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Conditional simulations of Brown–Resnick processes

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SUMMARY

Since many environmental processes such as heat waves or precipitation are spatial in extent, it is likely that a single extreme event affects several locations and the areal modelling of extremes is therefore essential if the spatial dependence of extremes has to be appropriately taken into account. Although some progress has been made to develop a geostatistic of extremes, conditional simulation of max-stable processes is still in its early stage. This paper proposes a framework to get conditional simulations of Brown–Resnick processes. Although closed forms for the regular conditional distribution of Brown–Resnick processes were recently found, sampling from this conditional distribution is a considerable challenge as it leads quickly to a combinatorial explosion. To bypass this computational burden, a Markov chain Monte–Carlo algorithm is presented. We test the method on simulated data and give an application to extreme rainfall around Zurich. Results show that the proposed framework provides accurate conditional simulations of Brown–Resnick processes and can handle real-sized problems.

Some key words: Brown–Resnick process; Conditional simulation; Gibbs sampler; Markov chain Monte–Carlo; Precipitation; Regular conditional distribution.

1. INTRODUCTION

Max-stable processes are a natural extension of the extreme value theory to the infinite dimensional case, i.e., extremes of stochastic processes, and therefore play a major role in the statistical modelling of spatial extremes (Padoan et al., 2010; Davison et al., 2011). Although a different spectral characterization of max-stable processes exists (de Haan, 1984), for our purposes the most useful representation is the one of Schlather (2002) that considers the process

$$Z(x) = \max_{i \geq 1} \zeta_i Y_i(x), \qquad x \in \mathbb{R}^d, \tag{1}$$

where $\{\zeta_i\}_{i\geq 1}$ are the points of a Poisson process on $(0, \infty)$ with intensity $\mathrm{d}\Lambda(\zeta) = \zeta^{-2}\mathrm{d}\zeta$ and $Y_i(\cdot)$ are independent replicates of a non-negative continuous sample path stochastic process $Y(\cdot)$ such that $\mathrm{E}[Y(x)] = 1$ for all $x \in \mathbb{R}^d$. It is well known that $Z(\cdot)$ is a max-stable process on $\mathbb{R}^d$ with unit Fréchet margins (de Haan & Fereira, 2006; Schlather, 2002). Although (1) amounts

to compute the pointwise maximum over an infinite number of points $\{\zeta_i\}$ and processes $Y_i(\cdot)$, it is possible to get (approximate) realizations from $Z(\cdot)$ (Schlather, 2002; Oesting et al., 2011).

Based on (1) several parametric max-stable models have been proposed (Schlather, 2002; Smith, 1990; Davison et al., 2011) but in this paper we focus on Brown–Resnick processes (Brown & Resnick, 1977; Kabluchko et al., 2009) for which

$$Y(x) = \exp\left\{W(x) - \gamma(x)\right\}, \qquad x \in \mathbb{R}^d, \tag{2}$$

where $W(\cdot)$ is a centered Gaussian process with continuous sample path, stationary increments, (semi) variogram $\gamma(\cdot)$ and such that $W(o) = 0$ almost surely. Closed forms for the bivariate distribution function of (2) are known for a long time (Brown & Resnick, 1977; Kabluchko et al., 2009; Davison et al., 2011), i.e.,

$$-\log \mathrm{pr}[Z(x_1) \leq z_1, Z(x_2) \leq z_2] = \frac{1}{z_1}\Phi\left(\frac{a}{2} + \frac{1}{a}\log\frac{z_2}{z_1}\right) + \frac{1}{z_2}\Phi\left(\frac{a}{2} + \frac{1}{a}\log\frac{z_1}{z_2}\right), \tag{3}$$

where $a = \{2\gamma(x_1 - x_2)\}^{1/2}$ and Φ denotes the standard normal cumulative distribution function. Inferential procedures for fitting max-stable processes have been missing for a long time but recently Padoan et al. (2010) suggest the use of the maximum pairwise likelihood estimator since closed forms for the k-variate distribution function when $k > 2$ are not available.

Paralleling the use of the variogram in classical geostatistics, the extremal coefficient function (Schlather & Tawn, 2003; Cooley et al., 2006) is a widely used summary statistic to analyze the spatial dependence of extremes. This function takes values in $[1, 2]$ and the lower bound indicates complete dependence while the upper one independence. From (3) it is straightforward to see that the extremal coefficient function for Brown–Resnick processes is $\theta(h) = 2\Phi[\{\gamma(h)/2\}^{1/2}]$ for all $h \in \mathbb{R}^d$.

As suggested by the preceding brief review on max-stable processes, the last decade has seen many advances to develop a geostatistic of extremes and software are already available to practitioners (Wang, 2010; Schlather, 2011; Ribatet, 2011). However one important tool is currently missing: conditional simulation of max-stable processes. In classical geostatistic based on Gaussian models, conditional simulations are well established (Chilès & Delfiner, 1999) and play a key role since it provides a framework to assess the distribution of a Gaussian random field given that some values have been observed at some fixed locations. For example, conditional simulations of Gaussian processes have been successfully used to model oil reservoirs (Delfiner & Chilès, 1997), land topography (Mandelbrot, 1982) or even the length of a submarine cable to be laid between two coastal cities (Alfaro, 1979).

Conditional simulation of max-stable processes is known to be a long-standing problem (Davis & Resnick, 1989, 1993) but recently Wang & Stoev (2011) provide a first answer to this problem. However their framework is limited to processes having a discrete spectral measure and might be too restrictive to appropriately model the spatial dependence in complex situations.

The aim of this paper is to provide a methodology to get conditional simulations of Brown–Resnick processes, which have a continuous spectral measure, based on the recent developments on the regular conditional distribution of infinitely divisible processes (Dombry & Eyi-Minko, 2011). More formally for a study region $\mathcal{X} \subset \mathbb{R}^d$, our goal is to derive an algorithm to sample from the regular conditional distribution of $Z(\cdot) \mid \{Z(x_1) = z_1, \ldots, Z(x_k) = z_k\}$ for some $z_1, \ldots, z_k > 0$ and k conditioning locations $x_1, \ldots, x_k \in \mathcal{X}$.

In Section 2 we provide an overview of the main results of Dombry & Eyi-Minko (2011) and propose a procedure to get conditional realizations of Brown–Resnick processes. Section 3 puts the emphasis on the combinatorial explosion of the regular conditional distribution and introduces a Markov chain Monte Carlo sampler to bypass this computational burden, which is

then analyzed on a simulation study in Section 4. The paper ends with an application on extreme rainfall around Zurich followed by a brief discussion.

2. CONDITIONAL SIMULATION OF BROWN–RESNICK PROCESSES

This section reviews some key results of Dombry & Eyi-Minko (2011) with a particular emphasis on Brown–Resnick processes. Our goal is to give a more practical interpretation of their results from a simulation perspective. To this aim, we recall two key results and propose a procedure to get conditional realizations of Brown–Resnick processes.

Let $\mathbb{C}_0$ be the space of positive continuous functions on $\mathcal{X} \subset \mathbb{R}^d$ and $\Phi = \{\varphi_i\}_{i\geq 1}$ a Poisson point process on $\mathbb{C}_0$ where

$$\varphi_i(x) = \zeta_i \exp\{W_i(x) - \gamma(x)\}, \qquad (i = 1, 2, \ldots)$$

with ζ_i and W_i as in (1) and (2). To shorten the notations we write $f(\mathbf{x}) = \{f(x_1), \ldots, f(x_k)\}$ for all (random) function $f\colon \mathcal{X} \to \mathbb{R}$ and $\mathbf{x} = (x_1, \ldots, x_k) \in \mathcal{X}^k$. It is not difficult to show that the Poisson point process $\{\varphi_i(\mathbf{x})\}_{i\geq 1}$ defined on $(0, +\infty)^k$ has intensity measure

$$\Lambda_{\mathbf{x}}(A) = \int_0^\infty \mathrm{pr}\left[\zeta \exp\{W(\mathbf{x}) - \gamma(\mathbf{x})\} \in A\right] \zeta^{-2} \mathrm{d}\zeta, \qquad A \subset (0, +\infty)^k \text{ Borel set.}$$

Dombry & Eyi-Minko (2011) show that provided the distribution of the random vector $W(\mathbf{x})$ is non degenerate, i.e., the covariance matrix $\Sigma_{\mathbf{x}} = \mathrm{E}[W(\mathbf{x})W(\mathbf{x})^T]$ is positive definite, the intensity measure $\Lambda_{\mathbf{x}}$ is absolutely continuous with respect to the Lebesgue measure and the density of $\Lambda_{\mathbf{x}}$ is

$$\lambda_{\mathbf{x}}(\mathbf{z}) = C_{\mathbf{x}} \exp\left(-\frac{1}{2}\log \mathbf{z}^T Q_{\mathbf{x}} \log \mathbf{z} + L_{\mathbf{x}} \log \mathbf{z}\right) \prod_{i=1}^k z_i^{-1}, \qquad \mathbf{z} \in (0, \infty)^k,$$

where

$$\begin{aligned}
Q_{\mathbf{x}} &= \Sigma_{\mathbf{x}}^{-1} - \frac{\Sigma_{\mathbf{x}}^{-1}\mathbf{1}_k\mathbf{1}_k^T\Sigma_{\mathbf{x}}^{-1}}{\mathbf{1}_k^T\Sigma_{\mathbf{x}}^{-1}\mathbf{1}_k},\\
L_{\mathbf{x}} &= \frac{1}{2}\left(\frac{\mathbf{1}_k^T\Sigma_{\mathbf{x}}^{-1}\sigma_{\mathbf{x}}^2 - 2}{\mathbf{1}_k^T\Sigma_{\mathbf{x}}^{-1}\mathbf{1}_k}\mathbf{1}_k^T - {\sigma_{\mathbf{x}}^2}^T\right)\Sigma_{\mathbf{x}}^{-1},\\
C_{\mathbf{x}} &= (2\pi)^{(1-k)/2}|\Sigma_{\mathbf{x}}|^{-1/2}(\mathbf{1}_k^T\Sigma_{\mathbf{x}}^{-1}\mathbf{1}_k)^{-1/2}\exp\left\{\frac{1}{2}\frac{(\mathbf{1}_k^T\Sigma_{\mathbf{x}}^{-1}\sigma_{\mathbf{x}}^2 - 1)^2}{\mathbf{1}_k^T\Sigma_{\mathbf{x}}^{-1}\mathbf{1}_k} - \frac{1}{2}{\sigma_{\mathbf{x}}^2}^T\Sigma_{\mathbf{x}}^{-1}\sigma_{\mathbf{x}}^2\right\},
\end{aligned}$$

and $\mathbf{1}_k = (1)_{i=1,\ldots,k}$, $\sigma_{\mathbf{x}}^2 = \{\sigma^2(x_i)\}_{i=1,\ldots,k}$.

Interestingly $\lambda_{\mathbf{x}}$ is closely related to a multivariate log-normal probability density function since for all $(\mathbf{s}, \mathbf{x}) \in \mathcal{X}^{(m+k)}$ and $\mathbf{z} \in (0, \infty)^k$, the function $\lambda_{\mathbf{s}|\mathbf{x},\mathbf{z}}(\mathbf{u}) = \lambda_{(\mathbf{s},\mathbf{x})}(\mathbf{u}, \mathbf{z})/\lambda_{\mathbf{x}}(\mathbf{z})$, $\mathbf{u} \in (0, \infty)^m$, is a multivariate log-normal density, i.e.,

$$\lambda_{\mathbf{s}|\mathbf{x},\mathbf{z}}(\mathbf{u}) = (2\pi)^{-m/2}|\Sigma_{\mathbf{s}|\mathbf{x}}|^{-1/2}\exp\left\{-\frac{1}{2}(\log \mathbf{u} - \mu_{\mathbf{s}|\mathbf{x},\mathbf{z}})^T\Sigma_{\mathbf{s}|\mathbf{x}}^{-1}(\log \mathbf{u} - \mu_{\mathbf{s}|\mathbf{x},\mathbf{z}})\right\}\prod_{i=1}^m u_i^{-1}, \tag{4}$$

where $\mu_{\mathbf{s}|\mathbf{x},\mathbf{z}} \in \mathbb{R}^m$ and $\Sigma_{\mathbf{s}|\mathbf{x}}$ are the mean and covariance matrix of the underlying normal distribution and are given by

$$\Sigma_{\mathbf{s}|\mathbf{x}}^{-1} = J_{m,k}^T Q_{(\mathbf{s},\mathbf{x})} J_{m,k}, \qquad \mu_{\mathbf{s}|\mathbf{x},\mathbf{z}} = \left(L_{(\mathbf{s},\mathbf{x})}J_{m,k} - \log \tilde{\mathbf{z}}^T \tilde{J}_{m,k}^T Q_{(\mathbf{s},\mathbf{x})} J_{m,k}\right)\Sigma_{\mathbf{s}|\mathbf{x}},$$

with

$$J_{m,k} = \begin{bmatrix} \mathrm{Id}_m \\ \mathbf{0}_{k,m} \end{bmatrix}, \qquad \tilde{\mathbf{z}} = \begin{bmatrix} \mathbf{z} \\ \mathbf{1}_m \end{bmatrix}, \qquad \text{and} \qquad \tilde{J}_{m,k} = \begin{bmatrix} \mathbf{0}_{m,k} \\ \mathrm{Id}_k \end{bmatrix},$$

where Id_k denotes the $k \times k$ identity matrix and $\mathbf{0}_{m,k}$ the $m \times n$ null matrix.

For our work, equation (4) is the first key result of Dombry & Eyi-Minko (2011) since it drives how the conditioning terms $\{Z(x_i) = z_i\}_{i=1,\dots,k}$ are met. The second key point is that, conditionally on $Z(\mathbf{x}) = \mathbf{z}$, the Poisson point process Φ can be decomposed into two independent Poisson point processes, say $\Phi = \Phi^- \cup \Phi^+$, where

$$\Phi^- = \{\varphi \in \Phi \colon \varphi(x_i) < z_i \text{ for all } i = 1, \dots, k\},$$
$$\Phi^+ = \{\varphi \in \Phi \colon \varphi(x_i) = z_i \text{ for some } i = 1, \dots, k\}.$$

Before introducing a procedure to get conditional realizations of Brown–Resnick processes, we introduce some notations and make some connections with the pioneer work of Wang & Stoev (2011) on the regular conditional distribution of spectrally discrete max-stable processes.

A function $\varphi \in \Phi^+$ such that $\varphi(x_i) = z_i$ for some $i \in \{1, \dots, k\}$ is called an extremal function associated to x_i and denoted by $\varphi^+_{x_i}$. Since Φ is a simple point process, there exists almost surely a unique extremal function associated to x_i. Although $\Phi^+ = \{\varphi^+_{x_1}, \dots, \varphi^+_{x_k}\}$ almost surely, it might happen that a single extremal function contributes to the random vector $Z(\mathbf{x})$ at several locations x_i, e.g., $\varphi^+_{x_1} = \varphi^+_{x_2}$. To take such repetitions into account, we define a (random) partition $\theta = (\theta_1, \dots, \theta_\ell)$ of the set $\{x_1, \dots, x_k\}$ into $\ell = |\theta|$ blocks and extremal functions $(\varphi^+_1, \dots, \varphi^+_\ell)$ such that $\Phi^+ = \{\varphi^+_1, \dots, \varphi^+_\ell\}$ and

$$\varphi^+_j(x_i) = z_i \text{ if } x_i \in \theta_j \quad \text{and} \quad \varphi^+_j(x_i) < z_i \text{ if } x_i \notin \theta_j, \quad (i = 1, \dots, k;\ j = 1, \dots, \ell).$$

Using the terminology of Wang & Stoev (2011), the partition θ is called the hitting scenario. The set of all possible partitions of $\{x_1, \dots, x_k\}$, denoted $\mathscr{P}_k$, identifies all possible hitting scenarios.

From a simulation perspective, the fact that, given $Z(\mathbf{x}) = \mathbf{z}$, Φ^- and Φ^+ are independent is especially convenient and suggests a three step procedure to sample from the conditional distribution of $Z(\cdot)$ given $Z(\mathbf{x}) = \mathbf{z}$.

As we will see, Φ^- and Φ^+ are conditionally independent given $Z(\mathbf{x}) = \mathbf{z}$. This is especially convenient from a simulation perspective and suggests a three step procedure to sample from the conditional distribution of $Z(\cdot)$ given $Z(\mathbf{x}) = \mathbf{z}$.

THEOREM 1. *Let $(\mathbf{x}, \mathbf{s}) \in \mathcal{X}^{k+m}$ and suppose that the covariance matrix $\Sigma_{(\mathbf{s},\mathbf{x})}$ is positive definite. For $\tau = (\tau_1, \dots, \tau_\ell) \in \mathscr{P}_k$ and $j = 1, \dots, \ell$, define $I_j = \{i \colon x_i \in \tau_j\}$ and note $\mathbf{x}_{\tau_j} = (x_i)_{i \in I_j}$, $\mathbf{z}_{\tau_j} = (z_i)_{i \in I_j}$, $\mathbf{x}_{\tau_j^c} = (x_i)_{i \notin I_j}$ and $\mathbf{z}_{\tau_j^c} = (z_i)_{i \notin I_j}$. Consider the following three step procedure:*

Step 1. Draw a random partition $\theta \in \mathscr{P}_k$ with distribution

$$\pi_{\mathbf{x}}(\mathbf{z}, \tau) = \mathrm{pr}\left[\theta = \tau \mid Z(\mathbf{x}) = \mathbf{z}\right] = \frac{1}{C(\mathbf{x}, \mathbf{z})} \prod_{j=1}^{|\tau|} \lambda_{\mathbf{x}_{\tau_j}}(\mathbf{z}_{\tau_j}) \int_{\{\mathbf{u}_j < \mathbf{z}_{\tau_j^c}\}} \lambda_{\mathbf{x}_{\tau_j^c} | \mathbf{x}_{\tau_j}, \mathbf{z}_{\tau_j}}(\mathbf{u}_j) \mathrm{d}\mathbf{u}_j,$$

where the normalization constant $C(\mathbf{x}, \mathbf{z})$ is given by

$$C(\mathbf{x}, \mathbf{z}) = \sum_{\tilde{\tau} \in \mathscr{P}_k} \prod_{j=1}^{|\tilde{\tau}|} \lambda_{\mathbf{x}_{\tilde{\tau}_j}}(\mathbf{z}_{\theta_j}) \int_{\{\mathbf{u}_j < \mathbf{z}_{\tilde{\tau}_j^c}\}} \lambda_{\mathbf{x}_{\tilde{\tau}_j^c} | \mathbf{x}_{\tilde{\tau}_j}, \mathbf{z}_{\tilde{\tau}_j}}(\mathbf{u}_j) \mathrm{d}\mathbf{u}_j.$$

Step 2. Given $\tau = (\tau_1, \ldots, \tau_\ell)$, draw ℓ independent random vectors $\varphi_1^+(\mathbf{s}), \ldots, \varphi_\ell^+(\mathbf{s})$ from the distribution

$$\operatorname{pr}\left[\varphi_j^+(\mathbf{s}) \in \mathrm{d}\mathbf{v} \mid Z(\mathbf{x}) = \mathbf{z}, \theta = \tau\right] = \frac{1}{C_j}\left\{\int 1_{\{\mathbf{u}<\mathbf{z}_{\tau_j^c}\}}\lambda_{(\mathbf{s},\mathbf{x}_{\tau_j^c})|\mathbf{x}_{\tau_j},\mathbf{z}_{\tau_j}}(\mathbf{v},\mathbf{u})\mathrm{d}\mathbf{u}\right\}\mathrm{d}\mathbf{v}$$

where $1_{\{\cdot\}}$ is the indicator function and

$$C_j = \int 1_{\{\mathbf{u}<\mathbf{z}_{\tau_j^c}\}}\lambda_{(\mathbf{s},\mathbf{x}_{\tau_j^c})|\mathbf{x}_{\tau_j},\mathbf{z}_{\tau_j}}(\mathbf{v},\mathbf{u})\mathrm{d}\mathbf{u}\mathrm{d}\mathbf{v},$$

and define the random vector $Z^+(\mathbf{s}) = \max_{j=1,\ldots,\ell}\varphi_j^+(\mathbf{s})$.

Step 3. Independently draw $\{\zeta_i\}_{i\geq 1}$ a Poisson point process on $(0,\infty)$ with intensity $\zeta^{-2}\mathrm{d}\zeta$ and $\{W_i(\cdot)\}_{i\geq 1}$ independent copies of $W(\cdot)$ and define the random vector

$$Z^-(\mathbf{s}) = \max_{i\geq 1}\zeta_i \exp\left\{W_i(\mathbf{s}) - \gamma(\mathbf{s})\right\} 1_{\{\zeta_i e^{W_i(\mathbf{x})-\gamma(\mathbf{x})}<\mathbf{z}\}}.$$

Then the random vector $\tilde{Z}(\mathbf{s}) = \max\left\{Z^+(\mathbf{s}), Z^-(\mathbf{s})\right\}$ *follows the conditional distribution of* $Z(\mathbf{s})$ *given* $Z(\mathbf{x}) = \mathbf{z}$.

It is not difficult to show that the corresponding conditional cumulative distribution function is given by

$$\operatorname{pr}\left[Z(\mathbf{s}) \leq \mathbf{a} \mid Z(\mathbf{x}) = \mathbf{z}\right] = \frac{\operatorname{pr}[Z(\mathbf{s}) \leq \mathbf{a}, Z(\mathbf{x}) \leq \mathbf{z}]}{\operatorname{pr}[Z(\mathbf{x}) \leq \mathbf{z}]}\sum_{\tau\in\mathscr{P}_k}\pi_{\mathbf{x}}(\mathbf{z},\tau)\prod_{j=1}^{|\tau|}F_{\tau,j}(\mathbf{a}), \qquad (5)$$

where $F_{\tau,j}$ is expressed in terms of log-normal distributions as follows

$$F_{\tau,j}(\mathbf{a}) = \operatorname{pr}\left[\varphi_j^+(\mathbf{s}) \leq \mathbf{a} \mid Z(\mathbf{x}) = \mathbf{z},\, \theta = \tau\right] = \frac{\int_{\{\mathbf{u}<\mathbf{z}_{\tau_j^c},\mathbf{v}<\mathbf{a}\}}\lambda_{(\mathbf{s},\mathbf{x}_{\tau_j^c})|\mathbf{x}_{\tau_j},\mathbf{z}_{\tau_j}}(\mathbf{v},\mathbf{u})\mathrm{d}\mathbf{u}\mathrm{d}\mathbf{v}}{\int_{\{\mathbf{u}<\mathbf{z}_{\tau_j^c}\}}\lambda_{\mathbf{x}_{\tau_j^c}|\mathbf{x}_{\tau_j},\mathbf{z}_{\tau_j}}(\mathbf{u})\mathrm{d}\mathbf{u}}.$$

Interestingly it is clear from (5) that the conditional random field $Z(\cdot) \mid \{Z(\mathbf{x}) = \mathbf{z}\}$ is not max-stable.

3. Markov chain Monte–Carlo sampler

The previous section introduced a procedure to get realizations from the regular conditional distribution of Brown–Resnick processes. We saw that this sampling scheme requires to be able to sample from a discrete distribution whose state space corresponds to all possible partitions of the set of conditioning points—see Theorem 1 step 1.

It is well known that the number of all possible partitions of a set with k elements corresponds to Bell numbers and results in a combinatorial explosion even for a moderate number of conditioning locations k. For example when $k = 10$ there are around 116000 possibilities. Even worse, the current computer capacities prevent the storage of all possible partitions in memory when $k > 12$.

Due to this combinatorial explosion, the distribution $\pi_{\mathbf{x}}(\mathbf{z},\cdot)$ cannot be computed and it seems sensible to use MCMC algorithms. It is questionable whether a Metropolis–Hastings algorithm will be efficient since we aim at sampling from a discrete distribution whose state space is huge and where typically only a few states have a significant probability to occur—see Figure 1; thus

resulting in a chain with poor mixing properties. A safest approach consists in using a Gibbs sampler as we shall describe now.

For $\tau \in \mathscr{P}_k$, let τ_{-j} be the restriction of τ to the set $\{x_1, \dots, x_k\} \setminus \{x_j\}$. As usual with Gibbs samplers, our goal is to simulate from the conditional distribution

$$\mathrm{pr}[\theta \in \cdot \mid \theta_{-j} = \tau_{-j}], \tag{6}$$

where $\theta \in \mathscr{P}_k$ is a random partition which follows the target distribution $\pi_{\mathbf{x}}(\mathbf{z}, \cdot)$ and τ is typically the current state of the Markov chain.

Since the number of possible updates is always less than k, the combinatorial explosion is avoided. Indeed for $\tau \in \mathscr{P}_k$ of size ℓ, the number of partitions $\tau^* \in \mathscr{P}_k$ such that $\tau^*_{-j} = \tau_{-j}$ for some $j \in \{1, \dots, k\}$ is

$$b^+ = \begin{cases} \ell & \text{if } \{x_j\} \text{ is a partitioning set of } \tau, \\ \ell + 1 & \text{if } \{x_j\} \text{ is not a partitioning set of } \tau, \end{cases}$$

since the point x_j may be reallocated to any partitioning set of τ_{-j} or to a new one.

To illustrate consider the set $\{x_1, x_2, x_3\}$ and let $\tau = (\{x_1, x_2\}, \{x_3\})$. Then the possible partitions τ^* such that $\tau^*_{-2} = \tau_{-2}$ are

$$(\{x_1, x_2\}, \{x_3\}), \qquad (\{x_1\}, \{x_2\}, \{x_3\}), \qquad (\{x_1\}, \{x_2, x_3\}),$$

while there exists only two partitions such that $\tau^*_{-3} = \tau_{-3}$, i.e.,

$$(\{x_1, x_2\}, \{x_3\}), \qquad (\{x_1, x_2, x_3\}).$$

The distribution (6) has nice properties. Since for all $\tau^* \in \mathscr{P}_k$ such that $\tau^*_{-j} = \tau_{-j}$ we have

$$\mathrm{pr}[\theta = \tau^* \mid \theta_{-j} = \tau_{-j}] = \frac{\pi_{\mathbf{x}}(\mathbf{z}, \tau^*)}{\displaystyle\sum_{\tilde{\tau} \in \mathscr{P}_k} \pi_{\mathbf{x}}(\mathbf{z}, \tilde{\tau}) 1_{\{\tilde{\tau}_{-j} = \tau_{-j}\}}} \propto \frac{\prod_{j=1}^{|\tau^*|} w_{\tau^*, j}}{\prod_{j=1}^{|\tau|} w_{\tau, j}}, \tag{7}$$

where

$$w_{\tau,j} = \lambda_{\mathbf{x}_{\tau_j}}(\mathbf{z}_{\tau_j}) \int_{\{\mathbf{u} < \mathbf{z}_{\tau^c_j}\}} \lambda_{\mathbf{x}_{\tau^c_j} | \mathbf{x}_{\tau_j}, \mathbf{z}_{\tau_j}}(\mathbf{u}) \mathrm{d}\mathbf{u},$$

it can be seen that in the right hand side of (7) many factors will cancel out except at most four of them. From a simulation perspective, it makes the Gibbs sampler especially convenient.

The most CPU demanding part of (7) corresponds to the computation of the multivariate log-normal probabilities

$$\int_{\{\mathbf{u} < \mathbf{z}_{\tau^c_j}\}} \lambda_{\mathbf{x}_{\tau^c_j} | \mathbf{x}_{\tau_j}, \mathbf{z}_{\tau_j}}(\mathbf{u}) \mathrm{d}\mathbf{u}.$$

Following Genz (1992), these probabilities are computed using a separation of variable method which provide a transformation of the original integration problem to the unit hyper-cube. Further variable ordering combined with a quasi Monte Carlo scheme and an antithetic variable sampling is used to improve integration efficiency.

Since it is not obvious how to implement a Gibbs sampler whose target distribution has support $\mathscr{P}_k$, the remainder of these section gives practical details on its implementation. For any fixed locations $x_1, \dots, x_k \in \mathcal{X}$, we first describe how each partition of $\{x_1, \dots, x_k\}$ is stored. To illustrate consider the set $\{x_1, x_2, x_3\}$ and the partition $\{(x_1, x_2); (x_3)\}$. With our convention,

this partition is defined as $(1,1,2)$ indicating that x_1 and x_2 belong to the same partitioning set labeled '1' and x_3 belongs to the partitioning set '2'. There exist several equivalent notations for this partition: for example one can use $(2,2,1)$ or $(1,1,3)$. However Orlov (2002) shows that there is a one-one mapping between $\mathscr{P}_k$ and the set

$$\mathscr{P}_k^* = \left\{ (a_1,\ldots,a_k),\, \forall i \in \{2,\ldots,k\} \colon 1 = a_1 \leq a_i \leq \max_{1\leq j<i} a_j + 1,\, a_i \in \mathbb{Z} \right\}.$$

Consequently we shall restrict our attention to the partitions that live in $\mathscr{P}_k^*$ and going back to our example we see that $(1,1,2)$ is valid but $(2,2,1)$ and $(1,1,3)$ are not.

For $\tau \in \mathscr{P}_k^*$ of size ℓ, let $r_1 = \sum_{i=1}^k \delta_{\tau_i = a_j}$ and $r_2 = \sum_{i=1}^k \delta_{\tau_i = b}$, i.e., the number of conditioning locations that belong to the partitioning sets 'a_j' and 'b' where $b \in \{1,\ldots,b^+\}$ and

$$b^+ = \begin{cases} \ell & (r_1 = 1), \\ \ell + 1 & (r_1 \neq 1). \end{cases}$$

Then the conditional probability distribution (7) satisfies

$$\mathrm{pr}[\tau_j = b \mid \tau_i = a_i,\, \forall i \neq j] \propto \begin{cases} 1 & (b = a_j), \quad \text{(8a)} \\ w_{\tau_*,b}/(w_{\tau,b} w_{\tau,a_j}) & (r_1 = 1, r_2 \neq 0, b \neq a_j), \quad \text{(8b)} \\ w_{\tau_*,b} w_{\tau_*,a_j}/(w_{\tau,b} w_{\tau,a_j}) & (r_1 \neq 1, r_2 \neq 0, b \neq a_j), \quad \text{(8c)} \\ w_{\tau_*,b} w_{\tau_*,a_j}/w_{\tau,a_j} & (r_1 \neq 1, r_2 = 0, b \neq a_j), \quad \text{(8d)} \end{cases}$$

where $\tau_* = (a_1,\ldots,a_{j-1},b,a_{j+1},\ldots,a_k)$. It is worth stressing that although τ_* does not necessarily belongs to $\mathscr{P}_k^*$, it corresponds to a unique partition of $\mathscr{P}_k$ and we can use the bijection $\mathscr{P}_k \to \mathscr{P}_k^*$ to recode τ_* into an element of $\mathscr{P}_k^*$.

In (8a)–(8d) the event $\{r_1 = 1, r_2 = 0, b \neq a_j\}$ is missing since $\{r_1 = 1, r_2 = 0\}$ implies that $\tau_* = \tau$, where the equality has to be understood in terms of elements of $\mathscr{P}_k$, and this case has been already taken into account with (8a). Practical details on the computation of these conditional weights are given in Algorithm 1 and deferred to Appendix 1.

Once these conditional weights have been computed, the Gibbs sampler proceeds as usual by updating each element of τ successively. However for our work we use a random scan implementation of the Gibbs sampler (Liu et al., 1995). More precisely, one iteration of the random scan Gibbs sampler selects an element of τ at random according to a given distribution, say $\mathbf{p} = (p_1,\ldots,p_k)$, and then updates this element. A widely used sampler is the uniform random scan Gibbs sampler for which the selection distribution is assumed to be a discrete uniform distribution, e.g., $\mathbf{p} = (k^{-1},\ldots,k^{-1})$.

Recently Latuszyński & Rosenthal (2010) show under mild regularity conditions the ergodicity of the adaptive random scan Gibbs sampler, i.e., a random scan Gibbs sampler such that the selection distribution $\mathbf{p}$ changes as the sampler proceeds. For our purposes the use of an adaptive Gibbs sampler might be appealing since typically only a few states of $\pi_{\mathbf{x}}(\mathbf{z},\cdot)$ have a significant probability to occur—see Figure 3. Although the quality of the simulated Markov chain could be largely improved, the implementation of such a sampler requires many manual tuning and we were not able to implement it appropriately to improve the quality of the simulated Markov chains.

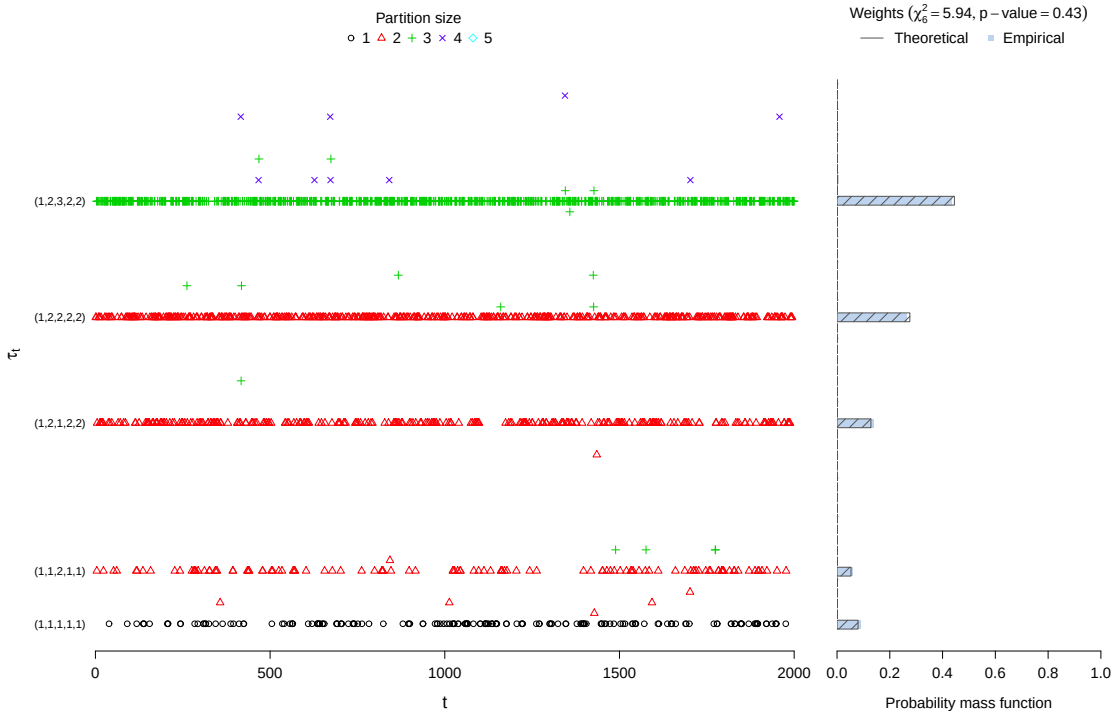

Fig. 1. Left: Trace plot of one Markov chain generated using the uniform random scan Gibbs sampler and whose target distribution is $\pi_{\mathbf{x}}(\mathbf{z}, \cdot)$ with $k = 5$ conditioning locations. The labels on the y-axis indicates the partitions having a probability greater than 0·01 to occur. Right: Comparison of the theoretical probabilities $\{\pi_{\mathbf{x}}(\mathbf{z}, \tau), \tau \in \mathscr{P}_k\}$ and the empirical ones estimated from the simulated Markov chain with an insert showing the sample χ^2 statistic and the associated p-value.

4. SIMULATION STUDY

4·1. *Gibbs Sampler*

In this section we check whether the Gibbs sampler is able to sample from $\pi_{\mathbf{x}}(\mathbf{z}, \cdot)$. To illustrate a typical sample path, Figure 1 shows the trace plot of a simulated chain of length 2000 with $k = 5$ conditioning locations and a thinning lag of 5 and compares the theoretical probabilities $\{\pi_{\mathbf{x}}(\mathbf{z}, \tau), \tau \in \mathscr{P}_k\}$ to the empirical ones estimated from the Markov chain. As mentioned in the previous section it can be seen that only a few states have a significant probability to occur and these states most often differs by a small bit. As expected for this particular simulation the empirical probabilities match the theoretical ones.

To better assess if our uniform random scan Gibbs sampler is able to sample from $\pi_{\mathbf{x}}(\mathbf{z}, \cdot)$ we simulate 250 Markov chains of length 1000—after removing a burn-in period and thinning the chain, and similarly to Figure 1, compare the theoretical probabilities $\{\pi_{\mathbf{x}}(\mathbf{z}, \tau), \tau \in \mathscr{P}_k\}$ to the empirical ones using a χ^2 test for each of these chains. Since the computation of these theoretical probabilities is CPU intensive, the number of conditioning locations is at most 5 in our simulation study.

Figure 2 plots the sample p-values of these χ^2 tests against the quantiles of a $U(0, 1)$ distribution for a varying number of conditional locations. This figure corroborates what we saw

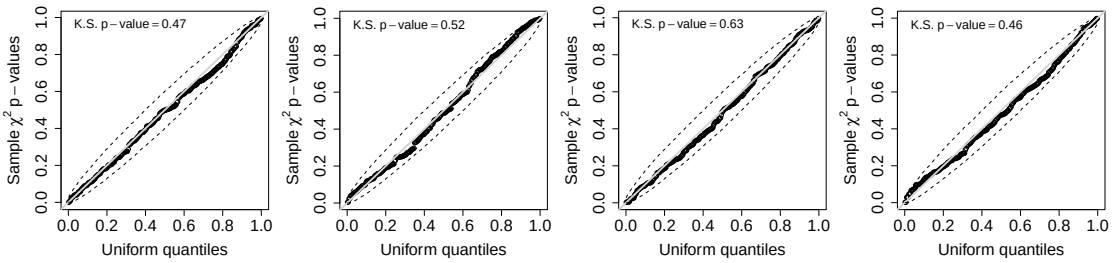

Fig. 2. QQ-plots for the sample χ^2 test p-values against $U(0,1)$ quantiles with a varying number of conditioning locations k with an insert showing the p-values of a Kolmogorov Smirnov test for uniformity—from left to right, $k = 2, 3, 4$ and 5. The dashed lines show the 95% confidence envelopes.

Table 1. *Spatial dependence structures of Brown–Resnick processes with (semi) variogram $\gamma(h) = (h/\lambda)^\nu$. The variogram parameters are set to ensure that the extremal coefficient function satisfies $\theta(115) = 1{\cdot}7$.*

	Sample path properties		
	γ_1: Wiggly	γ_2: Smooth	γ_3: Very smooth
λ	25	54	69
ν	0·5	1·0	1·5

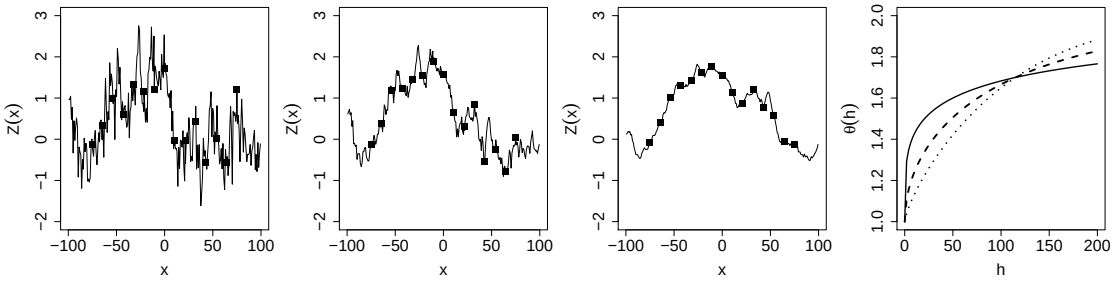

Fig. 3. Three realizations of a Brown–Resnick process with standard Gumbel margins and (semi) variograms γ_1, γ_2 and γ_3—from left to right. The squares correspond to the 15 conditioning values that will be used in the simulation study. The right panel shows the associated extremal coefficient functions where the solid, dashed and dotted lines correspond respectively to γ_1, γ_2 and γ_3.

in Figure 1 since the sample p-values seem to follow a $U(0,1)$ distribution indicating that the sampler is able to sample from $\pi_{\mathbf{x}}(\mathbf{z}, \cdot)$.

4·2. *Conditional simulations*

In this section we check if our algorithm is able to produce realistic conditional simulations of Brown–Resnick processes with (semi) variogram $\gamma(h) = (h/\lambda)^\nu$. To have a broad overview, we consider three different sample path properties as summarized in Table 1. Figure 3 shows one realization for each sample path configuration as well as the corresponding extremal coefficient function. These realizations will serve as the basis for our conditioning events.

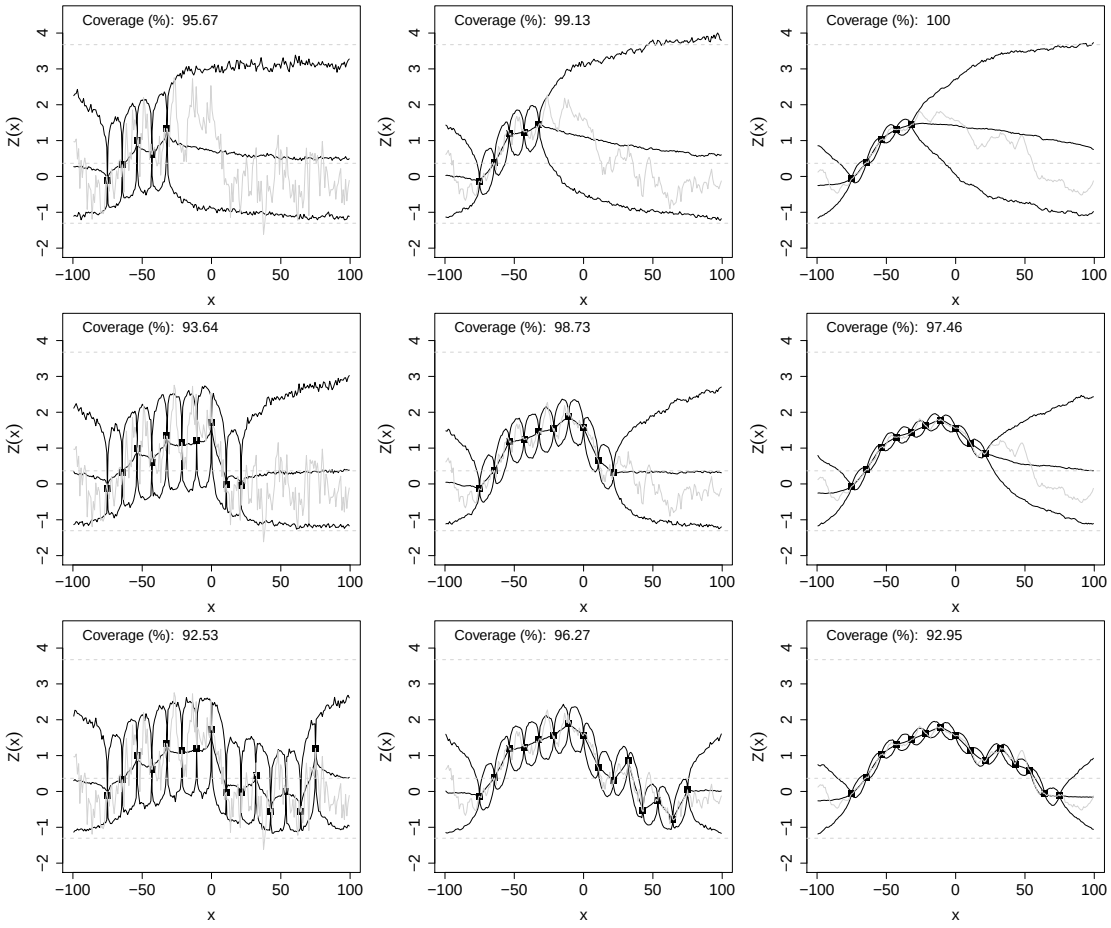

Fig. 4. Pointwise sample quantiles estimated from 1000 conditional simulations of Brown–Resnick processes with standard Gumbel margins and (semi) variograms γ_1, γ_2 and γ_3 (left to right) and with $k = 5, 10, 15$ conditioning locations—top to bottom. The solid black lines show the pointwise 0·025, 0·5, 0·975 sample quantiles and the dashed grey lines that of a standard Gumbel distribution. The squares show the conditional points $\{(x_i, z_i)\}_{i=1,\dots,k}$. The solid grey lines correspond the simulated paths used to get the conditioning events. The inserts give the proportion of points lying in the 95% pointwise confidence intervals.

In order to check if our sampling procedure is accurate and given a single conditional event $\{Z(\mathbf{x}) = \mathbf{z}\}$, we generated 1000 conditional realizations of a Brown–Resnick processes with standard Gumbel margins and (semi) variograms γ_j $(j = 1, 2, 3)$.

Figure 4 shows the pointwise sample quantiles obtained from these 1000 simulated paths and compare them to unit Gumbel quantiles. As expected the conditional sample paths inherit the regularity driven by the Hurst index $\nu/2$ of the process $Y(\cdot)$ in (2) and there is less variability in regions close to some conditioning locations. On the opposite, although for this specific type of variogram $\theta(h) \to 2$ as $h \to \infty$, for regions far away from any conditioning location the sample quantiles converges to that of a standard Gumbel distribution indicating that the conditional event

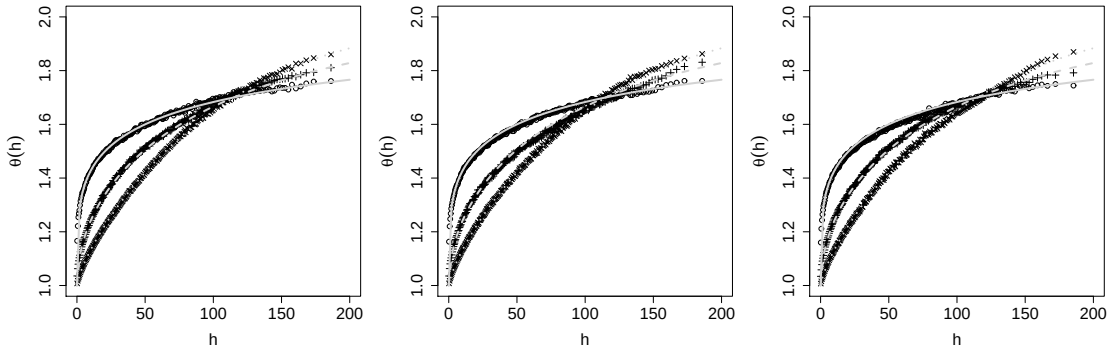

Fig. 5. Comparison of the extremal coefficient estimates (using a binned F-madogram with 250 bins) and the theoretical extremal coefficient function for a varying number of conditioning locations and different (semi) variograms. From left to right, $k = 5, 10, 15$. The 'o', '+' and 'x' symbols correspond respectively to γ_1, γ_2 and γ_3. The solid, dashed and dotted grey lines correspond to the theoretical extremal coefficient functions for γ_1, γ_2 and γ_3

does not have any influence anymore. In addition the sample paths used to get the conditional events, see Figure 3, lay most of the time in the 95% pointwise confidence intervals corroborating that our sampling procedure seems to be accurate—the coverage range between 0·93 and 1·00 with a mean value of 0·96.

So far we have checked that the proposed sampling procedure yields the expected coverage as well as the right marginal properties as we move far away from any conditioning location. The last point to be fulfilled is to assess whether the simulation procedure honours the spatial dependence driven by the (semi) variogram $\gamma(\cdot)$. To this aim we use the F-madogram (Cooley et al., 2006) to compare the pairwise extremal coefficient estimates to the theoretical extremal coefficient function. As mentioned in Section 2, since $Z(\cdot) \mid \{Z(\mathbf{x}) = \mathbf{z}\}$ is not max-stable the F-madogram cannot be used. However, by integrating out the conditional event we recover the original Brown-Resnick distribution and the max-stability property. So we generate independently 1000 conditional events $\{Z(\mathbf{x}) = \mathbf{z}\}$, $\mathbf{x}$, and for each conditional event one conditional realization of a Brown–Resnick process. Figure 5 compares the pairwise extremal coefficient estimates based on these simulations to the theoretical extremal coefficient function. As expected, whatever the number of conditioning location and the (semi) variograms are, the (binned) pairwise estimates match the theoretical curve indicating that the spatial dependence is honoured.

5. APPLICATION

In this section we apply our framework to get conditional simulations of extreme precipitation fields. The data considered here were previously analyzed by Davison et al. (2011) where it was shown that Brown–Resnick processes were one of the most competitive models among various statistical models for spatial extremes.

The data are summer maximum daily rainfall for the years 1962–2008 at 51 weather stations in the Plateau region of Switzerland, provided by the national meteorological service, MeteoSuisse. For our study we consider as conditional points the 24 weather stations that are at most 30km apart from Zurich and set as the conditional values the rainfall amounts recorded in the year 2000, i.e., the year of the largest precipitation event ever recorded in Zurich between 1962–2008—see

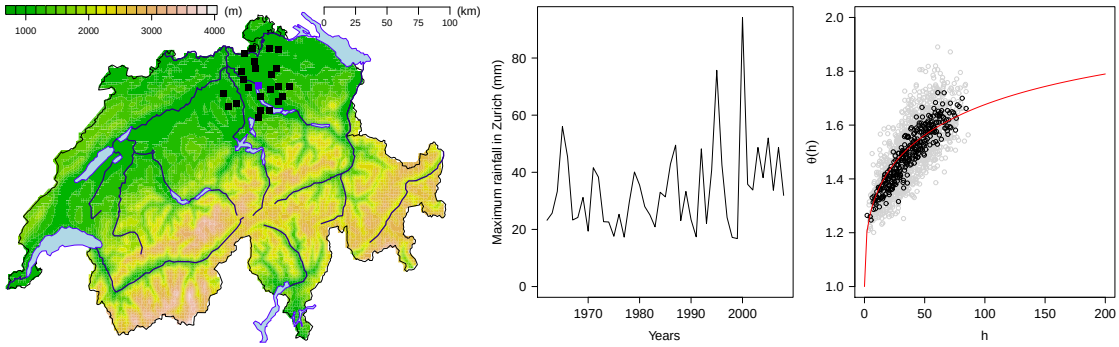

Fig. 6. Left: Map of Switzerland showing the stations of the 24 rainfall gauges used for the analysis, with an insert showing the altitude. The station marked with a blue square corresponds to Zurich. Middle: Summer maximum daily rainfall values for 1962–2008 at Zurich. Right: Comparison between the pairwise extremal coefficient estimates for the 51 original weather stations and the extremal coefficient function derived from a fitted Brown–Resnick processes having (semi) variogram $\gamma(h) = (h/\lambda)^\nu$. The grey points are pairwise estimates; the black ones are binned estimates and the red curve is the fitted extremal coefficient function.

Table 2. *Empirical distribution of the partition size for the rainfall data estimated from a simulated Markov chain of length 15000.*

Partition size	1	2	3	4	5	6	7–24
Empirical probabilities (%)	66·2	28·0	4·8	0·5	0·2	0·2	$<$0·05

Figure 6. The largest and smallest distances between the conditioning locations are around 55km and just over 4km respectively.

Prior to generate conditional realizations, a Brown–Resnick process having (semi) variogram $\gamma(h) = (h/\lambda)^\nu$ has to be fitted and in this work the maximum pairwise likelihood estimator introduced by Padoan et al. (2010) was used to simultaneously fit the marginal parameters and the spatial dependence parameters λ and ν. In accordance to the previous work of Davison et al. (2011), the marginal parameters were described by the following trend surfaces

$$\begin{aligned}\eta(x) &= \beta_{0,\eta} + \beta_{1,\eta}\mathrm{lon}(x) + \beta_{2,\eta}\mathrm{lat}(x),\\ \sigma(x) &= \beta_{0,\sigma} + \beta_{1,\sigma}\mathrm{lon}(x) + \beta_{2,\sigma}\mathrm{lat}(x),\\ \xi(x) &= \beta_{0,\xi},\end{aligned}$$

where $\eta(x), \sigma(x), \xi(x)$ are the location, scale and shape parameters of the generalized extreme value distribution and $\mathrm{lon}(x), \mathrm{lat}(x)$ the longitude and latitude of the stations at which the data are observed. The maximum pairwise likelihood estimates for λ and ν are 38 (14) and 0·69 (0·07) and give a practical extremal range, i.e., the distance h_+ such that $\theta(h_+) = 1{\cdot}7$, around 115km—see the right panel of Figure 6.

Table 2 shows the empirical distribution of the partition size. We can see that around 65% of the time the summer maxima observed at the 24 conditioning locations were a consequence of a single extremal function, i.e., only one storm event, and around 30% of the time a consequence of two different storms. Since the simulated Markov chain keeps a trace of all the simulated partitions, we looked at the partitions of size two and saw that around 65% of the time, at least

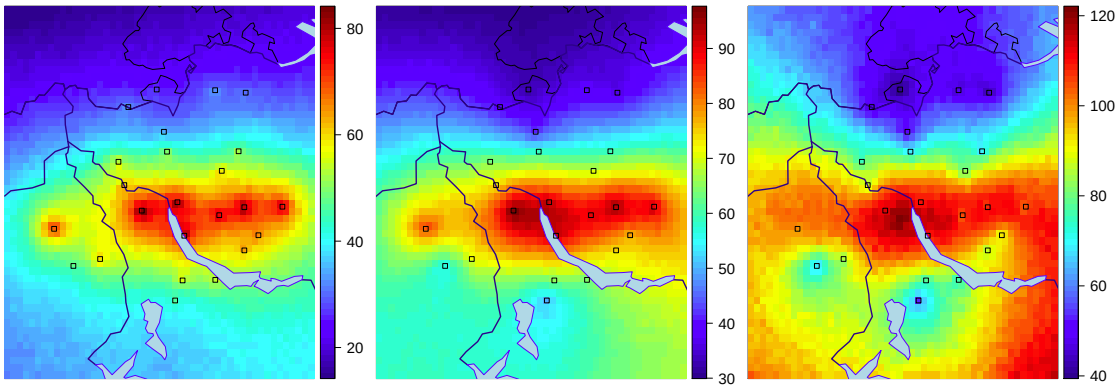

Fig. 7. From left to right, maps on a 50×50 grid of the pointwise 0·025, 0·5 and 0·975 sample quantiles for rainfall (mm) obtained from 1000 conditional simulations of Brown–Resnick processes having (semi) variogram $\gamma(h) = (h/38)^{0.69}$. The squares show the conditional locations.

one of the four up-north conditioning locations was impacted by one extremal function while the remaining 20 locations were always influenced by another one.

Figure 7 plots the pointwise 0·025, 0·5 and 0·975 sample quantiles obtained from 1000 conditional simulations of our fitted Brown–Resnick process. The conditional median provides a point estimate for the rainfall at an unknown location and the 0·025 and 0·975 conditional quantiles a 95% pointwise confidence interval. As indicated by our simulation study—see Figures 3 and 4, the Hurst index $\nu/2$ has a major impact on the regularity of paths and on the width of the confidence interval. Here, the value $\nu \approx 0.69$ corresponds to wiggly sample paths and wider confidence intervals. It is however reassuring that even on a complex case study like this one, i.e., simulation on a 50×50 grid and with $k = 24$ conditioning locations, the maps are consistent with one might expect.

6. Conclusion

The last decade has seen many major advances for building up a mathematically well founded geostatistic of extremes. This work makes a contribution to this field by allowing conditional simulations of Brown–Resnick processes. Although closed forms for the regular conditional distributions of max infinitely divisible processes were found recently, simulating conditional realizations of Brown–Resnick processes appears to be a considerable challenge since these closed forms are intractable even for a moderate number of conditioning locations.

To bypass this computational burden a Markov chain Monte–Carlo sampler was proposed. Using a simulation study and an application to extreme rainfall around Zurich, we show that our procedure is able to draw accurate conditional simulations for real sized problems and hence opens many avenues for a better description of spatial extremes. The simulations were performed using the statistical software `R` (R Development Core Team, 2011) and the implemented routines will be collected in the `SpatialExtremes` package (Ribatet, 2011).

Future works could focus on different conditioning events. For instance, an interesting open problem would be to get a procedure to sample from a max-stable process $Z(\cdot)$ conditionally on $\max_{x \in K} Z(x) = z$, $K \subset \mathcal{X}$. Indeed since regional/global circulation models are widely used to

assess the potential consequences of a global warming, K could typically represent a grid cell of a given atmospheric model.

ACKNOWLEDGEMENTS

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APPENDIX. ALGORITHM TO COMPUTE $\mathrm{pr}[\theta = \tau^* \mid \theta_{-j} = \tau_{-j}]$

Algorithm 1: Computing the probabilities of (7).

Input : A partition $\tau \in \mathscr{P}_k^*$ of size ℓ and $j \in \{1, \ldots, k\}$
Output: The conditional weights $w^* = (w_1^*, \ldots, w_{b^+}^*)$

`//Identify which partitioning set` x_j `belongs to`
$s \leftarrow \tau_j$;
`//Compute the size of this partition set`
$r_1 \leftarrow \sum_{m=1}^{k} \delta_{\tau_m = s}$;
`//Create a new partition that will be updated`
$\tau^* \leftarrow \tau$;
`//Get the number of possible states for` τ^*
$b^+ \leftarrow \ell + \delta_{r_1 \neq 1}$;
for $b \leftarrow 1$ **to** b^+ **do**
  `//`b `refers to the partitioning set where` x_j `is moved to`
  `//Update the partition` τ^*
  $\tau_j^* = b$;
  `//Compute the conditional weights for this new partition`
  $r_2 \leftarrow \sum_{m=1}^{k} \delta_{\tau_m = b}$;
  if $b = s$ **then**
    `//This is case` (8a)
    $w_b^* \leftarrow 1$;
    continue;
  end
  case $r_1 = 1$ *and* $r_2 \neq 0$
    `//This is case` (8b)
    $w_b^* \leftarrow w_{\tau^*,b} / \{w_{\tau,b} w_{\tau,s}\}$;

  case $r_1 \neq 1$ *and* $r_2 \neq 0$
    `//This is case` (8c)
    $w_b^* \leftarrow w_{\tau^*,b} w_{\tau^*,s} / \{w_{\tau,b} w_{\tau,s}\}$;

  case $r_1 \neq 1$ *and* $r_2 = 0$
    `//This is case` (8d)
    $w_b^* \leftarrow w_{\tau^*,b} w_{\tau^*,s} / w_{\tau,s}$;

end
Normalize the conditional weights to sum to 1;
return w^*;

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