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Slides at *www.lancs.ac.uk/∼jonathan*

Philip Jonathan
Statistics and Data Science

Acknowledgement

- Shell Statistics and Data Science
- Department of Mathematics and Statistics, Lancaster University

Motivation

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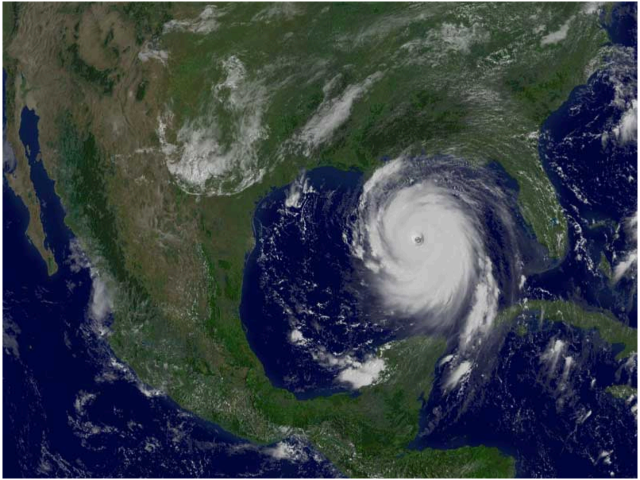

Motivation

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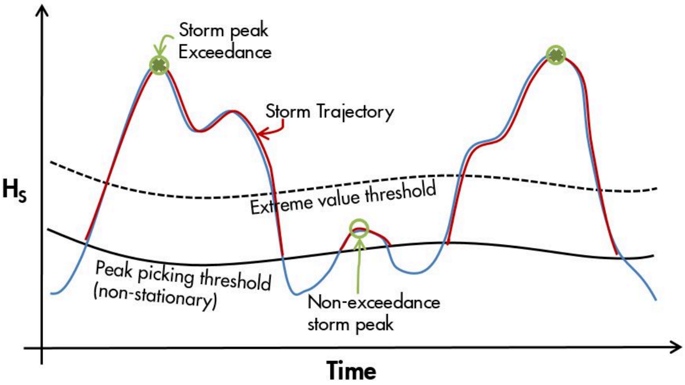
- Rational and consistent design and assessment of marine structures
  - Reduce bias and uncertainty in estimation of structural integrity
  - Quantify uncertainty as well as possible
- Non-stationary marginal, conditional and spatial extremes
  - Multiple locations, multiple variables, time-series
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

Motivation

- Environmental extremes vary smoothly with multidimensional covariates
  - Model parameters are functions of covariates
- Uncertainty quantification for whole inference
  - Data acquisition (simulator or measurement)
  - Data pre-processing (storm peak identification)
  - Extreme value threshold
  - Model form (marginal measurement scale effect, spatial extremal dependence)
- Statistical and computational efficiency
  - Slick algorithms
  - Parallel computation
  - Bayesian inference

Motivation: storm model

$H_S \approx 4\times$ standard deviation of ocean surface time-series at specific location corresponding to a specified period (typically three hours)



Outline

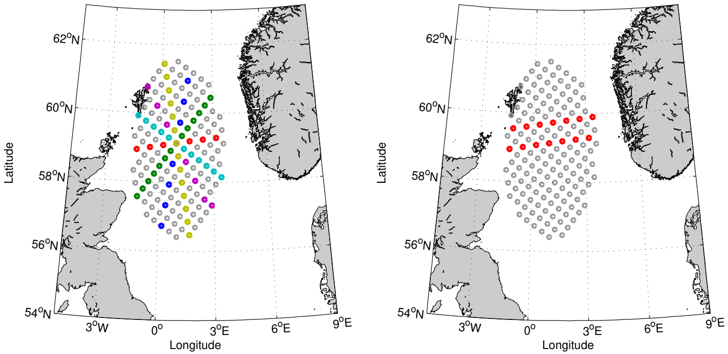
Covariate effects in:

- Marginal models
  - Simple introductory example (directional model)
  - Storm peak H_S with 2D, 3D and 4D covariates
- Conditional extremes models
  - Associated values of other wave field parameters given extreme stork peak H_S
- Spatial extremes models
  - Directional dependence in max-stable process parameters for storm peak H_S

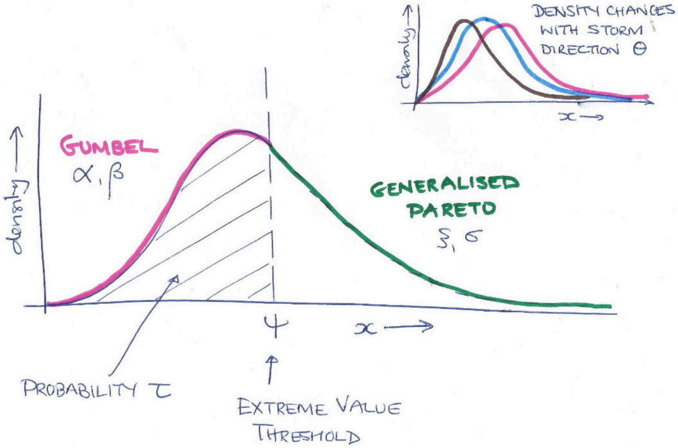
North Sea example used as "connecting theme"; other examples to embellish

Outline: North Sea application

Storm peak H_S from gridded NEXTRA *winter* storm hindcast for North Sea locations; directional variability in storm severity; "strips" of locations with different orientations; central location for directional model



Marginal: simple gamma-GP model



Marginal: simple gamma-GP model

- Sample of peaks over threshold y, with covariates θ
  - θ is 1D in motivating example : directional
  - θ is nD later : e.g. $4D$ spatio-directional-seasonal
- Below threshold ψ
  - y follows truncated gamma with shape α, scale $1/\beta$
  - Hessian for gamma better behaved than Weibull
- Above ψ
  - y follows generalised Pareto with shape ξ, scale σ
- ξ, σ, α, β, ψ all functions of θ
- ψ for pre-specified threshold probability τ
  - Generalise later to estimation of τ

- Frigessi et al. [2002], Behrens et al. [2004], MacDonald et al. [2011]
- Randell et al. [2016]

Marginal: simple gamma-GP model

- Density is $f(y|\xi,\sigma,\alpha,\beta,\psi,\tau)$

$$= \begin{cases} \tau \times f_{TG}(y|\alpha,\beta,\psi) & \text{for } y \leq \psi \\ (1-\tau) \times f_{GP}(y|\xi,\sigma,\psi) & \text{for } y > \psi \end{cases}$$

- Likelihood is $\mathcal{L}(\xi,\sigma,\alpha,\beta,\psi,\tau|\{y_i\}_{i=1}^{n})$

$$= \prod_{i:y_i\leq\psi} f_{TG}(y_i|\alpha,\beta,\psi) \prod_{i:y_i>\psi} f_{GP}(y_i|\xi,\sigma,\psi)$$

$$\times \quad \tau^{n_B}(1-\tau)^{(1-n_B)} \text{ where } n_B = \sum_{i:y_i\leq\psi} 1.$$

Estimate all parameters as functions of θ

Marginal: count rate c

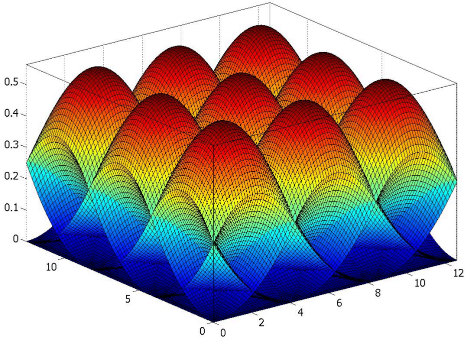
- Whole-sample rate of occurrence ρ modelled as Poisson process given counts c of numbers of occurrences per covariate bin
- Chavez-Demoulin and Davison [2005]

Marginal: P-splines

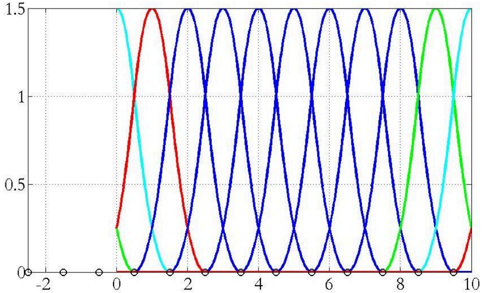
- Physical considerations suggest $\alpha, \beta, \rho, \xi, \sigma, \psi$ and τ vary smoothly with covariates θ
- Values of $\eta \in \{\alpha, \beta, \rho, \xi, \sigma, \psi, \tau\}$ on some index set of covariates take the form $\boldsymbol{\eta} = \boldsymbol{B}\boldsymbol{\beta}_\eta$
  - For nD covariates, $\boldsymbol{B}$ takes the form of tensor product $\boldsymbol{B}_{\theta_n} \otimes \ldots \otimes \boldsymbol{B}_{\theta_\kappa} \otimes \ldots \otimes \boldsymbol{B}_{\theta_2} \otimes \boldsymbol{B}_{\theta_1}$
- Spline roughness with respect to each covariate dimension κ given by quadratic form $\lambda_{\eta\kappa}\beta'_{\eta\kappa}\boldsymbol{P}_{\eta\kappa}\boldsymbol{\beta}_{\eta\kappa}$
- $\boldsymbol{P}_{\eta\kappa}$ is a function of stochastic roughness penalties $\delta_{\eta\kappa}$

- Brezger and Lang [2006]

Marginal: P-splines



Kronecker product



Periodic P-splines

Marginal: Bayesian inference on a page

POSTERIOR, LIKELIHOOD, PRIOR

$$p(\beta \mid y) = \frac{p(y \mid \beta)\; p(\beta)}{p(y)}$$

BAYES THEOREM

$p(y)$ ← EVIDENCE

$$\propto p(y \mid \beta)\, p(\beta) \text{ when data } y \text{ is fixed.}$$

We start by guessing $p(\beta)$, and specifying $p(y \mid \beta)$. Then we can "learn" what β is when we've observed y.

$$p(\beta_1, \beta_2 \mid y) \propto p(y \mid \beta_1, \beta_2)\, p(\beta_1, \beta_2)$$

ITERATE

$$p(\beta_1 \mid y, \beta_2) \propto p(y \mid \beta_1, \beta_2)\, p(\beta_2)$$

$$p(\beta_2 \mid y, \beta_1) \propto p(y \mid \beta_1, \beta_2)\, p(\beta_1)$$

GIBBS SAMPLING

GIBBS SAMPLING allows us to learn about LOTS OF βs in a computationally efficient way.

Marginal: priors and conditional structure

Priors

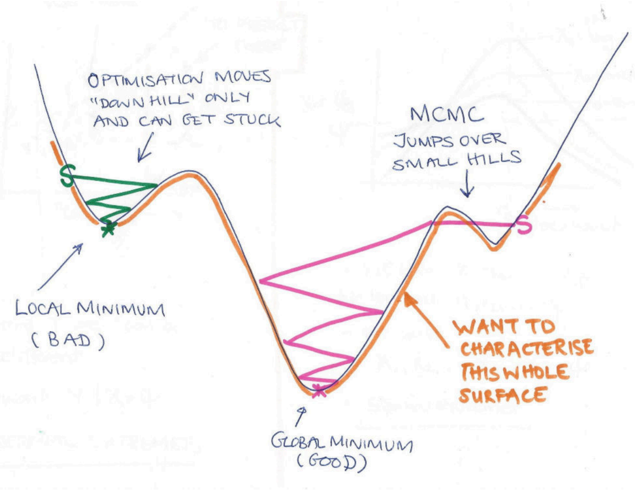
$$
\begin{aligned}
\text{density of } \boldsymbol{\beta}_{\eta\kappa} &\propto \exp\left(-\frac{1}{2}\lambda_{\eta\kappa}\boldsymbol{\beta}'_{\eta\kappa}\boldsymbol{P}_{\eta\kappa}\boldsymbol{\beta}_{\eta\kappa}\right) \\
\lambda_{\eta\kappa} &\sim \text{gamma} \\
(\text{ and } \tau &\sim \text{beta, when } \tau \text{ estimated })
\end{aligned}
$$

Conditional structure

$$
\begin{aligned}
f(\tau|\boldsymbol{y},\Omega\setminus\tau) &\propto f(\boldsymbol{y}|\tau,\Omega\setminus\tau)\times f(\tau) \\
f(\boldsymbol{\beta}_\eta|\boldsymbol{y},\Omega\setminus\boldsymbol{\beta}_\eta) &\propto f(\boldsymbol{y}|\boldsymbol{\beta}_\eta,\Omega\setminus\boldsymbol{\beta}_\eta)\times f(\boldsymbol{\beta}_\eta|\boldsymbol{\delta}_\eta,\boldsymbol{\lambda}_\eta) \\
f(\boldsymbol{\lambda}_\eta|\boldsymbol{y},\Omega\setminus\boldsymbol{\lambda}_\eta) &\propto f(\boldsymbol{\beta}_\eta|\boldsymbol{\delta}_\eta,\boldsymbol{\lambda}_\eta)\times f(\boldsymbol{\lambda}_\eta)
\end{aligned}
$$

$$\eta\in\Omega=\{\alpha,\beta,\rho,\xi,\sigma,\psi,\tau\}$$

Marginal: inference



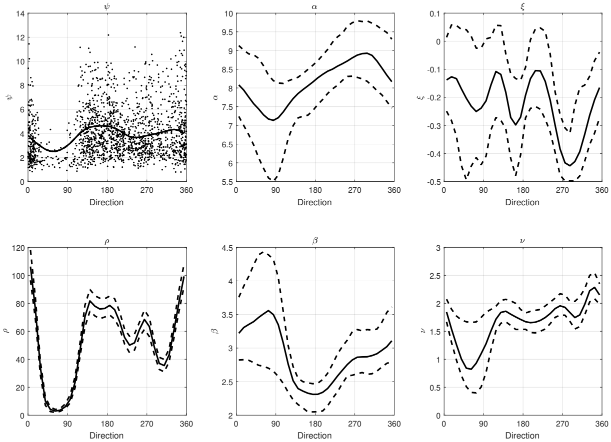
Marginal: inference

- Elements of β_η highly interdependent, correlated proposals essential for good mixing
- "Stochastic analogues" of IRLS and back-fitting algorithms for maximum likelihood optimisation used previously
- Estimation of different penalty coefficients for each covariate dimension

- Gibbs sampling when full conditionals available
- Otherwise Metropolis-Hastings (MH) within Gibbs, using suitable proposal mechanisms
  - mMALA where possible

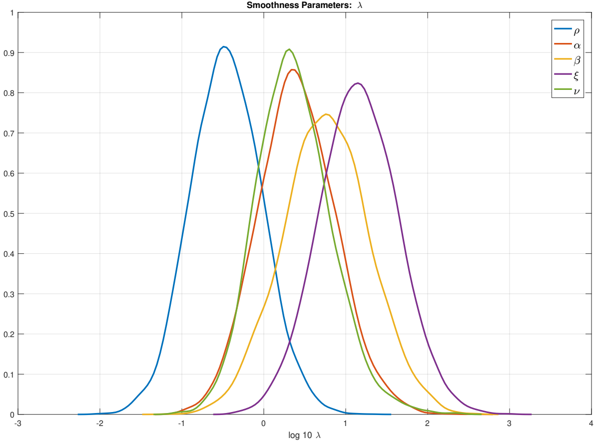
- Roberts and Stramer [2002], Girolami and Calderhead [2011], Xifara et al. [2014]

Marginal: posterior parameter



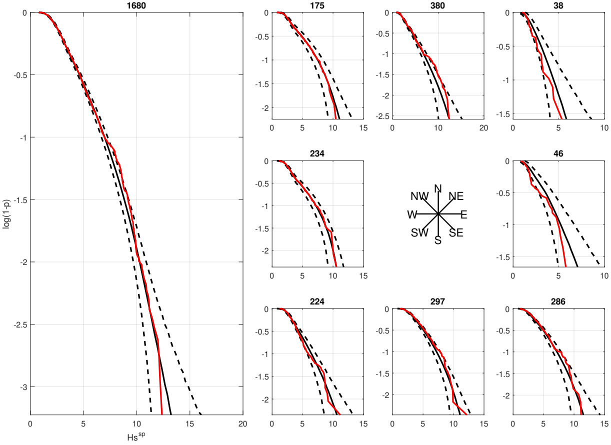
Marginal: posterior roughness penalty

Different scales so must be careful : rate is roughest, GP shape is smoothest

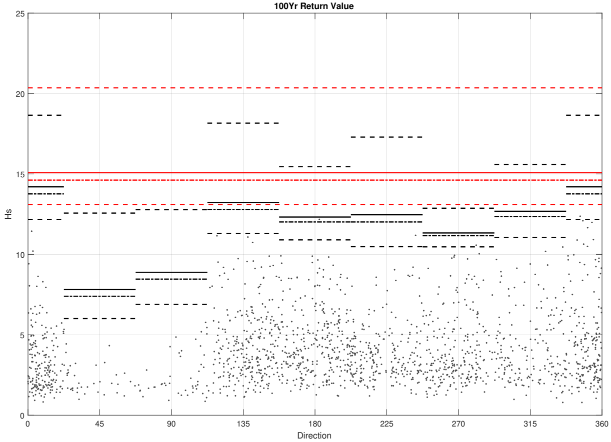


Marginal: validation

Compare sample with simulated values on partitioned covariate domain

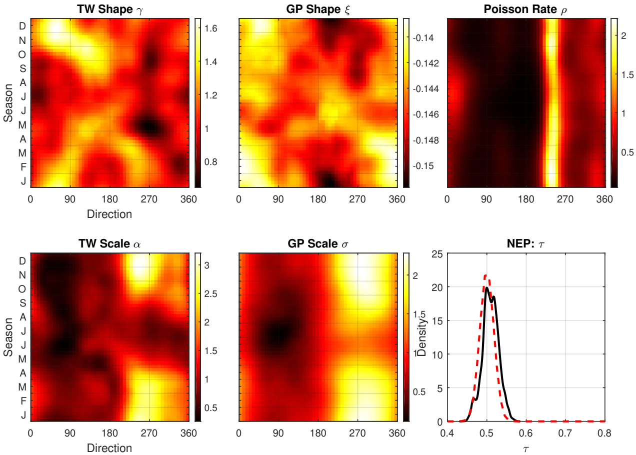


Marginal: return values



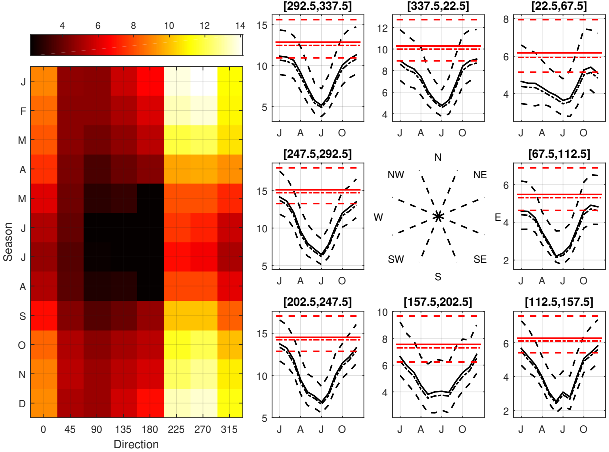
Marginal: extension to 2D

Directional-seasonal model for location in northern North Sea; τ estimated; land-shadow effect of Norway obvious; Randell et al. [2016]



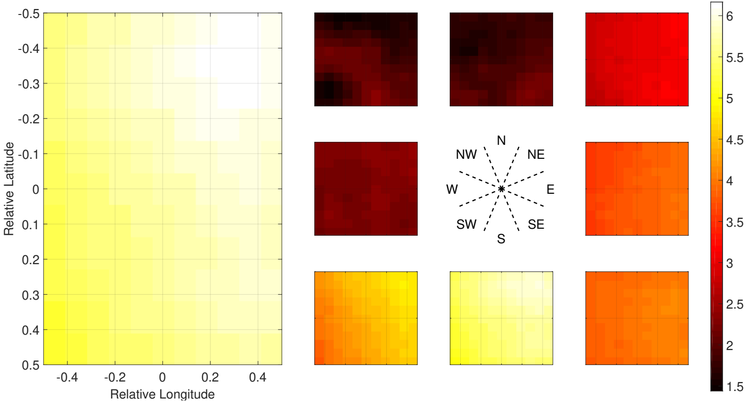
Marginal: extension to 2D

Summary statistics for return value distributions



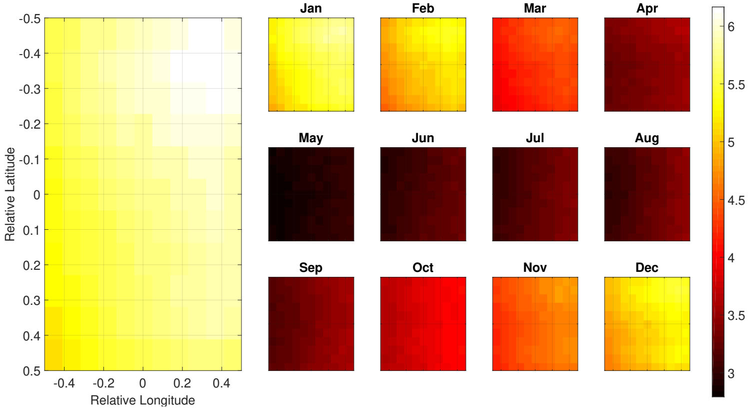
Marginal: extension to 4D

Spatio-directional-seasonal model for location in South China Sea; ML/CV/BS estimation; bootstrap median estimate after integration over season; clear spatial and directional effects; Raghupathi et al. [2016]

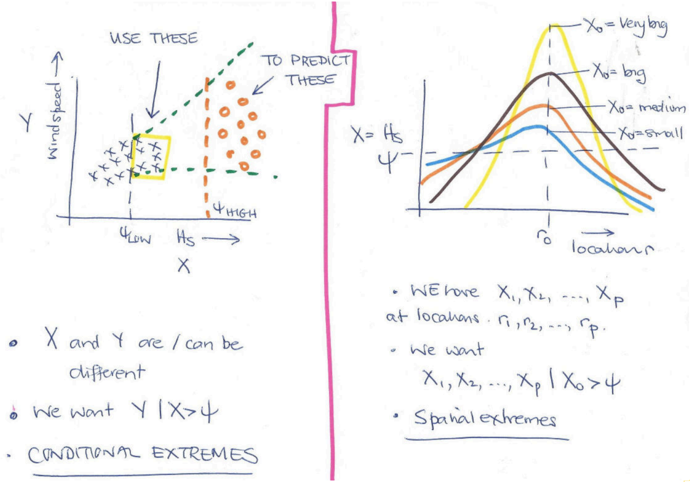


Marginal: extension to 4D

Bootstrap median estimate after integration over direction; clear spatial and seasonal effects



Conditional and spatial extremes



Conditional: summary

- Heffernan and Tawn [2004] and derivatives
- Evidence for covariate effects in conditional extremes of sea-state and storm peak variables
  - Marginal non-stationary extreme value model
  - Marginal transformation to standard scale removing marginal covariate dependence
  - Conditional dependence structure showing covariate effects
- Examples
  - Wave peak period | Significant wave height
  - Ocean current at one depth | Current at another depth
  - Significant wave height | Wind speed
  - Storm surge | Significant wave height

Conditional: $T_P|H_S$ example

On **Laplace** scale, extend with covariates θ

$$(Y_2|Y_1 = y, \theta) = \alpha_\theta y + y^{\beta_\theta}(\mu_\theta + \sigma_\theta Z) \text{ for } y > \psi_\theta(\tau)$$

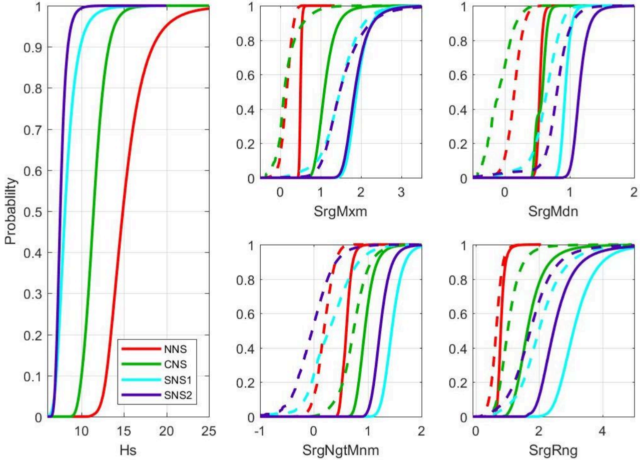
- $\psi_\theta(\tau)$ is a high non-stationary quantile of Y_1 on Gumbel scale, for non-exceedance probability τ, above which the model fits well
- $\alpha_\theta \in [0,1]$, $\beta_\theta \in (-\infty, 1]$, $\sigma_\theta \in [0, \infty)$
- Z is a random variable with **unknown** distribution G, assumed Normal for estimation

Application

- Estimate spectral peak wave period T_P for storm sea states with extreme severity (energy) H_S
- In T_P, H_S case, $\psi = \theta_j = \theta_k$
- Jonathan et al. [2014]

Conditional: Surge $|H_S$ example

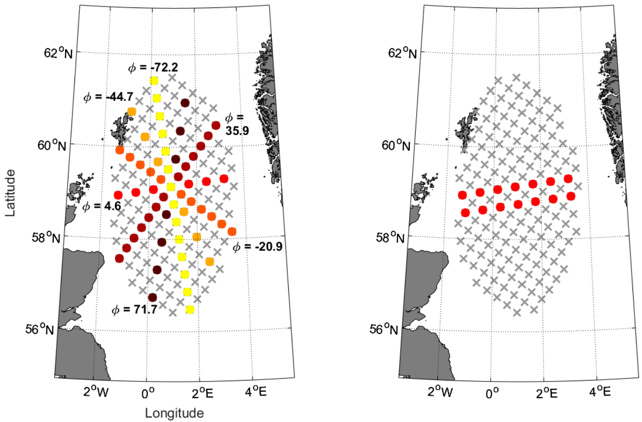
100-year storm peak H_S together with marginal and conditional surge characteristics



- Pre-print (Ross et al. 2018)

Spatial extremes

Storm peak H_S from gridded NEXTRA *winter* storm hindcast for North Sea locations; directional variability in storm severity; “strips” of locations with different orientations; central location for directional model



Modelling extremal spatial dependence : why bother?

- Improved inference for the characteristics of extremes at one location exploiting data from multiple locations in a spatial neighbourhood
- Improved estimation of risk for spatially-distributed structures (coastal defences, multiple installations) from spatially spread storm events

- Can we estimate spatial extremes models usefully from typical metocean hindcast data?
- Can we see evidence for covariate effects in extremal spatial dependence for ocean storm severity?

- Pre-print (Ross et al. 2017)

Modelling extremal spatial dependence : mathematically

- Locations $j = 1, 2, ..., p$, continuous random variables $\{X_j\}$ and values $\{x_j\}$
- Spatial distribution of storm peak H_S

$$f(x_1, x_2, ..., x_p) = [f(x_1)f(x_2)...f(x_p)]\,\mathcal{C}(x_1, x_2, ..., x_p)$$

- $\{f(x_j)\}$ are marginal densities, $\mathcal{C}(x_1, x_2, ..., x_p)$ is dependence "copula"
- Interested in estimating things like "the shape of an extreme storm"

$$f(x_1, x_2, ..., x_p | X_k = x_k > u_k) \text{ for large } u_k$$

- We know how to estimate extremes marginally, but what about extremal dependence?
- $\Rightarrow$ study spatial extremes, i.e. sensible models for $\mathcal{C}(x_1, x_2, ..., x_p)$

Modelling extremal spatial dependence : procedure

- Sample of peaks over threshold $\{x\}$ at p locations, with covariates $\{\theta\}$
- Simple marginal gamma-GP model
- Sample transformed ("whitened") to standard Fréchet scale per location
- Spatial extremes ("max-stable model") to estimate extremal spatial dependence
- Bayesian inference estimating joint distributions of parameters, uncertainties

Extremes basics : marginal

- Block maxima Y_k at location k have distribution F_{Y_k} which is max-stable in the sense that $F^n_{Y_k}(b'_{kn} + a'_{kn} y_k) = F_{Y_k}(y_k)$ for some sequences $\{a'_{kn} > 0\}$ and $\{b'_{kn}\}$
- Only possible limiting distribution for F_{Y_k} is generalised extreme value (GEV)

$$\begin{aligned} F_{Y_k}(y_k) &= \exp[-\exp\{(y_k - \eta)/\tau\}] \text{ for } \xi = 0 \\ &= \exp[-\{1 + \xi(y_k - \eta)/\tau\}_+^{-1/\xi}] \text{ otherwise} \end{aligned}$$

- For peaks over threshold, the equivalent asymptotic distribution is the generalised Pareto distribution.

Extremes basics : spatial

- Similarly, F_Y for block maxima Y at p locations "max-stable" when $F_Y^n(b'_{1n} + a'_{1n}y_1, b'_{2n} + a'_{2n}y_2, ..., b'_{pn} + a'_{pn}y_p) = F_Y(y_1, y_2, ..., y_p)$
- Transform to unit Fréchet $Z_k = \{1 + \xi(Y_k - \eta)/\tau\}^{1/\xi}$, $F_{Z_k}(z_k) = \exp(-1/z_k)$, for $z_k > 0$. Then

$$F_Z(z_1, z_2, ..., z_p) = F_Z(nz_1, nz_2, ..., nz_p)^n$$

- Only choices of F_Z exhibiting this homogeneity correspond to finite-dimensional distributions from max-stable processes (MSPs), and are hence valid for spatial extreme value modelling

Spatial : basic theory

- Max-stable process (MSP) : a means of extending the GEV for modelling maxima at one location, to multivariate extreme value distributions for modelling of component-wise maxima observed on a lattice
- On unit Fréchet scale, only choices of F_Z exhibiting homogeneity are valid for spatial extreme value modelling
- Terminology : exponent measure V_Z

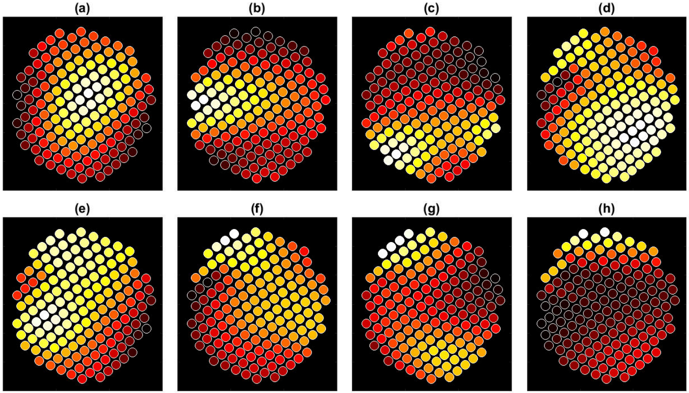
$$F_Z(z_1, z_2, ..., z_p) = \exp\{-V_Z(z_1, z_2, ..., z_p)\}$$

- Terminology : extremal coefficient θ_p

$$\begin{aligned} F_Z(z, z, ..., z) &= \exp\left(-V_Z(z, z, ..., z)\right) \\ &= \exp\left(-z^{-1} V_Z(1, 1, ..., 1)\right) \text{ from the homogeneity property} \\ &= \exp\left(-\theta_p / z\right) \end{aligned}$$

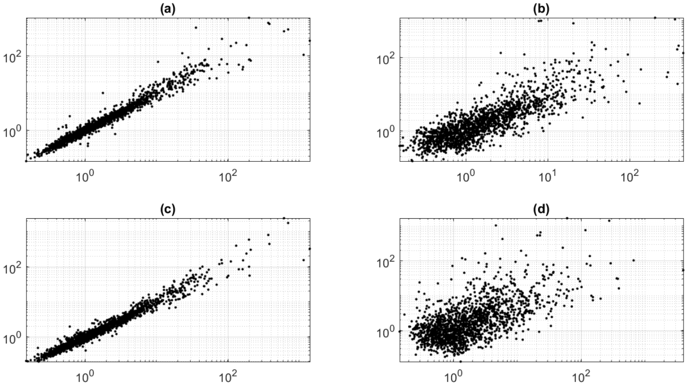
Spatial : data

Fréchet scale observations of the spatial distribution of storm peak H_S over the North Sea spatial grid for 8 typical events (a)-(h). The spatial maximum for each event is given as a white disc, and the spatial minimum as a black disc (with white outline). The white $\rightarrow$ yellow $\rightarrow$ red $\rightarrow$ black colour scheme indicates the spatial variation of relative magnitude of storm peak H_S



Spatial : data

Fréchet scale scatter plots of storm peak H_S for different pairs of locations. Panel (a) for the central location and its nearest neighbour to the West along the approximate West-East transect with angle $\phi = 4.6$; panel (b) for the end locations of the same transect. Panel (c) for the central location and its nearest neighbour to the North along the approximate North-South transect with angle $\phi = -72.2$; panel (d) for the end locations of the same transect



Spatial : V_Z for Smith, Schlather and Brown-Resnick processes

- **Smith** : For two locations s_k, s_l in $\mathcal{S}$, V_{kl} for Smith process given by

$$V_{kl}(z_k, z_l; h(\Sigma)) = \frac{1}{z_k}\Phi(\frac{m(h)}{2} + \frac{\log(z_l/z_k)}{m(h)}) + \frac{1}{z_l}\Phi(\frac{m(h)}{2} + \frac{\log(z_k/z_l)}{m(h)})$$

- $h = s_l - s_k$, $m(h)$ is Mahalanobis distance $(h'\Sigma^{-1}h)^{1/2}$ between s_k and s_l
- Σ is 2×2 covariance matrix (2-D space) to be estimated. Σ scalar in 1-D
- $V_{kl}(1, 1; h(\Sigma)) = 2\Phi(m(h)/2)$ by construction

- **Schlather** : similar likelihood, parameterised in terms of Σ only
- **Brown-Resnick** : identical likelihood, parameterised in terms of Σ and scalar Hurst parameter H (estimated up front)

Spatial : constructive representation

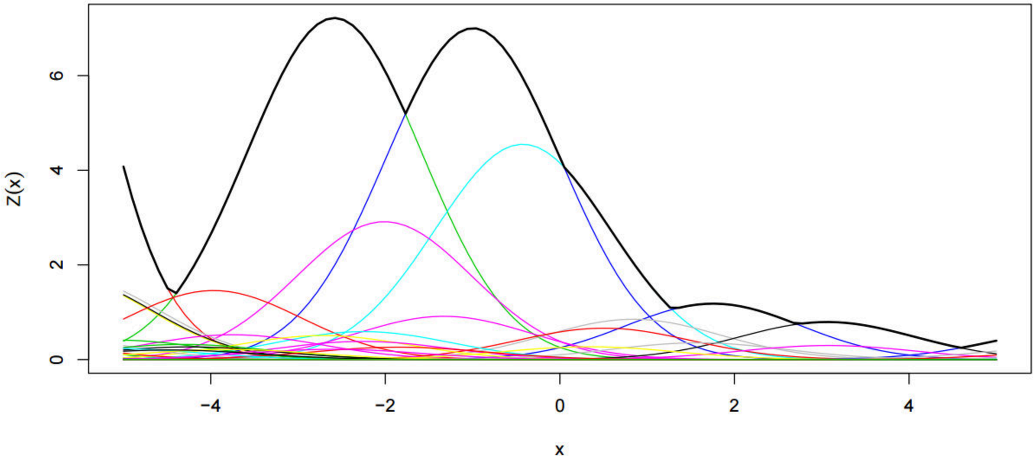
- MSP is maximum of multiple copies $\{W_i\}$ $(i \geq 1)$ of random function W
- Each W_i weighted using Poisson process $\{\rho_i\}$ $(i \geq 1)$

- The MSP $Z(s)$ for s in spatial domain $\mathcal{S}$ is $Z(s) = \mu^{-1} \max_i\{W_i^+(s)/\rho_i\}$

- $W_i^+ = \max\{W_i(s), 0\}$, $\mu = E(W^+(s)) = 1$ by construction typically
- $\rho_i = \epsilon_i$ for $(i = 1)$, $\rho_i = \epsilon_i + \rho_{i-1}$ for $(i > 1)$, and $\epsilon_i \sim \text{Exp}(1)$

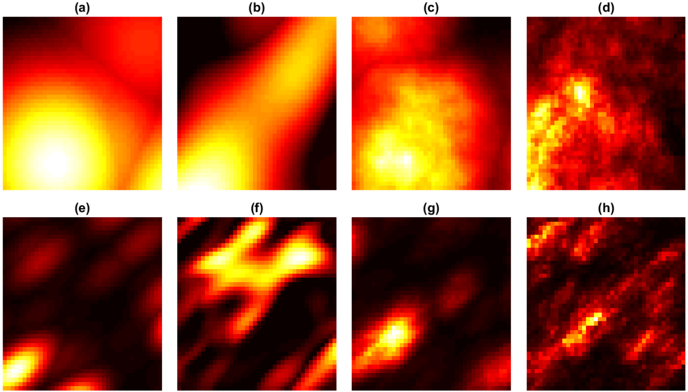
- Different choices of $W(s)$ give different MSPs
- Smith : $W_i(s; s_i, \Sigma) = \varphi(s - s_i; \Sigma)/f_S(s_i)$, with s_i sampled from density $f_S(s_i)$ on $\mathcal{S}$, with φ representing standard Gaussian density
- Schlather, Brown-Resnick : Similar

Spatial : constructive representation



Spatial : illustrations

Illustrative realisations of Smith (a,e), Schlather (b,f), and Brown-Resnick (c,d,g,h) processes for different parameter choices. The first row corresponds to parameter settings $(\Sigma_{11}, \Sigma_{22}, \Sigma_{12}) = (300, 300, 0)$ for all processes, and the second row to (30,20,15). For Brown-Resnick processes (c,g), Hurst parameter $H = 0.95$. For Brown-Resnick processes (d,h), $H = 0.65$. Each panel can be considered to show a possible spatial realisation of storm peak H_S, similar to those shown earlier



Spatial : estimation approximations

- Theory applies for (Fréchet scale) block maxima Z_Y, but we have (Fréchet scale) peaks over threshold Z_X. For $z_k, z_l > u$ for large u, approximate

$$\Pr\left[Z_{Xk} \leq z_k, Z_{Xl} \leq z_l\right] \approx \Pr\left[Z_{Yk} \leq z_k, Z_{Yl} \leq z_l\right]$$

- Theory gives us models for pairs of locations. Cannot write down full joint likelihood $\ell(\Sigma; \{z_j\})$. Approximate with composite likelihood $\ell_C(\Sigma; \{z_j\})$

$$\ell(\Sigma; \{z_j\}) \approx \ell_C(\Sigma; \{z_j\}) = \sum_{\{k,l\} \in \mathcal{N}} w_{kl} \log f_{kl}(z_k, z_l; h(\Sigma))$$

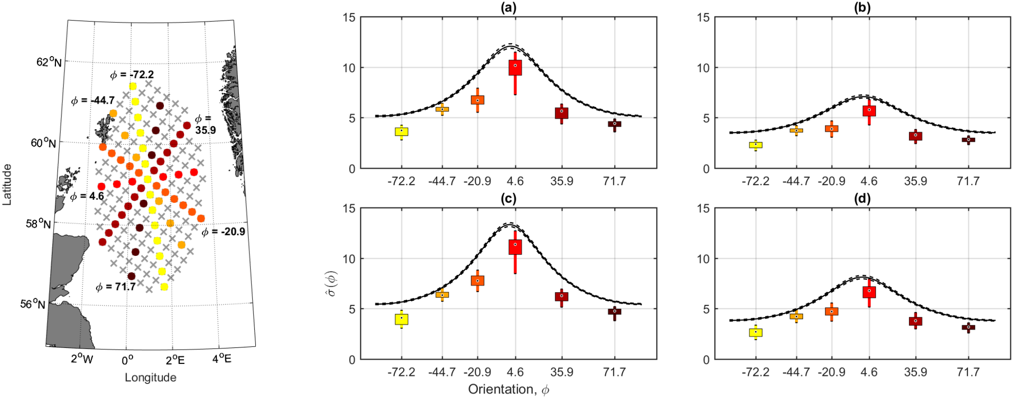
- Need $f_{kl}(z_k, z_l; h(\Sigma))$ for non-exceedances of u also, so make censored likelihood approximation

Spatial : estimation

- Estimate joint distribution of $\Omega = [\Sigma_{11}, \Sigma_{22}, \Sigma_{12}]$ (2-D space, or $\Omega = \Sigma$ in 1-D)
- MCMC using Metropolis-Hastings
  - Current state Ω_{r-1}, marginal posterior $f_M(\beta_M)$, original sample D of storm peak H_S.
  - Draw a set of marginal parameters β_{Mr} from f_M, independently per location.
  - Use β_{Mr} to transform D to standard Fréchet scale, independently per location, obtaining sample D_{Fr}.
  - Execute "adaptive" MCMC step from state Σ_{r-1} with sample D_{Fr} as input, obtain Σ_r.
- Adaptive MCMC candidates generated using $\Omega_r^c = \Omega_{r-1} + \gamma\epsilon_1 + (1-\gamma)\epsilon_2$
  - $\gamma \in [0,1]$, $\epsilon_1 \sim N(0, \delta_1^2 I_3/3)$, $\epsilon_2 \sim N(0, \delta_2^2 S_{\Omega_{r-1}}/3)$
  - $S_{\Omega_{r-1}}$ estimate of variance of Ω_{r-1} using samples to trajectory to date
  - Roberts and Rosenthal [2009]

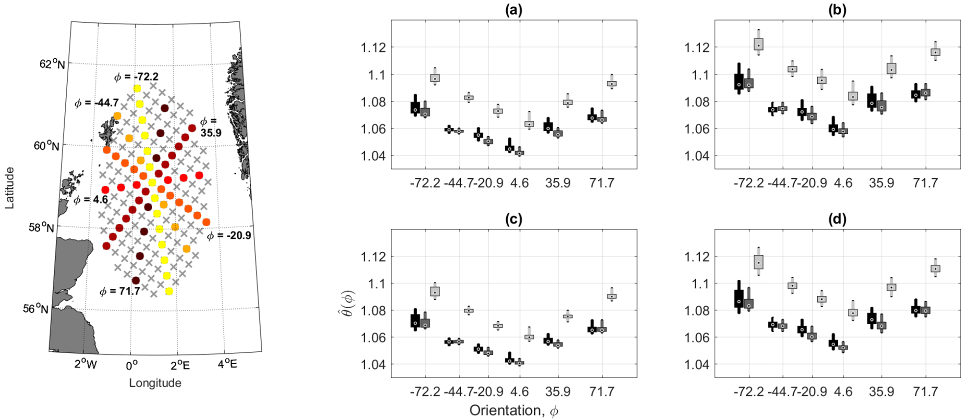
Spatial : $\hat{\sigma}(\phi)$ for Smith

For all transects with a given orientation ϕ estimated using 1-D (box-whisker) and 2-D (black) Smith processes. ϕ is quantified as the transect angle anticlockwise from a line of constant latitude. The first (second) row: marginal threshold non-exceedance probability 0.5 (0.8). The first (second) column: censoring threshold non-exceedance probability 0.5 (0.8). For 1-D estimates with a given ϕ, box centres = median, box edges = 0.25 and 0.75 quantiles across all parallel transects; whisker edges = 0.025 and 0.975 quantiles. For 2-D estimates, the 0.025, 0.5 and 0.975 quantiles are shown as a function of ϕ. Note that the colour coding of box-whisker plots corresponds to that of transect orientation



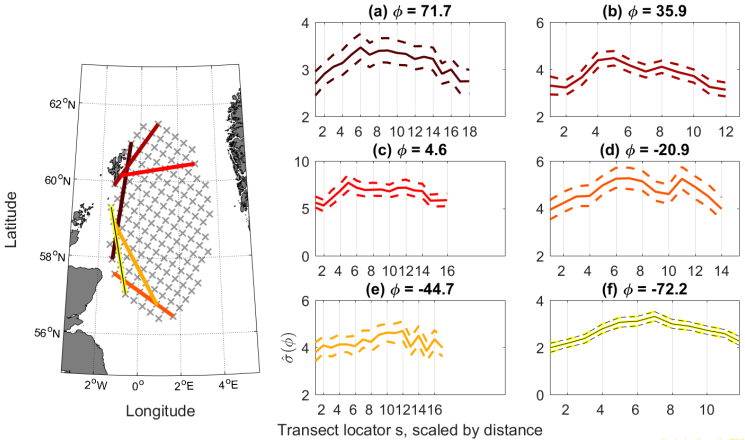
Spatial : extremal coefficient $\hat{\theta}(\phi)$

Estimated extremal coefficient $\hat{\theta}(\phi)$ for all transects with a given orientation ϕ, estimated using 1-D Smith (black), Schlather (dark grey) and Brown-Resnick (light grey) processes. The first (second) row corresponds = marginal threshold with non-exceedance probability 0.5 (0.8). The first (second) column = censoring threshold with non-exceedance probability 0.5 (0.8)



Spatial : spatial dependence parameter $\hat{\sigma}(\phi, s)$ for individual transects

Smith process with marginal and censoring thresholds = non-exceedance probability of 0.8. (b)-(g): $\hat{\sigma}(\phi, s)$ for fixed orientation ϕ (given in the panel title) as a function of transect locator s. (a): transects with $s = 1$ for different orientations ϕ. (b)-(g): abscissa values for transect locators are scaled to physical perpendicular distances between parallel transects



Summary

- Evidence for covariate effects in marginal, conditional and spatial extremes of ocean storms
  - Modelling non-stationarity essential for understanding extreme ocean storms, and estimating marine risk well
  - Non-parametric P-spline flexible basis for covariate description
  - Essential that non-stationary models are used for marginal, conditional and spatial extremes inference of ocean environment
  - Cradle-to-grave uncertainty quantification
- Further investigation of covariate effects in spatial ocean extremes needed
  - Anisotropy in North Sea hindcast, maybe absolute location (or fetch) effect?
  - Currently examining satellite altimeter measurements
  - Asymptotic independence?
- Goal : Bayesian inference for whole-basin spatial models with 4D covariates

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Diolch yn fawr iawn!