

Flexible covariate representations for extremes

Slides and draft paper at www.lancs.ac.uk/~jonathan

Elena Zanini, Emma Eastoe, Matthew Jones, David Randell, Philip Jonathan Shell & Lancaster University

Copyright of Shell Shell & Lancaster University September 2019 1

Thanks

- Colleagues at Shell: Vadim Anokhin, Graham Feld, Emma Ross
- Colleagues at Lancaster: Jonathan Tawn



Structural damage



Ike, Gulf of Mexico, 2008 (Joe Richard)



North Sea, Winter 2015-16 (The Inertia)

Motivation

- Rational and consistent design and assessment of marine structures
 - Reduce bias and uncertainty in estimation of structural integrity
 - Quantify uncertainty as well as possible
- Non-stationary marginal, conditional, spatial and temporal extremes
 - Multiple locations, multiple variables, time-series
 - Multidimensional covariates
- Improved understanding and communication of risk
 - Incorporation within established engineering design practices
 - Knock-on effects of improved inference

The ocean environment is an amazing thing to study ... especially if you like to combine beautiful physics, measurement and statistical modelling!



Motivation

- Environmental extremes vary smoothly with multidimensional covariates
 - Model parameters are non-stationary
- Environmental extremes exhibit spatial and temporal dependence
 - Characterise these appropriately
- Uncertainty quantification for whole inference
 - Data acquisition (simulator or measurement)
 - Data pre-processing (storm peak identification)
 - Hyper-parameters (extreme value threshold)
 - Model form (marginal measurement scale effect, spatial extremal dependence)
- Statistical and computational efficiency
 - Slick algorithms
 - Parallel computation
 - Bayesian inference



This work

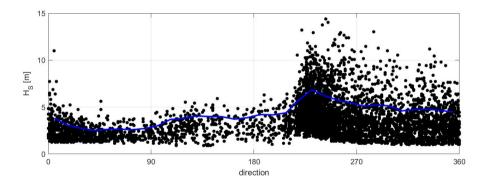
Directional models for storm peak H_S

- Different covariate representations
 - Penalised B-splines (or P-splines)
 - Bayesian adaptive regression splines
 - Voronoi partition
- Generic modelling framework
- Bayesian inference
- Northern North Sea case study as motivation
- Simulation study for comparison
- Focus on the generalised Pareto (GP) inference
- Extensions to multidimensional covariates



Motivating application

Typical data for northern North Sea. Storm peak H_S on direction, with $\tau=0.8$ extreme value threshold.



Model



Observational model

- Sample of peaks *Y* over threshold ψ , with covariates θ
 - \blacksquare θ is 1D in current work : directional
 - \bullet is nD later : e.g. 4D spatio-directional-seasonal
- **E**xtreme value threshold ψ assumed known
 - **E**stimated as the $\tau = 0.8$ quantile of a directional gamma model to full data
 - lacktriangle Essential in general to capture uncertainty in ψ
- *Y* assumed to follow generalised Pareto distribution with shape ξ , (modified) scale ν (= $\sigma(1 + \xi)$)
 - \blacksquare ξ , ν are functions of θ
- Frigessi et al. [2002], Behrens et al. [2004], MacDonald et al. [2011], Randell et al. [2016], Northrop et al. [2017]



Generalised Pareto

$$f_{\text{GP}}(y|\xi,\nu) = \frac{1}{\sigma} \left(1 + \frac{\xi}{\sigma} (y - \psi)^{-1/\xi - 1} \right)$$

- $\nu = \sigma(1+\xi)$
- $y > \psi, \psi \in (-\infty, \infty)$
- Shape parameter $\xi \in (-\infty, \infty)$ and scale parameter $\nu \in (0, \infty)$



10 / 33

Covariate representations

- Index set $\mathcal{I}_{\theta} = \{\theta_s\}_{s=1}^m$ on **periodic** covariate domain \mathcal{D}_{θ}
- **Each** observation belongs to exactly one θ_s
- \blacksquare On \mathcal{I}_{θ} , assume

$$\eta_s = \sum_{k=1}^n B_{sk} \beta_k, s = 1, 2, ..., m, \text{ or}$$

$$\eta = B\beta \text{ in vector terms}$$

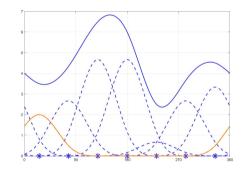
- $\eta \in (\xi, \nu)$
- $\mathbf{B} = \{B_{sk}\}_{s=1:k=1}^{m;n}$ basis for \mathcal{D}_{θ}
- $\beta = \{\beta_k\}_{k=1}^n$ basis coefficients
- Inference reduces to estimating n_{ξ} , n_{ν} , B_{ξ} , B_{ν} , β_{ξ} and β_{ν}
- P-splines, BARS and Voronoi are different forms of *B*



Copyright of Shell Shell & Lancaster University September 2019

P-splines

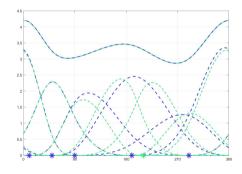
- *n* regularly-spaced knots on \mathcal{D}_{θ}
- \blacksquare *B* consists of *n* B-spline bases
 - Order d
 - Each using d + 1 consecutive knot locations
 - Local support
 - Wrapped on \mathcal{D}_{θ}
 - Cox de Boor recursion formula
- *n* is fixed and "over-specified"
- Knot locations $\{r_k\}_{k=1}^n$ fixed
- Local roughness of β penalised



Periodic P-splines

BARS basis

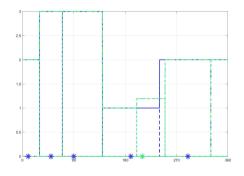
- *n* irregularly-spaced knots on \mathcal{D}_{θ}
- \blacksquare *B* consists of *n* B-spline bases
- Knot locations $\{r_k\}_{k=1}^n$ can change
- Number of knots n can change



Periodic BARS knot birth and death

Voronoi partition

- n irregularly-spaced centroids on \mathcal{D}_{θ}
 - Define *n* neighbourhoods or "cells"
- \blacksquare *B* consists of *n* basis functions
 - Piecewise constant on \mathcal{D}_{θ}
 - \blacksquare = 1 "within cell", = 0 "outside"
- Centroid locations $\{r_k\}_{k=1}^n$ can change
- \blacksquare Number of centroids n can change



Periodic Voronoi centroid birth and death



Prior for β (all representations)

prior density of
$$\beta \propto \exp\left(-\frac{1}{2}\beta'P\beta\right)$$

- $P = \lambda D'D$, D is a $n \times n$ (wrapped) differencing matrix
- P-splines: *D* represents first-difference; prior equivalent to local roughness penalty
- BARS and Voronoi: D is I_n ; prior is "ridge-type" for Bayesian regression

Prior for λ (all representations)

$$\lambda \sim \text{gamma}$$

Prior for *n* (BARS and Voronoi)

$$n \sim \text{Poisson}$$

Prior for r_k , k = 1, 2, ..., n (BARS and Voronoi)

$$r_k \sim \text{uniform}$$



Parameter set O

- P-splines: $\Omega = \{\beta_{\xi}, \lambda_{\xi}, \beta_{\gamma}, \lambda_{\gamma}\}$ with $n_{\xi}, r_{\xi}, n_{\gamma}$ and r_{γ} pre-specified
- BARS and Voronoi: $\Omega = \{n_{\xi}, r_{\xi}, \beta_{\xi}, \lambda_{\xi}, n_{\gamma}, r_{\gamma}, \beta_{\gamma}, \lambda_{\gamma}\}$
- where $r = \{r_k\}_{k=1}^n$, $\beta = \{\beta_k\}_{k=1}^n$,



16 / 33

Updating β , λ (all representations) and r (BARS and Voronoi)

- Gibbs sampling when full conditionals available
- Otherwise Metropolis-Hastings (MH) within Gibbs, using suitable proposal mechanisms, mMALA where possible
- Roberts and Stramer [2002], Girolami and Calderhead [2011], Xifara et al. [2014]

Conditional structure

$$f(\beta_{\eta}|y,\Omega\setminus\beta_{\eta}) \propto f(y|\beta_{\eta},\Omega\setminus\beta_{\eta}) \times f(\beta_{\eta}|\lambda_{\eta})$$

$$f(\lambda_{\eta}|y,\Omega\setminus\lambda_{\eta}) \propto f(\beta_{\eta}|\lambda_{\eta}) \times f(\lambda_{\eta})$$

$$f(r_{\eta}|y,\Omega\setminus r_{\eta}) \propto f(y|r_{\eta},\Omega\setminus r_{\eta}) \times f(r_{\eta}),$$

■ where $\eta \in (\xi, \nu)$



Dimension-jumping (BARS and Voronoi)

- Update n, and birth or death elements of r, β using reversible-jump MCMC
- Green [1995], Richardson and Green [1997], Biller [2000], Zhou and Shen [2001], DiMatteo et al. [2001], Wallstrom et al. [2008], Costain [2008], Bodin and Sambridge [2009]

Birth-death Metropolis-Hastings acceptance probability

- Jump from current $\Omega = (n_n, r_n, \lambda_n, \beta_n)$ to proposed $\Omega^* (=(\Omega \setminus \omega, \omega^*))$
- $\omega = (n_n, \beta_n, r_n)$ in current and $\omega^* = (n_n^*, \beta_n^*, r_n^*)$ in proposed

$$\min\left(1, \frac{f(\boldsymbol{y}|\Omega^*)}{f(\boldsymbol{y}|\Omega)} \frac{f(\omega^*)}{f(\omega)} \frac{q(\omega|\omega^*)}{q(\omega^*|\omega)} \left| \frac{\partial(\omega^{a*})}{\partial(\omega^a)} \right| \right)$$

- $f(y|\Omega)/f(y|\Omega^*)$ sample lik. ratio
- $f(\omega)/f(\omega^*)$ prior ratio

- $= q(\omega^*|\omega)/q(\omega|\omega^*)$ proposal ratio
- Final term Jacobian for transformation

■ Sample from prior!



September 2019

Dimension-jumping birth for β

- Location r^+ of the new knot is sampled uniformly on \mathcal{D}_{θ}
- Current knot locations $r = \{r_k\}_{k=1}^n$ and proposed $r^* = (\{r_k\}_{k=1}^n, r^+)$
- Establish bijection between augmented coefficient vector $\boldsymbol{\beta}^a = (\boldsymbol{\beta}, u_{\boldsymbol{\beta}})$ $(u_{\boldsymbol{\beta}} \sim N(0, \bullet))$ for current state, and vector $\boldsymbol{\beta}^*$ for proposed
- Motivation: make $B\beta$ and $B^*\beta^*$ as similar as possible
- Regression solution is $\hat{\beta}^* = [(B^{*'}B^*)^{-1}B^{*'}B]\beta = G_j\beta$
- Set

$$oldsymbol{eta}_j^* = \left[egin{array}{ccc} G_j & \left[egin{array}{c} 0 \ dots \ 0 \ 1 \end{array}
ight] imes \left[egin{array}{c} eta_j \ u_eta \end{array}
ight] = F_j oldsymbol{eta}_j^a.$$

- Jacobian for a birth is |G|
- For death transition, essentially use F^{-1}
- Zanini et al. [2019]



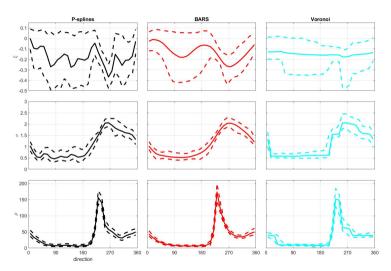
North Sea application



20 / 33

Posterior parameter estimates for ξ , ν and ρ for northern North Sea

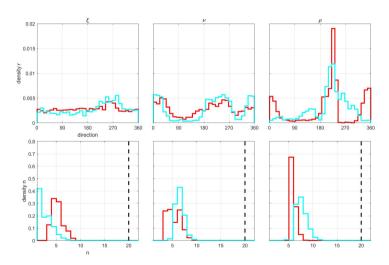
- Note colour scheme
- Rate ρ and ν very similar
- Voronoi gives almost constant ξ
- Voronoi piecewise constant
- Land shadow effects
- General agreement





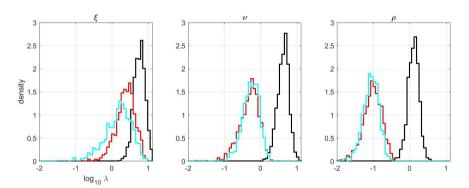
Posterior densities for locations r and numbers n

- Knot placement uniform for ξ , clear effect for ρ
- n close to 1 for Voronoi ξ
- General agreement
- Effect of different priors on *n* checked





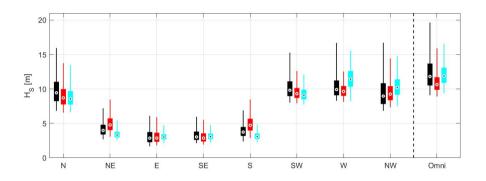
Posterior densities for penalty coefficients λ



- Ridge penalties for BARS and Voronoi, but roughness for P-splines
- \blacksquare λ somewhat lower for Voronoi, but also this has smaller n
- General consistency



Directional posterior predictive distribution of T = 1000-year maximum

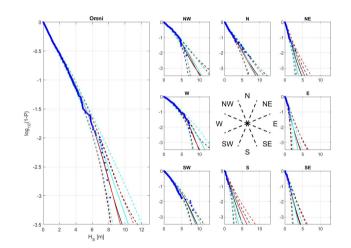


- Box-whiskers with 2.5%, 25%, 50%, 75% and 97.5% percentiles
- Uncertainties larger for P-splines?
- General consistency



Fit diagnostic

- Empirical tail (blue)
- Posterior means and 95% credible intervals for quantile levels from different models
- General consistency





Simulation study

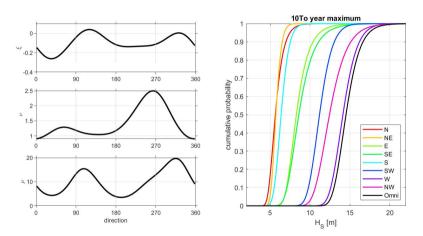


Set-up

- n_S = 100 samples, each containing exactly n_O = 1000 observations of threshold exceedances with a generalised Pareto distribution
- True Poisson rate ρ , shape ξ and scale ν vary systematically with covariate θ .
- Functional forms of $\xi(\theta)$, $\nu(\theta)$ and $\rho(\theta)$ generated using sum of 10 weighted (wrapped) Gaussian kernels of standard deviation 30°, randomly located on the periodic covariate domain
- Weights drawn at random from suitable distributions, so that $\xi(\theta)$, $\nu(\theta)$ and $\rho(\theta)$ like North Sea sample
- Distribution of *T*-year maxima ($T = 10 \times$ the period of sample, T_O) estimated



Illustrative realisation

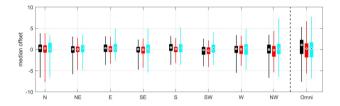


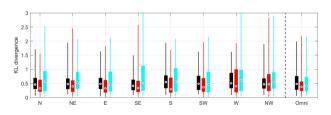
- True $\xi(\theta)$, $\nu(\theta)$ and $\rho(\theta)$ for typical realisation
- Directional distribution of 10*T*_O-year maximum for 8 octants, and "omni"

September 2019

Performance summary

- Compare posterior predictive distribution for $10T_O$ -year maximum with truth
- Median offset small
- KL divergence more variable for Voronoi
- BARS slightly better?
- General consistency

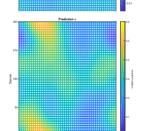




Where next?

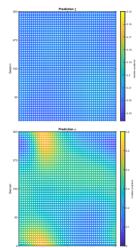






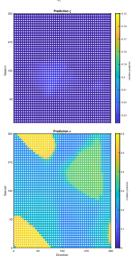
Direction

BARS:
$$n_{\xi}^{mo} = 3 \times 3, n_{\chi}^{mo} = 4 \times 4$$



Direction

Voronoi:
$$n_{\xi}^{mo} = 1, n_{V}^{mo} = 7$$



Summary

- Covariate effects important in environmental extremes
- Need to tackle big problems ⇒ need efficient models
- Need to provide solutions as "end-user" software ⇒ stable inference
- P-splines: straightforward, global roughness per dimension
- BARS: optimally-placed knots
- All splines: nD basis is tensor product of marginal bases
- Voronoi: piecewise constant, naturally nD
- Combinations useful
- Conditional, spatial and temporal extremes



References

- C N Behrens, H F Lopes, and D Gamerman. Bayesian analysis of extreme events with threshold estimation. Stat. Modelling, 4:227–244, 2004.
- C. Biller. Adaptive Bayesian regression splines in semiparametric generalized linear models. J. Comput. Graph. Statist., 9:122–140, 2000.
- Thomas Bodin and Malcolm Sambridge. Seismic tomography with the reversible jump algorithm. Geophysical Journal International, 178:1411–1436, 2009.
- D. A. Costain. Bayesian partitioning for modeling and mapping spatial case-control data. Biometrics, 65:1123–1132, 2008.
- I. DiMatteo, C. R. Genovese, and R. E. Kass. Bayesian curve-fitting with free-knot splines. Biometrika, 88:1055-1071, 2001.
- A. Frigessi, O. Haug, and H. Rue. A dynamic mixture model for unsupervised tail estimation without threshold selection. Extremes, 5:219-235, 2002.
- M. Girolami and B. Calderhead. Riemann manifold Langevin and Hamiltonian Monte Carlo methods. J. Roy. Statist. Soc. B, 73:123–214, 2011.
- P.J. Green. Reversible jump Markov chain Monte Carlo computation and Bayesian model determination. Biometrika, 82:711-732, 1995.
- A. MacDonald, C. J. Scarrott, D. Lee, B. Darlow, M. Reale, and G. Russell. A flexible extreme value mixture model. Comput. Statist. Data Anal., 55:2137–2157, 2011.
- P. Northrop, N. Attalides, and P. Jonathan. Cross-validatory extreme value threshold selection and uncertainty with application to ocean storm severity. J. Roy. Statist. Soc. C, 66: 93–120, 2017.
- D. Randell, K. Turnbull, K. Ewans, and P. Jonathan. Bayesian inference for non-stationary marginal extremes. Environmetrics, 27:439–450, 2016.
- S Richardson and P. J. Green. On bayesian analysis of mixtures with an unknown number of components (with discussion). J. Roy. Statist. Soc. B, 59(4):731–792, 1997.
- G. O. Roberts and O. Stramer. Langevin diffusions and Metropolis-Hastings algorithms. Methodology and Computing in Applied Probability, 4:337–358, 2002.
- G. Wallstrom, J. Liebner, and R. E. Kass. An implementation of Bayesian adaptive regression splines (BARS) in C with S and R wrappers. Journal of Statistical Software, 26, 2008.
- T. Xifara, C. Sherlock, S. Livingstone, S. Byrne, and M Girolami. Langevin diffusions and the Metropolis-adjusted Langevin algorithm. Stat. Probabil. Lett., 91(2002):14–19, 2014.
- E. Zanini, E. Eastoe, M. Jones, D. Randell, and P. Jonathan. Covariate representations for non-stationary extremes. Environmetrics (draft at www.lancs.ac.uk/~jonathan), 2019.
- E. Zahimi, E. Lastoe, M. Jones, D. Rahden, and I. Johathan. Covariate representations for non-stationary extremes. Environments (unique a www.aures.ac.uk/~johathan. Covariate representations for non-stationary extremes.
- S. Zhou and X. Shen. Spatially adaptive regression splines and accurate knot selection schemes. J. Am. Statist. Soc., 96:247–259, 2001.



Copyright of Shell Shell & Lancaster University September 2019 33 / 33