comparing the numerators

$$\tau^* = \arg \max_{\tau} \{Q_1(\tau) Q_2(\tau) \pi(\tau)\}.$$

The prior weight $\pi(\tau)$ in the nominator sum in Formula (3.2.5) shrinks each alternative likelihood value, still every element in the sum will be positive, and the greater the nominator is, the more likely it is to reject H_0 . We choose a more conservative condition:

$$\gamma_{\tau^*} = \frac{\pi(\tau^*)Q_1(\tau^*)Q_2(\tau^*)}{L_0} \quad (3.2.7)$$

where τ^* is the best changepoint position a posteriori.

Equivalently, we can use log-likelihood values:

$$\gamma'_{\tau^*} = \log(\pi(\tau^*)) + q_1^* + q_2^* - l_0 = \log(\pi(\tau^*)) + l_1^* - l_0 \quad (3.2.8)$$

where $q_1^* = \log(Q_1(\tau^*))$ and $q_2^* = \log(Q_2(\tau^*))$. For Formula (3.2.8) the value 0 is a threshold for rejecting the null model of no changepoint and, at the same time, find the changepoint position: if $\gamma'_{\tau^*} > 0$, the null hypothesis is rejected and the changepoint occurs at τ^* .

This conservative version of a Bayes Factor is particularly suitable for testing known potential changepoints. In the special case of a known changepoint position, computations can be reduced: the model is run only once under each hypothesis, the position tested can be called τ^* and the Bayes Factor automatically reduces to the more conservative version we have chosen, as in Formula (3.2.8) or its equivalent (3.2.7).

Method 2: Schwartz Information Criterion method

Another option for taking decisions about the presence of changepoints in a temporal series is to use the Schwartz Information Criterion (SIC), also known as Bayesian Information Criterion (BIC).

Under H_0

$$SIC_{H_0} = -2l_0 + \log T$$

while under H_1

$$SIC_{H_1}^* = -2l_1^* + 2 \log T$$

where again $l_1^* = q_1^* + q_2^*$ and $SIC_{H_1}^*$ is the value corresponding to the most likely changepoint position (*i.e.* producing the smallest SIC value under the alternative hypothesis). This criterion incorporates a penalty for the number of parameters included in the model and is therefore expected to behave

analogously to the BF method.

As for all information criteria, smaller values are preferred, hence the condition for rejecting the null hypothesis of no changepoint is

$$SIC_{H_0} > SIC_{H_1}^*.$$

As we show in Chapter 4, results for this method are indeed very similar to results produced by the BF method.

Method 3: Posterior Threshold method

An alternative option we explored is another typical Bayesian way of taking decisions, *i.e.* by looking at the posterior distribution and fixing a posterior probability threshold for significant values.

In the changepoint analysis context, the posterior distribution concerns the potential changepoint position: once data are observed, every time point of the series is assigned a probability of being a changepoint. Once the resulting curve is plotted, a threshold needs to be fixed in order to take decisions on what time points are to be considered changepoints.

As for the threshold choice, it is to bear in mind that greater values (closer to 1) will lead to more conservative conclusions, and smaller values (closer to 0) will detect changepoints more easily. The choice of the threshold can be knowledge-driven, if information is available on the diffusion of changepoints in the data series. Note that useful knowledge can also be incorporated in the posterior probability via the prior distribution. Another important notion is that the height of peaks in the posterior distribution depends on the length of the time series: since the curve must integrate to 1, longer T s will flatten its peaks. For example, Park et al. (2012) use a threshold of 0.1 for a data series of $T = 1000$; the same value would certainly lead to the acceptance of too many changepoints in a shorter series.

In order to find a sensible and not too arbitrary threshold h , we propose to use simulated data under the null hypothesis for assessing the probability of committing type I errors based on different values of h . Once we find a value for h such that the significance level α does not exceed a certain limit (usually $\alpha \leq \alpha_0$, $\alpha_0 \in \{0.01, 0.05, 0.1\}$), we use h on data generated under

the alternative hypothesis in order to evaluate the Posterior Threshold (PT) method's power level, the ability to detect the correct changepoints and the accuracy of the produced estimates.

In the special case of a known changepoint position to test, the method does not change: a posterior probability curve will be estimated all the same, and the threshold will be only used to evaluate the significance of the candidate changepoint position.

3.3 Multiple changepoint detection

We now extend the method to an unknown number of changepoints, the most complicated type of changepoint analysis. The hypotheses become:

H_0 : no changepoints

H_1 : ≥ 1 changepoint.

As for the single changepoint detection, note that H_1 is not tied to a specific changepoint position, nor to a number of changepoints; the alternative hypothesis is very complex because it considers the presence of changepoints first, but then the precise number and positions also have to be estimated. If H_0 is rejected, the final result is $\tau^* = (\tau_1^*, \dots, \tau_M^*)$, a $M \times 1$ vector containing the estimated changepoint positions, a subset of $(1, \dots, T)$.

Multiple changepoints can be searched with two approaches: an iterative search aims at finding one changepoint at every step, while a simultaneous search aims at finding all the significant changepoints in one step.

Iterative changepoint search via binary segmentation algorithms

The simplest and more straightforward way of running an iterative multiple changepoint analysis is to use a binary segmentation method. For a general introduction to these methods we refer to Eckley et al. (2011), and in particular for point processes to Park et al. (2012). The idea of a binary segmentation procedure, and the key to its simplicity, is to split the multiple search into a series of subsequent single changepoint searches. In general, the algorithm can be explained as:

1. Run a changepoint analysis on the whole data series Y , testing the simple hypotheses
 - H_0 : no changepoints
 - H_1 : one changepoint.
2. a) If no changepoint is found, stop the algorithm.
 b) If one changepoint is found, let its position be τ_0^* , and split data in correspondence of τ_0^* into two segments, Y_A ($[S \times \tau_0^*] \times 1$) and Y_B ($[S \times (T - \tau_0^*)] \times 1$). Note that the changepoint position τ_0^* marks the end of segment Y_A . For each of the two resulting segments, go back to step 1.
3. a) If no more changepoints are found, the dataset has a single changepoint in τ_0^* .
 b) If changepoints τ_A^* and/or τ_B^* are detected, go back to step 2b and repeat the procedure for each segment containing a changepoint.
4. Repeat until some criterion is met:
 - no more changepoints are detected in any segment
 - a pre-fixed number of changepoints is reached
 - a minimum segment length is reached.

Many binary segmentation methods can be built, according to the criterion for detecting a changepoint (*e.g.* the BF or PT method); what they have in common is that at each step the algorithm carries out a single changepoint search for every segment. When running such an algorithm, number and positions of changepoints are estimated sequentially at the same time: at every step, if a changepoint is found, its position is immediately chosen before moving on to the next step, as we need to know where to split data into further segments.

Intuitively, the analysis can become computationally very demanding as T and M become large (Killick et al., 2012), and methods are available for reducing time and memory storage requirements. The computational efficiency of INLA makes this algorithm feasible even for complex spatio-temporal data.

Simultaneous changepoint search

The alternative option is to run a simultaneous changepoint search. A non naïf algorithm must be effectively able to identify all changes even if they have different magnitudes.

The procedure we build follows the two level prior in Section 2.3.4: first of all, we estimate the number of changepoints, and then, conditional on that number, we identify the most likely positions. We then follow Wyse et al. (2011) as introduced from Section 2.3.5 on, with an extension to spatio-temporal models. The method consists of two steps, irrespective of the number of changepoints found:

1. first of all, the number of changepoints is estimated by comparing data marginal likelihoods under a given number m of changepoints, for different values of $m = 0, \dots, M$. We then obtain $M + 1$ conditional likelihoods, which are computed using recursive equations, and give evidence for the model with m changepoints. The highest likelihood value corresponds to the chosen number of changepoints, say \hat{M} ;
2. conditional on \hat{M} , the positions for the changepoints are then estimated, by computing the conditional posterior probabilities for each changepoint given the previous one, the data and \hat{M} as shown in Section 2.3.6.

With this technique, the criterion for the detection of changepoints is incorporated in the method itself, therefore there are no alternative choices (such as the BF or PT method). Different results can be compared by fitting different models to the data segments, and model selection and choice can be carried out.

3.3.1 Prior distribution

A prior distribution is first set on the number of changepoints. In practical changepoint analyses, a maximum number of changepoints M is usually fixed; if not, then potentially $M = T$, which could lead to nonsensical conclusions, as all time points could be changepoints. To avoid this, usually

$M = \lfloor \frac{T}{d} \rfloor$ where d is a minimum set segment length, and $\lfloor \cdot \rfloor$ denotes the integer part of the ratio. Other reasons due to the specific context or to prior knowledge can lead to different choices for M .

Again, given M we use non informative priors, by assigning the same probability mass to all values:

$$\begin{aligned} \pi(m) &= \frac{1}{M+1} & m = 0, \dots, M \\ \pi(m) &= 0 & m > M. \end{aligned} \tag{3.3.1}$$

The prior for the position of the changepoint(s) depends on the technique used for the changepoint search. If an iterative binary segmentation algorithm is used, the prior distribution can be built analogously to what shown in Sec 3.2.1, as the analysis concerns a single changepoint at each step. Again, we set a minimum segment length d and at each step

$$\begin{aligned} \pi(\tau^*) &= \frac{1}{T_{1:2}} & \tau^* \in \{t_1, t_1 + 1, \dots, t_2 - 1, t_2\} \\ \pi(\tau^*) &= 0 & \tau^* < t_1 \vee \tau^* > t_2. \end{aligned}$$

where t_1 and t_2 are the extremes of the considered range given d , of length $T_{1:2} = t_2 - t_1 + 1$. If during the iterative procedure a segment is found to be shorter than $2d$, it means it cannot be further split into sub segments of an acceptable length, therefore the analysis is stopped on that segment.

If a simultaneous search is performed, the prior distribution for changepoint number and positions follows what explained in Section 2.3.4. In particular, for the changepoint number it can be the same as in Formula (3.3.1). As for the positions, for every possible m conditional probabilities on the changepoint positions given the following changepoint are built:

$$\pi_m(\tau_1, \dots, \tau_m) = \pi_m(\tau_m) \times \pi_m(\tau_{m-1} | \tau_m) \times \pi_m(\tau_{m-2} | \tau_{m-1}) \times \dots \times \pi_m(\tau_1 | \tau_2).$$

Note that this implies the assumption that the changepoints follow a Markov process.

A discussion regarding the choice of priors is left to Chapter 6.

3.3.2 Segment likelihood

For each data segment, the same four models listed in Sec 3.2.2 are fitted. The general formulation for the four models is a more complicated version

of what presented for the single changepoint search.

Let us assume we have a maximum $M = \lfloor \frac{T}{d} \rfloor$ fixed, and that the chosen number of detected changepoints is $\hat{M} \leq M$. Under the alternative hypothesis, every model is fitted separately to each of the $\hat{M} + 1$ data segments.

Model 1: model with fixed effect

The model equation is

$$\log \lambda = \mu + \epsilon$$

and under each hypothesis

$$\begin{aligned} H_0 : \log \lambda(t) &= \mu + \epsilon_t && \text{for } t = 1, \dots, T \\ H_1 : \log \lambda(t) &= \mu_1 + \epsilon_t && \text{for } t \leq \tau_1^* \\ &= \mu_2 + \epsilon_t && \text{for } \tau_1^* < t \leq \tau_2^* \\ &\dots && \dots \\ &= \mu_{\hat{M}} + \epsilon_t && \text{for } \tau_{\hat{M}-1}^* < t \leq \tau_{\hat{M}}^* \\ &= \mu_{\hat{M}+1} + \epsilon_t && \text{for } t > \tau_{\hat{M}}^* \end{aligned}$$

where μ is an offset term and the detected changepoints are reordered so that $\tau_1^* < \tau_2^* < \dots < \tau_{\hat{M}}^*$. We have $\hat{M} + 1$ time segments, *i.e.* $\hat{M} + 1$ values of μ_t to estimate.

Model 2: model with temporal effect

The model equation changes, including a temporal effect called ϕ , as

$$\log \lambda = \mu + \phi + \epsilon$$

and specifically

$$\begin{aligned} H_0 : \log \lambda(t) &= \mu + \phi + \epsilon_t && \text{for } t = 1, \dots, T \\ H_1 : \log \lambda(t) &= \mu_1 + \phi_1 + \epsilon_t && \text{for } t \leq \tau_1^* \\ &= \mu_2 + \phi_2 + \epsilon_t && \text{for } \tau_1^* < t \leq \tau_2^* \\ &\dots && \dots \\ &= \mu_{\hat{M}} + \phi_{\hat{M}} + \epsilon_t && \text{for } \tau_{\hat{M}-1}^* < t \leq \tau_{\hat{M}}^* \\ &= \mu_{\hat{M}+1} + \phi_{\hat{M}+1} + \epsilon_t && \text{for } t > \tau_{\hat{M}}^*. \end{aligned}$$

Within each time segment, ϕ is a random effect modelled as an AR(1) as for the single changepoint detection, and again under H_1 there are $\hat{M} + 1$ values of ϕ to estimate.

Model 3: model with spatial effect

In this model the spatial effect is called ψ :

$$\log \lambda = \alpha + \psi + \epsilon$$

and specifically, for $s = 1, \dots, S$

$$\begin{aligned} H_0 : \log \lambda(t, s) &= \delta + \psi_s + \epsilon_{t,s} && \text{for } t = 1, \dots, T \\ H_1 : \log \lambda(t, s) &= \delta + \psi_{1s} + \epsilon_{t,s} && \text{for } t \leq \tau_1^* \\ &= \delta + \psi_{2s} + \epsilon_{t,s} && \text{for } \tau_1^* < t \leq \tau_2^* \\ &\dots && \dots \\ &= \delta + \psi_{\hat{M}s} + \epsilon_{t,s} && \text{for } \tau_{(\hat{M}-1)}^* < t \leq \tau_{\hat{M}}^* \\ &= \delta + \psi_{(\hat{M}+1)s} + \epsilon_{t,s} && \text{for } t > \tau_{\hat{M}}^*. \end{aligned}$$

Here, δ is a time invariant intercept, and ψ is again modelled as a Random Walk in two dimensions, as for the single changepoint model.

Model 4: general model

We here include both effects, and the model can be written as

$$\log \lambda = \alpha + \phi + \psi + \epsilon$$

and for each hypothesis

$$\begin{aligned} H_0 : \log \lambda(t, s) &= \delta + \phi + \psi_s + \epsilon_{t,s} && \text{for } t = 1, \dots, T \\ H_1 : \log \lambda(t, s) &= \delta + \phi_1 + \psi_{1s} + \epsilon_{t,s} && \text{for } t \leq \tau_1^* \\ &= \delta + \phi_2 + \psi_{2s} + \epsilon_{t,s} && \text{for } \tau_1^* < t \leq \tau_2^* \\ &\dots && \dots \\ &= \delta + \phi_{\hat{M}} + \psi_{\hat{M}s} + \epsilon_{t,s} && \text{for } \tau_{(\hat{M}-1)}^* < t \leq \tau_{\hat{M}}^* \\ &= \delta + \phi_{\hat{M}+1} + \psi_{(\hat{M}+1)s} + \epsilon_{t,s} && \text{for } t > \tau_{\hat{M}}^*. \end{aligned}$$

The total number of parameters to estimate (hyperparameters excluded) is $2(\hat{M} + 1) + 4$: all the ϕ s and ψ s, plus the three precisions and δ .

3.3.3 Posterior distribution

In multiple changepoint analysis, the generation of likelihood values and, eventually, of the posterior distribution, depends on whether the search is simultaneous or iterative.

As for the binary segmentation algorithm, a criterion for decision making must be chosen first in order to proceed with the iterations. Any of the methods proposed in 3.2.4 can be used. Once chosen, the posterior distribution for each potential changepoint position is obtained for every step and for every time segment the same way as in Sec 3.2.3, as we have a single changepoint search at every step. As time is discrete, a final posterior distribution for the whole time series can be obtained by averaging values pointwise, and then rescaling in order to integrate to 1 and deal with a proper distribution. If a simultaneous search is carried out, the method follows what presented in Section 2.3.5. First of all $M + 1$ data likelihoods are obtained conditional on different values for $m = 0, \dots, M$: we obtain $L(Y|m = 0)$, $L(Y|m = 1)$, $L(Y|m = 2)$, \dots , $L(Y|m = M)$, where $Y = y_{1:T}$ is the whole dataset. Following the Bayes Rule we have

$$P(m|Y) \propto L(Y|m)\pi(m)$$

therefore, if the prior is uniform then the likelihood values are proportional to the posterior probability values for m . This means that, under a non informative prior, the highest conditional likelihood determines the chosen \hat{M} *a posteriori*

$$\hat{M} = \arg \max_m \{L(Y|m), m = 1, \dots, M\}.$$

Conditional on \hat{M} , the posterior positions for the \hat{M} changepoints need to be found. Assuming the changepoint process is a Markov process

$$P(\tau_1, \dots, \tau_{\hat{M}}|Y, \hat{M}) = P(\tau_1|Y, \hat{M}) \times P(\tau_2|\tau_1, Y, \hat{M}) \times \dots \times P(\tau_{\hat{M}}|\tau_{\hat{M}-1}, Y, \hat{M})$$

and we find one changepoint position at a time, following Formula 2.3.8:

$$Pr(\tau_j|\tau_{j-1}, Y, \hat{M}) \propto \frac{P(\tau_{j-1} + 1, \tau_j)L_j^{(\hat{M})}(\tau_j + 1)\pi_{\hat{M}}(\tau_{j-1}|\tau_j)}{L_{j-1}^{(\hat{M})}(\tau_{j-1} + 1)}.$$

3.3.4 Methods for changepoint detection

In a multiple changepoint analysis, the choice of the search technique (simultaneous or iterative), the choice of the methods for detecting significant changepoints if an iterative technique is used and the generation of the posterior distribution are tightly linked.

As explained in Section 3.3.3, for a binary segmentation algorithm the detection method is chosen before the analysis starts, as the algorithm only goes on if a changepoint is detected. Any of the methods can be used (BF, SIC or PT) but once the choice is made it cannot be changed in further steps for consistency reasons. After a proper posterior distribution is obtained, using the same criterion chosen for the algorithm steps decisions are made on the presence/absence, number and positions of changepoints in the data series. If a simultaneous search following Wyse et al. (2011) is carried out, as previously said the detection method is incorporated in the analysis. As the algorithm is quite computationally intensive, despite INLA's efficiency, when a dataset is too long or complex techniques for increasing the computational speed, such as the Reduced Filtering Recursion method, can be used.

Reduced Filtering Recursion

The simultaneous changepoint detection algorithm in Wyse et al. (2011) consists in combining recursive techniques with INLA, in order to produce estimates for the segment marginal likelihoods and approximations for the posterior of both number of changepoints and their positions. Issues that may arise if every segment has a very small amount of data or if the total amount of data is very large, can be overcome by Reduced Filtering Recursions (RFR). In a nutshell, the idea of RFR is to take a subset of points from the data and to look for changepoints inside that small series; if the subset is well chosen, the detected changepoints should be close to the true ones. The main principle is to reduce computations by running the recursive equations on a small number of time points; the assumption is that data segments have a 'reasonable' length, therefore even if a subset of points is chosen, changepoints should be found close to where they have occurred. A number $N < T$ is chosen and ordered time points $\{t_1, \dots, t_N\}$ extracted (where we

define $t_0 = 0$ and $t_{N+1} = T$). Then, the recursive equation method is implemented as if this were the complete data series.

Intuitively, the spacing between chosen time points is an issue. As in all our work, we assume there is no prior knowledge on the number or length of the data segments. Therefore, a natural choice is $t_i = id$, *i.e.* equal spacing, where d must be fixed in order to reach the desired trade off between computational speed and precision. If points are well chosen, each true changepoint should lie in the interval $]t_i - \frac{d}{2}; t_i + \frac{d}{2}[$. The greater d is, the faster the algorithm, but the greater error will be allowed for the detected changepoint location, with a risk of totally missing some points. Details on the computational cost saving and techniques for refining the detected changepoints' estimated locations are available in Wyse et al. (2011).

3.4 Intensity estimates

Obtaining a good summary of the posterior distribution of the parameter whose changes are under analysis (in our case, λ) in order to produce estimates for each time segment is often a secondary, non required step in a changepoint analysis. In many situations, the interest only lies in detecting the positions of the changepoints; sometimes there is a focus on understanding what type of change occurs (an increase or a decrease in the parameters) but without special attention to the accuracy of the estimated values. Nevertheless, in a complete changepoint analysis not only the location but also the magnitude of the change has to be detected, therefore parameter estimates for every time segment are needed.

The INLA algorithm produces estimates for all model effects and for each potential changepoint location, thus once the changepoints are detected the corresponding means of the parameters of the identified segments are chosen as estimates, since we are working on a Gaussian field. In the simulation study presented in Chapter 4, a comparison of the INLA estimates to the true values is carried out, showing that the estimates are satisfactorily accurate for our data under all scenarios.

For the spatially homogeneous models (Model 1 and 2) the estimated value

for the intensity will result in a stepwise linear function, as a single intensity value over space is representative of the point pattern at every time point. For the inhomogeneous models (model 3 and 4), the intensity is assumed constant inside each cell, due to the discretization necessary for the approximation, therefore at every time point the resulting estimate will be a (two-dimensional) pixel image. As the intensity strength is constant within each time segment, for m changepoints $m + 1$ images will be produced, where each image contains values averaged/synthesized over the corresponding segment.

If desired, any synthetic measure (mean, median, ...) can be chosen for the estimate as the INLA approximation provides the whole posterior distribution for all (both fixed and random) effects. Estimates are also provided for the precision hyperparameters.

As recent literature about INLA proves (Rue et al., 2009), if the assumptions hold then the produced estimates are very accurate and outperform MCMC estimates for any given computational time.

3.5 Discussion

In this Chapter, we presented all the models we fit to the data segments and we showed how to obtain the posterior distribution and detect changepoints with different algorithms and methods. In Chapter 4, all the proposed methods will be tested and evaluated in a complex simulation study. We now give some hints for discussion and further work concerning the methodological choices.

3.5.1 Time dependent data

A note is necessary about data with strong time dependence. A substantial advantage of our method is that it works even when data are space and time dependent, irrespective of the dependence strength; nevertheless, it must not be forgotten that time dependence inevitably affects the detection of changepoints.

When data are *i.i.d.* or show a weak time dependence, changepoints usually

correspond to effective changes in the intensity strength, *e.g.* due to external factors or changes in environmental conditions. When dependence is strong, though, the data series can drift far away from the initial values, and changes might be detected that are not due to a real change of time segment, but to the time dependence itself. In general, a higher number of changepoints will be detected in a time dependent temporal series with regard to an *i.i.d.* time series with the same initial conditions.

The risk is an overestimation of the number of changepoints, and on real data where changepoints are unknown and not set a priori, it is not certain if the two resulting time segments be effectively independent of each other. Therefore, to protect results against overestimation, conservative versions of the above illustrated methods (*e.g.* higher thresholds) should be adopted. Anyway, abrupt changes due to external/environmental changes should still be detectable in the series. We show results for strong time dependent data as well as *i.i.d.* data in our simulation study in Chapter 4, we highlight the difference in the results and propose a method for choosing thresholds when dealing with strong time dependent data.

3.5.2 Abrupt vs gradual change

All the work done here concerns abrupt changes in the intensity function of a process. Abrupt changes are often of interest in many changepoint studies and in a simple homogeneous case or in the case of a standard time series they generate a stepwise function representing the behaviour of the process parameter. Other studies consider gradual changes, producing a smoother function and covering a wider range of problems, up to what is referred to as trend analysis. We choose to focus on abrupt changes as the issue of where to locate the changepoint and of the linked uncertainty is simpler to deal with; this work brings many novelties to the fields of changepoint analysis and spatio-temporal point processes, and these new techniques need to be assessed on a process with well defined changes first. Further work might extend the methods to gradual changes.

3.5.3 Model definition

The four models proposed in this Chapter include few effects, therefore they appear rather simple. It is to remember that in this work the aim is not to build a complex model, but to be able to fit this class of models to complex data, which is currently an open challenge. Despite looking simple, these models contain the key elements for the analysis, that is to say spatial heterogeneity, spatial dependence and temporal dependence within segments. Once our methodology has proved itself well performing on time and space dependent spatio-temporal point processes, it is straightforward to add fixed and random effects up to very complicated models, thanks to the additive structure of Log-Gaussian Cox models and to INLA. The addition of effects has to respect the INLA assumptions: a latent Gaussian field and a small number of hyperparameters. For example, further extensions to this work can include covariates; in particular, constructed covariates based on the distance between points can be used in order to account for interpoint interaction and small scale variation which is in general not considered in LGCPs (see Illian (2012)). The key point of this study remains the ability to obtain results for such models fitted on spatio-temporal point process data. In our work, spatial dependence is modelled as a Random Walk in two dimensions and temporal dependence as an autoregressive of order 1. This choice is due to prior knowledge on the motivating dataset and to the availability of these models in the `R-INLA` package; they define a smooth spatial structure and a strong short-time dependence. Other dependence structures can be tried among the ones provided by the `R` package or by defining new ones; as long as the assumptions underlying the use of INLA hold, accurate results will be obtained under any model specification.

3.5.4 Model selection

Our primary interest lies in testing the models on our data, in order to understand if it is possible to obtain results by progressively adding effects. The main goal is to be able to fit models allowing for spatial and temporal dependence. In this work, we do not focus on the issue of selecting the best model for the data. When this is of interest, the usual Bayesian tool for model

comparison and selection can be used, which is the Deviance Information Criterion (DIC). If specified when running the code, INLA computes and returns DIC values for every model. It will be of interest to compare models as a further step, once the ability of fitting such models is successfully tested, and realistically good models for the data can be built, that include not only dependence but also covariates, marks and extra information. Some further work towards model selection is given in Section 5.5.

3.5.5 Methodological discussion

Single changepoint detection techniques

When running a single search (and within binary segmentation techniques) in Chapter 4 we highlight the difference between BF, SIC and PT method. Note that irrespective of its performance, the PT method has some advantages: it is visually immediate and easy to explain to non-statisticians, besides it is very flexible as the threshold choice can be adapted to the model fitting the data and to the analysis context. The threshold choice is undoubtedly an issue as it strongly affects the results. If there is prior knowledge, it can be used when fixing the threshold. A method for reducing the arbitrariness in absence of external knowledge is proposed in Chapter 4. If the PT method is selected in a multiple changepoint search, a further note on the choice of the threshold is needed: if the whole data series is not very long, as in our simulated data presented in Chapter 4, the threshold value can be kept constant throughout the detection algorithm with negligible consequences. If the series is very long, say $T = 1000$, then the time segments can become much shorter than the original data length, and keeping a constant threshold can lead to overestimation of the number of changepoints, as posterior distribution peaks, once rescaled for short segments, will more easily raise quite high in order to integrate to 1. In conclusion, it can be considered to weight the initial threshold by a value inversely proportional to the segment length. This is left to further studies.

Multiple changepoint detection techniques

As we introduce in Section 3.3, two possible classes of algorithms can be used when carrying out a multiple analysis: binary segmentation iterative algorithms, or a simultaneous changepoint search. We decided to try both techniques as comments in the literature concerning the performance of the two methods are contradictory. In many studies, the simultaneous changepoint search is discarded as it proved to perform poorly, showing tendency to underestimate the number of changepoints. This can be intuitively explained: different changepoints will refer to changes of different magnitudes in the intensity function; when the posterior probability curve is normalised to integrate to 1, posterior peaks will tend to flatten and changepoint positions corresponding to smaller, but not negligible, changes may be considered non-significant. A binary segmentation algorithm allows local maxima to be found and has proved itself better performing in many analyses. On the other hand, Wyse et al. (2011) state that when running multiple changepoint analysis on data with dependence within segments, some binary segmentation methods can perform poorly with regard to the recursive techniques. In Chapter 4 and 5, we show results and performance of the above methods on both simulated and real data for both techniques.

A further note on binary segmentation algorithms is needed. Since the method is iterative, at every step a single changepoint is found; on data with multiple changepoints this implies that in the first steps some changepoints will be 'hidden'. What is temporarily treated as a single segment actually contains changepoints that have not yet been detected; this means that an error is included, as the 'segment' likelihood should actually be a product of segment likelihoods. The likelihood we are using at that step is therefore not strictly correct. This should not prevent people from using such techniques, as what is done at each step is a comparison among different likelihoods conditional on different changepoint positions, in order to choose the best one before moving on with the search. Indeed, if a changepoint is found, a finer analysis will be carried out on each segment. The 'correct' segment likelihoods will only be found at the last step of the algorithm, still every step is meant to bring the greatest possible improvement given a sin-

gle changepoint search. In other words, the meaning of a single step is not 'we just computed the correct segment likelihood'; it is 'splitting data at a specific location returns the best possible marginal likelihood, given the hypotheses H_0 (no changepoint) versus H_1 (a single changepoint)'.

Chapter 4

Methods Assessment via Simulation Study

Our simulation study is designed to explore the validity and properties of the changepoint detection methods proposed in Section 3.2.4 and the behaviour of the INLA algorithms in this context; once the performance is evaluated through a number of simulation replicates and under different scenarios, it will be possible to apply them to real data and answer to research questions.

In this Chapter, we first show how we plan our complex simulation study, highlighting what aspects and characteristics we change over the scenarios. Secondly, we present in detail all the simulation results for every single model and scenario. We then propose an extension of the simulation study for a restricted scenario, where we allow the intensity function to change in a more general way. A final discussion with comments and remarks is in Section 4.4. All the analyses in this Chapter are carried out with the statistical software R (R Development Core Team, 2008); the main packages used are `spatstat` (Baddeley and Turner, 2005) for defining point processes and `R-INLA` for computations (www.r-inla.org). There is no use of the currently available packages for changepoint analysis in this work, as they do not support spatio-temporal data.

4.1 Simulation design

Our simulation study is quite complex as it aims at covering a wide range of point process scenarios.

We fix a time series of $T = 50$ time points, and a grid of $S = 20 \times 20 = 400$ cells. Both shorter and longer time series lengths have been tested and mainly differ in computational time; the chosen value for T is a good trade off between reliability of the results and computational speed; moreover, the series length is enough to cover many real datasets.

The observation window W is a square of area 100; choosing a regularly shaped window makes code writing simpler, and many software functions for point processes only work on this type of windows. In our case, though, a more complicated version allowing for irregular polygonal windows is available, which does not lead to substantially different conclusions and is therefore not presented here.

As for the choice of the scenarios to cover, we first present a synthetic summary of the simulation structure in Section 4.1.1; then, we explain each aspect in more details in Section 4.1.2.

4.1.1 Summary of the simulation plan

We build data for both single and multiple changepoint detection.

For a **single changepoint search** we have

- *i.i.d.* and strong time dependent (AR(1)) data (see Section 4.1.3 for details on the data generation) with
 - no changepoint ($\lambda = 1$)
 - one big change (from $\lambda_1 = 1$ to $\lambda_2 = 2$)
 - one small change (from $\lambda_1 = 1$ to $\lambda_2 = 1.2$)

100 replicates generated for each case

- four model scenarios (Section 3.2.2):
 1. Model 1 - fixed effect (homogeneous process)
 2. Model 2 - fixed and temporal effect (homogeneous process)
 3. Model 3 - spatial effect, with intercept (inhomogeneous process)
 4. Model 4 - spatial and temporal effect, with intercept (inhomogeneous process)
- three detection methods (Section 3.2.4)
 1. BF - Bayes Factor method
 2. SIC - SIC criterion
 3. PT - Posterior Threshold method.

For a **multiple changepoint search** we have

- *i.i.d.* and strong time dependent (AR(1)) data (see Section 4.1.4 for details on the data generation) with
 - no changepoint
 - three changepoints of different magnitude ($\lambda_1 = 1$, $\lambda_2 = 1.4$, $\lambda_3 = 2.3$, $\lambda_4 = 2$)

100 replicates generated for each case

- four model scenarios (Section 3.2.2):
 1. Model 1 - fixed effect (homogeneous process)
 2. Model 2 - fixed and temporal effect (homogeneous process)
 3. Model 3 - spatial effect, with intercept (inhomogeneous process)
 4. Model 4 - spatial and temporal effect - with intercept (inhomogeneous process)
- two detection algorithms (Section 3.3)
 1. simultaneous changepoint search

2. binary segmentation algorithms, with
 - (a) BF method
 - (b) SIC criterion
 - (c) PT method.

A summary of the simulation design is in Table 4.1; the SIC results are not reported as they replicate the BF results in nearly all cases. Comments can be found in Section 4.2.2. In Section 4.1.2 we present in further detail how the simulation structure has been designed and planned.

Table 4.1: Structure of the simulation study

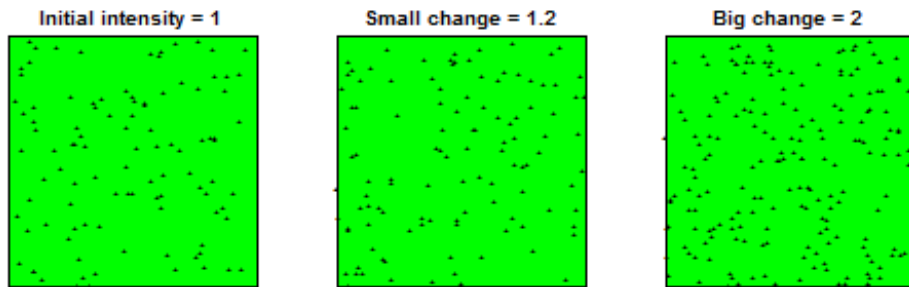
			Homogeneous data				Inhomogeneous data			
			Model 1		Model 2		Model 3		Model 4	
			BF	PT	BF	PT	BF	PT	BF	PT
IID	H_0	$\lambda = 1$	100r	100r	100r	100r	100r	100r	100r	100r
	H_1	$\lambda_2 = 2$	100r	100r	100r	100r	100r	100r	100r	100r
		$\lambda_2 = 1.2$	100r	100r	100r	100r	100r	100r	100r	100r
		multiple	100r	100r	100r	100r	100r	100r	100r	100r
AR(1)	H_0	$\lambda = 1$	100r	100r	100r	100r	100r	100r	100r	100r
	H_1	$\lambda_2 = 2$	100r	100r	100r	100r	100r	100r	100r	100r
		$\lambda_2 = 1.2$	100r	100r	100r	100r	100r	100r	100r	100r
		multiple	100r	100r	100r	100r	100r	100r	100r	100r

4.1.2 Details of the simulation design

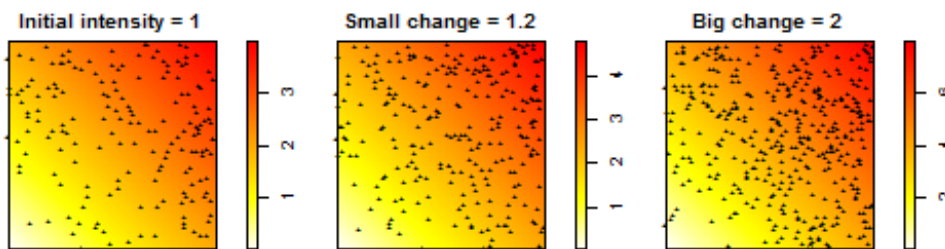
In this Section, we present all the aspects we choose to tune and test in the simulation study. First of all, the spatial and temporal structure of the intensity function is introduced. Then, we show how to build the data series and choose different dependence structures; technical details on how the data series are generated are in Sections 4.1.3 and 4.1.4. Lastly, number and magnitude of changepoints for both a single and a multiple search are set. Details on the models and detection methods can be found in Sections 3.2.2 and 3.2.4.

Choice of the intensity function

As for the intensity function structure, in the simplest case we assume the intensity function to be constant over space, *i.e.* we have a spatially homogeneous process; this means the intensity function at each time point can be represented by a single value. Therefore, point pattern series are generated with a spatially homogeneous intensity structure (a single value for λ over the window) and a inhomogeneous spatial structure. As for the inhomogeneous case, the overall value for $\Lambda = \sum_{s \in W} \lambda(s)$ gives the average number of points at each time point, but the spatial structure changes over the window and is indexed by s . More precisely, we build a smooth spatial trend which is more intense in the top-right corner of the square window and then progressively decreases toward the bottom-left corner. Figure 4.1 shows an example before and after the changepoint for both homogeneous and inhomogeneous patterns, with both a small and a big change.



(a) Homogeneous pattern, three different intensity levels



(b) Inhomogeneous pattern, three different intensity levels

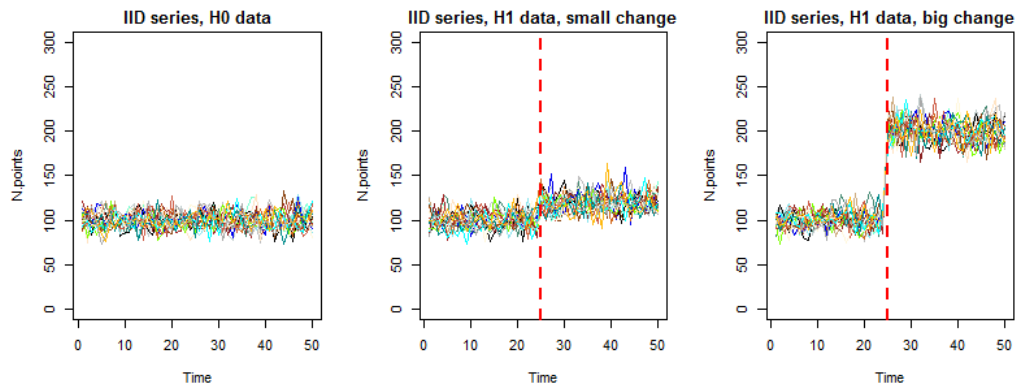
Figure 4.1: Simulated patterns - examples

We build the inhomogeneous series assuming that the spatial structure is the same over time up to a scale parameter whose change defines the changepoint in the series, thus the changepoint detection identifies the time point that corresponds to the change of scale in our data. We are here focusing on changes in the intensity strength, not on changes in its spatial structure. This scenario fits many real situations where the point distribution is mainly due to an underlying driver whose structure remains constant over time, but whose strength may vary. As a further step, we also study the performance of the detection methods when a change in the spatial distribution of points occurs (see Section 4.3).

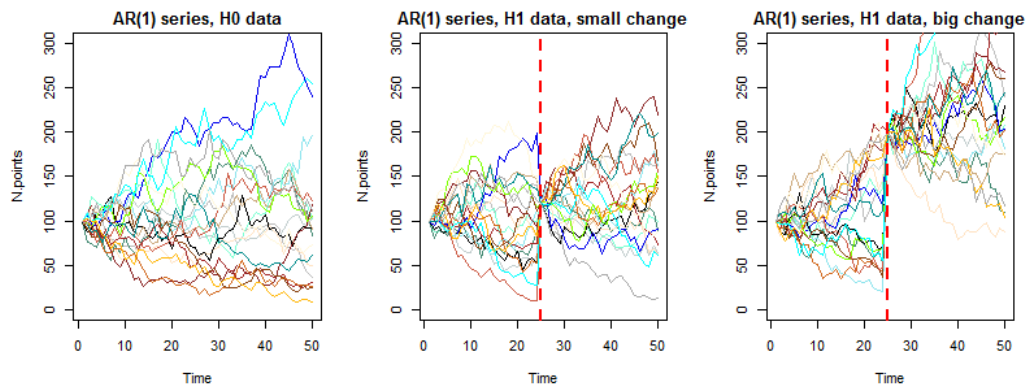
Dependence structure of the data series

As for the type of time series, we generated data with no temporal dependence and data with a strong temporal dependence to the previous time point, in order to check the method performance over both situations. We generate both *i.i.d.* and autoregressive (AR(1)) data series. *I.i.d.* data keep the same parameter value for the intensity over each segment, while for time dependent data the set values are initial values for each time segment, and the following values inside the same segment are generated using the number of points in the previous time instant (divided by the window area) as intensity parameter. The same thing has been done for time dependent inhomogeneous data, keeping the same spatial structure over time and using the number of generated points as intensity strength for the following pattern. We choose to generate both *i.i.d.* and time dependent data as their behaviour is very different as regards changepoint detection. Figure 4.2 shows some time series built by counting the number of points for each time point.

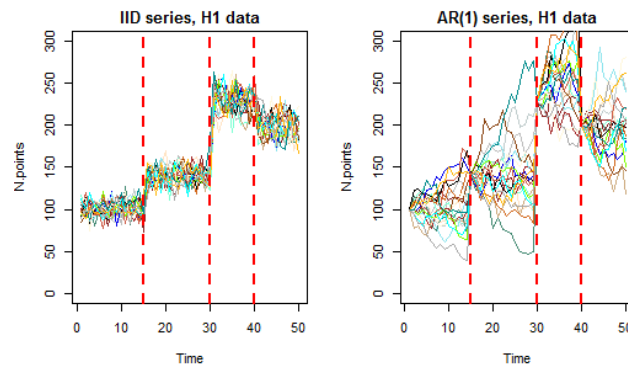
As can be seen, *i.i.d.* data keep very close to the initial set value over the series, and the changepoints are easily recognizable, while AR(1) data tend to drift far away from the initial value, and are far more variable. On one hand, this can result in the detection of spurious changepoints, *i.e.* changepoints that are due to the variability of the series and not to external factors; on the other hand, changes set in the simulation may not be easy to identify. It is therefore of interest to test the methods on both types of data.



(a) Iid time series with no change, small change, big change



(b) AR(1) time series with no change, small change, big change



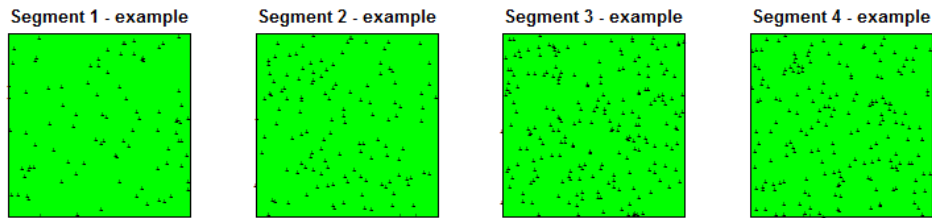
(c) Multiple change points, iid and AR(1) time series

Figure 4.2: Simulated time series with zero, one and three change points

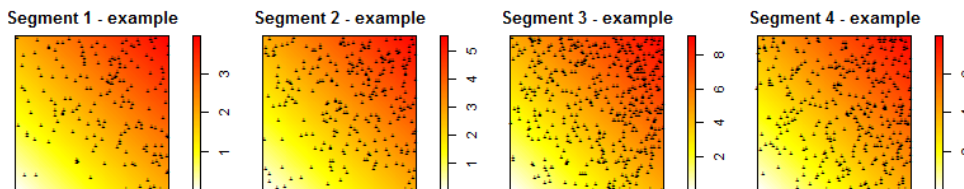
Number and magnitude of changepoints

As for the number of changepoints, we start with a single changepoint with a large magnitude change, the easiest case to detect; we then check the performance of our methods on a small magnitude change. Besides, we generate data with three changepoints of varying size and quality (increasing/decreasing intensity strength).

Let $\lambda(j)$ be the parameter for segment j , where for m changepoints we have $j = 1, \dots, m + 1$. For the single changepoint series, we tried two different change magnitudes: a big one, from $\lambda(1) = 1$ to $\lambda(2) = 2$, and a small one, from $\lambda(1) = 1$ to $\lambda(2) = 1.2$. Given the window area, $\lambda = 1$ produces patterns with an expected number of points equal to 100, $\lambda = 1.2$ generates 120 points and $\lambda = 2$ generates 200 points on average. Bigger changes have been tested and lead to analogous conclusions as $\lambda(2) = 2$. As for the multiple changepoint series, we set two positive changes and a negative one, all with different magnitudes: the segment intensity values are $\lambda(1) = 1$, $\lambda(2) = 1.4$, $\lambda(3) = 2.3$ and $\lambda(4) = 2$. Figure 4.3 shows data with multiple changes.



(a) Homogeneous pattern, 3 changepoints, 4 data segments



(b) Inhomogeneous pattern, 3 changepoints, 4 data segments

Figure 4.3: Examples of data segments patterns for series with multiple changepoints

The last change is extremely small, to further test the performance of the detection methods. Each one of these time series was replicated 100 times. For the inhomogeneous models, the same values are used for Λ . Once all the time series are generated, we fit the four models described in Section 3.2.2 on all of them and try to detect changepoints with both methods described in Section 3.2.4. All model fitting is done using INLA.

4.1.3 Single changepoint data generation

As for the homogeneous models (Models 3.2.1 and 3.2.2), data are generated from a stationary Poisson process, with an initial intensity value of $\lambda = 1$. Data generated under H_0 keep the same value for λ all throughout the series; data generated under H_1 have a change in the intensity value in $t = 24$, the fixed changepoint. Since the intensity function is constant within segments, in a homogeneous process $\lambda(j)$ is the single parameter value for the intensity at time segment j ; for 1 changepoint we have $j = 1, 2$. In all replicates $\lambda(1) = 1$, while in one scenario $\lambda(2) = 2$ and in the other one $\lambda(2) = 1.2$.

As for the non uniform case, data were generated from a spatially inhomogeneous function, whose structure is constant over time up to a scale factor, using an inhomogeneous Poisson process (this is analogous to generating from a LGCP, but fixing the latent field). Let now $\lambda(j, s)$ be the value for the intensity of time segment j at location s , and $\Lambda(j) = \sum_s \lambda(j, s)$ be the overall value for the observation window in segment j . Here too, the initial setting for the intensity function $\Lambda(1) = 1$ produced patterns with 100 points on average over the window, and for alternative data from $t = 24$ on there have been again two change magnitude possibilities: $\lambda(2, s) = 2\lambda(1, s)$ or $\lambda(2, s) = 1.2\lambda(1, s)$, resulting in $\Lambda(2) = 2$ and an expected number of points equal to 200, or $\Lambda(2) = 1.2$ and an expected number of points equal to 120. Under these conditions, both *i.i.d.* and AR(1) data were generated.

Therefore, for *i.i.d.* **homogeneous patterns**

$$H_0 \left\{ \begin{array}{l} Y_t \sim Poi(1) \quad \text{for } t = 1, \dots, 50 \end{array} \right.$$

$$H_1 \left\{ \begin{array}{ll} Y_t \sim Poi(1) & \text{for } t \leq 24 \\ Y_t \sim Poi(\lambda(2)) & \text{for } t > 24 \end{array} \right.$$

where $\lambda(2) \in \{1.2, 2\}$.

For **AR(1) homogeneous patterns**, let $\hat{\lambda}(t) = \frac{N(X_t)}{|W|}$ be the maximum likelihood (ML) estimate for the intensity of the process at time t , where $N(X_t)$ is the number of points of the pattern, and $|W| = 100$ is the window area.

$$H_0 \left\{ \begin{array}{ll} Y_t \sim Poi(1) & \text{for } t = 1 \\ Y_t \sim Poi(\hat{\lambda}(t-1)) & \text{for } t = 2, \dots, 50 \end{array} \right.$$

$$H_1 \left\{ \begin{array}{ll} Y_t \sim Poi(1) & \text{for } t = 1 \\ Y_t \sim Poi(\hat{\lambda}(t-1)) & \text{for } t = 2, \dots, 24 \\ Y_t \sim Poi(\lambda(2)) & \text{for } t = 25 \\ Y_t \sim Poi(\hat{\lambda}(t-1)) & \text{for } t = 26, \dots, 50 \end{array} \right.$$

For *i.i.d.* **inhomogeneous patterns**

$$H_0 \left\{ Y_{ts} \sim Poi(\lambda(1, s)) \quad \text{for } t = 1, \dots, 50, s = 1, \dots, 400 \right.$$

$$H_1 \left\{ \begin{array}{ll} Y_{ts} \sim Poi(\lambda(1, s)) & \text{for } t \leq 24, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(\lambda(2, s)) & \text{for } t > 24, s = 1, \dots, 400 \end{array} \right.$$

where $\lambda(2, s) \in \{1.2\lambda(1, s), 2\lambda(1, s)\}$.

For **AR(1) inhomogeneous patterns**, now let $\hat{\lambda}(t, s) = \frac{N(X_{ts})}{|C|}$ be the ML estimate for the intensity of the process at time t in cell s , where $N(X_{ts})$ is the number of points at time t inside cell s , and $|C| = \frac{|W|}{S}$ is the (time

invariant) cell area.

$$H_0 \begin{cases} Y_{ts} \sim Poi(\lambda(1, s)) & \text{for } t = 1, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(\hat{\lambda}(t-1, s)) & \text{for } t = 2, \dots, 50, s = 1, \dots, 400 \end{cases}$$

$$H_1 \begin{cases} Y_{ts} \sim Poi(\lambda(1, s)) & \text{for } t = 1, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(\hat{\lambda}(t-1, s)) & \text{for } t = 2, \dots, 24, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(\lambda(2, s)) & \text{for } t = 25, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(\hat{\lambda}(t-1, s)) & \text{for } t = 26, \dots, 50, s = 1, \dots, 400 \end{cases}$$

An example of homogeneous and inhomogeneous data can be again found in Figure 4.1 and Figure 4.2.

4.1.4 Multiple changepoint data generation

For the multiple changepoint analysis, data are generated using the same methods as the single changepoint data: homogeneous and inhomogeneous process, *i.i.d.* and AR(1) time series. There is no difference with regard to a single changepoint search in H_0 data, while H_1 data have three changepoints instead of one. For both homogeneous and inhomogeneous data, changepoints are set at $t = 15, 30, 40$. In a general inhomogeneous process, with $M = 3$ changepoints $\lambda(j, s)$ is now defined for $j = 1, \dots, 4$. Following the fixed values, the expected number of points at every time point is 100 for segment 1 ($\Lambda(1) = 1$), 140 for segment 2 ($\Lambda(2) = 1.4$), 230 for segment 3 ($\Lambda(3) = 2.3$) and 200 for segment 4 ($\Lambda(4) = 2$); they are randomly scattered in a homogeneous dataset, and randomly distributed given the intensity at each location for a inhomogeneous dataset. The same technique as in Section 4.1.3 is used for generating time dependent data.

For *i.i.d.* homogeneous patterns

$$H_0 \begin{cases} Y_t \sim Poi(1) & \text{for } t = 1, \dots, 50 \end{cases}$$

$$H_1 \begin{cases} Y_t \sim Poi(1) & \text{for } t \leq 15 \\ Y_t \sim Poi(1.4) & \text{for } 15 < t \leq 30 \\ Y_t \sim Poi(2.3) & \text{for } 30 < t \leq 40 \\ Y_t \sim Poi(2) & \text{for } 40 < t \leq 50 \end{cases}$$

For **AR(1) homogeneous patterns**

$$H_0 \begin{cases} Y_t \sim Poi(1) & \text{for } t = 1 \\ Y_t \sim Poi(\hat{\lambda}(t-1)) & \text{for } t = 2, \dots, 50 \end{cases}$$

$$H_1 \begin{cases} Y_t \sim Poi(1) & \text{for } t = 1 \\ Y_t \sim Poi(\hat{\lambda}(t-1)) & \text{for } t = 2, \dots, 15 \\ Y_t \sim Poi(1.4) & \text{for } t = 16 \\ Y_t \sim Poi(\hat{\lambda}(t-1)) & \text{for } t = 17, \dots, 30 \\ Y_t \sim Poi(2.3) & \text{for } t = 31 \\ Y_t \sim Poi(\hat{\lambda}(t-1)) & \text{for } t = 32, \dots, 40 \\ Y_t \sim Poi(2) & \text{for } t = 41 \\ Y_t \sim Poi(\hat{\lambda}(t-1)) & \text{for } t = 42, \dots, 50 \end{cases}.$$

For ***i.i.d.* inhomogeneous patterns**

$$H_0 \left\{ Y_{ts} \sim Poi(\lambda(1, s)) \quad \text{for } t = 1, \dots, 50, s = 1, \dots, 400 \right.$$

$$H_1 \left\{ \begin{array}{ll} Y_{ts} \sim Poi(\lambda(1, s)) & \text{for } t \leq 15, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(1.4\lambda(1, s)) & \text{for } 15 < t \leq 30, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(2.3\lambda(1, s)) & \text{for } 30 < t \leq 40, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(2\lambda(1, s)) & \text{for } 40 < t \leq 50, s = 1, \dots, 400 \end{array} \right. .$$

For **AR(1) inhomogeneous patterns**

$$H_0 \begin{cases} Y_{ts} \sim Poi(\lambda(1, s)) & \text{for } t = 1, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(\hat{\lambda}(t-1, s)) & \text{for } t = 2, \dots, 50, s = 1, \dots, 400 \end{cases}$$

$$H_1 \left\{ \begin{array}{ll} Y_{ts} \sim Poi(\lambda(1, s)) & \text{for } t = 1, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(\hat{\lambda}(t - 1, s)) & \text{for } t = 2, \dots, 15, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(1.4\lambda(1, s)) & \text{for } t = 16, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(\hat{\lambda}(t - 1, s)) & \text{for } t = 17, \dots, 30, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(2.3\lambda(1, s)) & \text{for } t = 31, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(\hat{\lambda}(t - 1, s)) & \text{for } t = 32, \dots, 40, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(2\lambda(1, s)) & \text{for } t = 41, s = 1, \dots, 400 \\ Y_{ts} \sim Poi(\hat{\lambda}(t - 1, s)) & \text{for } t = 42, \dots, 50, s = 1, \dots, 400 \end{array} \right.$$

An example of both homogeneous and inhomogeneous data series with multiple changes is in Figure 4.3.

4.1.5 Simulation models and methods

We use the simulated data to run all four model scenarios described in Section 3.2.2: a simple one assuming a spatially homogeneous process and introducing a fixed effect to describe the intensity level over time (Model 1, Formula 3.2.1), a model adding a temporal random effect (Model 2, Formula 3.2.2), a model including an intercept, spatial dependence and heterogeneity (Model 3, Formula 3.2.3), and finally a more complex model for spatially inhomogeneous intensity with two smooth effects allowing for both spatial and temporal dependence within segments (Model 4, Formula 3.2.4).

Since the window is discretized into 400 cells and we have 50 time points, for each scenario and under each hypothesis the response vector is Y (50×400) $\times 1 = 20,000 \times 1$.

Models are fitted separately to different parts of the data, according to the hypotheses. Under the null hypothesis, each model is fitted to the whole data vector to obtain the marginal data log-likelihood. Under the alternative hypothesis, for a single changepoint search we

1. choose a minimum segment length of $d = 4$ to make the changepoint search more effective and improve the INLA algorithm performance (see Section 3.2.3)
2. run each model $T - 2d + 1$ times for each simulation replicate; in each run, we condition on the changepoint occurring at a location

- $\tau \in \{4, 6, \dots, 44, 46\}$ (remember that τ marks the end of a segment) and fit the considered model to every data segment using INLA; for every τ , we obtain two log-likelihood values $q_1(\tau)$ and $q_2(\tau)$ (see Section 3.2.4)
3. sum $q_1(\tau)$ and $q_2(\tau)$ to obtain the marginal data log-likelihood under a specific changepoint $l_1(\tau)$
 4. since we do the same for every possible τ , for every single replicate we obtain $T - 2d + 1$ marginal log-likelihood values under the alternative hypothesis of one changepoint; they all refer to the whole data series Y , but they are conditional on different positions for the potential changepoint
 5. use the log-likelihood vector to build the posterior distribution of the potential changepoint positions for a specific replicate as explained in Chapter 3
 6. for every model, we do the same over 100 data series replicates, thus we have 100 posterior curves
 7. for every curve, we use one of the methods described in Section 3.2.4 to take decisions on the occurrence of a changepoint
 8. evaluate the performance of each detection method, for each scenario, by summarising the results over 100 posterior curves.

For a multiple changepoint search, we can follow either an iterative or a simultaneous technique, as introduced in Section 3.3. If we use a binary segmentation algorithm, the same procedure is repeated at every step for the multiple changepoint detection; we set the algorithm to find maximum 4 changepoints, but different maxima can easily be fixed. When we run a simultaneous changepoint search, we follow what explained in Chapter 3: we first obtain a few data likelihoods conditional on different numbers of changepoints and choose the number of changepoints that corresponds to the highest likelihood; then, we infer the position of every single changepoint via conditional posterior distributions of every changepoint given the previous

one, the data and the chosen number of changepoints.

We use all detection methods proposed in Chapter 3 in order to assess their performance and choose the most suitable one(s) for the analysis on real data presented in Chapter 5.

4.2 Simulation results

After running all the analyses, we obtain results for each of the cases listed in Section 4.1.1, and we show a few graphs:

- a histogram showing the probability of committing type I errors for H_0 data and type II errors for H_1 data
- a histogram of the number of changepoints found, where the mode is chosen as the correct number of changepoints
- a posterior probability plot: conditioning on the chosen number of changepoints, we obtain the averaged (over 100 replicates) pointwise posterior probability for each time point to be a changepoint
- an estimate for the intensity function for each time segment produced by the INLA algorithm, together with a few synthetic measures and a comparison with the true values.

As for Section 4.1, a summarised overview of the results with general comments is given first in Section 4.2.1; detailed comments can be found in the following Sections. A few representative results are displayed in figures along the Chapter. For all the remaining results, we refer to figures in the Appendix. As a note, data without changepoints are labelled as $H0$, single big change data as $H1b$ and single small change data as $H1s$ in all graphs; multiple changepoint data are simply labelled as $H1$.

4.2.1 Summary of the simulation results

The BF (and SIC) and PT methods' performance was evaluated according to type I and type II errors, number and position of detected changepoints and values of the intensity estimates.

Type I and II errors

A summary of the methods performance is in Table 4.2.

Table 4.2: Significance levels (H_0 data) and power levels (H_1 data)

		Homogeneous data					Inhomogeneous data			
		Model 1		Model 2		Model 3		Model 4		
		BF	PT	BF	PT	BF	PT	BF	PT	
IID	H_0	$\lambda = 1$	0	≤ 0.05	0	≤ 0.05	0	≤ 0.1	0	≤ 0.01
	H_1	$\lambda_2 = 2$	1	1	1	1	1	1	0	1
		$\lambda_2 = 1.2$	1	1	1	0.98	0	0.34	0	0.3
		mult BinSeg	1	1	0.99	1	0	0.93	0	0.26
		mult Simult	1		1		0		0	
AR(1)	H_0	$\lambda = 1$	0.96	0.66	0.38	0.24	0.15	0.26	0	0.18
	H_1	$\lambda_2 = 2$	1	0.97	0.81	0.75	0.53	0.81	0	0.52
		$\lambda_2 = 1.2$	1	0.73	0.43	0.36	0.19	0.54	0	0.37
		mult BinSeg	1	0.98	0.94	0.91	0.55	0.84	0	0.67
		mult Simult	1		1		0		0	

In general, the Bayes Factor method (and, analogously, the simultaneous approach) performs very well as regards the first two models: in most cases type I errors are very small (with the exception of one case with time dependent data, but we expect poorer performance on these data, for the reasons introduced in Section 3.1) and type II errors are negligible in all cases. When we fit more complicated models including a spatial effect, though, the performance is very poor: the method is too conservative and does not detect changepoints, irrespective of their magnitude.

The Posterior Threshold method gives a better performance over all models; this is sensible, as the threshold value can be tuned according to the model. A few 'grey' zones are produced, but the overall conclusions are correct in most cases, and there is at least some ability to detect changes in all situations (unlike the Bayes Factor method).

A further summary of this performance can be found in Table 4.3: the first row in each table concerns data generated under H_0 and the second row concerns data generated under H_1 , therefore numbers have to sum to 100 by row. It is very plain that the PT method has a better overall performance: as regards null data (first row), the behaviour of the two methods is very similar,

but the PT method is 20 percentage points better in finding changepoints in H_1 data (second row).

Table 4.3: Summary of type I and type II errors

H_0 correct result	False positive
False negative	H_1 correct result

BF method (%)		PT method (%)	
81.38	18.63	79.75	20.25
43.79	56.21	23.92	76.08

Number and location of changepoints

As for the number of detected changepoints, results are linked, but not necessarily identical, to the previous ones: committing or not a type II error only concerns the rejection of H_0 and tells nothing on the number and positions of the detected changepoints, which is of special interest in a multiple changepoint search. Table 4.4 shows a summary of the results.

We can see that as far as H_0 data are concerned, results are correct in all cases: even in situation where some changepoints were found, as in AR(1) data, all the positions were different, and this indicates they are spurious changepoints and not 'true' ones. As regards the detection in H_1 data, the BF method suffers from the above mentioned issue: it is very precise in detecting the true change(s) in the first two models, but too conservative when spatial dependence and inhomogeneity is introduced. The PT method performs much better: when changepoints are not detected in the majority of replicates, it is due to the small magnitude of the change, which means the method is not too sensible; despite the small size, a percentage of replicates still had a change detected. The only wrong conclusion concerns the multiple changepoint *i.i.d.* data series under the most complicated model; in all other cases, conclusions are very sensitive and the detected positions are correct or as close as it makes no difference. It is interesting to note that spurious changes in time dependent data do not affect conclusions.

Table 4.4: Position of the detected changepoints

		Homogeneous data				Inhomogeneous data				
		Model 1		Model 2		Model 3		Model 4		
		True	BF	PT	BF	PT	BF	PT	BF	PT
IID	H_0	No chp	–	–	–	–	–	–	–	–
	H_1	24	24	24	24	24	24	24	–	24
		24	24	24	24	24	–	–	–	–
		15 30 40 BinSeg	15	15	15	15	–	15	–	–
			30	30	30	30		30		
	40	40	40	40						
	15 30 40 Simult	28		28 16		–		–		
AR(1)	H_0	No chp	–	–	–	–	–	–	–	
	H_1	24	24	24	24	24	24	–	24	
		24	24	24	–	–	–	24	–	–
		15 30 40 BinSeg	15	15	15	15	15	15	–	15
			30	30	30	30	30	30		30
	41	41	40	40		41		40		
	15 30 40 Simult	28 13		28 13 40		–		–		

Intensity estimates

Lastly, a few comments about the intensity estimates, which again depend on the above presented results. A summary of the estimated values is given in Table 4.5. Note that the intensity is an inhomogeneous function which takes different values over space. In this table, for brevity reasons, only the mean value is reported, but the mean range (over the replicates) and credibility bands are also available as in every Bayesian inference output. Given the detected changepoints, estimates are very accurate over all the simulated scenarios: when a changepoint is not detected, values are an average between the two segments' true values, and when a changepoint is only detected in part of the replicates (as it happens with very small changes), the true magnitude of the change is shrunk. In all cases the correct (increasing or decreasing) trend is captured.

Table 4.5: Estimates for the segment intensity

		True intensity	Homogeneous data				Inhomogeneous data				
			Model 1		Model 2		Model 3		Model 4		
			BF	PT	BF	PT	BF	PT	BF	PT	
IID	H_0	1.00	1.00	1.01	1.00	1.01	0.99	1.00	1.00	1.00	
	H_1	1.00 2.00	0.99	1.04	1.00	1.04	0.99	1.00	1.50	1.00	
		1.00 1.20	2.00	2.00	2.00	2.00	2.00	2.00		2.00	
		1.00 1.20	1.00	1.01	1.00	1.01	1.09	1.10	1.10	1.10	
AR(1)	H_0	1.00	1.00	1.01	1.00	1.01	1.00	1.58	1.20	1.51	1.60
	H_1	1.00 1.40 2.30 2.00	1.40	1.38	1.40	1.38		1.50			
		1.40 1.38	2.17	2.22	2.12	2.15		2.20			
		2.07 2.05	2.10	2.08							
AR(1)	H_0	1.00	0.99	1.01	0.96	0.99	0.92	0.98	0.87	0.98	
	H_1	1.00 2.00	1.05	1.05	1.09	1.11	1.18	1.08	1.41	1.20	
		2.04 2.03	2.10	2.05	1.90	1.99				1.78	
		1.00 1.20	1.01	1.01	1.06	1.06	1.10	1.01	1.07	1.09	
AR(1)	H_1	1.00 1.20	1.14	1.14			1.18				
		1.00 1.40 2.30 2.00	1.02	1.02	1.05	1.07	1.12	1.10	–	1.15	
		1.40 1.40	1.39	1.38	1.40	1.42				1.41	
		2.21 2.22	2.15	2.14	2.13	2.18				2.03	
		1.08	2.07	2.02	2.04		2.08		1.97		

In the next Sections, detailed comments about the simulation results are presented, along with some representative graphs; a complete list of the figures is in Appendix A.

4.2.2 Single changepoint detection with Bayes Factor method

In this Section, we summarise results for a single changepoint search on both *i.i.d.* and time dependent data. Bayes Factor (BF) and SIC method (SIC) perform extremely similarly; the SIC method tends to be ever so slightly less conservative, but the difference is negligible in most cases, and never substantial. We will therefore not explicitly report results for the SIC

method.

As we say in Section 3.2.4, the Formula (3.2.8) we apply to simulated data is a conservative version of the commonly used Bayes Factor. This is for two main reasons: first of all, a positive but small value for the Bayes Factor is usually interpreted as 'small evidence', and we would like to protect results against type I errors. Secondly, as log-likelihoods are returned by the INLA algorithm, when computing the sum in the numerator of the Bayes Factor exponents have to be taken and issues due to software numerical rounding arise, as number easily go to infinity or 0. The version in Equation 3.2.8 is instead perfectly computable with no need to convert logarithms.

On both *i.i.d.* and time dependent data, the BF method performs very well over three of the four model scenarios as regards detection and location of the change.

Homogeneous models

In the fixed and temporal effect models the statistic correctly rejects H_0 in all *i.i.d.* replicates, even when a very small change occurs; moreover, the detected changepoint position is correct in all replicates with a big change, and in most with a small change (very close in the remaining ones). The estimated values produced by INLA are compactly distributed around the true value, and both their mean and median are a good choice for the intensity parameter posterior estimate, being always less than 0.05 away from the correct values. An example of the simulation output is in Figure 4.4. Predictably, results are not so neat on time dependent data, and the main cause is data variability that will lead to the detection of changepoints that have not been set *a priori* in H_0 data; nevertheless, introducing the temporal effect in the model has a high positive effect on the statistic performance on null data, as the mode of the detected number of changepoints is correctly set to 0. For both models, the performance is very good for data generated under the alternative hypothesis as regards both power and location. As for the estimated values, the variability among the replicates is much higher than the *i.i.d.* data one, still both mean and median are very close enough to the initial intensity values. Some results for AR(1) data are in Figure 4.5.

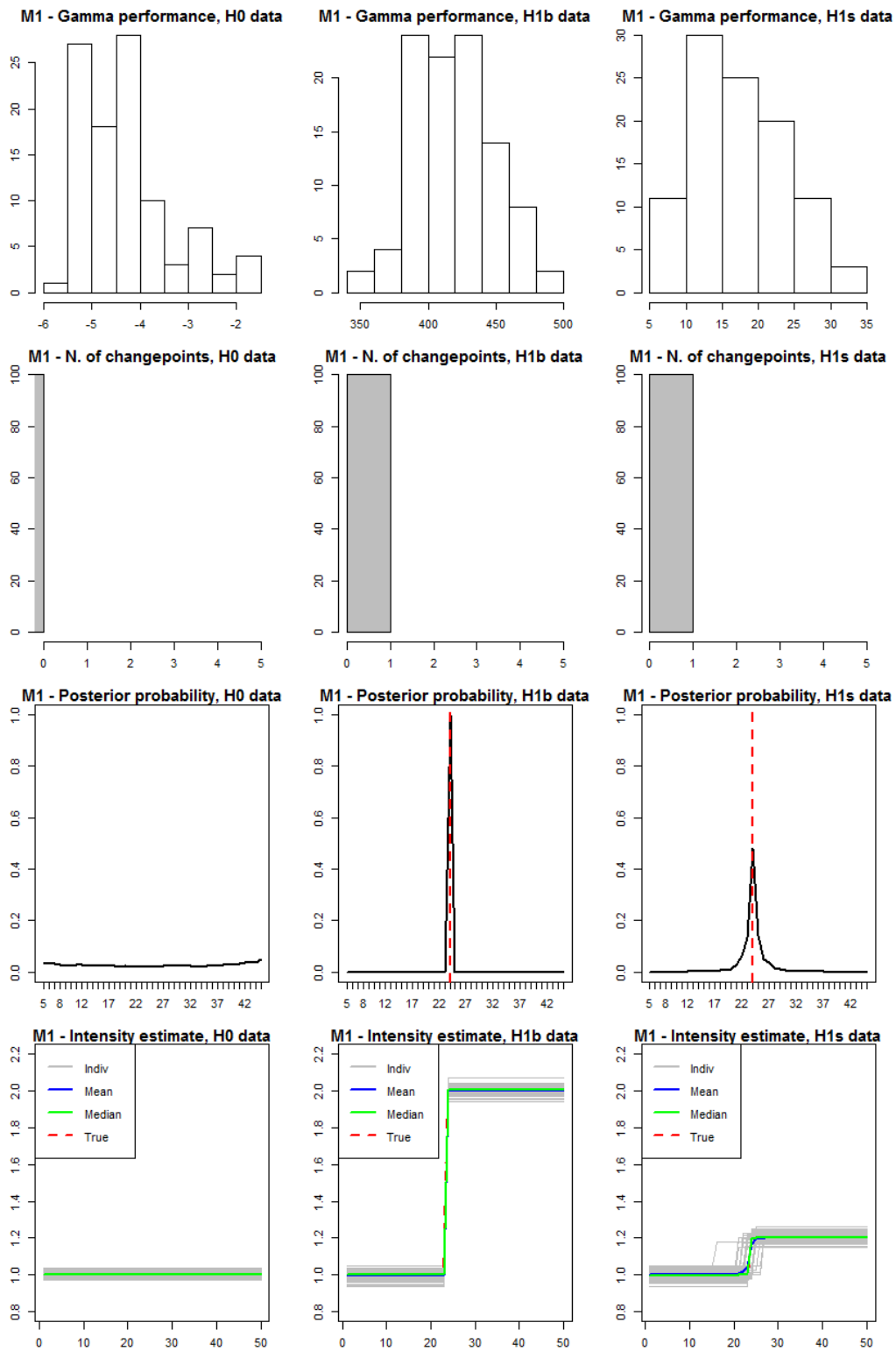


Figure 4.4: Single changepoint search on iid data, with the fixed effect model and the BF method

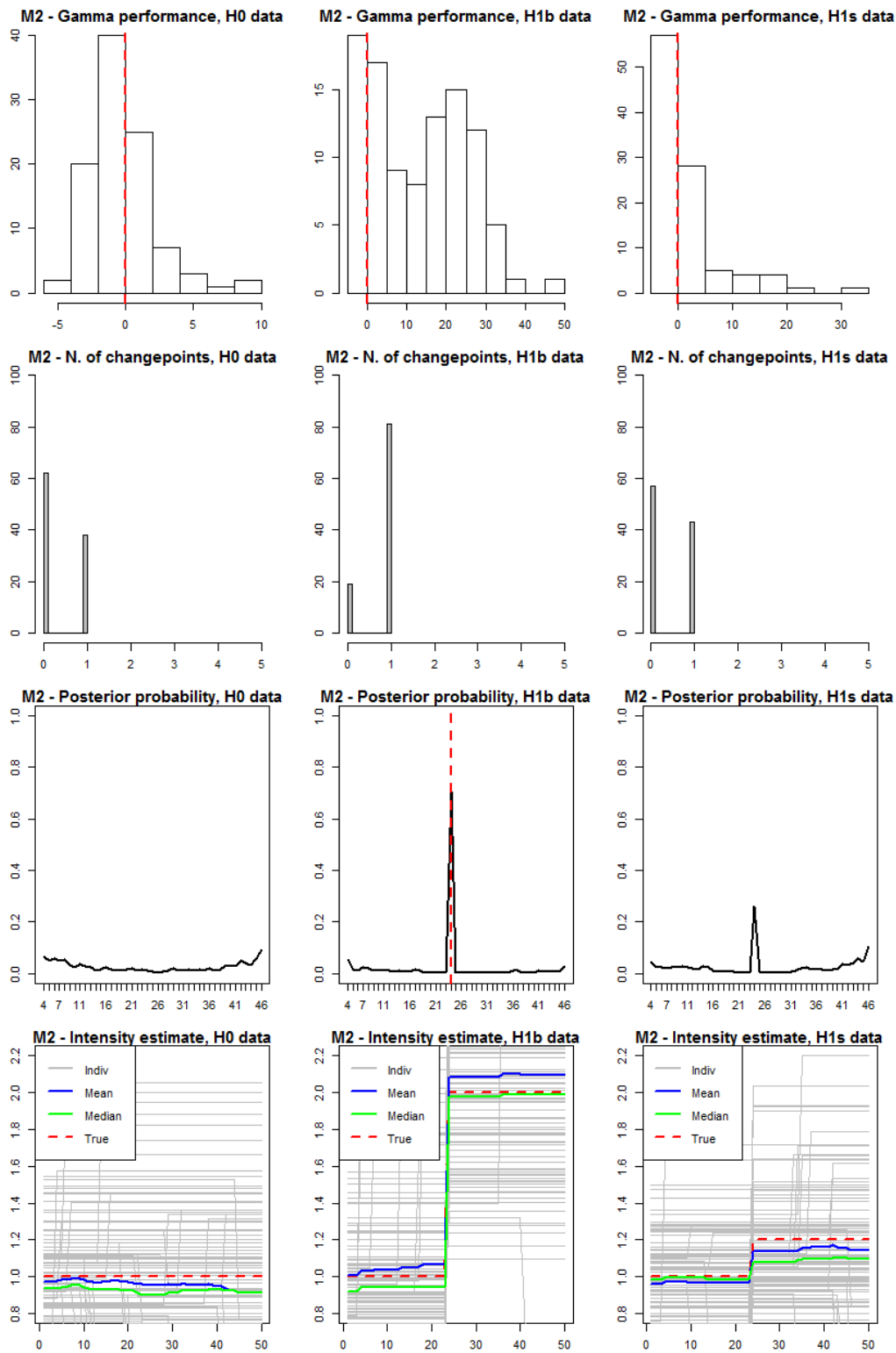


Figure 4.5: Single changepoint search on AR(1) data, with the temporal effect model and the BF method

Inhomogeneous models

The third and fourth models allow for spatially inhomogeneous intensity functions and a spatial random effect, and are therefore applied to data generated following an inhomogeneous process. An example of the resulting graphs is in Figure 4.6.

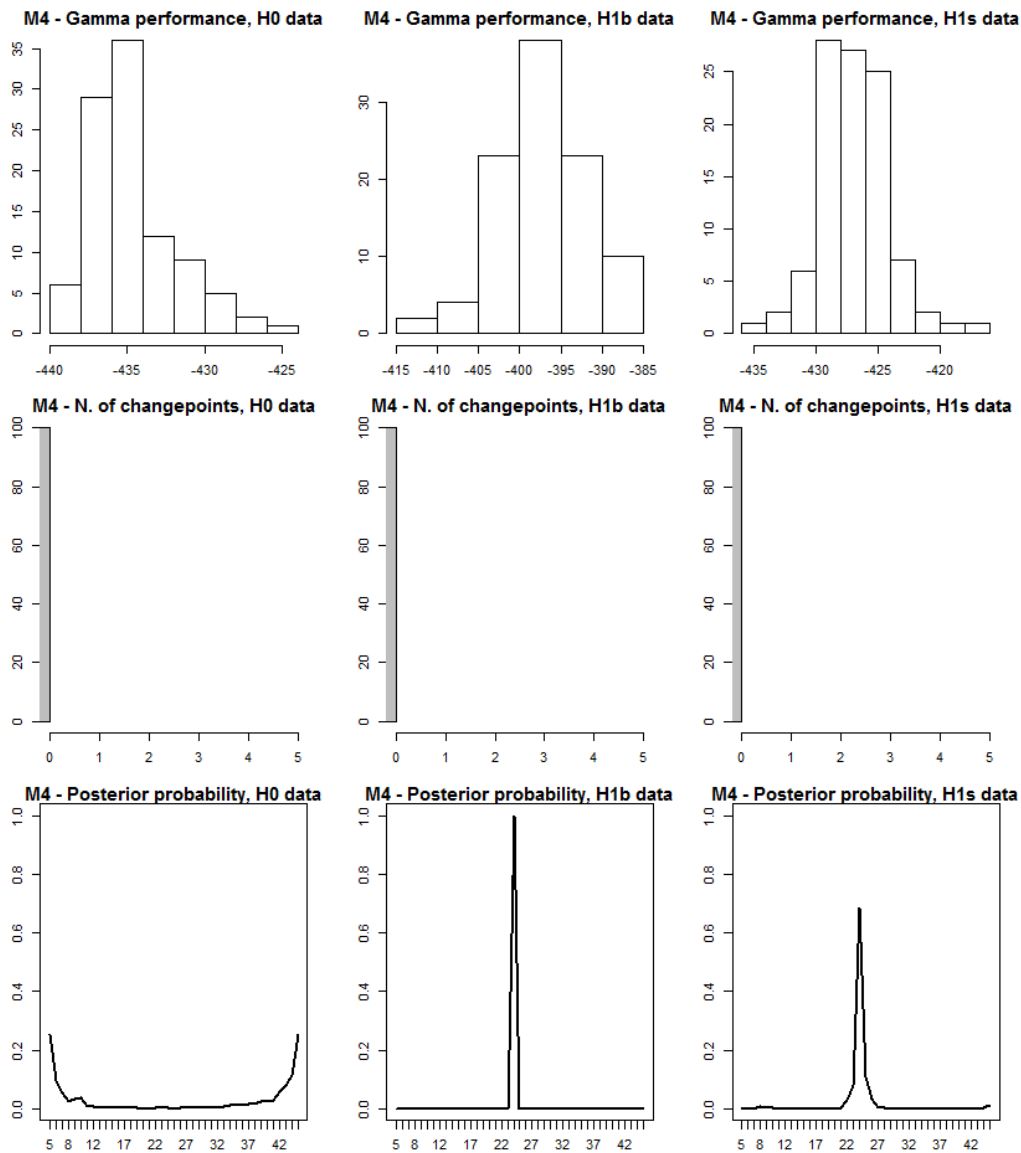


Figure 4.6: Single changepoint search on iid data, with the spatio-temporal effect model and the BF method - Power level and location of the changepoint

The significance level is correctly set to 0 over all replicates for both models, but a conservatism issue raises here, as the big change is the only one detected (in the correct location) with the spatial model, while with the spatio-temporal model no change is detected over all the data series, despite high peaks corresponding to $t = 24$ in all posterior distributions. The most interesting novelty with inhomogeneous models is the intensity estimate: we obtain a value for every grid cell, hence the estimate is shown as a pixel image where for every cell values are averaged over the corresponding time segment (we choose the mean as synthetic value, and the median would lead to extremely similar results in all cases). In all cases (both spatial and spatio-temporal model, and both *i.i.d.* and AR(1) data) the estimates are very accurate given the detected changepoints: they not only capture the true range of values very well, but also produce a smooth image that correctly estimates the spatial trend. When changepoints are not detected, the range of the estimated values is correctly set in between the two segment's values (see *e.g.* Figure 4.7). In AR(1) data, some small drifts with respect to the set values occur, due to the strong time dependency and variability in the data.

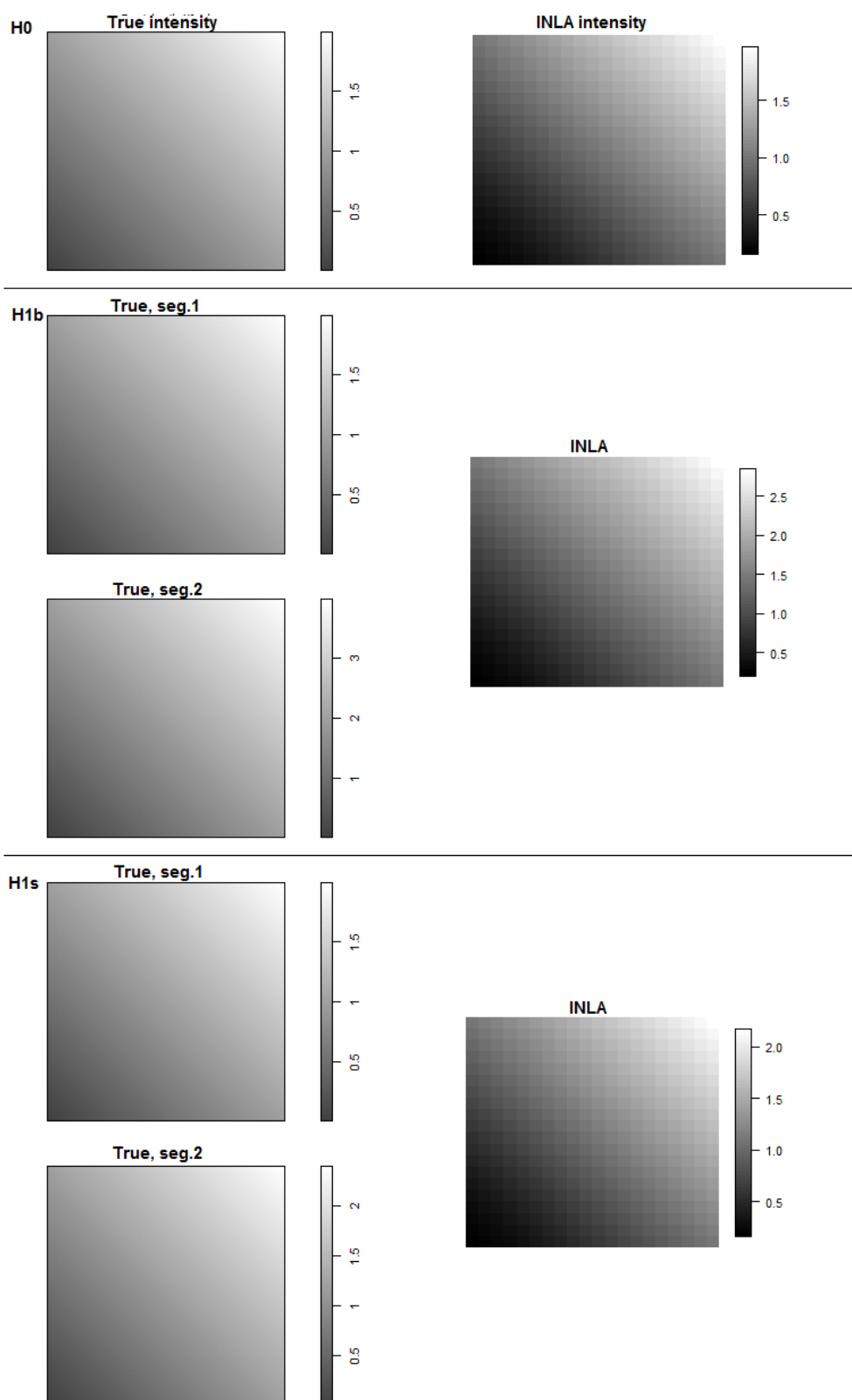


Figure 4.7: Single changepoint search on iid data, with the spatio-temporal effect model and the BF method - Estimated intensities

4.2.3 Single changepoint detection with Posterior Threshold method

The method consisting in fixing a threshold for posterior probability values can be adapted to the model, in order to be able to recognise changepoints even when spatial and/or temporal dependence are considered and lead to higher data variability, *e.g.* by raising the threshold with respect to a simpler model. Having simulated data, we bound the choice of the threshold to a certain significance level, giving an objective threshold value that will still depend on the model applied to our data.

We use a threshold corresponding to $\alpha \leq 0.05$ for the fixed and temporal effect models, and one corresponding to $\alpha \leq 0.1$ for the spatial and spatio-temporal inhomogeneous models. The different choice for α is due to the fitted model: for the inhomogeneous models, fixing a lower α would result in a threshold equal to 1, which is not a sensible choice. For dependent data, fixing a threshold based on the significance level obtained on such variable data is tricky. We decide to fix the threshold referring to *i.i.d.* data, keeping, where possible, a stricter criterion: this results in a choice of $\alpha \leq 0.01$ for the two homogeneous models and in $\alpha \leq 0.1$ for the inhomogeneous ones for the same reasons explained above.

The performance of this method on a single changepoint search is, in general, preferable to the BF method on alternative data.

Homogeneous models

The threshold for these two models for *i.i.d.* data is 0.2 with the fixed effect model and 0.25 for the temporal model; for time dependent data, it is 0.55 with the fixed effect model and 0.65 for the temporal model. A significance level not greater than 0.05 is set on *i.i.d.* data; on AR(1) data, it is higher and, as for the BF method, leads to an overall wrong conclusion with a fixed model but a correct conclusion when the temporal effect is introduced; the significance level is anyway much better on time dependent data than the one obtained by the BF method.

As for *i.i.d.* data, the changepoint is correctly detected and the right location is identified as with the BF method, since the choice of the method only

concerns the number of changepoints, while the correct location is given by the posterior probability distributions, irrespective of the method used. The same conclusions concern the intensity estimate. A summary of the results is in Figure 4.8.

As far as time dependent data are concerned, no evidence for a specific change is shown by the $H0$ data posterior distribution, while conclusions regarding both number and location of changepoints are correct in most $H1b$ data and not significant in $H1s$ data. As said in the BF method results, single replicate estimates are extremely variable, still both mean and median perform well as estimates for λ . In $H1s$ data, there is a small underestimation of the second segment value, due to the difficulty in detecting the small change. Results for the fixed effect model are in Figure 4.9.

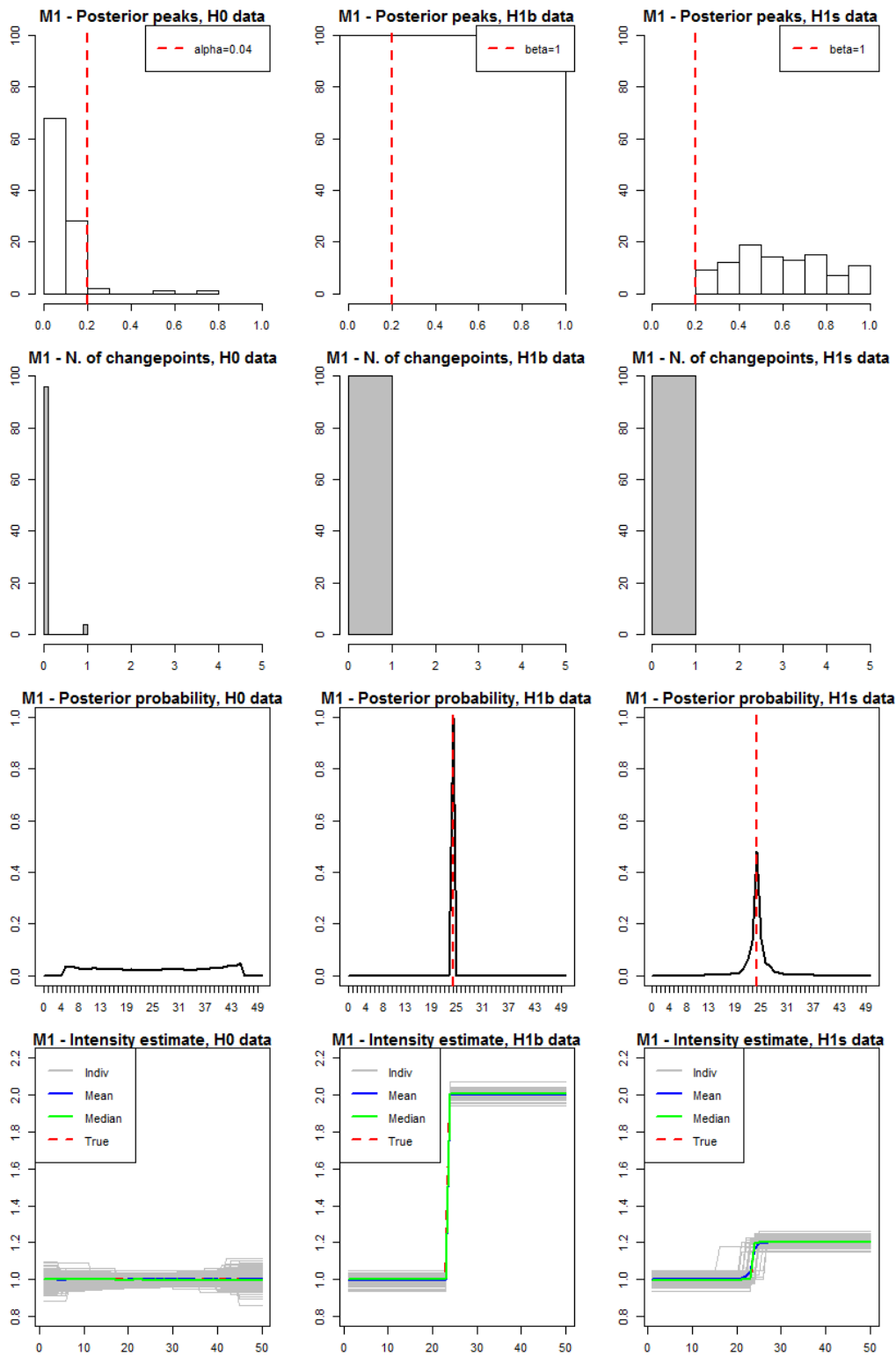


Figure 4.8: Single changepoint search on iid data, with the fixed effect model and the PT method

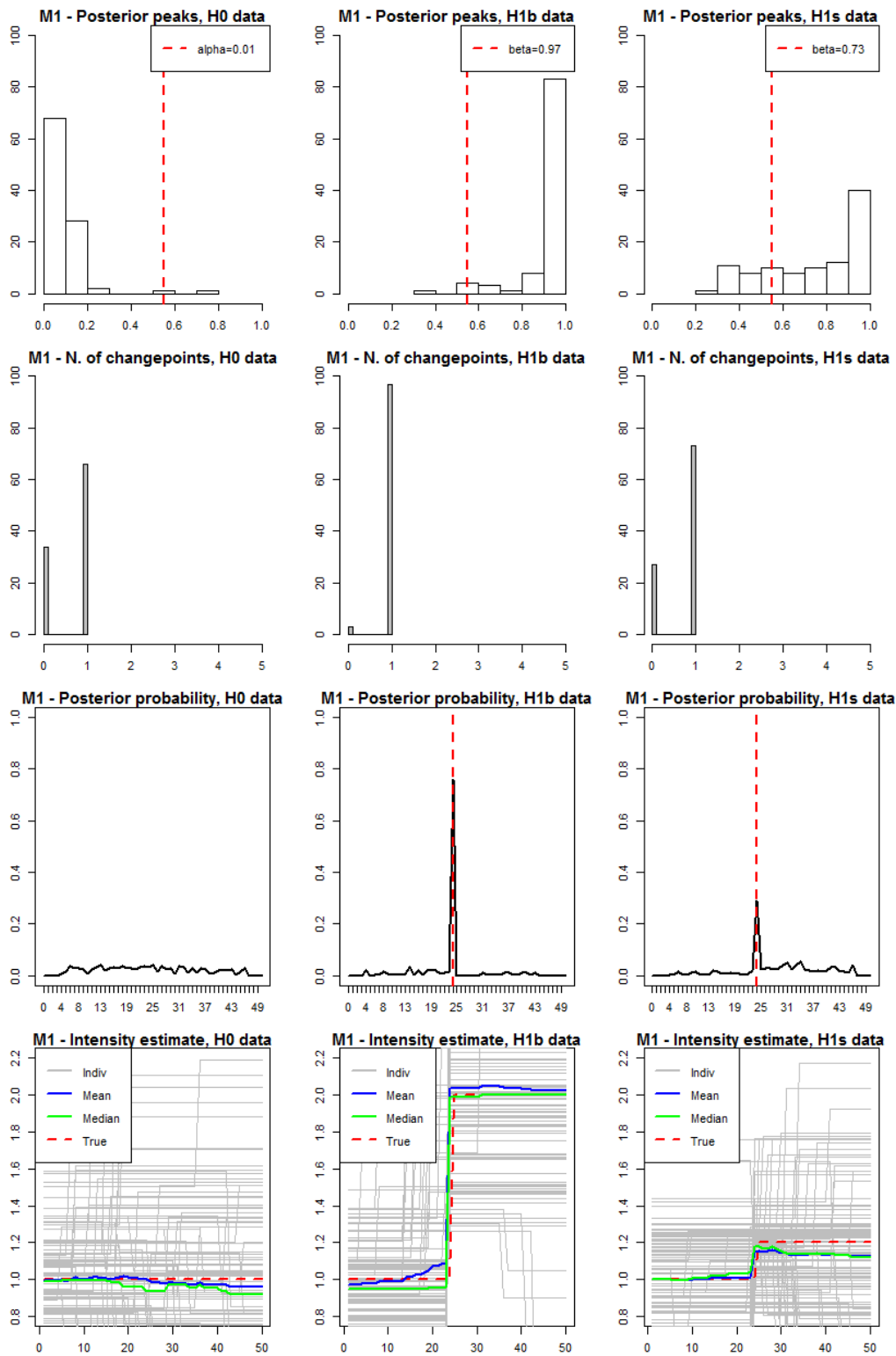


Figure 4.9: Single changepoint search on AR(1) data, with the fixed effect model and the PT method

Inhomogeneous models

The threshold for the inhomogeneous models is 0.95 for all data, corresponding to a significance level not greater than 0.1 on *i.i.d.* data and low enough to reach the overall correct conclusion on AR(1) data.

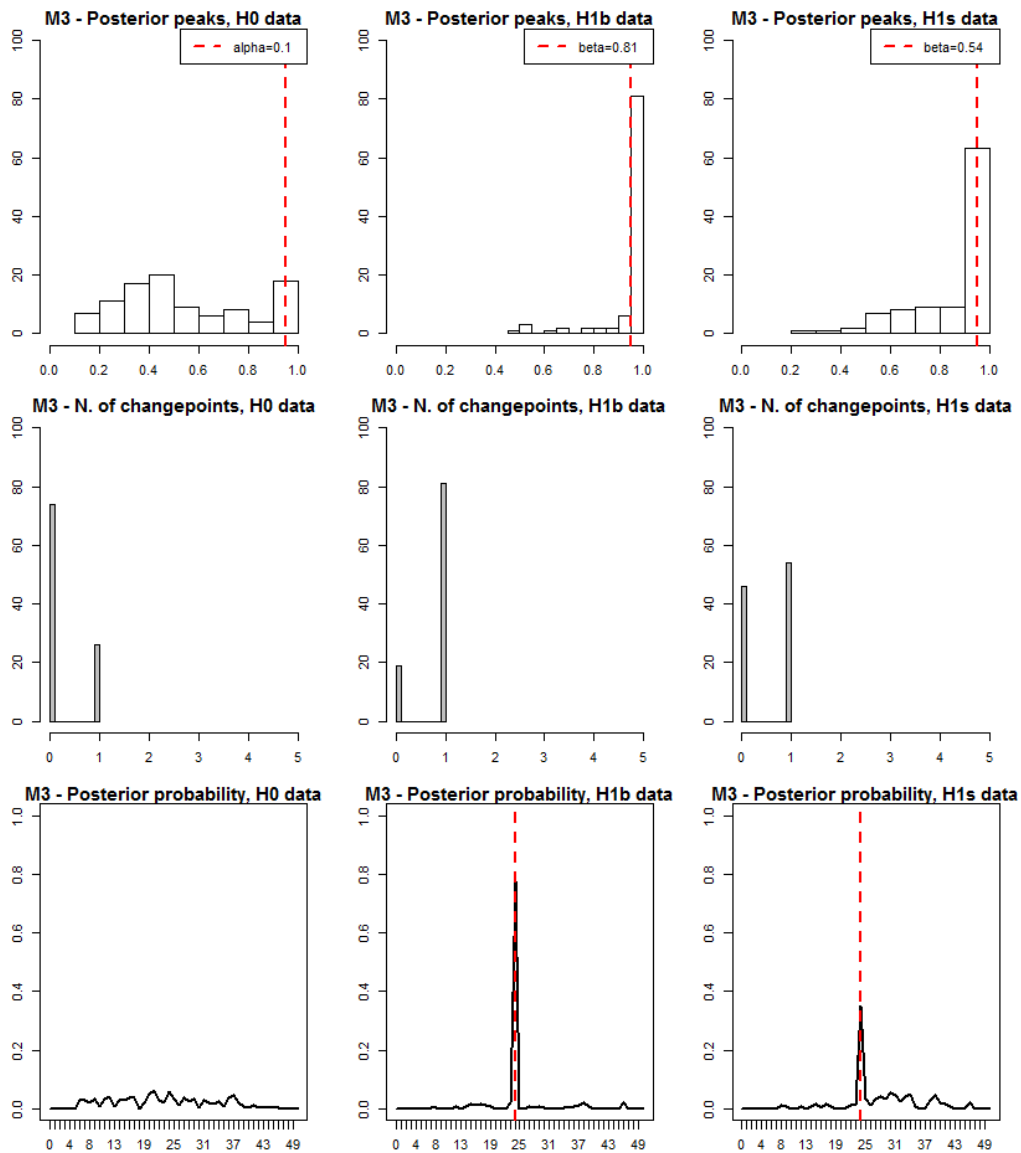


Figure 4.10: Single changepoint search on AR(1) data, with the spatial effect model and the PT method - Power level and location of the changepoint

The most important comparison to the BF method conclusions concern data with a changepoint; with the spatial model results are similar on *i.i.d.* data: one changepoint in *H1b* data, no changepoint in *H1s* data. On time dependent data, though, a changepoint is correctly detected even when it has a small magnitude with the spatial model. The spatio-temporal model also leads to better conclusion as the big change is detected on both *i.i.d.* and time dependent data. See Figure 4.10 for a summary of the results.

Again, location estimates are correct and the intensity estimates are very accurate given the changepoint locations and the variability in the data, as shown in Figure 4.11. When the changepoint is not detected in a consistent part of the replicates, its actual size will be shrunk in the estimates.

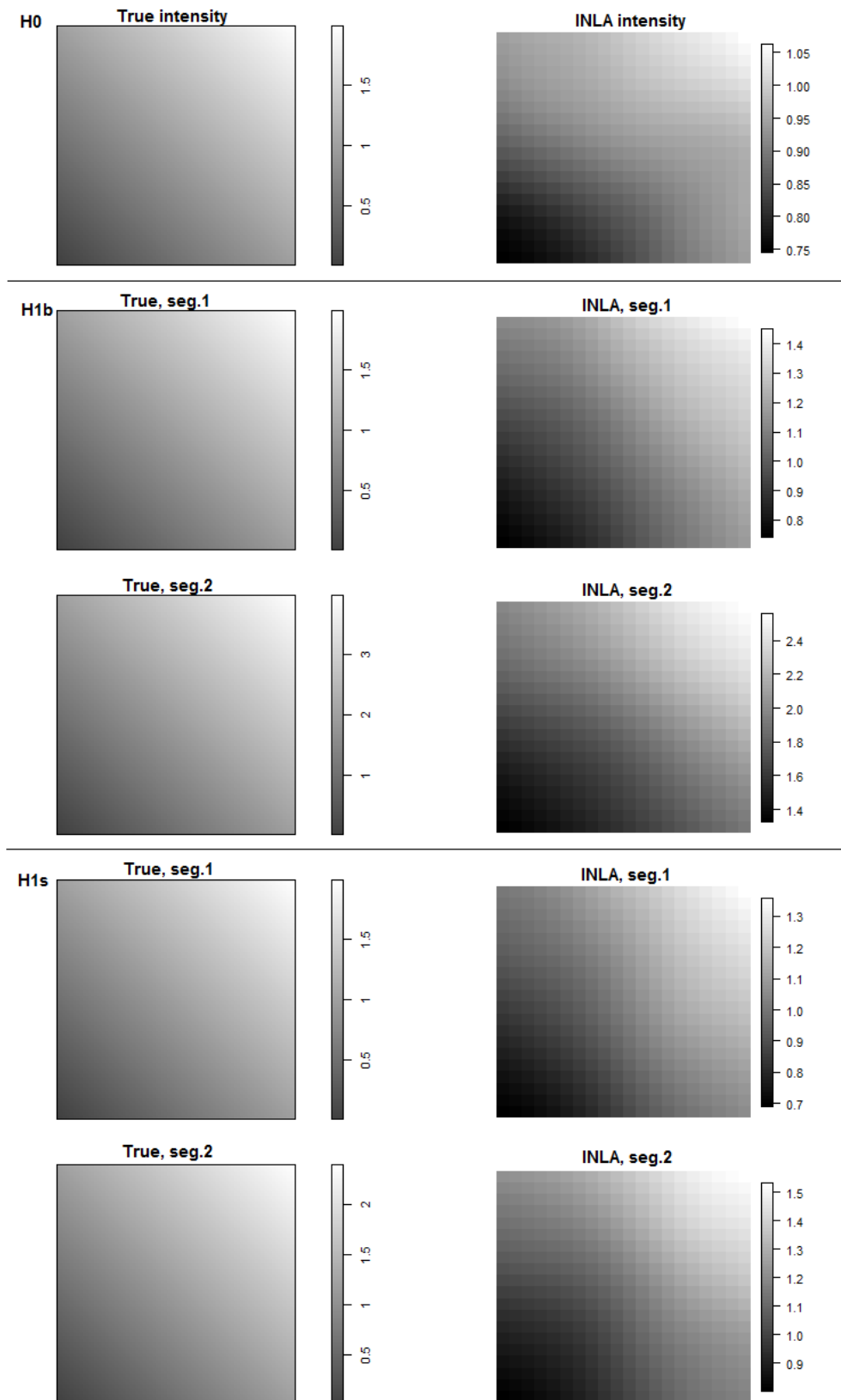


Figure 4.11: Single changepoint search on AR(1) data, with the spatial effect model and the PT method - Estimated intensities

4.2.4 Iterative multiple changepoint detection with Bayes Factor method

When applied to a multiple changepoint search, the BF method performs more poorly than in the single changepoint case: its results are good for the first two homogeneous models, but not for the inhomogeneous ones. The greater difficulty in detecting changepoints in more complex models in this analysis can also be imputed to the very small change magnitudes that have been set over these datasets. It is interesting to notice that the range of γ values is in all cases very consistent: either nearly all values are negative or they are positive, the power level is 1 or 0, there is no grey zone. Perhaps, as the posterior threshold is tuned according to the fitted model, the γ'_{τ^*} statistic (Formula 3.2.8) decision threshold should also be changed according to the model. There is anyway no reference we are aware of about giving a different threshold than zero to the logarithm of the Bayes Factor. As the method does not perform well on time dependent data, we only use the Posterior Threshold method on those ones.

The significance level is of course very similar to the single changepoint results over all data, as it only concerns the rejection of H_0 . Moreover we already know the INLA estimates are very good given the detected changepoints. What is of interest here is then the actual number of detected changepoints and their location. for every model. Remember that with multiple changes we only have one type of data generated under H_1 .

As for the fixed effect model, 3 changepoints were correctly found in 15, 30 and 40. The peak in 40 is smaller as this changepoint has the lowest change magnitude along with the highest data variability (from $\lambda = 2.3$ to $\lambda = 2$). Consistently, the INLA estimate are very accurate in the first two segments, and then a bit lower than 2.3 on the third and a bit higher than 2 in the fourth, shrinking the actual magnitude for the last changepoint. Nevertheless, the general behaviour of the intensity function is very well captured.

Introducing a temporal effect on *i.i.d.* generated data does not substantially modify the results with respect to the first model, except it flattens the third peak in 40 even more, even if this time point will still be detected.

In the INLA estimates it is of interest to see that the abruptness of all steps is softened, giving more gradual changes, and that best suits real data situations.

When moving on to inhomogeneous processes, problems in the BF method begin, as no changepoints are identified in any data series. Since the first potential changepoint found (the one returning the maximum log-likelihood value) is considered non significant, the binary segmentation algorithm stops running; nevertheless, the posterior distribution curve shows a very high peak at position $t = 30$, where the change with the largest magnitude is set. Due to the lack of changepoint detections, the estimate images are very precise for $H0$ data, but the range of values for $H1$ data has a mean of 1.7, which is a good average across all segments.

All figures can be found in Appendix A.

4.2.5 Iterative multiple changepoint detection with Posterior Threshold method

We finally fit the four models on both *i.i.d.* and AR(1) data, looking for multiple changepoints in the series and making decisions based on the posterior probability distribution and a fixed threshold. On *i.i.d.* data, we detect different possibilities for the threshold corresponding to a probability of committing the type I error equal to 0.01, 0.05, 0.1, when possible. Then, for *i.i.d.* data when homogeneous models are fitted, we choose the threshold corresponding to $\alpha = 0.05$. In the two inhomogeneous models, the only sensible threshold corresponds to $\alpha = 0.1$ as lower values for α would result in a threshold equal to 1. For the same reason, the threshold is maintained at the same value for AR(1) data, while in the homogeneous models we choose a stricter threshold, corresponding to $\alpha = 0.01$ on *i.i.d.* data, as it is much more likely to detect changepoints even in $H0$ data series when data are time dependent.

Homogeneous models

The threshold for the first model is 0.25 for *i.i.d.* data and 0.45 for AR(1) data; for the second model, it is the same for *i.i.d.* data and 0.4 for AR(1) series.

Conclusions concerning the detection of multiple changes are very good: the two greatest changes in $t = 15$ and $t = 30$ are detected over all cases, and the small one in $t = 40$ is still detected on all data series, except for the AR(1) data with the temporal model, where most likely the data variability together with the inclusion of a time dependence hides the small change. As for the location, the only conclusion that is slightly wrong concerns the last small change that is sometimes detected in $t = 41$ instead, but in the greatest majority of practical studies, this result will be considered precise enough to make correct description and inference on the phenomenon under study.

The estimated stepwise function for the intensity is a little smoothed at the step angles, but very close to the true one. Even on time dependent data, despite the variability of the estimates, a stepwise process is identifiable through the series, across all replicates, and the synthetic measure chosen for estimation are both performing well.

An output example is in Figure 4.12.

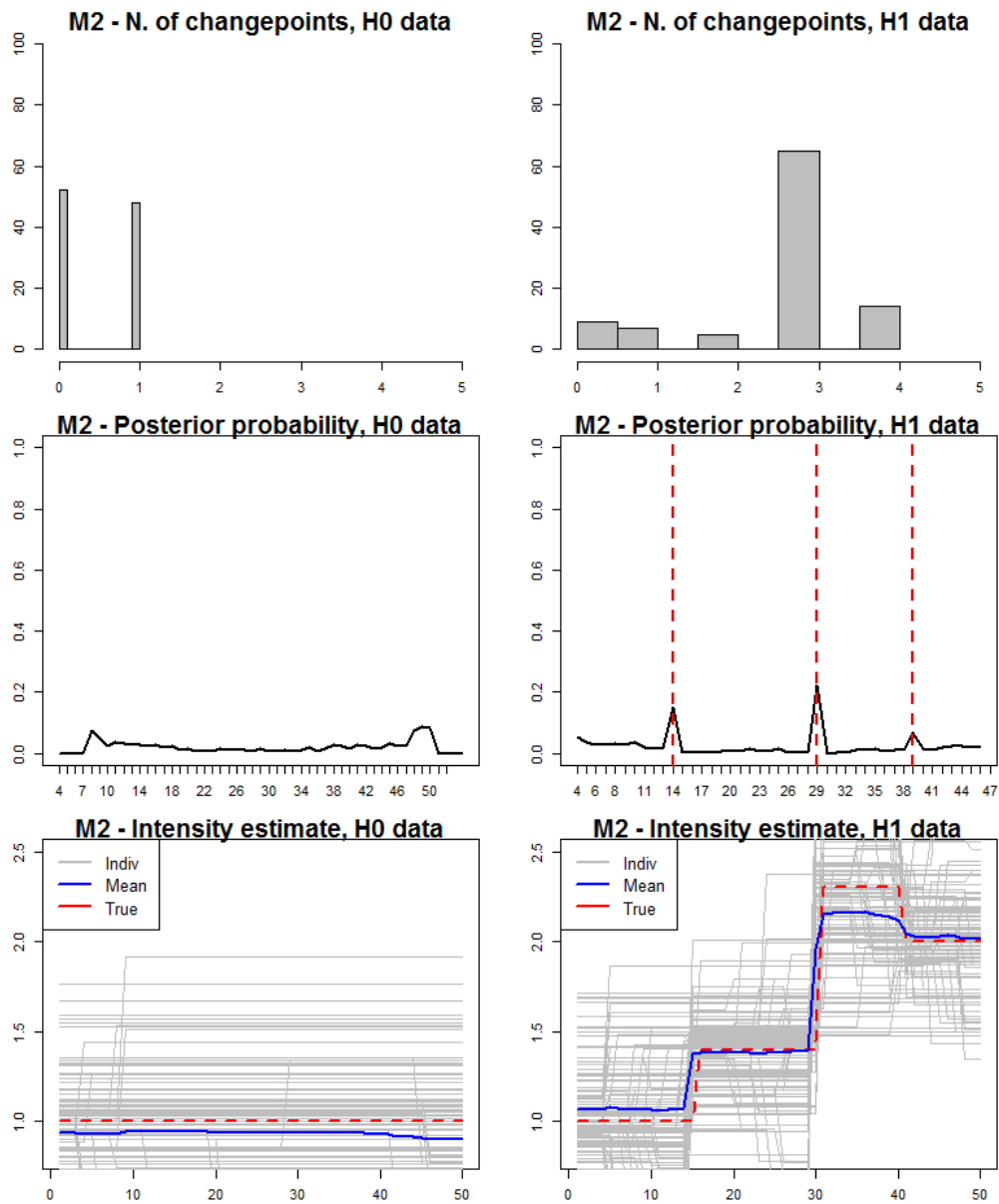


Figure 4.12: Multiple changepoint search on AR(1) data, with the temporal effect model and the PT method

Inhomogeneous models

As for the single search, the threshold is 0.95 for all data and the spatial model, and 0.9 for the spatio-temporal model.

As for the spatial model, on *i.i.d.* data the number of changepoints is underestimated, as the mode is 2; a third non significant peak corresponds to $t = 40$. In AR(1) H_0 data, correct overall conclusions are drawn; on H_1 data the mode for the number of changes is 3, and all three peaks in the posterior distribution correspond to the correct locations. As for the estimated images, the spatial trend is correct over all segments, the range is a little overestimated over the first two segments and then, as usual, the estimated distance between third and fourth segment is smaller than the true one.

When fitting the last model on *i.i.d.* data the power, is much lower, therefore the main decision is not to reject H_0 . The second option would be to have 2 changepoints, correctly identified in the posterior distribution by two peaks at 15 and 30, nevertheless they are not considered significant in the majority of cases. The estimate is therefore a single image, with the correct spatial trend and a mean value close to 1.6, a good average of the four time segments. Time dependent data show sensibly better results, as the model suits them better: a correct conclusion of no changepoints is drawn in H_0 data, and the mode of the number of changepoint is now correctly situated at 3 for H_1 data, where the three peaks in the posterior correspond to the true changes in 15, 30, 40. Therefore the conclusion is overall correct despite the strong time dependence, when using a high strict threshold and accounting for both spatial and temporal dependence within segments. Again, the estimated images produce a good imitation of the set values. An example figure is in Figure 4.13 and 4.14.

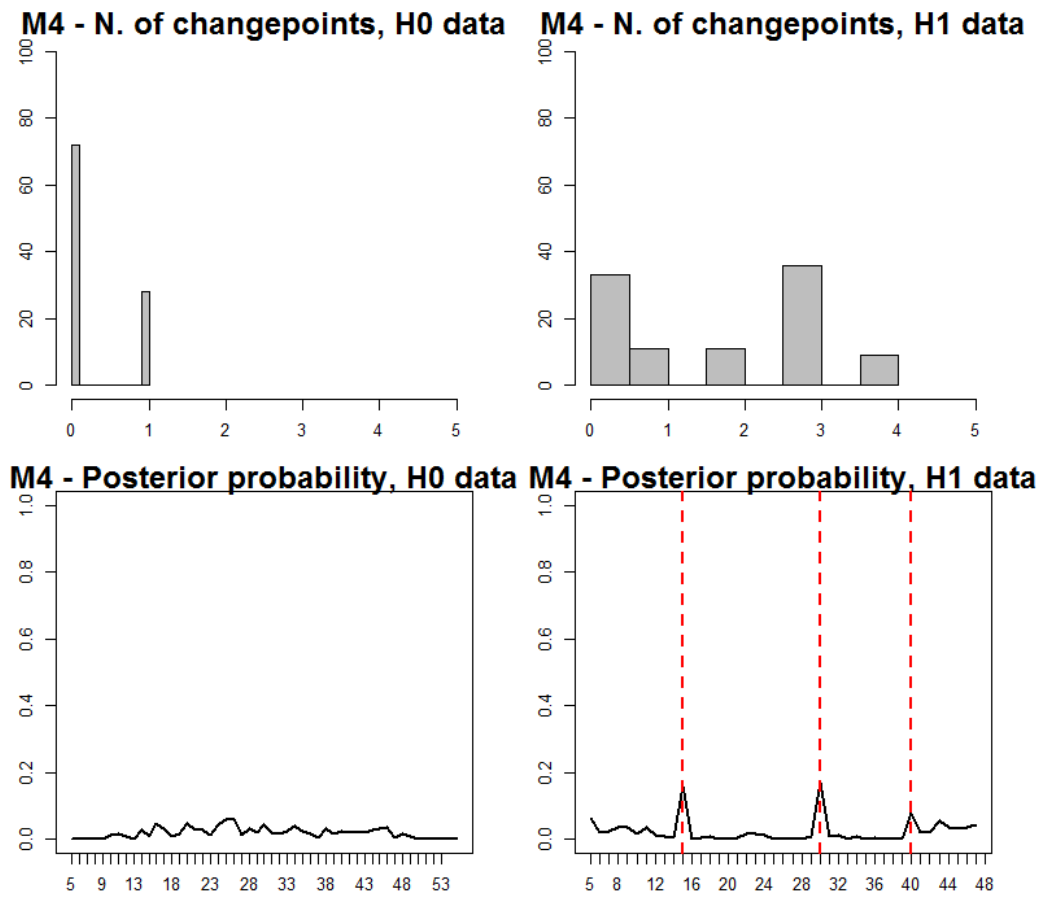


Figure 4.13: Multiple changepoint search on AR(1) data, with the spatio-temporal effect model and the PT method - Power level and location of the changepoint

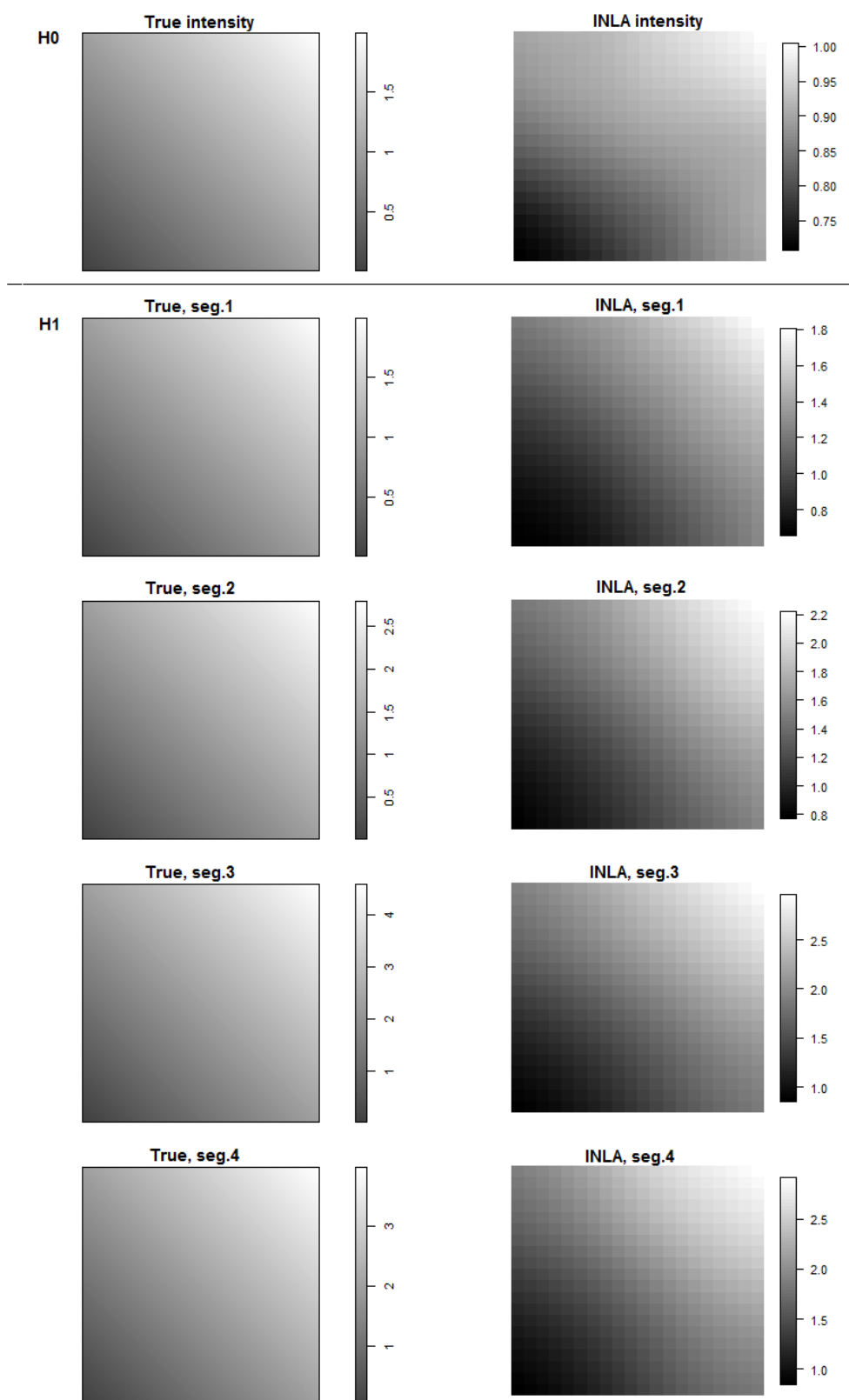


Figure 4.14: Multiple changepoint search on AR(1) data, with the spatio-temporal effect model and the PT method - Estimated intensities

4.2.6 Simultaneous multiple changepoint detection

Results have been presented so far that concern both a single and a multiple unknown changepoint search; therefore, they cover a wide range of changepoint questions. Additional information on our methods' performance would derive from a comparison of the iterative algorithms to a simultaneous detection approach.

In this study, we are particularly interested in understanding the ability of the methods to detect changepoints. Therefore, we focus on the results of the simultaneous search method on $H1$ data with multiple changes, and we present a summary of the results regarding the number and locations of detected changes. We do not focus on the estimated values, since, as we pointed out already, they depend on the INLA algorithm and not on the detection method, and are always very accurate given the changepoints.

As for the changepoint location, with this method it will be only approximately detected. Indeed, as introduced in Section 3.3.4, computations become relatively intense when all the possible segment likelihoods have to be computed, therefore we used Reduced Filtering Recursions (RFR). In particular, we drew a subset of the 50 time points by choosing equispaced points with an interpoint distance equal to 3. This generated a sample of 17 time points, namely 1, 4, 7, \dots . Changepoints will be looked for within the subset, therefore their location will not be exact; if the method performs well, though, it should be very close to some, or all, the set changepoints $\tau_1 = 15$, $\tau_2 = 30$, $\tau_3 = 40$.

A summary of the detected changes is in Table 4.6 for *i.i.d.* data and Table 4.7 for AR(1) data.

Table 4.6: Simultaneous search - detected changepoints on *iid* data

Model	No of changepoints	Location (no of repl.)
Fixed	1	28 (96/100)
Temporal	1	28 (63/100), 16 (33/100)
Spatial	0	—
Sp-temp	0	—

Table 4.7: Simultaneous search - detected changepoints on AR(1) data

Model	No of changepoints	Location (no of repl.)
Fixed	1	28 (58/100), 13 (30/100)
Temporal	1	28 (43/100), 13 (33/100), 40 (10/100)
Spatial	0	—
Sp-temp	0	—

As regards *i.i.d.* data, first of all, we immediately see that the method shows to be more conservative than the binary segmentation algorithms, as it detects at most one change over data that actually have three changes. Its performance is extremely similar to the BF method: one changepoint for the homogeneous models, no changepoints for the inhomogeneous ones. Indeed, we have pointed out the relationship with the Bayes Factor in Section 2.3.5. As for the detected location, results are very sensible. In the fixed model, the changepoint is identified as very close to $t = 30$, which is the location of the change with the largest magnitude (from $\lambda_2 = 1.4$ to $\lambda_3 = 2.3$). As soon as the temporal effect is included, a second possible location is highlighted (though only by a minority of replicates) that is the closest point to the true changepoint location $\tau_1 = 15$. The small changepoint in 40 is never detected. As happened more than once over the simulation study, the spatial effect and spatio-temporal effect model lead to the detection of no significant changepoints when combined with the simultaneous approach.

When time dependent data are analysed, there is no change in the conclusions as regards the inhomogeneous models: again, as happens with all the analyses carried out using the BF method, no changepoint is considered significant. Nevertheless, results improve when working with the homogeneous models. The number of detected changepoints is still 1, but the locations are more evenly distributed close to the three true changes. The majority of the locations are close to the change with the largest magnitude, *i.e.* $\tau_2 = 30$, but there is a consistent percentage of replicates where the second largest change, $\tau_1 = 15$, is (approximately) detected instead, and with the temporal effect some of the replicates show a changepoint correspondent to the third one, $\tau_3 = 40$. Further comments can be found in Section 4.4.

4.3 Changes in the spatial structure

We now briefly check the performance of the proposed methods with a more general inhomogeneous intensity function. As explained in Chapter 1, we still look for changepoints over time, not over space, but we now aim at detecting changes not only in the scale of the intensity function, but also in its spatial structure.

4.3.1 General framework

So far, all the simulated data series are generated by choosing a constant spatial structure for the intensity function and allowing for a change in scale, *i.e.* a changepoint corresponds to a greater or smaller number of points, which follow the same spatial distribution. We generate such data for two main reasons: first of all, the real dataset that motivated the work presents a spatial structure that is roughly constant over time, therefore changes mainly concern the number of points. Secondly, this scenario represents a step towards the analysis of inhomogeneous processes, without being too general, and we consider it a good starting point for evaluating the performance of the proposed methods.

Nevertheless, we would ideally like a methodology that is able to detect any type of change over time in the intensity function of a inhomogeneous process. Hence, we are now interested in relaxing the spatial assumption and allowing the intensity function to change in space as well as in time, as happens in many real situations. This might lead to two more different types of change: a change in structure, when the overall number of points remains approximately the same but the spatial distribution changes, and a change in both scale and structure.

We believe our methods to hold over this general situation as well: when looking for a change with the proposed algorithms, we never specify that we are looking for a different number of points; we try and split the data at all different time points and look for the single equation (no changepoint) or the product of $M + 1$ equations (M changepoints) that describe the dataset best, irrespective of the type of change that occurred. Therefore, if we use a

model that includes a spatial effect, we expect our methodology to be able to identify changepoints in both space and time.

4.3.2 Design

We do not replicate the whole complex simulation study we carried out and reported in this Chapter so far. We only want to test the performance of our methods in detecting changes in the spatial structure as well as scale on a restricted scenario. Indeed, for studying this situation we only work on inhomogeneous *i.i.d.* data generated under the alternative hypothesis of one changepoint. The spatially homogeneous case is of no interest here, and if the method works for a single changepoint search it is straightforward to extend it to multiple changes with the tools we provide. We use the same values for $T = 50$, $S = 400$ and the same window W , and the changepoint is again set in the centre of the time series, at $t = 24$. We cover both the case of only spatial change and the case of spatial plus scale change. For data presenting a change in both scale and spatial structure, we use the large magnitude change, therefore we have 100 data series with $\Lambda(1) = 1$ for segment $y_{1:24}$ and $\Lambda(2) = 2$ for segment $y_{25:50}$. In conclusion, we have

1. Data with only a spatial change

- 100 replicates of data series with $T = 50$ time points
- 1 changepoint in $t = 24$
- same overall intensity strength across segments:

$$\Lambda(1) = \sum_s \lambda(1, s) = \Lambda(2) = \sum_s \lambda(2, s) = 1$$
- different spatial structure
 - segment 1: higher values for top-right cells, lower values for bottom-left cells
 - segment 2: higher values for bottom-left cells, lower values for top-right cells

2. Data with both spatial and scale change

- 100 replicates of data series with $T = 50$ time points

- 1 changepoint in $t = 24$
- different overall intensity strength across segments:
 - segment 1: $\Lambda(1) = \sum_s \lambda(1, s) = 1$
 - segment 2: $\Lambda(2) = \sum_s \lambda(2, s) = 2$
- different spatial structure
 - segment 1: higher values for top-right cells, lower values for bottom-left cells
 - segment 2: higher values for bottom-left cells, lower values for top-right cells

An example of generated data can be seen in Figure 4.15.

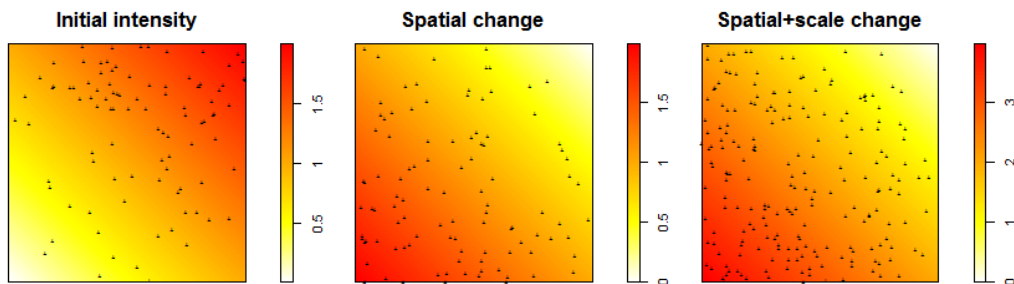


Figure 4.15: Examples of generated data with a change in the spatial structure and in both spatial structure and scale

4.3.3 Results

Results for this extended simulation study are very good and show that the proposed methods are able to detect all types of change, making them even more valuable. A summary of the performance of the methods in terms of power is displayed in Table 4.8.

Table 4.8: Results summary for data with a change in spatial structure

		Homogeneous data				Inhomogeneous data			
		Model 1		Model 2		Model 3		Model 4	
		BF	PT	BF	PT	BF	PT	BF	PT
Spatial	Power	0.38	0.44	0.42	0.26	1.00	1.00	1.00	1.00
	Location	–	–	–	–	24	24	24	24
	Estimate	0.95	0.95	0.97	0.97	1.05 1.00	1.03 1.01	1.06 1.02	1.04 1.00
Spatial and scale	Power	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
	Location	24	24	24	24	24	24	24	24
	Estimate	1.00 1.95	1.00 1.95	0.99 1.96	0.99 1.97	1.06 2.00	1.01 2.00	1.03 2.01	1.02 2.00

Results for the first two models, with fixed and temporal effect, are very similar for the BF and PT method. An example of the simulation output is in Figure 4.16 concerning both data with only a change in spatial structure (labelled as $H1sp$ data) and data with change in scale and structure (labelled as $H1ss$) for the fixed model with the PT method; for more (similar) results, see Appendix A.

As regards data with only a change in the spatial structure, as expected the first two models do not perform very well in detecting the change, since the spatial effect is not included and they ignore the inhomogeneity in the intensity function, *i.e.* they assume that the intensity function is constant over space. It is nevertheless interesting to point out that, in the minority of cases where the changepoint is detected, it is in the correct location $t = 24$. For what concerns data with a change in both spatial structure and scale, the change is correctly detected in all replicates even in the homogeneous models, as a change in the number of points is recognized as changepoint over all models.

As soon as spatial inhomogeneity and dependence are included (Models 3 and 4), results show that a changepoint is correctly detected in all replicates (Figure 4.17 for a representative graph, and the Appendix for more graphs). The power level is 1, and the location is correctly estimated in all datasets.

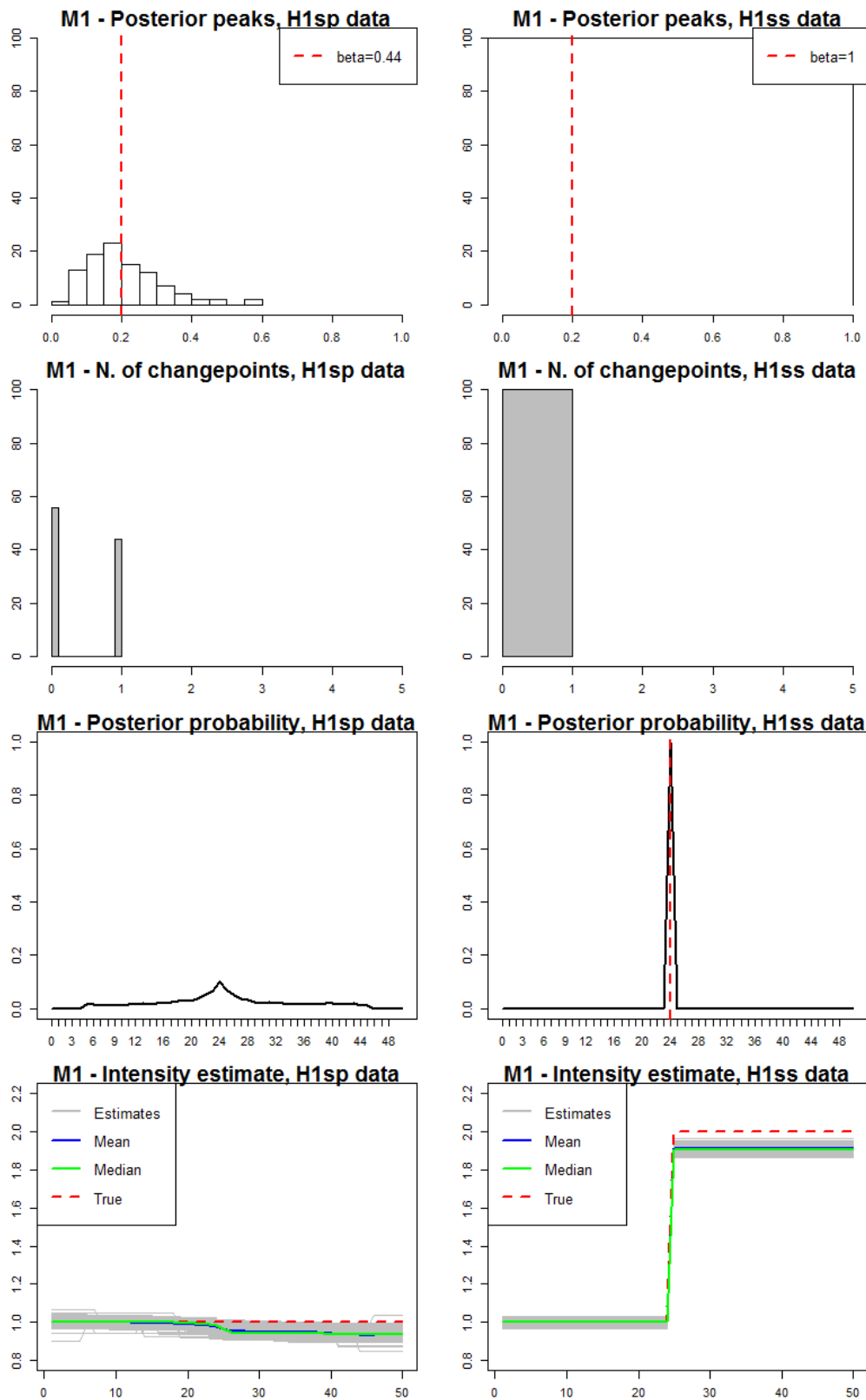


Figure 4.16: Results for a changepoint search on data with a change in the spatial structure, with the fixed effect model and the PT method

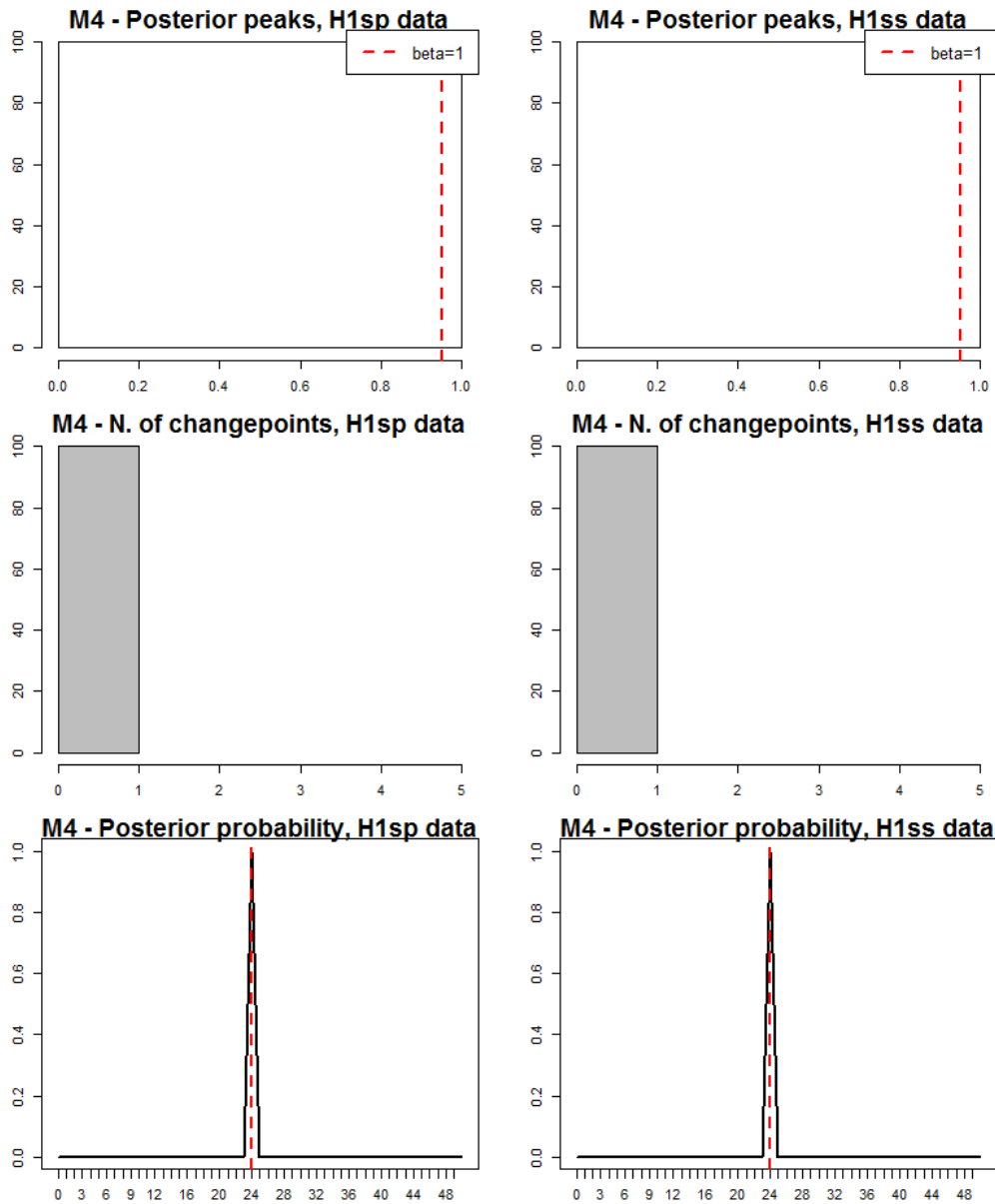


Figure 4.17: Change point search on data with a change in the spatial structure, with the spatio-temporal model and the PT method - Power level and location of the change point

As for the intensity estimates (*e.g.* Figure 4.18), since only a spatial change takes place, the values for $\Lambda(1)$ and $\Lambda(2)$ are extremely similar.

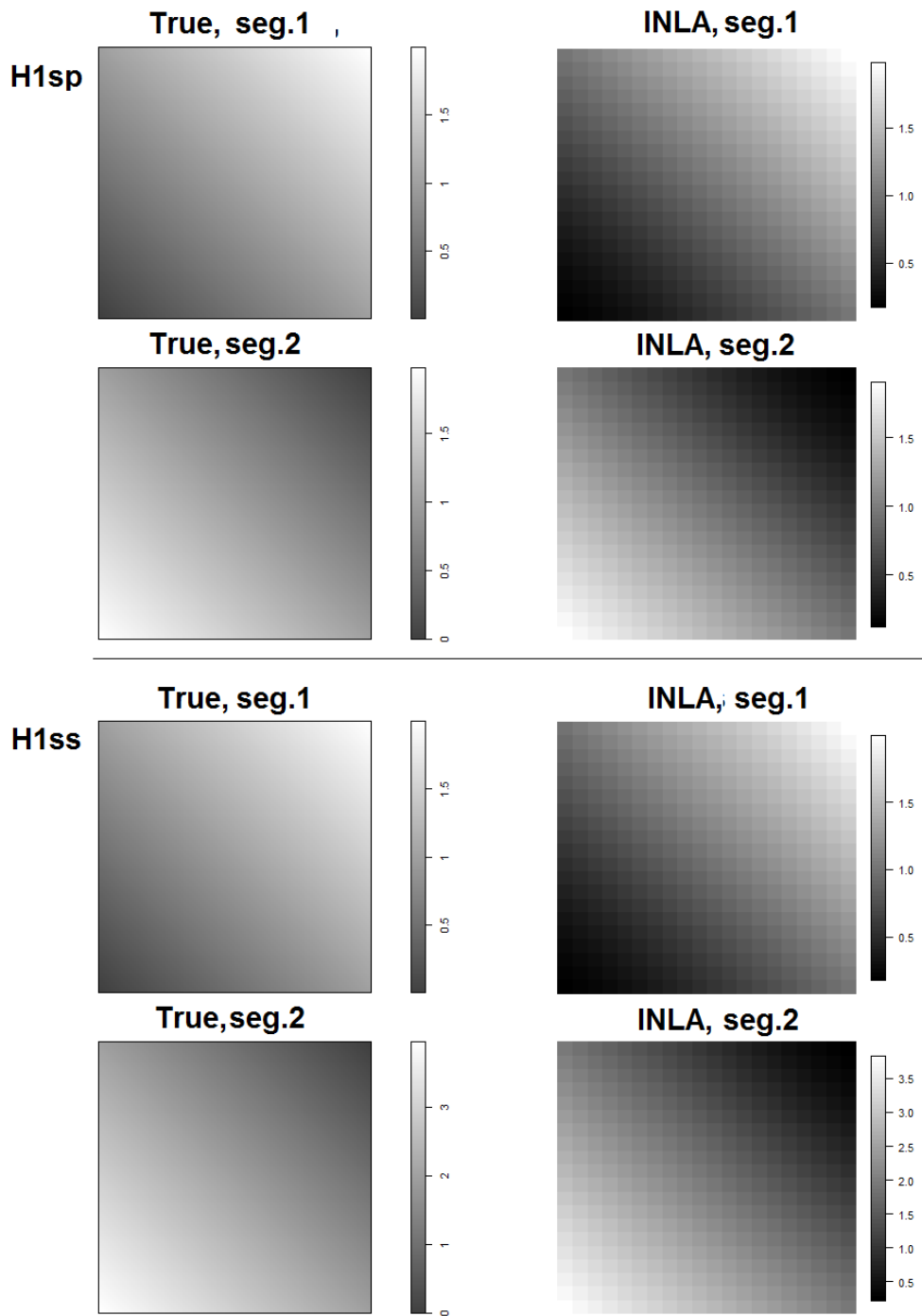


Figure 4.18: Changepoint search on data with a change in the spatial structure, with the spatio-temporal model and the PT method - Estimated intensities

We can appreciate a slight decrease in the estimated values from segment 1 to segment 2; this happens in all results as the original dataset is the same (100 replicates of a inhomogeneous process under H_1) and must be imputed to the uncertainty linked to the single process realizations. However, all estimates are very close to 1, the initial set value. Over all cases the power is 1, the location is in 24 and the estimated values are close around 1 for the first time segment and around 2 for the second segment. In particular, the estimate for the second segment is very precise for the two inhomogeneous models, while it is slightly underestimated in the first two models, due to the lack of spatial effects.

There are no substantial differences in the performance of the BF and PT method; the BF method performs even better than in the only-scale change situation (previous simulation study), as it does not suffer from too much conservatism and gives sensibly good results over all models, therefore generalising the type of change improves the BF method results.

4.4 Discussion

Our simulation study consisted in fitting four different model scenarios over both *i.i.d.* and time dependent data, generated with single or multiple changepoints and with a homogeneous or inhomogeneous intensity function; 100 replicates were produced for each case, over a square observation window. Once the models were fitted, Bayes Factor, SIC and Posterior Threshold methods were applied to detect a single changepoint in the process intensity; as for multiple changes, both some iterative techniques and a simultaneous search have been carried out. The first model, including only a fixed effect, was more suitable for homogeneous *i.i.d.* series; the temporal effect model for time dependent homogeneous data; the spatial effect model for *i.i.d.* inhomogeneous data; finally, the spatio-temporal model fits the AR(1) inhomogeneous time series best.

4.4.1 Methodological discussion

Both the BF and the PT method results coincide with likelihood-based results if we choose non informative priors in all cases; the likelihood for each potential changepoint position is then rescaled so that the final distribution integrates to one and is a proper posterior distribution. However, they show two advantages with respect to likelihood-based methods: first of all, they can be extended to any prior setting and exploit external knowledge; secondly, with this approach (approximate) results can be obtained even for complex models including spatial and temporal dependence, which is not currently the case with likelihood-based approaches.

The difference between the two methods is that the BF focuses on comparing values under both hypotheses and has an absolute threshold, while the PT looks at the posterior distribution of the potential changepoint positions and has a tunable threshold.

The BF method is essentially the Bayesian likelihood ratio test: the values under H_0 and H_1 are compared, in order to look for substantial evidence in favour of the alternative model and detect the presence of changepoints. Given that small positive values for the BF test are considered non substantial, and given some computational issues linked to taking the exponent of log-likelihood values, a more conservative version of the BF has been chosen, and the value 0 considered an absolute threshold for rejecting (positive values) or non rejecting (negative values) H_0 . This conservative version has also the advantage of easily reducing to the case of known potential changepoint positions.

The PT method does not require the computation of the likelihood value under H_0 : once the posterior distribution is produced, peaks raising above a certain threshold are considered significant changepoints. This lack of comparison between null and alternative model can be unacceptable under a frequentist approach, but is often used in Bayesian statistics. However, doubts can be raised about the arbitrariness of the method. When available, prior knowledge on the presence, possible number or locations of changepoints can be incorporated in the threshold choice. As an alternative option, in order to reduce the arbitrariness in choosing the threshold, this has been fixed as the

lowest possible value allowing the probability of committing the type I error to be kept below the usual limits (0.01, 0.05 and 0.1). This technique returns a different threshold according to the model, which is a sensible choice considering that models including dependence allow for higher data variability, and this must be kept in mind when fitting models to real data.

As a note on the PT method, the reader might notice that some of the posterior distribution peaks do not raise above the threshold. This is due to normalisation of the posterior curve: the threshold value is applied to every single data segment throughout the algorithm implementation, as a proper posterior distribution is obtained for every single segment. Once the change-points are detected, the final posterior distribution is obtained by averaging over the values for every segment pointwise, and rescaling in order to integrate to one. This might flatten some peaks, that do not appear to raise above the threshold in the final posterior, but are significant when the segments are analysed separately. This is how a binary segmentation algorithm works, and is one of the reasons why these iterative approaches are often able to detect more changes than simultaneous techniques.

The BF method proves to perform very well in simpler models, up to the spatial one for the single changepoint detection and up to the temporal one for the multiple changepoint detection. Results are in general very precise and neat, with significance levels very close to zero and power levels very close to one. When moving on to more complex models, though, the method proves unable to detect changepoints, despite the high peaks shown in the posterior distribution; again results are very neat as the power level abruptly decreases from 1 to 0. It could be improved by substituting the segment likelihood with more complex recursive methods for computing the overall likelihood, as shown in Fearnhead (2006) and Wyse et al. (2011). The PT method is more flexible, therefore its results, given the threshold choice, produce more grey zones but also more sensible conclusions, and hold over all models. Different choices for the threshold can be made due to *ad hoc* necessities/knowledge, and our figures show the significance and power levels corresponding to any threshold choice between 0 and 1. A summary of all results for comparison purposes can be found in Table 4.2, 4.3, 4.4 and 4.5. In the extension of our simulation study to changes in the intensity spatial

structure (Section 4.3), though, both methods have a really good performance (Table 4.8), therefore either can be used when a spatial change is hypothesised.

4.4.2 Time dependent data

It is interesting to observe the difference between data generated as independent replicates within time segments and data showing a very strong time dependence. The values taken by the latter are much less under control once the series develops further away from the initial set values, therefore the time dependent data variability is much higher and estimated values are sometimes different from the initial ones. Moreover, changepoints other than the fixed ones can be detected in the series. Indeed, in many cases they are detected in H_0 data and the locations are evenly distributed along the series: on simulated data it is then easy to conclude that there is no specific changepoint. Nevertheless, if there is no prior knowledge on the number or nature of changepoints, and if only a single data series is available, this will lead to the detection of a changepoint along the series. Note that this is not necessarily a wrong conclusion, as a shift in the intensity value actually takes place, but this changepoint is driven by the time dependence itself and not by some external factor, therefore, depending on the analysis context, the statistician must be careful in interpreting the phenomenon under study. When more than one data series is available, though, little doubt remains as the changepoints due to time dependence will change from one replicate to the other, while the other ones will keep the same position. A positive result given by the PT method is that when changepoints fixed *a priori* are present, they are still detected above the other ones in most data series. This means that changes due to external conditions are more recognisable than changes due to the series variability, and if it is known that such changepoints are present in a series, then our method will be able to identify them.

As for data generated under the alternative hypothesis, sometimes the posterior distribution shows a peak in the correct location which is considered non significant, but is still much higher than all other values. In such cases, if the analysis focuses on locating a changepoint when it is expected or known that

one is present in the series, despite the time dependence conclusions will still be correct. In addition, an informative prior over the expected changepoint will probably raise the peak above the threshold.

4.4.3 Multiple detection algorithms

For the multiple changepoint detection, for performance comparison purposes, firstly a binary segmentation algorithm was implemented, then two simultaneous changepoint searches were carried out.

For what concerns the iterative multiple changepoint search, we fix the maximum number of detectable changepoints to 4 for computational reasons, but the method works for any number of changepoints. It is advisable to fix a minimum segment length, though, as the INLA performance becomes unreliable if segments have very few data, besides in most studies it is not sensible to detect changepoints too close to each other. As a further note, choosing a binary segmentation algorithm means that at each step we carry out a single changepoint search. This way, the BF method performance suffers from the same problems as the single search: no detection of changepoints in models with spatial dependence, when only a change in scale is considered. Indeed, Wyse et al. state that if testing for more than one changepoint then binary segmentation procedures can perform poorly.

As regards the simultaneous approaches, two have been implemented but one of them has not been mentioned so far as it brought no methodological novelty and was simply meant to check the performance of the PT method further; indeed, we simply used the PT method to detect more than one changepoint (*i.e.* more than one significant peak in the posterior distribution) in one single step. This simultaneous search method performs poorly: if one change magnitude is higher than the others, the posterior mass will concentrate at that position, and other peaks will not be detected. In the simplest model one changepoint was detected in all replicates, and its position located at an intermediate time point between 15 and 30, the two greater changes; for the second model, the mode for the number of detected changes is 1, and the highest peak is located in 30, though a few replicates also found a second changepoint in 15; in the spatial model only the changepoint in 30

was detected; even if the final model posterior distributions shows two peaks, these have not been considered significant so no changepoints are detected. The binary segmentation algorithm allows a deeper search which includes minor but still interesting changes. This first simultaneous search method has therefore been discarded.

The more complex simultaneous changepoint detection algorithm we implemented exploits recursive equations following the idea of Wyse et al. (2011). The authors argue that for data with temporal dependence within segments, the approach performs better than a binary segmentation algorithm, though they do not bring proof of that. As regards our spatio-temporal data series, the simultaneous approach performs poorly with respect to iterative procedures, since it only detects one change when combined with the homogeneous models and no changes with the inhomogeneous ones. The (approximate) detected location is close to the true changes, with a preference for the one with the largest magnitude. The best performing model in finding the right locations is the temporal one, and is the type of model Wyse et al. work on: on *i.i.d.* data, 30 and 15 are both identified, and on AR(1) data even the small change in 40 is found in a few replicates. The concentration of the resulting values around a few points over the replicates is a hint for multiple changes. Possibly, better results (namely more than one significant change per replicate) can be found when imposing informative priors.

As a final note on the multiple changepoint detection techniques, we would like to highlight that these methods work similarly to the Information Criteria used with likelihood-based approaches, *i.e.* they incorporate a penalty for the number of parameters so that models with more changepoints are not necessarily chosen. Indeed, as an example, in the binary segmentation algorithm up to 4 changepoints were detectable, but a fourth one was hardly ever found; moreover, in many scenarios less than three changes (*i.e.* two, or even zero) were detected, meaning that a model allowing for more data segments does not always describe data better. The same happens with the simultaneous approach, that proves to be even too conservative on our data.

4.4.4 INLA performance

The use of the INLA algorithm means all results are approximate, but since the latent field is Gaussian the approximation is in general very accurate; all estimated values computed with INLA are very precise and accurate, given the detected changepoints. In all scenarios and cases the spatial structure of the intensity function and its smoothness have been perfectly captured; as for the estimated value (homogeneous process) or range of values (inhomogeneous process) for the intensity, this is extremely close to the true one in most cases, with departures from the initial values due to the lack of detection of a changepoints, or to the time dependence within a segment. We are therefore very satisfied with the INLA performance, for both computational time and produced results. A comparison to non parametric estimates has been run for all scenarios, and in all inhomogeneous processes INLA performs sensibly better as for reproducing the smooth spatial trend: the non parametric estimates are generally reasonably good as far as the range of values is concerned, but much more noisy as for the spatial structure. In addition, it is to keep in mind that when producing a non parametric estimate only a single value for each cell is available, while INLA returns the whole posterior probability and we may choose any synthesis for the parameters (in our work, mean and median). An example of the difference between INLA and non parametric estimates is in Figure 4.19.

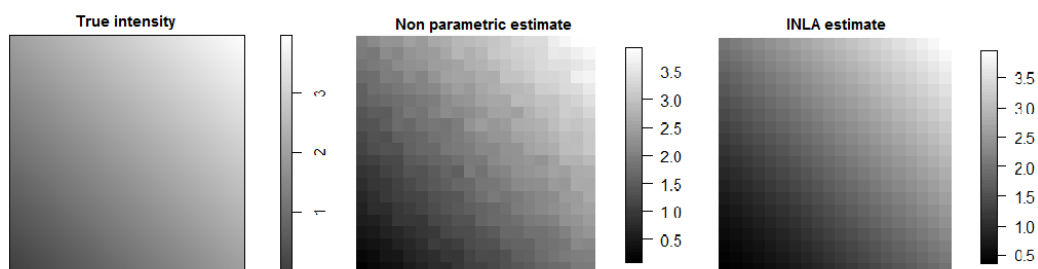


Figure 4.19: Comparison between a non parametric and a INLA estimate for the segment intensity function

One of the issues that is commonly raised when working with INLA concerns the resolution of the grid and the computational speed. The two aspects

are closely connected, as in general a finer grid will lead to more accurate but slower results. One of the INLA advantages, though, is that it assumes a sparse covariance matrix; therefore, computational issues that are normally linked to a dense matrix are not a problem here. This means that in many situations a grid can be as fine as the statistician wishes, with a feasible increase in computational effort. If computations are not prohibitive, it is sufficient to choose a grid resolution that allows response data (counts) to be 'sufficiently sparse', meaning that a finer resolution will not affect the conclusions substantially. In our work, we tried different grid sizes, and a grid of 20x20 proved to be a good trade off between accuracy and time.

If an application needs an extremely fine grid and this leads to a prohibitive computational time, there are other tools that allow the algorithm's fastness to be increased while keeping the information about the exact location of the points. This is commonly referred to as the Stochastic Partial Differential Equation (SPDE) approach ((Lindgren et al., 2011)).

A further issue concerns the validity of the Gaussian assumption. Questions can be raised about how accurate/wrong estimates would be with a non-Gaussian field. This is currently under study by the INLA team, that would like to extend the range of models that can be fitted with INLA. At the moment, though, assuming a Gaussian Field is the only way to obtain a fast solution for data with dependence. The advantage is that a Gaussian distribution is a reasonable approximation in many applications.

4.4.5 Choice of the priors

In our work, prior distributions need to be set on many different parameters. First of all, they can concern both number of changepoints and location conditional on the number. This depends on prior knowledge on the occurrence of changes in a specific dataset. Moreover, prior distributions concern the model hyperparameters, in particular for the temporal effect ϕ and the spatial effect ψ . Since our present goal is not to test the sensitivity of results to changes in priors, we keep the default setting given by the R-INLA package: for both effects, the only hyperparameter is the precision ν which follows, as usual, a Gamma distribution $\nu \sim \text{Gamma}(\alpha, \beta)$. For both

ϕ and ψ , the default values are set in order to give a non informative prior: $\nu \sim \text{Gamma}(1, 5e^{-5})$. This standard setting gives a good performance for both the temporal and the spatial effect: in particular, the smoothness of the spatial trend is well reproduced over time. We tried different options for the hyperparameters; none of them were informative as this was not our point, and we found no substantial change in the results, apart from the occurrence of some spatial noise when the smoothness was not enough.

The choice of the smoothness is not always trivial: if a spatial random effect is too smooth, it becomes flat and changes in the spatial structure can be missed, while the opposite might lead to an overdetection of the changes. Different settings should be tried when working with real data, that should also incorporate knowledge on the phenomenon under study; thanks to the computational efficiency of INLA, it is feasible to fit a model more than once in a reasonable time, and this allows a proper sensitivity analysis to be carried out for every specific situation.

It needs to be pointed out that the spatial smoothness also depends on the grid resolution, and if this changes, in general the smoothness will change as well. A very recent option has been added to the `inla` function, that rescales the priors according to a change in the grid size, in order to keep a constant spatial structure. For further information on this topic, we refer to Sørbye (2013).

Chapter 5

Radioactive Particle Data Analysis

After all the methodology is developed and a simulation study carried out to assess the validity of the proposed methods, it is time to go back to the original research questions.

In this Chapter, we present the real problem that is our motivating example for the need of a changepoint analysis on the behaviour of the intensity function and of a detection technique for point processes. Questions concern both a multiple known changepoint and a multiple unknown changepoint detection problem, as presented in Chapter 1.

The Chapter starts with a general introduction to the environmental problem and an historical review of the decommissioning process. Afterwards, a standard preliminary analysis on the point pattern is carried out, in order to detect clustering or repulsing behaviour and choose the most suitable class of models. Then, the changepoint analysis results are shown; the Section is quite brief as all models and methods are presented and discussed in Chapter 3, and their practical implementation and the assessment of their performance is in Chapter 4. Sections 5.5 and 5.6 present some extensions of our work that might be of interest on real data application, such as the introduction of covariates and of informative prior distributions on number and location of the changepoints. Finally, some concluding remarks are presented.

Please note that in this Chapter the time point (*i.e.* the year) labelled as the changepoint is the first year of a new segment, as experience told this was more intuitive when presenting a real application. For instance, if we mark a change in 2003 this means the previous segment ends in 2002 and 2003 corresponds to the beginning of a new segment.

5.1 Introduction to particle data

The data we are working with are a collection of radioactive particles that have been retrieved from Sandside beach, around Dounreay site, North of Scotland. They present a hazard to the environment and individuals who come in contact with them. From the early 1980s a retrieval process started but is not finished yet. An analysis of the behaviour of particles over time will help our understanding of the environmental processes whereby particles arrive on the beach, and the longevity of the problem.

Our temporal data series is made of yearly point pattern realizations that show the particles' locations over the years on a single beach; additional information about the retrieval location and time and radioactivity level also labels each particle once it has been collected and examined.

Birth of Dounreay nuclear reactor

Dounreay is on the north coast of Caithness, in the Highland area of Scotland, and was originally the site of a castle. Since the 1950s, it has been the site of several nuclear research establishments, including a prototype fast breeder reactor and a test for submarine reactors (www.dounreay.com). The site was used by the United Kingdom Atomic Energy Authority (UKAEA, Dounreay Nuclear Power Development Establishment) and the Ministry of Defence (Vulcan Naval Reactor Test Establishment), and is well known for its five nuclear reactors, three owned and operated by the UKAEA and two by the Ministry of Defence. Dounreay was chosen as the reactor location because of its isolation for safety reasons, in case of an explosion.

In 1994, the last reactor ceased operation. Dounreay Site Restoration Ltd (DSRL) is the Site Licence Company (SLC) that manages and operates on

Dounreay site in order to restore its previous conditions.

A map of the former nuclear area can be seen in Figure 5.1.

On April 1st 2005, the Nuclear Decommissioning Authority (NDA) became the owner of the site, with the UKAEA remaining as operator. Decommissioning of Dounreay is planned to bring the site to an interim care and surveillance state by 2036, and as a brownfield site by 2336, at a total cost of £2.9 billions (Dounreay Particle Advisory Group, 2006).



Figure 5.1: Dounreay nuclear area (UK)

Source: www.dounreay.com

Decommissioning and particle clean up

Approximately 180 fuel processing facilities were built at the site. Some are very straightforward to dismantle, while others require great care because of chemical or radiological hazards. About 50 facilities have a presence of radioactive materials, and special controls are needed to contain radiation. Areas of ground have been polluted by radioactive materials and chemicals, and need to be remediated. Apart from decommissioning reactors, reprocessing plant, and associated facilities, one of the main environmental issues to be dealt with are radioactive particles on the seabed near the plant, estimated (in terms of the potential number retrieved) about several hundreds

of thousands in number (Dounreay Particle Advisory Group, 2006).

Radioactive particles are fragments of irradiated nuclear fuel discharged into the sea during the 1960s and 1970s by a nuclear discharge outlet, located approximately 600 metres offshore on the seabed: through this undersea pipe, old fuel rod fragments were released into the sea. The belief is that the significant ($> 10^6$ bequerels of Caesium-137) particles are physically larger, that they may be buried on the seabed and then brought to the surface by storms; these larger particles might then physically fragment to give smaller particles, less radioactive and more likely to be moved by tides and waves, hence there is a winnowing. The further from the outlet point, the more likely small and less radioactive particles are believed to be.

The firstly investigated areas, from the early 1980s, are the foreshore area directly in front of the site, and the closest beach on the West, Sandside beach, as tides and currents are likely to bring particles there: the very first particle was retrieved in Sandside beach in 1984 (Tyler et al., 2010). The particle population density is at its highest at Dounreay foreshore and Sandside beach. Other surrounding areas have been monitored, but the number of particles recovered was extremely small (1 or 2). The Sandside beach has been closed to public access since 1983 due to this danger. In 1999, vehicular based beach monitoring was introduced (Tyler et al., 2010); prior to this, the beach was monitored using hand held devices. The introduction of this monitoring provided a time series of data which helped understanding the distribution and movement of the particles. From 2008, a clean-up project using Geiger counter-fitted robot submarines searches out and retrieves each particle offshore individually, a process that will take years.

Presently, not all offshore areas have been surveyed yet. The most hazardous particles are located within an area shaped as a 'plume'; the overall clean-up is targeted at an area of seabed measuring 60 hectares with depth of water up to 30 metres. By the end of 2012, all 60 hectares should have been covered by the underwater detection and retrieval system, with some areas repeated. The total coverage is 90 hectares. The last datasets used for the analysis were updated in February 2013.

We focus on the Sandside beach area. Here are a few highlights in the cleaning process history.

- 1984: starting of recovery of particles on Sandside beach with hand-held Geiger counters
- 1999: starting of vehicular-based beach monitoring
- 2002, November: major change in equipment for Sandside beach
- 2007, January: change in equipment for Sandside beach

The changes in equipment appear to be followed by an increase in the number of retrievals, with a higher number of detected particles with lower activities. The observed Sandside area is (approximately) 526,400 m². Particles recovered from the seabed are returned to Dounreay and analysed, thus no particle remains in the seabed or beach after being detected; particles are extremely small, typically less than 2 mm in size (Figure 5.2 shows a particularly large one).



Figure 5.2: One of the largest retrieved particles

Source: www.dounreay.com

The dataset consisting of all up to date particle retrievals is publicly available, together with notes and reports, at www.dounreay.com. For each particle, the Sandside beach dataset reports

- ID number
- Date of finding
- Easting coordinate (in metres)
- Northing coordinate (in metres)
- Depth in the sediment in centimetres (this could be considered as a third dimension in the point pattern)

- The Caesium-137 concentration (measured in bequerels, which is a continuous mark)
- Radioactivity category (depending on Cs-137 activity): Minor/ Relevant/ Significant (categorical mark)
- Further comments

Coordinates are provided in UK national grid. We have also converted them in decimal degrees (Latitude-Longitude) to plot them on GIS software (www.arcgis.com).

The underlying intensity function behaviour of the Sandside beach dataset is of interest, with particular focus on potential changes in its scale and/or structure. The point patterns are given by the particles' locations over the years (we have used the annual cumulative cover).

The dataset presents some difficulties when a changepoint analysis is carried out: the time series is not long ($T = 15$) and some annual patterns present very few points, since in certain years the monitoring was limited. Still, the questions presented in Chapter 1 are of interest, and the methods' performance has already been tested over simulated data, therefore we are ready to try to give them an answer.

5.2 Exploratory analysis

All analyses in this Section are run using the R package `spatstat` (Baddeley and Turner, 2005).

The observation window has been plotted around the particle data, accounting for the retrieval criteria: the Sandside beach area covers beach and low water area (up to a depth of 300 mm).

The polygonal boundary has then been used in R to create the point pattern and the (irregularly shaped) observation window. Both the selected area and the point pattern plot in R can be see in Figure 5.3.

As an exploratory tool, we have produced a kernel intensity estimate of the area. The single estimated value for λ does not look very representative, as

we can see from the kernel plot in Figure 5.4 that the intensity is spatially variable, *i.e.* inhomogeneous.

A plot of the data series is shown in Figure 5.5: every single datum is a point pattern and they range from 1999 to 2013. Previous years have been discarded as they contain an insufficient number of particles (< 5).

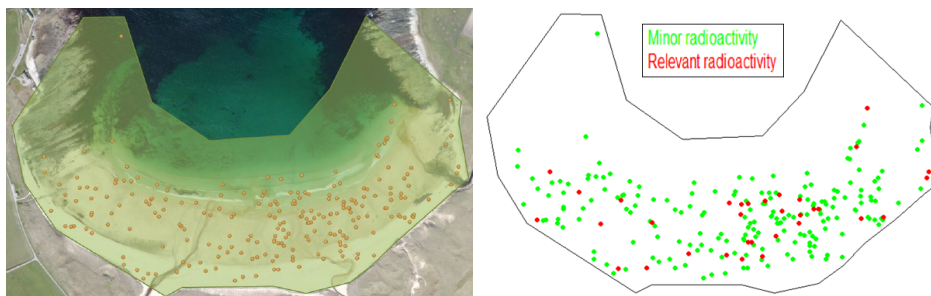


Figure 5.3: Selected observation window, Sandside beach
Source: www.dounreay.com

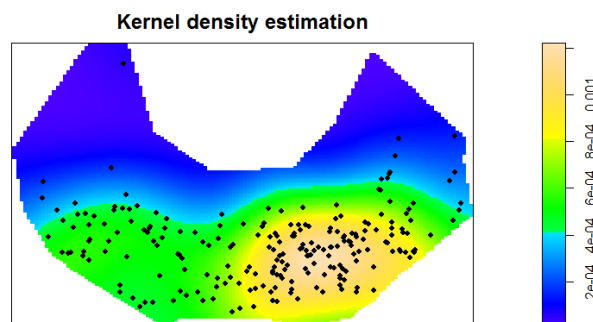


Figure 5.4: Kernel density estimate, Sandside beach

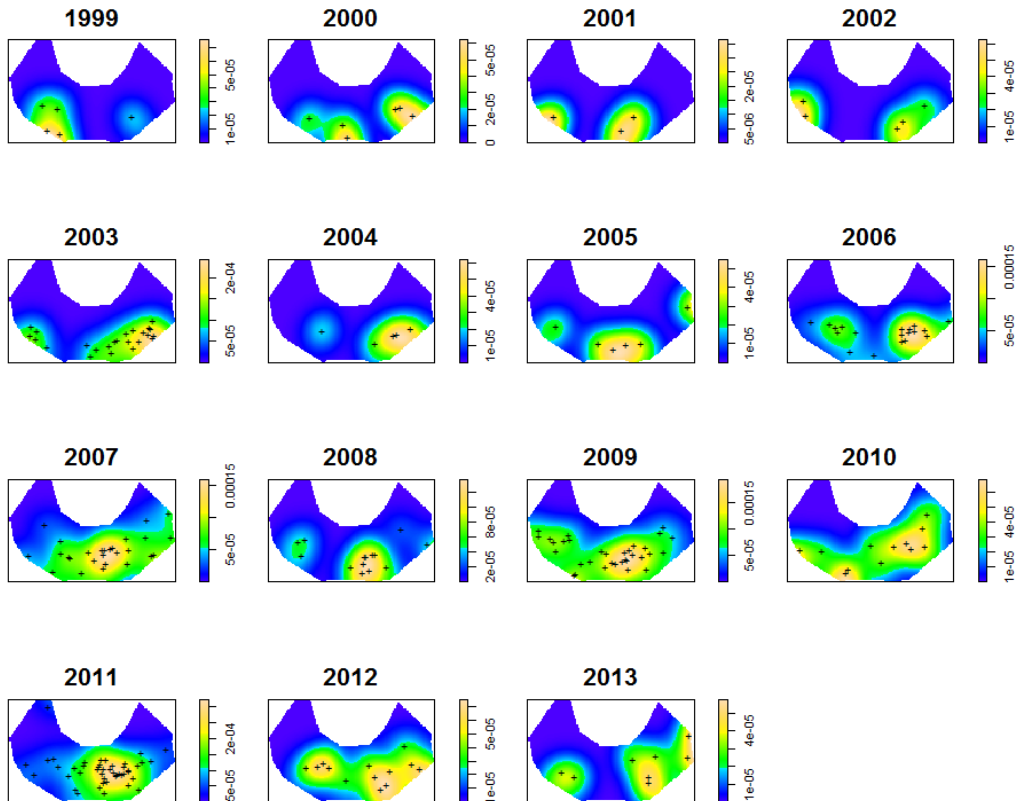


Figure 5.5: Sandside beach data, yearly patterns

The following usual step in the analysis of a point pattern consists in checking complete spatial randomness (CSR), regularity or clustering. The results give hints about what kind of process we are facing and what kind of models can, or can not, fit our data. The most common tests for CSR are MCMC based and look for repulsive or clustering behaviour by measuring the distance between points (see Section 2.1.2). The credibility intervals are called *envelopes* and are created by repeated MCMC simulations from a homogeneous Poisson model with the same intensity value as the dataset. There are three different tests, one based on the empty-space distance (*i.e.* the distance between an arbitrary location in the region and the nearest point of the pattern), one on the pairwise distance (*i.e.* the distance between all possible pairs of points of the pattern) and one on the nearest neighbour distance

(*i.e.* the distance between each point and its nearest neighbour). All plots are shown in Figure 5.6.

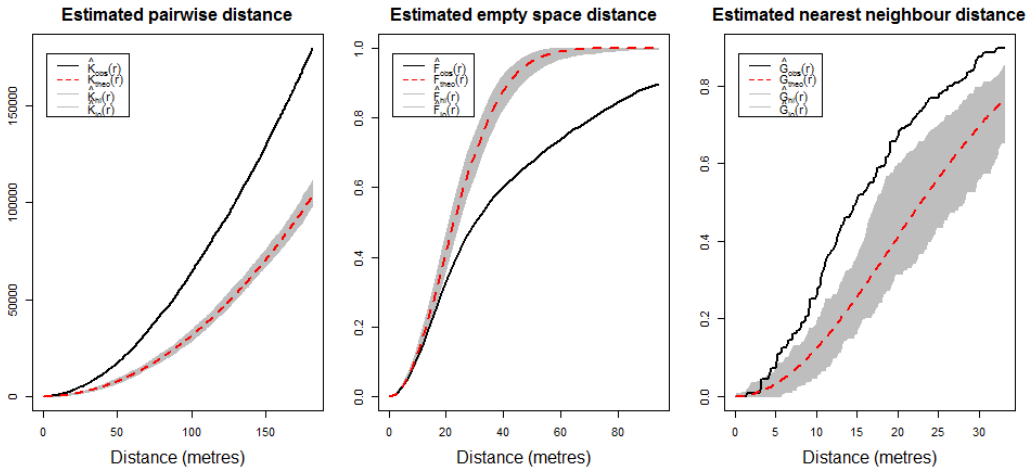


Figure 5.6: MCMC tests for Complete Spatial Randomness

All tests are run on the overall dataset, *i.e.* on the spatial point pattern containing all the points of the data series. From the plots it is possible to see that in all tests the empirical curve lies well outside the bands: this says the overall Sandside pattern is not randomly scattered in the area and gives hints for clustering.

Other non parametric, not simulation-based tests are presented in Section 2.1.2 for checking CSR. Some examples are Pearson's Chi square test and the Kolmogorov-Smirnov test, usually more powerful than the Chi square test, which compares the distribution of a spatial covariate (as the spatial coordinates themselves, or another available covariate) under the null hypothesis of CSR with its empirical curve. All tests led to the same result: rejection of the null hypothesis in favour of clustering. Plots are shown in Figure 5.7.

In conclusion, the exploratory analysis shows some clustering which may be mainly due to environmental reasons (discharge outlet, water stream etc.) and possibly to particle interaction (*e.g.* the generation of sub-particles). This suggests a Cox process should be particularly suitable for the data.

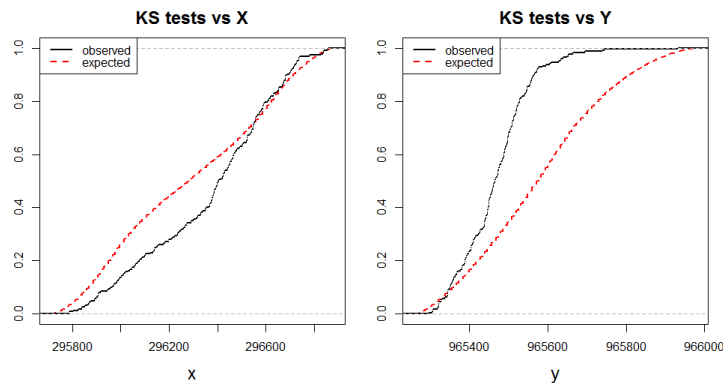


Figure 5.7: Kolmogorov-Smirnov tests for Complete Spatial Randomness

5.3 Fitting Cox models

We fit a few different models mentioned in Section 2.1.1 (inhomogeneous Poisson processes, Poisson cluster processes, area interaction processes; results not reported here) and then choose the more flexible and general class of Cox processes, particularly suitable for modelling data with clustering due to an underlying environmental driver.

We first fit a stationary Thomas process to the data, as it is a very common Cox model, it is quite simple and it seems sensible to fit this model to the particles (see an introduction to this process in Section 2.1.1). Indeed, the model seems to fit the data very well, according to an MCMC goodness of fit test based on 39 simulations (significance level $\alpha = 0.025$). The goodness-of-fit plot is shown in Figure 5.8.

A more flexible type of Cox models is the Log-Gaussian Cox Process (LGCP, see Section 2.1.4). A stationary LGCP model with no effects fitted to our data has a very similar performance to the Thomas model, with even better results when the distance between points becomes really huge: see Figure 5.8 for a comparison. This similarity suggests that, as the Thomas process fits the data so well, the LGCP is also very good for them.

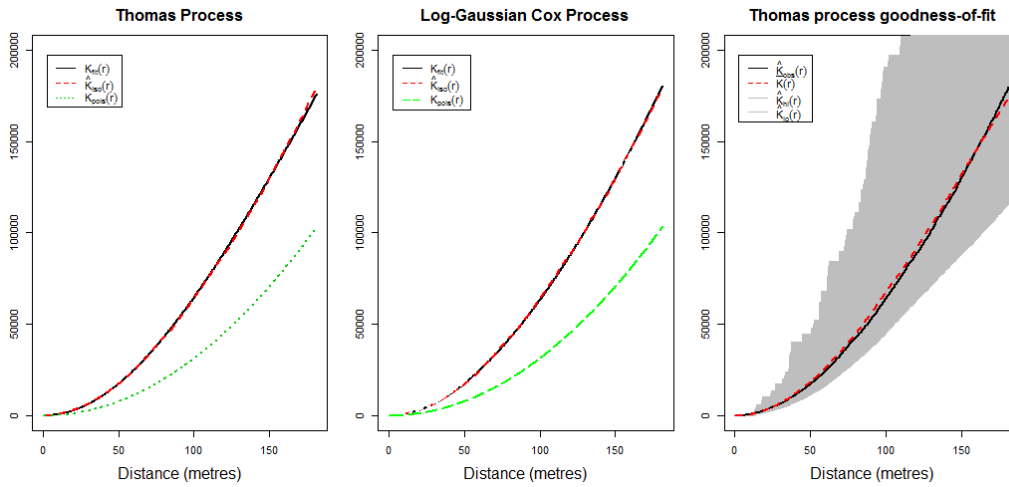


Figure 5.8: Thomas process and Log-Gaussian Cox process: a comparison

It is worth using LGCPs rather than Thomas processes because

- it is very straightforward to complicate these models by adding fixed or random/smooth effects to the structured predictor (see Section 2.2.4);
- they can be estimated with INLA so the estimation is very fast (and precise) even for complex models and this allows many different models to be fitted without high computational effort;
- they look well-fitting the data and also realistically suitable for the problem as the distribution of particles could be due to an underlying driver.

The use of LGCPs is then motivated, and in the next Section we proceed with the changepoint analysis using the methods presented in Chapter 3.

5.4 Changepoint analysis on particle data

In Section 2.2, we showed how INLA works in general and how to fit LGCPs with this approach. In this Section, we fit all the LGCP models with INLA and apply all the detection techniques presented in Chapter 3 to the real dataset. We use the same practical procedures and functions presented

in Chapter 4 for the simulated data. Where further notes are needed on how to implement the methods, they are presented in this Section.

5.4.1 Preparing the data

The first task when dealing with a practical spatial problem and INLA is to adapt the window to the INLA functions: having an irregular polygonal window is an issue that we have not faced during the simulation study in Chapter 4. Most of the R functions and commands for point process analysis are created for a rectangular window, therefore a few preliminary steps are needed for adapting the code. The procedure consists in

1. creating a rectangular box bounding the polygonal window (Figure 5.9, panel 1);
2. building a regularly distributed dummy process that discretizes the rectangular window into a cell grid: every point of the dummy process is the centroid of a cell (Figure 5.9, panel 2);
3. counting the number of true process points in each cell; a vector of counts Y is produced with the same dimension as the number of cells, and this becomes the dataset of interest, as explained in detail in Section 3.1 (Figure 5.9, panel 3);
4. selecting the polygonal window area out of the bounding box (Figure 5.9, panel 4).

In conclusion, we have

- W , an irregular shaped observation window;
- $T = 15$ yearly time points from 1999 to 2013, renumbered 1 to 15;
- $S = 698$ cells: the rectangular box was cut into $30 \times 40 = 1200$ cells and all the cells with a centroid outside W were discarded;
- Y , a $15 \times 698 = 10470$ -dimensional response vector.

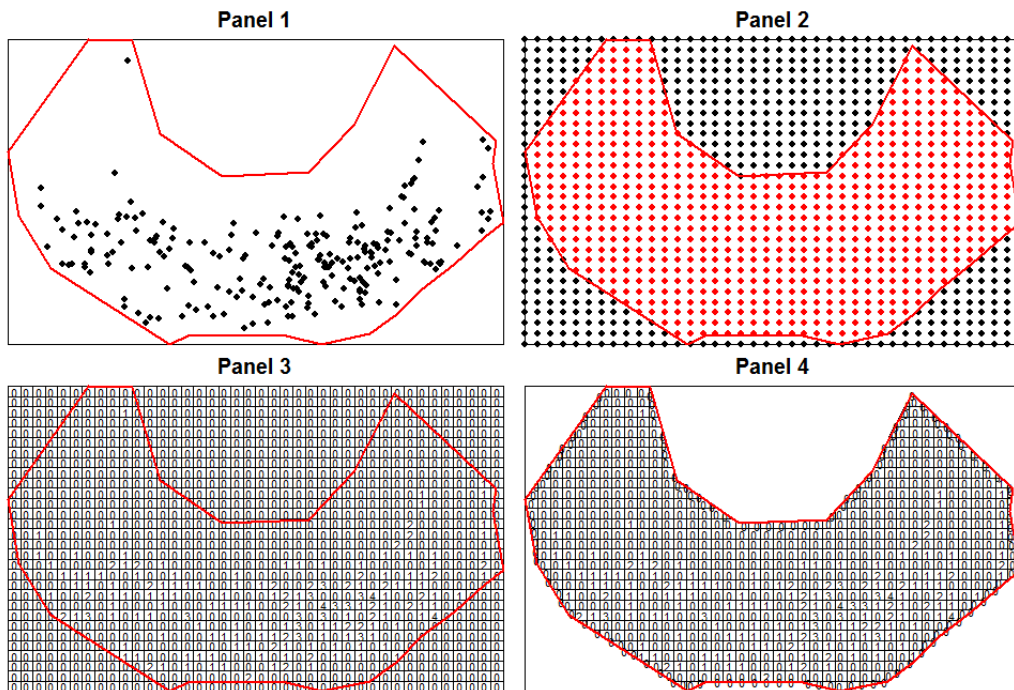


Figure 5.9: Building the response variable with an irregular window
 In this picture, the resolution of the grid is very rough in order to make it readable. The actual resolution is much finer.

After adapting the functions to an irregular window, all the models used in the simulation study can be fitted to real data; we run both a single and a multiple changepoint analysis, keeping the maximum number of changepoints to look for set to 3 as more than 3 would be too many for such a short time series. We used both the Bayes Factor method and the Posterior Threshold method presented in Section 3.2.4 for detecting single changepoints, and both the binary segmentation and the recursive equations approach as in Section 3.3 for multiple changes. As in Chapter 4, at the beginning non informative prior distributions are taken on number and position for the changepoints and on all hyperparameters. An extension using different prior distributions is given in Section 5.6.

5.4.2 Single changepoint search results

For a single changepoint analysis, results are available for the four models introduced in Section 3.2.2, using both the BF and the PT detection methods. We recall here that Model 1 assumes a spatially homogeneous process and only includes a fixed effect, Model 2 adds a random temporal effect modelled as an AR(1), Model 3 allows for spatial heterogeneity and dependence thanks to a random spatial effect modelled as a Random Walk in two dimensions, and Model 4 includes both smooth effects. In general, two major peaks are detected, both leading to an increase in the intensity function, and they are very close to the changes in the equipment used to find and retrieve the particles.

Bayes Factor method

When moving from one model to the following one and using the BF method, results change, as it can be seen in the summary in Figure 5.10. Models 1 and 3, which do not include a temporal effect, detect a change in 2006, while Models 2 and 4, with a temporal effect, show a higher peak in 2003. In particular, with the fixed effect model, a changepoint in 2006 is detected, with an increase in the particle intensity. We know there has been a change in equipment at the beginning of 2007, so this might give a hint for an effective improvement in the ability of detecting particles. The time points in the data series are quite different as for number of points, therefore the changepoint might be detected a year earlier because of a random positive oscillation, after which the increase in the intensity level is due to the equipment improvement. As can be seen from the changepoint posterior distribution, though, there is another high peak corresponding to 2003, only slightly lower than the 2006 one. This peak becomes significant when fitting the second model, introducing temporal dependence, which leads to a detection of a changepoint in 2003, and perfectly coincides with the first change in equipment at the end of 2002.

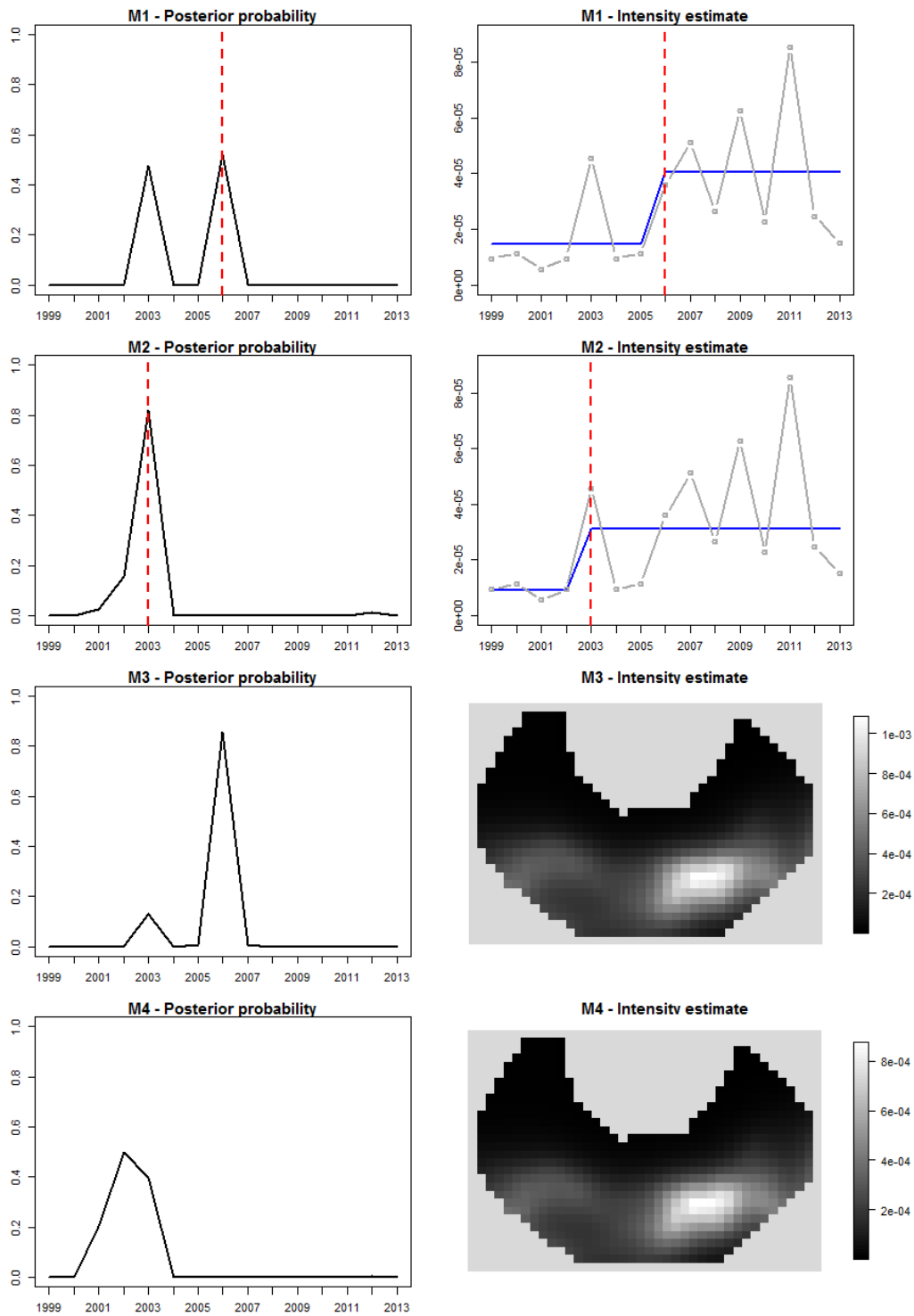


Figure 5.10: BF performance, single changepoint search

As happens when using the BF method with simulated data, there are no changepoints detected in the two inhomogeneous models, despite the fact that the spatial model posterior shows a very high peak, above 0.8, in 2006 and a second one in 2003, while the spatio-temporal model posterior has a peak around 0.5 between 2002 and 2003. They are considered non-significant using the BF method, therefore changepoints are present in the data series only if fitting the two homogeneous models.

Posterior Threshold method

As for the PT method, threshold values are chosen based on the simulation results: a low threshold of 0.2 for the first model, an only slightly greater one, 0.25, for the second model, and much higher values, 0.85, for the third and fourth model. In general, results are consistent with the simulation results: coherent conclusions with respect to the BF method results for the two homogeneous models, but more changepoints detected when moving to the inhomogeneous models. Results are all shown in Figure 5.11. Indeed, a significant changepoint in 2006 is detected when fitting the fixed effect model, with a peak raising high above the threshold; the second peak in 2003 is also above the threshold, so, even if discarded at the moment because we are looking for a single changepoint, it suggests the usefulness of a multiple changepoint search. Coherent results with regard to the BF method are also achieved with the second model: a major changepoint in 2003, determining an increase in the particle intensity. Results change with respect to the BF method conclusions when fitting the spatial inhomogeneous model: the peak in 2006 is considered significant, therefore the INLA estimates are split into two images for the two segments, with a similar spatial structure and a different scale. Here too, a visible second peak in 2003 hints at the need to look for further changes. The posterior distribution of the fourth model, showing a peak that reaches 0.5, does not raise above the threshold, therefore no changepoints are detected when allowing for both spatial and temporal dependence.

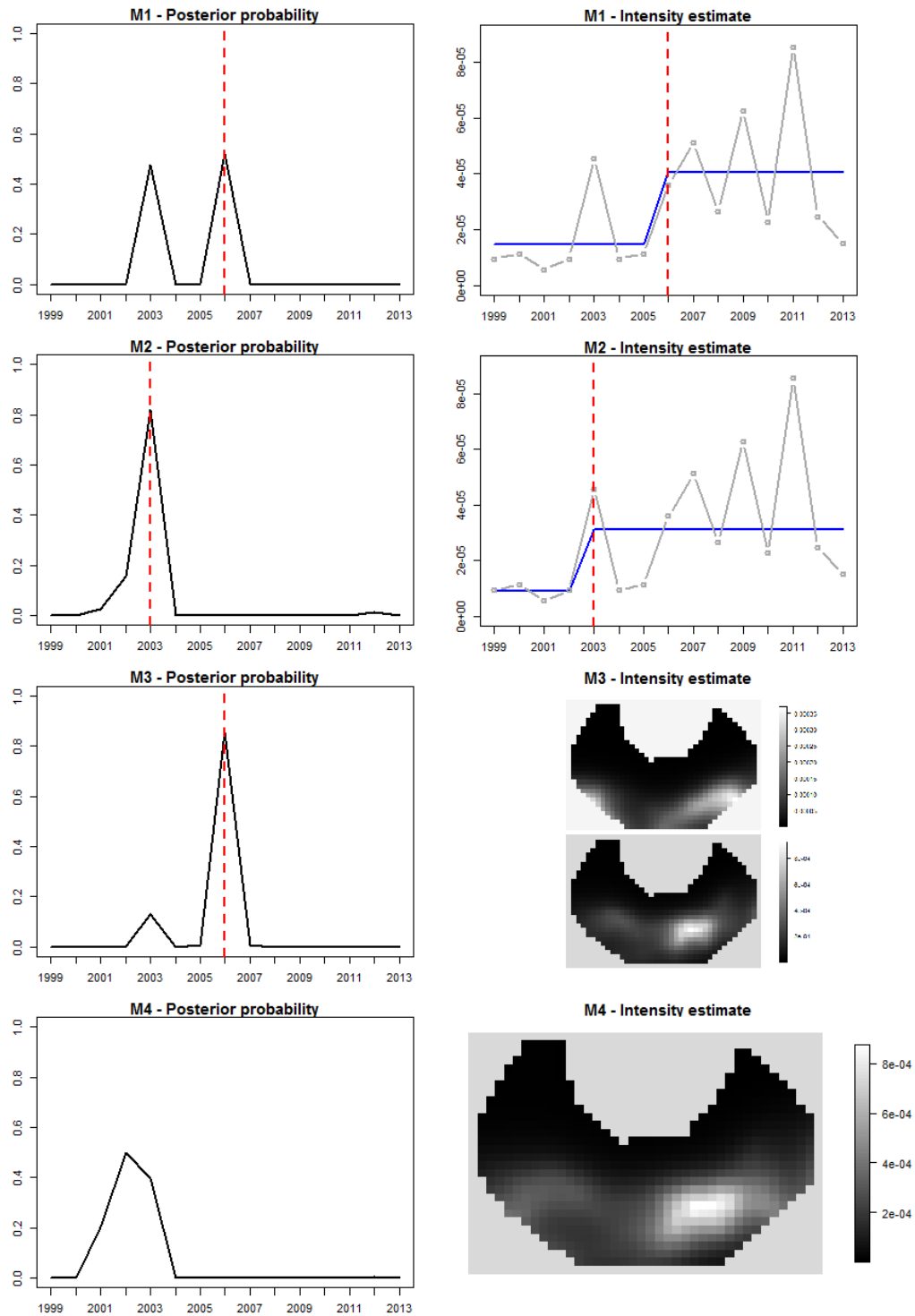


Figure 5.11: PT performance, single changepoint search

Results for the single changepoint search are summarised in Table 5.1.

Table 5.1: Single search - detected changepoints

Model	Changepoint (BF)	Changepoint (PT)
Fixed	2006	2006
Temporal	2003	2003
Spatial	—	2006
Sp-temp	—	—

When looking at the data behaviour, models assuming a homogeneous intensity do not seem very suitable for our data: the kernel intensity estimates (Figure 5.5) show an inhomogeneous behaviour, whose structure is substantially constant over time up to a scale parameter, with a main hot spot in the bottom-right area and a second one in the bottom-left part, and lower density in the top half of the window. This visual approach suggests data are better described with the third or fourth model, and show a similar behaviour to the simulated data presented in Chapter 4, which kept a constant spatial structure and only showed a change in scale. If further investigation is of interest about the best model for the data, the Deviance Information Criterion can be used as introduced in Section 3.5.

5.4.3 Multiple changepoint search results

Again, we follow the same procedure used for the simulation study, *i.e.* we implement a binary segmentation algorithm combined with both BF and PT methods, and then we try a simultaneous multiple changepoint search with the recursive equation approach.

A summary of the resulting changepoints is given in Table 5.2.

Table 5.2: Multiple search - detected changepoints

Model	Binseg-BF	Binseg-PT	Simultaneous
Fixed	2003, 2006, 2012	2003, 2006, 2012	2006
Temporal	2003	2003, 2006, 2012	2003
Spatial	—	2006, 2012	—
Sp-temp	—	—	—

Binary segmentation algorithm and BF method

All results for a multiple search with the BF method are in Figure 5.12. The most interesting result obtained by the BF method is found when fitting the fixed effect model: three changepoints are considered significant, corresponding to 2003, 2006 and 2012. The first two of them correspond to (or are close to) the equipment changes and mark an increase in the point intensity; this means the change in equipment has significantly improved the ability of detecting particles. The third changepoint is very close to the end of the series, therefore conclusions must be drawn carefully; it gives a hint for a decreasing intensity, and might be a sign that the offshore retrieval campaign has recently efficiently reduced the arrival of particles in the Sandside area. When adding a temporal effect, the analysis produces the same results as for a single changepoint search, with the only changepoint detected in 2003; the second step of the algorithm identifies a potential change in 2006 but it is discarded by the method as non significant. As for the two inhomogeneous models, the single changepoint search had not produced any significant detection, so there is no change in the conclusion when running the multiple changepoint detection algorithm, and no changepoints are identified.

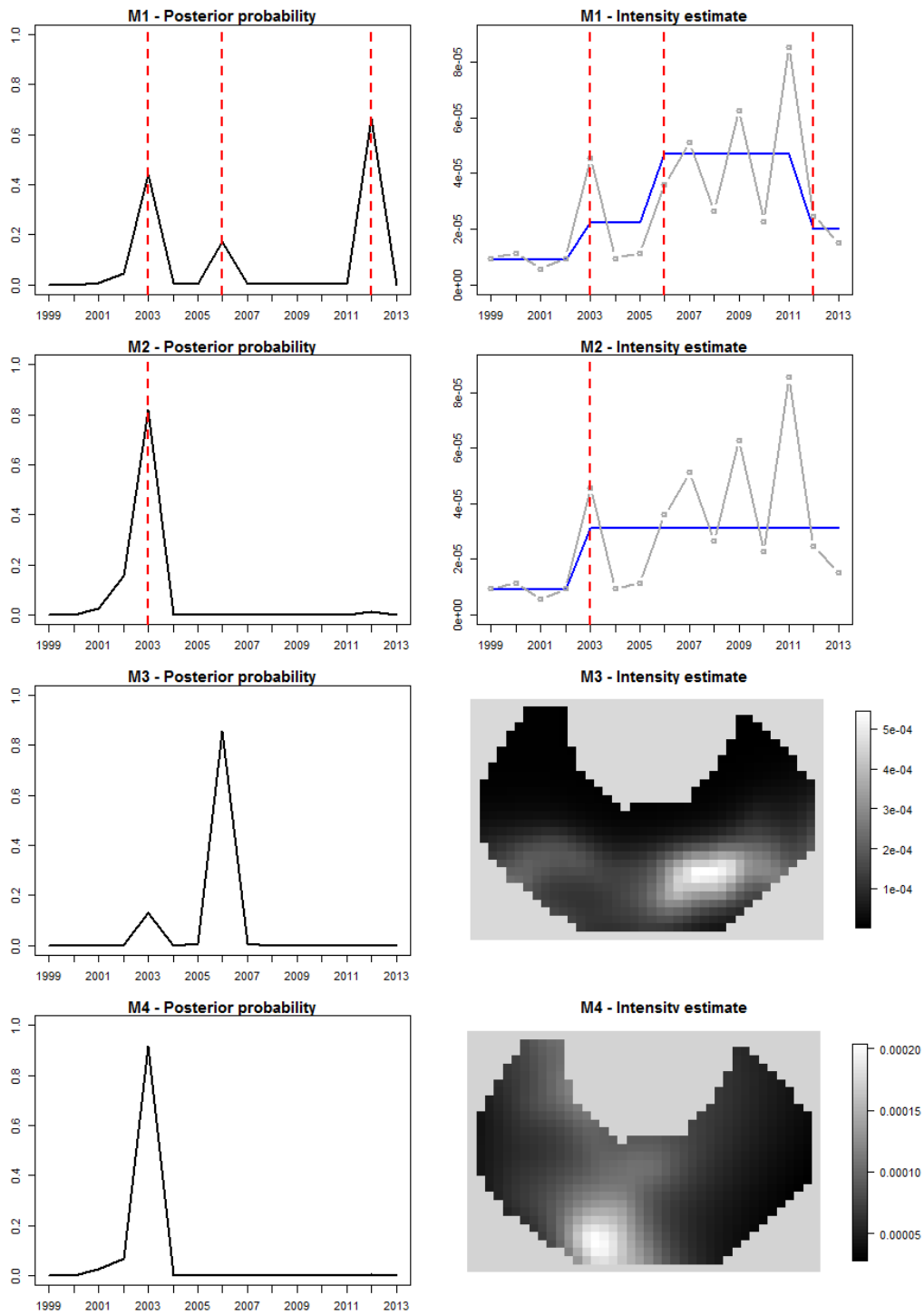


Figure 5.12: BF performance, multiple changepoint search

Binary segmentation algorithm and PT method

The fixed effect model fitting again leads to the same conclusions as the BF method: three changepoints detected in 2003, 2006, 2012, the first two marking an increasing intensity, and the last one corresponding to a decrease. This time, the same conclusions are drawn when adding a temporal effect: 3 changepoints, two increasing and one decreasing, in 2003, 2006, 2012. Fitting the spatial model and plotting the posterior curve with a threshold of 0.85 leads to the detection of two changepoints in 2006 and 2012; there is a third peak between 2002 and 2003 but it remains below the threshold. As in the single search, when fitting the last model with a threshold of 0.85 there are no changepoints. Given the similarity between fixed and temporal model, and the absence of novelty brought by the spatio-temporal model, graphs are only displayed for the temporal and the spatial model in Figure 5.13; in order to distinguish them from non significant peaks, all the detected changepoints are identified by a dashed vertical red line.

Simultaneous changepoint search

As we have seen for the simulation results in Chapter 4, here too the simultaneous changepoint detection approach (Wyse et al., 2011 and Section 2.3.5) suffers from too much conservatism. Again, this is probably due to the connection with the BF method. Results are nonetheless consistent with what detected with the other methods. Indeed, a changepoint in 2006 is detected with the fixed effect model and one in 2003 when including the temporal effect. The other two models do not lead to the detection of significant changepoints, even if year 2006 is a borderline value with the spatial effect.

Since all computations here are based on the INLA approach, given the detection of the changepoint there are no differences as regards the estimated intensity functions. We therefore do not report results for the estimates.

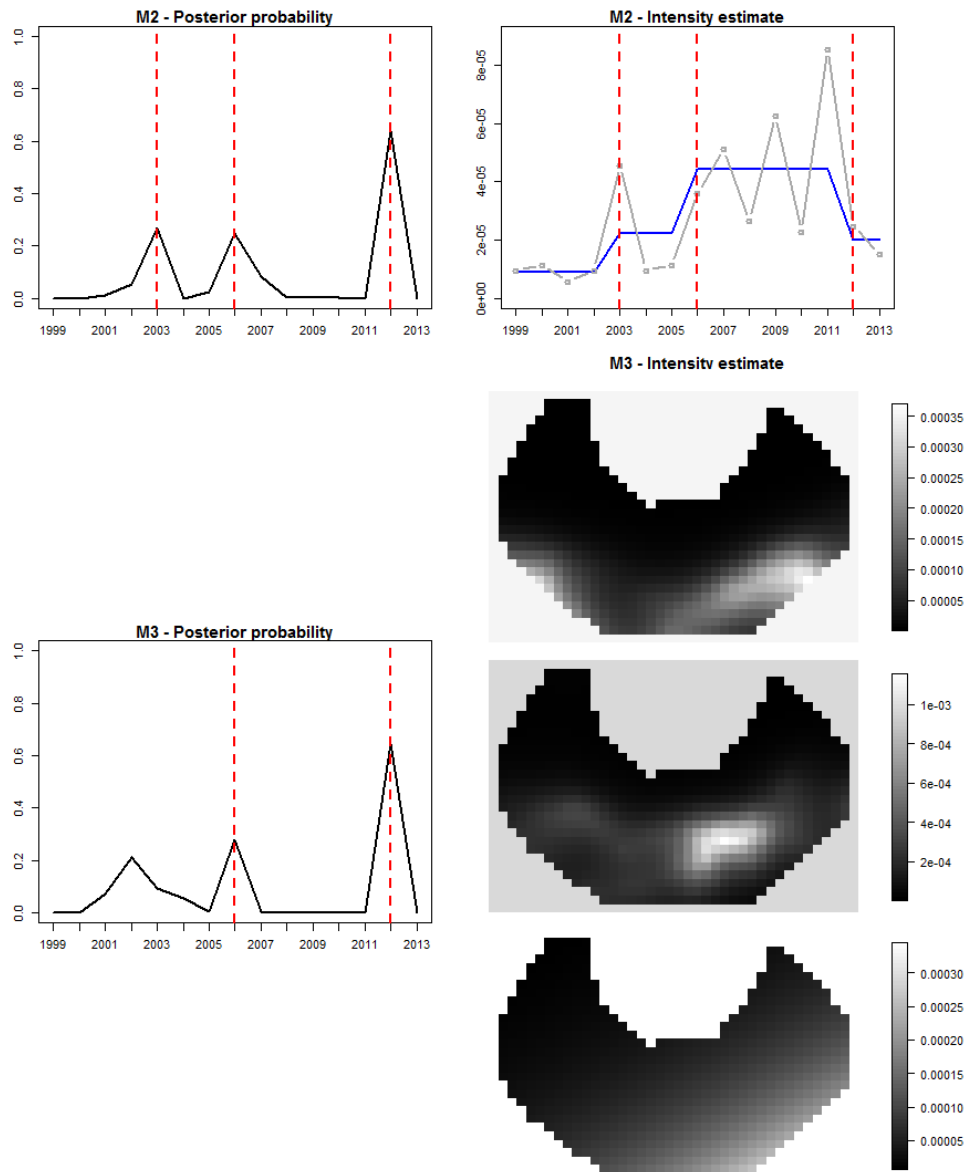


Figure 5.13: PT performance, multiple changepoint search

5.5 Inclusion of covariates

When introducing the dataset (Section 5.1), we listed the available information including data on the radioactivity level and depth in the sediment of the retrieved particles. This is part of the response and is usually referred to in point process analysis as *marks*. Additional information is also available, though, that is contextual and does not depend on the particles themselves; it can be exploited to improve the models and further check the methods' performance.

5.5.1 Introducing covariates

Two covariates in particular may be useful for analysing the particle distribution over Sandside beach: the distance from the nuclear discharge outlet, that is considered the main source for particle dispersion, and the distance from the 'low water level', *i.e.* the northern boundary of the observation window, since the particle arrival from the offshore area must depend on tides and currents.

Figure 5.14 shows both distances; as can be seen, the range of values is very different as the low water level is part of the window border, while the nuclear discharge outlet is far away from the beach in the North-East direction. We are inclined to believe that the nuclear discharge does not have a significant effect on the distribution of particles, because the distance is high and there are several intervening environmental processes; for instance, the U-shaped coast around the beach (Figure 5.1) is likely to nullify potential long-distance effects. Nevertheless, we test both covariates separately on our data in order to check their ability to add useful information for describing the phenomenon under study.

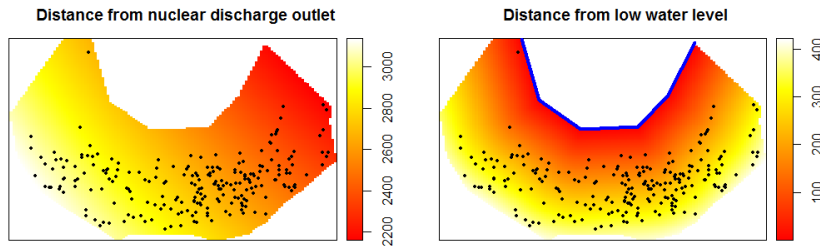


Figure 5.14: Covariates (distance in metres)

5.5.2 Extensions of the models

We introduce the two covariates in our models, one at a time, as fixed effects. The models become:

- Model 1: fixed effect and covariate
 $\log \lambda(t) = \mu_t + \beta_t z + \epsilon_t$ for $t = 1, \dots, T$
- Model 2: fixed effect, covariate and temporal effect
 $\log \lambda(t) = \mu_t + \beta_t z + \phi_t + \epsilon_t$ for $t = 1, \dots, T$
- Model 3: intercept, covariate and spatial effect
 $\log \lambda(t, s) = \delta + \beta_t z + \psi_{ts} + \epsilon_{ts}$ for $t = 1, \dots, T$ and $s = 1, \dots, S$
- Model 4: intercept, covariate, temporal effect and spatial effect
 $\log \lambda(t, s) = \delta + \beta_t z + \phi_t + \psi_{ts} + \epsilon_{ts}$ for $t = 1, \dots, T$ and $s = 1, \dots, S$.

We refer to Section 3.2.2 for details on the notation; here, z indicates the single covariate. As usual, under H_0 each effect takes a single value over time, while under H_1 it takes $m + 1$ values where $m \geq 1$ is the unknown number of changepoints. We apply all our detection methods considering each covariate separately.

5.5.3 Results and discussion

A summary of the obtained results is in Tables 5.3 for a single changepoint search and 5.5 for a multiple changepoint search.

Single search: comparison and comments

Table 5.3: Single search - detected changepoints with either covariate

Model	Nuclear discharge		Low water level	
	BF	PT	BF	PT
Fixed	2003	2003	2006	2006
Temporal	—	2003	—	2003
Spatial	—	2006	—	2006
Sp-temp	—	—	—	—

When comparing Table 5.3 to Table 5.1, the first thing to note is that with Model 1 (fixed) results depend on the covariate. Using the distance from the low water level leads to the same results as the analysis without covariates, while including the distance from the nuclear discharge outlet has a similar effect to including a temporal component: year 2003 is chosen as the changepoint. Besides, including a covariate in Model 2 (temporal) has a negative effect on the BF method, since it is now unable to detect any changepoint. Results remain the same as regards Model 2 with the PT method and Model 3 (spatial) and 4 (spatio-temporal) with either method and covariate. In conclusion, when covariates are included in a single changepoint search no increase in the ability to find changepoints takes place: the PT method seems unaffected by covariates, and the BF method tends to be even more conservative.

It would be of interest to carry out a model comparison and see if a model with one of the covariates is preferred to the corresponding one with no covariate. The Deviance Information Criterion (DIC) may be used as it is frequently used in Bayesian analysis for model selection. Since this is not the main focus of our work, we only show an example of the DIC for a single search and leave a deeper analysis for further studies; values are in Table 5.4.

In this Table, we can see that when using Model 1 the addition of the distance from the nuclear discharge improves the DIC, while the distance from the low water level has no effect. As for Model 2, no improvements take place: when using the BF method, no changepoints are found, so the DIC

Table 5.4: Single search - DIC values

Model	No covariate		Nuclear discharge		Low water level	
	BF	PT	BF	PT	BF	PT
Fixed	599	599	234	234	598	598
Temporal	239	239	2080	243	2077	243
Spatial	1949	1864	1951	1081	1951	648
Sp-temp	1853	1853	1855	1855	1855	1855

under H_0 is far higher than the other ones; when using the PT method, there are no substantial changes. The DIC for Model 2 shows a consistent improvement with respect to Model 1 when no covariate is used (the temporal model would be chosen as the best model among the four of them), but the best performance is given by the fixed model with the inclusion of the distance from the nuclear discharge outlet. As regards Model 3, the inclusion of the covariates has a strong positive effect, especially with the distance from the low water level, if combined with the PT method: the model performs much better than the one without covariates. No changepoints are detected with Model 4 irrespective of the method and of the inclusion of covariates; H_0 is never rejected and all DICs are very high.

Multiple search: comparison and comments

The detected changepoint location for a binary segmentation procedure with either the BF or the PT method and for a simultaneous approach are reported in Table 5.5.

Table 5.5: Multiple search - detected changepoints with either covariate

Model	Nuclear discharge			Low water level		
	Binseg-BF	Binseg-PT	Simult	Binseg-BF	Binseg-PT	Simult
Fixed	2003	2003 2006 2012	2003	2006	2003 2006 2012	2006
Temporal	—	2003 2006 2012	—	—	2003 2006 2012	—
Spatial	—	2006 2012	—	—	2006 2012	—
Sp-temp	—	—	—	—	—	—

The binary segmentation combined with the PT method is unaffected by either covariate: results are exactly the same as in Table 5.2 for all models. The binary segmentation with the BF method and the simultaneous search lead to the same results, which are roughly the same as for the single search in Table 5.3: in Model 1, the inclusion of the distance from the nuclear discharge outlet shifts the changepoint from 2006 to 2003, while in Model 2 considering any of the two covariates leads to the detection of no changepoint. No other change occurs with respect to Table 5.2, and conclusions are extremely similar to the simple single search ones.

Concluding remarks

This Section is only a first step towards the inclusion of covariates and the search for a good model for the data. Different options for including covariates can be tested: for instance, they can be modelled as smooth effects or can be included jointly. In this work, we do not aim at a complete analysis on the covariates; the scope of our work has already been clarified and focuses on spatial and temporal dependence. Since the available information is of interest on real data, though, we choose to give a hint of what can be done to improve our models and to show that our methods still produce good results. Indeed, linear dependence on a covariate does not substantially affect results on these data. We are in general still able to detect changes and the only relevant differences concern BF-based detection techniques: a changepoint is detected in 2003 instead of 2006 when fitting Model 1 with the distance from the nuclear discharge outlet, and no changepoint is detected in Model 2. A comparison of the DIC values for the single search highlights a preference for the first model combined with the distance from the nuclear discharge outlet, or (with very close values) for the second model.

5.6 Informative prior settings

In the simulation study presented in Chapter 4, all prior distributions are non informative, as the scope of the study is to test the ability of the methods to detect changepoints irrespective of the prior setting. When working

with real data, though, prior knowledge can be of help in obtaining sensible results. In particular, one of the research questions presented in Section 1.1.2 concerns two known potential changepoints corresponding to equipment changes. So far, we focused on the more general case of unknown locations, but it is of interest to check the performance of our methods in the presence of informative priors. Non vague prior distribution may, in this context, regard the number of changepoints and/or their positions. We try both cases separately.

5.6.1 Number of changepoints

Firstly, we focus on prior knowledge concerning the number of changepoints. Since we believe that there are two main changepoints, we focus on multiple changepoint detection techniques, in particular on the simultaneous search for two main reasons. First of all, the approach presented in Section 2.3.4 allows separate prior distributions on number and locations to be set; secondly, the simultaneous approach produced conservative results on our data (Section 5.4.3), so we are interested in improving the method by including extra information. Moreover, the binary segmentation algorithms do not need different prior distributions, as they have already detected the two changepoints of interest in most cases with no addition of extra knowledge. We compare results with four different prior settings: a non informative one (presented in Section 5.4.3) and three different belief strengths:

1. Prior 1 - vague
 $\pi(m) = 0.25$ for $m = 0, 1, 2, 3$
2. Prior 2 - weak
 $\pi(2) = 0.4$
 $\pi(m) = 0.2$ for $m = 0, 1, 3$
3. Prior 3 - medium
 $\pi(2) = 0.6$
 $\pi(m) = 0.13$ for $m = 0, 1, 3$
4. Prior 4 - strong

$$\pi(2) = 0.8$$

$$\pi(m) = 0.07 \text{ for } m = 0, 1, 3$$

The four prior distributions are shown in Figure 5.15.

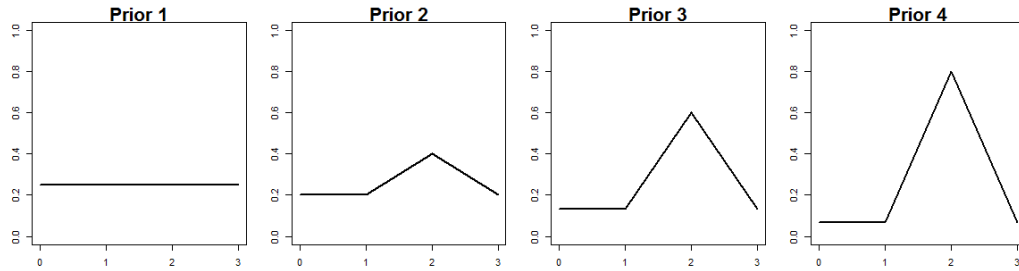


Figure 5.15: Prior settings on the number of changepoints

After choosing the priors, the same simultaneous changepoint search is run; then, the conditional likelihoods $L(Y|m)$, $m = 0, \dots, 3$ are multiplied by the corresponding prior probability before choosing the highest one. Results are displayed in Table 5.6. Note that the column referring to Prior 1 is the same as the results displayed in Table 5.2, since the prior is non informative.

Table 5.6: Simultaneous search with different prior settings

Model	Prior 1	Prior 2	Prior 3	Prior 4
Fixed	2006	2003,2006	2003,2006	2003,2006
Temporal	2003	2003,2006	2003,2006	2003,2006
Spatial	—	—	2003,2006	2003,2006
Sp-temp	—	—	2000,2003	2000,2003

With the first two models, a weak belief that there are two changepoints is sufficient for detecting the changes in the equipment, while Model 3 and 4 allow for more data variability, therefore they need a strongly informative prior setting in order to detect any change. When fitting Model 3, conclusions are consistent with the rest of the results, while Model 4 leads to the detection of a different changepoint in 2000, which had never been found before. In conclusion, the use of an informative prior setting allows the first

research question to be fully answered by detecting positive changes in the intensity of the process corresponding, in most cases, to the improvements in the equipment. The simultaneous approach is substantially improved by the addition of extra knowledge via informative prior distributions, as its conservatism is overcome.

5.6.2 Changepoint positions

Another option is to use information about the changepoint positions (in a changepoint search with an unknown number of changepoints the two options can be combined). Since the two equipment changes took place at the end of 2002 and at the beginning of 2007, we fix peaks in the prior distributions corresponding to 2003 and 2007, firstly one at a time (for a single search), then jointly (for a multiple search). Three prior distributions with different peak heights are set for each case, where the first one is non informative and coincides with the previous analysis. For a single search with a prior peak in 2003

1. Prior 1 - vague

$$\pi(\tau) = 0.083 \text{ for } \tau = 2000, \dots, 2011$$

$$\pi(\tau) = 0 \text{ for } \tau = 1999, 2012, 2013$$

2. Prior 2 - weak

$$\pi(\tau) = 0.2 \text{ for } \tau = 2003$$

$$\pi(\tau) = 0.073 \text{ for } \tau = 2000, 2001, 2002, 2004, \dots, 2011$$

$$\pi(\tau) = 0 \text{ for } \tau = 1999, 2012, 2013$$

3. Prior 3 - strong

$$\pi(\tau) = 0.5 \text{ for } \tau = 2003$$

$$\pi(\tau) = 0.045 \text{ for } \tau = 2000, 2001, 2002, 2004, \dots, 2011$$

$$\pi(\tau) = 0 \text{ for } \tau = 1999, 2012, 2013$$

The same setting is replicated for a changepoint in 2007. Extreme values have a null prior probability as we set a minimum segment length of 2 time points.

For a multiple search

1. Prior 1 - vague

$$\pi(\tau) = 0.083 \text{ for } \tau = 2000, \dots, 2011$$

$$\pi(\tau) = 0 \text{ for } \tau = 1999, 2012, 2013$$

2. Prior 2 - weak

$$\pi(\tau) = 0.2 \text{ for } \tau = 2003, 2007$$

$$\pi(\tau) = 0.06 \text{ for } \tau = 2000, 2001, 2002, 2004, 2005, 2006, 2008, 2009, 2010, 2011$$

$$\pi(\tau) = 0 \text{ for } \tau = 1999, 2012, 2013$$

3. Prior 3 - strong

$$\pi(\tau) = 0.4 \text{ for } \tau = 2003, 2007$$

$$\pi(\tau) = 0.02 \text{ for } \tau = 2000, 2001, 2002, 2004, 2005, 2006, 2008, 2009, 2010, 2011$$

$$\pi(\tau) = 0 \text{ for } \tau = 1999, 2012, 2013$$

All prior distributions are displayed in Figure 5.16 (single peak) and 5.18 (multiple peaks).

Single changepoint detection

We fit Model 1 to 4 with six different prior settings, three for 2003 and three for 2007, as shown in Figure 5.16. Then, we look for a changepoint with both the BF and the PT method.

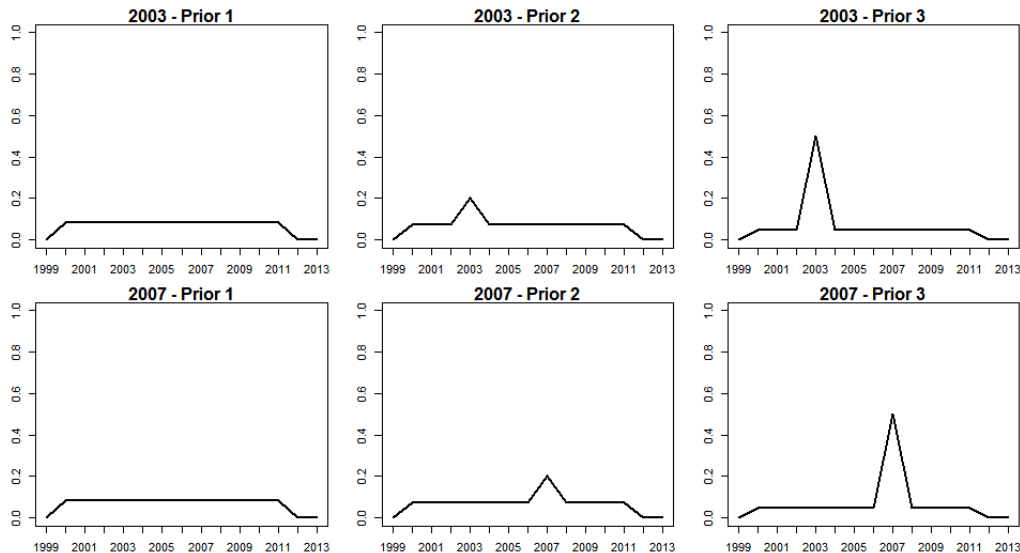


Figure 5.16: Prior settings on the changepoint position

Results for the BF method are summarized in Table 5.7, while results for the PT method are in Table 5.8.

In both Tables, it is immediate to see that the inclusion of an informative

Table 5.7: Single search with different prior settings and the BF method

Model	Vague prior	Prior on 2003		Prior on 2007	
		Prior 2	Prior 3	Prior 2	Prior 3
Fixed	2006	2006	2006	2006	2006
Temporal	2003	2003	2003	2003	2003
Spatial	—	—	—	—	—
Sp-temp	—	—	—	—	—

Table 5.8: Single search with different prior settings and the PT method

Model	Vague prior	Prior on 2003		Prior on 2007	
		Prior 2	Prior 3	Prior 2	Prior 3
Fixed	2006	2006	2006	2006	2006
Temporal	2003	2003	2003	2003	2003
Spatial	2006	—	—	2006	—
Sp-temp	—	—	2003	—	—

prior with a single peak does not affect the result in most cases. When using the BF method, no difference in the results occurs. With the PT method, changes in Model 3 results decrease the ability to find changes, as the changepoint in 2006 is not detectable when imposing a prior peak on 2003 (or a very strong one on 2007); indeed, showing a preference for 2003 flattens the other peaks so that 2006 becomes non significant, still the preference is not powerful enough to raise the posterior probability in 2003 above the threshold. The only new changepoint occurs when fitting Model 4 with a strong prior on 2003: the posterior distribution raises above the threshold thus, for the first time with respect to results deriving from non informative priors, we have a significant changepoint with the spatio-temporal model. We can see how posterior distributions change as we take different prior distributions in Figure 5.17; the threshold for the PT method is also reported.

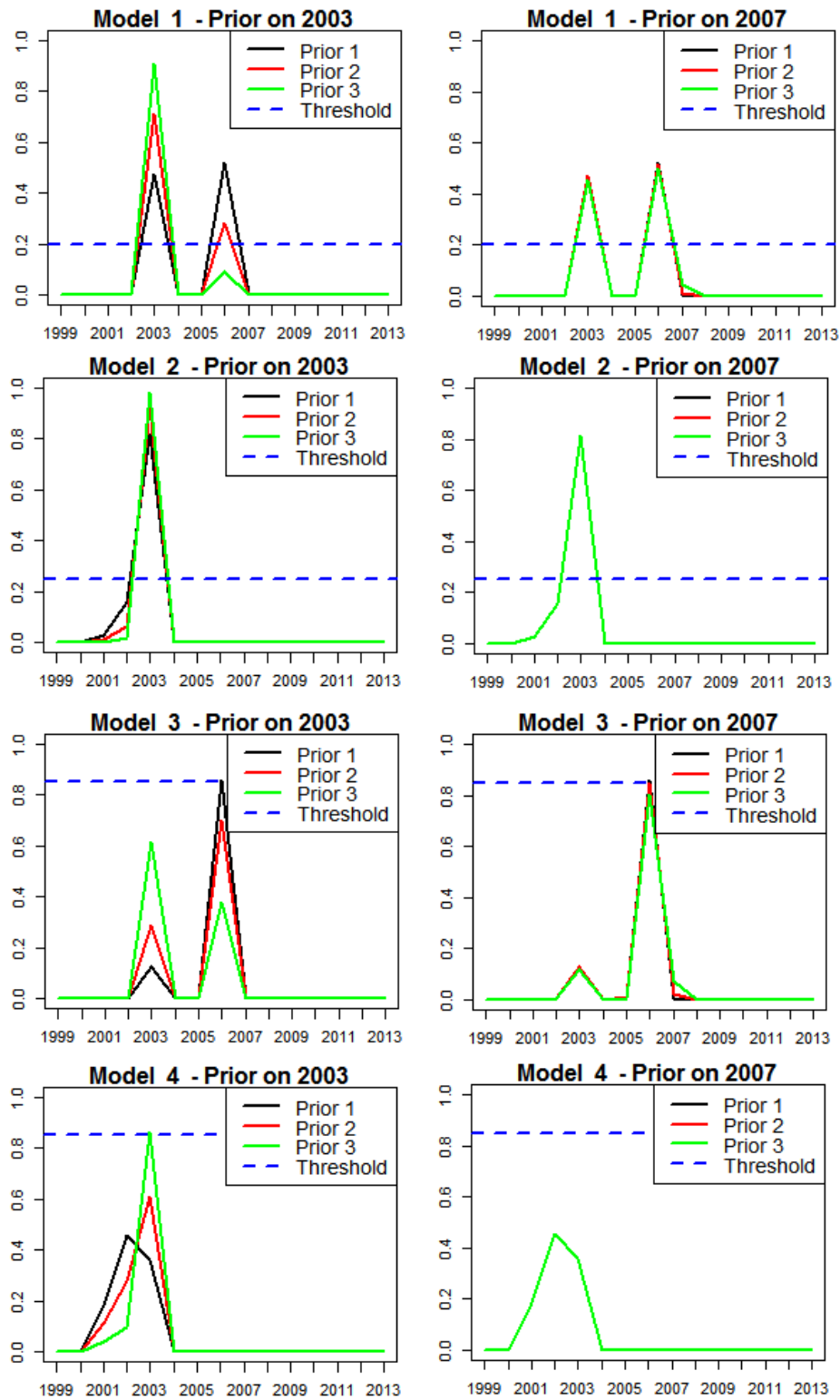


Figure 5.17: Posterior distributions resulting from different priors

Multiple changepoint detection

We again fit Model 1 to 4 with different prior settings for two changepoints corresponding to the equipment changes (Figure 5.18). We use both the binary segmentation algorithm and the simultaneous approach to look for changepoints.

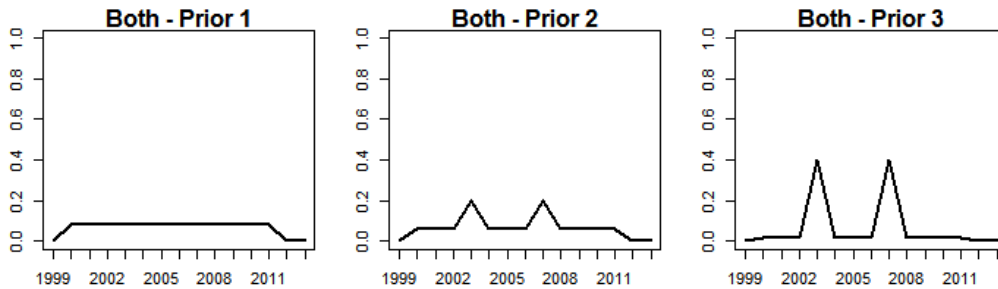


Figure 5.18: Prior settings for two changepoints

Results for the binary segmentation method are in Tables 5.9 and 5.10, while changepoints detected with the simultaneous approach are summarised in Table 5.11.

Table 5.9: Multiple changepoint search with different prior settings, the binary segmentation algorithm and the BF method

Model	Vague prior	Prior on 2003 and 2007					
		Prior 2			Prior 3		
Fixed	2003 2006 2012	2003 2006 2012	2003 2006 2012	2003 2006 2012	2003 2006 2012	2003 2006 2012	
Temporal	2003	2003	2003	2003	2003	2003	
Spatial	—	—	—	—	—	—	
Sp-temp	—	—	—	—	—	—	

As for the single search with the BF method, a multiple changepoint analysis with the binary segmentation and the BF method (Table 5.9) does not depend on the prior distributions on the changepoint locations: results are identical to what obtained with a vague prior (see also Table 5.2). Again, there is an analogy to the single search when using the PT method; fitting

Table 5.10: Multiple changepoint search with different prior settings, the binary segmentation algorithm and the PT method

Model	Vague prior	Prior on 2003 and 2007	
		Prior 2	Prior 3
Fixed	2003 2006 2012	2003 2006 2012	2003 2006 2012
Temporal	2003 2006 2012	2003 2006 2012	2003 2006 2012
Spatial	2006 2012	—	—
Sp-temp	—	—	2003

Table 5.11: Simultaneous multiple changepoint search with different prior settings

Model	Vague prior	Prior on 2003 and 2007	
		Prior 2	Prior 3
Fixed	2006	2003	2003
Temporal	2003	2003	2003
Spatial	—	—	—
Sp-temp	—	—	—

Model 3 with an informative prior on 2003 and 2007 decreases the ability to detect changes, which become non significant. The improvement in Model 4 also occurs with a multiple search: when imposing strong peaks, the changepoint in 2003 raises above the threshold.

With a simultaneous approach, there is no improvement in the ability to detect changepoints; it is to remark that a non vague prior leads to preferring a changepoint in 2003 rather than in 2006 even with the fixed model.

5.7 Discussion

In this Chapter, we go back to the original research questions that motivated the whole study, after providing all the needed methodology and method assessment: since the performance of the methods has already been evaluated with simulated data, we know when to rely on the results and when

they can be, *e.g.*, too conservative.

We first follow the usual preliminary steps in a point process analysis. We test Complete Spatial Randomness with MCMC distance based tests and reject it in favour of a clustering behaviour. We motivate the use of Log-Gaussian Cox processes via goodness of fit tests and privilege this class of models over others for reasons such as flexibility and compatibility with INLA, which provides fast estimates even for complex models. After choosing the right class of models, we can apply our new changepoint methods and draw conclusions on the data behaviour. As a last step, we add some external information such as including covariates and trying informative prior settings on the number or locations of the changepoints.

According to the overall results, both the improvements in the equipment and the offshore retrieval process have had positive effects in the intensity of the process. The constance in the spatial structure of the intensity suggests that future search of radioactive particles should emphasise the bottom part of the Sandside beach, where the greater number of particles tends to concentrate.

5.7.1 Remarks on standard changepoint analysis

Firstly, we carried out the same changepoint analysis as in Chapter 4, with no addition/change in the models.

Results must be interpreted carefully since the time series is very short, but they are sensible given the context, and there is a general, comforting consistency over all the results: two major changes are detected, corresponding to two peaks in the posterior probability of the changepoint position. They correspond to 2003 and 2006, and they both mark an increase in the intensity function. The spatial structure of the function remains approximately the same, with higher values in the bottom half of the observation window and lower values in the top half; its strength, or scale, increases after the two changes. We know from the data history that two major changes in the equipment used to detect the particles have taken place, one at the end of 2002 and the following at the beginning of 2007. We then hoped to find two positive significant changes in 2003 and 2007; results are very close to what

expected, with a shift of one year in the second change that might be due to natural random oscillation in the data. When running a single changepoint analysis, there are no different changepoints found. For both BF and PT methods, we note that the peak in 2003 is favoured when including temporal dependence in the model, while the change in 2006 is detected for the fixed and spatial models. This supports the thesis of a positive random increase in the data just before the second change: if we do not consider time dependence in the data series, the peak in 2006 is detected first, probably because it is the greatest in terms of scale shift. When including time dependence, though, this peak becomes smaller than the one in 2003, thus the temporal model results suggest that part of the change in 2006 is imputable to time dependence. Despite this, the second peak is still visible in all models and must not be discarded. Therefore, there is good support for stating that the changes in the equipment have been effective in improving the ability to find nuclear particles in the area.

As for the multiple changepoint search, the two peaks in 2003 and 2006 are still among the detected ones, with, again, a preference for the first one in the temporal model and for the second one in the fixed effect and spatial model. In addition, a further change in 2012 is detected when a binary segmentation algorithm is implemented. The third change point is very close to the end of the series, therefore conclusions must be drawn with a special care; it gives a hint of a decreasing intensity, which could be related to the offshore retrieval campaign, suggesting a reduction of the arrival of particles on Sandside beach.

5.7.2 Inclusion of extra information

In this Chapter, we also bring some novelty with regard to what has been done so far, as we take a first step towards the inclusion of external knowledge to potentially improve the models in order to explain the phenomenon under study better.

First of all, we add two possible covariates, the distance to the nuclear discharge outlet that is presumably responsible for the particle spreading offshore, and the distance from the low water level; we refit all the models and

apply all our methods including one covariate at a time. In general, we can say the distance from the low water level has a scarce effect on the changepoint detection, while the distance from the nuclear discharge outlet leads to a preference for the changepoint in 2003. Apart from this effect, the PT method (both in a single and multiple detection context) shows no changes when either covariate is included. The effect on the BF based search and on the simultaneous approach is negative as results become even more conservative. A comparison of the DIC values (that depend on the number and location of the detected changepoints) shows the preferred options are the temporal model with no covariate or with the distance from the low water level, or the fixed model with the distance from the nuclear discharge outlet. Model 3 and 4 have higher DICs because of the inability to detect significant changes.

Then, we exploit knowledge concerning the two changes in the equipment to set informative prior distributions on the number or locations of the changepoints. As for their number, different peak heights on $m = 2$ are tested with the simultaneous approach. This leads to a substantial increase in the method performance, as regards the number of changes: the conservatism is overcome, two changepoints are detected, results are consistent about the changepoint locations and, above all, when imposing a stronger prior the changes in the equipment become significant even with more complex models. For the first time, we detect changepoints with the spatio-temporal model. Fixing an informative prior on the number of changepoints has a more positive effect than a prior on the changepoint locations. When setting peaks corresponding to 2003 and 2007, the only remarkable modification in the results concerns the PT method: with a strong prior, a changepoint in 2003 is detected with Model 4. No other substantial changes or improvements take place; in general, the changepoint in 2003 is preferred to the one in 2006/2007. This is probably also due to the fact that the change in the equipment that took place at the end of 2002 is more radical than the second one (see Section 5.1).

Further steps in the analysis of the process should extend the inclusion of available information to marks, such as the depth in the sediment or the radioactivity level, and focus on finding the best model for the data.

Chapter 6

Conclusions and Final Discussion

Detailed concluding remarks regarding specific aspects of our work can be found at the end of each Chapter. In this final Chapter, we firstly summarise the project and the main findings. Afterwards, we highlight the novelty and contribution of our work to the fields of changepoint analysis and of point process analysis and we motivate the choice of a Bayesian approach. Lastly, a few hints at possible further directions for the study and the most recent developments are outlined.

6.1 Work review

Our work aims at developing new methods for a changepoint analysis on the inhomogeneous intensity function of a spatio-temporal point process. We consider the most general case of multiple unknown changes, and are interested in both detecting the change locations and estimating the change type and its magnitude. Dealing with spatio-temporal data, the estimated intensity for each time segment is a two dimensional pixel image. Estimates of the segment parameters are not always the first goal of a changepoint analysis, as sometimes the interest only lies in detecting where the changepoint lies, however our method also provides accurate estimates for a wide range of problems.

6.1.1 Assumptions

The assumptions and restrictions that need to be made when using our methods are not strong. The process can be inhomogeneous and the intensity function is only constrained to be smooth. Any type of change over time can be detected: in scale, in spatial distribution or in both. Any prior setting is acceptable and only influences the total computational time, which is still feasible and can be further improved thanks to recent developments in the INLA methodology, if needed. Data are Poisson distributed in our work but may follow any distribution. There is no independence assumption except between time segments. Dependence can be both spatial and temporal, either small scale dependence or wide and smooth, either strong or weak, as long as all the parameters can be assumed to belong to a Gaussian Field. There is no limitation on the number of changepoints and reasonably weak assumptions on their locations (they have to be 'not too close' to each other). Therefore, this method covers a very wide range of real situations.

6.1.2 Work summary

We start by presenting the motivating issues which include both theoretical and practical questions.

As for the theory, we want to know what happens if a changepoint analysis is run on a spatio-temporal point process instead of traditional time series: first of all we have three dimensions, two spatial and one temporal, and we want our method to be able to keep the information about all of them; secondly, we can have different types of change over time and our method should be able to detect any of them and, ideally, to distinguish between them; besides, the dataset is quite complex and a long computational time may be required to obtain results. The other theoretical assumption that is usually made in changepoint analysis is that data are *i.i.d.*. If they are not, spatio-temporal data can show many types of dependence, both in space (between events at a specific time point) and in time (within time segments); in particular, when temporal dependence is allowed, traditional changepoint detection techniques do not offer a solution as, except for trivial situations, the segment marginal likelihood is not tractable. This generates a need for

fast and accurate approximate computational methods.

As for the practical aspect, we have an interesting dataset concerning the collection of radioactive particles on a beach, and the objective consists in understanding the behaviour of the underlying process over time, with particular focus on two changes in the particle detection equipment that have desirably marked an increased ability to find the particles, and on an offshore retrieval campaign that should have recently reduced the arrival of particles onshore.

As a second step in our work, we briefly present the three main topics our study is built on: point processes, INLA and changepoint analysis. We give a general introduction to all of them and present the most recent works in those fields, then we focus on the aspects that are most useful for our project. As for point processes, we introduce the class of spatio-temporal Log-Gaussian Cox Processes, a broad and flexible class of models particularly suitable for environmental applications. As for INLA, after a general introduction we explain in detail how the fitting of a LGCP works and how it is possible to overcome the intractability issue. As regards changepoint analysis, the most recent challenge is of particular interest for us, concerning how to include temporal dependence in time series data.

From Chapter 3 on, the contribution of our work is presented. We first give a few options for setting the prior distributions on number and locations of the changepoints; we introduce four increasingly complex LGCPs for both a single and a multiple changepoint detection; then, after obtaining the posterior distribution of the changepoint locations we propose some different methods for taking decisions on which changepoints are significant and which are not. Lastly, we present two methods, an iterative and a simultaneous one, to carry out a multiple changepoint search.

A complex simulation study follows, where the performance of our models and methods, the accuracy and the computational time of the INLA methodology are evaluated. We cover a wide range of real situations by generating both *i.i.d.* and time dependent data, both from a homogeneous and an inhomogeneous process, with zero, one or multiple changes; we also try all types of temporal change, in scale, in spatial structure and in both. In general, our method proves to work; it suffers from too much conservatism when using

some of the methods, still it is overall satisfactory; whenever changepoints are detected, the methods are very accurate in estimating the changepoint location(s) and producing good estimates for the process intensity at every time segment.

As a last stage, all the proposed models and methods are applied to the motivating dataset in order to answer the motivating practical questions. Firstly, we reproduce the study carried out on simulated data, then we extend it by adding covariates and introducing informative prior distributions on number and locations of the changes. In general, we find sensible results, as the equipment changes correspond to a significant increase in the intensity function of the process, while a decrease toward the end of the series gives a hint for effectiveness in reducing the quantity of particles that arrive onshore.

6.1.3 Meeting the research questions

We have positively answered all our research questions, both theoretical and practical. Our approach is effectively able to detect any type of changepoint over time in the intensity of a spatio-temporal point process, even when spatial heterogeneity, spatial dependence and temporal dependence within segments are allowed. The computational time is satisfactory, as results only take a few minutes for every dataset, and this is very useful because it allows many different models to be fit and model comparison and selection to be run in a feasible time despite the complexity of the data. Results are in general good (improvements in some of the methods are left to further studies) and the application to real data leads to sensible interpretation of the phenomenon under study.

One of our motivating questions is to look for potential changepoints at known locations (equipment changes). We firstly address the question using the general technique for unknown locations for two main reasons. First of all, the other practical question concerns unknown changes and needs to be addressed this way; secondly, the case of known changepoints can easily be derived as a special case of our method by imposing informative priors (see Section 6.3 for a discussion), thus we prefer to propose a method that is able to cover a wider range of issues. We also showed an example of what happens

in the special case of an informative prior on 2 changepoints and of a high prior probability of having a changepoint corresponding to the equipment changes. In general, results have not been affected by the priors as they were already very good; it is worth mentioning that an informative prior on the number of changepoints has substantially increased the ability of the simultaneous approach to detect changes.

6.2 Contribution of the work

Spatial statistic and changepoint analysis are two well established areas of statistical research, but they do not meet often. A combination of changepoint analysis and point processes is even rarer, and we have very few examples of this in recent literature. These examples all deal with a temporal process, and it usually is a simple Poisson process; nevertheless, analyses are complex. The extension of changepoint analysis to spatial studies is uncommon, therefore it is even rarer to find works focused on looking for changepoints in the parameters of a spatio-temporal model, irrespective of the type of available data. In particular, as far as changepoints in spatio-temporal point processes are concerned the subject is totally unexplored. Nevertheless, questions and issues are raised, as is the case of our motivating dataset, that need to be answered by developing new methods and extending the existing ones.

A changepoint analysis on spatio-temporal point processes, therefore, would be a novelty itself in statistical studies. It would extend the currently used methods even if it were dealing with a very simple case, like a homogeneous Poisson process with *i.i.d.* point patterns within segments. Our work aims at doing more than providing an extension of simple models: it aims at developing methods able to cover a wide range of real situations.

The second novelty is the inclusion of dependence within time segments; as we deal with spatio-temporal data, we include both spatial and temporal dependence between data points. In the simulation study presented in Chapter 4, we show results for models allowing for temporal dependence between point patterns, for spatial dependence between the points of a single point

pattern, and for both.

The third novelty is the class of models we use, Log-Gaussian Cox Processes, thanks to which we cover the case of inhomogeneous processes, and the possibility of spatial clustering and/or repulsion.

Moreover, we study changes in the scale of the intensity function (*i.e.* a change in the expected number of points per pattern), in its spatial structure (*i.e.* a change in the spatial distribution of points, with the same expected number of events) and in both. This means our methods are able to cover an extremely wide variety of real situation, and in particular many datasets with a complex behaviour that are not easy to model and describe.

In addition to all this, our work provides a useful new case study of the INLA performance. INLA is a young methodology and it is still unknown to a wide part of the global statistical community. The number of case studies is increasing but currently limited. In particular, there is a very small number of published papers on point process models fitted with INLA and hardly any work on changepoint analysis using INLA. Therefore, our work shows a new way of exploiting the power and potential of the INLA approach.

As mentioned in Chapter 1, in the special case of a spatially homogeneous spatio-temporal point process, the same results can be obtained in a simpler way by running a changepoint analysis on the time series made by the number of points at every instant. This is hardly ever the case in real situations, though, and our method is much more general as it not only considers how many changepoints are present, but also where they occur. Therefore, if a process is inhomogeneous or if we are not sure about what kind of process we are facing, the use of our method avoids the risk of missing changes in the spatial distribution of the points and brings more information by maintaining the spatial dimension of the dataset.

Lastly, we add a few details that are often avoided in Bayesian inference: despite our methods should theoretically work with any prior distribution, we show it by running some sensitivity analysis on our real dataset and comparing posterior distributions deriving from different prior settings.

A further topic might be to face the issue of dependence across segments. This is scarcely of interest in the situation of an abrupt change, where it is sensible to assume independence after a changepoint occurs, but can open up

to other possibilities such as gradual changes. Still, our study is a consistent step forward and a big challenge even without covering the case of dependence across segments; moreover, as we use Log-Gaussian Cox Processes and assume changes to be due to an external factor such as a change in the equipment, the assumption of dependence within segments only fits the situation well.

6.3 Discussion on the Bayesian approach

We build a Bayesian approach to face this complex changepoint issue. The main reason is that we want to be able to incorporate external prior knowledge in the model. In many real applications, experts of the phenomenon under study have ideas of where, or approximately where, a changepoint might be. Frequentist approaches, though, are very rigid, since only two possibilities are considered. In an unknown changepoint search, all time points have exactly the same probability of being a changepoint; in known changepoint testing, only one (or a small number of) changepoint location(s) is tested, and if there is an extra, unexpected changepoint it will be missed. With a Bayesian approach, prior belief on the changepoint location(s) can be included and the strength of this belief specified, as we do in our real data application; in an extreme case, the prior mass may be concentrated on very few points, but if knowledge is not that strong, a higher prior probability can be assigned to a set of specific points, without excluding the other time points from the analysis. This avoids the risk to miss significant unexpected changes. A Bayesian setting substantially enriches the crude information given by the data and allows for more flexibility.

Secondly, the issue of including dependence is recent and challenging, and very few techniques are currently available; we have no knowledge of a fully likelihood-based approach able to produce accurate results in such situations. A Bayesian approach, combined with reliable approximate methods such as INLA, returns posterior distributions and estimates for any kind of model as long as the underlying assumptions hold. This way, we provide a method that is able to give results that, in the worst case (*i.e.* total absence of prior

knowledge) will equal the frequentist results that are currently unachievable in this context; in any case where even weak prior knowledge is available, likelihood-based conclusions will be improved by a Bayesian approach.

6.4 Hints for further studies

Our work combines recent literature from many different fields of statistics, therefore it can be faced from different perspectives; this is very stimulating, as each perspective gives suggestions for future directions and further developments.

First of all, our work consists in a Bayesian approach. Doubtless, the most important aspect of Bayesian statistics is the role of the prior distributions; still, in most works this is hidden under the carpet. In our study, the main goal that has been fulfilled is to be able to fit models with spatial and temporal dependence, and a sensitivity analysis has been hinted at in Chapter 5. One of the next natural steps is therefore to carry out a complete work on the priors that can concern the number of changepoints, their locations and all the effects hyperparameters; it would certainly be of interest to test different, more informative prior settings and check how strongly conclusions are affected by them. As for the priors on number and positions of changepoints, an alternative option is given in Fearnhead (2006) and Wyse et al. (2011); no motivation is given for that specific setting, though, apart from its property to reduce computation and increase the algorithm speed. Consequences on the ability to detect changes should be further investigated. Another, more informative setting can be given when there is knowledge about a possible location for the change: one value, or a small set of adjacent values, can be given a high *a priori* probability of being a changepoint.

A second filter for looking at our work is INLA. This approximate approach is proving so effective in many situations that is now often used even for non fully Bayesian analyses. People interested in cases studies where INLA is employed will find an original contribution here, as there is very little done in recent literature on point processes and even less on spatio-temporal extensions or changepoint detection. As for further work in this field, improve-

ments in the INLA settings can be made; in particular, it may be possible to use the recent Stochastic Partial Differential Equation (SPDE) approach to increase computational efficiency and precision of the approximations, and also to keep the information about the exact locations of the pattern points, that is only approximated with the grid approach. Work can be done about improving the Laplace approximation or trying different ways to approximate the integrals. In a broader perspective, alternative approaches to INLA can be tried, that allow more flexibility in the choice of the models for the effect (*e.g.* exploiting techniques from the field of regime-switching models).

Moreover, this work is of interest for all statisticians dealing with point process analysis. Spatio-temporal point processes are not widely used yet, and we provide a case study here. Note that in our work we assume the spatio-temporal process to have a separable structure; an extension to non separable models would certainly be of interest. When the perspective regards point process models, the interest often lies in finding good models for real data. As for the model effects, once the ability to include dependence is assessed it is possible to add any other effect easily, thanks to the additive structure of the chosen class of models. For instance, it can be of interest to add covariates, when available, and other fixed effects. Moreover, if the process is marked the mark can be included in the model as part of the response, and further studies can be carried out on the distribution of the mark(s) and its potential changes over time. Trying different models and adding effects also gives the opportunity to run model comparison and selection, where traditional (DIC) or new Bayesian tools can be proposed.

A wider perspective can also be taken, including our work in the general field of spatial statistics. It would then be interesting to consider the boundary issue. Spatial point process analysis already has tools for considering the so-called 'edge effect', when for example observations lack neighbours because of the limit of the observation window; they should be extended to the spatio-temporal case. Other border issues should be analysed, such as the presence of physical boundaries (*e.g.* in the particle dataset the presence of a cliff) that actually prevent the points from spreading in the corresponding direction and that may cause *e.g.* an involuntary accumulation of points.

Furthermore, this piece of work is of interest for temporal studies in gen-

eral, and changepoint analysis in particular. This is a specific field in time series analysis that does not often meet with other traditional approaches, for instance what is called trend analysis. It would be interesting to further extend the analysis to gradual changes in the intensity function, and compare its performance with a study of the spatio-temporal trend of the series.

Lastly, as the work is motivated by practical questions on a real dataset, it is possible to face this study from an applied perspective. This work can find applications in many fields: ecology, forestry, epidemiology, crime, Since the methodology has been well developed but the application only concerns a short time series with few points, we suggest the production of another case study with a larger spatio-temporal point process dataset.

Appendix A

Simulation - all figures

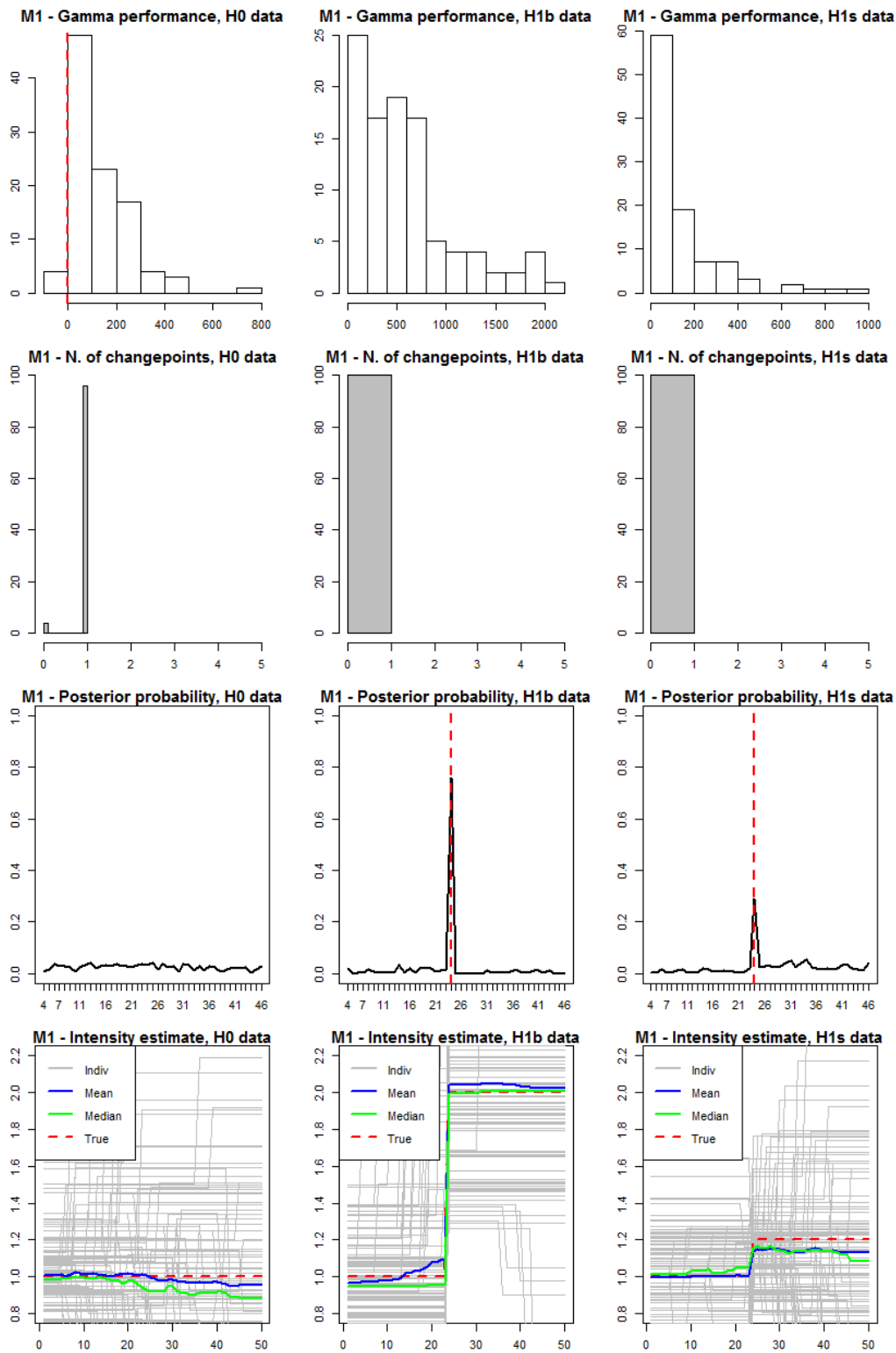


Figure A.1: Single changepoint search on AR(1) data, with the fixed effect model and the BF method

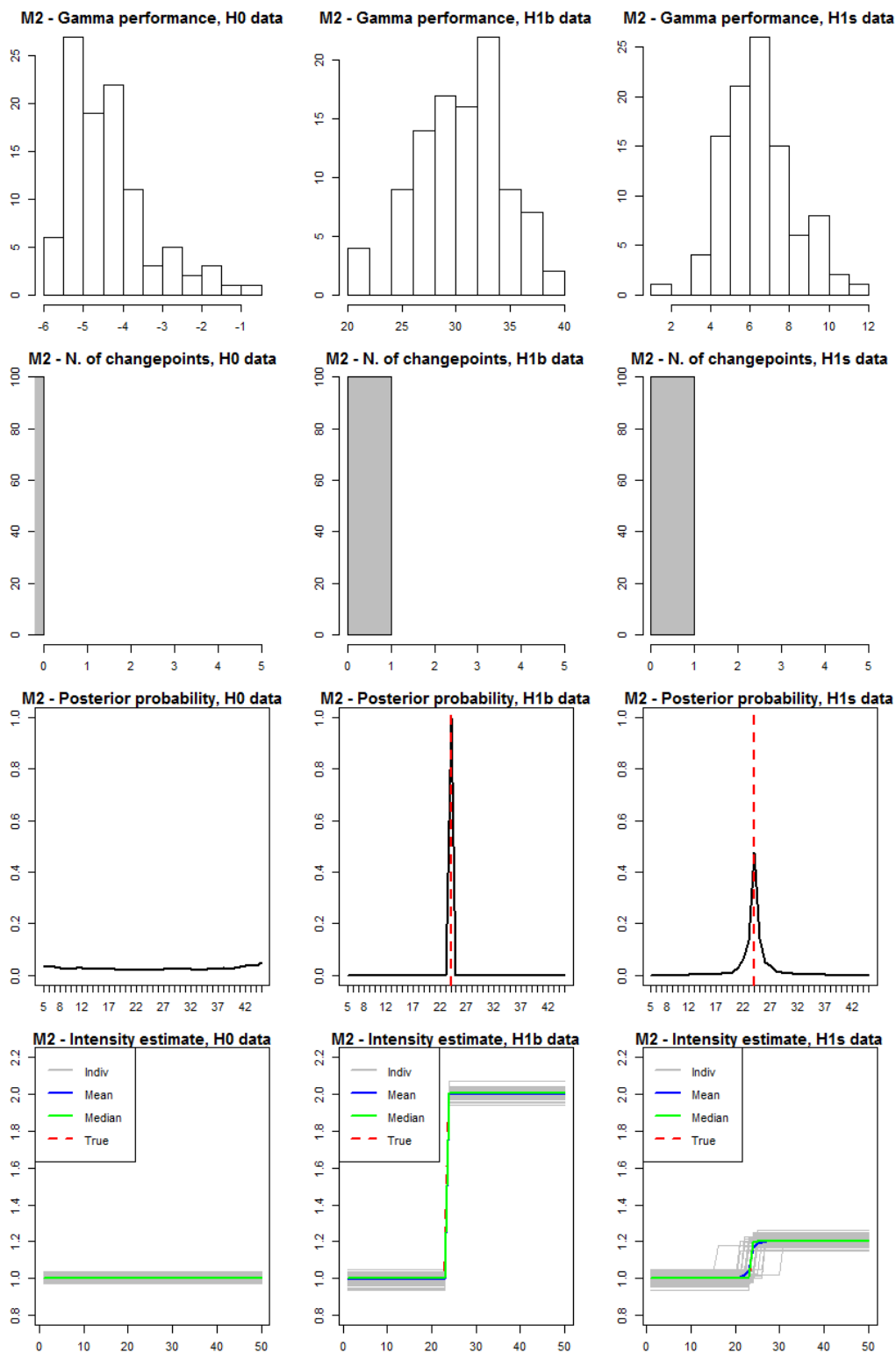


Figure A.2: Single changepoint search on iid data, with the temporal effect model and the BF method

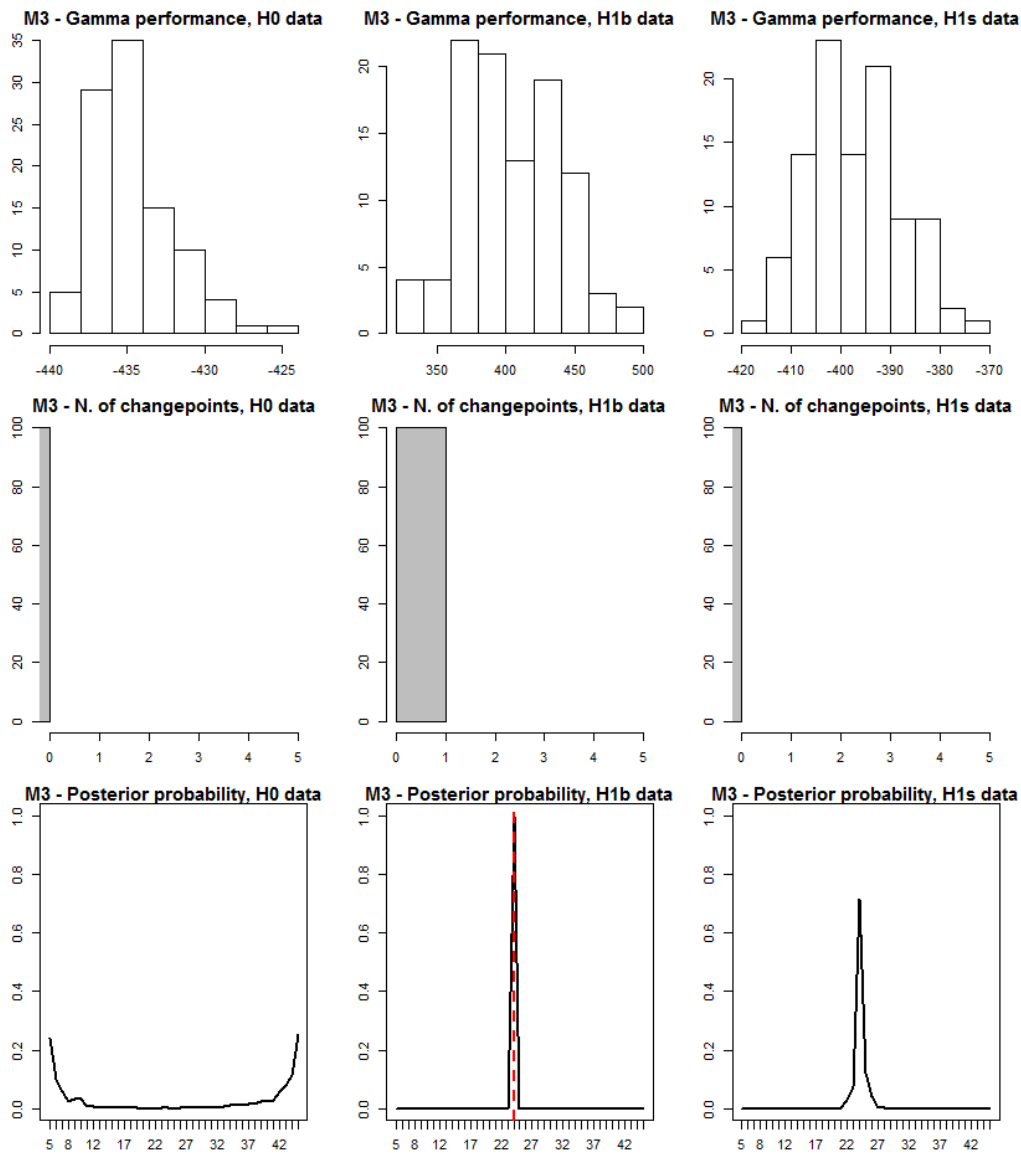


Figure A.3: Single changepoint search on iid data, with the spatial effect model and the BF method - Power level and location of the changepoint

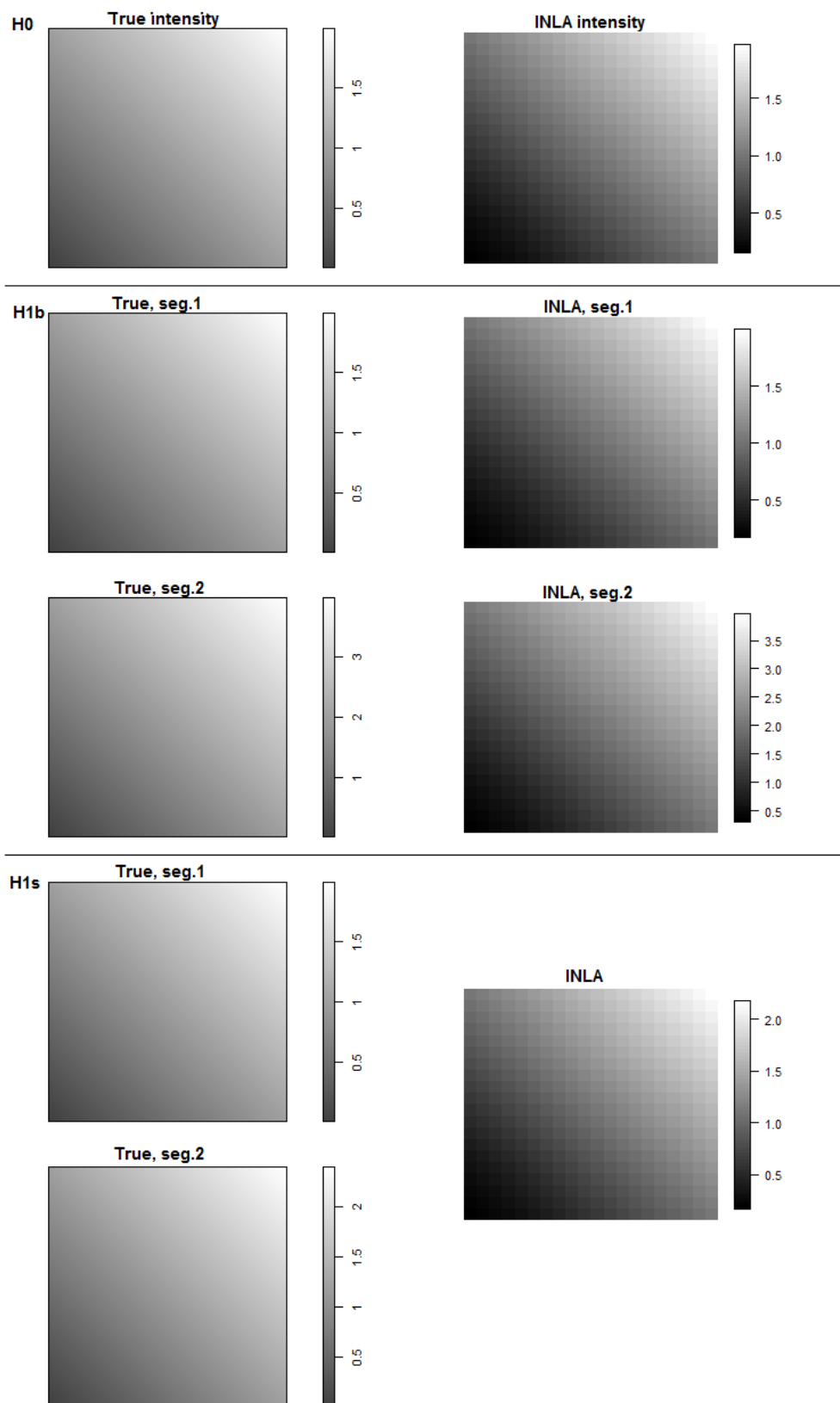


Figure A.4: Single changepoint search on iid data, with the spatial effect model and the BF method - Estimated intensities

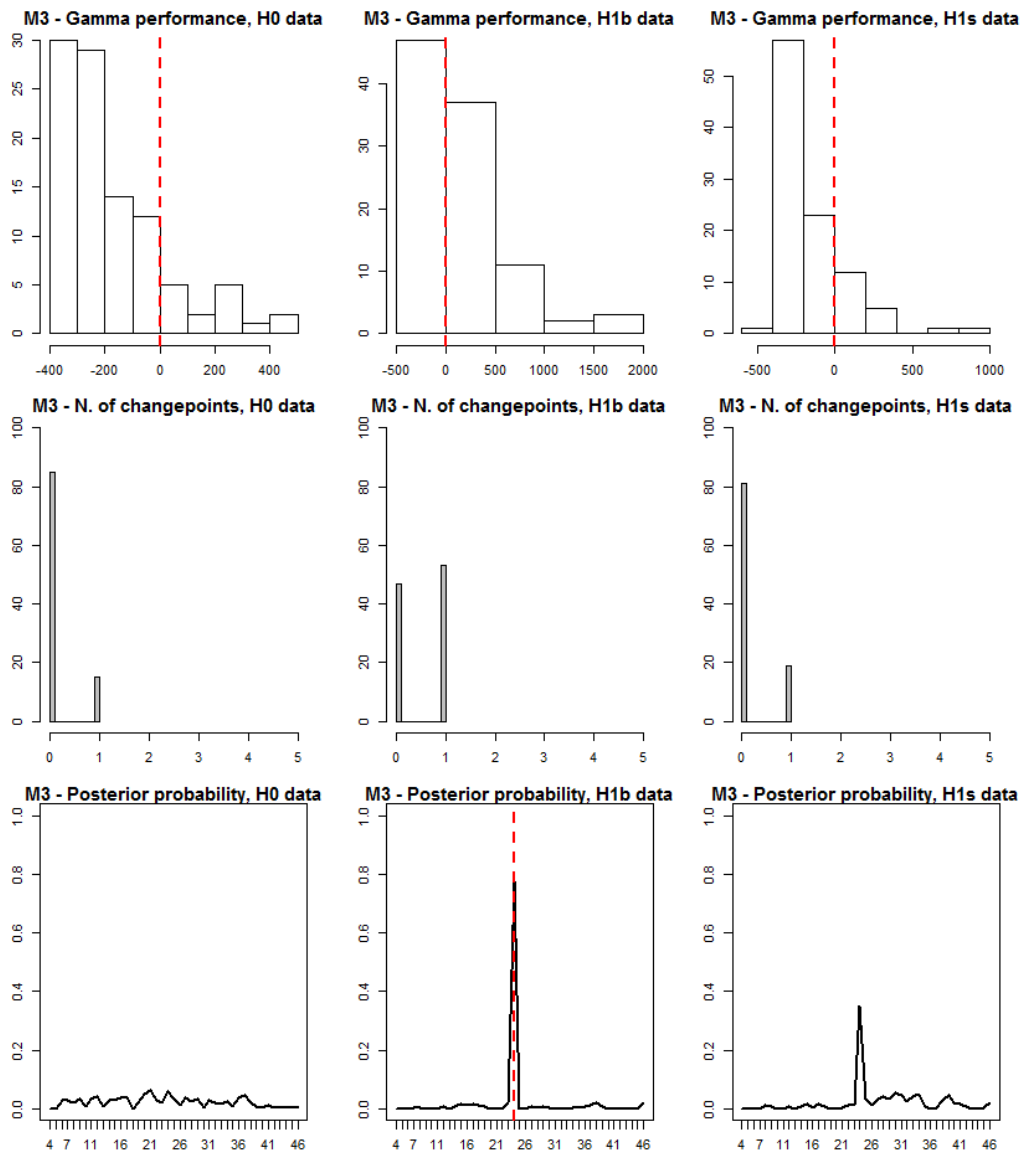


Figure A.5: Single changepoint search on AR(1) data, with the spatial effect model and the BF method - Power level and location of the changepoint

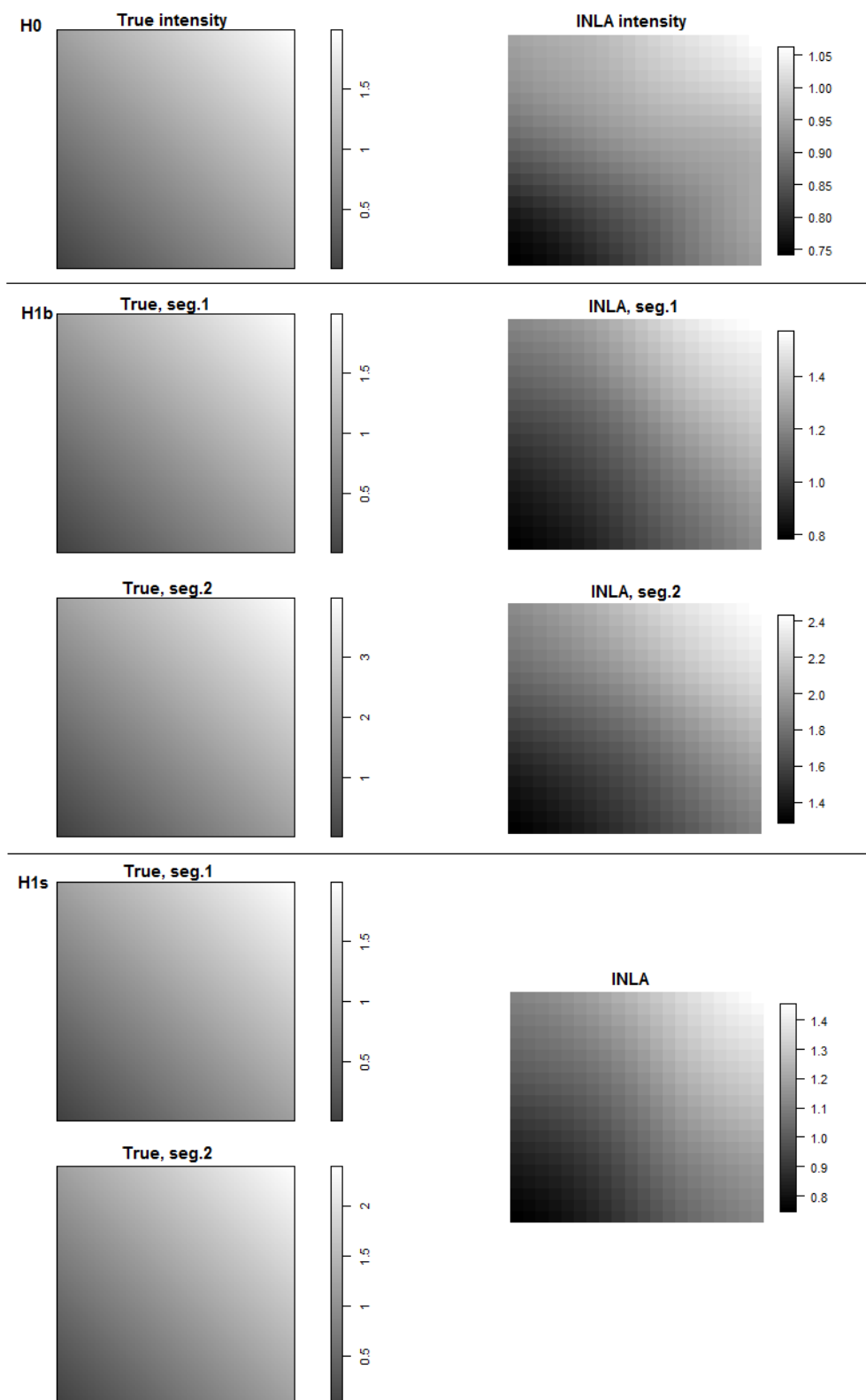


Figure A.6: Single changepoint search on AR(1) data, with the spatial effect model and the BF method - Estimated intensities

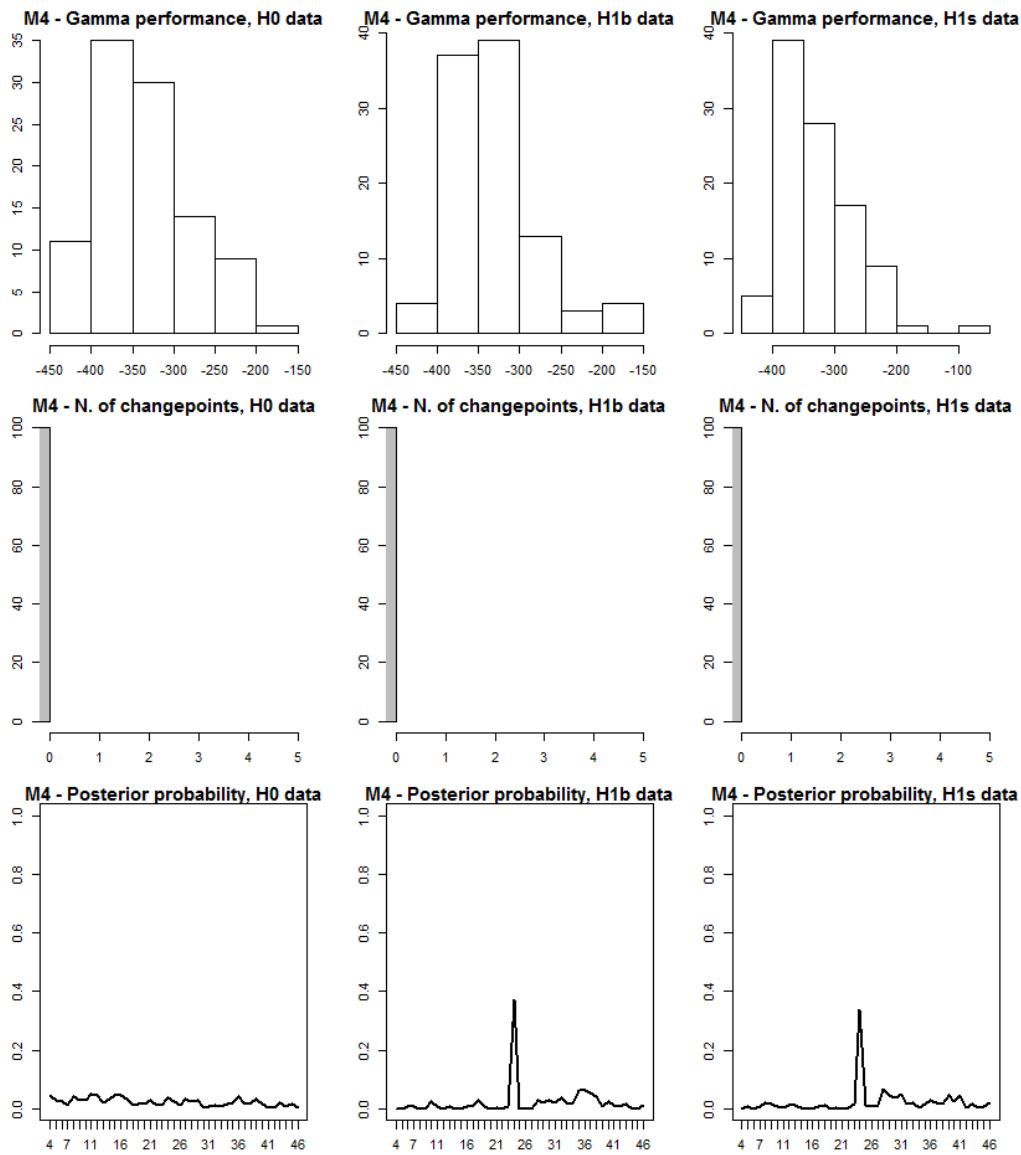


Figure A.7: Single changepoint search on AR(1) data, with the spatio-temporal effect model and the BF method - Power level and location of the changepoint

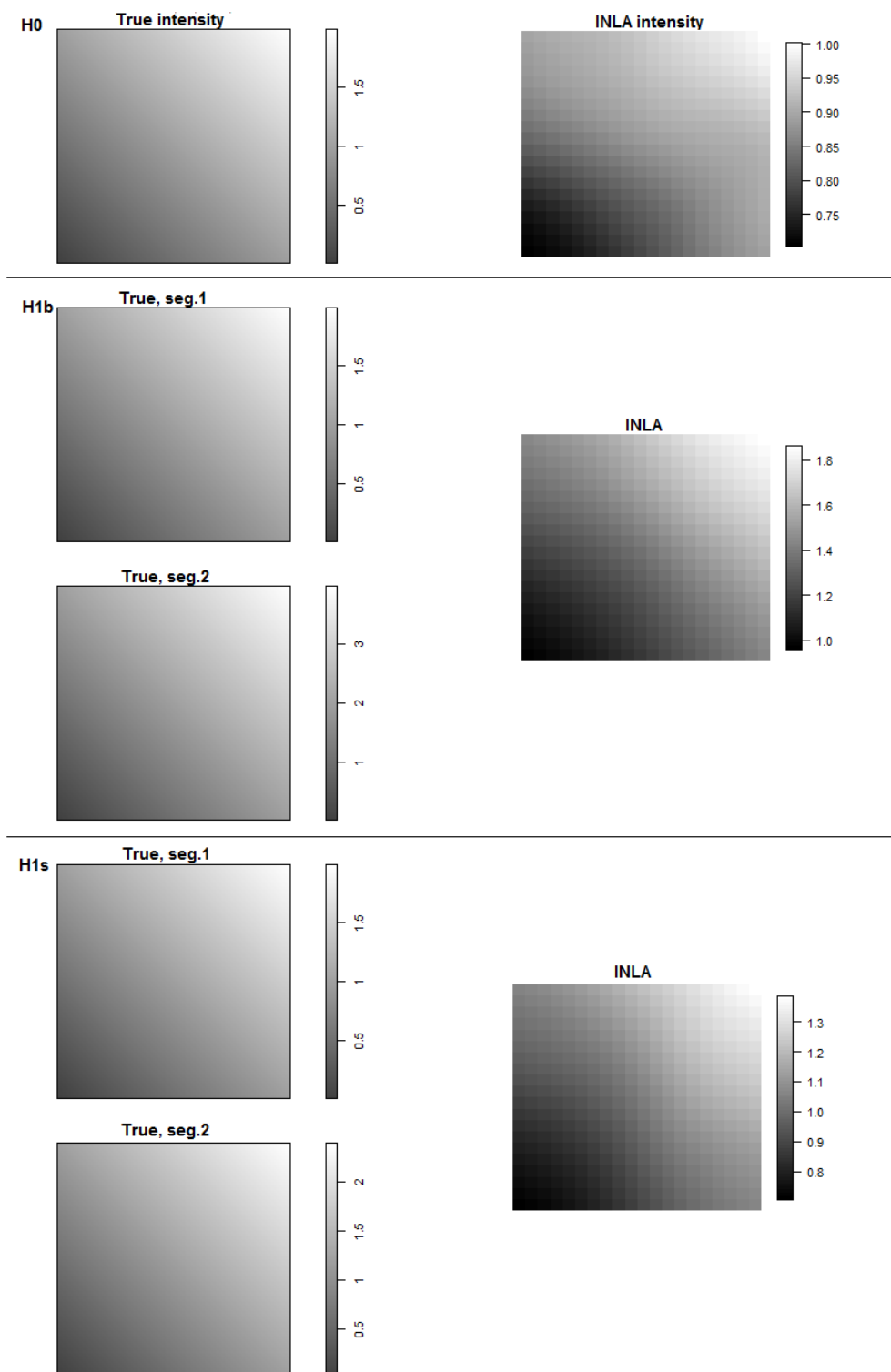


Figure A.8: Single changepoint search on AR(1) data, with the spatio-temporal effect model and the BF method - Estimated intensities

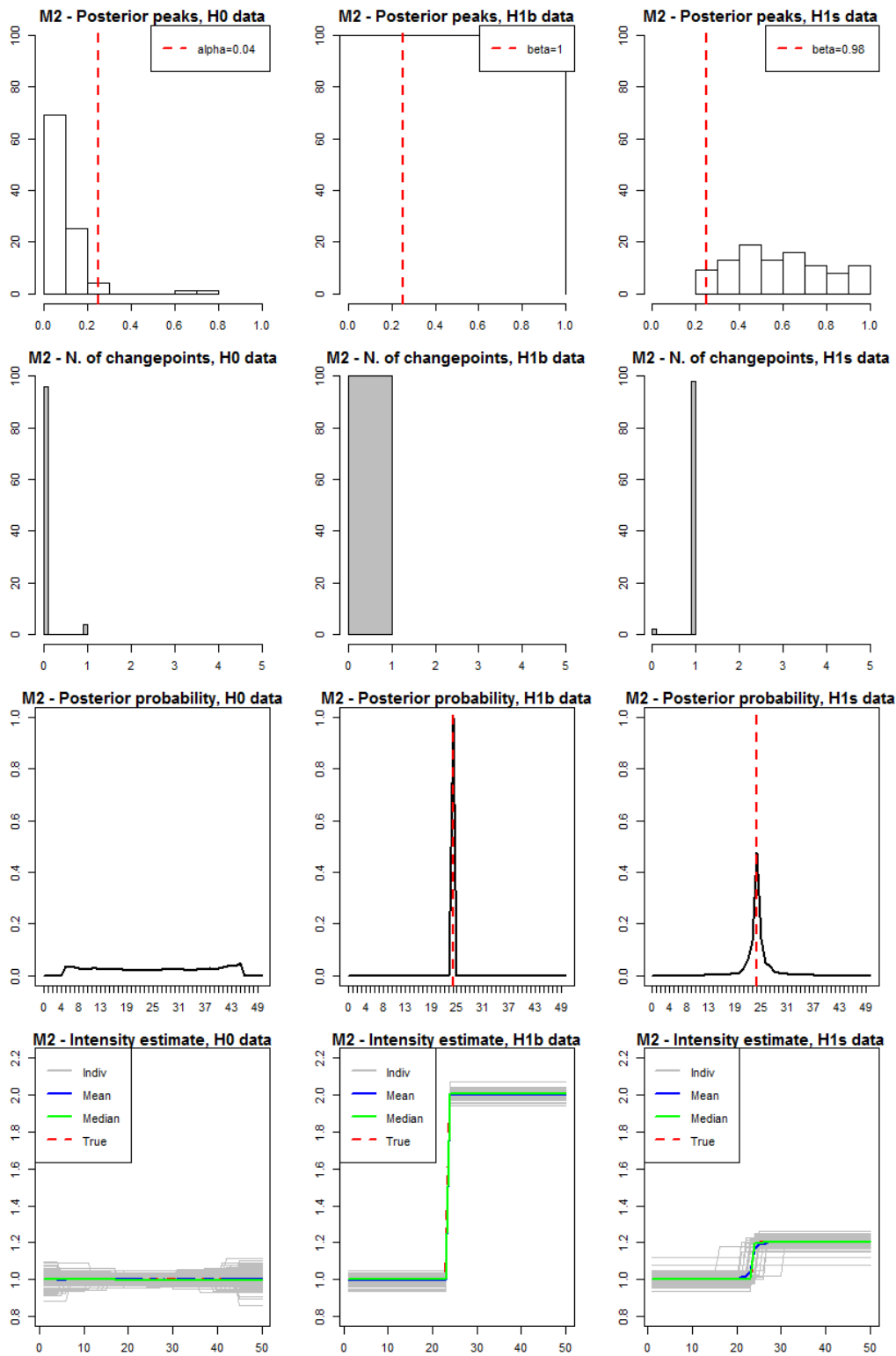


Figure A.9: Single changepoint search on iid data, with the temporal effect model and the PT method

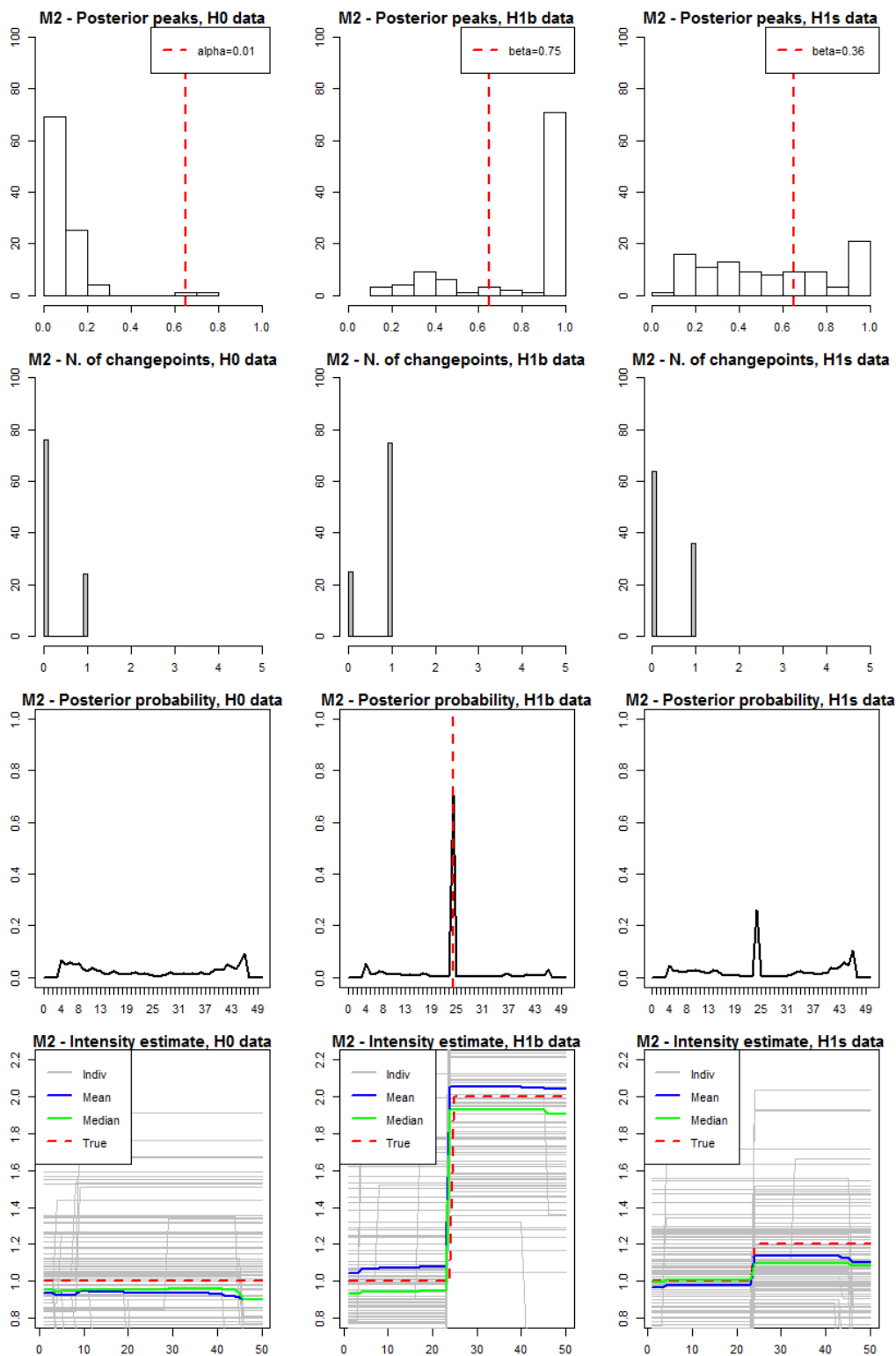


Figure A.10: Single changepoint search on AR(1) data, with the temporal effect model and the PT method

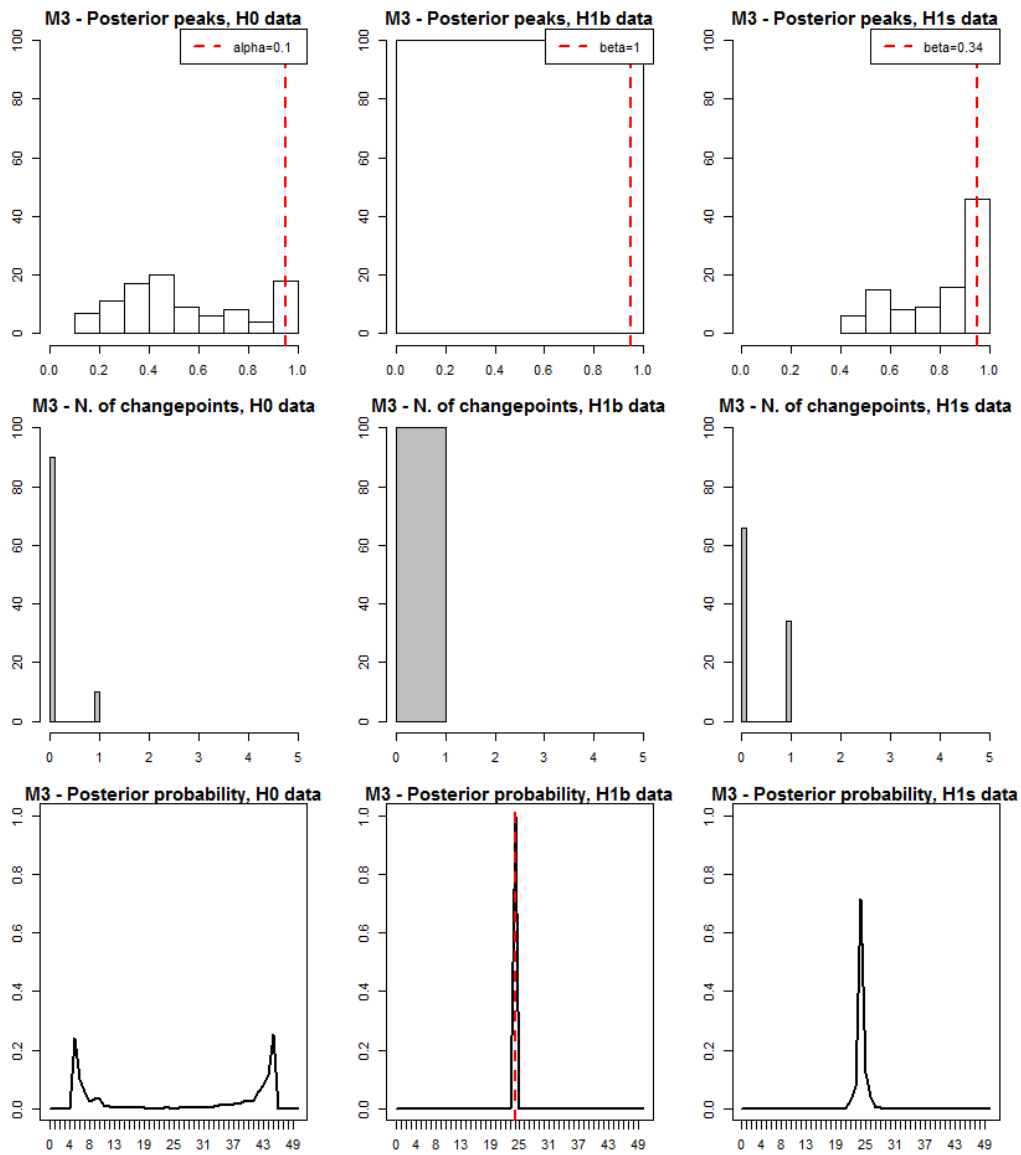


Figure A.11: Single changepoint search on iid data, with the spatial effect model and the PT method - Power level and location of the changepoint

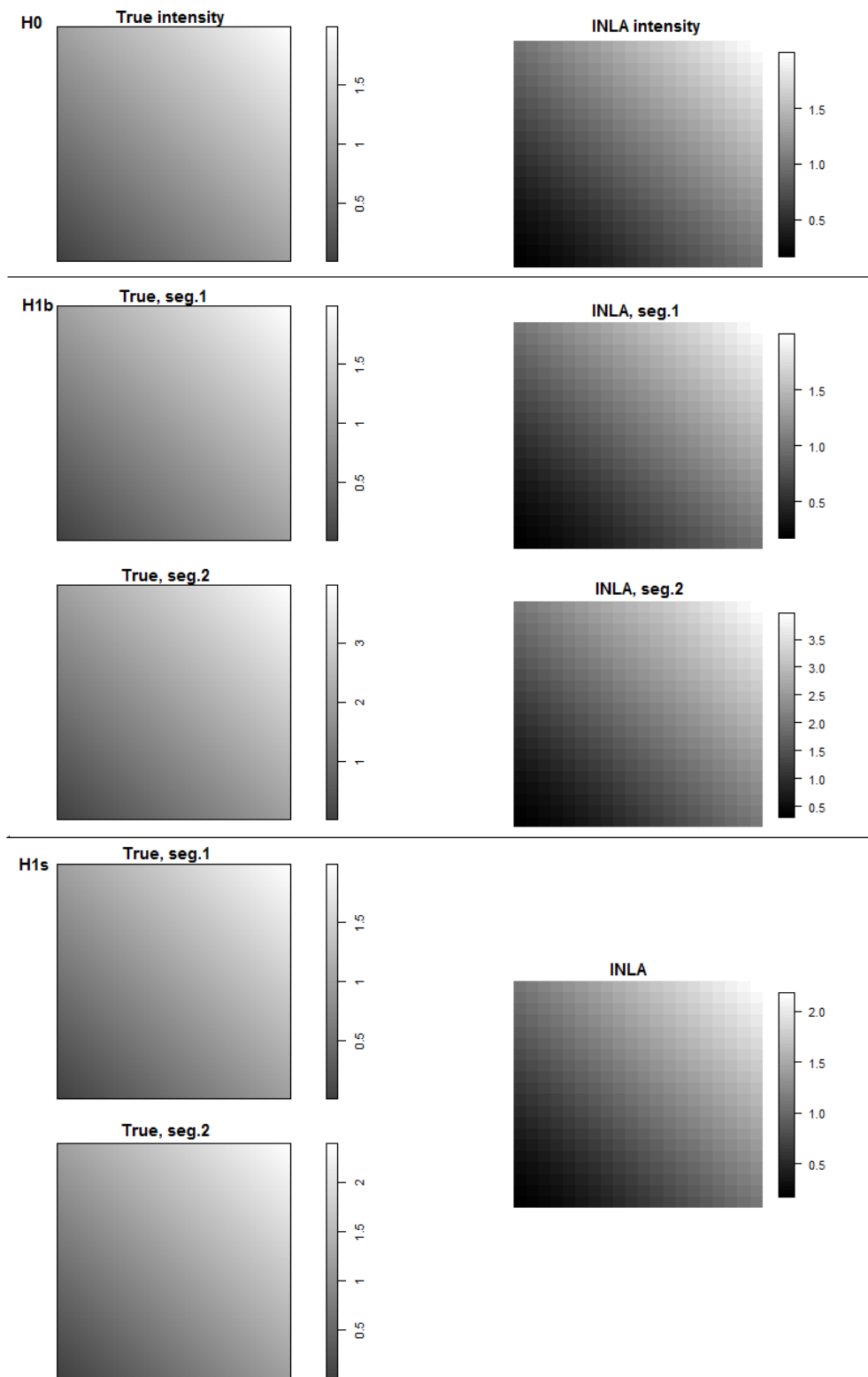


Figure A.12: Single changepoint search on iid data, with the spatial effect model and the PT method - Estimated intensities

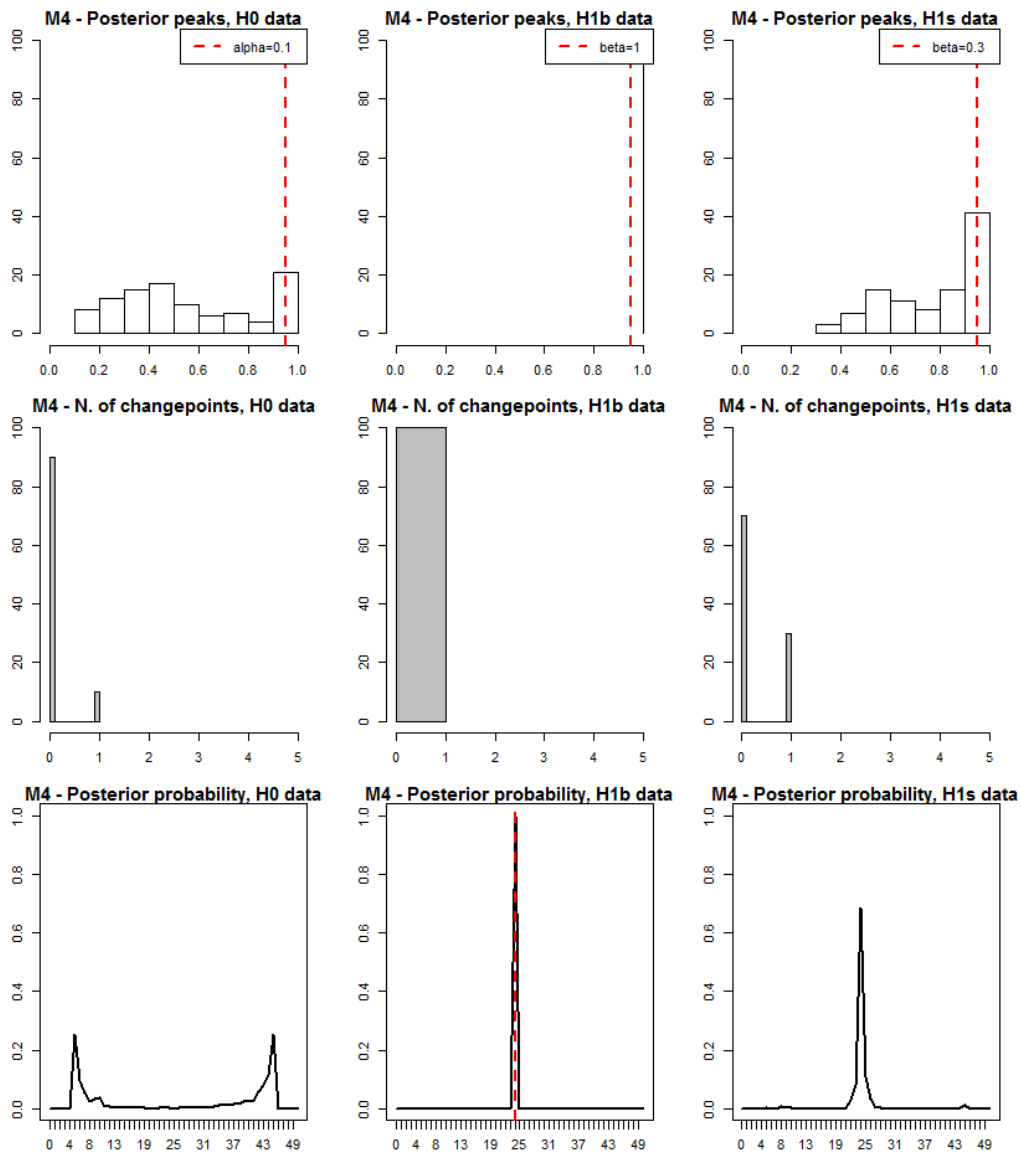


Figure A.13: Single changepoint search on iid data, with the spatio-temporal effect model and the PT method - Power level and location of the changepoint

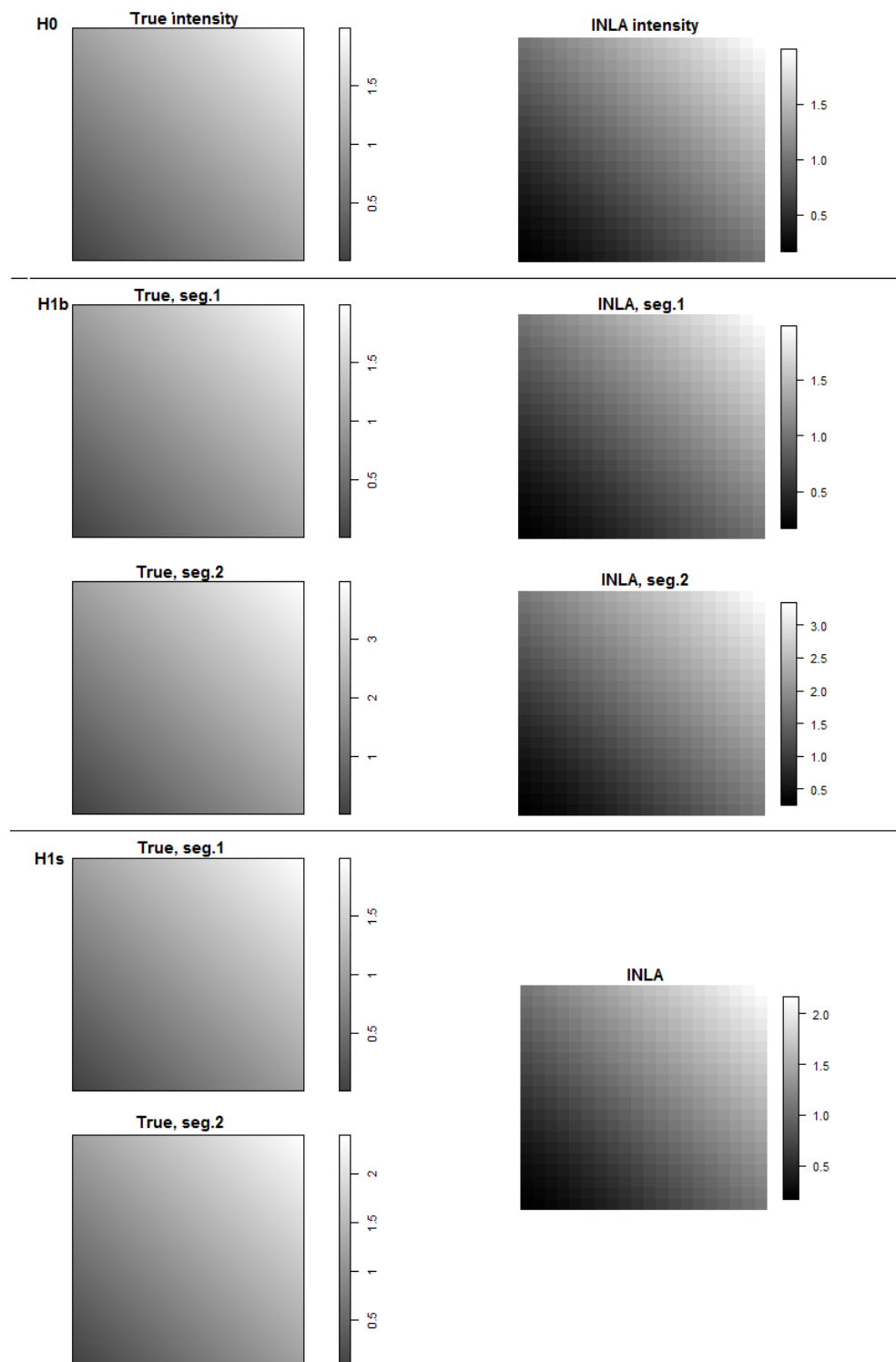


Figure A.14: Single changepoint search on iid data, with the spatio-temporal effect model and the PT method - Estimated intensities

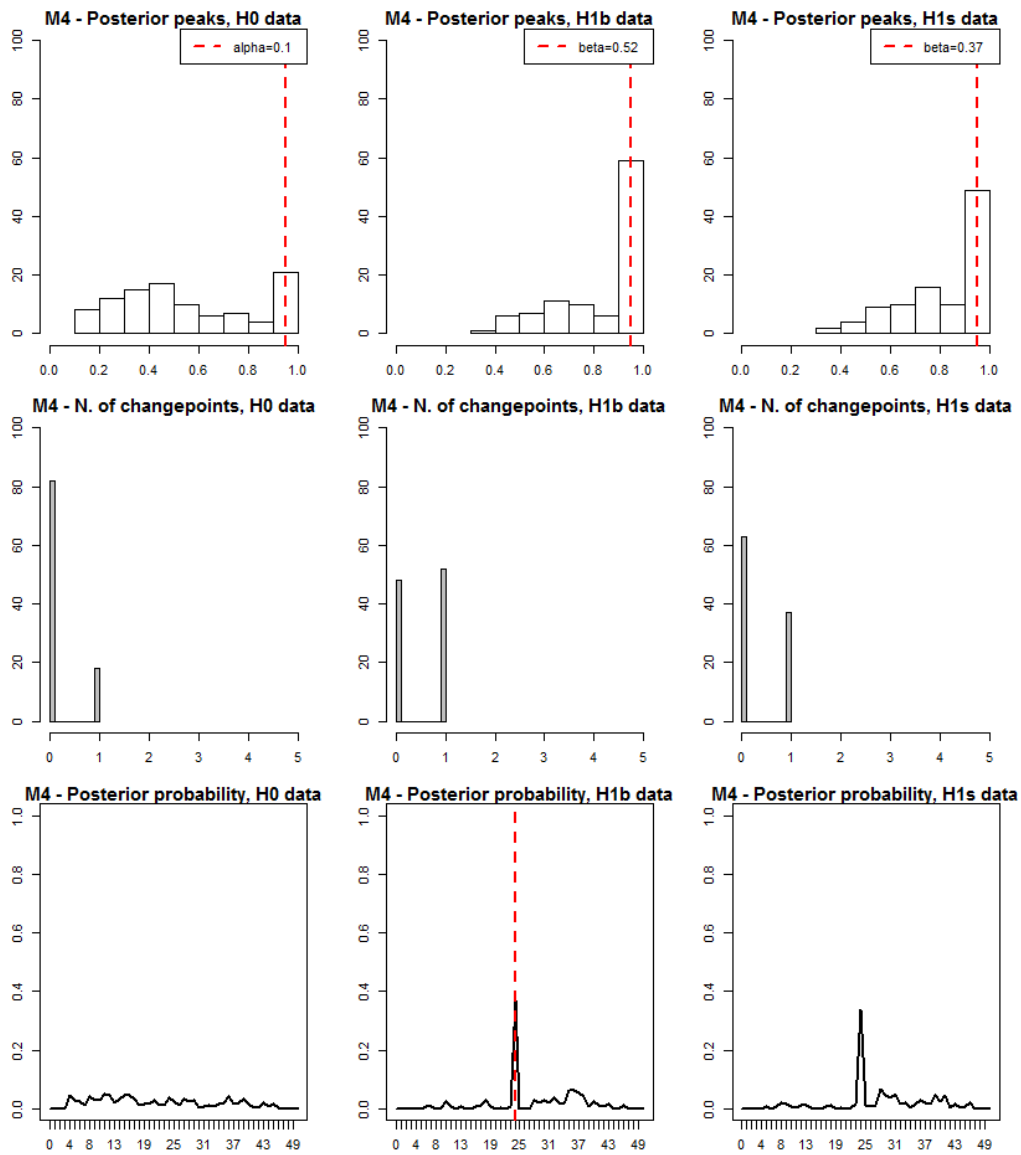


Figure A.15: Single changepoint search on AR(1) data, with the spatio-temporal effect model and the PT method - Power level and location of the changepoint

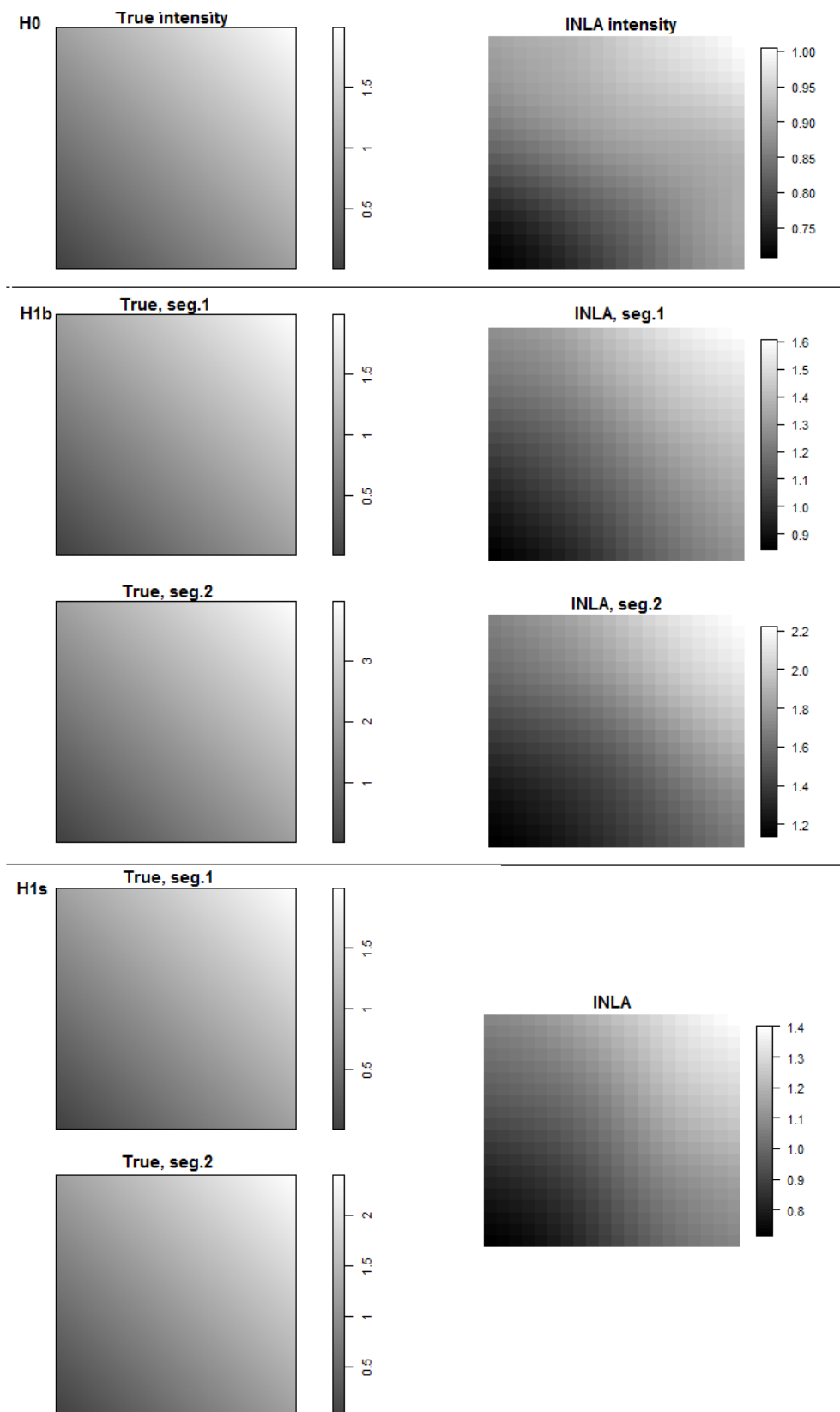


Figure A.16: Single changepoint search on AR(1) data, with the spatio-temporal effect model and the PT method - Estimated intensities

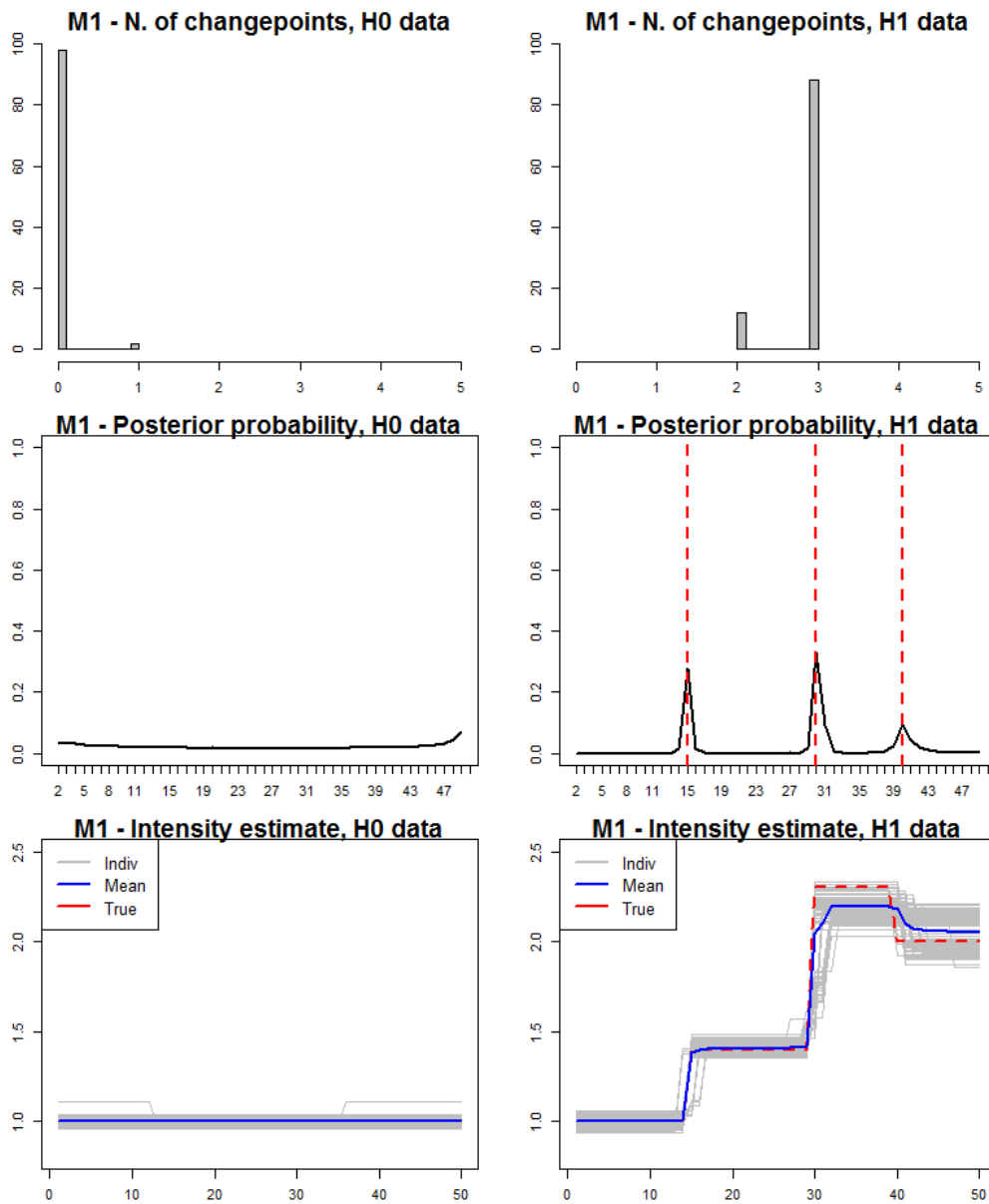


Figure A.17: Multiple changepoint search on iid data, with the fixed effect model and the BF method

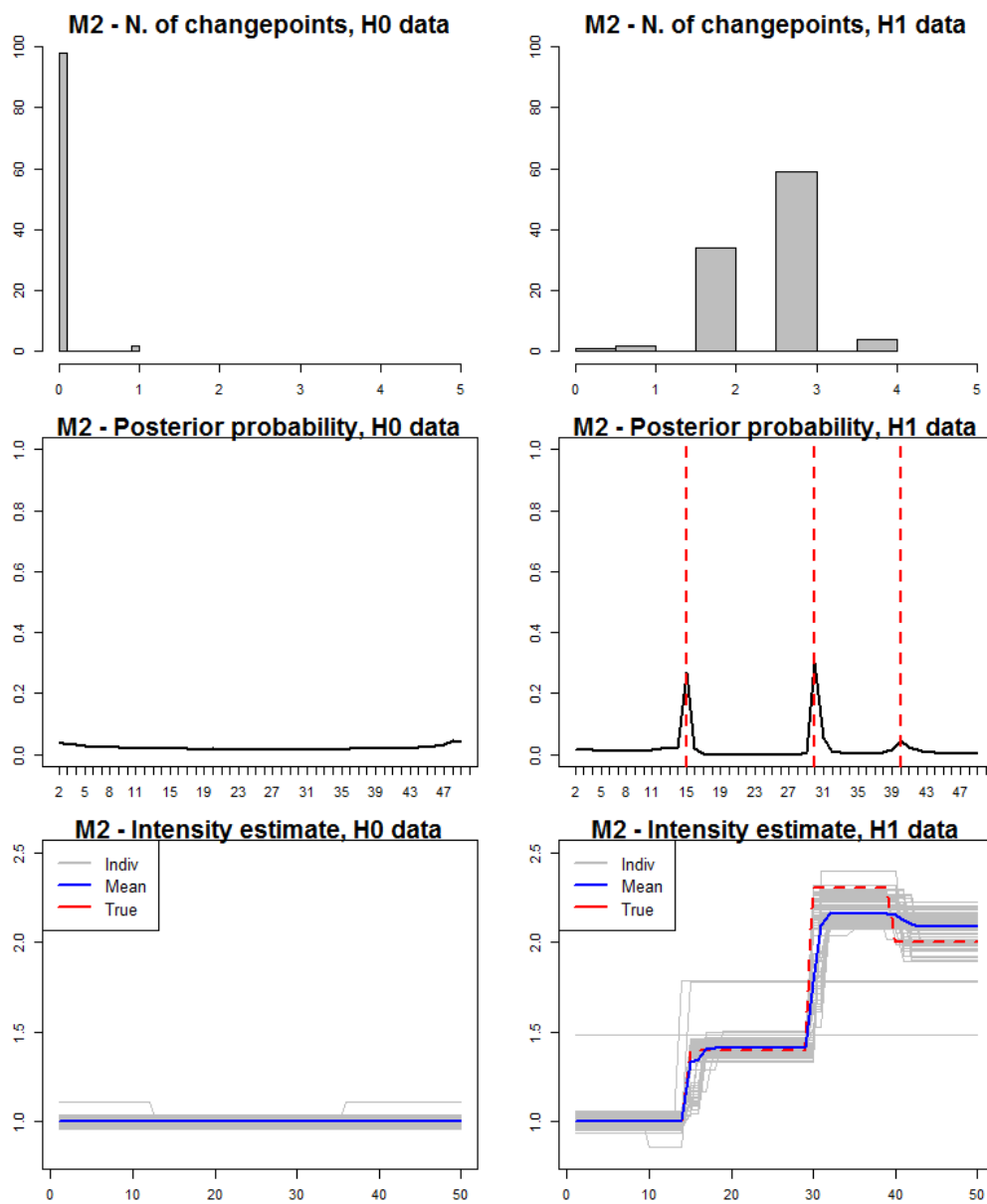


Figure A.18: Multiple changepoint search on iid data, with the temporal effect model and the BF method

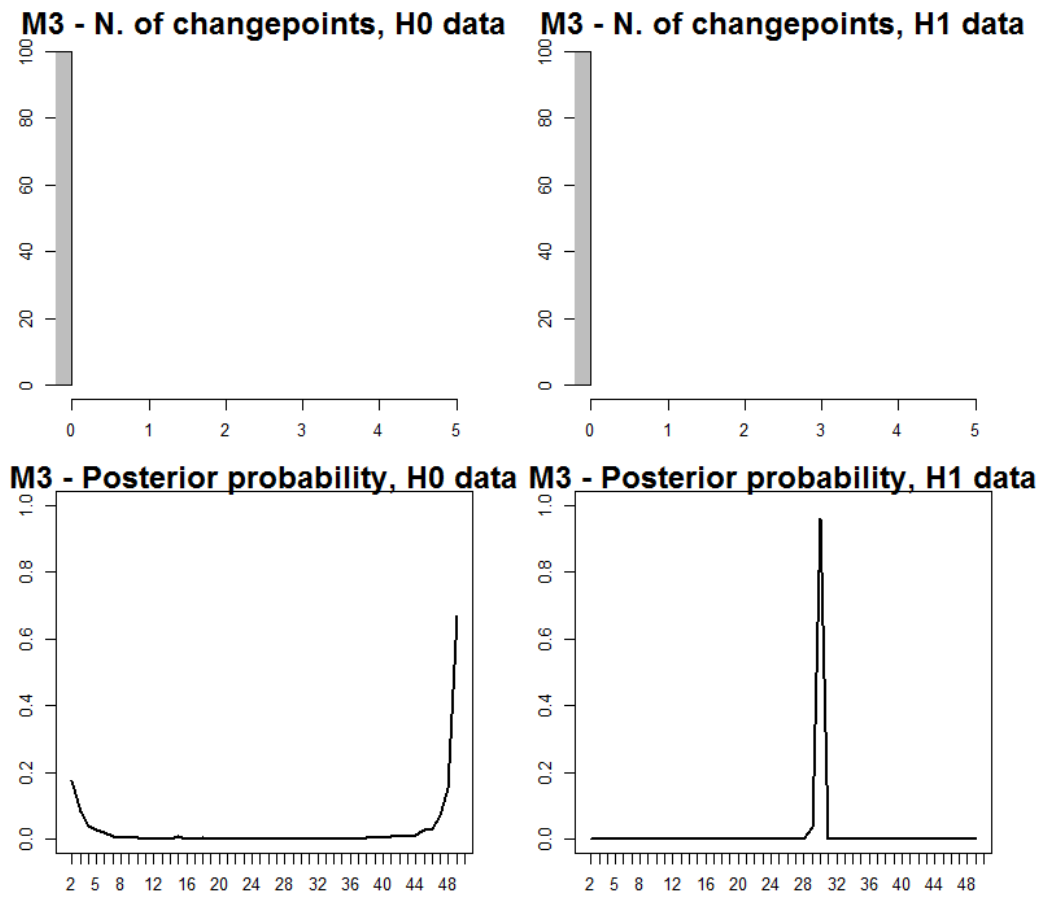


Figure A.19: Multiple changepoint search on iid data, with the spatial effect model and the BF method - Power level and location of the changepoint

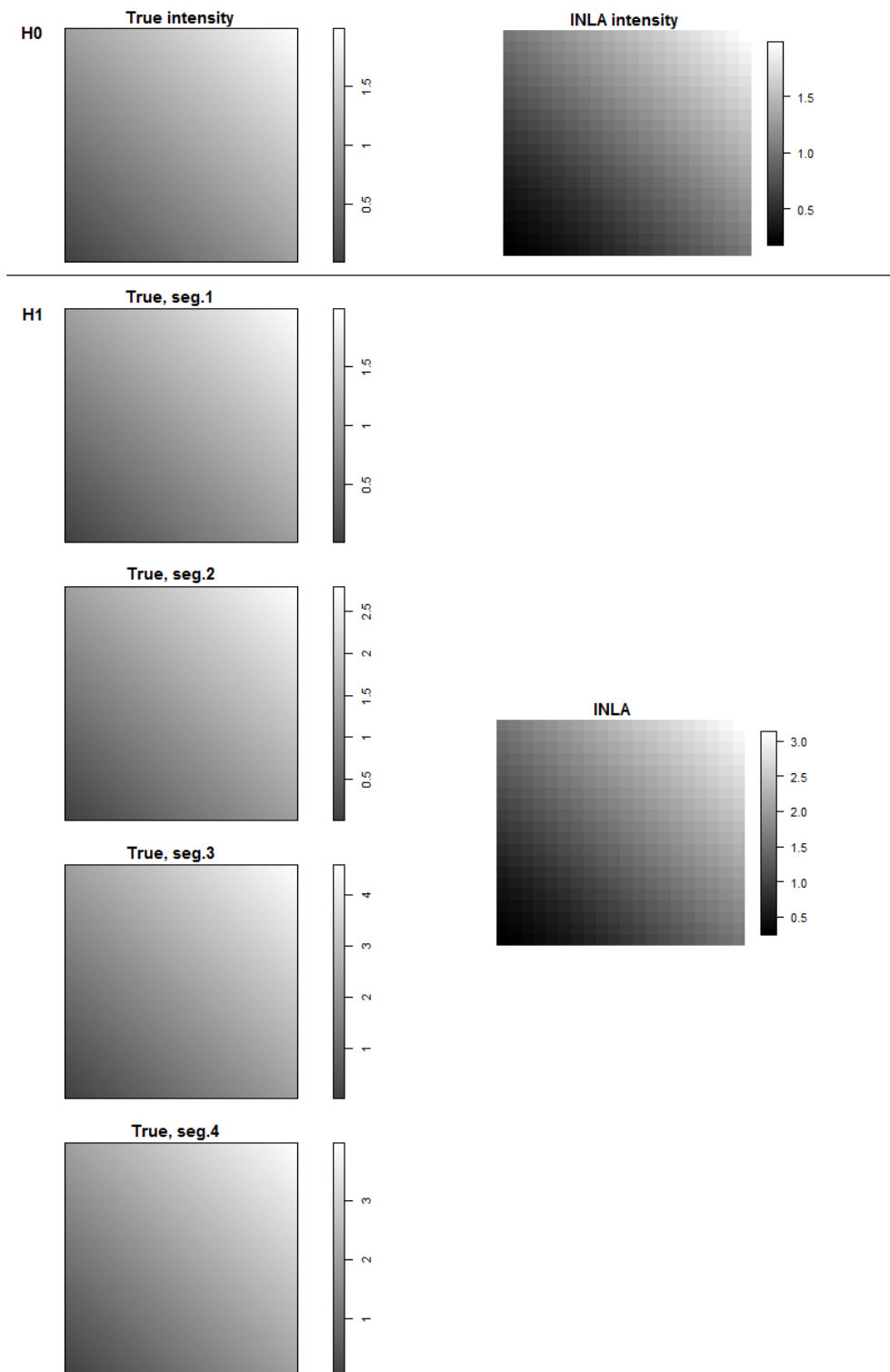


Figure A.20: Multiple changepoint search on iid data, with the spatial effect model and the BF method - Estimated intensities

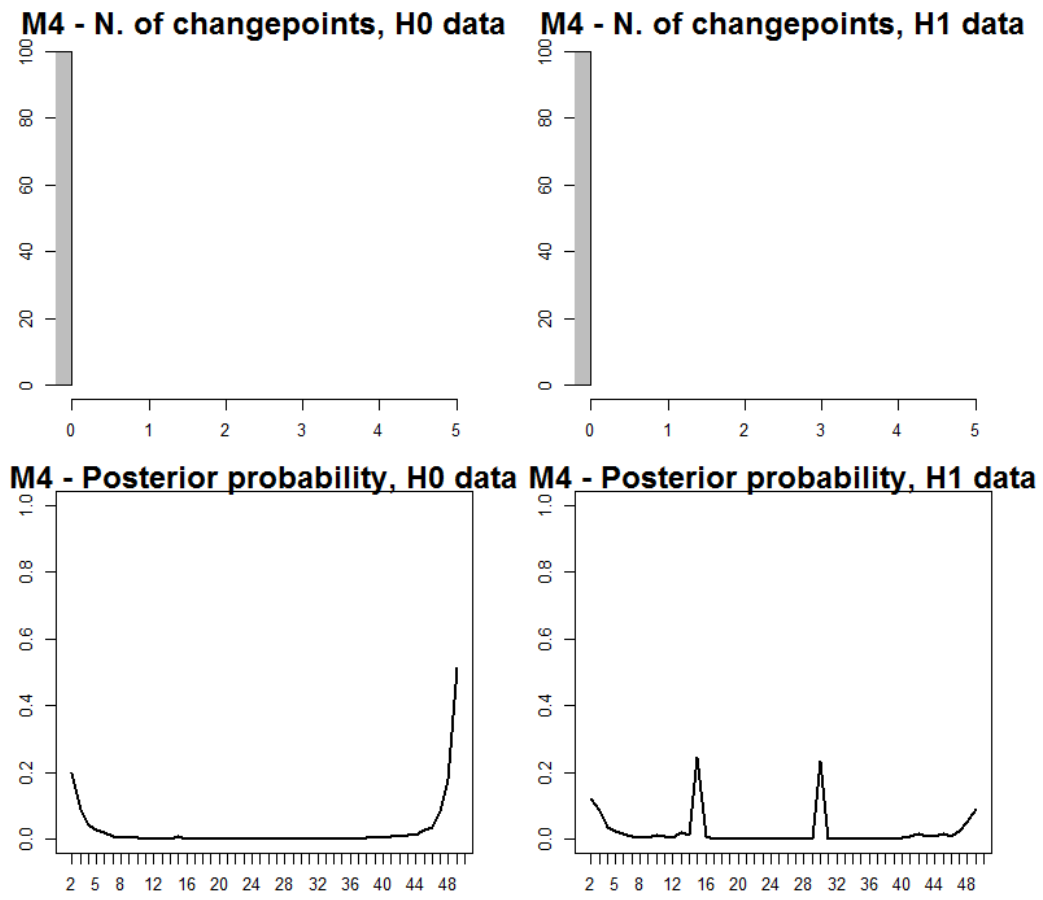


Figure A.21: Multiple changepoint search on iid data, with the spatio-temporal effect model and the BF method - Power level and location of the changepoint

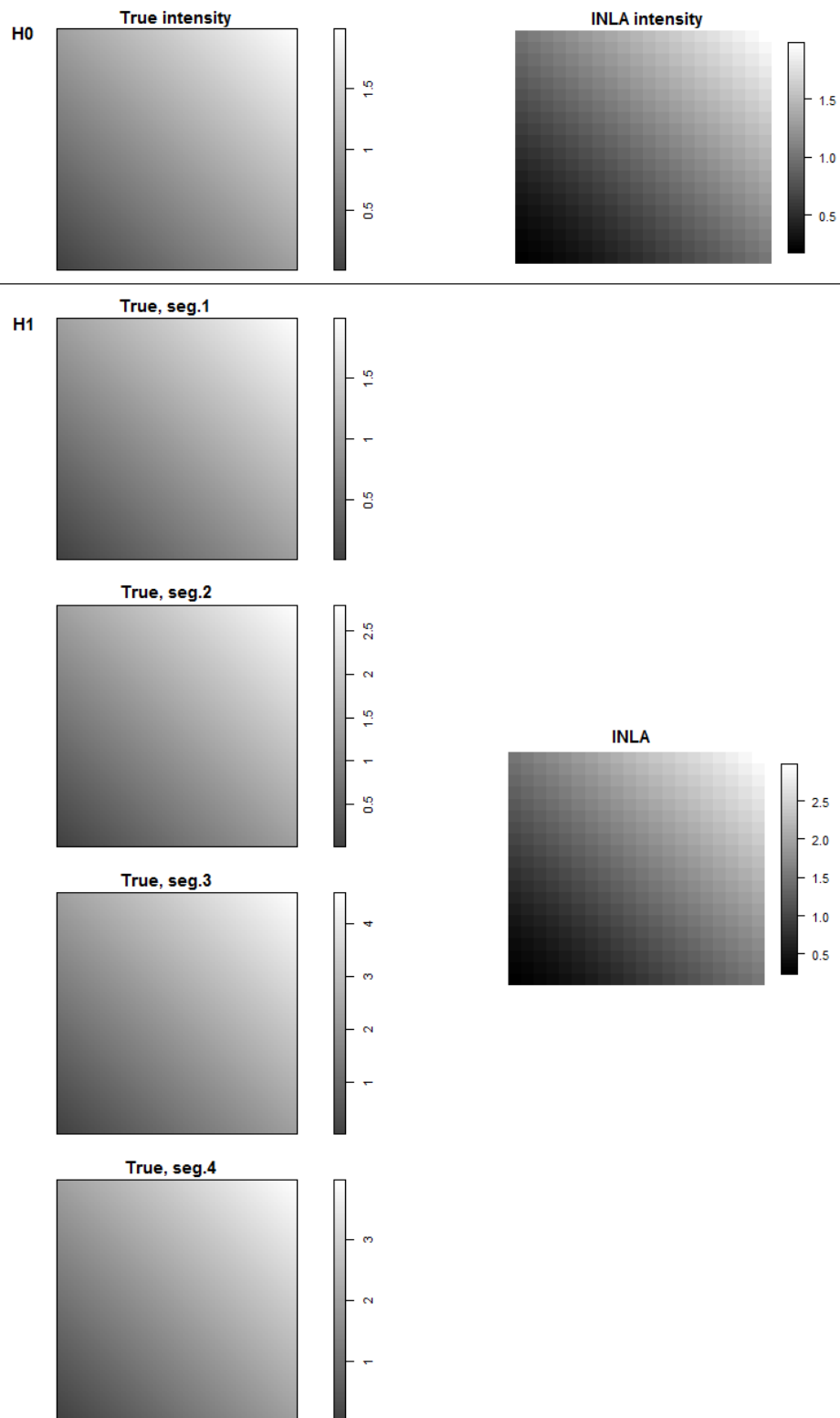


Figure A.22: Multiple changepoint search on iid data, with the spatio-temporal effect model and the BF method - Estimated intensities

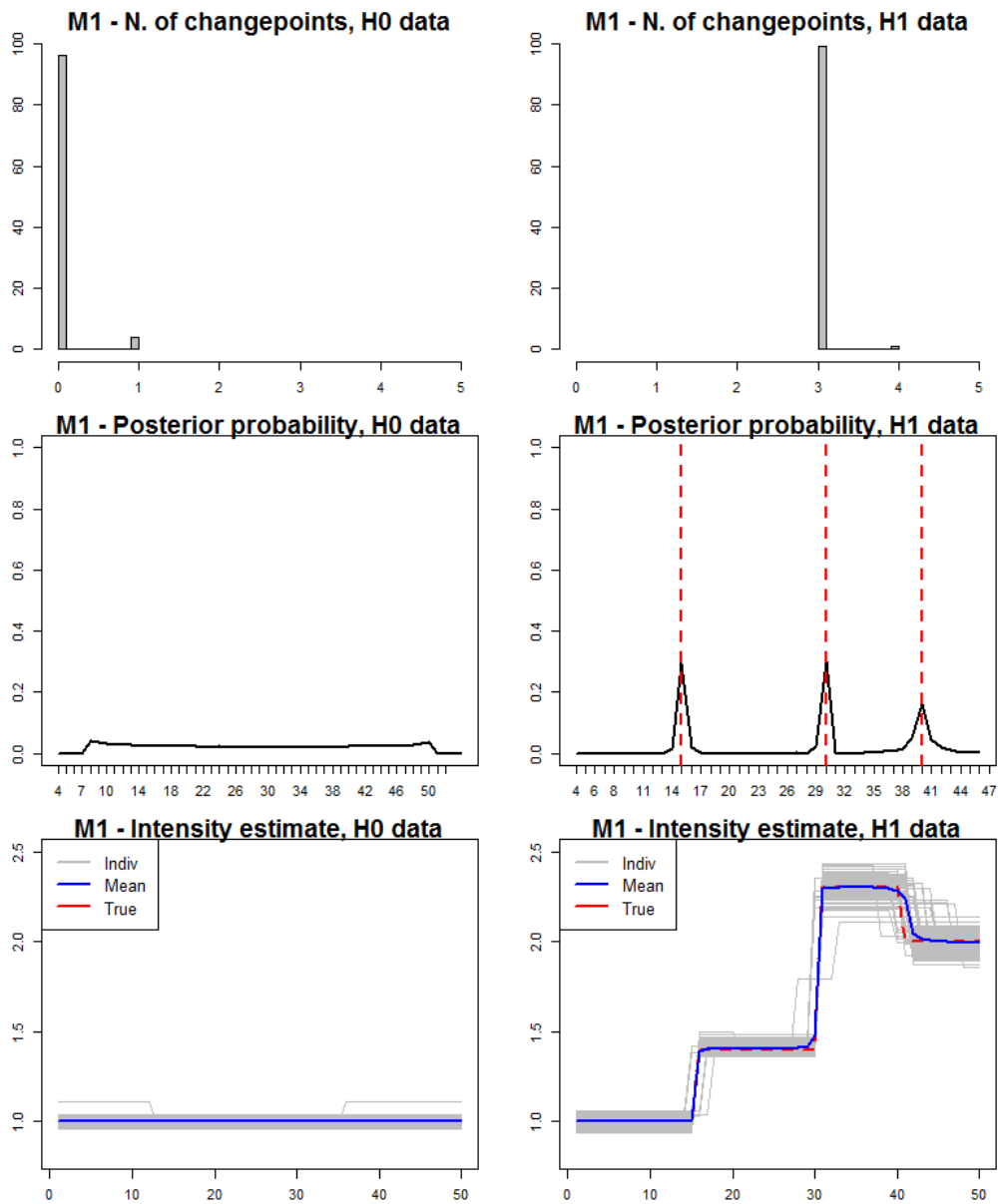


Figure A.23: Multiple changepoint search on iid data, with the fixed effect model and the PT method

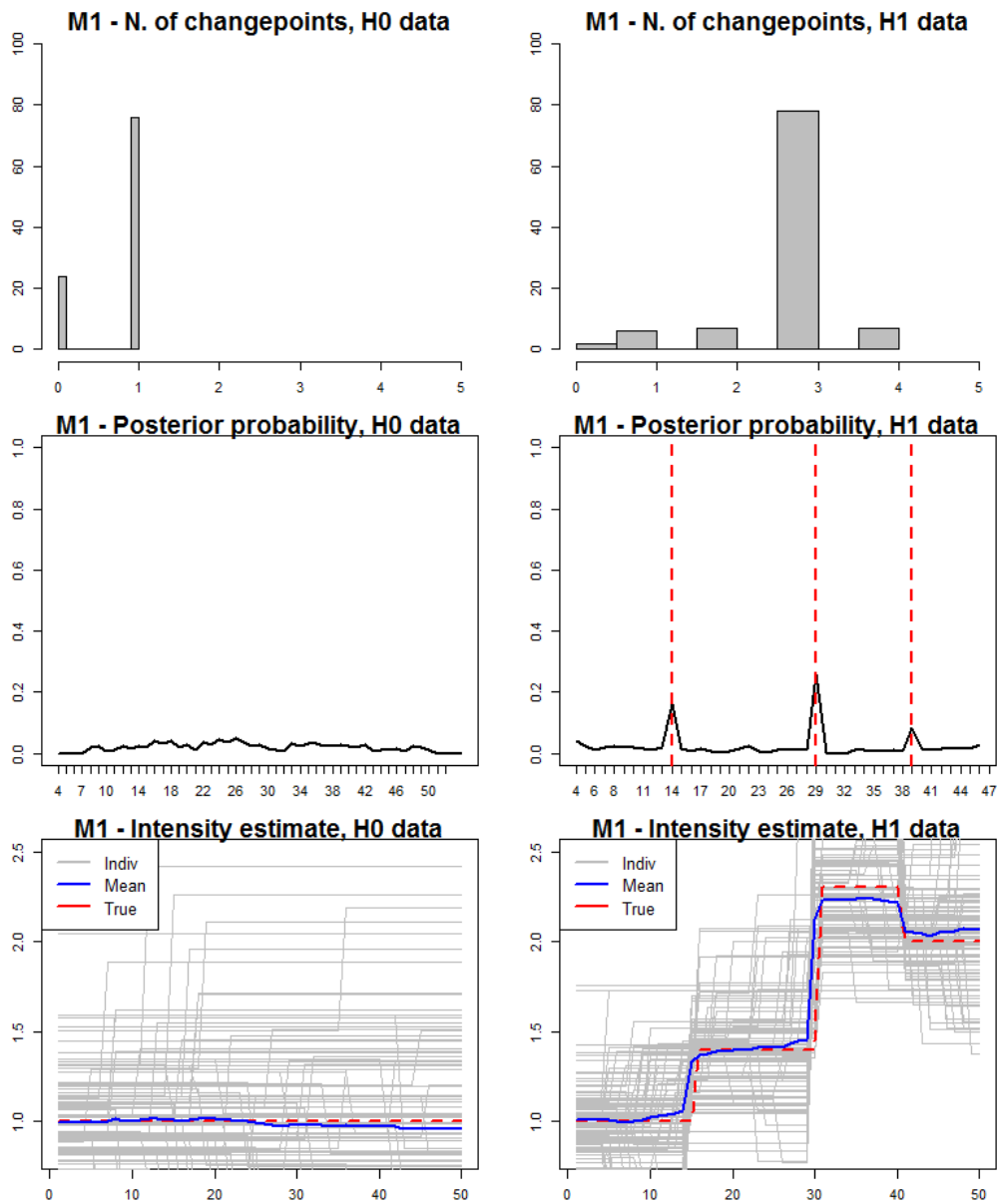


Figure A.24: Multiple changepoint search on AR(1) data, with the fixed effect model and the PT method

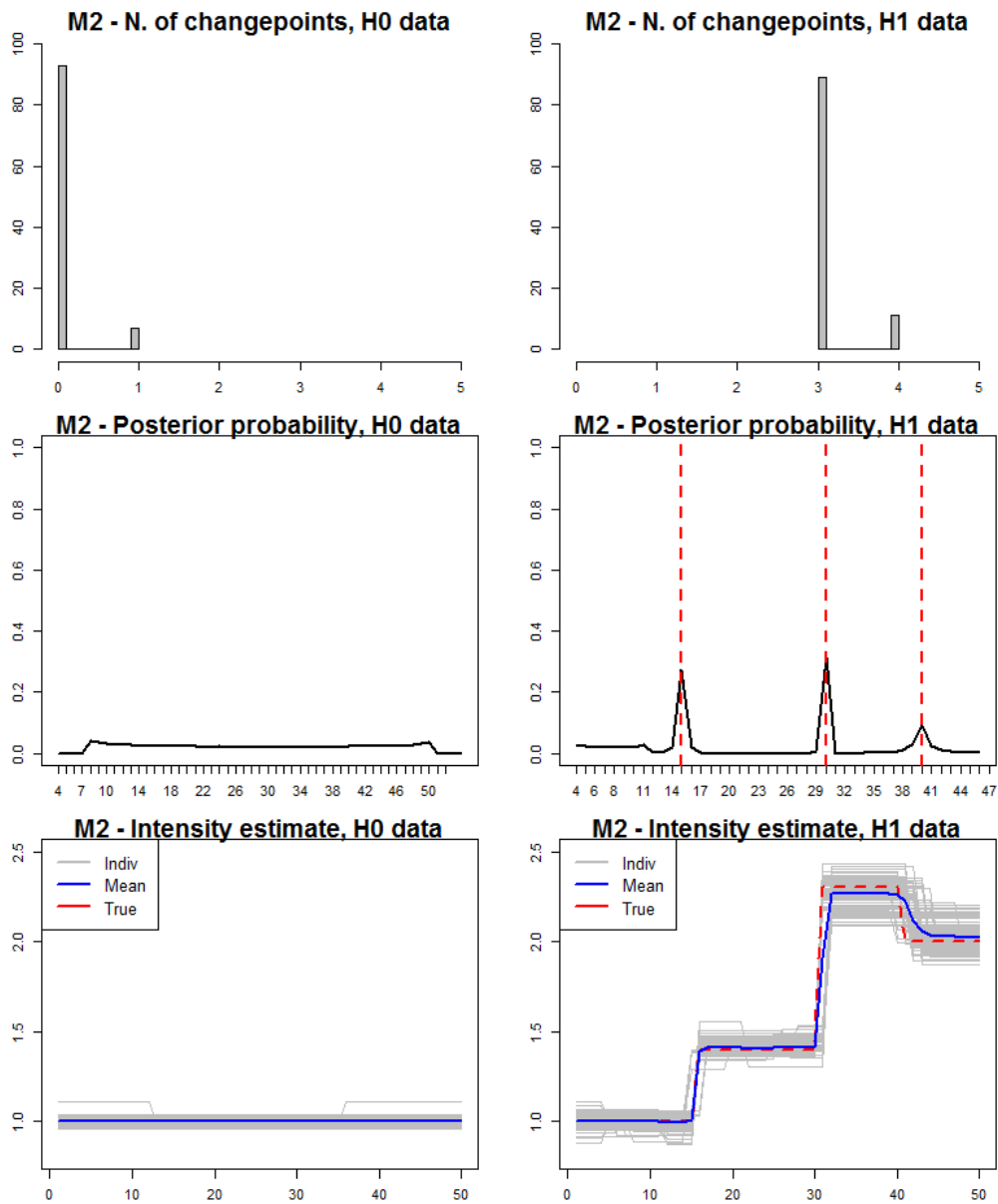


Figure A.25: Multiple changepoint search on iid data, with the temporal effect model and the PT method

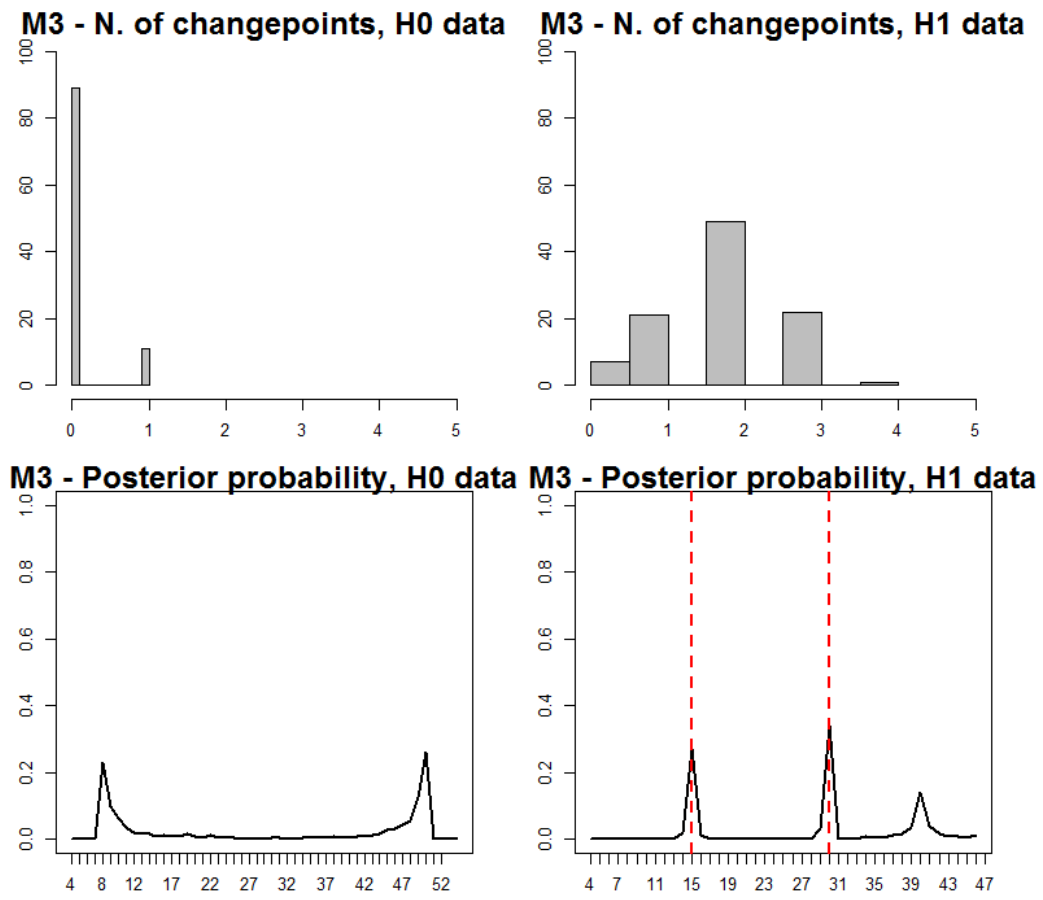


Figure A.26: Multiple changepoint search on iid data, with the spatial effect model and the PT method - Power level and location of the changepoint

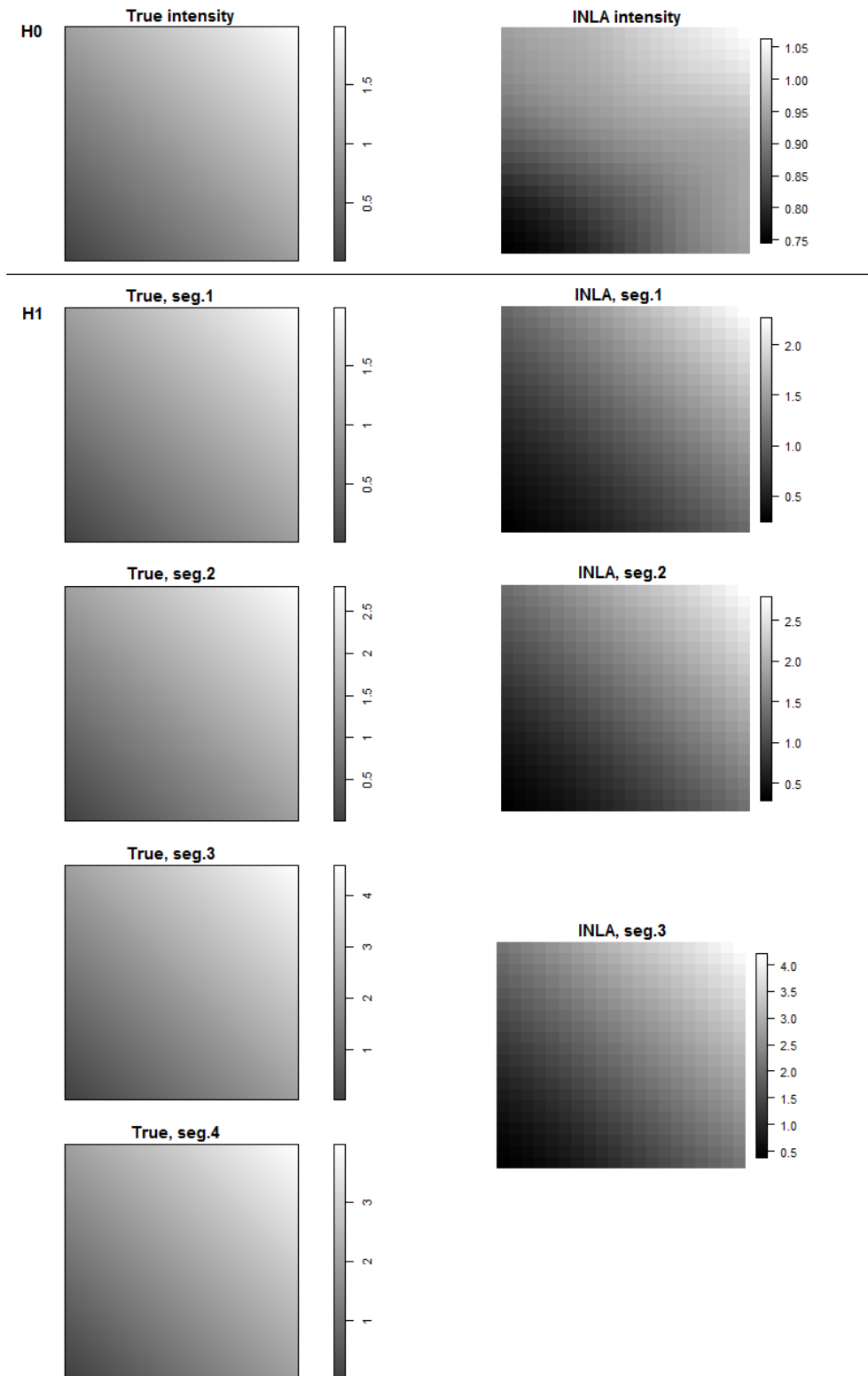


Figure A.27: Multiple changepoint search on iid data, with the spatial effect model and the PT method - Estimated intensities

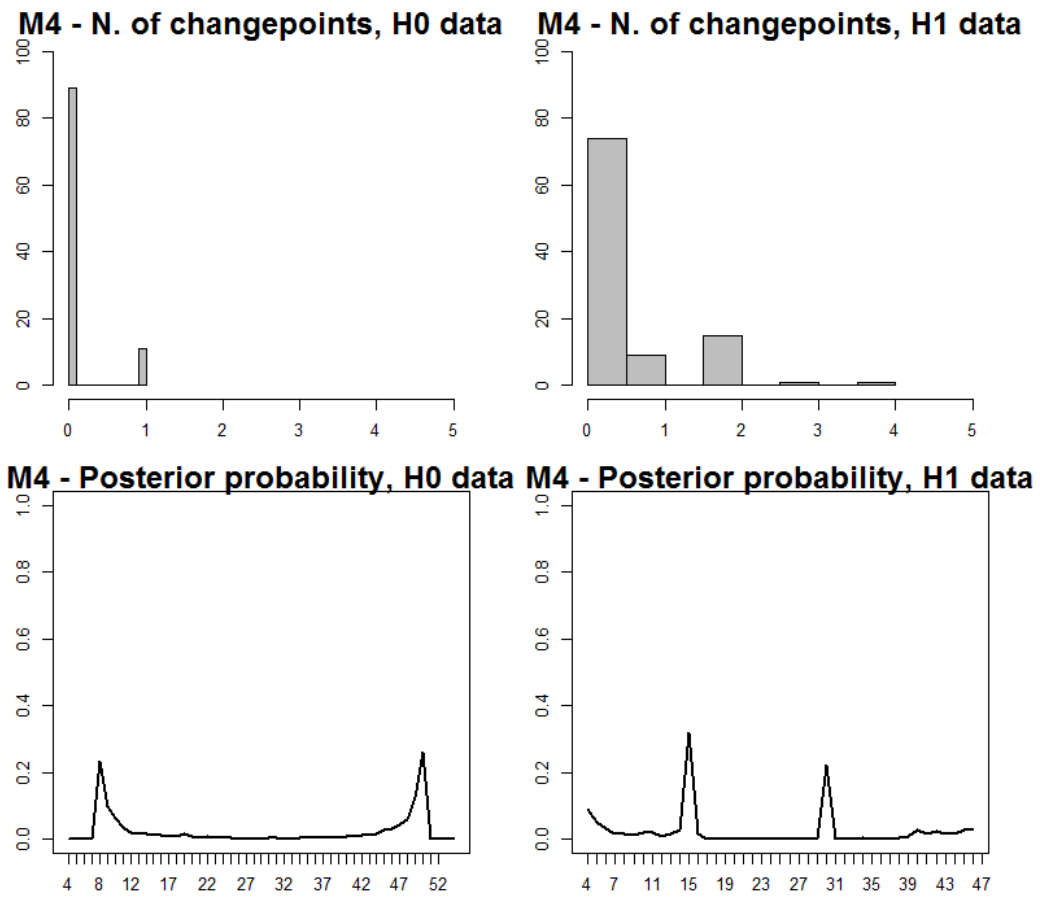


Figure A.28: Multiple changepoint search on iid data, with the spatio-temporal effect model and the PT method - Power level and location of the changepoint

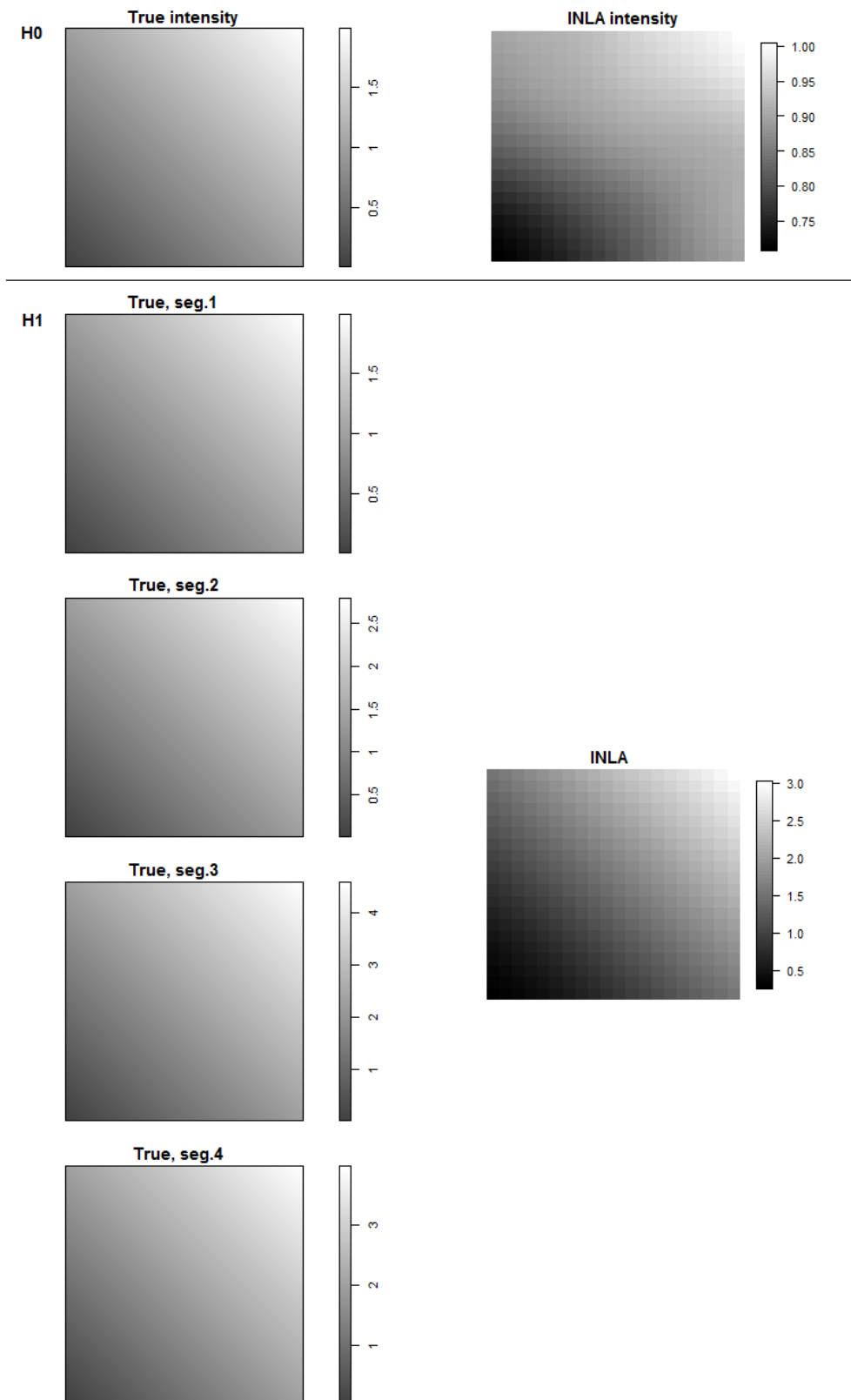


Figure A.29: Multiple changepoint search on iid data, with the spatio-temporal effect model and the PT method - Estimated intensities

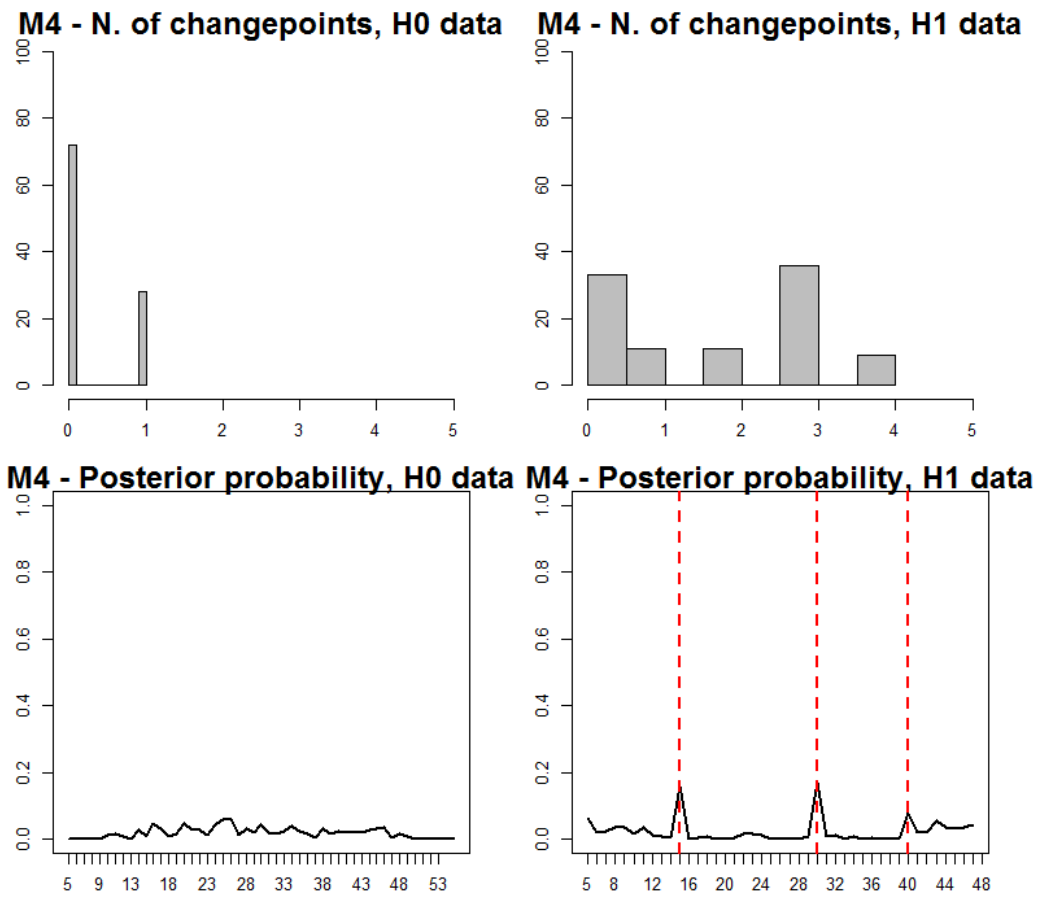


Figure A.30: Multiple changepoint search on AR(1) data, with the spatio-temporal effect model and the PT method - Power level and location of the changepoint

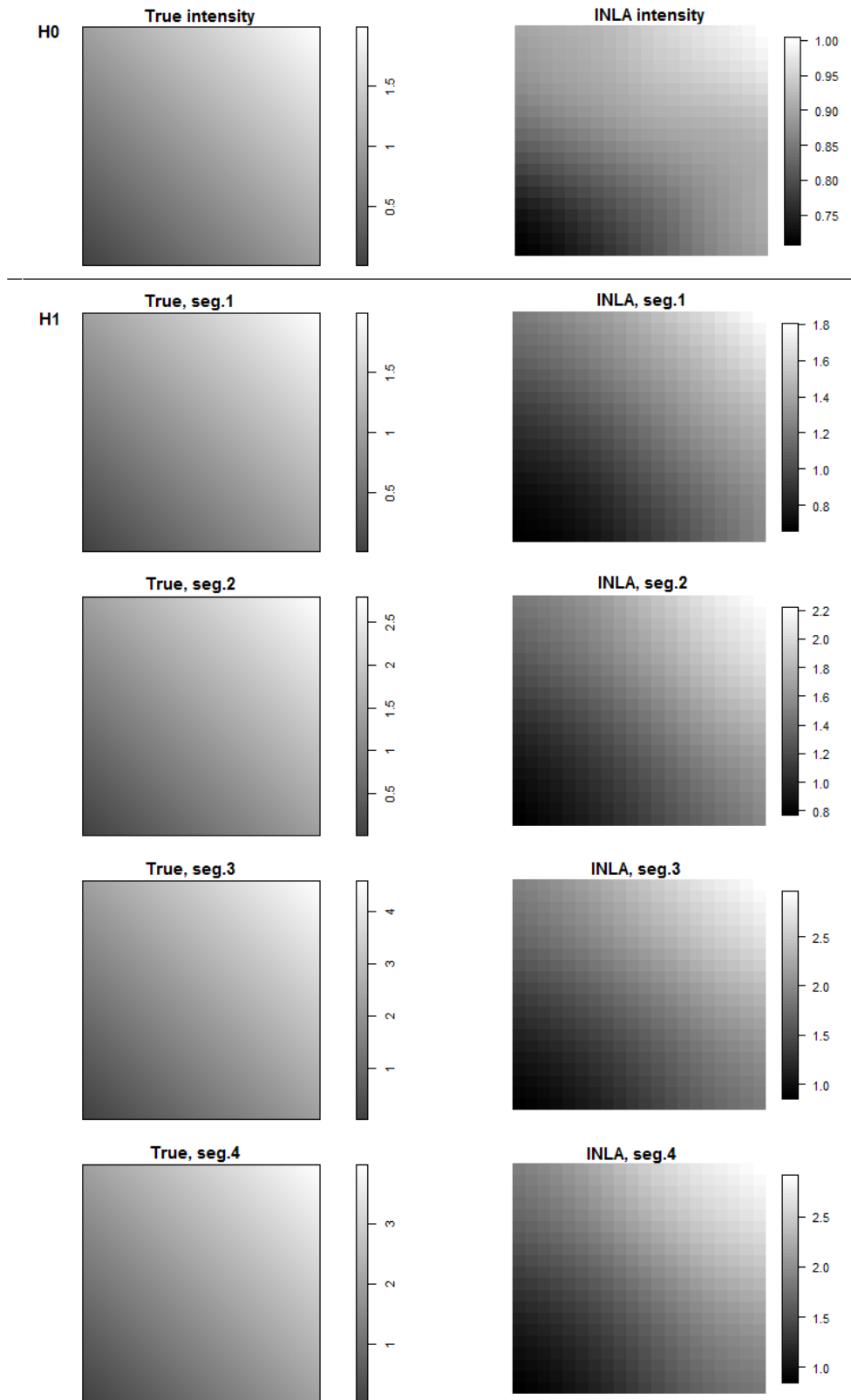


Figure A.31: Multiple changepoint search on AR(1) data, with the spatio-temporal effect model and the PT method - Estimated intensities

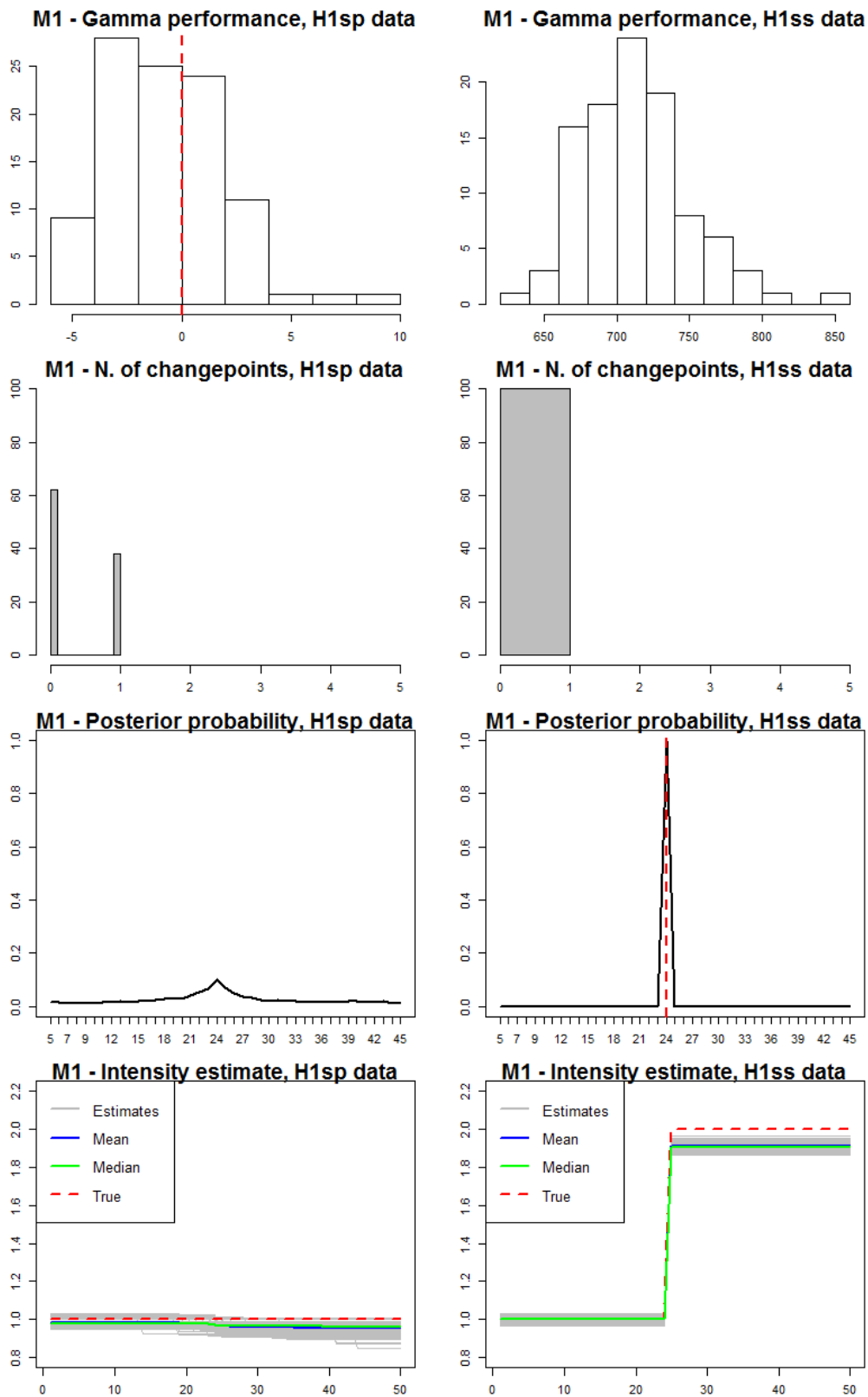


Figure A.32: Changepoint search on data with a change in the spatial structure, with the fixed effect model and the BF method

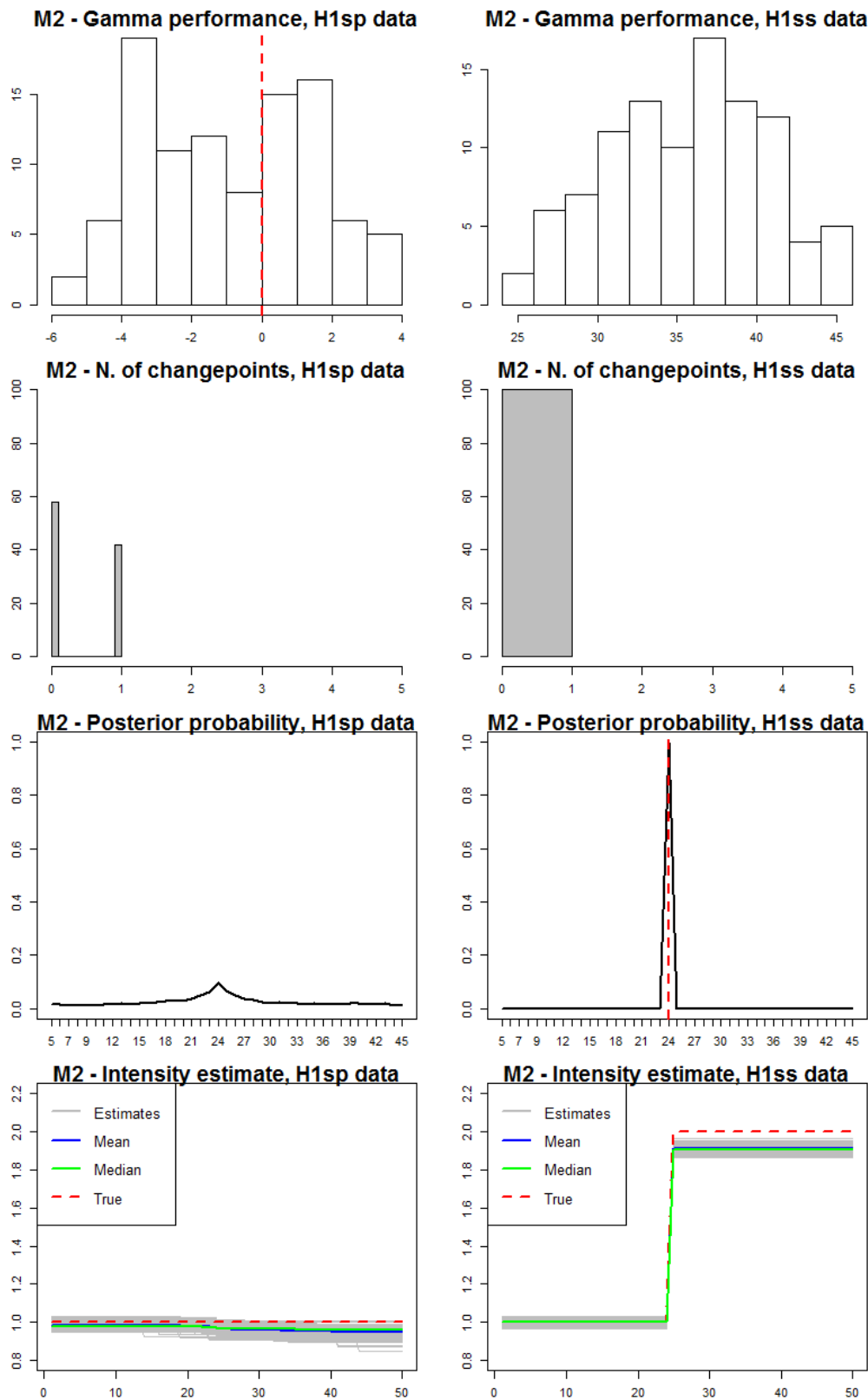


Figure A.33: Changepoint search on data with a change in the spatial structure, with the temporal effect model and the BF method

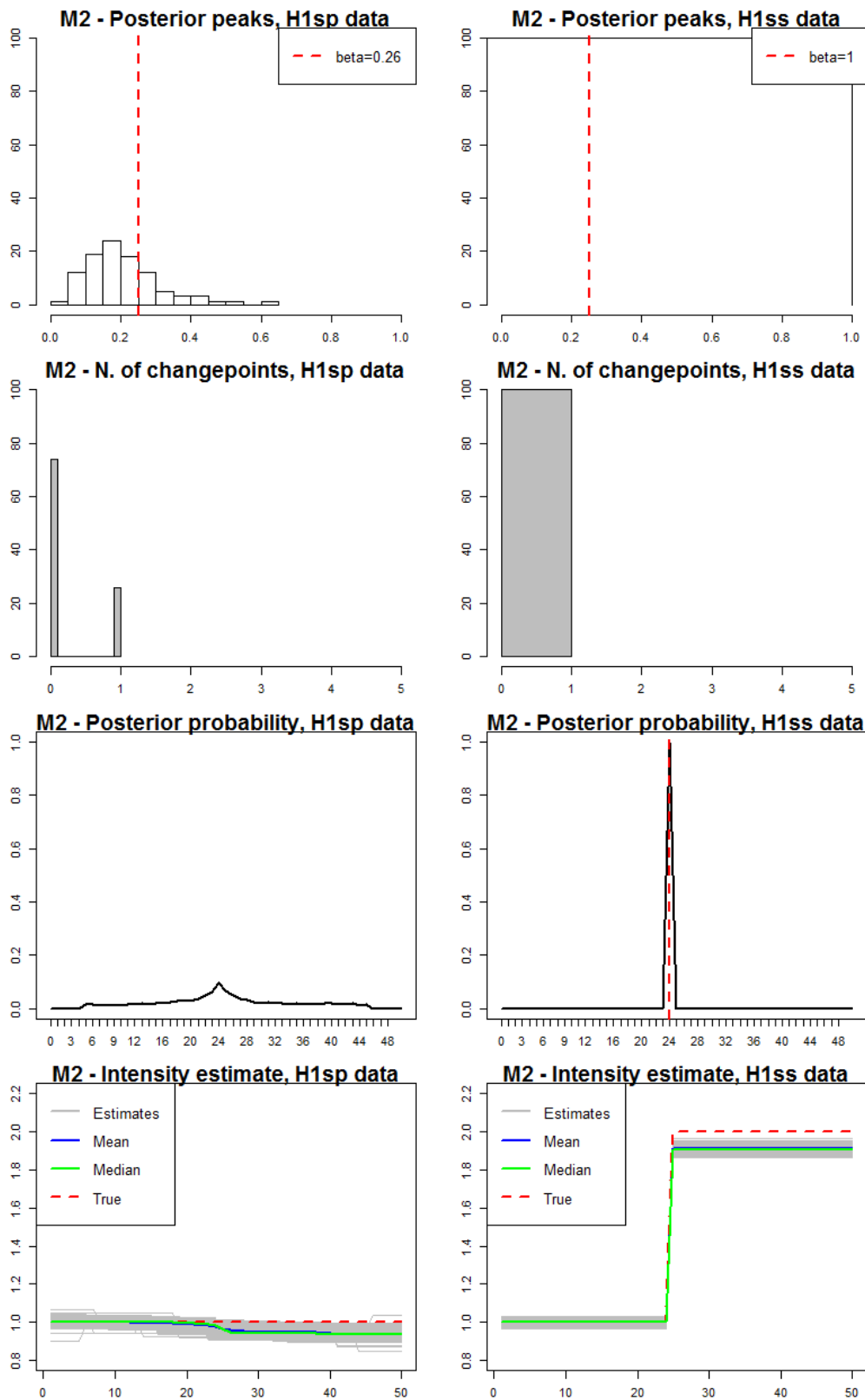


Figure A.34: Changepoint search on data with a change in the spatial structure, with the temporal effect model and the PT method

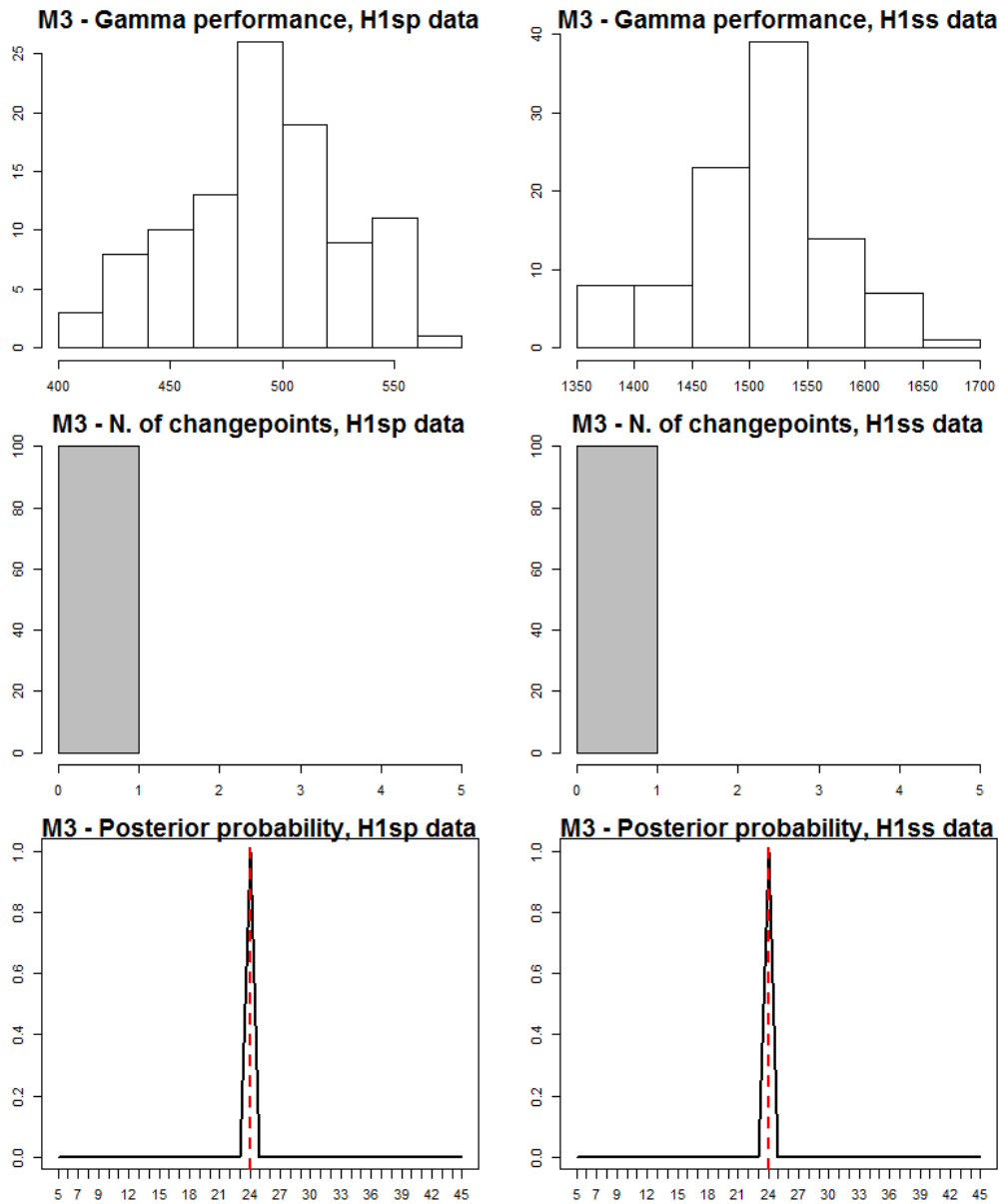


Figure A.35: Changepoint search on data with a change in the spatial structure, with the spatial model and the BF method - Power level and location of the changepoint

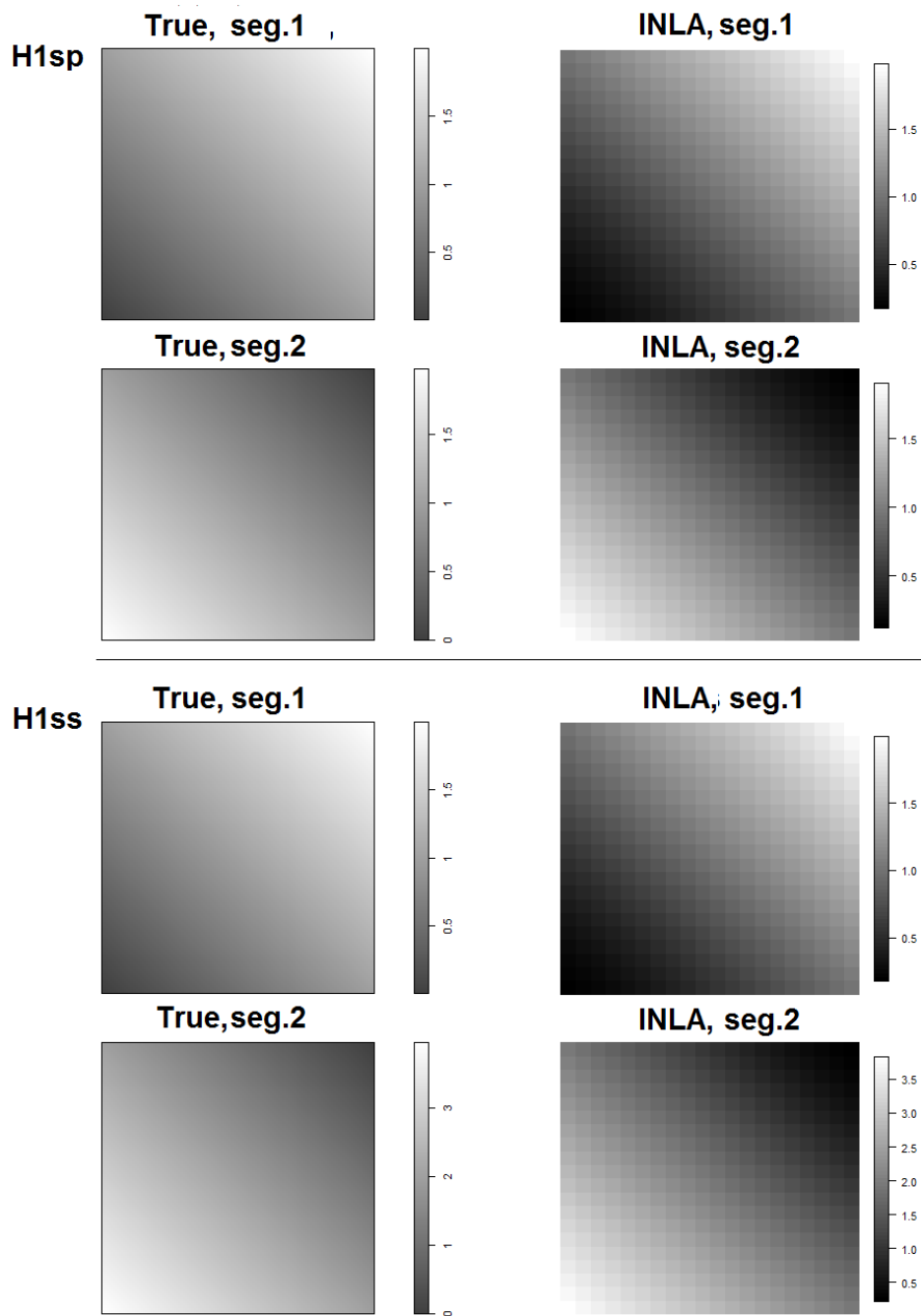


Figure A.36: Changepoint search on data with a change in the spatial structure, with the spatial model and the BF method - Estimated intensities

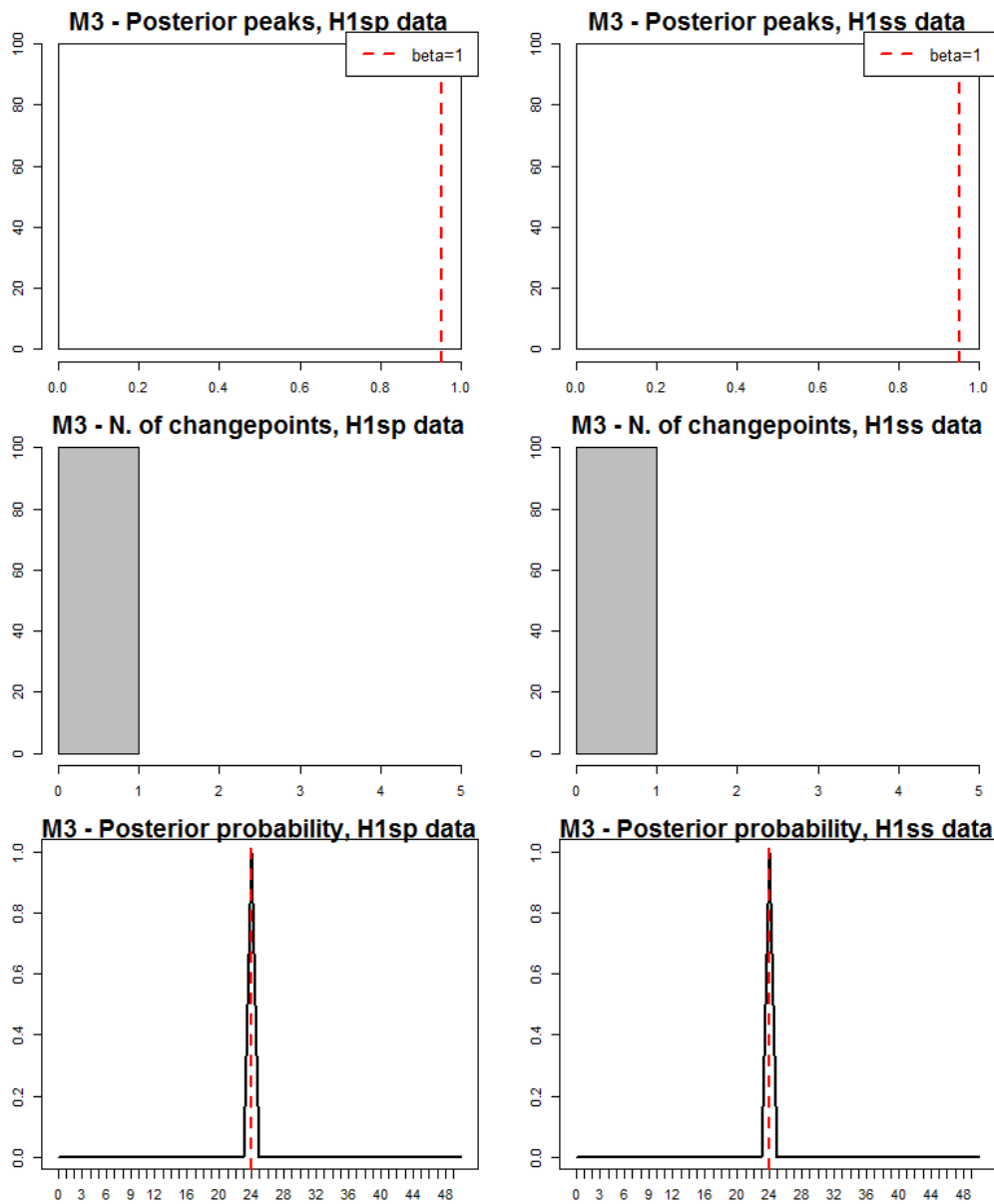


Figure A.37: Changepoint search on data with a change in the spatial structure, with the spatial model and the PT method - Power level and location of the changepoint

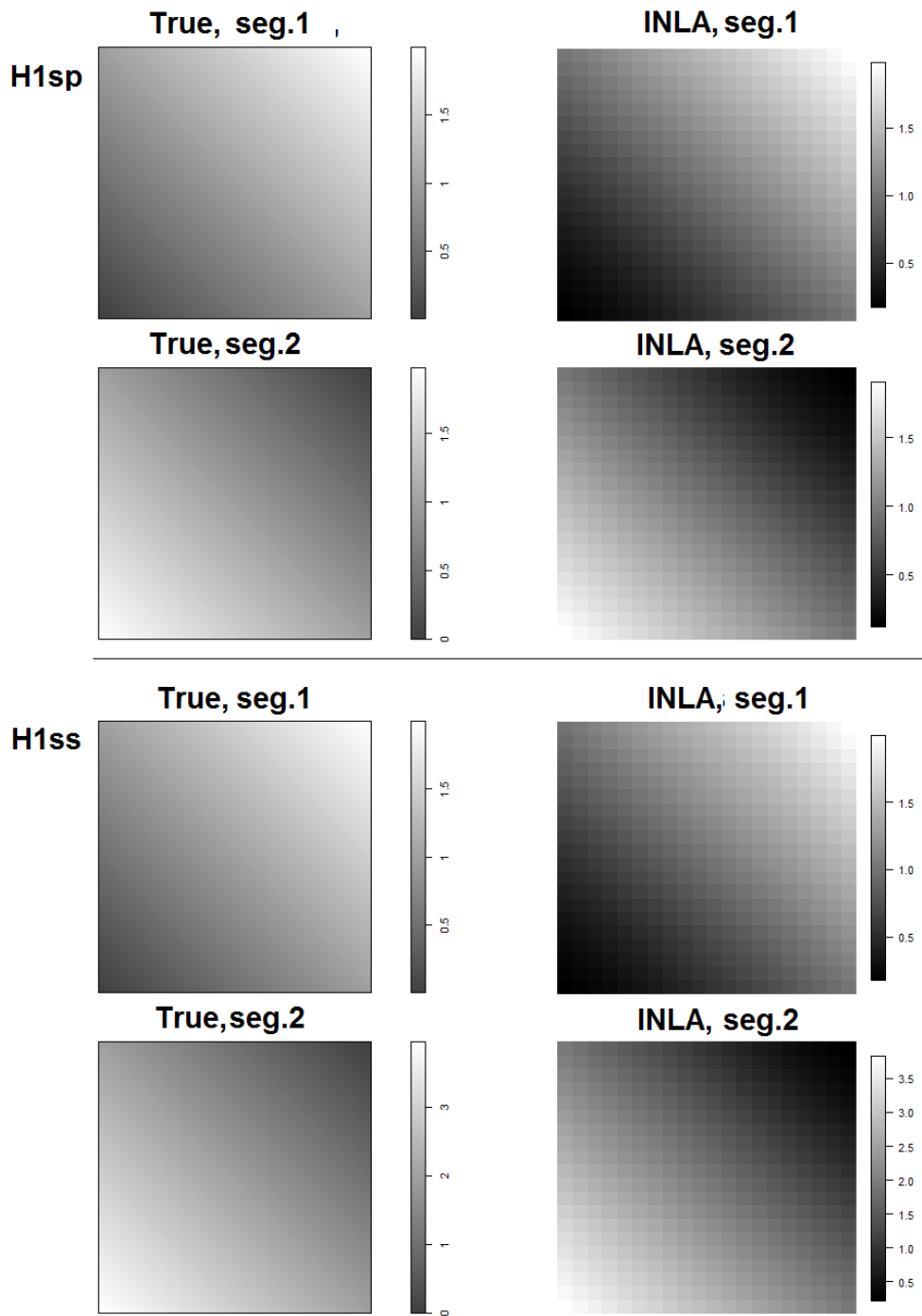


Figure A.38: Changepoint search on data with a change in the spatial structure, with the spatial model and the PT method - Estimated intensities

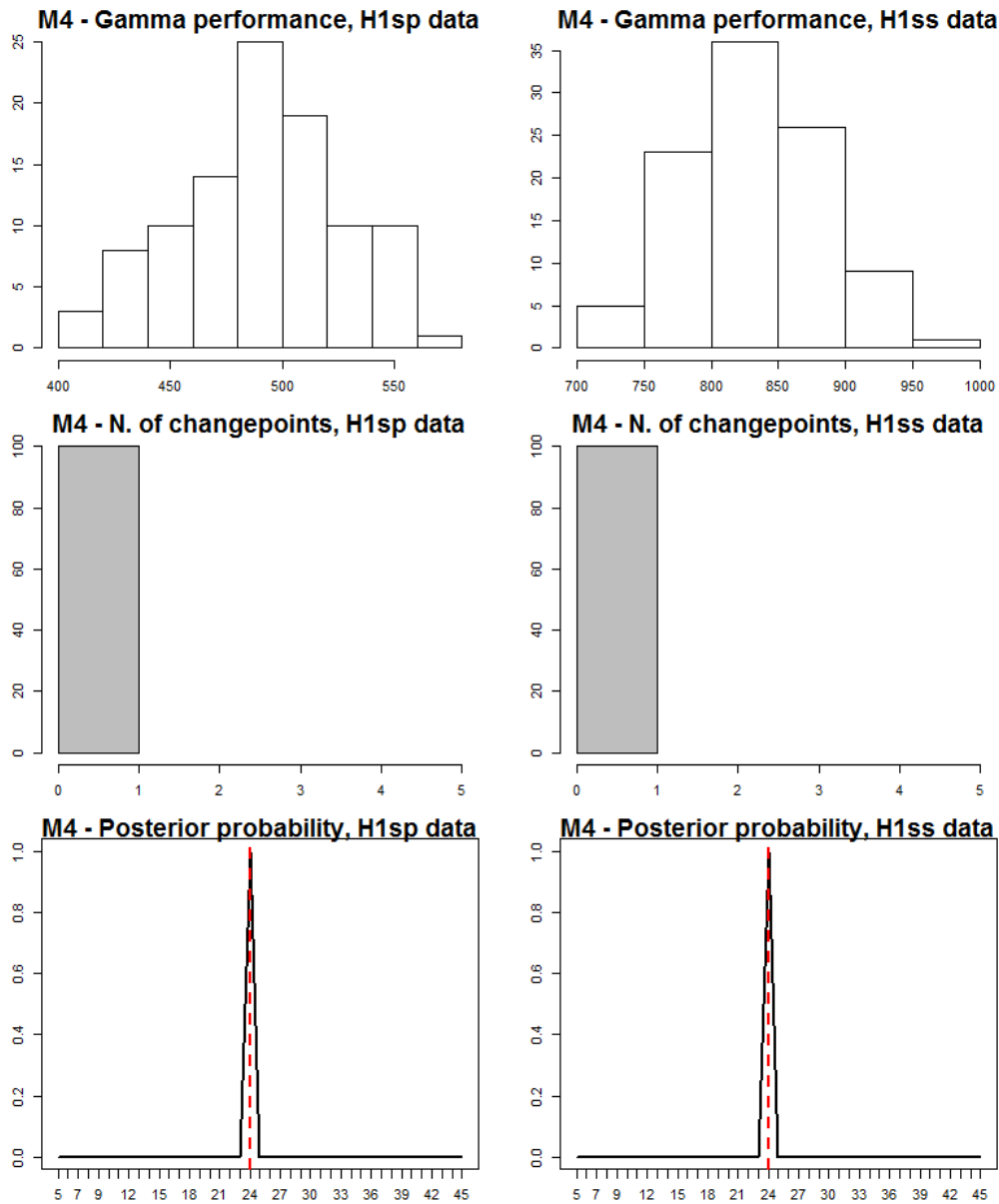


Figure A.39: Changepoint search on data with a change in the spatial structure, with the spatio-temporal model and the BF method - Power level and location of the changepoint

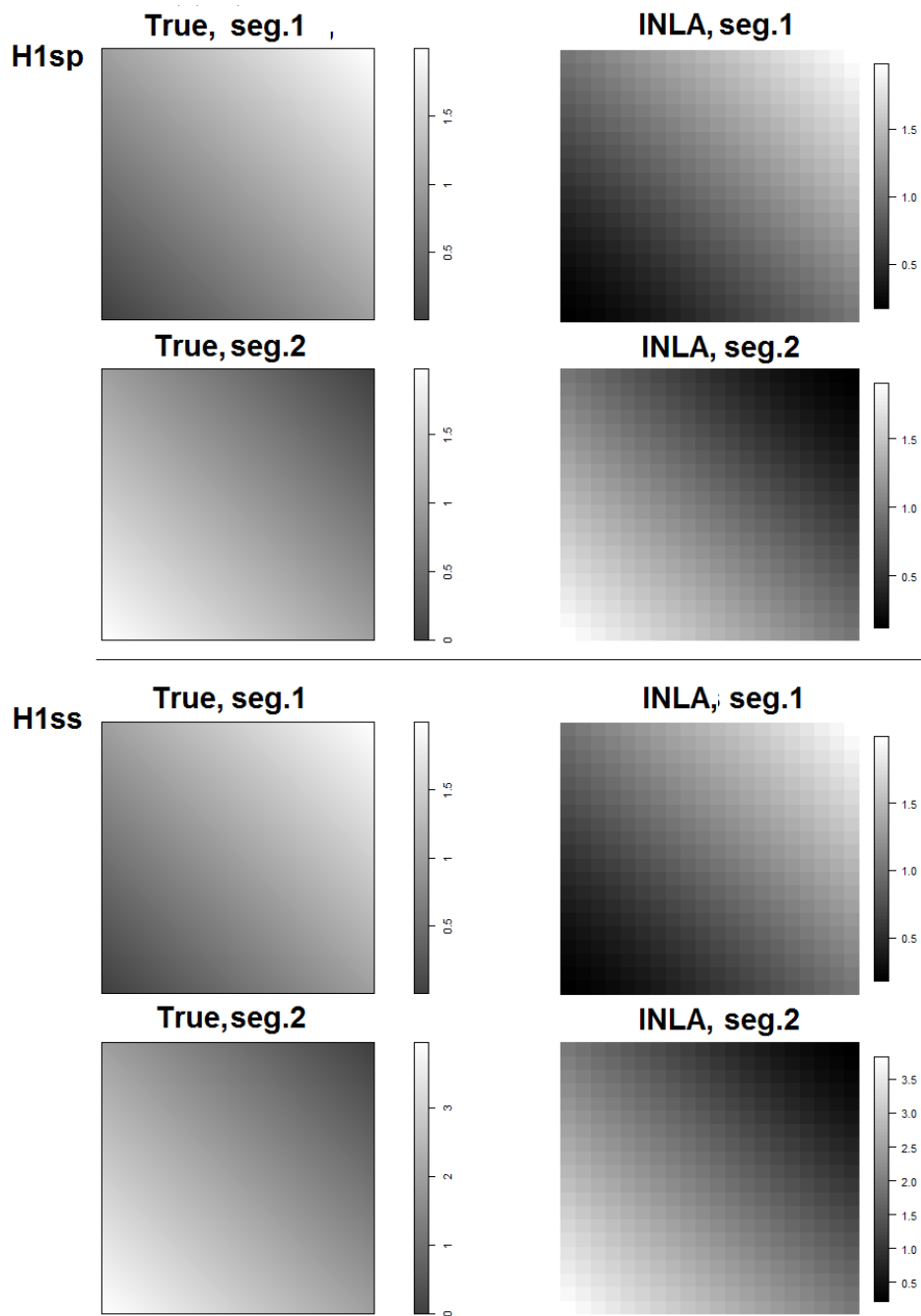


Figure A.40: Changepoint search on data with a change in the spatial structure, with the spatio-temporal model and the BF method - Estimated intensities

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