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Flexible integro-difference equation modeling for spatio-temporal data

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ABSTRACT

The choice of kernel in an integro-difference equation (IDE) approach to model spatio-temporal data is studied. By using approximations to stochastic partial differential equations, it is shown that higher order cumulants and tail behavior of the kernel affect how an IDE process evolves over time. The asymmetric Laplace and the family of stable distributions are presented as alternatives to the Gaussian kernel. The asymmetric Laplace has an extra parameter controlling skewness, whereas the class of stable distributions includes parameters controlling both tail behavior and skewness. Simulations show that failing to account for kernel shape may lead to poor predictions from the model. For an illustration with real data, the IDE model with flexible kernels is applied to ozone pressure measurements collected biweekly by radiosonde at varying altitudes. The results obtained with the different kernel families are compared and it is confirmed that better model prediction may be achieved by electing to use a more flexible kernel.

1. Introduction

A spatio-temporal data set refers to data collected across a spatial field and over several time points. Climatological and environmental variables provide several common and abundant examples of data recorded in space and time. In addition to traditional examples of environmental space–time variables, such as temperature or precipitation, there is an increasing ability to store and monitor the dynamics of different types of georeferenced processes. Data for housing costs, crime rates, population growth, soil content, and disease incidence, are some of the many examples of variables that are of interest in areas as diverse as spatial econometrics, epidemiology, and geography, to mention a few.

The field of time series has produced a rich body of literature during at least the last 50 years (Hamilton, 1994; Shumway and Stoffer, 2011). Spatial statistics, despite the seminal work by Matheron (1963), was a fringe area as recently as the early 1990s (Cressie, 1993), but has since received a great deal of attention within the statistical community. Spatio-temporal models stem naturally from these areas, but a systematic treatment of spatio-temporal statistical models has only recently been developed (Cressie and Wikle, 2011). Compared to times series and spatial statistics, the fundamental challenge of spatio-temporal models is to capture the interactions between the spatial and temporal components.

Three general methods are currently used to analyze data from spatio-temporal processes of the form $\{X_t(s) : s \in \mathcal{S}, t \in \mathcal{T}\}$, where s indexes the spatial domain $\mathcal{S}$ and t indexes the time domain $\mathcal{T}$. The first involves an extension of the traditional approach to modeling random fields, focusing on the first and second moment of the process. The goal is to find general

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families of space–time correlation functions of the form $Cov(X_t(s), X_u(v)) = C(s, v, t, u)$, which are "smooth everywhere" and yet "allow different degrees of smoothness" (Stein, 2005). In this setting, both s and t are considered as continuous indexes. This lends flexibility to the models, but requires dealing with potentially large covariance matrices. This approach can thus have important computational drawbacks when large spatial domains or long time periods are considered.

A second common modeling approach for spatio-temporal data is an extension of deterministic dynamical models that incorporates stochastic components. This leads to stochastic partial differential equation (SPDE) models. For instance, Jones and Zhang (1997) consider the SPDE $\frac{\partial}{\partial t}X_t(s) - \beta\frac{\partial^2}{\partial s^2}X_t(s) + \alpha X_t(s) = \delta_t(s)$, where $\delta_t(s)$ is a zero mean error process. This SPDE is called a diffusion–injection equation and is just one of the various SPDE-based models commonly used for naturally occurring physical processes (Heine, 1955; Zheng and Aukema, 2010).

The third method is to obtain an explicit description of the dynamics of the process by specifying its evolution as a function of the spatial distribution of the process. A dynamic spatio-temporal model can be written as

$$X_t(s) = \mathcal{M}(X_{t-1}(s), s, \boldsymbol{\theta}) + \varepsilon_t(s), \quad t = 1, \dots, T,$$

where $\mathcal{M}$ represents a specific model configuration, governing the transfer of information from time $t-1$ to time t. Here, $\boldsymbol{\theta}$ is a parameter vector, and $\varepsilon_t(s)$ is a zero mean noise process which may have a spatially dependent covariance structure. In these models, the process evolves as an entire spatial field over a discrete time component. Cressie and Wikle (2011) strongly support this approach, and suggest a "hierarchical dynamical spatio-temporal model" of the form

$$\boldsymbol{Y}_t = \boldsymbol{B}_t\boldsymbol{X}_t + \boldsymbol{\varepsilon}_t, \quad \boldsymbol{\varepsilon}_t \sim N(\mathbf{0}, \boldsymbol{V}_t),\ t = 1, \dots, T, \tag{1}$$

and

$$\boldsymbol{X_t} = \mathcal{M}_t(\boldsymbol{X}_{t-1}, \boldsymbol{\theta}) + \boldsymbol{\omega}_t, \quad \boldsymbol{\omega}_t \sim N(\mathbf{0}, \boldsymbol{W}_t),\ t = 1, \dots, T, \tag{2}$$

where $\boldsymbol{Y}_t$ is the vector of data, and $\boldsymbol{X}_t$ is a vector of latent variables representing an underlying process that is linked to $\boldsymbol{Y}_t$ through the incidence matrix $\boldsymbol{B}_t$. Moreover, $\boldsymbol{\varepsilon}_t$ and $\boldsymbol{\omega}_t$ are noise terms with specified covariances $\boldsymbol{V}_t$ and $\boldsymbol{W}_t$, respectively.

A specific case of the model described by Eqs. (1) and (2) is the integro-difference equation (IDE) spatio-temporal model. We consider IDE models of the form

$$X_t(s) = e^{\lambda} \int k(s-u|\boldsymbol{\theta})X_{t-1}(u)du + \omega_t(s), \tag{3}$$

where $k(\cdot)$ is a redistribution kernel with parameter vector $\boldsymbol{\theta}$, and $\omega_t(s)$ is an error process which may be spatially colored. This kernel weights the contribution of the process at time $t-1$ to the process at time t at location s. The scaling term λ controls the growth or decay of the process. Typically, the center of the kernel for each location is somewhere near s, resulting in nearby values being weighted more heavily than others. The spatial dependency in the IDE model arises from nearby observations sharing large contributions from many of the same observations of the previous time point. Thus, the spatial and temporal relationships interact with each other as the process evolves,producing a non-separable process. Furthermore, the kernel width affects the smoothness of the resulting process.

Originally used by ecologists studying the growth and spread of species (Kot et al., 1996), integro-difference equations were introduced for general spatio-temporal processes in Wikle and Cressie (1999). In Wikle (2002), the IDE kernel is specified parametrically through a Gaussian distribution with unknown location and scale parameters. The stochastic properties of the process that results from an IDE, such as stationarity and separability, are explored in Brown et al. (2000) and Storvik et al. (2002). An important extension where the mean of the kernel is spatially indexed is presented in Wikle (2002) and Xu et al. (2005).

Overall, the literature is dominated by IDE models based on Gaussian kernels. Though there is some mention of non-Gaussian kernels, it is without exploring the modeling benefits and inferential issues arising from the use of more general kernel families. Spatio-temporal data can have a variety of features that may not be represented well by a Gaussian kernel IDE model. As shown here, these features include dispersion, extra-diffusion, and flexibility in local behavior. In this paper, we focus on the exploration of the properties and the development of inferential methods to deal with IDE models based on relatively simple non-Gaussian parametric families of kernels. Our main purpose is to show how using non-Gaussian kernels in IDE modeling can add value to spatio-temporal modeling. We will show that, for hierarchical models as in Eqs. (1) and (2), an IDE with a kernel more flexible than the Gaussian can lead to improved model performance and prediction, and capture a wider array of process dynamics. We restrict the scope of this paper to one-dimensional space for ease in computation, but we expect that the same advantages arising from the use of non-Gaussian kernels in one dimension will also emerge when using non-Gaussian kernels in two dimensions.

The rest of the paper is organized as follows. In Section 2, we use two approximations of the IDE to differential equations to theoretically justify the use of more flexible kernels. Section 3 provides modeling techniques for the IDE model and presents two alternatives to the Gaussian kernel. Direct comparison of model fit and prediction is performed for each kernel choice in Section 4, for both real and synthetic data. Concluding remarks are made in Section 5, and the four Appendices collect technical details.