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Non-homogeneous Poisson models with a change-point: an application to ozone peaks in Mexico city

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Abstract In this paper, we use some non-homogeneous Poisson models in order to study the behavior of ozone measurements in Mexico City. We assume that the number of ozone peaks follows a non-homogeneous Poisson process. We consider four types of rate function for the Poisson process: power law, Musa–Okumoto, Goel–Okumoto, and a generalized Goel–Okumoto rate function. We also assume that a change-point may or may not be present. The analysis of the problem is performed by using a Bayesian approach via Markov chain Monte Carlo methods. The best model is chosen using the DIC criterion as well as graphical approach.

Keywords Non-homogeneous Poisson process · Bayesian inference · Change-point · MCMC methods · Air pollution data

1 Introduction

High levels of pollution certainly is one of the most important problems in large cities throughout the world. One of the most common pollutants that affect the inhabitants

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of those cities is ozone. When ozone concentrations stay above a certain threshold for a given period of time, individuals exposed to the pollutant may experience serious health problems (see for example Bell et al. 2004; Loomis et al. 1996; Wilson et al. 1980). It is well known that a very sensitive population such as the elderly, newborn and ill, may experience a deterioration in their health when exposed to ozone levels above 0.11 parts per million (0.11 ppm) for a period of one hour or more. Therefore, modelling and predicting such exceedances are very important issues. If they are predicted well in advance, then environmental authorities can take preventive measures to avoid that susceptible population are exposed to high levels of ozone.

Several methods have been used in order to predict the violation of an air quality standard. A common method is to apply extreme values theory to perform predictions (Horowitz 1980; Roberts 1979a,b; Smith 1989). However, other techniques may be used to study this type of problem, such as, multivariate analysis (Guardani et al. 2003), neural networks (Comrie 1997; Guardani et al. 1999), Poisson models (Achcar et al. 2008; Javits 1980; Leadbetter 1991; Raftery 1989; Smith 1989), time series analysis (Loomis et al. 1996) and Markov chain models (see for instance Álvarez et al. 2005; Austin and Tran 1999; Larsen et al. 1980).

Another important issue to be considered when studying problems related to environmental policy is the impact that actions taken by environmental authorities have on the behavior of a given pollutant. One of the impacts is related to the probability of occurrence or not of a violation of a given environmental standard. Hence, it is important to know when a change in the behavior of a pollutant happens, because in that way it is possible to have an idea when is necessary to make changes in the model used to perform predictions.

The results obtained in this work are applied to a data set collected from the monitoring network of Mexico City (www.sma.df.gob.mx/simat/) corresponding to seven years of measurements (from January 1, 1998 to December 31, 2004) of the overall daily maximum measurements for the city. This data set will be referred to MAMC and is obtained as follows. The measurements are obtained minute by minute and the averaged hourly result is reported at each station. The MAMC data is obtained by taking the daily maximum among the averaged values reported by all monitoring stations in the city. The average measurement of this data set is 0.154 ppm with standard deviation of 0.05. The Mexican ozone standard of 0.11 ppm (NOM 2002) was violated in 2063 days. The daily peaks were double the Mexican standard on 237 days.

Remark Note that even though the Mexican environmental standard for ozone is 0.11 ppm and the threshold for declaring a situation of emergency in Mexico City is 0.22 ppm, we will not consider those values in the present analysis. Since the Mexican standard is violated almost every day and the Mexico City standard is rarely surpassed, we have chosen to work with the threshold 0.17 ppm. We have chosen this threshold because it is an intermediate value between 0.11 and 0.22 ppm. Hence, we remove the two extreme cases. Therefore, from now on a violation of an environmental standard occurs if the daily maximum measurement is greater than 0.17 ppm. Note that this threshold was surpassed 980 days during the 7-year period considered. We would like to call attention to the fact that there is a will of lowering the threshold at which situations of emergency are declared in Mexico City. The threshold 0.23 ppm

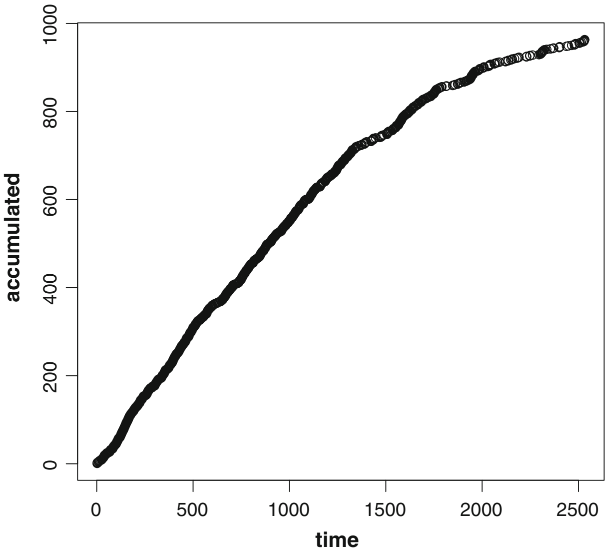

Fig. 1 Accumulated number of ozone violations versus time of occurrence. Time is measured in days

was lowered to 0.22 ppm. A decrease that would not be so slim as this and not so drastic as to 0.11 ppm (at which the city would have to stop practically every day) could be 0.17 ppm. This is another reason for choosing this threshold, to analyze how ozone peaks might behave when this value is considered.

In Fig. 1, we have the plot of the accumulated number of violations versus time (day of occurrence). It is possible to observe a candidate for a change-point close to time 1300, which corresponds to approximately the middle of the year 2001.

Remark It is worth calling attention to the fact that in the year 1999 strict measures were implemented when considering the standard at which cars sold in Mexico City were manufactured. Since the year 2000, cleaner cars were produced and people were encouraged to buy and use them instead of not so clean ones. Hence, it is natural that shortly after in the future some changes in the behavior of the number of violations of ozone should occur.

Even though some authors have used Poisson processes to model the number of violations of ozone, they either allowed the presence of change-points in a time homogeneous model (see Raftery 1989 and Smith 1989, for instance) or they used a non-homogeneous model but without allowing the presence of a change-point (see for example Achcar et al. 2008).

The novelty of this work is that we use a non-homogeneous Poisson process to model the number of violations of an ozone environmental standard and include the possibility of a presence of a change-point. Identifying a change-point is important in that it may indicate a possible new source of environmental disturbance, a sudden and systematic change in the environment or if a given preventive measure, taken by the environmental authorities, has an impact on the behavior of the number of exceedances of ozone measurements. Recall that in this work we are taking into account the threshold 0.17 ppm. (Note that other threshold parameters may be considered, but we will not include any other in this work.) In many applications as the one considered here it is possible to observe the presence of a change-point for the intensity function of the non-homogeneous Poisson process. In those cases as well as in the present work, the interest is in inferring this point where the non-homogeneous Poisson process changes.

This paper is organized as follows. In Sect. 2, a description of the mathematical formulation of the model is made. In Sect. 3, the Bayesian estimation of the parameters is made considering four special classes of intensity functions and taking into account the presence or not of a change-point. An application to ozone measurements in Mexico City in the presence or not of a change-point is given in Sect. 4. Finally, in Sect. 5, we conclude and present a discussion of the results obtained.

2 Description of the model

In order to model the number of times that a violation of an ozone environmental standard occurs in Mexico City, we consider a point process to count these violations. Let $N = \{N_t : t \in [0, T]\}$ be the process that registers the cumulative number of ozone violations that are observed during the interval $[0, T]$, i.e., for each $t \in [0, T]$, N_t is the number of ozone peaks that occurred during the time interval $(0, t)$. Assume that N is modelled by a non-homogeneous Poisson process (NHPP) with intensity function

$$\lambda(t) = \frac{\mathrm{d}}{\mathrm{d}t} m(t) = \frac{\mathrm{d}}{\mathrm{d}t} \mathrm{E}(N_t)$$

where $m(t)$ is the mean value function. (Note that this means that the inter-event times, i.e., the time between two consecutive ozone peaks are exponentially distributed.)

Remark The overall ozone measurements for Mexico City are such that there were 216, 194, 191, 144, 121, 67, and 47 days in the years 1998, 1999, 2000, 2001, 2002, 2003, and 2004, respectively, in which the threshold 0.17 ppm was surpassed. Hence, it is possible to see that the number of ozone exceedances has decreased throughout the years. Therefore, it is interesting to have an intensity function $\lambda(t)$, $t \geq 0$, that is a monotonic decreasing function of t.

Different parametric forms introduced in the literature can be used. Those parametric forms for monotonic intensity functions are very popular within the framework of software reliability studies (see for example Cox and Lewis 1996; Musa and Okumoto 1984; Musa et al. 1987). A popular form for the monotonic intensity functions is given by power law processes (PLP) or the Weibull intensity function. An alternative to monotonic functions is to consider the superposition of several independent NHPP with simple intensity functions (see for example Kuo and Yang 1999). The latter will not be considered here.

Remark Other forms for the intensity function are introduced in the literature considering software reliability studies such as: the exponentiated-Weibull intensity function which generalizes PLP models (Mudholkar et al. 1995); the Yamada intensity function

(Yamada and Osaki 1984, 1985); the logistic growth intensity function or the modified Duane intensity function (see for example Huang et al. 2003). Some of these models have more than two parameters, and this makes it difficult to obtain inference for the parameters of the model using standard classical inference procedures. Hence, Bayesian methods based on Monte Carlo algorithms could be a suitable way of obtaining inference for these parameters. Other inference procedures, such as kernel (i.e., non-parametric) estimation methods could be used to estimate the intensity or the mean function. However, this in not the goal here and therefore, this methodology will not be used in the present work.

2.1 Definitions, notations and assumptions

Let $N^{(\boldsymbol{\theta})} = \{N_t^{(\boldsymbol{\theta})} : t \in [0, T]\}$ be a non-homogeneous Poisson process with mean value function $m(t \mid \boldsymbol{\theta})$ where $\boldsymbol{\theta}$ is a vector of parameters. The function $m(t \mid \boldsymbol{\theta})$ represents the expected number of events registered by $N^{(\boldsymbol{\theta})}$ up to time t. (In here, events are the violations of the ozone environmental standard when the threshold is 0.17 ppm.) The full characterization of a process of this type is achieved by specifying the functional form of $m(t \mid \boldsymbol{\theta})$, or equivalently, of its intensity function

$$\lambda(t \mid \boldsymbol{\theta}) = \frac{\mathrm{d}}{\mathrm{d}t} m(t \mid \boldsymbol{\theta}).$$

In the present work we explore the use of some special cases of NHPP to analyze the ozone pollution data of Mexico City. The cases considered here are the power law (PLP), the Musa–Okumoto (MOP) (Musa and Okumoto 1984), the Goel–Okumoto (GOP) (Goel and Okumoto 1978) and a generalized form of a Goel–Okumoto (GGOP) processes defined, respectively, by the following mean value functions,

$$\begin{aligned} m^{(\mathrm{PLP})}(t \mid \boldsymbol{\theta}) &= (t/\beta)^{\alpha}, \qquad \alpha, \beta > 0 \\ m^{(\mathrm{MOP})}(t \mid \boldsymbol{\theta}) &= \beta \log\left(1 + \frac{t}{\alpha}\right), \qquad \alpha, \beta > 0 \\ m^{(\mathrm{GOP})}(t \mid \boldsymbol{\theta}) &= \alpha\left[1 - \exp\left(-\beta t\right)\right], \qquad \alpha, \beta > 0 \\ m^{(\mathrm{GGOP})}(t \mid \boldsymbol{\theta}) &= \alpha\left[1 - \exp\left(-\beta t^{\gamma}\right)\right], \qquad \alpha, \beta, \gamma > 0, \end{aligned} \tag{1}$$

where $\boldsymbol{\theta} = (\alpha, \beta)$ for the PLP, MOP and GOP models and $\boldsymbol{\theta} = (\alpha, \beta, \gamma)$ for the GGOP model. The intensity functions associated with those processes are given, respectively, by

$$\begin{aligned} \lambda^{(\mathrm{PLP})}(t \mid \boldsymbol{\theta}) &= (\alpha/\beta)\,(t/\beta)^{\alpha-1}, \\ \lambda^{(\mathrm{MOP})}(t \mid \boldsymbol{\theta}) &= \beta/(t+\alpha), \\ \lambda^{(\mathrm{GOP})}(t \mid \boldsymbol{\theta}) &= \alpha\beta \exp\left(-\beta t\right), \\ \lambda^{(\mathrm{GGOP})}(t \mid \boldsymbol{\theta}) &= \alpha\beta\gamma t^{\gamma-1} \exp\left(-\beta t^{\gamma}\right). \end{aligned} \tag{2}$$

Remark 1 Note that the intensity functions given by (2) define the hazard rates of the time between occurrence of events in the respective models.

Remark 2 We observe from (2) that the intensity function $\lambda^{(\mathrm{PLP})}(t \mid \boldsymbol{\theta})$ gives a different behavior for the PLP depending on the value of α. We have that as a function of time this intensity function can be constant, decreasing or increasing depending on whether $\alpha = 1, \alpha < 1$ or $\alpha > 1$, respectively. The intensities $\lambda^{(\mathrm{MOP})}(t \mid \boldsymbol{\theta})$ and $\lambda^{(\mathrm{GOP})}(t \mid \boldsymbol{\theta})$ present a decreasing behavior as functions of t; and $\lambda^{(\mathrm{GGOP})}(t \mid \boldsymbol{\theta})$ describes the situation where the intensity increases slightly at the beginning and then begins to decrease with t.

Since two situations are considered (presence or not of a change-point for the NHPP) we have two different forms for the likelihood function of the model (one for each formulation). First, we define the notation and expressions for the case where no change-points are present and then we do the same for the case where a presence of a change-point is allowed.

2.1.1 No change-points are present

In this case the data set is denoted by $\mathbf{D_T} = \{n\,;\ t_1, \ldots, t_n\,;\ T\}$ where n is the number of observed occurrence times which are such that $0 < t_1 < t_2 < \cdots < t_n < T$. In the application considered here these values are the epochs of occurrence of ozone environmental standard violations up to time T and are obtained by taking into account the MAMC data.

The likelihood function for $\boldsymbol{\theta}$ considering the time truncated model is (see for example Cox and Lewis 1996) given by,

$$L(\boldsymbol{\theta} \mid \mathbf{D_T}) = \left(\prod_{i=1}^{n} \lambda(t_i \mid \boldsymbol{\theta}) \right) \exp\left(-m(T \mid \boldsymbol{\theta})\right) \tag{3}$$

2.1.2 Presence of a change-point

Sometimes the counting process undergoes changes over the time range $(0, T)$ due to some kind of intervention (e.g., political decision that has as possible consequence either a decrease or an increase in the emission of ozone precursors and therefore a similar effect may occur on the daily measurements). In that case we have a single change-point τ making a transition between two NHPP models of the same type but with different parameters. In this way, the intensity function of the overall process is written by,

$$\lambda(t \mid \boldsymbol{\theta}) = \begin{cases} \lambda(t \mid \boldsymbol{\theta}_1), & 0 \le t \le \tau \\ \lambda(t \mid \boldsymbol{\theta}_2), & t > \tau, \end{cases} \tag{4}$$

where $\lambda(t \mid \boldsymbol{\theta}_j)$, $j = 1, 2$ are intensity functions related to those defined in (2) and $\boldsymbol{\theta}_j$, $j = 1, 2$ are the parameters associated to the NHPP before and after the change-point. Equivalently, for $m(t \mid \boldsymbol{\theta}_j)$, $j = 1, 2$, the corresponding mean value functions, we have that,

$$m(t \mid \boldsymbol{\theta}) = \begin{cases} m(t \mid \boldsymbol{\theta}_1), & 0 \leq t \leq \tau \\ m(\tau \mid \boldsymbol{\theta}_1) + m(t \mid \boldsymbol{\theta}_2) - m(\tau \mid \boldsymbol{\theta}_2), & t > \tau. \end{cases} \tag{5}$$

The data set for the formulation (4) and (5) is given by $\mathbf{D_T} = \{n\,;\, t_1, \ldots, t_{N_\tau^{(\boldsymbol{\theta})}}, t_{N_\tau^{(\boldsymbol{\theta})}+1}, \ldots, t_n\,;\, T\}$, where t_k, $k = 1, 2, \ldots, n$ is the time of occurrence of the kth event (in the present case is the kth violation of the environmental standard) and where $N_s^{(\boldsymbol{\theta})}$ stands for the number of events occurred during the time interval $(0, s]$. Therefore, the likelihood function of the model is given by,

$$L(\boldsymbol{\theta}, \tau \mid \mathbf{D_T}) = \left(\prod_{i=1}^{N_\tau^{(\boldsymbol{\theta})}} \lambda(t_i \mid \boldsymbol{\theta}_1)\right) \exp\left(-m(\tau \mid \boldsymbol{\theta}_1)\right)$$
$$\left(\prod_{i=N_\tau^{(\boldsymbol{\theta})}+1}^{N_T^{(\boldsymbol{\theta})}} \lambda(t_i \mid \boldsymbol{\theta}_2)\right) \exp\left(-m(T \mid \boldsymbol{\theta}_2) + m(\tau \mid \boldsymbol{\theta}_2)\right). \tag{6}$$

Remark 1 Observe that (3) is a special case of (6) when a change-point is not present (e.g., $\tau = T$). On the other hand, (6) can be straightforwardly extended to cover the scenario where more than one change-point is assumed.

Remark 2 Observe that considering PLP models in the presence of a change-point, the intensity function (4) is given by,

$$\lambda(t \mid \boldsymbol{\theta}) = \begin{cases} (\alpha_1/\beta_1)\,(t/\beta_1)^{\alpha_1 - 1}, & 0 \leq t \leq \tau \\ (\alpha_2/\beta_2)\,(t/\beta_2)^{\alpha_2 - 1}, & t > \tau, \end{cases}$$

with corresponding mean value function given by,

$$m(t \mid \boldsymbol{\theta}) = \begin{cases} (t/\beta_1)^{\alpha_1}, & 0 \leq t \leq \tau \\ (\tau/\beta_1)^{\alpha_1} + (t/\beta_2)^{\alpha_2} - (\tau/\beta_2)^{\alpha_2}, & t > \tau. \end{cases}$$

In a similar way, we may obtain the intensity and mean value functions for the MOP, GOP and GGOP models in the presence of a change-point τ using (4) and (5).

Remark 3 It is important to point out that different parametric forms for the intensity function before and after the change-point could be considered when using the Bayesian approach presented here. In this case the change-point should be estimated in advance and be fixed. Note that for each parametric form we have a different change-point. Hence, one would have to estimate the possible change-point using some other methodology. After this estimation is performed, then one could consider different parametric forms before and after the estimated change-point. Even though, the same parametric form is used in both time interval induced by the presence of a change-point, the methodology considered here allow to estimate simultaneously the possible change-point as well as the parameters of the model before and after the change-point. Hence, here we are not going to pursue the case where we estimate the change-point first and then use different parametric forms before and after this change-point.

Remark 4 Note that, we could use maximum likelihood methods to estimate the parameters of the model. However, the Bayesian approach using Markov chain Monte Carlo methods have some advantages that maximum likelihood methods do not have, such as inclusion of expert opinion and prior knowledge given by prior studies. Additionally, when using classical inference methods we could have difficulties in obtaining inference of interest when dealing with the case of non-homogeneous Poisson models in the presence of change-points.

3 A Bayesian estimation of the parameters

The aim of this work is to estimate the parameter $\boldsymbol{\theta}$ corresponding to the parameters of the different intensity functions considered here and to jointly estimate $(\boldsymbol{\theta}, \tau)$ when the presence of a change-point is allowed. Inference is made under a Bayesian point of view and we propose the use of Markov chain Monte Carlo (MCMC) methods to estimate the parameters of the models. Additionally, we want to decide which model best fit the ozone environmental standard violation data provided by the overall measurements of the Mexico City monitoring network when the threshold 0.17 ppm is considered. Hence, in this section a Bayesian analysis for the PLP, MOP, GOP, and GGOP models is made. Posterior summaries of interest are obtained using MCMC methods.

Bayesian inference for NHPP has been discussed by many authors (see for example Kuo and Yang 1996; Pievatolo and Ruggeri 2004; Ramírez-Cid and Achcar 1999). Those processes have been used by different authors to get inference for change-point models (see for example Achcar and Bolfarine 1989; Achcar and Loibel 1998; Carlin et al. 1992; Dey and Purkayastha 1997; Matthews and Farewell 1982). Raftery and Akman (1986) consider a Bayesian analysis for homogeneous Poisson processes (HPP) in the presence of a change-point. Ruggeri and Sivaganesan (2005) introduce a Bayesian analysis for change-points in non-homogeneous Poisson processes considering PLP and dealing with a random number of change-points.

In this paper, the use of MCMC methods is made (see for example Chib and Greenberg 1995; Gelfand and Smith 1990 or Smith and Roberts 1993) to develop a Bayesian analysis for the change-point in NHPP when PLP, MOP, GOP, and GGOP models are considered.

We are going to use an empirical Bayesian type analysis of the proposed models. Hence, we first consider that the NHPP does not have a change-point. In this way, we assume uniform $\mathrm{U}[a, b]$ prior distributions for the parameters of each model, choosing a and b in an appropriate way to have approximately non-informative prior distributions. For the special case of the PLP model, we assume a uniform $\mathrm{U}[0, 1]$ prior distribution for the parameter α in order to have decreasing intensity functions. We further assume prior independence among the parameters. Other prior distributions may also be considered to analyze the pollution data of Mexico City. In this way, in some cases, we also consider $\mathrm{Gamma}[c, d]$ prior distributions with mean c/d and variance c/d^2, where c and d are known hyperparameters.

The joint posterior distribution for $\boldsymbol{\theta}$ given the data $\mathbf{D_T}$ is,

$$P(\boldsymbol{\theta} \mid \mathbf{D_T}) \propto L(\boldsymbol{\theta} \mid \mathbf{D_T})\, P(\boldsymbol{\theta}) \tag{7}$$

where $P(\boldsymbol{\theta})$ denotes the joint prior distribution of the parameter $\boldsymbol{\theta}$ and $L(\boldsymbol{\theta} \mid \mathbf{D_T})$ is the likelihood function given in (3).

Simulated samples for the joint posterior distribution for $\boldsymbol{\theta}$ are obtained, using standard MCMC methods, from the full conditional posterior distributions $P(\theta_{(i)} \mid \boldsymbol{\theta}_{(-i)}, \mathbf{D_T})$, $i = 1, 2, \ldots, d$ (see for example Gelfand and Smith 1990), where $\theta_{(i)}$ is the ith coordinate of the vector $\boldsymbol{\theta}$, $\boldsymbol{\theta}_{(-i)}$ is the vector $\boldsymbol{\theta}$ without its ith coordinate and d is the dimension of $\boldsymbol{\theta}$. A great simplification is obtained using the software WinBugs (Spiegelhalter et al. 1999) where only the joint distribution for the data and the prior distributions for the parameters need to be specified.

In a second stage of the Bayesian analysis, we consider the PLP, MOP, GOP and GGOP models in the presence of a change-point τ. Hence, we also consider a prior distribution for τ which in this case could either be a uniform distribution in a subinterval $[e, f]$ of $(0, T)$, large enough to have an approximate non informative prior, or be a Gamma distribution with a sufficiently large variance, and an informative prior distribution for $\boldsymbol{\theta}$ for each NHPP model. Those informative prior distributions are obtained using the environmental information gathered from prior opinion from researchers from the Ministry of Environment in Mexico and using the information for each parameter obtained from the case where we assume NHPP models without the presence of a change-point.

We take either uniform U$[a, b]$ or Gamma$[c, d]$ prior distributions for each parameter assuming that a, b, c and d are known hyperparameters. We further assume prior independence among the parameters.

The joint posterior distribution for $\boldsymbol{\theta}$ and τ is given by,

$$P(\boldsymbol{\theta}, \tau \mid \mathbf{D_T}) \propto L(\boldsymbol{\theta}, \tau \mid \mathbf{D_T})\, P(\boldsymbol{\theta}, \tau) \tag{8}$$

where $P(\boldsymbol{\theta}, \tau)$ denotes the joint prior distribution for $\boldsymbol{\theta}$ and τ and $L(\boldsymbol{\theta}, \tau \mid \mathbf{D_T})$ is the likelihood function of the model with the presence of a change-point τ and it is given by (6).

4 An application to the case of ozone in Mexico City

Consider the ozone pollution data corresponding to the daily maximum measurements of ozone provided by the monitoring network of Mexico City during the period of January 1, 1998 and December 31, 2004. This corresponds to a total of $T = 2557$ days. The Bayesian analysis is made considering two cases. In the first case, we consider NHPP models with PLP, MOP, GOP, and GGOP intensity functions without the presence of a change-point. In the second case, we consider the same NHPP model but now assuming the presence of a change-point τ.

The selection of the best model is made using some existing Bayesian adequacy measures such as the deviance information criterion (DIC) (Spiegelhalter et al. 2002) which is an approximation for the Bayes factor. Smaller values of DIC indicate better models. The DIC is the Bayesian equivalent the the AIC (Akaike Information Criterion) (see Akaike 1974). In general, DIC is suitable to discriminate hierarchical models. DIC is given by

$$\mathrm{DIC} = D^{*} + 2\,p_D$$

where D^{*} is the deviance evaluated at the posterior mean and $p_D = D^{a} - D^{*}$ is the effective number of parameters in the model with D^{a} the posterior mean deviance. DIC can be estimated by the sample generated by the MCMC algorithm and is given automatically by the software WinBugs (Spiegelhalter et al. 1999). We also discriminate the models by comparing plots of the accumulated number of ozone violations with the estimated mean value functions versus time of occurrence.

The Bayesian analysis for all models was made using WinBugs. Convergence of the Gibbs sampling algorithm was monitored by usual time series plots for the simulated samples and also using some existing Bayesian convergence methods considering different initial values (see for example Gelman and Rubin 1992).

4.1 NHPP models without the presence of change-points

Assuming the PLP model, we consider a uniform U[0, 100] non-informative prior distribution for the parameter β and a uniform U[0, 1] prior distribution for the parameter α in order to have a decreasing intensity function. A burn-in sample of size 1000 was considered to eliminate the effect of the initial values. The posterior summaries of interest and the Monte Carlo estimate for DIC based on 2000 simulated Gibbs samples are given in Table 1. This 2000 Gibbs sample as well as the sample for the MOP, GOP, and GGOP models were produced by taking every 10th simulated value.

If we consider the MOP model, we take informative prior distributions for the parameters α and β using empirical Bayesian methods to have convergence of the

Table 1 Posterior mean, standard deviation (SD), and 95% credible interval of the parameters of each intensity function of the NHPP process when the presence of change-point is not taken into account

Model	Parameters	Mean	SD	95% Credible interval	DIC
PLP	α	0.7491	0.02397	(0.7033,0.7957)	3713.69
	β	0.2761	0.08194	(0.145,0.4592)	
MOP	α	49900	69.86	(49770,50050)	38508.6
	β	18270	41.55	(18190,18350)	
GOP	α	1198	28.75	(1145,1260)	3604.47
	β	0.00064	0.000039	(0.00057,0.00072)	
GGOP	α	1064	41.83	(989.1,1152)	3585.08
	β	0.00019	0.000058	(0.000106,0.00033)	
	γ	1.206	0.04466	(1.116, 1.289)	

Gibbs sampling algorithm. We assume a Gamma[500000, 10] prior distribution for α and a Gamma[200000, 10] prior distribution for β. In Table 1, we also have the posterior summaries and Monte Carlo estimate for DIC based on 2000 simulated Gibbs samples. In this case, we considered a burn-in sample of size 1000 to have a stationary distribution for each parameter. It is important to point out that the convergence of the Gibbs sampling algorithm was obtained only when using a very informative prior for the parameters of the MOP model.

Assuming the GOP model, we consider a Gamma[1200, 1] non-informative prior distribution for the parameter α and a Gamma[0.1, 1] prior distribution for the parameter β. In this case, convergence was obtained after a burn-in sample of size 1000. Posterior summaries of interest and the DIC estimate based on 2000 simulated Gibbs samples are also given in Table 1.

Finally, assuming the GGOP model, informative prior distributions based on the information from a Bayesian analysis for the GOP model are considered. In this case, we assume a uniform U[300, 2000] prior distribution for α, a Gamma[0.1, 1] prior distribution for β and a uniform U[0.5, 1.5] prior distribution for γ. We would like to point out that convergence of the Gibbs sampling algorithm considering the GGOP model was obtained using the same prior distribution for β as the one assumed for the GOP model. However, in the case of the parameter α in the GGOP model it was necessary a more informative prior distribution in order to obtain convergence of the MCMC algorithm internally implemented in the WinBugs software. In Table 1, we also have the posterior summaries and the DIC estimate based on 2000 simulated Gibbs samples taken after a burn-in sample of size 1000.

In Fig. 2, we have the plots for the accumulated number $N_t^{(\boldsymbol{\theta})}$, $t \in (0, T)$ of ozone violations and for the estimated mean value functions $m(t \mid \boldsymbol{\theta})$ versus time t for each non-homogeneous Poisson model assumed here. (Plots were made using the estimated posterior mean of the parameters of the mean value function.) Observing the plots of Fig. 2, we see a much better fit of the GGOP model. The GOP model also gives a very good fit.

Note that the Monte Carlo estimates for DIC (see Table 1) indicates that the GGOP model gives better fit for the ozone data of Mexico City, since it is the one with smaller DIC value. This result is in close agreement with the plots presented in Fig. 2. In that figure we observe that the GOP and GGOP models are the ones giving better fit for the data. Observe that the DIC value for the GOP and GGOP models are very close to each other. However, since the value one is not included in the 95% credible interval for the parameter γ in the GGOP model, we conclude that the GGOP model is the best model, since GOP is a particular case of GGOP model (setting $\gamma = 1$).

Remark Note that besides the use of DIC we are also taking into account the plots of the accumulated number of ozone violations and estimated mean value functions to check the fit of the models involved. This is performed in the case where the presence of a change-point is not considered as well as when the presence of a change-point is allowed.

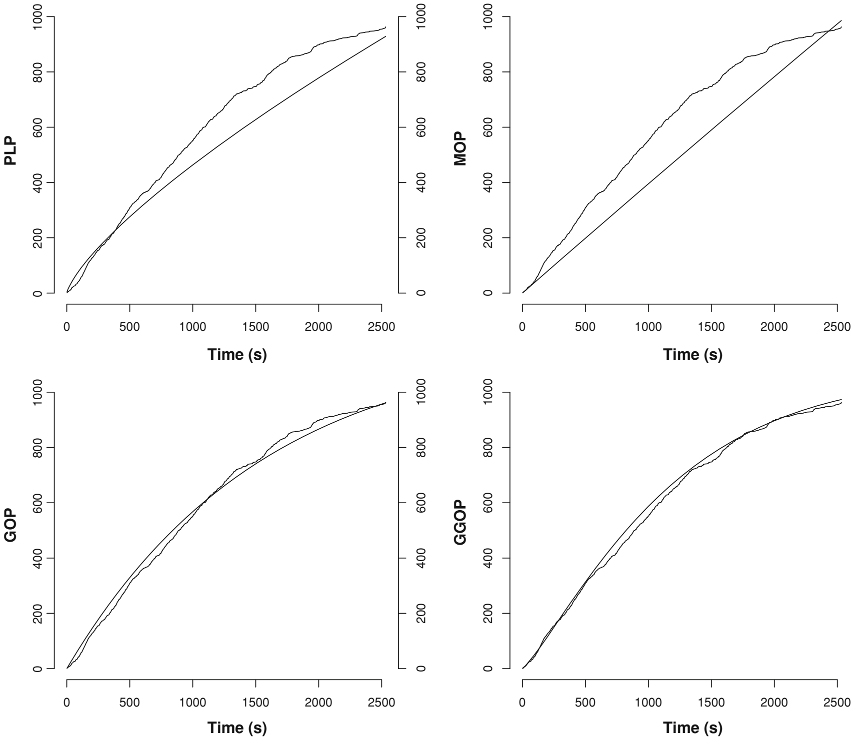

Fig. 2 Accumulated number of ozone violations and estimated mean value functions versus time without the presence of a change-point when the PLP, MOP, GOP, and GGOP models are considered. Time is measured in days

4.2 NHPP models with the presence of a change-point

In the second stage of the Bayesian analysis, we assume the presence of a change-point τ in the NHPPs with PLP, MOP, GOP and GGOP intensity functions.

The consideration of a model that includes the presence of a change-point could be justified by a careful preliminary analysis of the data or by political decision to improve the air quality in Mexico City. In this way, we could consider graphical plots (see Fig. 1). Alternatively, we could assume in the first step of the statistical analysis of the MAMC ozone data, a HPP model in the presence or not of a change-point (see Raftery and Akman 1986). Pursuing in that direction, we have the following. If a change-point, is considered to be present, then the intensity function is given by

$$\lambda(t \mid \boldsymbol{\theta}) = \begin{cases} \lambda_1, & \text{if } 0 \leq t \leq \tau \\ \lambda_2, & \text{if } t > \tau, \end{cases} \tag{9}$$

where λ_1 and λ_2 are strictly positive constants. The corresponding mean value functions are given by

$$m(t \mid \boldsymbol{\theta}) = \begin{cases} t\,\lambda_1, & \text{if } 0 \le t \le \tau \\ \tau\,\lambda_1 + t\,\lambda_2 - \tau\,\lambda_2, & \text{if } t > \tau. \end{cases} \tag{10}$$

The likelihood function for $\boldsymbol{\theta} = (\lambda_1, \lambda_2)$ and τ is a special case of (6) where $\lambda(t \mid \boldsymbol{\theta}_1) = \lambda_1$ and $\lambda(t \mid \boldsymbol{\theta}_2) = \lambda_2$. Hence, $L(\boldsymbol{\theta}, \tau \mid \mathbf{D_T})$ is given by,

$$L(\boldsymbol{\theta}, \tau \mid \mathbf{D_T}) = \lambda_1^{N_\tau^{(\boldsymbol{\theta})}}\, \lambda_2^{N_T^{(\boldsymbol{\theta})} - N_\tau^{(\boldsymbol{\theta})}}\, \mathrm{e}^{-\lambda_1 \tau - \lambda_2 (T-\tau)}. \tag{11}$$

When a HPP model without the presence of a change-point is considered, the likelihood function for $\boldsymbol{\theta} = \lambda$ is a special case of (3) and it is given by

$$L(\lambda \mid \mathbf{D_T}) = \lambda^n \mathrm{e}^{-\lambda T}. \tag{12}$$

Note that in order to discriminate between the models with and without the presence of a change-point, we may also use the Bayesian Information Criterion (BIC) (Schwarz 1978), given by,

$$\ln\left(L(\hat{\boldsymbol{\theta}} \mid \mathbf{D_T})\right) - \frac{1}{2}\mathrm{d}\, \ln(n) \tag{13}$$

where $\hat{\boldsymbol{\theta}}$ is the maximum likelihood estimator for $\boldsymbol{\theta}(\boldsymbol{\theta} = (\lambda_1, \lambda_2, \tau)$ or $\boldsymbol{\theta} = \lambda)$, d is the dimension of the vector $\boldsymbol{\theta}$ and n is the sample size.

In this way, considering the HPP model we obtain the value -3500.84 for the BIC approximation when no change-point is present, and obtain the value -1809.30 for the BIC approximation when the presence of a change-point is taken into account. Clearly, there is an indication that a model with a change-point gives better fit to the ozone pollution data of Mexico City since it presents a bigger value for BIC. (Note that in here we use the maximum likelihood estimator of $\boldsymbol{\theta}$ to calculate (13).)

Returning to the NHPP formulation and assuming the PLP model, we take a uniform U[1, 2557] non-informative prior distribution for the change-point τ, uniform U[0, 1] prior distributions for α_1 and α_2, in order to have decreasing intensity functions, Gamma[50, 100] prior distribution for β_1 and Gamma[27, 100] prior distribution for β_2. The choice of the hyperparameters for the Gamma prior distributions for β_1 and β_2 was based on the information obtained from the first stage of analysis (NHPP without the presence of a change-point). A burn-in sample of size 1000 was considered in the simulation of the Gibbs samples for the parameters. The posterior summaries of interest and the DIC estimate based on 1000 Gibbs samples, taking every 10th sampled value to have approximately uncorrelated values, are given in Table 2.

Considering a GOP model, we take a Gamma[1200, 1] prior distribution for the change-point τ. The choice of the hyperparameters of the gamma prior distribution for the change-point τ was based on a preliminary analysis of the plot for the accumulated number of ozone violations versus time (see Fig. 1). This choice of prior was motivated by observing that using non-informative uniform prior distributions, we did not get convergence of the Gibbs sampling algorithm using the software WinBugs. We also assume a Gamma[1, 1000] prior distribution for the parameters β_1 and β_2 and a Gamma[120000, 100] prior distribution for the parameters α_1 and α_2. A burn-in

Table 2 Posterior mean, standard deviation (SD), and 95% credible interval of the parameters of each intensity function of the NHPP process in the presence of a change-point

Model	Parameters	Mean	SD	95% Credible interval	DIC
PLP	α_1	0.5943	0.07263	(0.4528,0.742)	3613.01
	α_2	0.2627	0.04875	(0.1728,0.368)	
	β_1	0.8528	0.01427	(0.8235,0.8802)	
	β_2	0.7071	0.01402	(0.6795,0.734)	
	τ	1341	41.43	(1318,1371)	
MOP	α_1	49840	214.7	(49410, 50280)	3788.22
	α_2	50180	230.4	(49720, 50650)	
	β_1	20150	142.9	(19870, 20420)	
	β_2	19820	146.3	(19540, 20100)	
	τ	1211	360.4	(376.6, 1769)	
GOP	α_1	1201	3.463	(1194,1207)	3598.13
	α_2	1999	3.444	(1193,1206)	
	β_1	0.000612	0.0000344	(0.000549,0.000684)	
	β_2	0.00085	0.0000794	(0.000689,0.001001)	
	τ	1197	35.74	(1130,1267)	
GGOP	α_1	1441	259.7	(1010,1949)	3575.54
	α_2	1389	197.5	(1007,1791)	
	β_1	0.000252	0.0000791	(0.000135, 0.000433)	
	β_2	0.000582	0.000262	(0.000054,0.000975)	
	γ_1	1.106	0.05779	(1.001,1.227)	
	γ_2	1.104	0.09028	(1.004,1.386)	
	τ	1202	34.26	(1137, 1268)	

sample of size 1000 was needed to obtain convergence of the Gibbs sampling algorithm. The posterior summaries of interest and the DIC estimate based on 2000 Gibbs samples, taking every 10th sampled value to have approximately uncorrelated values, are given in Table 2.

Assuming the GGOP model, we consider a Gamma[1200, 1] prior distribution for the change-point τ; uniform U[300, 2000] prior distribution for α_1 and α_2; uniform U[0.000001, 0.001] prior distribution for β_1 and β_2; and Gamma[0.5, 1.5] prior distribution for γ_1 and γ_2. The choice of the hyperparameters for the GGOP model was based on the information obtained during the first stage of analysis using the GGOP model. When considering non-informative prior distributions for the parameters of the GGOP model, we did not get convergence of the Gibbs sampling algorithm using the software WinBugs. A burn-in sample of size 1000 was needed to obtain convergence of the Gibbs sampling algorithm. The posterior summaries of interest and the DIC estimate based on 2000 Gibbs samples, taking every 10th sample to have approximately uncorrelated values, are given in Table 2.

Considering a MOP model, we take a uniform U[200, 1800] prior distribution for the change-point τ, a Gamma[50000, 1] prior distribution for both α_1 and α_2, and a

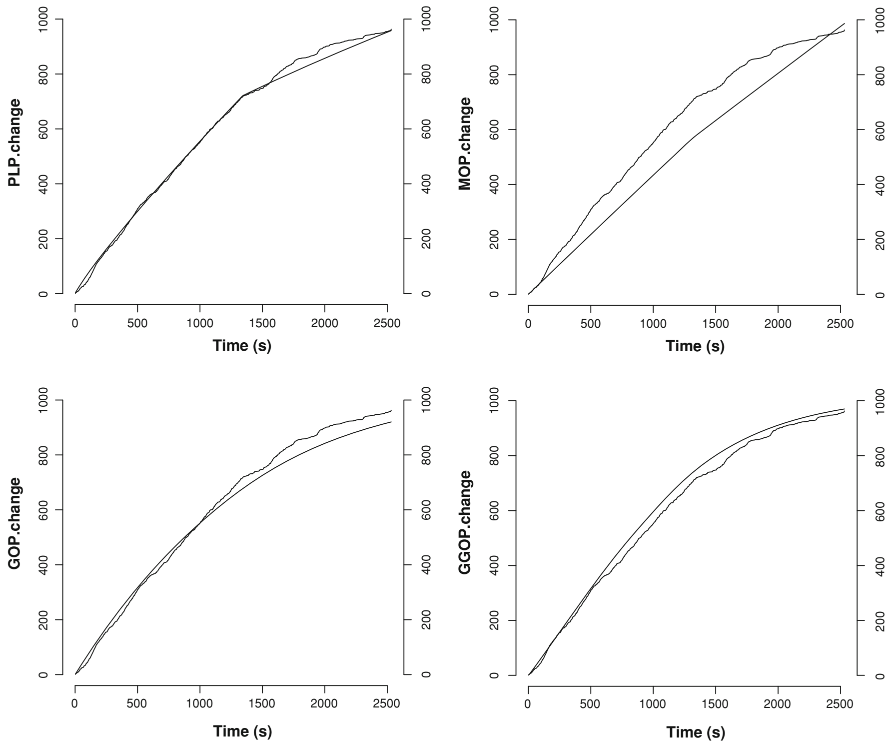

Fig. 3 Accumulated number of ozone violations and estimated mean value functions versus time with the presence of a change-point when the PLP, MOP, GOP and GGOP models are considered. Time is measured in days

Gamma[20000, 1] prior distribution for β_1 and β_2. We have considered informative prior distributions in order to obtain convergence of the Gibbs sampling algorithm. The choice of the hyperparameters and prior distributions were made using the information provided by the use of MOP model without the presence of a change-point. A burn-in period of 1000 samples was considered. The posterior summaries of interest and the DIC based on 2000 Gibbs samples, taking every 10th sample to have approximately uncorrelated values, are given in Table 2.

Remark We would like to point out that the choice of different prior distributions for τ for different models was needed in order to obtain convergence of the Gibbs sampling algorithm using the WinBugs software.

In Fig. 3, we have the plots for the accumulated number $N_t^{(\boldsymbol{\theta})}$, $t \in (0, T)$ of ozone violations and for the estimated mean value function $m(t \mid \boldsymbol{\theta})$ versus time t considering each non-homogeneous Poisson model assumed here. It is possible to see from the results of Table 2 and Fig. 3 that the PLP, GOP and GGOP models give good fit for the ozone violation data of Mexico City. Note that both the graphical and DIC results obtained using these models and the MOP model, corroborate the fact that either in

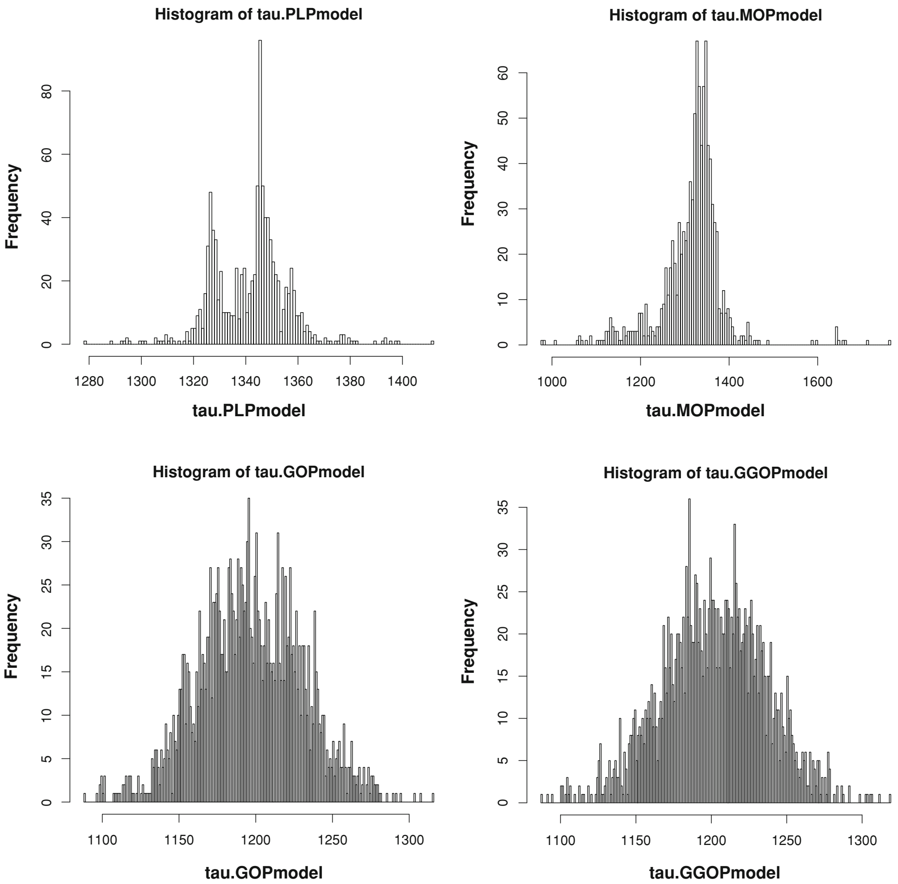

Fig. 4 Marginal posterior distribution for the change-point when the PLP, MOP, GOP and GGOP models are considered. The horizontal axis represents time which is measured in days

the presence of a change-point or not, the GGOP model with a change-point has the overall better fit, as can be seen in Fig. 3.

Note that there is practically no difference in the fit obtained when using the MOP model either with or without the presence of a change-point. Perhaps the MOP model is not an adequate model to be used with the data set considered here, specially when a change-point is present.

In Fig. 4, we have the plot of the marginal posterior distribution for the change-point τ for all the non-homogeneous Poisson models considered here.

5 Discussion

The use of non-homogeneous Poisson processes could be very useful to analyze pollution data of cities throughout the world. The use of some existing parametric forms for the intensity function for the NHPP commonly used in software reliability studies could give great flexibility of fit for the pollution data. This data would provide information about the epochs of occurrence of pollution violations of environmental standards during a specific period of time, as is the case of the pollution data of Mexico City analyzed in this paper. Using Markov Chain Monte Carlo methods, we obtain in a simple way the posterior distribution summaries of quantities of interest.

The use of the WinBugs software gives a great simplification in the computational work to simulate the samples from the posterior distributions of interest. This software could be an important tool to analyze large amount of pollution data as it is common in cities where data is collected daily in different monitoring stations.

The use of models with more than two parameters, usually requires information of experts or the use of empirical Bayesian methods in different stages to have convergence of the Gibbs sampling algorithm. Other common problem with pollution data is the presence of one or more change-points, since the pollution is expected to decrease or increase after political decisions to control or not the sources of pollution in the cities. In this case, we also observe that better NHPP models, like the GOP or the GGOP models could be of great use. However, the analysis of the case where multiple change-points are present is not going to be addressed here. This is the aim of another work. One methodology that may be used in the case where multiple change-points are present is the empirical Bayesian analysis. One could assume at first that no change-points are present. Using the information obtained in this stage, one may assume the presence of one change-point. Again, using the information obtained in this stage one may assume the presence of two or more change-points and so on. After, considering the different possibilities that are compatible with the data set at hand, one may use the preferred criterion to select the model that best adjust to the data set used.

The MOP model does not seem to be a model that should be used to describe the data set considered here, either with or without the presence of a change-point. We would like to point out that the convergence of the algorithm, when the MOP model with change-point is considered, only happened when we used very informative prior distributions for the parameters α and β. This possibly happens due to non identification of the parameters associated to the model. The informative prior distributions were obtained from information provided by results when the presence of a change-point was not considered. If we consider the MOP model with the presence of a change-point and use uniform prior distributions for α and β, then convergence of the WinBugs software is not achieved. Note that for the MOP model without the change-point, we have used Gamma[500000, 10] and Gamma[200000, 10] prior distributions for α and β, respectively.

Therefore, based on the DIC results shown in Tables 1 and 2, we have an indication that the best model is given by the GGOP (generalized Goel–Okumoto) model with a change-point. Its DIC value is the smallest when compared to all models either in the case where a change-point is present or in the case where there is no change-point. This conclusion is in close agreement with the plots given by Figs. 2 and 3.

The lack of convergence of the Monte Carlo algorithm unless informative prior distributions are used as well as large variance of the posterior distributions of the parameters, are very important issues in the Bayesian paradigm. More complex models give better fit for the data. However, in many cases, including some presented in this paper, convergence problems of the Monte Carlo algorithm may occur when using non informative prior distributions. In the present paper we have used prior expert environmental information and empirical Bayesian methods to choose informative prior distributions for the parameters of the models. It is possible that more informative priors could improve the variance for the GOP and GGOP models.

When we consider the GGOP model allowing the presence of a change-point τ we have that the Monte Carlo estimate for the posterior mean of τ produces the value 1202. This corresponds roughly to a day in March 2001. We would like to point out the strict environmental measures were implemented in Mexico City in the years 1999 and 2000. Besides, regulatory measures have been taken since 1990. We have that the ozone concentrations in 2005 was 30% smaller than those in 1990. The rate at which ozone peaks occurred has also decreased. Note that de GGOP model selected to explain the data set used here, also captures the decrease in concentration and of the rate of occurrence. When plotting the rate function $\lambda^{(\mathrm{GGOP})}(t)$, $t \geq 0$ using the estimated parameters we have that using the values of the estimated parameters before the change-point, the rate function has values larger than when we use the values of the estimated parameters after the change-point. Around the estimated change-point the relation is reversed, i.e., the values of the rate function is smaller when using the parameters estimated after the change-point than when using the parameters estimated before the change-point. Therefore, the mean inter-occurrence times between consecutive peaks increases and therefore the mean number os peaks decreases. This captures the ozone behavior that may be observed in the Mexico City ozone data (see for instance Figs. 1 and 3). The change in behavior of the mean function can also be explained by the change in the ozone pollution behavior caused in part by the preventive measures implemented by the environmental authorities.

We would like to call attention to the fact that even though the models considered here are for ozone exceedances, one could also model the daily ozone records. However, the latter was not pursued here. The reason for that is that the interest is in obtaining ways of estimating the probability of having emergency situations declared a certain number of times in a time interval of interest. This estimation may be performed by using the fact that $N_t^{(\boldsymbol{\theta})}$, $t \geq 0$ is such that

$$P(N_{t+s}^{\boldsymbol{\theta}} - N_t^{\boldsymbol{\theta}} = k) = \frac{[m(t+s|\boldsymbol{\theta}) - m(t|\boldsymbol{\theta})]^k}{k!} \exp\left(-[m(t+s|\boldsymbol{\theta}) - m(t|\boldsymbol{\theta})]\right),$$

for $s, t \geq 0$ and $k = 0, 1, 2, \ldots$. The mean function $m(t|\boldsymbol{\theta})$, $t \geq 0$ is the one obtained by substituting the estimated posterior means of the parameters involved in the model that best fit the data (in the present case the GGOP model).

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Appendix

In this appendix, we present the WinBugs code used to obtain the estimates for the parameters of the rate function $\lambda(t), t \geq 0$, when the GGOP model is taken into account and the presence of a change-point is allowed.

Generalized Goel–Okumoto model in the presence of a change-point.

```
model{
    for (i in 1 : N){
    zeros[i] <- 0
    phi[i] <- -log(L[i])
    zeros[i] ~ dpois(phi[i])
    log(lambda[i]) <- log(alpha[J[i]]) + log(beta[J[i]])
        +log(gamma[J[i]]) + (gamma[J[i]] - 1) * log(t[i])
        -(beta[J[i]]) * pow(t[i], gamma[J[i]])
    L[i] <- lambda[i] * m
    J[i] <- 1 + step(t[i] - tau - 0.5)
    }
    m <- exp(-((alpha[1]) * (1 - exp(-(beta[1]) * (pow(tau, gamma[1]))))
        +(alpha[2]) * (1 - exp(-(beta[2]) * (pow(T, gamma[2]))))
        -(alpha[2]) * (1 - exp((beta[2]) * (powtau, gamma[2])))))/N)
    tau ~ dgamma(1200, 1)
    beta[2] ~ dunif(0.000001, 0.001)
    alpha[1] ~ dunif(300, 2000)
    alpha[2] ~ dunif(300, 2000)
    beta[1] ~ dunif(0.000001, 0.001)
    gamma[1] ~ dunif(0.5, 1.5)
    gamma[2] ~ dunif(0.5, 1.5)
    }
```

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