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# Spatio-temporal modelling of hydrological return levels. A quantile regression approach

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## Abstract

Extreme river flows can lead to inundation of floodplains, with consequent impacts for society, the environment and the economy. Extreme flows are inherently difficult to model, being infrequent, irregularly spaced and affected by non-stationary climatic controls. To identify patterns in extreme flows a quantile regression approach can be used. This paper introduces a new framework for spatio-temporal quantile regression modelling, where the regression model is built as an additive model that includes smooth functions of time and space, as well as space-time interaction effects. The model exploits the flexibility that P-splines offer and can be easily extended to incorporate potential covariates. We propose to estimate model parameters using a penalized least squares regression approach as an alternative to linear programming methods, classically used in quantile parameter estimation. The model is illustrated on a data set of flows in 98 rivers across Scotland.

**Keywords:** P-splines; PIRLS; hydrometric time series; extreme values

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# 18 1 Introduction

19 The occurrence of extreme events in the environment, i.e. those that deviate considerably from  
20 expected average levels, for example extreme temperatures, river flows, wave heights, or pollutant  
21 concentrations, has received increasing interest over the last decade. The last report by the  
22 Intergovernmental Panel on Climate Change (IPCC) recognizes the effect that climate change  
23 may have on the “frequency, intensity, spatial extent, duration, and timing of extreme events”  
24 (IPCC, 2014). Understanding the spatial and temporal structure of extremes is essential for  
25 planning purposes. An example of the severe consequences of extreme events, including loss of  
26 life, are the floods that hit the UK, especially Northern England and Scotland, in December  
27 2015. These events prompted the National Flood Resilience Review (HM Government, 2016), a  
28 “review of how we assess flood risk, reduce the likelihood of flooding, and make the country as  
29 resilient as possible to flooding” and the latest in a series of reviews following damaging events  
30 in the UK and internationally (Evans et al., 2004; Pitt, 2008; Georgi et al., 2016).

31 It is now recognized that statistical methods specifically developed to analyze extreme values  
32 (over time and/or space) are needed. One common approach for dealing with spatial data is the  
33 use of geostatistical models (Diggle and Ribeiro Jr., 2007) that assume the data to be a realization  
34 of an underlying spatial Gaussian random field; these kinds of models have also been extended to  
35 the spatio-temporal case (see, e.g. Cressie and Wikle (2011)). However, the Gaussian assumption  
36 is not realistic when modelling extreme values, whose distribution is known to be skewed (Coles,  
37 2004). The increasing interest in extreme values, especially in environmental applications, has  
38 led to the development of new statistical models specifically designed for spatial (and spatio-  
39 temporal) extremes. These include latent variables (Davison et al., 2012; Cooley et al., 2007),  
40 copula models (Fuentes et al., 2012) and the more recent max-stable processes (Davison et al.,  
41 2012; Davison and Gholamrezaee, 2012). A max-stable process can be thought of as the limiting  
42 distribution of the pointwise maxima of independent copies of a process. Max-stable processes  
43 are best characterized via their spectral representation, for which several models have been

44 proposed. In particular, the Smith (Smith, 1990), Schlather (Schlather, 2002) and Brown-Resnick  
45 (Brown and Resnick, 1977) models are widely used, where a composite marginal likelihood, built  
46 using the pairwise marginal distributions, is used for parameter estimation (Davison et al., 2012;  
47 Davison and Gholamrezaee, 2012; Wadsworth and Tawn, 2012). Good reviews of these models  
48 can be found in Davison et al. (2012) and Davison and Gholamrezaee (2012). More recently,  
49 several authors have considered the extension of max-stable processes to model extremes over  
50 space and time (Davis et al., 2013; Embrechts et al., 2016). Max-stable processes are based  
51 on asymptotic extreme value theory and hence can be useful when the aim is to estimate very  
52 extreme events. When interest lies in less extreme values, a further approach is that of quantile  
53 regression (Koenker, 2005). An extreme event in this case is characterized as a value falling  
54 in the upper (or lower, e.g. to model drought conditions) tail of the distribution. Quantile  
55 regression allows estimation of the relationship between response and explanatory variables at  
56 any percentile of the distribution of the response (conditioned on the explanatory variables). As  
57 a result, rates of change in the response variable can be estimated for the whole distribution  
58 and not only at the mean. The regression coefficients are estimated minimizing an objective  
59 function that is defined in terms of the sum of weighted absolute residuals. Quantile regression  
60 has been mostly developed in the case of independent observations, but a number of approaches  
61 for spatial and spatio-temporal quantile regression can be found in the literature. The paper  
62 by He et al. (1998) is, to our knowledge, the first one to extend the 1-dimensional quantile  
63 regression problem into a 2-dimensional context; the objective function can be re-written in  
64 terms of bivariate smoothing splines (Koenker, 2005; He et al., 1998) and then minimized using  
65 linear programming methods. Penalization and fitting of splines coefficients becomes considerably  
66 more complex. This initial paper on bivariate quantile regression was followed by the work of  
67 Hallin et al. (2009), who propose using a local linear regression approach in which the regression  
68 coefficients are allowed to vary spatially. Quantile regression has also been considered from a  
69 Bayesian perspective; Lee and Neocleous (2010) and Neelon et al. (2015) develop a quantile  
70 regression model for spatial and spatio-temporal count data respectively, incorporating a spatial

71 autoregressive term in the predictor to deal with spatial correlation. Reich et al. (2011) and Reich  
72 (2012) propose, respectively, spatial and spatio-temporal quantile regression models, in which  
73 the spatial structure is introduced via the covariance function of the Gaussian spatial processes  
74 associated with the parameters of the model; regarding the temporal structure, the quantile  
75 function at each spatial location is defined as a linear function of time within a hierarchical  
76 model. Any residual spatial correlation is then modelled via a spatial copula. More recently, Sun  
77 et al. (2016) introduce temporal and spatial dependence using a fused adaptive Lasso penalty.

78 In this paper, we propose a spatio-temporal quantile regression model for river flow data; by  
79 re-expressing the quantile model as a weighted linear regression, parameter estimates can be ob-  
80 tained using penalized iterative re-weighted least squares (PIRLS). The paper introduces a new  
81 framework for spatio-temporal quantile regression modelling, where the regression model is built  
82 as an additive model that includes smooth functions of time and space, as well as space-time  
83 interaction effects. While inclusion of bivariate smooth functions in a quantile regression setting  
84 has been considered before (He et al., 1998), the case of higher dimensional smooth functions,  
85 needed, for example, for the space-time interaction term, has not been addressed in the literature.  
86 The model exploits the flexibility that P-splines offer and can be easily extended to incorporate  
87 potential covariates. We propose to estimate model parameters using a penalized least squares  
88 regression approach as an alternative to linear programming methods classically used in quantile  
89 parameter estimation. The fitting procedure is simple and computationally efficient and allows  
90 modelling strategies already available for mean regression (e.g. varying coefficient models) to  
91 be adapted to the case of quantile regression. This presents a clear advantage over linear pro-  
92 gramming methods given the increasing complexity and availability of data and the interest in  
93 extreme events. By considering a fully spatio-temporal model rather than modelling one river  
94 a time, information is borrowed across rivers; this means a more efficient use of the available  
95 data, fundamental when dealing with short records and/or aiming to estimate very high (low)  
96 quantiles.

97 In particular, quantile regression can be a useful modelling strategy for extreme river flow

98 values, given the direct link between quantile estimates and return levels, which, in turn, are used  
99 in risk assessment. In the extreme value theory (Coles, 2004) the quantile  $z_p$  of a generalized  
100 extreme value distribution  $G$  is defined as the return level with return period  $1/(1-p)$ ; the latter,  
101 also known as recurrence interval, is defined as the amount of time (on average) until the value  
102  $z_p$  is likely to be equalled or exceeded; i.e. the long term average of the time intervals between  
103 successive exceedances of a peak of magnitude  $z_p$  (Coles, 2004). The flexible spatio-temporal  
104 regression model introduced in Section 3 can be seen as a tool for modelling return levels under  
105 non-stationary conditions. Such a tool is valuable as environmental variables often exhibit non-  
106 stationarity; for example, ongoing climate change has been shown to affect both the means and  
107 extreme values of climatic and river flow time series (Arnell and Gosling, 2013, 2016). By fixing  
108 the quantile to be estimated, we are fixing the probability of the estimated value being exceeded  
109 and hence the return period, to then estimate the associated return level, that is allowed to vary  
110 both in time and space. The proposed model is illustrated on a large set of Scottish rivers.

111 In Scotland, the Scottish Flood Risk Management Act (The Scottish Government, 2010)  
112 was introduced in 2010 following the requirements of the European Union Directive on Flood  
113 Risk Management (2007/60/EC). This new piece of legislation was partly motivated by changes  
114 in Scotland's river flow and rainfall regimes. Evidence from a number of published studies  
115 (Black, 1996; Black and Burns, 2002; Werritty, 2002) reports increased variability and statistically  
116 significant changes in annual peak-over-threshold magnitude and frequency of events and in  
117 annual maxima trends in Scotland during 1956-1995. In particular, dry (1960s-1970s) and wet  
118 periods (late 1980s-early 1990s) have been identified. However, no general trend seems to hold  
119 across the country as observed changes are not homogeneous, neither in frequency, with estimates  
120 of changes in return periods changing with location, nor in time, with seasonal changes in extreme  
121 rainfall being more pronounced than annual ones, especially in autumn (Fowler and Wilby,  
122 2010). Climate model predictions (Fowler and Kilsby, 2003; Fowler and Wilby, 2010; Fowler  
123 and Ekström, 2009) suggest that these differences are likely to continue and/or increase in the  
124 near future, with fairly reliable estimates over the winter months but greater uncertainty over

125 the summer. Despite these concerns, there seems to be a research gap in the recent literature  
126 on Scottish hydrology; the most complete paper on Scottish rivers dates back to 1997 (Black  
127 and Werritty, 1997), while most UK based studies are limited to England and Wales (Hannaford  
128 and Buys, 2012) and are focused on individual catchments. The work done by Prosdocimi  
129 et al. (2013) includes a relatively large number of Scottish gauging stations, but analysis is  
130 limited to one gauging station at a time and autumn and spring are disregarded, even though  
131 significant rainfall increases in western Scotland have been identified in those seasons (Jenkins  
132 et al., 2009; Werritty, 2002). The study by Hannaford and Buys (2010) includes twenty Scottish  
133 gauging stations, but the analysis is performed on the UK as a whole. Results from some of  
134 the previously mentioned studies suggest regional variation in hydrological trends across the  
135 UK as a whole and also within Scotland. Although the focus of this paper is development of a  
136 spatio-temporal modelling methodology, the results presented here also update the literature and  
137 extend understanding of extreme river flows in Scotland. Rather than working on one gauging  
138 station at a time, we follow a spatio-temporal modelling approach that takes into account possible  
139 dependencies among stations. Further, important changes in river flow may not be detected at  
140 the annual scale (Hannaford and Buys, 2012); we use daily data, without restricting the series to  
141 annual maxima or peak-over-threshold data, the usual practice in extreme value analysis. The  
142 dataset considered is very rich, with nearly 100 gauging stations, and the results show how the  
143 spatio-temporal trend in extreme flows has changed in recent years (1996-2013), helping to fill  
144 in the current research gap. Identifying these changes is important to understand the effect of  
145 climate change (Prosdocimi et al., 2013) and to investigate the validity of model projections or  
146 for historical model run validation (Hannaford and Buys, 2012).

147 The paper is organized as follows. The dataset is introduced in Section 2. Section 3 de-  
148 scribes the proposed methodology for fitting a spatio-temporal quantile regression model. The  
149 performance of the model is illustrated in Section 4 on a set of Scottish rivers, for which the 95%  
150 quantile of river flow is estimated. A simulation study is presented in Section 5. Finally, the  
151 main results and discussion are summarized in Section 6.

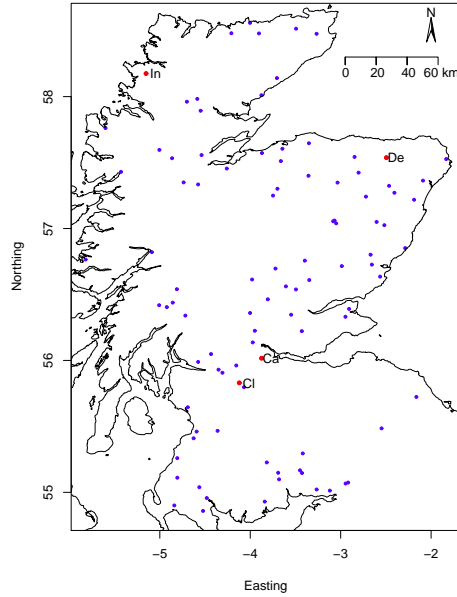


Figure 1: Location of the 98 selected gauging stations. In red, location of rivers Inver (In), Clyde (Cl), Carron (Ca) and Deveron (De).

## 152 2 Data

153 Data, in the form of daily river flow ( $\text{m}^3/\text{s}$ ), were provided by the Scottish Environment Pro-  
 154 tection Agency (SEPA) and the National River Flow Archive (NRFA). Most of the records are  
 155 available online on the NRFA webpage. Our data set consists of 98 gauging stations, selected  
 156 on the basis of geographical location, quality and length of the records, covering the period 1<sup>st</sup>  
 157 January 1996- 31<sup>st</sup> December 2013. The spatial locations can be seen in Figure 1. Forty-three  
 158 series contained missing values. However, the missing proportions ( $< 0.1\%$ ) were small enough  
 159 not to be a concern, and missing values were imputed using linear interpolation. The interpo-  
 160 lation was done separately for each month to better reproduce the variability of the series; i.e.  
 161 missing values in January were imputed using only recorded values in January, and so on. Since  
 162 the distribution of river flow is very skewed, a log transformation was used.

163 In particular, four rivers have been chosen for illustrative purposes and are discussed in more  
 164 detail in Section 4: the river Inver (North West), Clyde (South West), Carron (South East)  
 165 and Deveron (North East). The gauging stations are marked in red in Figure 1 while data are



166 shown in Figure 2. The main characteristics of these rivers (catchment area, maximum elevation,  
167 mean flow, 95th (Q95) and 99th (Q99) quantiles of river flow and mean flow/catchment area)  
168 are summarized in Table 1. Rivers Clyde and Deveron have higher flow values on average, as  
169 they are the largest rivers out of the four rivers considered, with a catchment area of 1903.1 km<sup>2</sup>  
170 and 954.9 km<sup>2</sup> respectively. Rivers Inver and Carron, on the other hand, have a catchment area  
171 of 137.5 km<sup>2</sup> and 122.3 km<sup>2</sup> respectively. All four rivers exhibit a clear strong seasonal pattern,  
172 with greater variability in rivers Clyde and Carron, which are located on the southern part of  
173 the country. While there is no apparent long term trend, Figure 2 shows extreme flows in all  
174 four rivers, but these are not all coincident. This suggests that a simple statistical model with  
175 only a time trend and a spatial trend will probably not be enough to capture the complexity of  
176 the data, but inclusion of a time-space interaction may be required. Spatial differences can be  
177 partly explained by the predominant rainfall pattern in Scotland, wetter in the West and dryer  
178 in the East, as seen in Figure 3.

179 Prior to model fitting, the mean flow was removed at each individual location as a way of  
180 standardizing the data. This was done to account for differences in flow values due to catchment  
181 size.

### 182 **3 Methodology**

183 We introduce a new approach that builds upon the idea of approximating the absolute residuals  
184 with the squared residuals, as suggested in Reiss and Huang (2012). This approximation, mo-  
185 tivated by the fact that the check function in Equation (1) is not differentiable at zero, ensures  
186 differentiability everywhere. This way, instead of using linear programming methods to estimate  
187 the model parameters, a weighted least squares approach is preferred, exploiting the fact that  
188 the objective function in Equation (1) is a weighted sum of absolute residuals. In their paper,  
189 Reiss and Huang (2012) consider a very simple model where the response depends on a single  
190 covariate, while we introduce a flexible spatio-temporal model in a generalized additive model

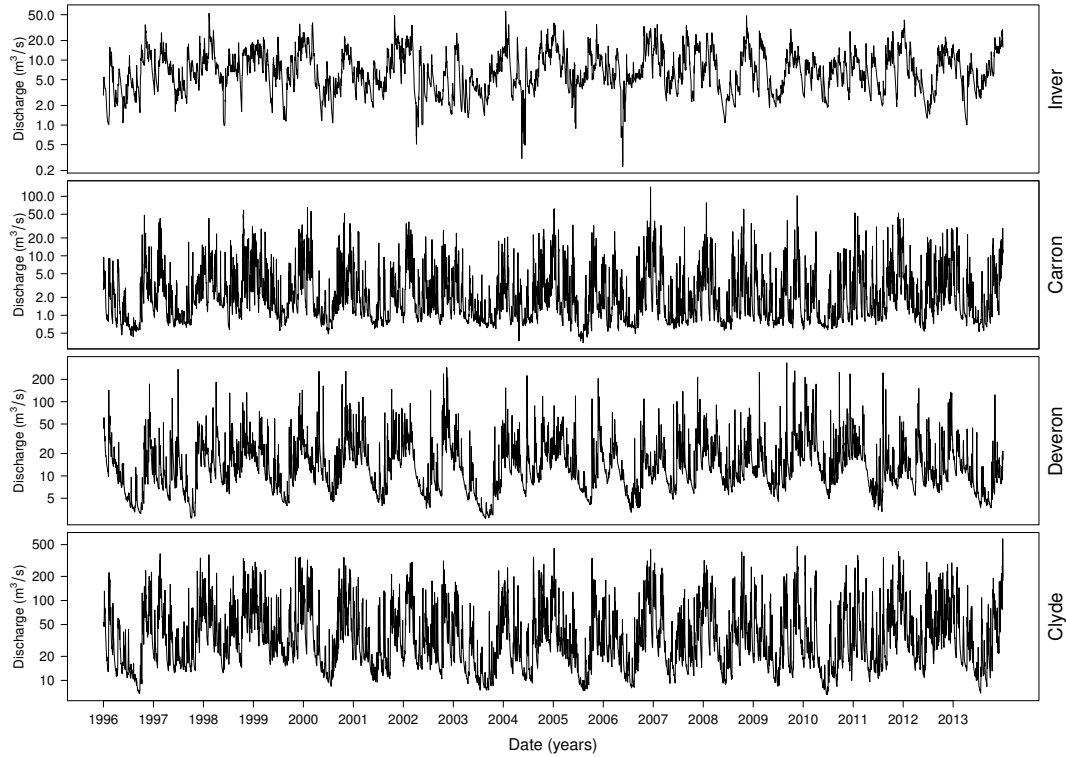


Figure 2: Time series of flow ( $\text{m}^3/\text{s}$ ) ordered by flow magnitude for the rivers Inver, Carron, Deveron and Clyde.

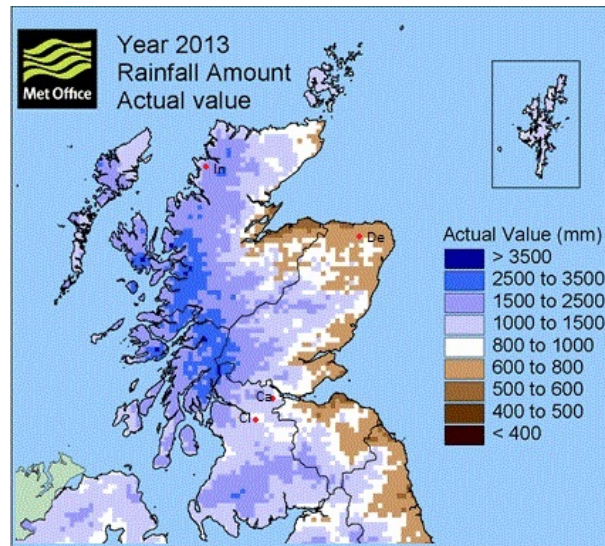


Figure 3: Average annual rainfall in 2013 (*Source:* modified from <https://www.metoffice.gov.uk/climate/uk/summaries>). In red, location of rivers Inver (In), Clyde (Cl), Carron (Ca) and Deveron (De).

191 framework.

192 The classic simple linear regression model of  $y$  over  $x$  aims to estimate  $E[Y|X = x] = \alpha + \beta x$ .  
193 Instead, the aim now is to estimate a quantile of the distribution of  $Y|X = x$  rather than the  
194 mean. The conditional quantile of a random variable  $Y$  with cumulative distribution function  $F_Y$   
195 can be expressed as  $Q_Y(\tau|\mathbf{X} = \mathbf{x}) = F_Y^{-1}(\tau|\mathbf{X} = \mathbf{x})$ , where  $\tau \in (0,1)$ , and  $\mathbf{X} = (X_1, \dots, X_p)$   
196 is a vector of explanatory variables (Koenker, 2005; Cade and Noon, 2003). As in classic linear  
197 regression, the errors are assumed to be independent, but here no assumptions are made regarding  
198 their distribution. The general objective function in a quantile linear regression model is defined  
199 as:

$$R(\boldsymbol{\beta}) = \sum_{i=1}^n \rho_{\tau}(y_i - (x_{1,i}\beta_1 + \dots + x_{p,i}\beta_p)), \quad (1)$$

200 where  $\boldsymbol{\beta} = (\beta_1, \dots, \beta_p)^T$ ,  $\rho_{\tau}(u) = u(\tau - I(u < 0))$  is the check function and  $I$  is an indicator  
201 function (Koenker, 2005; Koenker and Hallock, 2001; Koenker and Bassett, 1978). Estimating the  
202 parameters  $\boldsymbol{\beta}$  in Equation (1) involves minimizing a sum of weighted absolute deviations, where  
203 the weights are asymmetric functions of  $\tau$ . The function  $R(\boldsymbol{\beta})$  is piecewise linear and continuous,  
204 being differentiable at every point except at those whose residuals are zero. Until now, linear  
205 programming methods, like the simplex method or the interior point method (Koenker, 2005;  
206 Koenker and Hallock, 2001) are used to estimate  $\boldsymbol{\beta}$ .

### 207 3.1 A spatio-temporal quantile regression model

208 A simple spatio-temporal additive model (main effects model) for river flow can be expressed as:

$$Q_{\log(\text{flow})_i}(\tau|t_i, d_i, z_i) = s_1(t_i) + s_2(d_i) + s_3(z_i), \quad i = 1, \dots, n \quad (2)$$

209 where  $Q_{\log(\text{flow})}(\tau|t, d, z)$  is the  $\tau^{\text{th}}$  quantile of the (conditional) distribution of  $\log(\text{flow})$ ,  $s_1(t)$ ,  
210  $s_2(d)$  are smooth functions of time and day of the year and  $s_3(z)$  is a bivariate smooth function  
211 of easting and northing coordinates. These three terms represent the temporal, seasonal and  
212 spatial trends in river flow respectively. In our particular application, the trend ( $s_1(t)$ ), seasonal

213 ( $s_2(d)$ ) and spatial ( $s_3(z)$ ) terms were built as smooth functions of  $t$ =time (1996 to 2013),  $d$ =day  
 214 within the year (1 to 365) and  $z$ =(easting, northing), respectively. The model assumes the  
 215 seasonal component  $s_2(d)$  to be constant over the years and the temporal trend to be the same  
 216 at all spatial locations (or similarly, the spatial trend is assumed to be constant over time). A  
 217 preliminary exploratory analysis of the data revealed a seasonal cycle that changes from year to  
 218 year, suggesting that this might be too simple a model for the Scottish river flow dataset. We  
 219 introduce an interaction term  $s_4(t, d)$  to adjust for yearly changes in the seasonal pattern:

$$Q_{\log(flow)_i}(\tau|t_i, d_i, z_i) = s_1(t_i) + s_2(d_i) + s_3(z_i) + s_4(t_i, d_i). \quad (3)$$

220 Similarly, Model (3) can be further extended to include space-time  $s_5(t, z)$  and space-season  
 221  $s_6(d, z)$  interactions so that the full model becomes:

$$Q_{\log(flow)_i}(\tau|t_i, d_i, z_i) = s_1(t_i) + s_2(d_i) + s_3(z_i) + s_4(t_i, d_i) + s_5(t_i, z_i) + s_6(d_i, z_i). \quad (4)$$

222 Each of the univariate smooth functions can be rewritten as a linear combination of  $k$  cubic  
 223 B-spline basis functions  $B_1(t), \dots, B_k(t)$  (Eilers and Marx, 2009, 2010), so that  $s_1(t) = \mathbf{B}_1\boldsymbol{\theta}_1$   
 224 and  $s_2(d) = \mathbf{B}_2\boldsymbol{\theta}_2$ , where  $\boldsymbol{\theta}_1, \boldsymbol{\theta}_2$  are  $k_1 \times 1, k_2 \times 1$  vectors of coefficients respectively,  $\mathbf{B}_1, \mathbf{B}_2$  are  
 225 the matrices of basis functions ( $\dim(\mathbf{B}_1) = n \times k_1, \dim(\mathbf{B}_2) = n \times k_2$ ),  $k_1, k_2$  are the number of  
 226 basis functions used in each case and  $n$  is the total number of observations.

227 The bivariate smooth function  $s_3(z) = s_3(easting, northing)$  can be expressed in terms of the  
 228 tensor product of the marginal B-splines basis on the individual variables *easting* and *northing*  
 229 (Wood, 2006; Eilers and Marx, 2003, 2010; He et al., 1998) so that  $s_3(z) = \mathbf{B}_3\boldsymbol{\theta}_3$  where  $\boldsymbol{\theta}_3$  is a  
 230  $(k_{east} \times k_{north}) \times 1$  vector of coefficients and  $\mathbf{B}_3$  is a  $n \times (k_{east} \times k_{north})$  matrix. The interaction  
 231 terms  $s_4(t, d)$ ,  $s_5(t, z)$  and  $s_6(d, z)$  can be built in a similar way in terms of the tensor product  
 232 of the corresponding marginal basis matrices as detailed above.

233 The full model can be expressed in matrix form as:

$$\mathbf{y} = \mathbf{B}\boldsymbol{\theta} + \boldsymbol{\epsilon}$$

234 where the design matrix  $\mathbf{B} = [\mathbf{B}_1 \ \mathbf{B}_2 \ \mathbf{B}_3 \ \mathbf{B}_4 \ \mathbf{B}_5 \ \mathbf{B}_6]$  is the matrix that results from  
 235 combining the individual matrices column-wise and  $\boldsymbol{\theta} = [\boldsymbol{\theta}_1 \ \boldsymbol{\theta}_2 \ \boldsymbol{\theta}_3 \ \boldsymbol{\theta}_4 \ \boldsymbol{\theta}_5 \ \boldsymbol{\theta}_6]^T$  is the vec-  
 236 tor of coefficients. By expressing the model as a linear model, the parameters can be estimated  
 237 easily using efficient matrix-vector operations. A penalty term can be added to control for the  
 238 amount of smoothness, which can be tuned individually for each term in the model. This means  
 239 that a vector of smoothing parameters  $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \boldsymbol{\lambda}_3, \boldsymbol{\lambda}_4, \boldsymbol{\lambda}_5, \boldsymbol{\lambda}_6)$  needs to be specified. In this  
 240 case, a second order different penalty on the spline coefficients is used following Eilers and Marx  
 241 (2009); further, a periodicity constraint can be imposed on the seasonal term  $s_2(d)$  to ensure  
 242 continuity of the seasonal cycle over the years. This can be implemented, for cubic B-splines,  
 243 by forcing the first and last three spline coefficients to be the same. The penalty term can be  
 244 expressed as  $\boldsymbol{\theta}^T \mathbf{P} \boldsymbol{\theta}$  where  $\mathbf{P}$  is a block diagonal penalty matrix, each block corresponding to  
 245 the penalization of the individual smooth terms included in the model. For the univariate terms  
 246  $s_1(t)$ ,  $s_2(d)$  the corresponding penalty matrix can be easily built as  $\mathbf{D}_{do}^T \mathbf{D}_{do}$  following Eilers and  
 247 Marx (2009), where  $\mathbf{D}_{do}$  is a difference matrix of order  $do$  ( $do = 2$  for a second order penalty)  
 248 of dimension  $(k - 2) \times k$  with  $k$  the number of basis functions.

249 For the spatial term  $s_3(east, north)$ , the penalty is constructed by penalizing individually  
 250 the rows and columns of matrix  $\mathbf{B}_3$  (Wood, 2006; Eilers and Marx, 2003, 2010; He et al., 1998).  
 251 Penalty terms for  $s_4(t, d)$ ,  $s_5(t, z)$  and  $s_6(d, z)$  can be built similarly.

252 The vector of model parameters  $\boldsymbol{\theta}$  is estimated using the penalized iterative weighted regres-  
 253 sion approach described below. Assuming the vector of smoothing parameters  $\boldsymbol{\lambda}$ , to be fixed,

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta} \in \mathbb{R}^k}{\operatorname{argmin}} \left[ \sum_{i=1}^n \rho_{\tau}(y_i - \mathbf{B}_i \boldsymbol{\theta}) + \boldsymbol{\lambda} \boldsymbol{\theta}^T \mathbf{P} \boldsymbol{\theta} \right] \quad (5)$$

254 where  $k$  is the total number of coefficients and  $\mathbf{B}_i$  represents the  $i^{th}$  row of matrix  $\mathbf{B}$ . We

255 propose translating the minimization problem in Equation (5) into a penalized least squares  
 256 problem that can be solved using penalized iterative reweighted least squares (PIRLS, Wood  
 257 (2006)). The (approximate) objective function expressed in matrix form becomes:

$$\|\mathbf{W}(\mathbf{y} - \mathbf{B}\boldsymbol{\theta})\|^2 + \boldsymbol{\lambda}\boldsymbol{\theta}^T \mathbf{P}\boldsymbol{\theta} \quad (6)$$

258 where  $\mathbf{W}$  is a diagonal matrix of weights calculated iteratively following Equation (7):

$$w_i^{(j)} = \frac{\tau - I \left[ (y_i - \mathbf{B}_i \hat{\boldsymbol{\theta}}^{(j)}) < 0 \right]}{2(y_i - \mathbf{B}_i \hat{\boldsymbol{\theta}}^{(j)})} \quad (7)$$

259 for  $i = 1, \dots, n$ . A large upper bound is set for the weights to avoid residuals close to zero,  
 260 which would result in the check function not being differentiable. Truncating all weight values  
 261 above the given upper bound does not have a large effect on the fitting process as we are just  
 262 forcing very small residuals, whose contribution to the objective function is negligible, to be even  
 263 smaller. The estimated vector of parameters  $\hat{\boldsymbol{\theta}}$  at iteration ( $j$ ) can be computed as:

$$\hat{\boldsymbol{\theta}}^{(j)} = (\mathbf{B}^T \mathbf{W}^{(j-1)} \mathbf{B} + \boldsymbol{\lambda} \mathbf{P})^{-1} \mathbf{B}^T \mathbf{W}^{(j-1)} \mathbf{y} \quad (8)$$

264 Convergence of the algorithm is defined based on the objective function  $R(\boldsymbol{\theta})$  defined in Equa-  
 265 tion (1); the algorithm stops when the difference between  $R(\boldsymbol{\theta}^{(j-1)})$  and  $R(\boldsymbol{\theta}^{(j)})$  is smaller than  
 266 some predefined small tolerance. Results from a simulation study suggest no differences in the  
 267 fitted model for tolerance values of  $10^{-2}$  and above. Identifiability of the single components of  
 268 the model is ensured by including a ridge penalty (Eilers and Marx, 2002).

269 The smoothing parameters are chosen to minimize a modified version of the Schwarz infor-  
 270 mation criterion (SIC, Koenker et al. (1994)):

$$SIC(\boldsymbol{\lambda}) = \log \left[ \frac{1}{n} \sum_{i=1}^n \rho_{\tau}(y_i - \hat{y}_i) \right] + \frac{1}{2n} df_{\boldsymbol{\lambda}} \log n \quad (9)$$

271 where the approximated degrees of freedom  $df_\lambda$  can be calculated as the trace of the smoothing  
 272 matrix  $\mathbf{S} = \mathbf{B}(\mathbf{B}^T\mathbf{W}\mathbf{B} + \lambda\mathbf{P})^{-1}\mathbf{B}^T\mathbf{W}$  (Hastie and Tibshirani, 1990). As previously stated,  
 273 Model (4) is fitted assuming independent observations. In this case, standard errors for the fitted  
 274 values  $\hat{\mathbf{y}}$  can be obtained as:

$$se(\hat{\mathbf{y}}) = \sqrt{diag(\mathbf{S}\mathbf{S}^T)\hat{\sigma}^2}$$

275 where  $\mathbf{S}$  is the smoothing matrix at the last iteration and  $\hat{\sigma}^2$  is an estimate of the residual variance  
 276 that can be obtained as  $\hat{\sigma}^2 = \frac{RSS}{df_{error}}$ , with  $RSS = \mathbf{Y}^T(\mathbf{I} - \mathbf{S})\mathbf{W}(\mathbf{I} - \mathbf{S})\mathbf{Y}$  and  $df_{error} = n - df_\lambda$ .  
 277 However, if some spatio-temporal dependence structure is left in the residual term, standard  
 278 error calculation needs to be adjusted accordingly. Let  $\mathbf{V}$  be the correlation matrix. Adjusted  
 279 standard errors can be estimated as:

$$se(\hat{\mathbf{y}}) = \sqrt{diag(\mathbf{S}\mathbf{V}\mathbf{S}^T)\hat{\sigma}^2}. \tag{10}$$

## 280 4 Results

281 Model (4) was fitted to the data set described in Section 2, comprising 98 rivers with 6570  
 282 daily observations per river spanning 18 years, from 1<sup>st</sup> January 1996 to 31<sup>st</sup> December 2013  
 283 ( $n = 643860$  observations in total). The 29th of February was removed from the dataset after  
 284 ensuring that no relevant information (i.e. no extreme values) was lost. Since we are mostly  
 285 interested in extreme values, a value of  $\tau=0.95$  was chosen to fit a model for the 95<sup>th</sup> quantile  
 286 of logged river flow. The trend ( $s_1(t)$ ), seasonal ( $s_2(d)$ ) and spatial ( $s_3(z)$ ) terms in Model (4)  
 287 were built as smooth functions of  $t$ =time (1996 to 2013),  $d$ =day within the year (1 to 365)  
 288 and  $z$ =(easting, northing), respectively. When using penalized splines, the usual practice is to  
 289 choose an arbitrary large number of basis functions and then control the amount of smoothness  
 290 by penalizing the spline coefficients. The definition of *large*, however, depends on the application  
 291 at hand. We fitted the model using an increasing number of basis functions until the percentage  
 292 change in SIC was smaller than 1%. In this case, the number of basis functions was chosen to

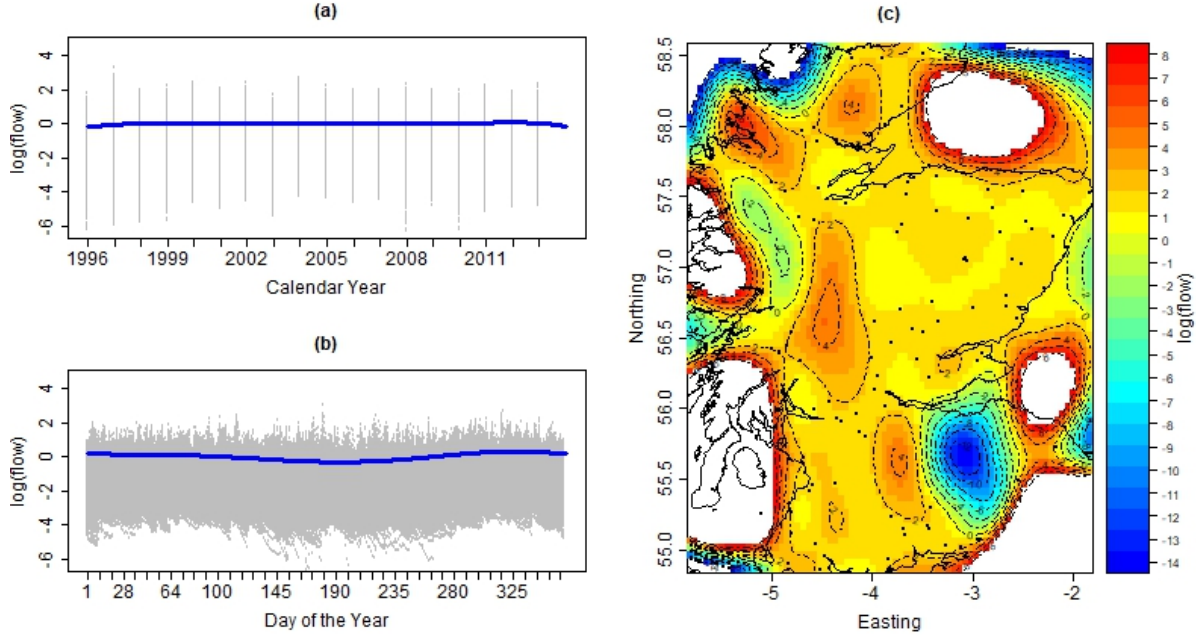


Figure 4: Estimated trend (a), seasonal (b) and spatial (c) components along with partial residuals.

293 be  $k_1 = 12$  for the trend component,  $k_2 = 6$  for the seasonal component and  $k_3 = 12^2$  for the  
 294 space component, while  $k_4 = 12 \times 6$ ,  $k_5 = 12^3$  and  $k_6 = 6 \times 12^2$  were used for the interaction  
 295 terms  $s_4(t, d)$ ,  $s_5(t, z)$  and  $s_6(d, z)$  respectively. A second order penalty was imposed on the  
 296 spline coefficients. This is a commonly used smoothness penalty that corresponds to penalizing  
 297 the roughness of a curve, measured as the integral square of the second derivative of the curve  
 298 (Eilers and Marx, 1996). Smoothing parameters were chosen based on the Schwarz Information  
 299 Criteria (Equation (9)), using a restricted grid of values for  $\lambda$ . The trend, seasonal and spatial  
 300 main effects are shown in Figure 4.

301 Overall, the estimated trend (Figure 4 (a)) appears to be fairly flat. There is a seasonal  
 302 effect (Figure 4 (b)), as expected, with lower values during the summer (reaching a minimum  
 303 at the beginning of July) and higher values during the winter months. The estimated spatial  
 304 pattern (Figure 4 (c)) suggests a slight East-West gradient, with greater values on the Western  
 305 side. Figure 5(a) shows the seasonal adjustment that needs to be made to the overall seasonal  
 306 pattern ( $s_4(t, d)$ ) in four different years (1998, 2000, 2003 and 2012); it can be seen that there is



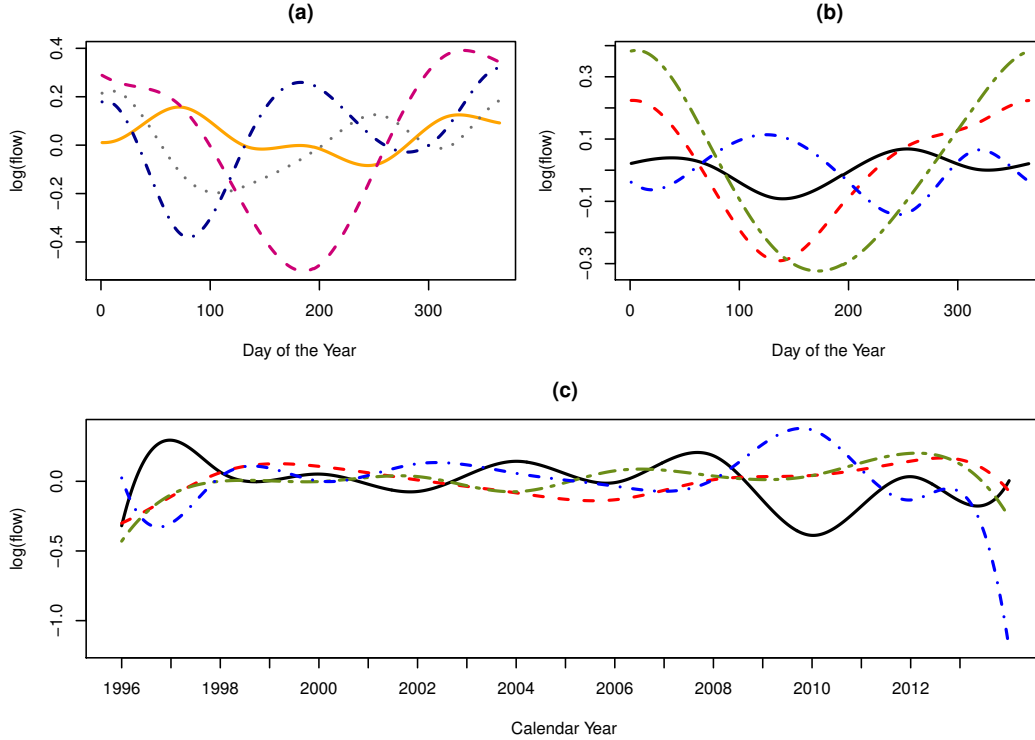


Figure 5: (a) Season-year interaction for 4 different years (1998 (orange), 2000 (pink), 2003 (grey) and 2012 (dark blue)), (b) season-space interaction and (c) trend-space interaction for rivers Inver (black), Clyde (red), Carron (blue) and Deveron (green).

307 variation from year to year and, in particular, that the seasonal pattern in 2000 (pink curve) is  
 308 very different from the rest.

309 Following Model (4), we can identify not only long term trends over the whole period/spatial  
 310 region but also assess how the spatial distribution of extreme flows has changed over time by  
 311 visual inspection of the interaction term  $s_5(t, z)$ , that can also be interpreted as the adjustment  
 312 that needs to be made to the temporal trend  $s_1(t)$  shown in Figure 4(a) at each location; these  
 313 adjustments can be seen in Figure 5(c) for the four rivers described in Section 2, while the  
 314 corresponding seasonal adjustment (interaction term  $s_6(d, z)$ ) can be seen in Figure 5(b). While  
 315 the trend appears to be very homogeneous over space, with little adjustment needed with respect  
 316 to the overall trend shown in Figure 4(a), seasonality varies considerably among the different  
 317 rivers (Figure 5(b)), supporting the idea that no unique seasonal pattern is valid over the whole  
 318 country.

319 One can graphically show the fitted values from a spatial or a temporal point of view. The  
320 estimated 95<sup>th</sup> quantile of river flow over Scotland is shown in Figure 6 for four different time  
321 points, namely 1<sup>st</sup> of January, April, July and October, over years 1996 to 2000. These dates  
322 were chosen to illustrate possible differences between seasons. We can see how the contrast  
323 between East and West is more pronounced in some periods than others, and that there is a  
324 clear difference in the summer (1<sup>st</sup> of July) and winter (1<sup>st</sup> of January) values between 1996 and  
325 the remaining years. A model without a time-space interaction term would not have been able  
326 to identify a spatial pattern changing over time.

327 Even though the data were log transformed initially, it is possible to show the fitted model  
328 at each gauging station in the original scale as quantile regression is invariant to monotonic  
329 transformations. An example for the fitted model (with and without interaction) can be seen  
330 in Figure 7 for four different rivers located in various parts of the country (see Figure 1 for  
331 locations). While for River Carron the fitted models with and without interaction are very close,  
332 for the River Inver there are clear differences between the two models, especially at the beginning  
333 and end of the record.

334 Model (4) was estimated assuming independence; residual correlation was investigated by  
335 means of empirical variograms and autocorrelation plots. Once the spatial trend is taken into  
336 account, there is no spatial structure left in the residuals, as suggested by the flat empirical  
337 variograms (not included here). This is expected given the spatial flexibility that we have allowed  
338 for in the model by incorporating the interaction terms space-time and space-season. On the other  
339 hand, the residual autocorrelation plots indicated the presence of temporal correlation. Hence, an  
340 AR(1) process was assumed on the residuals, a common choice for environmental processes. The  
341 standard errors of the fitted model were adjusted for residual correlation following Equation (10)  
342 and are illustrated in Figure 7. As expected, the pointwise confidence bands become wider once  
343 correlation is taken into account.

344 The full model includes 2826 parameters. With these specifications, running the model took  
345  $\approx 10$  hours on a CPU with 2.0Ghz (128Gb RAM). The PIRLS algorithm converged after 43

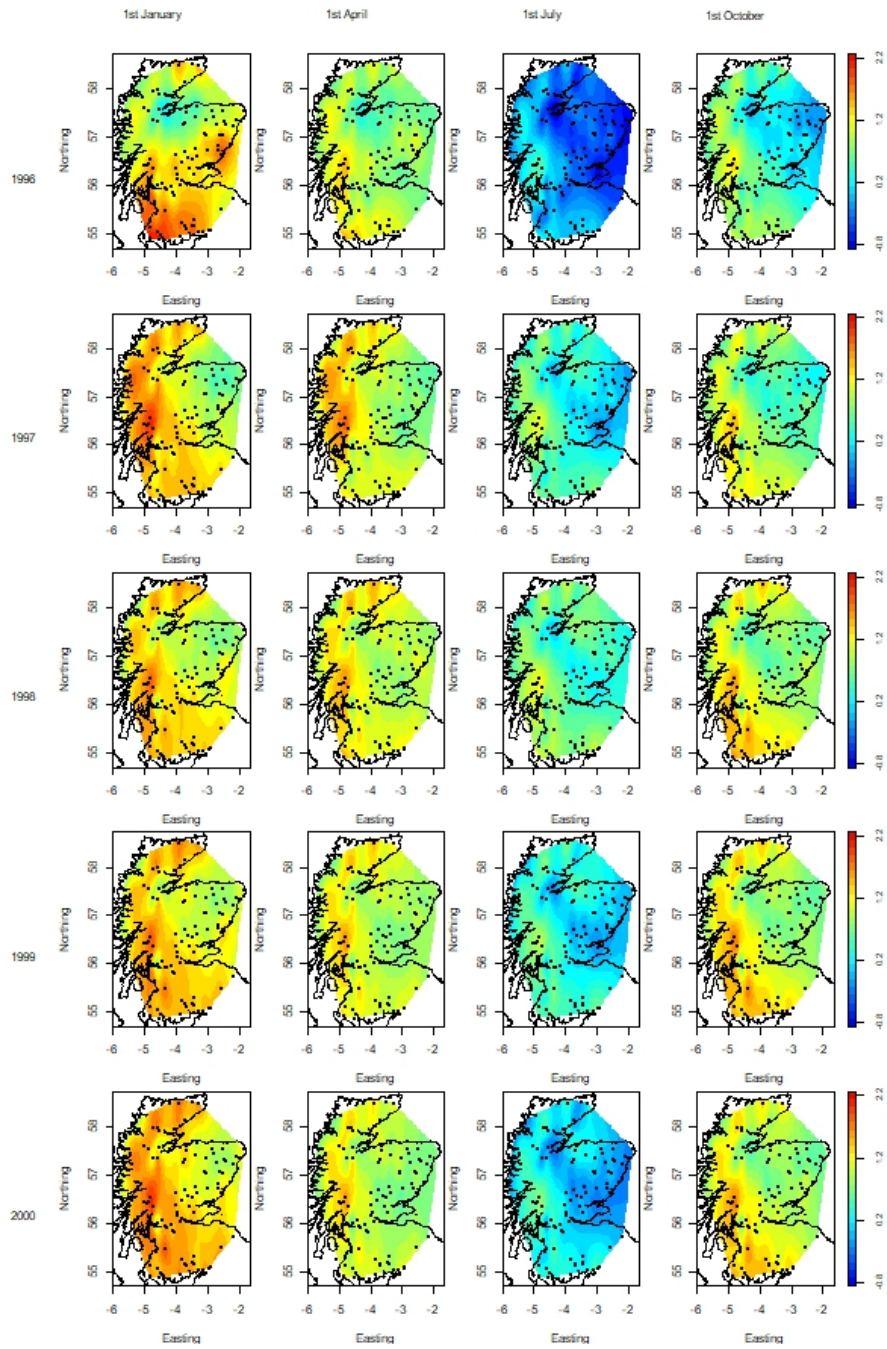


Figure 6: Estimated 95<sup>th</sup> quantile of (logged) river flow at four different dates (columns) and five different years (rows)

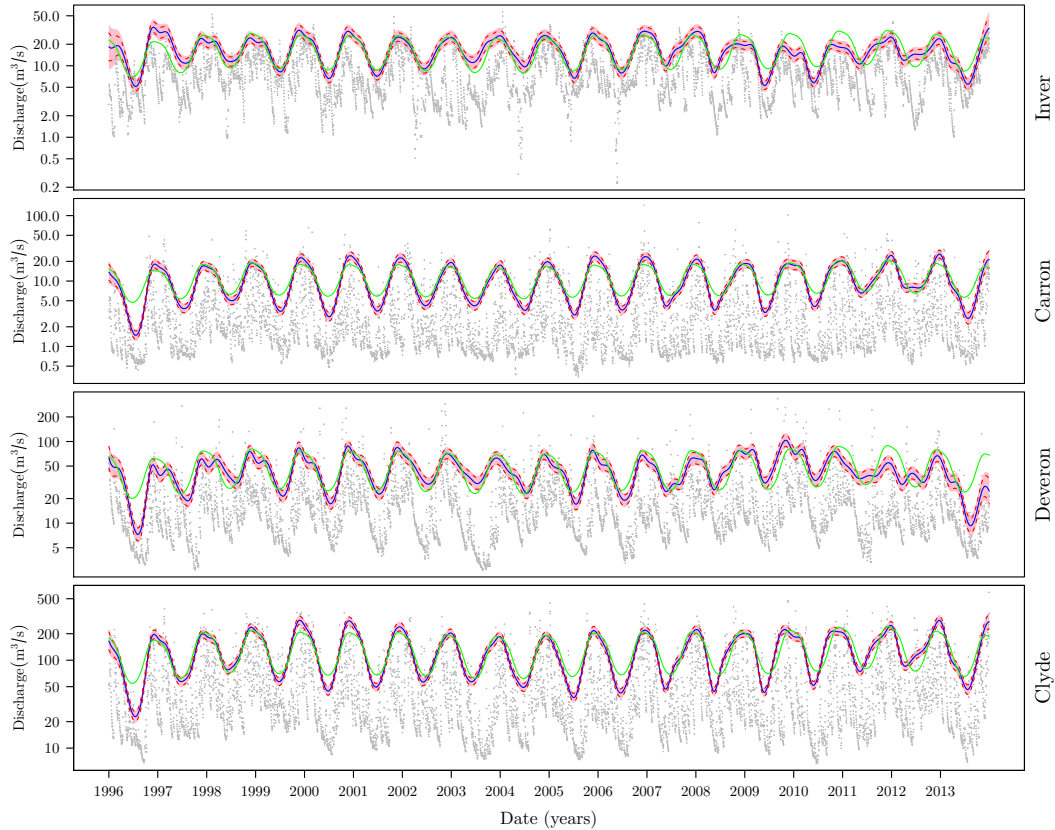


Figure 7: Fitted model (blue), 95% approximated confidence interval under independence (red) and dependence (pink) and fitted model without the interaction terms (green) for rivers Inver (North West), Carron (South East), Deveron (North East) and Clyde (South West).

346 iterations, with a tolerance value set to  $10^{-2}$ . The approximation of the check-function as a  
 347 weighted sum of squared residuals was also investigated. At the last iteration, the weighted  
 348 residuals (i.e. using the approximation) were similar to those obtained using the check function.  
 349 As a way of informally assessing whether the model was appropriate or not, the proportion of  
 350 residuals above and below the fitted surface was calculated; these were equal to 5.2% and 94.8%  
 351 respectively, not far from the theoretical expected values of 5% and 95%.

## 352 5 Simulation Study

353 A simulation study was run in order to evaluate the performance of the model proposed in  
 354 Section 3.1 and compare it to that of the R package `quantreg` (Koenker, 2018) for the 95<sup>th</sup>  
 355 quantile. We simulated daily data under 4 different scenarios with varying sample size in time  
 356 and space. For the time component, we consider 5 and 10 years of data, while for the space  
 357 component we consider 20 and 50 locations on a spatial irregular grid on  $[0, 1] \times [0, 1]$ . Data were  
 358 generated as the sum of a smooth time trend  $s(t)$ , a seasonal cycle  $s(d)$  and a spatial component  
 359  $s(z)$  as follows:

$$\begin{aligned} s(t) &= 1 + 0.3t + 0.7t^2, \\ s(d) &= \sin(2\pi d/365 + \pi/2), \\ s(z) &= s(z_1, z_2) = 0.2z_1 + 0.25z_2 + 3z_1z_2. \end{aligned}$$

360 Random noise was simulated from an asymmetric Laplace distribution  $ALD(\mu, \sigma, q)$ , a com-  
 361 monly used distribution in quantile regression, with  $\mu = 0$  and  $q = 0.95$ . Regarding  $\sigma$ , two  
 362 different levels of noise were considered in each scenario, corresponding to a signal to noise ratio  
 363 (SNR) of two and four. Table 7 summarizes the different scenarios considered while and example  
 364 of simulated data is illustrated in Figure 8.

365 Model (2) was fitted for the 95<sup>th</sup> quantile to 100 simulated data sets under each scenario  
 366 using the method described in Section 3.1 with  $k = 5$  for all terms. The `rqss` function from  
 367 the `quantreg` R package was also used to estimate the same model. Smoothing parameters

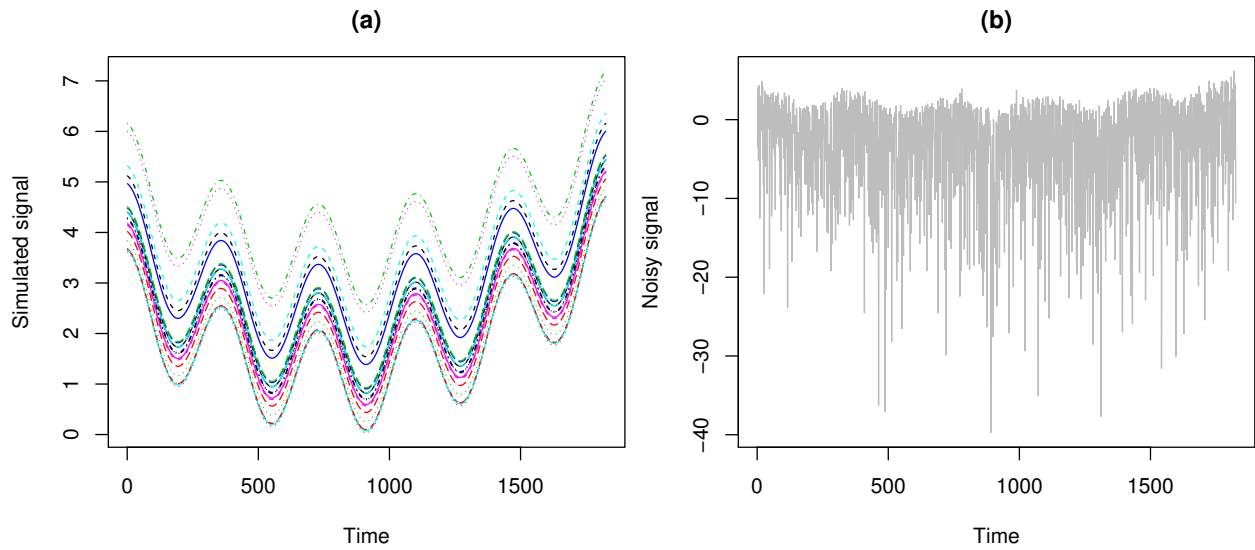


Figure 8: (a) Simulated signal under scenario A, (b) noisy signal simulated at one spatial location under scenario A4.

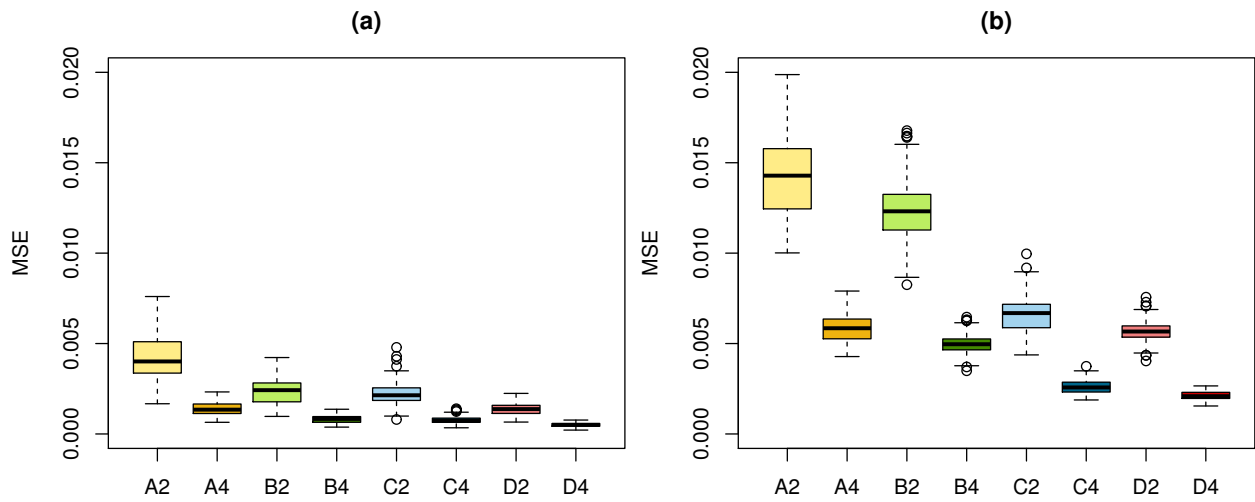


Figure 9: Boxplots of MSE under the different simulation scenarios when the 95<sup>th</sup> quantile model is estimated using the method proposed in this paper (a) and the `quantreg` package (b).

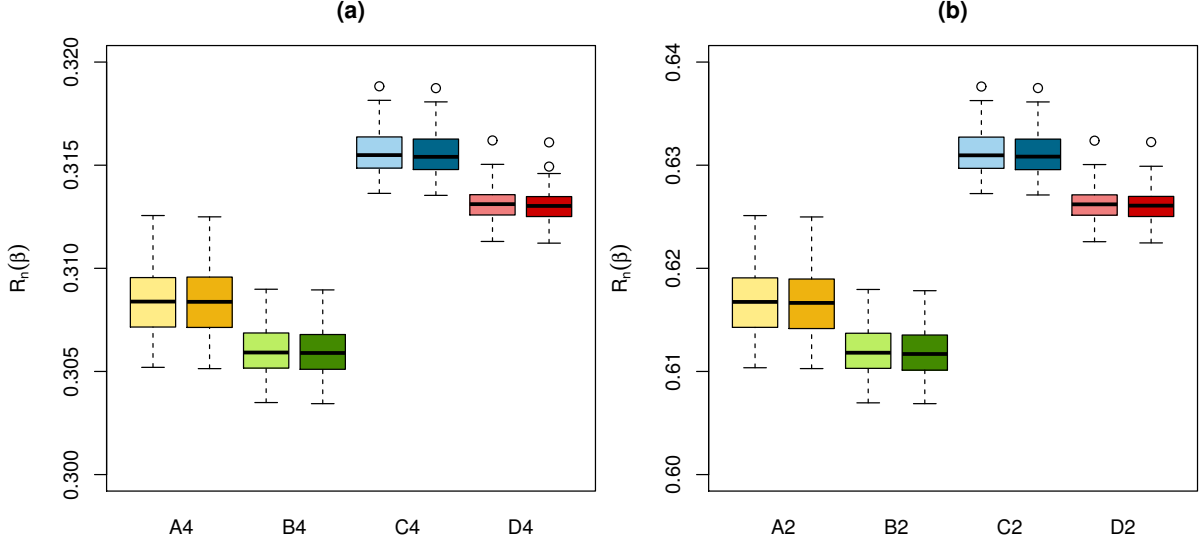


Figure 10: Boxplots of  $R_n(\beta)$  under the different simulation scenarios when the 95<sup>th</sup> quantile model is estimated using the method proposed in this paper (lighter colours) and the `quantreg` package (darker colours) with SNR=4 (a) and SNR= 2 (b).

368 in both cases were chosen based on SIC. Boxplots of the mean square error (MSE) between  
 369 the simulated and estimated signal are shown in Figure 9, where it can be clearly seen that  
 370 the MSE is considerably lower for the proposed method (panel (a)) in all simulation scenarios.  
 371 In both panels (a) and (b) the MSE is smaller when the signal to noise ratio is greater and  
 372 decreases as the sample size increases (both in time and space), as one would expect. From  
 373 this simulation study, it can be concluded that for nonparametric spatio-temporal modelling our  
 374 method performs better than classical quantile regression estimation. The poorer performance  
 375 obtained using `quantreg` might be partly explained by the fact that is not possible to constrain  
 376 the seasonal component to be cyclic.

377 To assess how good the approximation that the proposed method makes is (Equation (6)),  
 378 we compared the following quantity for both approaches:

$$R_n(\beta) = \frac{1}{n} \sum_{i=1}^n \rho_\tau(y_i - \hat{y}_i)$$

379 where  $\rho_\tau$  is the check function in Equation (1),  $y_i$  are the (noisy) simulated values,  $\hat{y}_i$  are the

380 fitted values and  $n$  is the total number of observations. As can be seen in Figure 10, there are  
381 no differences in  $R_n(\beta)$  between the two approaches, suggesting very good agreement between  
382 the original check function and its approximated version.

383 For the more complex model including the interaction terms, it is not possible to compare  
384 the performance of the proposed method with `quantreg` as the latter does not allow inclusion of  
385 smooth functions of dimension greater than two.

## 386 **6 Discussion**

387 Environmental processes are highly variable in both space and time and, as such, investigation  
388 of trends in their means may not be sufficiently informative, especially when the interest is  
389 in extreme values. On the other hand, river flow records tend to be relatively short, usually  
390 spanning about 20-30 years of data; modelling extremes, such as the 1 in 100 year design event,  
391 from such short records using the classical extreme value theory approach can be problematic, as  
392 the number of observations is dramatically reduced when considering the annual maxima series  
393 or only the peaks above a certain threshold. This paper proposes a spatio-temporal quantile  
394 regression approach for modelling extreme river flow values. Although the work was motivated  
395 by a case study on river flow in Scotland, the proposed model is applicable to other areas where  
396 quantiles might be of interest, e.g. air pollution. The model is built in a generalized additive  
397 model framework that allows inclusion of three-variate smooth functions to account for space-  
398 time interaction effects. The number of observations is crucial for reliable estimation in a quantile  
399 regression setting, especially when building models for very high (or very low) quantiles. Rather  
400 than modelling one river at a time, we use a single model for the whole dataset; this way we  
401 borrow information across locations, particularly important when dealing with short records.

402 Despite quantile regression being increasingly popular in environmental applications (see  
403 e.g. Weerts et al. (2011); Reich (2012); Planque and Buffaz (2008)), applications on spatio-  
404 temporal data are still very limited. We propose a flexible spatio-temporal model that takes into



405 account potential space-time interactions with the novelty that model parameters are estimated  
406 via penalized iterative re-weighted least squares. We believe this has two main advantages with  
407 respect to using linear programming methods; first, it is a more intuitive way of thinking about  
408 parameter estimation for those familiar with classic regression and least squares estimation.  
409 Second, this regression-like framework can be easily extended to incorporate covariates or to  
410 build more complex models, e.g. varying coefficient models. Further, estimating such a complex  
411 model is not possible using the classical quantile regression approach as currently implemented in  
412 the R package `quantreg`, where neither smooth functions depending on more than two covariates  
413 nor periodicity constraints can be included in the model. For a simpler spatio-temporal model  
414 with no interaction terms, results from a simulation study showed that our proposed method  
415 outperforms the standard quantile regression approach.

416 The focus of this work is on extreme values and hence we have only considered modelling  
417 single quantiles high up in the tail of the distribution (e.g. 90<sup>th</sup>, 95<sup>th</sup> quantile) separately. Even  
418 though the modelling approach used here does not allow fitting various quantiles simultaneously,  
419 it is easy to implement and therefore can be fitted for a range of quantiles independently to  
420 investigate, for instance, how the spatial distribution of extreme values changes with respect to  
421 the mean. Nevertheless, the issue of quantile crossing was not investigated and is left for further  
422 research. Schnabel and Eilers (2013) proposed the so-called “quantile sheets” to estimate a  
423 range of quantiles simultaneously by means of a bivariate smooth function of a covariate and the  
424 probability  $\tau$  using P-splines; non-crossing of quantile curves is ensured by forcing monotonicity  
425 in the  $\tau$  direction in the penalty. Finally, assessing goodness of fit for quantile models remains  
426 an area of open research; usual indices of performance such as the root mean square error or the  
427 correlation coefficient between observed and predicted values are of no use here. In this paper,  
428 goodness of fit was informally assessed based on the expected and observed proportion of positive  
429 and negative residuals. For linear quantile regression models, an equivalent to the coefficient of  
430 determination  $R^2$  was proposed by Koenker and Machado (1999).

431 The proposed model was applied to a set of Scottish rivers spanning 18 years of data. In

432 Scotland, studies assessing changes in extreme river flows have been carried out mostly in the time  
433 domain. Spatially, differences in frequency and magnitude of river flow extreme events have been  
434 found between the East and the West (Black and Burns, 2002; Black, 1996), as well as in trends  
435 in annual maxima series (Black, 1996). In particular, two ‘micro-climates’ have been identified  
436 over 1980-2000, wetter in the North-West, with significant spring and autumn increases in the  
437 West and winter increases in the North, and drier in the South-East, especially in the summer  
438 months (Jenkins et al., 2009; Werritty, 2002). Even though we only have data for years 1996-2000  
439 within the time frame 1980-2000, our results (partially shown in Figure 6) also support a clear  
440 East/West gradient in the 95<sup>th</sup> quantile. Downscaled projections from global circulation models  
441 for the 2050s predict that observed trends are to continue in the near future (Fowler and Wilby,  
442 2010; Werritty, 2002); however, while estimates over the winter months are fairly reliable there is  
443 great uncertainty over the summer. Regional climate models predict increases in winter extreme  
444 rainfall (Fowler and Kilsby, 2003) and an increase of annual runoff of 5-15% across the country  
445 for the 2050s but that could locally exceed 25% (Werritty, 2002). Given the uncertainty of the  
446 predictions and the heterogeneity of the observed changes over time and space, it is important to  
447 gain a better understanding of the spatio-temporal pattern of extreme river flows and we believe  
448 that the model proposed in this paper could prove useful in doing so. Given the observed and  
449 projected seasonal differences in river flow, it is common practice to divide the year into seasons  
450 to then model each season independently, see e.g. Hannaford and Buys (2012), where seasonal  
451 quantiles were calculated to investigate the presence of trends in the quantiles. Our approach  
452 avoids this division of the years into seasons, for which there is no general agreement (and hence  
453 a different division of the year may yield different results) and which may be changing due to  
454 climate change, and directly models the quantile of interest across time so that the temporal  
455 evolution of the spatial trend in extremes can be assessed.

456 Since estimates of flood risk derived from river flow data are usually based on relatively short  
457 records, the current procedure recommends adding a safety margin of 20% of the expected flow  
458 level to ensure that design infrastructure (e.g. flood barriers) can cope with an unexpected

459 extreme flow (HM Government, 2016). On the other side, after the 2007 UK floods (Pitt, 2008),  
460 action was taken and the plan was to lower the threshold at which alarms were issued. The results  
461 from the Scottish data presented in this paper suggest that neither of these adjustments may  
462 be sufficient to provide accurate flood warning as trends for high quantiles have not changed in  
463 a homogeneous way spatially. These spatial differences have potentially important implications  
464 for decision making, where optimizing the balance between expenditure and risk reduction is a  
465 critical part of the decision process.

466 Additional information and supporting material for this article is available online at the  
467 journal's website.

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River	Catchment area (km <sup>2</sup> )	Max elevation (mAOD)	Mean flow (m <sup>3</sup> /s)	Q95 <sup>a</sup> (m <sup>3</sup> /s)	Q99 <sup>b</sup> (m <sup>3</sup> /s)	mean flow/catchment area
Inver	137.5	1108.6	8.182	20.500	28.852	0.060
Clyde	1903.1	745.2	49.362	159.710	263.334	0.026
Carron	122.3	561.9	3.664	13.821	28.569	0.030
Deveron	954.9	754.2	18.605	50.921	107.931	0.019

<sup>a</sup> 95th quantile of river flow, <sup>b</sup> 99th quantile of river flow

Table 1: Main characteristics of rivers Inver, Clyde, Carron and Deveron.

Scenario	Time	Space	n	SNR	
				2	4
A	5 years	20 locations	36500	A2	A4
B	10 years	20 locations	73000	B2	B4
C	5 years	50 locations	91250	C2	C4
D	10 years	50 locations	182500	D2	D4

Table 2: Scenarios considered in the simulation study.