

- This draft version of the article (to be submitted to Environmental Modelling & Software) is provided to accompany the talk given at the RSS conference 2023
- The user guide will be provided in due course (end of Section 1)
- The location of the GitHub repository will be provided in due course (reference to Towe et al. 2023)

Highlights

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- Generalised Pareto marginal models of peaks over threshold are estimated, using a piecewise-constant representation for the variation of GP threshold and scale parameters on the (potentially multidimensional) covariate domain of interest.
- The conditional variation of one or more associated variates, given a large value of a single conditioning variate, is described using the conditional extremes model of Heffernan and Tawn, the slope term of which is also assumed to vary in a piecewise constant manner with covariates.
- Optimal smoothness of marginal and conditional extreme value model parameters with respect to covariates is estimated using cross-validated roughness-penalised maximum likelihood estimation.
- Estimates of environmental contours using various schemes, including the direct sampling approach of Huseby et al. 2013, are calculated by simulation or numerical integration under fitted models.
- Multiple models are estimated for plausible selections of marginal and dependent thresholds, and for bootstrap resamples of the original data, to provide uncertainty quantification.

covXtreme : MATLAB software for non-stationary penalised piecewise constant marginal and conditional extreme value models

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ABSTRACT


The covXtreme software provides functionality for estimation of marginal and conditional extreme value models, non-stationary with respect to covariates, and environmental design contours. Generalised Pareto (GP) marginal models of peaks over threshold are estimated, using a piecewise-constant representation for the variation of GP threshold and scale parameters on the (potentially multidimensional) covariate domain of interest. The conditional variation of one or more associated variates, given a large value of a single conditioning variate, is described using the conditional extremes model of Heffernan and Tawn (2004, HT), the slope term of which is also assumed to vary in a piecewise constant manner with covariates. Optimal smoothness of marginal and conditional extreme value model parameters with respect to covariates is estimated using cross-validated roughness-penalised maximum likelihood estimation. Uncertainties in model parameter estimates due to marginal and conditional extreme value threshold choice, and sample size, are quantified using a bootstrap resampling scheme. Estimates of environmental contours using various schemes, including the direct sampling approach of Huseby et al. 2013, are calculated by simulation or numerical integration under fitted models. The software was developed in MATLAB for metocean applications, but is applicable generally to multivariate samples of peaks over threshold. The software can be downloaded from GitHub, with an accompanying user guide.

1. Introduction

Reasonable estimation of the characteristics of extreme environments is essential to quantify natural hazards, and assure the reliability and safe operability of man-made infrastructure. For example, the extreme ocean environment can be thought of as a multivariate random process in space and time, describing interacting wind, wave, current, tide and surge phenomena. Accurate theoretical modelling of *extremes* from the ocean environment is problematic, because of the complexity of the numerical calculations involved. Practical risk assessment for marine and coastal structures and operations therefore typically requires the development of a statistical model from observational data for the joint behaviour of multiple meteorological-oceanographic (“metocean”) variables.

Physical intuition and previous work has demonstrated that the marginal distribution of a variable such as ocean storm severity (quantified in terms of significant wave height, H_S) is dependent on covariates such as the direction in which the storm evolves, and the time of year in which the storm occurs (e.g. Randell, Turnbull, Ewans and Jonathan 2016). Over the long term, there is evidence that storm severity also evolves slowly in time due to anthropogenic climate change as well as natural climate cycles (e.g. Ewans and Jonathan 2023). It is important therefore that any statistical model for the extreme environment captures covariate non-stationarity. The nature and extent of covariate dependence varies across metocean variables. Experience also suggests that it is reasonable to assume that typical metocean variables are drawn from so-called “max-stable” distributions (e.g. Coles 2001). Therefore, typically conditional on covariates, the conditional distribution of threshold exceedances will be well approximated by the generalised Pareto (GP) distribution, provided that the threshold level is sufficiently high. This suggests that the marginal characteristics of metocean variables can be described reasonably using a non-stationary GP model (e.g. Davison and Smith

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1990, Chavez-Demoulin and Davison (2005), Randell et al. (2016)).

In addition we require that the statistical model also describes the *joint* tail of all metocean variables in general. However the nature of extremal dependence between different metocean variables is generally unknown. The specification of the statistical model therefore needs to be sufficiently general to admit different extents of extremal dependence, the specifics of which are then estimated by fitting the model to data. The conditional extremes model of Heffernan and Tawn (2004) is an attractive candidate, because it admits different classes of extremal dependence, it has a simple form and is relatively easily interpretable. There is evidence that the nature and extent of extremal dependence also varies systematically with covariates (e.g. Jonathan, Ewans and Randell 2013, Ross, Sam, Randell, Feld and Jonathan 2018, Shooter, Ross, Ribal, Young and Jonathan 2021).

The sizes of data samples available (e.g. from direct observation of the environment) for modelling are typically small relative to the time-scales of the inference task. For example, in engineering design we typically need to characterise events which occur on average once in 1,000 or 10,000 years based on a sample of at most the order of 100 years of observation. In these circumstances, our estimate of the joint tail of the distribution of metocean variables is typically uncertain. It is critical that this uncertainty is captured and incorporated appropriately in our hazard assessment.

For individual metocean variables, the size of a rare occurrence is often quantified in terms of a *return value* associated with some return period N (=1000 years, say). The return value is defined straightforwardly as the quantile of the distribution of the annual maximum of the metocean variable with exceedance probability $1/N$, or (for large N , see Jonathan, Randell, Wadsworth and Tawn 2021) the quantile of the distribution of the N -year maximum with non-exceedance probability $\exp(-1)$. In engineering design, the joint tail of the distribution of two (or sometimes three) metocean variables is often quantified in terms of an *environmental design contour*; points on the contour are “equally rare” with respect to some criterion, related to the joint cumulative distribution function or density of the variables (e.g. Ross, Astrup, Bitner-Gregersen, Bunn, Feld, Gouldby, Huseby, Liu, Randell, Vanem and Jonathan 2020, Haselsteiner, Coe, Manuel, Chai, Leira, Clarindo, Guedes Soares, Hannesdóttir, Dimitrov, Sander, Ohlendorf, Thoben, de Hauteclouque, Mackay, Jonathan, Qiao, Myers, Rode, Hildebrandt, Schmidt, Vanem and Huseby 2021)). Therefore estimates for the distribution of the annual maximum or that of the N -year maximum for individual metocean variables, and environmental contours for pairs or triplets of variables, are key outputs from the statistical analysis.

There are many software tools available for applied extreme value analysis; Stephenson and Gilleland (2006), Gilleland, Ribatet and Stephenson (2012), Gilleland (2016) and Belzile, Dutang, Northrop and Opitz (2023) provide reviews. The discussion of Belzile et al. (2023) notes the lack of good “off the shelf” software for practitioners, particularly incorporating more recent advances in methodology. Some software has been published for environmental contour estimation (e.g. Haselsteiner, Lehmkuhl, Pape, Windmeier and Thoben 2019). The purpose of the covXtreme software introduced here is to provide the environmental practitioner with a straightforward means to estimate marginal and joint tails of distributions of random variables, and quantify extremes in terms of return values and environmental design contours. covXtreme accommodates covariate non-stationarity in both marginal and dependence behaviour, provides flexibility in estimating extremal dependence, and careful uncertainty quantification in inferences.

The sophistication of the methodology underpinning covXtreme has been set deliberately, based on the authors’ experience of metocean applications, to accommodate necessary complexity in a pragmatic manner, whilst avoiding unnecessary complexity. Extreme value analysis is in some senses a less mature research area (e.g. Davison and Huser 2015) with numerous pressing challenges. For example, there are many approaches to modelling non-stationary marginal extremes; the work of Biller (2000), Wood (2004), Brezger and Lang (2006), Huser and Genton (2016), Wood, Pya and Safken (2016), Wood, Li, Shaddick and Augustin (2017), Youngman (2019), Youngman (2020), Shao, Hazra, Richards and Huser (2022) provide examples. With sufficiently rich data, complex extreme value models can be well estimated. However, in practice, typical samples tend only to support the adoption of relatively simple covariate models; for example, Zanini, Eastoe, Jones, Randell and Jonathan (2020) show that a simple piecewise constant covariate representation (used by covXtreme) provides marginal inferences competitive with those from more sophisticated P-spline (e.g. Eilers and Marx 2010) and Bayesian adaptive regression spline models (e.g. Biller 2000) for a metocean application.

An early version of the covXtreme software was published alongside Ross et al. (2018) for modelling of storm surge, and Ross et al. (2020) for estimation of environmental contours. Bore, Amdahl and Kristiansen (2019) suggest that covXtreme is useful for analysis of extreme ocean current profiles with depth. Vanem, Guo, Ross and Jonathan (2020) using covXtreme to compare different contour methods with response-based methods for extreme ship response analysis. Guerrero, Huser and Ombao (2023) have used their enhancement of an earlier version of covXtreme for analysis of electrical signals in the human brain. The software has motivated the development of analogous prototype

software PPL for marginal extreme value modelling with penalised piecewise-linear covariate representations (Barlow, Mackay, Eastoe and Jonathan 2023). The software has also been used as a pre-processor for transformation of data to standard marginal scale, allowing joint and conditional extreme value analysis (e.g. Shooter et al. 2021; Shooter, Ross, Ribal, Young and Jonathan 2022), and in metocean consultancy work.

Objectives and layout of article

The objective of the current article is to provide motivation and description of the covXtreme software, and illustrations of its use in the development of design conditions for ocean engineering. The layout of the article is as follows. Section 2 provides an overview of the software and the statistical methodology on which it is based. Sections 3 and 4 present case studies, involving a bivariate response and single covariate (Section 3), and trivariate response with 2-D covariate (Section 4). An accompanying user guide will be made available in due course, providing a detailed step-by-step description of developing a covXtreme model for ocean engineering data sets provided with the software.

2. Overview of software and statistical methodology

covXtreme provides simple software for multivariate non-stationary extreme value analysis of peaks over threshold. The modelling framework of covXtreme (a) is statistically straightforward to understand and use without sacrificing rigour, (b) is computationally efficient, (c) provides good estimation of key quantities of interest to the extreme value practitioner, and (d) provides realistic quantification of modelling uncertainties.

Extreme value analysis of peaks over threshold of metocean (meteorological-oceanographic) variables requires the satisfactory completion of a number of analysis steps. Inference typically involves using a sample of time-series data for a number of variables (corresponding to some period P years of observation) as the basis for estimating the characteristics of extreme environments. These might include return values, associated values (e.g. Towe, Randell, Kensler, Feld and Jonathan (2023a)) and design contours (e.g. Haselsteiner et al. 2021) corresponding to a return period of T years, $T \gg P$. For reasonable extreme value inference of a single variable (such as significant wave height), key features of the data must be accommodated carefully in the analysis, including the serial correlation of time-series, the dependence of values of metocean variables on covariates such as direction and season. Appropriate model forms for tails of distributions should also be adopted. For peaks over threshold analysis of a single variable, choice of threshold level can be source of considerable uncertainty. Moreover, different metocean variables (such as wind speed and significant wave height) are likely to be intercorrelated, and the nature of this dependence must be characterised carefully especially for *extremes* of one or more variables, using appropriate model forms; in these models, choice of threshold is again not always straightforward. Further, since samples of peaks over threshold are generally small (e.g. for high thresholds), it is critical to quantify uncertainty in return values and associated extremal quantities thoroughly using well-understood estimators.

The structure of the covXtreme software is written to reflect the sequential nature of practical extreme value analysis, as a set of MATLAB functions (see Section 2.6). For a given application, these are executed sequentially, leading the user through the inference, addressing important analysis considerations in order. A typical analysis stage involves the specification of tuning parameters, the appropriate choice of which is informed by diagnostic information generated at that stage; generally it will therefore be necessary to repeat the analysis stage until satisfactory diagnostics are achieved, before moving on to the next analysis stage.

Given a sample of multivariate time-series of metocean variables, a typical analysis would proceed as described below. Note, for ease of reference, that subsection numbering 2.1-2.5 here corresponds to the numbering of stages 1-5 of the analysis procedure, and also to the numbering of sections in the covXtreme user guide.

2.1. Data preparation

The main aspect of data preparation is the isolation of storm peak events. Storm peak events correspond to peaks over threshold for a dominant variable (e.g. significant wave height for a wave-dominated metocean application), *associated* values of all other variables of interest (e.g. wind speed) per event, and storm peak covariate values for all relevant covariates (e.g. direction and season). Storm peak events are isolated using the procedure described by Ewans and Jonathan (2008), and discussed in Section 1 of the covXtreme user guide. Storm peak events are then assumed to be conditionally independent given (storm peak) covariates.

Mathematically, consider a sample $\check{Y}_1(t_i), \check{Y}_2(t_i), \dots, \check{Y}_D(t_i)$ of multivariate time-series for D metocean variables observed at regularly-spaced time points t_i , $i = 1, 2, 3, \dots$ over some period. Data preparation requires the isolation

of a sample $\{\dot{y}_{i1}, \dot{y}_{i2}, \dots, \dot{y}_{iD}\}_{i=1}^N$ of N storm peak events (by convention for the first variable) and associated events (for the remaining variables) summarising the peak characteristics of each of N storms observed, and corresponding storm peak covariate values $\{x_{i1}, x_{i2}, \dots, x_{iC}\}_{i=1}^N$ for C storm peak covariates X_1, X_2, \dots, X_C defined on some domain \mathcal{X} . Storm peak and associated values are taken to be conditionally-independent given covariates, in the sense that \dot{y}_{id} can be viewed as an independent draw from $\dot{Y}_d | (X_1 = x_{i1}, X_2 = x_{i2}, \dots, X_C = x_{iC})$, for $i = 1, 2, \dots, N, d = 1, 2, \dots, D$.

2.2. Specification of covariate bins

covXtreme adopts a piecewise-constant parameterisation for the distribution of peaks over threshold on a partition of the covariate domain comprised of elements referred to as ‘‘covariate bins’’. Covariate bins are not estimated as part of the analysis, but must be specified carefully by the user prior to the analysis, for reasonable inference. Briefly, the user is required to partition the domain of each covariate (independently) into a set of intervals. The resulting covariate bins over all covariates are then simply Cartesian products of these intervals. covXtreme assumes, *within* a given covariate bin, that the statistical properties of a storm peak or associated variable are no longer dependent on covariates. Diagnostic plots illustrating features such as the variation of storm peak and associated variables with individual covariates, are provided to inform reasonable choice of marginal partitions. Illustrations of the specification of covariate bins are given in Section 2 of the covXtreme user guide.

Mathematically, each observation $\dot{y}_{i1}, \dot{y}_{i2}, \dots, \dot{y}_{iD}$ is allocated to one of B covariate bins by means of an allocation vector A , with $A(i) = b$ mapping observation (with index) i to bin (with index $B = b$), $i = 1, 2, \dots, N, b = 1, 2, \dots, B$. All observations within a specified covariate bin are assumed to have common extreme value characteristics, specified in terms of the parameters of the marginal model for peaks over threshold from that bin for each of the D components of the observation. Hence in particular, all threshold exceedances of storm peak variable \dot{Y}_d , $d = 1, 2, \dots, D$ from covariate bin b can be viewed as independent draws from a generalised Pareto distribution with common shape, scale and threshold parameter values.

2.3. Marginal modelling

A two-stage modelling procedure is used to describe the marginal distribution of storm peak and associated variables. First a three-parameter gamma distribution is fitted independently to all the data for each covariate bin in turn, providing a good description of the bulk of the distribution of storm peak and associated variables on the covariate domain. The extreme value threshold for each covariate bin is then set to the quantile of the corresponding gamma distribution with pre-specified non-exceedance probability. Finally the distribution of threshold exceedances per covariate bin is estimated using a non-stationary generalised Pareto distribution. Since generalised Pareto shape parameter is typically more difficult to estimate than scale, its value is assumed fixed but unknown across all covariate bins. Moreover, variation of the generalised Pareto scale parameter on the covariate domain is regulated using roughness penalisation, set to maximise the predictive performance of the generalised Pareto model on a hold-out sample within a cross-validation scheme. We judge from prior experience that these assumptions regarding the variation of generalised Pareto parameters are reasonable, and confirm using diagnostics during analysis that the assumptions give reasonably well-fitting models. By reducing the number of degrees of freedom for model fitting, the assumptions are a possible source of estimation bias, but also a reduction in variance in estimated model parameters and return values. Further details and illustrations of marginal modelling are given in Section 3 of the covXtreme user guide.

Mathematically, for each variable \dot{Y}_d , $d = 1, 2, \dots, D$, and covariate bin $B = b$, $b = 1, 2, \dots, B$ independently, we estimate a three-parameter gamma distribution using maximum likelihood estimation with sample likelihood

$$\mathcal{L}_{\text{Gmm}}(\omega_{bd}, \kappa_{bd}, l_{bd}; \{\dot{y}_{id}\}_{i=1}^N) = \prod_{i: A(i)=b} f_{\text{Gmm}}(\dot{y}_{id}; \omega_{bd}, \kappa_{bd}, l_{bd})$$

for sample $\{\dot{y}_{id}\}_{i=1}^N$, where f_{Gmm} is the density of the gamma distribution with shape $\omega_{bd} \in \mathbb{R}$, scale $\kappa_{bd} > 0$ and location $l_{bd} \in \mathbb{R}$ given by

$$f_{\text{Gmm}}(\dot{y}_{id}; \omega_{bd}, \kappa_{bd}, l_{bd}) = (\kappa_{bd}^{-\omega_{bd}} / \Gamma(\omega_{bd})) (\dot{y}_{id} - l_{bd})^{\omega_{bd}-1} \exp((\dot{y}_{id} - l_{bd}) / \omega_{bd}).$$

where $\Gamma(\bullet)$ is the gamma function. In practice for fitting the gamma model, the location parameters $\{l_{bd}\}$ are first estimated using a low empirical quantile of the sample per variate per covariate bin, and the remaining shape and scale parameters estimated using likelihood. Next we calculate the extreme value threshold as $\psi_{bd} = F_{\text{Gmm}}(\tau_d; \hat{\omega}_{bd}, \hat{\kappa}_{bd}, \hat{l}_{bd})$ using the estimated gamma parameters, for the pre-specified non-exceedance probability τ_d , where F_{Gmm} is the cumulative distribution function of the gamma distribution. The marginal sample likelihood for threshold exceedances

of ψ_{bd} for variable \dot{Y}_d over all covariate bins can therefore be written

$$\mathcal{L}_{\text{GP}}(\xi_d, \{v_{bd}\}_{b=1}^B; \{\dot{y}_{id}\}_{i=1}^N, \{\psi_{bd}\}_{b=1}^B) = \prod_{b=1}^B \prod_{i: A(i)=b; \dot{y}_{id} > \psi_{bd}(\tau_d)} f_{\text{GP}}(\dot{y}_{id}; \xi_d, v_{bd}, \psi_{bd})$$

where f_{GP} is the density of the generalised Pareto distribution with shape $\xi_d \in \mathbb{R}$ and scale $v_{bd} > 0$ given by

$$f_{\text{GP}}(\dot{y}_{id}; \xi_d, v_{bd}, \psi_{bd}) = (1/v_{bd})[1 + (\xi_d/v_{bd})(\dot{y}_{id} - \psi_{bd})]^{-1/\xi_d - 1}.$$

The corresponding cumulative distribution functions of the gamma and generalised Pareto distributions are

$$F_{\text{Gmm}}(\dot{y}_{id}; \omega_{bd}, \kappa_{bd}, l_{bd}) = (1/\Gamma(\alpha)) \gamma(\omega_{bd}, \kappa_{bd}(\dot{y}_{id} - l_{bd}))$$

where $\gamma(\bullet, \bullet)$ is the lower incomplete gamma function, and

$$F_{\text{GP}}(\dot{y}_{id}; \xi_d, v_{bd}, \psi_{bd}) = 1 - (1 + (\xi_d/v_{bd})(\dot{y}_{id} - \psi_{bd}))^{-1/\xi_d}.$$

Optimal predictive performance for the marginal generalised Pareto model is achieved using roughness-penalisation for the scale parameters $\{v_{bd}\}_{b=1}^B$ across covariate bins. The corresponding penalised negative log likelihood takes the form

$$\begin{aligned} & -\log \mathcal{L}_{\text{GP}}^*(\xi_d, \{v_{bd}\}_{b=1}^B; \{\dot{y}_{id}\}_{i=1}^N, \{\psi_{bd}\}_{b=1}^B) \\ &= -\log \mathcal{L}_{\text{GP}}(\xi_d, \{v_{bd}\}_{b=1}^B; \{\dot{y}_{id}\}_{i=1}^N, \{\psi_{bd}\}_{b=1}^B) + \lambda_d \left(\frac{1}{B} \sum_{b=1}^B v_{bd}^2 - \left[\frac{1}{B} \sum_{b=1}^B v_{bd} \right]^2 \right). \end{aligned} \quad (1)$$

The smoothness penalty λ_d controls the extent to which the generalised Pareto scale varies across covariate bins. Parameters can be estimated to minimise the penalised negative log likelihood for each variable \dot{Y}_d , $d = 1, 2, \dots, D$ in turn for each of a set of pre-specified values for λ_d . The optimal value λ_d° of λ_d is chosen to maximise predictive likelihood for a hold-out sample within a k -fold cross-validation procedure. Gamma parameter estimates per covariate bin, and generalised Pareto parameter estimates evaluated using the full sample for $\lambda_d = \lambda_d^\circ$ are carried forward to subsequent inference.

Since the numbers of parameters in the various marginal models above are relatively small, a simplex search procedure provides a straightforward approach to parameter estimation by minimisation of (penalised) negative log likelihoods.

Threshold selection for extreme value analysis of peaks over threshold is an important consideration (e.g. Northrop and Jonathan 2011, Scarrott and MacDonald 2012, Wadsworth 2016). Within a covXtreme analysis, multiple marginal models based on different random choices of threshold non-exceedance probabilities $\tau_d \in \mathcal{I}_{\tau_d} \subseteq [0, 1)$ are constructed, $d = 1, 2, \dots, D$. The user's task is to specify the interval \mathcal{I}_{τ_d} for each variable \dot{Y}_d . As explained in Section *** of the user guide, this choice is aided by numerous diagnostic plots, including examination of the stability of the estimated value of ξ_d as a function of τ_d .

Uncertainty quantification for marginal inference is performed using a non-parametric bootstrap procedure. The original sample of storm peak and associate values is resampled with replacement. For each variable \dot{Y}_d , $d = 1, 2, \dots, D$, the full marginal extreme value analysis is then repeated using the bootstrap resample together with a new random selection of τ_d . The outcome of the complete marginal inference is then quantified in terms of sets of parameter estimates $(\{\xi_d^r, \{v_{bd}^r, \psi_{bd}^r, \omega_{bd}^r, \kappa_{bd}^r, l_{bd}^r\}_{b=1}^B; \tau_d^r, \lambda_d^\circ\}_{d=1}^D)$ for each of R (typically = 100 or 250) bootstrap resamples (where superscript r indicates an estimate from a resample). Typically, the value of λ_d° estimated using the original sample is adopted for all bootstrap resamples also, although the option to estimate a new optimal roughness coefficient per bootstrap resample is provided.

The **distribution of the T -year maximum event** per covariate bin, and over all covariate bins can then be estimated (or sampled from) under the fitted marginal model. From above, the full marginal model for storm peak or associated variate \dot{Y}_d in covariate bin $B = b$ is

$$\begin{aligned} F_{\text{GmmGP}}(y; \omega_{bd}, \kappa_{bd}, l_{bd}, \xi_d, v_{bd}, \psi_{bd}) &= F_{\text{Gmm}}(y; \omega_{bd}, \kappa_{bd}, l_{bd}) && \text{for } A(i) = b, \dot{y}_{id} \leq \psi_{bd} \\ &= \tau_d + (1 - \tau_d) F_{\text{GP}}(y; \xi_d, v_{bd}, \psi_{bd}) && \text{for } A(i) = b, y > \psi_{bd} \end{aligned} \quad (2)$$

Then under the model, the distribution of a random occurrence of \dot{Y}_d from any covariate bin is

$$F_{\dot{Y}_d}(y; \{\omega_{bd}, \kappa_{bd}, l_{bd}, \nu_{bd}, \psi_{bd}\}_{b=1}^B, \xi_d) = \sum_{b=1}^B p_b F_{\text{GmmGP}}(y; \omega_{bd}, \kappa_{bd}, l_{bd}, \xi_d, \nu_{bd}, \psi_{bd}) \quad (3)$$

where p_b is an empirical estimate of the probability of observing a storm event in covariate bin b . If we further assume that the number N of storms in T -years is Poisson-distributed with mean $T\rho$, where ρ is an empirical estimate for the number of storms per annum, and suppressing parameter dependence for brevity, the distribution of the T -year maximum is simply

$$\begin{aligned} F_{\dot{Y}_d T\text{-year}}(y) &= \sum_{k=0}^{\infty} \mathbb{P}(N = k) F_{\dot{Y}_d}^k(y) = \sum_{k=0}^{\infty} (\exp(-T\rho)(T\rho)^k / k!) F_{\dot{Y}_d}^k(y) \\ &= \exp\left(-T\rho(1 - F_{\dot{Y}_d}(y))\right). \end{aligned} \quad (4)$$

We can use a similar approach to estimate and sample from the distribution of the T -year maximum of \dot{Y}_d for any combination of covariate bins, by restricting the set of covariate bins over which the summation is performed in Equation 3 (and linearly scaling the values of $\{p_b\}$ so that they sum to unity).

2.4. Extremal dependence modelling

Given non-stationary marginal models for storm peak and associated variables, we next seek to describe the nature of the dependence between them for large values of the storm peak variable. This is achieved using the conditional extremes model of [Heffernan and Tawn \(2004\)](#). Under the fitted conditional extremes model, we can then estimate the characteristics of the joint distribution of all associated variables given a large storm peak, and thereby estimate joint environmental design conditions and design contours. The conditional extremes model is specified for sets of variables on a common standard Laplace marginal scale, rather than their original physical scales. For this reason, a necessary first step is to transform the sample of storm peak and associated values to this scale, using the fitted marginal models. Incorporation of covariate effects is generally important for extremal dependence modelling, and these can be accommodated using conditional extremes models of different complexities with respect to covariates. The `covXtreme` software allows any or all parameters of the conditional extremes model to vary with covariates. Nevertheless, experience suggests that the data indicate the need for covariate non-stationarity of just one model parameter (the “linear” parameter, see below) for typical met-ocean applications. We therefore describe this specific model form as a recommended “default” approach below. Further details and illustrations of extremal dependence modelling are given in Section 4 of the `covXtreme` user guide.

Mathematically, `covXtreme` provides a model for the joint conditional tail $(Y_2, Y_3 \dots Y_D | \dot{Y}_1 = y)$ for large y , using an extension of the conditional extremes model of [Heffernan and Tawn \(2004\)](#) on standard Laplace (and optionally, as originally, on standard Gumbel) scale. Inference therefore requires that we transform the storm peak and associate value sample $\{\dot{y}_{i1}, \dot{y}_{i2}, \dots, \dot{y}_{iD}\}_{i=1}^N$ of variables $\{\dot{Y}_1, \dot{Y}_2, \dots, \dot{Y}_D\}$ to the corresponding Laplace scale sample $\{y_{i1}, i2, \dots, y_{iD}\}_{i=1}^N$ for variables $\{Y_1, Y_2, \dots, Y_D\}$.

2.4.1. Marginal transformation to standard Laplace scale

The marginal transformation to standard Laplace scale is achieved using the probability integral transform such that for $i = 1, 2, \dots, N$, $d = 1, 2, \dots, D$, $b = 1, 2, \dots, B$

$$F_{\text{GmmGP}}(\dot{y}_{id}; \omega_{bd}, \kappa_{bd}, l_{bd}, \xi_d, \nu_{bd}, \psi_{bd}) = F_{\text{Lpl}}(y_{id}) \text{ for } A(i) = b$$

where F_{GmmGP} is the marginal cumulative distribution function of storm peak variable \dot{Y}_d , for sets of parameters of marginal gamma and generalised Pareto models from Equation 2, and F_{Lpl} is the cumulative distribution function of the standard Laplace distribution given by $F_{\text{Lpl}}(y) = 0.5y \exp(-|y|)$ for $y \leq 0$ and $= 1 - 0.5y \exp(-|y|)$ otherwise.

2.4.2. Conditional extremes modelling

The Laplace-scale sample $\{y_{i1}, y_{i2}, \dots, y_{iD}\}_{i=1}^N$ from random variables $\{Y_1, Y_2, \dots, Y_D\}$ is next characterised using the conditional extremes model, for values y of the conditioning variate Y_1 above a dependence threshold $\phi(\tilde{\tau}) =$

$F_{Lpl}^{-1}(\tilde{\tau})$, for which the conditional extremes model is assumed to hold, for carefully specified non-exceedance probability $\tilde{\tau}$. For $y > \phi(\tilde{\tau})$, in covariate bin indexed $B = b$, the recommended non-stationary model takes the form

$$(Y_2, Y_3 \dots Y_D) | (Y_1 = y, B = b) = (\alpha_{b2}, \alpha_{b3}, \dots, \alpha_{bD})y + y^{(\beta_2, \beta_3, \dots, \beta_D)} \mathbf{Z} \quad (5)$$

with linear parameters $\alpha_{bd'} \in [-1, 1]$, $d' = 2, 3, \dots, D$ varying across covariate bins, scalar exponent parameters $\beta_{d'} \in [-\infty, 1]$ common to all covariate bins, and residual random variable $\mathbf{Z} = (Z_2, Z_3, \dots, Z_D) \in \mathbb{R}^{D-1}$ whose distribution is unknown.

For estimation of linear and exponent parameters, we assume that each component $Z_{d'}$ of \mathbf{Z} is independently distributed according to

$$Z_{d'} = \mu_{d'} + \sigma_{d'} W_{d'}$$

for mean $\mu_{d'} \in \mathbb{R}$, scale $\sigma_{d'} > 0$ and random variable $W_{d'} \in \mathbb{R}$ following a generalised Gaussian (or delta-Laplace) distribution with zero mean, unit variance and shape $\delta_{d'}$. For general mean m and variance s^2 , the corresponding density f_{GG} is

$$f_{GG}(w; m, s^2, \delta_{d'}) = \frac{\delta_{d'}}{2\kappa(\delta_{d'})s\Gamma(1/\delta_{d'})} \exp \left\{ - \left| \frac{w - m}{\kappa(\delta_{d'})s} \right|^{\delta_{d'}} \right\},$$

where $\kappa(\delta_{d'})^2 = \Gamma(1/\delta_{d'})/\Gamma(3/\delta_{d'})$. The value of $\delta_{d'} \in \{1, 2\}$ is user-specified in `covXtreme`. $\delta_{d'} = 1$ imposes a Laplace distribution (with zero mean and unit variance) on $W_{d'}$, appropriate when the dependence between $Y_{d'}$ and Y_1 is low. $\delta_{d'} = 2$ imposes a standard Gaussian distribution on $W_{d'}$, the original assumption of [Heffernan and Tawn \(2004\)](#) appropriate otherwise. For estimation purposes therefore, from the properties of the generalised Gaussian distribution, $Y_{d'} | (Y_1 = y)$ is assumed to follow a generalised Gaussian distribution with mean $m_{bd'} = \alpha_{bd'}y + \mu_{d'}y^{\beta_{d'}}$ and standard deviation $\zeta_{d'} = y^{\beta_{d'}}\sigma_{d'}$.

The conditional dependence likelihood $\tilde{\mathcal{L}}_{d'}$ for the model $Y_{d'} | (Y_1 = y)$ and $y > \phi(\tilde{\tau})$ can then be written

$$\tilde{\mathcal{L}}_{d'} \left(\{\alpha_{bd'}\}_{b=1}^B, \beta_{d'}, \mu_{d'}, \sigma_{d'}; \{y_{id}\}_{i=1, d=1}^{N, D}, \delta_{d'}, \tilde{\tau} \right) = \prod_{b=1}^B \prod_{\substack{i: b=A(i) \\ y_{i1} > \phi(\tilde{\tau})}} f_{GG} \left(y_{id}; \alpha_{bd'}y_{i1} + \mu_{d'}y_{i1}^{\beta_{d'}}, (y_{i1}^{\beta_{d'}}\sigma_{d'})^2, \delta_{d'} \right).$$

As for marginal models, we regulate the smoothness of $\{\alpha_{bd'}\}_{b=1}^B$ optimally on the covariate domain using a cross-validation procedure, selecting a value $\tilde{\lambda}_{d'}^\circ$ for roughness coefficient $\tilde{\lambda}_{d'}$ in roughness-penalised negative log likelihood

$$\begin{aligned} & -\log \tilde{\mathcal{L}}_{d'}^* \left(\{\alpha_{bd'}\}_{b=1}^B, \beta_{d'}, \mu_{d'}, \sigma_{d'}; \{y_{id}\}_{i=1, d=1}^{N, D}, \delta_{d'}, \tilde{\tau} \right) \\ &= -\log \tilde{\mathcal{L}}_{d'} \left(\{\alpha_{bd'}\}_{b=1}^B, \beta_{d'}, \mu_{d'}, \sigma_{d'}; \{y_{id}\}_{i=1, d=1}^{N, D}, \delta_{d'}, \tilde{\tau} \right) + \tilde{\lambda}_{d'} \left(\frac{1}{B} \sum_{b=1}^B \alpha_{bd'}^2 - \left[\frac{1}{B} \sum_{b=1}^B \alpha_{bd'} \right]^2 \right). \end{aligned} \quad (6)$$

to maximise predictive performance on cross-validation hold-out samples. Further, it is important to confirm reasonable choice of the dependence threshold $\tilde{\tau}$ by inspection of diagnostic plots.

Two algorithms are provided to minimise the penalised negative log likelihood in Equation 6. The default is a Newton-Raphson approach exploiting gradients; the alternative is a simplex search procedure.

Once parameter estimates are available, we represent the distribution of the $(D - 1)$ -dimensional residual random variable \mathbf{Z} using the set $\mathcal{E}_b = \{e_{i'bd'}\}$, for all $d' = 2, 3, \dots, D$, and all $i' = 1, 2, \dots, N$ such that $y_{i'1} > \phi(\tilde{\tau})$, $b = A(i')$, of residuals from the fit per covariate bin, with elements

$$e_{i'bd'} = \left(y_{i'd'} - \hat{\alpha}_{bd'}y_{i'1} - \hat{\mu}_{d'}y_{i'1}^{\hat{\beta}_{d'}} \right) / \left(\hat{\sigma}_{d'}y_{i'1}^{\hat{\beta}_{d'}} \right).$$

During subsequent simulation under the fitted conditional extremes model, these residuals are resampled jointly as $\{e_{i'b2}, e_{i'b3}, \dots, e_{i'bD}\}$, thereby preserving the dependence between them, and hence the dependence between variables $Y_2, Y_3, \dots, Y_D | (Y_1 = y, y > \phi(\tilde{\tau}), B = b)$ per covariate bin. Similarly, simulation below threshold $\phi(\tilde{\tau})$ is achieved simply by resampling from the original Laplace-scale storm peak sample. We note that `covXtreme` also facilitates estimation of variants of this dependence model, for which any number of conditional extremes model parameters α ,

β , μ and σ are allowed to vary between covariate bins, and their overall roughness penalised for good performance by extending the penalty term in Equation 6 to include all “non-stationary” parameters; see Section 4.2 of the user guide. It is also possible to pool estimates of residuals across covariate bins, useful when covariate bins with low occupancy are present.

Uncertainty quantification for extremal dependence inference is performed by extending the bootstrap procedure described in Section 2.3. Conditional extremes models are estimated for each of the bootstrap resamples based on which marginal models were estimated. The combined marginal and conditional extremes analysis therefore produces the set $\{\{\xi_d^r, \{v_{bd}^r, \psi_{bd}^r, \omega_{bd}^r, \kappa_{bd}^r, l_{bd}^r\}_{b=1}^B\}_{d=1}^D, \{\{\alpha_{bd'}^r\}_{b=1}^B, \beta_{d'}^r, \mu_{d'}^r, \sigma_{d'}^r\}_{d'=2}^D, \{\mathcal{E}_b^r\}_{b=1}^B; \{\tau_d^r, \lambda_d^\circ\}_{d=1}^D, \{\tilde{\tau}_{d'}^r, \tilde{\lambda}_{d'}^\circ\}_{d'=2}^D\}$ of parameter estimates and residuals for each of R bootstrap resamples indexed by superscript r . As for marginal modelling, the value of roughness coefficient $\tilde{\lambda}_{d'}^\circ$ is typically estimated using the original sample only, and adopted for all bootstrap resamples also, although the option to estimate a new optimal roughness coefficient per bootstrap resample is provided.

A sampling procedure is used to estimate the **conditional return value** distribution of the associated value for $\dot{Y}_{d'}$ given a T -year maximum event for \dot{Y}_1 per covariate bin, and over unions of covariate bins. The approach combines importance sampling from the marginal T -year maximum distribution of \dot{Y}_1 (exploiting Equation 4) with Monte Carlo sampling under the fitted conditional extremes model, managing transformations between marginal and standard Laplace scales.

2.5. Estimation of design contours

Using the estimated marginal and conditional extremes models, covXtreme allows estimation of quantities such as return values for the dominant variable, associated return values for associated variables, and environmental design contours. Haselsteiner, Ohlendorf, Wosniok and Thoben (2017), Ross et al. (2020) and Haselsteiner et al. (2021) provide recent reviews of contour estimation, encompassing a range of approaches. Algorithms to estimate three types of design contour are implemented in covXtreme. These are (a) constant exceedance contours; (b) direct sampling contours; and (c) conditional extremes (or “HT”, in acknowledgement of the authors of the conditional extremes model, Heffernan and Tawn) constant density contours. Each of the three contour methods estimates a line (in 2-D) or surface (in 3-D) on which certain characteristics of the distributions of $\dot{Y}_2 | (\dot{Y}_1 = y)$ (in 2-D, or $(\dot{Y}_2, \dot{Y}_3) | (\dot{Y}_1 = y)$ in 3-D) for large y are preserved. For example, the constant exceedance contour in 2-D is a line on which the probability of exceedance in an “outward” sense (e.g. $\mathbb{P}(\dot{Y}_1 > \zeta_1, \dot{Y}_2 > \zeta_2)$ in the first quadrant) is constant, for points (ζ_1, ζ_2) on the contour; see Jonathan, Ewans and Flynn (2014) for details. The direct sampling contour of Huseby, Vanem and Natvig (2015) is similar, except that now the probability in the half plane defined by the tangent to the contour at any point of interest is constant, and the contour itself must be convex. In 2-D, the conditional extremes constant density contour defines a line on which the joint density of the pair (\dot{Y}_1, \dot{Y}_2) is constant. By construction, all contours pass through a so-called “lock point”, defined as an extreme quantile (e.g. the T -year return value) of \dot{Y}_1 and the corresponding conditional median of $\dot{Y}_2 | (\dot{Y}_1 = T\text{-year value})$. The lock point defines the value of the distributional characteristic preserved on the contour. Further discussion and illustrations are provided in Section 5 of the covXtreme user guide.

Mathematically, in 2-D, the constant exceedance contour $\zeta(\theta) = (\zeta_1(\theta), \zeta_2(\theta))$ for $\theta \in \Theta \subseteq [0, 360)$ can be defined by the equation

$$\mathbb{P}\left(\bigcap_{d=1}^2 (r_d(\theta)\dot{Y}_d > r_d(\theta)\zeta_d(\theta))\right) = p$$

where $\mathbf{r}^\circ = (r_1^\circ, r_2^\circ)$ is a reference location (see e.g. Jonathan et al. 2014), and $r_d(\theta) = \zeta_d(\theta) - r_d^\circ$, $d = 1, 2$, for some small probability $p > 0$. The direct sampling contour is defined analogously, using the equation

$$\mathbb{P}\left(\left(\dot{\mathbf{Y}} - \zeta(\theta)\right) \cdot \mathbf{n}(\theta)\right) = p$$

where $\dot{\mathbf{Y}} = (\dot{Y}_1, \dot{Y}_2)$ and $\mathbf{n}(\theta)$ is the outward-pointing normal to the contour at θ , relative to \mathbf{r}° . The conditional extremes constant density contour consists of the set of points $\zeta \in \mathbb{R}^2$ for which the joint density $f_{\dot{\mathbf{Y}}}(\zeta) = c$ for some small value $c > 0$. Algorithms for estimation of the three contour types exploit importance sampling (e.g. Section 3.4 of Towe, Zanini, Randell, Feld and Jonathan 2021) for computational efficiency where possible. Contours can be estimated per covariate bin (e.g. as “directional” or “seasonal” contours), or integrated over covariate bins (e.g. to provide “omni” estimates).

The constant exceedance and direct sampling contours are convex curves by definition, in the sense that they enclose a convex region (of \mathbb{R}^2 for 2-D contours), possibly with the help of the coordinate axes. Depending on the nature of the joint density, the conditional extremes constant density “contour” could exist in the form of a set of disjoint curves, some of which may be closed. The constant exceedance and direct sampling contours are invariant to transformations of variables, whereas the conditional extremes constant density contour is not (e.g. Ross et al. 2020).

2.6. Accessing the software, and performing a typical analysis

The covXtreme is available for download from GitHub at Towe, Ross, Randell and Jonathan (2023b). Software is written using MATLAB object-oriented programming. Full specifications of classes, properties and methods are therefore provided, and available for user inspection.

A typical analysis involves executing each of the MATLAB scripts Stage1_PeakPicking, Stage2_SetBinEdges, Stage3_FitMargin (for each variable marginally), Stage4_FitHeffernanTawn and Stage5_Contour in sequence. As explained in detail in the user guide, each stage of the analysis involves the specification of control parameters for that stage. Default values for control parameters are provide, but it is necessary for the user at each stage to confirm that values are appropriate by confirming that diagnostic plots generated have reasonable characteristics. It may be necessary to repeat a given stage multiple times until acceptable diagnostic characteristics are found, before proceeding to the next stage.

Sections 3 and 4 below provide brief descriptions of the application of covXtreme to a pair of random variables (specifically significant wave height and spectra peak period) varying with directional covariate (Sections 3) and to four random variables (significant wave height, spectral peak period, wind speed and overturning moment) varying with 2-D directional-seasonal covariate.

3. Case study : Single covariate, bivariate response

This section outlines to application of covXtreme to estimation of design contours for extreme storm peak significant wave height and associated spectral peak period, both varying with storm direction. The analysis follows the five stages discussed in Section 2. The data correspond to approximately 35 years of time-series output from a hindcast simulator for a location in the northern North Sea.

Following isolation of storm peak significant wave height H_S , associated spectral peak period T_P and storm peak direction using Stage 1, Figure 1 illustrates the output of Stage 2 of the analysis, showing storm peak H_S and associated T_P as a function of the direction from which storms emanate, in degrees clockwise from north. The figure also shows the user-input bin edges at 0° , 20° , 60° , 225° , 270° and 315° , specified so that the variation of H_S and T_P is approximately independent of direction within each bin, but different between bins. Thus e.g. the bin including 45° corresponds to the land shadow of Norway, with resulting low values of storm peak H_S , whereas the bins including 250° and 340° contain large storms from the Atlantic and Norwegian Sea. Figure 2 provides scatter plots of associated T_P on storm peak H_S for each of the six directional bins. The rates of occurrence of storms, and the marginal characteristics of H_S and T_P are clearly different between bins. In directional bin $[225, 270)$, the dependence between T_P and H_S appears to be particularly strong.

Figure 3 illustrates marginal extreme value models for storm peak H_S , the panels describing the variation of the estimates of generalised Pareto scale ν , gamma shape ω and scale κ with direction, in terms of means (solid) and 95% uncertainty bands (dashed) over bootstrap resamples and random choices of marginal threshold non-exceedance probabilities drawn from the interval $[0.7, 0.9]$. The empirical density of corresponding (stationary) estimates of generalised Pareto shape ξ is shown in Figure 9 of the user guide to be a Gaussian-like with a mean at approximately -0.2. The variation of ν and κ with direction appears consistent with expectations given Figures 1 and 2. In particular, given estimated ν , the largest return values for storm peak H_S would be expected to emanate from the Atlantic Ocean and Norwegian Sea. Indeed, inspection of directional maxima for storm peak H_S for return periods of 10 and 100 years in Figure 4 confirms this: the largest contributors to the omni-directional maximum (in black) are the covariate bins corresponding to the Norwegian Sea ($[315, 0)$, magenta) and Atlantic ($[225, 270)$, cyan).

It is critical to assess the diagnostic plots generated by covXtreme to confirm that model fit is adequate. A number of illustrative diagnostic plots corresponding to this case study are shown in the user guide. For the current application, a plot of the predictive negative log likelihood from the cross-validation procedure (see Equation 1) suggests that the optimal choice λ° of roughness penalty lies at around three. The goodness of fit of the marginal model is assessed by examining the stability of the estimate for generalised Pareto shape parameter ξ as a function of extreme value

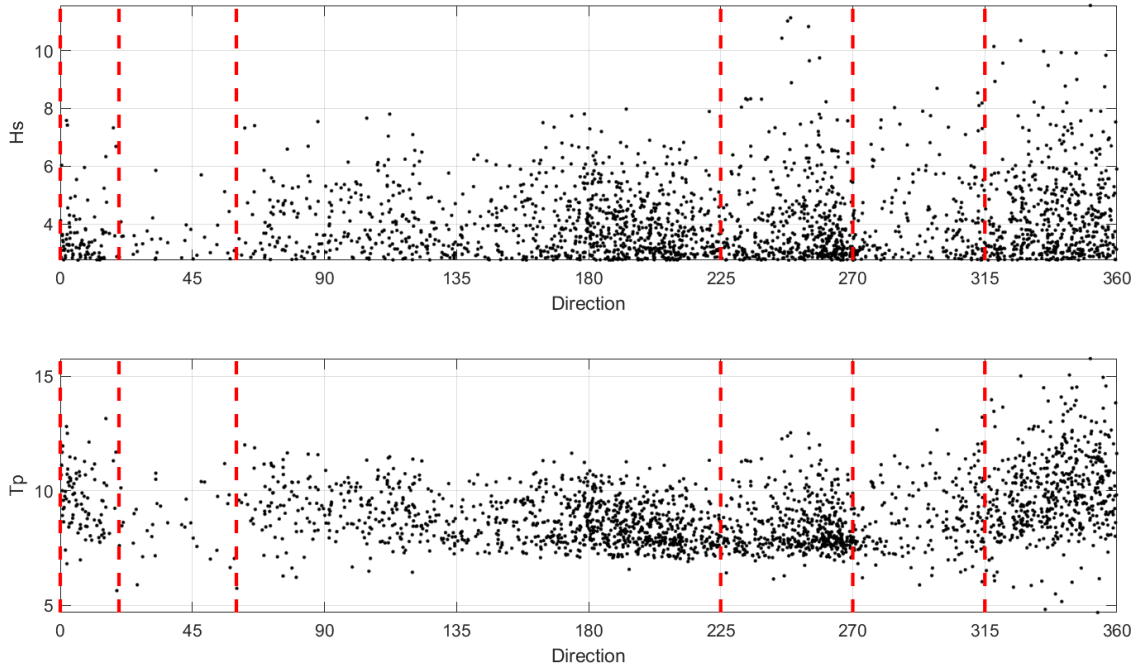


Figure 1: Directional variation of storm peak significant wave height (H_S , top) and associated spectral peak period (T_p , bottom). Also shown are directional bin edges (red) for 6 bins. The variation of H_S and T_p is approximately independent of direction within each bin, but different between bins.

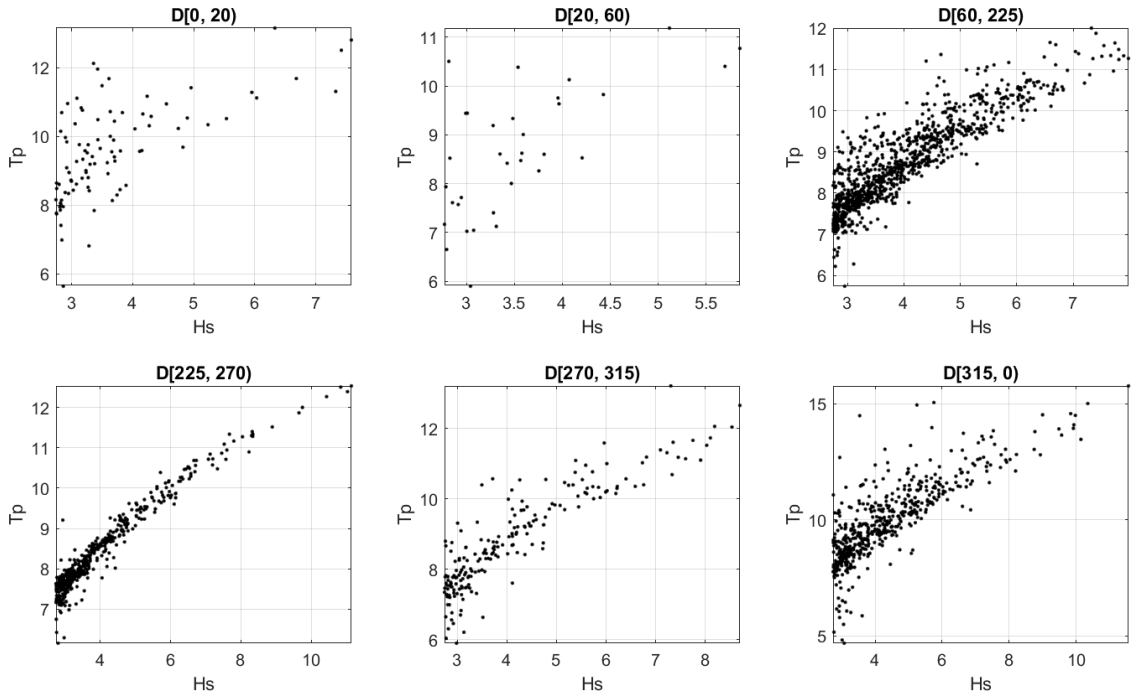


Figure 2: Associated spectral peak period on storm peak significant wave height per directional bin. Panel titles indicate that the covariate is direction “D”, and give the angular interval corresponding to the bin. It is apparent that the dependence between H_S and T_p varies between bins.

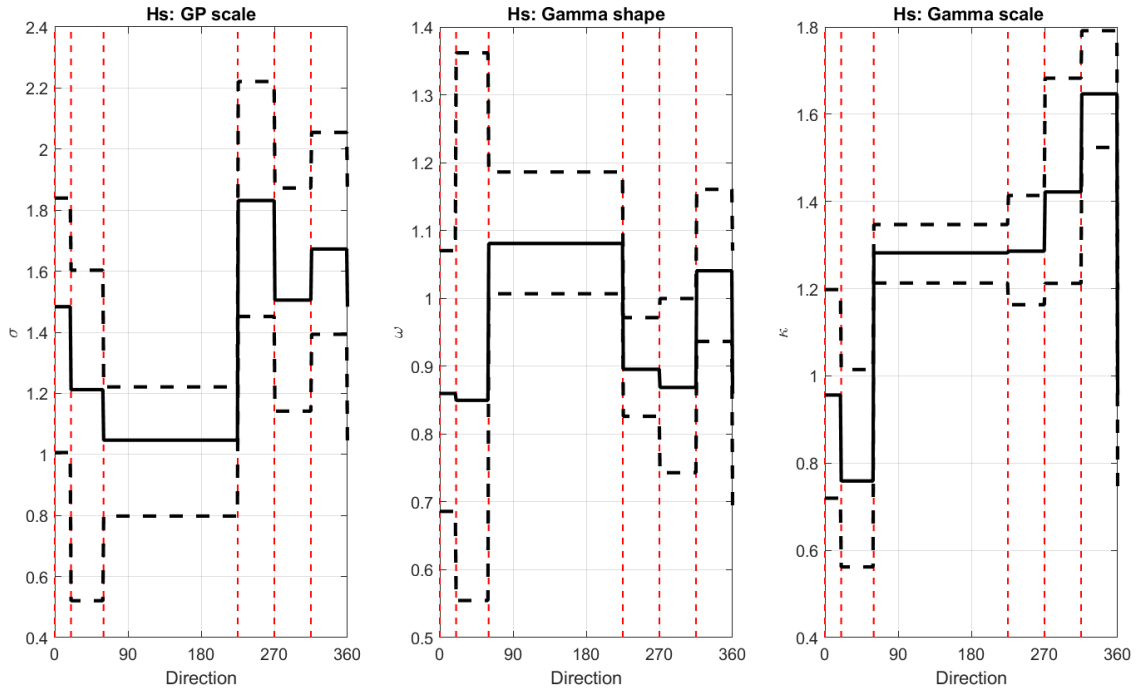


Figure 3: Marginal directional extreme value model for storm peak significant wave height. Variation of parameter estimates for GP scale σ , gamma shape ω and scale κ with direction. Mean estimates in solid black, and bootstrap 95% uncertainty bands in dashed black. Also shown are directional bin edges (red). Directional dependence is particularly clear for σ and κ .

threshold τ . Comparison of empirical tails directly from the sample, with corresponding tails (and their uncertainty) estimates from the extreme value model, per covariate bin and omni-directionally, also suggests the marginal model is reasonable. The corresponding full marginal analysis must also be performed for associated T_P with direction.

Using the marginal models, Figure 5 illustrates parameter estimates for the conditional extremes model for associated T_P given storm peak H_S on standard Laplace margins. The non-stationary estimate for linear parameter α suggests that dependence between the variables is high (near the maximum possible of unity), especially in the covariate bin corresponding to Atlantic storms. The value of exponent parameter β is slightly larger than zero, indicating that the sizes of residuals “ $y^\beta Z$ ” from the conditional extremes model fit (Equation 5) grow very slowly with the conditioning value y on Laplace scale. The empirical densities for residual parameters μ and σ are typical in our experience; unimodal densities, with roughly Gaussian shape.

Diagnostic plots are again assessed to confirm reasonable goodness of fit for the conditional extremes model. For the current application, parameter estimates from α per covariate bin are reasonably stable as a function of dependence threshold $\tilde{\tau}$ on the interval $[0.7, 0.85]$ (see Figure 20 of the User Guide). Further, the distribution of residuals \mathcal{E} from the model fit do not appear to be obviously dependent on the directional covariate (see Figure 18 of the User Guide). The overall distribution of residuals from the model fit (see Figure 17 of the User Guide) is typical; a Gaussian-like density with some positive skew.

We simulate under the fitted models to generate the environmental design contours (see Section 2.5) shown in Figure 6 omni-directionally (i.e. over all directional covariate bins) and Figure 7 per directional bin. The three different contour methods produce estimates which have similar characteristics in terms of describing the “outside” of the data cloud, reflecting the positive dependence between H_S and T_P , and passing through the appropriate lock points. However the methods also use different definitions of the environmental contour; it is not surprising therefore that the contours estimates do not agree fully. The HTDNs contour in particular produces a more variable estimate, especially when sample size is small (e.g. in the $[20,60)$ directional bin in Figure 7). For engineering design, points on the contour with large values of H_S would typically be adopted to test the integrity of models for the offshore or coastal structure of interest.

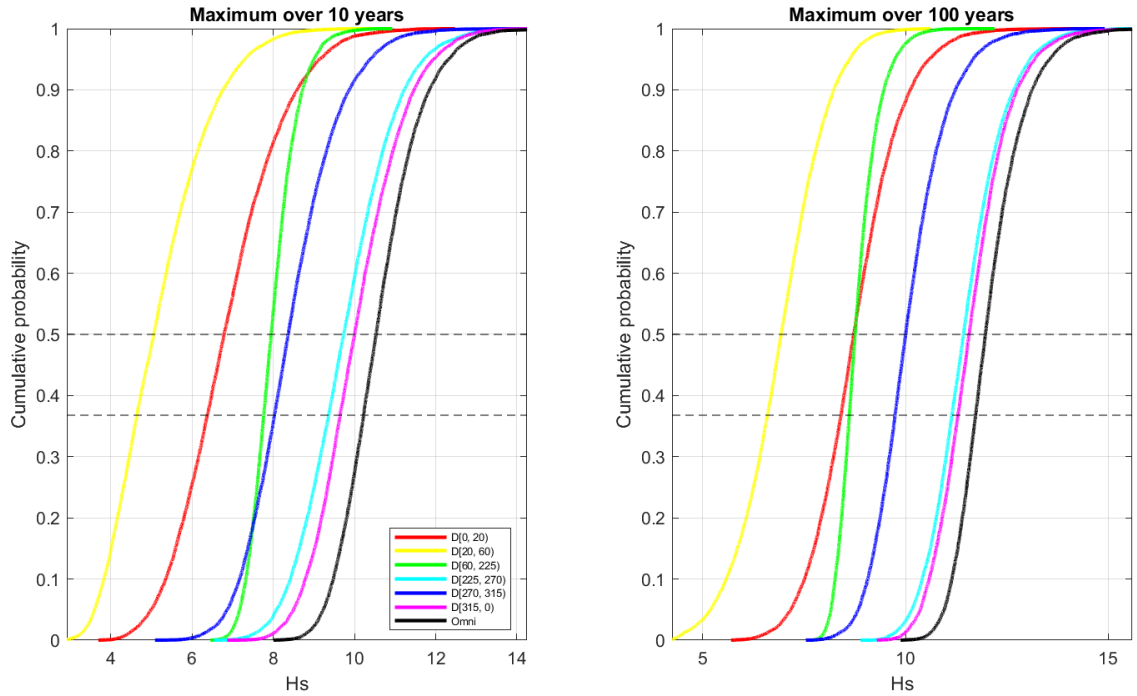


Figure 4: Cumulative distribution functions for the 10-year (left) and 100-year (right) maximum of storm peak significant wave height per directional bin and over all bins (“omni”, black). Horizontal dashed lines drawn at the $\exp(-1)$ quantile and median.

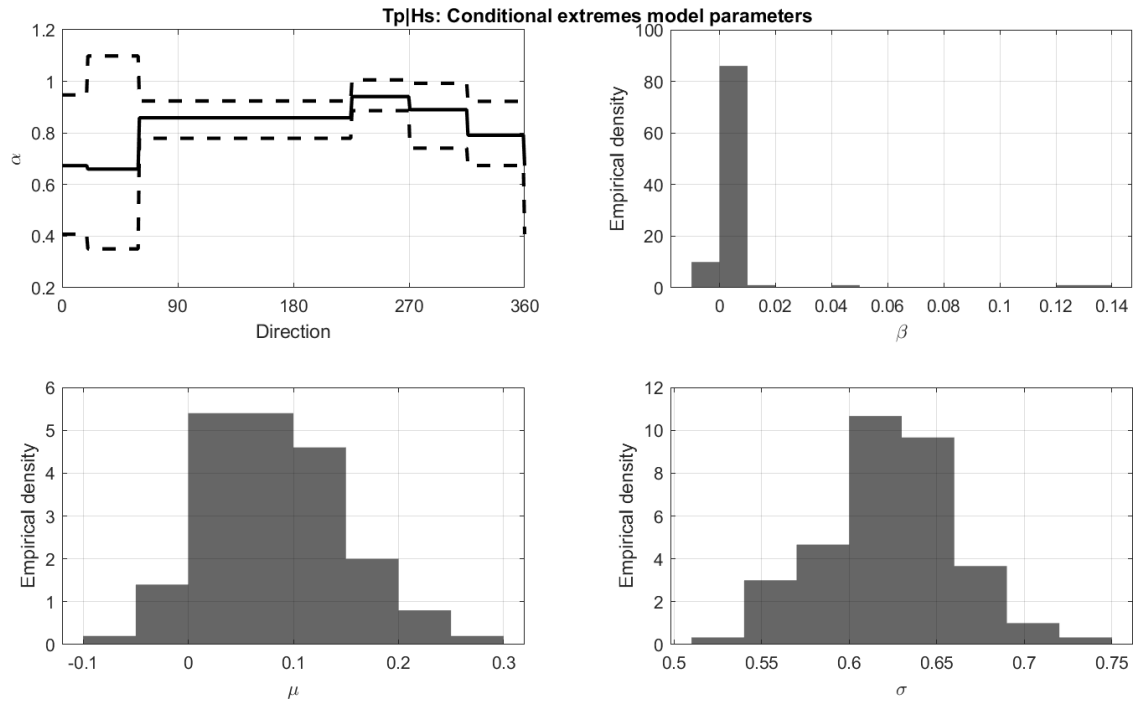


Figure 5: Parameter estimates from the conditional extreme value model for associated peak period given storm peak significant wave height. Top left: directional variation of α summarised as mean and 95% bootstrap uncertainty band; top right: histogram of β ; bottom left: histogram of μ ; bottom right: histogram of σ .

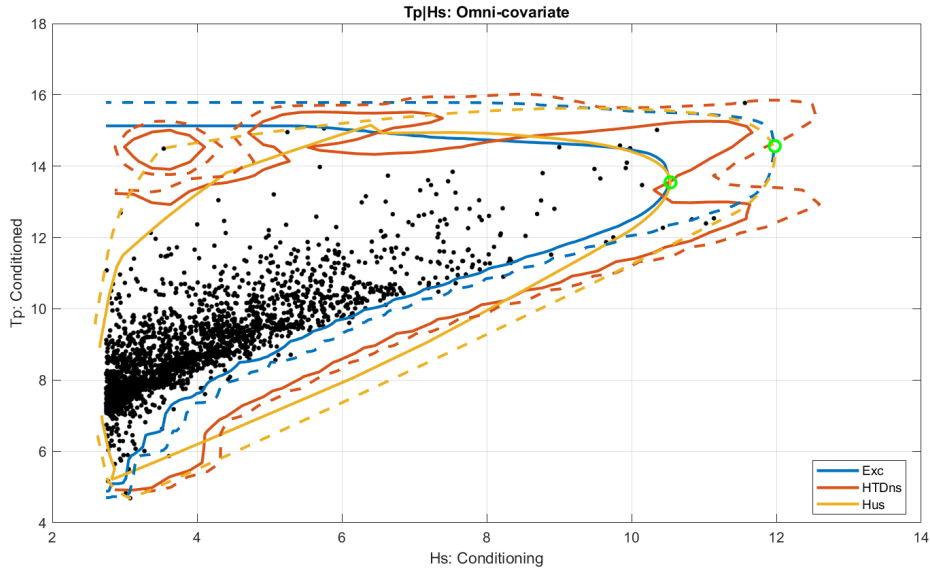


Figure 6: Omni-directional environmental contours of associated peak period and storm peak significant wave height, for 10- and 100-year return values of storm peak significant wave height shown as solid and dashed lines respectively, corresponding to the Exceedance (blue), Heffernan-Tawn density (HTDns, orange) and Huseby (yellow) contours.

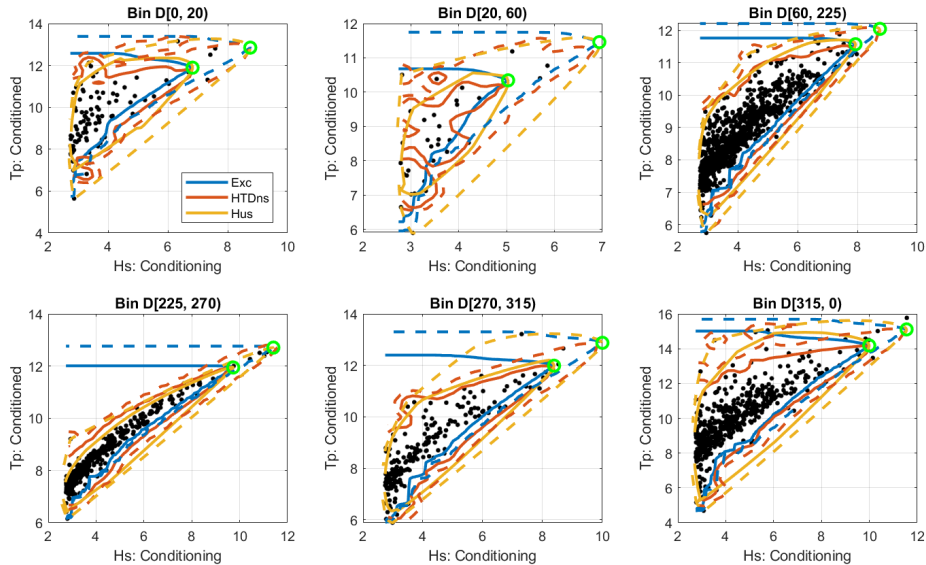


Figure 7: Environmental contours of associated peak period and storm peak significant wave height, for individual directional bins. Contours shows for 10- and 100-year return values of storm peak significant wave height, shown as solid and dashed lines respectively, corresponding to the Exceedance (blue), Heffernan-Tawn density (HTDns, orange) and Huseby (yellow) contours.

4. Case study : 2-D covariate, multivariate response

The second case study is an extension of that reported in Section 3, which incorporates the over-turning moment (OTM) experienced by an offshore structure subjected to wind and wave loading. Specifically, we seek to characterise

the joint distribution of (storm peak) H_S and wind speed (WS) conditional on extreme values of OTM, subject to directional and seasonal covariate effects. The analysis again follows the 5 stages described in Section 2.

Stage 1 of the analysis is isolation of storm peak events from the underlying storm H_S time-series data, following the same procedure as in Section 3. For Stage 2, Figure 8 shows the directional and seasonal variation of the conditioning variates OTM, H_S and WS together with the directional and seasonal bin edges specified. Note that a smaller number of directional bins is used for this case study, to limit the total number of directional-seasonal bins for the analysis. Nevertheless, we are careful to allow for possible directional effects due to storms from the Atlantic Ocean and Norwegian Sea. There are clear directional and seasonal effects present.

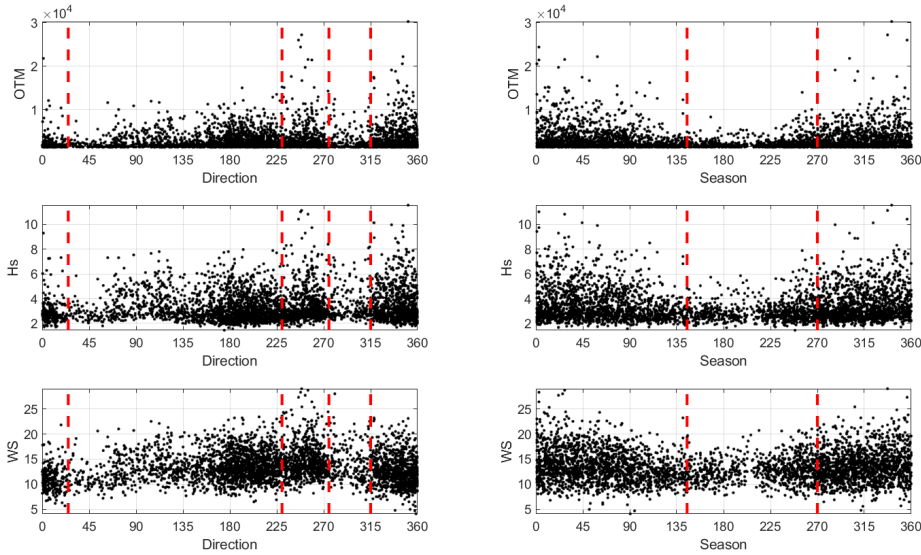


Figure 8: Directional (left) and seasonal (right) variation of overturning moment (OTM, top), storm peak significant wave height (H_S , second row) and associated wind speed (WS, bottom). Also shown are bin edges for four directional bins coupled with two seasonal bins (and hence a total of $8 = 4 \times 2$ directional-seasonal bins). The variation of OTM, H_S and WS is approximately independent of covariates within bins, but different between bins.

The resulting scatter plots of WS on OTM per covariate bin are shown in Figure 9 (and the corresponding plot for H_S on OTM in Figure 28 of the User Guide). Illustrative diagnostic plots for the estimation of marginal models for each of H_S , OTM, and WS with direction and seasonal covariates are given in Figures 30-32 of the User Guide. Marginal model parameters show clear directional and seasonal variation, and comparison of empirical and model-based tails suggest reasonable model fit. The fitted marginal models are then used to estimate the cumulative distribution functions for T -year maxima of interest; estimates for 10- and 100-year maximum of WS are given in Figure 10. Unsurprisingly, the “omni” distribution (estimated over all directional and seasonal bins) is dominated by winter storms from the Atlantic sector, and the 1000-year return value for WS is approximately 28 ms^{-1} .

Following transformation to standard Laplace scale, a non-stationary conditional extremes model is estimated for H_S and WS jointly, conditional on large OTM, given directional and seasonal covariates. Figure 11 gives parameter estimates for WS, showing directional and seasonal dependence of the conditional extremes slope parameter α ; as would be expected perhaps, the dependence between WS and OTM is strongest for winter storms emanating from the North-West. The estimates for index β , common over covariate bins, is somewhat larger than found in Case Study 1. The empirical densities of nuisance parameters μ and σ are approximately Gaussian-shaped. Supporting diagnostic plots for the conditional extremes model fit are given in Figures 33-38 of the User Guide. In particular, Figure 27 indicates that the value of the α parameter is relatively stable for conditional extremes threshold levels $\tilde{\tau} \in [0.8, 0.9]$, and that a minimum roughness penalty for predictive lack of fit is achieved at around 10.

Figure 12 gives estimated conditional return value distributions for H_S and WS given 10-year and 100-year maximum OTM for individual directional-seasonal covariate bins, and “omni” over all covariate bins. For H_S , conditional

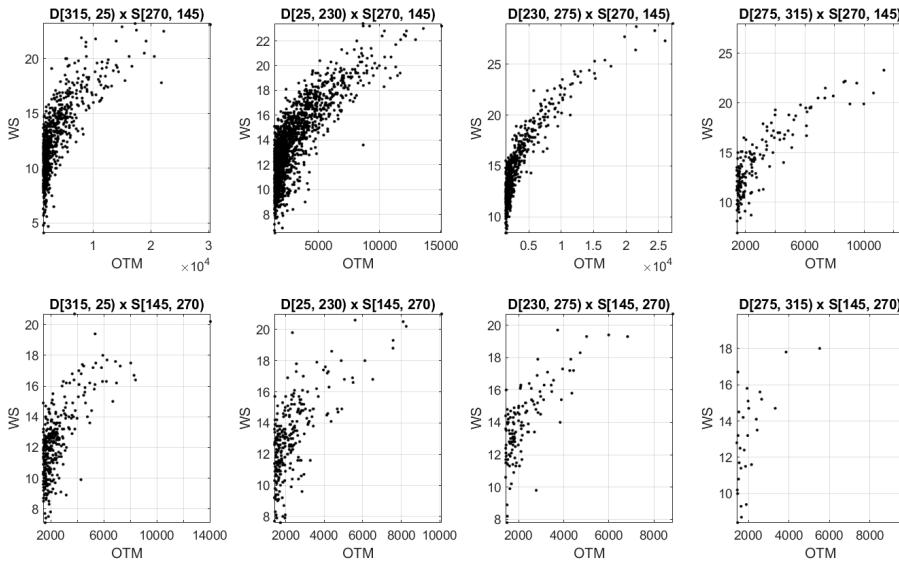


Figure 9: Associated wind speed on storm peak overturning moment per directional-seasonal bin. Panel titles indicate that the angular intervals of direction “D” and season “S” for the bin “D”. It is apparent that the dependence between WS and OTM varies between bins, with obvious non-linearity in some bins. A similar plot is generated for associated significant wave height on storm peak overturning moment.

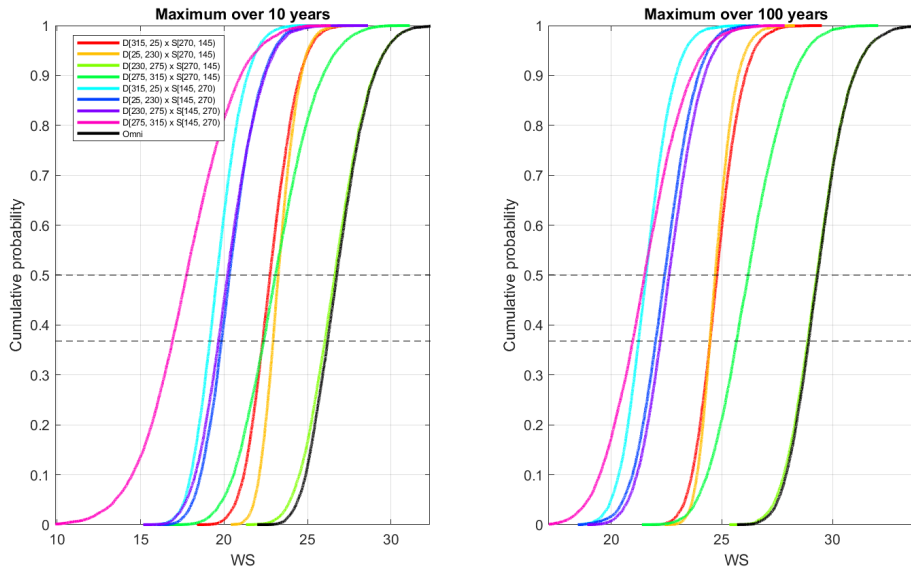


Figure 10: Cumulative distribution functions for the 10-year (left) and 100-year (right) maximum of associated wind speed per covariate bin and over all bins (“omni”, black). Horizontal dashed lines drawn at the $\exp(-1)$ quantile and median.

return values are again largest for Atlantic winter storms. For WS however, we observe an interesting transition involving winter storms from directional sectors [275,315] to [230,275].

The resulting omni-covariate environmental design contours for H_S and WS, given occurrences of the 10-year and 100-year maximum OTM, are shown in Figure 13. The general features of the contours are similar to those of Figure 6. Corresponding illustrative plots of contours per covariate bin for WS are given in Figure 40 of the User Guide.

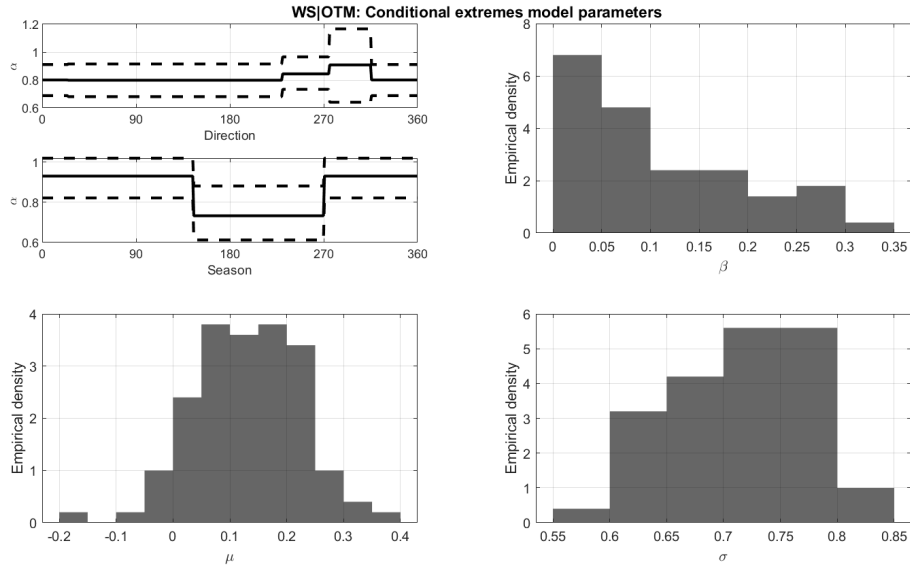


Figure 11: Parameter estimates from the conditional extreme value mode for associated wind speed given storm peak overturning moment. Top left: directional and seasonal variation of α summarised as mean and 95% bootstrap uncertainty band; top right: histogram of β ; bottom left: histogram of μ ; bottom right: histogram of σ . Note the very high directional dependence for α at around 280° .

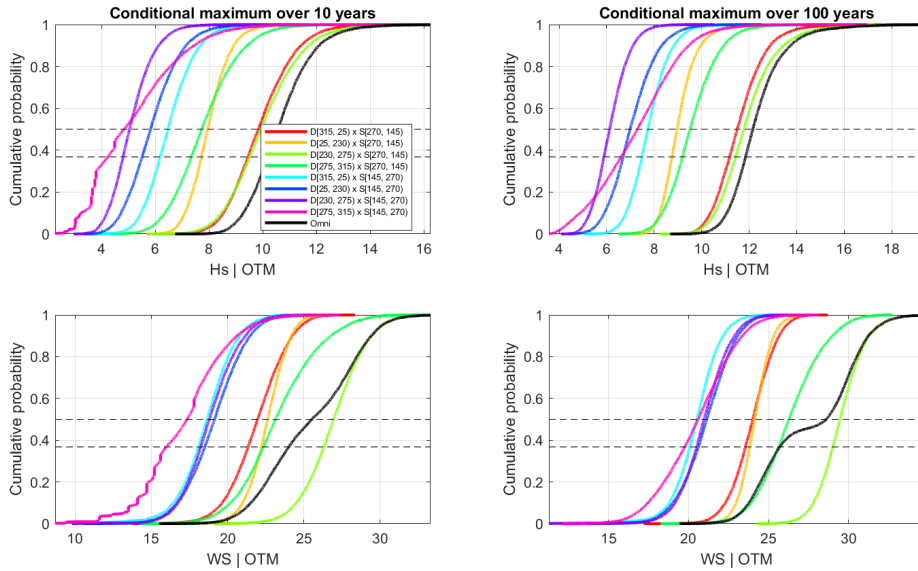


Figure 12: Conditional cumulative distribution functions of associated significant wave height (top) and associated wind speed (bottom) per directional bin and over all bins ("omni", black), conditional on the 10-year (left) and 100-year (right) maximum of storm peak overturning moment. Horizontal dashed lines drawn at the $\exp(-1)$ quantile and median.

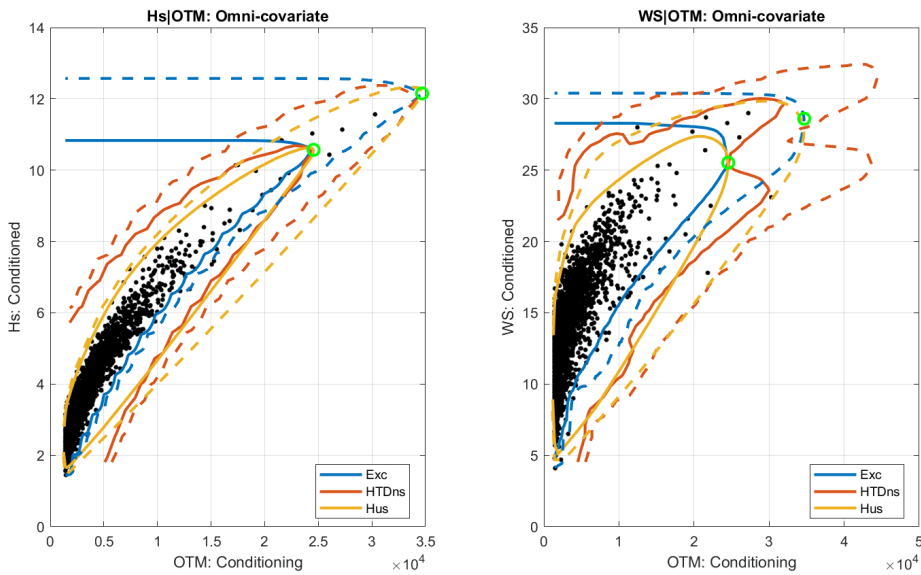


Figure 13: Omni-directional-seasonal environmental contours of associated significant wave height (left) and associated wind speed (right) and storm peak overturning moment. Contours show for 10- and 100-year return values of storm peak significant wave height, shown as solid and dashed lines respectively, corresponding to the Exceedance (blue), Heffernan-Tawn density (HTDns, orange) and Huseby (yellow) contours. Corresponding contours per covariate bin are also generated.

5. Discussion

This article introduces the covXtreme software for pragmatic multivariate extreme value analysis with covariate non-stationarity. The MATLAB software provides functionality to isolate temporal peaks from time-series, and to define an appropriate partition of the covariate domain. Using this partition, marginal generalised Pareto models are estimated for each variate independently assuming piecewise constant threshold and scale parameterisations within a penalised likelihood framework; optimal scale parameter roughness is estimated using cross-validation. Marginal models are then used to transform the sample to standard Laplace margins. A non-stationary conditional extremes model is then estimated with piecewise constant parameterisation for the slope (“ α ”) parameter, again using penalised likelihood estimation with cross-validation to estimate optimal roughness. Simulations and importance sampling are then used to estimate the distribution of T -year maxima for each variate, and environmental design contours conditional on a single conditioning variate. Uncertainty due to marginal and dependence threshold selection is quantified by fitting multiple models with randomly chosen thresholds within user-specified plausible intervals of threshold non-exceedance probability. Uncertainties in parameter estimates and subsequent inferences from model fitting are estimated using bootstrap resampling. As noted in Section 1, the software has already been used in a number of studies, mostly but not exclusively metocean-related.

The covXtreme methodology makes a number of simplifying assumptions, motivated by the authors’ experience of extreme value analysis applied to the ocean environment using a range of methodologies of difference complexities. For example, covXtreme relies on sensible user-specified partitioning of the covariate domain into bins within which it is reasonable to assume common marginal tails and a common dependence structure; this simplifies inference considerably compared with competitor approaches. Moreover, we believe that inferences using covXtreme with good partitioning are competitive with alternatives using more sophisticated tools. Specifically, covXtreme marginally is equivalent to a Voronoi set representation with pre-specified covariate partition, which was demonstrated by Zanini et al. (2020) to be competitive with P-spline and Bayesian adaptive regression spline covariate representations. covXtreme further assumes that the generalised Pareto shape parameter ξ in each marginal model is constant with covariate; because of the relative difficulty of estimating the shape parameter compared with the scale, this would appear reasonable in the absence of strong evidence to the contrary. Likewise, the β , μ and σ parameters of the conditional extremes model are assumed stationary. This appears reasonable since β is a power index and notoriously difficult to estimate. Moreover, μ and σ are essentially nuisance parameters; any model misspecification caused by the assumption of stationarity will be accommodated to some extent by the adoption of residuals from model fitting for inferences under the model. It might be appropriate to relax some of the assumptions for specific applications, for example (a) when there is strong evidence that generalised Pareto ξ is unlikely to be constant (e.g. due to land shadow and fetch limitation effects on H_S), or (2) since parameter estimates for conditional extremes α and μ are highly correlated when β is close to unity.

We anticipate that covXtreme might provide a pragmatic starting point to studies of spatial and temporal dependence of extremes, since the underlying methodology of both conditional spatial extremes (e.g. Shooter, Ross, Tawn and Jonathan 2019, Shooter et al. 2022, Wadsworth and Tawn 2019) and Markov extremal and similar time-series models (e.g. Winter and Tawn 2017, Tendijck, Ross, Randell and Jonathan 2019, Tendijck, Jonathan, Randell and Tawn 2023) involves each of Stages 1-4 of the covXtreme approach.

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