Latent Gauss-Markov models for spatial and spatiotemporal conditional extremes

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joint work with

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INRAE

Bayesian modeling and specificity of extremes

- Extreme-value setting: extensive probabilistic theory but **data are scarce!**
- **Bayesian benefits:**
  - Incorporation of physical constraints and expert opinion
  - Pooling of information, e.g. across space and time:
    - Hierarchical structures for parameters
    - Regularization/smoothing

Today's talk: Focus on **spatial dependence modeling**
(marginal distributions are normalized beforehand)

Reviews of Bayesian modeling and software for extremes:

- *Coles, S. G., & Powell, E. A. (1996). Bayesian methods in extreme value modelling: a review and new developments. International Statistical Review/Revue Internationale de Statistique, 119-136.*
- *Stephenson A.G. (2016) Bayesian inference for extreme value modelling. In: Dey DK, Yan J (eds) Extreme Value Modeling and Risk Analysis: Methods and Applications, CRC Press, Boca Raton, FL, pp 257–280*
- *Belzile, L. R., Dutang, C., Northrop, P. J., & Opitz, T. (2022). A modeler's guide to extreme value software. arXiv preprint arXiv:2205.07714.*

Modeling spatially dependent extremes

Spatial extent and duration of extreme episodes often matter
(*e.g.*, heatwaves, storms, precipitation cumulated over a catchment)

⚠ Plain Gaussian processes usually inappropriate for extreme events

- **Extreme-value limit theory** for linearly rescaled **maxima** or **threshold exceedances**
  $\rightarrow$ Max-stable processes, Peaks-over-threshold stable processes

- **Strong assumptions on dependence stability** in such classical limit models

  ⚠ Dependence strength does not change with the level of extremeness:

  $$t \times \Pr(\boldsymbol{X}^\star \in tE) = \Pr(\boldsymbol{X}^\star \in E) \quad \text{for extreme events } E \text{ and any } t > 0$$

Conditional extremes framework [Heffernan and Tawn, 2004]

Principle: Condition the process $X(s)$ on exceedance $X(s_0) > u$ at fixed location s_0

$\Rightarrow$ **Higher flexibility** with respect to extremal dependence structures

$\Rightarrow$ Recent **spatial and spatiotemporal extensions**
[Simpson and Wadsworth, 2020, Wadsworth and Tawn, 2022]

The "big-n problem" in spatial modeling

Spatial: $n =$ number of observation locations
Spatiotemporal: $n =$ number of spatial locations $\times$ number of time steps

- Likelihoods require costly computations involving **large variance-covariance matrices**
- **Low-rank representations** of matrices can alleviate the problem
- **Latent Gaussian fields**: number of latent variables $\ll$ number of observations
- **Markov structures** in latent Gaussian fields $\Rightarrow$ **Sparse precision matrices**
- **Bayesian INLA–SPDE framework** leverages latent Gauss–Markov fields

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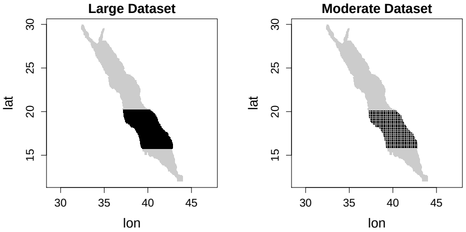
Example: OSTIA reanalysis data
$\rightarrow$ Red Sea Surface Temperatures
$\rightarrow$ 16703 pixels



Scope of today's talk

- Framework of **spatial conditional extremes**:
  certain **nonstationary Gaussian processes** flexibly capture extremal dependence

- **INLA-SPDE framework:**
  flexible Bayesian modeling **with many observation locations**

- Application to **marine heatwaves in the Red Sea**

1. Modeling spatial conditional extremes
2. High-dimensional Bayesian spatial conditional extremes
3. Application to Red Sea surface temperatures

The general spatial conditional extremes framework

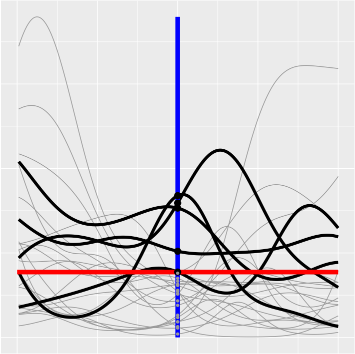
Spatial conditional extremes [Wadsworth and Tawn, 2022]

$\Rightarrow$ A flexible modeling framework beyond asymptotic dependence stability

- Observations $X_t(s)$ at regular time steps $t = 1, 2, \dots$
- Process is modeled conditional on threshold exceedance at fixed location s_0 (i.e. an extreme event occurs at time t if $X_t(s_0) > u$)

Illustration in $\mathbb{R}^1$:

- Conditioning location s_0 (blue)
- Threshold u (red)
- Extreme episodes (black)



Asymptotic formulation of conditional extremes

[⚠ We drop the time replicate index t to simplify notations!]

Assume a stationary spatial process $\{X(s)\}$ with **exponential upper tails** :

$$\exp(x) \times \Pr(X(s) > x) \to 1, \quad x \to \infty$$

$\Rightarrow$ In practice, we **pretransform to standard Laplace distribution**

Asymptotic assumption

Given a threshold $u \to \infty$, we assume that there exist **deterministic normalizing functions** $a_{s-s_0}(X(s_0))$ and $b_{s-s_0}(X(s_0))$ such that

$$\left(\frac{X(s) - a_{s-s_0}(X(s_0))}{b_{s-s_0}(X(s_0))}, X(s_0) - u \right) \Bigg| \, (X(s_0) > u) \xrightarrow{d} (Z^0(s), E), \quad u \to \infty$$

- $E \sim \mathrm{Exp}(1)$ at the conditioning location s_0
- **Residual stochastic process** $Z^0(s)$: independent of E, with constraint $Z^0(s_0) = 0$
- For coherence, we need $a_0(x) = x$ and $a_{s-s_0}(x) \leq x$
- No dependence stability if we can define $a_{s-s_0}(x) < x$ for $s \neq s_0$

Modeling assumption in practice [Wadsworth and Tawn, 2022]

$$X(s) \mid (X(s_0) = x) \quad \stackrel{d}{=} \quad a_{s-s_0}(x) + b_{s-s_0}(x)\, Z^0(s), \quad x > u$$

[Wadsworth and Tawn, 2022] develop parametric models:

- Residual process $Z^0(s)$ based on parametric stationary Gaussian process $Z(s)$, *e.g.*

  $$Z^0(s) = Z(s) - Z(s_0)$$

  with the flexible **Mátern covariance**

- Parametric forms of mean function $a_{s-s_0}(x)$ and scaling function $b_{s-s_0}(x)$

$\Rightarrow$ Frequentist full likelihood inference is tractable with up to hundreds of locations

⚠ **We want to handle data with thousands of locations!**

Modeling extensions to the Wadsworth–Tawn models

New extensions:

- **Semi-parametric conditional mean** $a_{s-s_0}(x)$ using basis expansions
- **Higher-dimensional inference:** work with latent Gaussian processes to allow for

  number of latent Gaussian variables $\ll$ number of observations

- **Bayesian inference** using **Penalized Complexity priors** for hyperparameters (variances, correlations) [Simpson et al., 2017]

Implementation:

- **Stochastic Partial Differential Equation** for latent Gauss–Markov process $Z(s)$
- **Integrated Nested Laplace Approximation** for Bayesian estimation

The Stochastic Partial Differential Equation approach

SPDE approach $\Rightarrow$ computationally convenient representations of Matérn covariance

Theoretical result [Whittle, 1954]:

Gaussian process $Z(s)$ with **Matérn covariance** (regularity ν) is stationary solution to

$$\left(\kappa^2 - \Delta\right)^{\zeta/2} Z(s) = B(s), \quad s \in \mathbb{R}^D, \quad \zeta = \nu + D/2$$

with

- Laplacian operator $\Delta y = \sum_{j=1}^{D} \partial^2 y / \partial^2 x_j$
- Gaussian white noise process $B(s)$

From SPDEs to high-dimensional spatial statistics

Approximate Gauss–Markov solution [Lindgren et al., 2011]

- Triangulation of space using a mesh with knots $\tilde{s}_\ell$, $\ell = 1, \ldots, m$
- Finite-element basis representation $Z(s) = \sum_{\ell=1}^{m} Z(\tilde{s}_\ell)\psi_\ell(s)$
- Solve SPDE on mesh to obtain

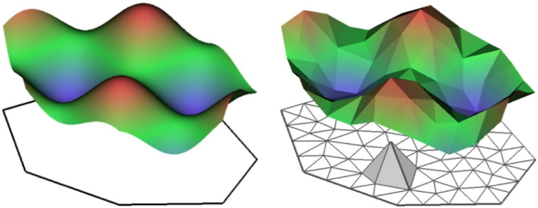
$$(Z(\tilde{s}_1), \ldots, Z(\tilde{s}_m)) \sim \mathcal{N}(\mathbf{0}, \boldsymbol{Q}^{-1})$$

with **sparse precision matrix** $\boldsymbol{Q}$

Spatial interpolation (towards any set of locations $s_1, \ldots, s_d$):

$$(Z(s_1), \ldots, Z(s_d))^T = \boldsymbol{A}(Z(\tilde{s}_1), \ldots, Z(\tilde{s}_m))^T$$

with **observation matrix** $\boldsymbol{A}$ having entries $a_{i,k} = \psi_k(s_i)$



“INLA models” are Bayesian hierarchical models

Integrated Nested Laplace Approximation [Rue et al., 2009]:
allows estimating **latent Gaussian models** through **Laplace approximations**

General Bayesian hierarchical structure

Given a generic observation vector $\boldsymbol{V}$, we assume:

$$\begin{aligned} \boldsymbol{\theta} &\sim \pi(\cdot) && \text{hyperparameters} \\ \boldsymbol{W} \mid \boldsymbol{\theta} &\sim \mathcal{N}_m(\mathbf{0}, Q(\boldsymbol{\theta})^{-1}) && \text{latent Gaussian components} \\ V_i \mid \boldsymbol{W}, \boldsymbol{\theta} &\overset{\text{ind.}}{\sim} \pi(\cdot \mid \eta_i(\boldsymbol{W}), \boldsymbol{\theta}) && \text{likelihood of observations} \end{aligned}$$

- Laplace approximation is deterministic and is used to
  - integrate out $\boldsymbol{W}$ in the posterior $\pi(\boldsymbol{\theta} \mid \boldsymbol{V})$, and
  - integrate out $\boldsymbol{\eta}_{-j}$ in the posterior $\pi(\eta_j, \boldsymbol{\theta} \mid \boldsymbol{V})$
- Numerical integration to integrate out small number of hyperparameters $\boldsymbol{\theta}$

$\Rightarrow$ **Accurate deterministic approximations** for all **univariate posteriors**

Spatial conditional extremes in INLA

Considered model structure ($\beta \in [0,1]$ controls residual variance depending on x):

$$X(s_i) \mid [X(s_0) = x] = x \times \alpha(\|s_i - s_0\|) + \gamma(\|s_i - s_0\|) + x^\beta Z^0(s_i)$$

Model formulation in INLA

$$V_i \mid \eta_i \sim \mathcal{N}(\eta_i, \sigma^2) \quad \text{with} \quad \eta_i = x \cdot \alpha(s_i - s_0) + \gamma(s_i - s_0) + x^\beta Z^0(s_i)$$

- Residual process $Z^0(s) = Z(s) - Z(s_0) \to$ SPDE in 2D for $Z(s)$
- Spline functions α and $\gamma \to$ SPDE in 1D with boundary constraints at $s_i - s_0 = 0$
- Small i.i.d. noise with variance σ^2 to "match" η_i and V_i

Observation matrix $A \in \mathbb{R}^{n\times m}$ with $\boldsymbol{\eta} = \boldsymbol{\eta}(\boldsymbol{W}) = A\boldsymbol{W}$

- $\boldsymbol{W} = (\boldsymbol{W}_\alpha^\top, \boldsymbol{W}_\gamma^\top, \boldsymbol{W}_Z^\top)^\top \in \mathbb{R}^{m_\alpha} \times \mathbb{R}^{m_\gamma} \times \mathbb{R}^{m_Z}$, with $m_\alpha + m_\gamma + m_Z = m$
- A is the concatenation of $A_\alpha \in \mathbb{R}^{d\times m_\alpha}$, $A_\gamma \in \mathbb{R}^{d\times m_\gamma}$, and $A_S^0 \in \mathbb{R}^{d\times m_Z}$
- To model $Z^0(s) = Z(s) - Z(s_0)$, we set $A_S^0 = A_{s_1,\dots,s_d} - \begin{pmatrix} A_{s_0} \\ \vdots \\ A_{s_0} \end{pmatrix} \in \mathbb{R}^{d\times m_Z}$

Recap of the full algorithm

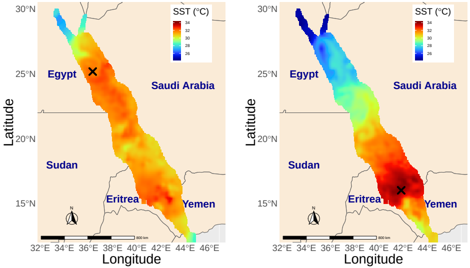
1. Estimate univariate model and normalize margins to standard Laplace $X_t(s)$
2. Fix a conditioning site s_0 and a high threshold u
3. Extract extreme episodes occuring at times $\tilde{t}$ with $X_{\tilde{t}}(s_0) > u$
4. Fit spatial INLA-SPDE Gaussian model to replicates of extreme episodes

1. Modeling spatial conditional extremes
2. High-dimensional Bayesian spatial conditional extremes
3. Application to Red Sea surface temperatures

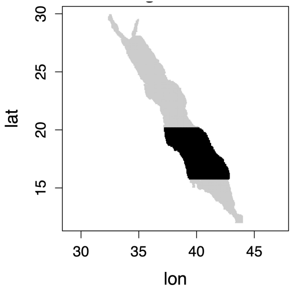
Red Sea surface temperature hotspots

- The Red Sea is a rich ecosystem with many endemic species and coral reefs
  ⚠ Climate change impacts (*e.g.*, coral bleaching due to marine heatwaves)
- **Dataset:** OSTIA gridded daily SST data (1985–2015, 16,703 pixels)
- Focus on southern Red Sea with many coral reefs (6239 grid cells)
- Conditioning location s_0 far from the coast
- Using the 95%-quantile as threshold, we extract **141 extreme episodes**

Examples of extreme episodes



Dataset



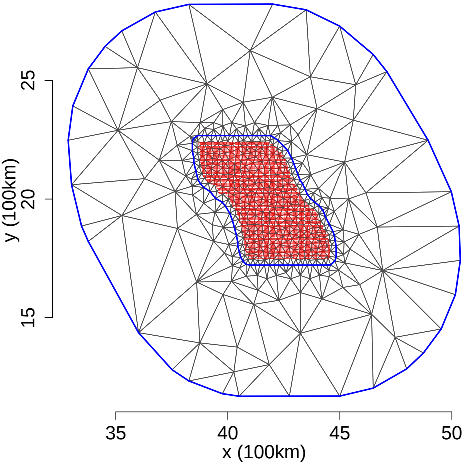
Model variants of conditional extremes

Various submodels of the most complex model are considered:

$$
\begin{aligned}
&(1) \quad x \cdot \alpha(\|s - s_0\|) + Z^0(s) \\
&(2) \quad x + \gamma(\|s - s_0\|) + Z^0(s) \\
&(3) \quad x \cdot \alpha(\|s - s_0\|) + \gamma(\|s - s_0\|) + Z^0(s) \\
&(4) \quad x \cdot \alpha(\|s - s_0\|) + \gamma(\|s - s_0\|) + x^\beta \, Z^0(s)
\end{aligned}
$$

Finite-element mesh for Gauss–Markov $Z(s)$

- Mesh extension beyond the study area to mitigate SPDE boundary conditions
- 541 mesh nodes ($= 8.7\%$ of number of observation pixels n)
- Total of $541 \times 141 = 76281$ **latent Gaussian variables** for residual process Z^0



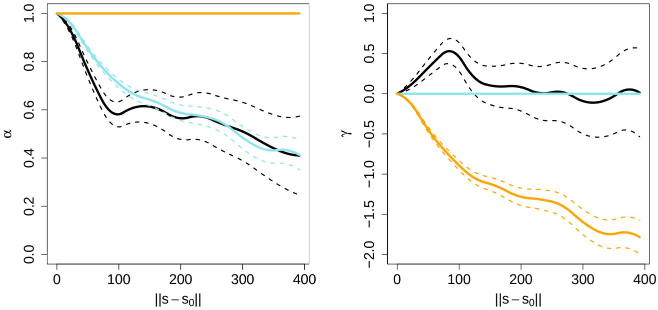
Estimation results

- INLA computation times between 20 and 110 minutes
- WAIC selects most complex models 3 and 4 (approximately equivalent)

Parameter (Model 3)	Posterior mean	95% credible interval
Noise variance σ^2	0.0107	(0.0106,0.0107)
Standard deviation of $Z(s)$	1.56	(1.50,1.62)
Correlation range of $Z(s)$ in km	428	(410, 447)

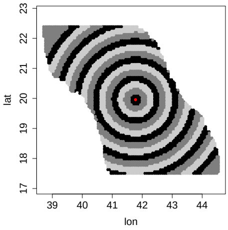
Estimated splines in the conditional mean: α (left), γ (right)

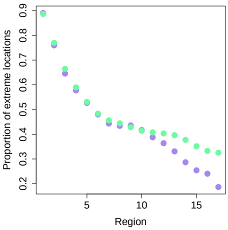
$\rightarrow$ Black curves for Model 3



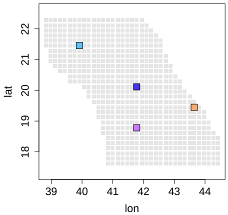
Validation of key properties

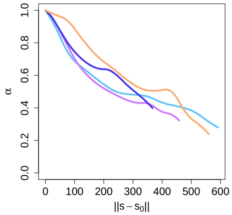
Joint exceedance probabilities: Model 3 (green) vs. Empirical (purple)





Spatial stationarity (when shifting s_0): function α estimated for different s_0





Take-home messages

- Flexible models to assess **extent of extreme-event episodes**
- **Latent variable approach** to decouple latent and observed vector dimensions
- **INLA-SPDE** for fast Bayesian estimation at high spatial resolution
- Extensions to **extreme space-time episodes** spanning $T > 1$ consecutive days:
  - Conditioning location (s_0, t_0) at first day t_0 of episode
  - Tensor-product spline functions $\alpha(\mathrm{dist}, \mathrm{day})$ and $\gamma(\mathrm{dist}, \mathrm{day})$ for $\mathrm{day} \in 1, \ldots, T$
  - $Z(s, t)$ has first-order autoregressive structure (AR1) in time

$\Rightarrow$ Tensor products and AR1 preserve sparse precision matrices $\boldsymbol{Q}$!

Simpson, Opitz, Wadsworth, 2022+, in revision for Extremes
arXiv: `https://arxiv.org/abs/2011.04486`
Code (Github): `https://github.com/essimpson/INLA-conditional-extremes`

— Thank you for your attention —

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