Gaussian Copulas for Large Spatial Fields

Modeling Data-Level Spatial Dependence in Multivariate Generalized Extreme Value Distributions

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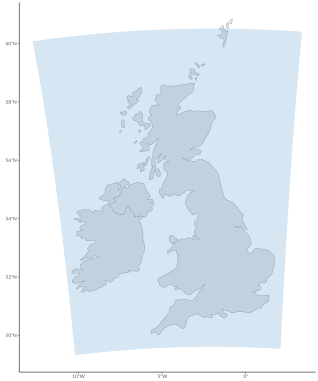
Introduction

- UKCP Local Projections on a 5km grid over the UK (1980-2080)
- Challenge: Modeling maximum daily precipitation in yearly blocks
  - 43,920 spatial locations on a 180 x 244 grid
- Two aspects of spatial dependence:
  1. GEV parameters (ICAR models)
  2. Data-level dependence (Copulas)



Calculating Multivariate Normal Densities

Log Density Formula

$$\log f(\mathbf{x}) \propto \frac{1}{2}\left(\log|\mathbf{Q}| - \mathbf{x}^T\mathbf{Q}\mathbf{x}\right)$$

Key Components

1. **Log Determinant**: $\log|\mathbf{Q}|$
   - Constant for a given precision matrix
2. **Quadratic Form**: $\mathbf{x}^T\mathbf{Q}\mathbf{x}$
   - Needs calculation for each density evaluation

Computational Challenges

- Log determinant calculation
  - Time complexity: $O(n^3)$ for naive methods
  - Memory complexity: $O(n^2)$
- Quadratic form calculation
  - Time complexity: $O(n^2)$
  - Critical for performance in large spatial fields

Spatial Model Considerations

- Some models (e.g., ICAR) avoid log determinant calculation
- Efficient computation crucial for large-scale applications

Spatial Models

Conditional Autoregression (CAR)

- $\mathbf{D}$ is a diagonal matrix with $D_{ii} = n_i$, the number of neighbours of i
- $\mathbf{A}$ is the adjacency matrix with $A_{ij} = A_{ji} = 1$ if $i \sim j$
- τ models overall precision

$$\mathbf{x} \sim N(\mathbf{0}, \tau \mathbf{Q})$$
$$\mathbf{Q} = \mathbf{D}\left(\mathbf{I} - \alpha \mathbf{A}\right)$$

Besag's Intrinsic Conditional Autoregression (ICAR)

- $\alpha = 1$, so $\mathbf{Q}$ is singular, but constant
- Don't have to calculate $\log |\mathbf{Q}|$
- τ is a precision parameter

$$\mathbf{x} \sim N(\mathbf{0}, \tau \mathbf{Q})$$
$$\mathbf{Q} = \mathbf{D} - \mathbf{W}$$

Spatial Models

BYM (Besag-York-Mollié) Model

- $\mathbf{u}$ is the structured spatial component (Besag model)
- $\mathbf{v}$ is the unstructured component (i.i.d. normal)
- τ_u and τ_v are precision parameters for each component

$$\mathbf{x} = \mathbf{u} + \mathbf{v}$$
$$\mathbf{u} \sim \mathrm{ICAR}(\tau_u)$$
$$\mathbf{v} \sim N(\mathbf{0}, \tau_v^{-1})$$

BYM2 Model

- Rewrite the combination to get proper scaling
- ρ models how much of variance is spatial
- s is a scaling factor chosen to make $\mathrm{Var}(\mathbf{u}_i) \approx 1$

$$\mathbf{x} = \left(\left(\sqrt{\rho/s}\right)\mathbf{u} + \left(\sqrt{1-\rho}\right)\mathbf{v}\right)\sigma$$
$$\mathbf{u} \sim \mathrm{ICAR}(1)$$
$$\mathbf{v} \sim N(\mathbf{0}, n)$$

Spatial Modeling on Parameter-level

- $\mu = \mu_0 \left(1 + \Delta \left(t - t_0\right)\right)$, location
- σ: scale
- ξ: shape

$$\log(\mu_0) = \psi \sim \mathrm{BYM2}(\mu_\psi, \rho_\psi, \sigma_\psi)$$

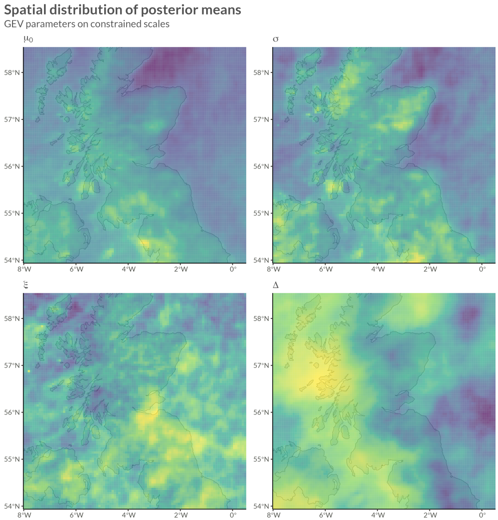
$$\log(\mu_0) - \log(\sigma) = \tau \sim \mathrm{BYM2}(\mu_\tau, \rho_\tau, \sigma_\tau)$$

$$f_\xi(\xi) = \phi \sim \mathrm{BYM2}(\mu_\phi, \rho_\phi, \sigma_\phi)$$

$$f_\Delta(\Delta) = \gamma \sim \mathrm{BYM2}(\mu_\gamma, \rho_\gamma, \sigma_\gamma)$$

Our BYM2 hyperparameters point to a large degree of spatial variation

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
σ_ψ	0.072	0.072	0.001	0.001	0.070	0.074	1.012	137	387
μ_ψ	2.133	2.133	0.001	0.001	2.131	2.135	1.001	5,029	3,417
ρ_ψ	0.998	0.998	0.001	0.001	0.997	0.999	1.000	3,161	3,218
σ_τ	0.102	0.102	0.002	0.002	0.098	0.106	1.015	381	973
μ_τ	−0.923	−0.923	0.001	0.001	−0.926	−0.921	1.000	4,130	3,507
ρ_τ	0.997	0.998	0.001	0.001	0.996	0.999	1.001	3,192	2,903
σ_ϕ	0.358	0.358	0.009	0.009	0.343	0.372	1.008	401	730
μ_ϕ	0.341	0.341	0.004	0.004	0.335	0.347	1.001	3,728	3,049
ρ_ϕ	0.996	0.997	0.001	0.001	0.994	0.998	1.002	1,995	2,677
σ_γ	0.332	0.333	0.011	0.011	0.313	0.351	1.029	105	208
μ_γ	1.438	1.438	0.012	0.012	1.419	1.458	1.001	2,517	3,053
ρ_γ	0.996	0.996	0.002	0.001	0.993	0.998	1.000	3,823	2,875



From Parameter-level to Data-level Dependence

Parameter-level Dependence

- Assumes conditional independence
- Biased joint probability estimates
- Underestimates parameter variance

Copula

- Improves joint probabilities
- Enhances spatial risk assessment
- Better variance estimates

Sklar's Theorem: For any multivariate distribution H, there exists a unique copula C such that:

$$H(\mathbf{x}) = C(F_1(x_1), \dots, F_d(x_d))$$

where F_i are marginal distributions. We can also write this as a log-density

$$\log h(x) = \log c(F_1(x_1), \dots, F_d(x_d)) \sum_{i=1}^{d} \log f_i(x_i)$$

Our Approach: Matérn-like Gaussian Copula

Marginal CDFs, $F_i(x_i)$, is $\mathrm{GEV}(\mu_i, \sigma_i, \xi_i)$

$$\log h(\mathbf{x}) = \log c(u_1, \ldots, u_d) + \sum_{i=1}^{d} f_{\mathrm{GEV}}(x_i | \mu_i, \sigma_i, \xi_i)$$
$$u_i = F_{\mathrm{GEV}}(x_i | \mu_i, \sigma_i, \xi_i)$$

Gaussian Copula

$$\log c(\mathbf{u}) \propto \frac{1}{2} \left(\log |\mathbf{Q}| - \mathbf{z}^T \mathbf{Q} \mathbf{z} + \mathbf{z}^T \mathbf{z} \right)$$
$$\mathbf{z} = \Phi^{-1}(\mathbf{u})$$

The Precision Matrix

$\mathbf{Q}$ defined as Kronecker sum of two AR(1) precision matrices

$$\mathbf{Q} = \left(\mathbf{Q}_{\rho_1} \otimes \mathbf{I_{n_2}} + \mathbf{I_{n_1}} \otimes \mathbf{Q}_{\rho_2}\right)^{\nu+1}, \quad \nu \in \{0, 1, 2\}$$

$$\mathbf{Q}_\rho = \frac{1}{1-\rho^2} \begin{bmatrix} 1 & -\rho & 0 & \cdots & 0 \\ -\rho & 1+\rho^2 & -\rho & \cdots & 0 \\ 0 & -\rho & 1+\rho^2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

Eigendecomposition

Because of how $\mathbf{Q}$ is defined, we know that

$$\begin{aligned}\mathbf{Q} &= \mathbf{V}\Lambda\mathbf{V} \\ &= (\mathbf{V}_1 \otimes \mathbf{V}_2)(\Lambda_{\rho_1} \otimes \mathbf{I} + \mathbf{I} \otimes \Lambda_{\rho_2})^{\nu+1}(\mathbf{V}_1 \otimes \mathbf{V}_2)^T \\ \mathbf{Q}_{\rho_1} &= \mathbf{V}_1\Lambda_{\rho_1}\mathbf{V}_1{}^T \qquad \& \qquad \mathbf{Q}_{\rho_2} = \mathbf{V}_2\Lambda_{\rho_2}\mathbf{V}_2{}^T\end{aligned}$$

Spectral decomposition defined by value/vector pairs of smaller matrices

$$\left\{\lambda_{\rho_1}\right\}_i + \left\{\lambda_{\rho_2}\right\}_j \qquad\qquad \left\{\mathbf{v}_{\rho_1}\right\}_i \otimes \left\{\mathbf{v}_{\rho_2}\right\}_j$$

- Problem: $\Sigma_{ii} = \left(\mathbf{Q}^{-1}\right)_{ii} \neq 1$
- Solution: $\tilde{\mathbf{Q}} = \mathbf{DQD}$, where $\mathbf{D}_{ii} = \sqrt{\Sigma_{ii}}$

Marginal Standard Deviations

$$\Sigma = \mathbf{Q}^{-1} = (\mathbf{V}\Lambda\mathbf{V}^T)^{-1} = \mathbf{V}\Lambda^{-1}\mathbf{V}$$

We know that if $A = BC$ then $A_{ii} = B_{i,.}C_{.,i}$, so

$$\Sigma_{ii} = \sum_{k=1}^{n} v_{ik}\frac{1}{\lambda_k}(v^T)_{ki} = \sum_{k=1}^{n} v_{ik}\frac{1}{\lambda_k}v_{ik} = \sum_{k=1}^{n} v_{ik}^2\frac{1}{\lambda_k}$$

Compute vector σ^2 containing all marginal variances

$$\sigma^2 = \sum_{i=1}^{n_1}\sum_{j=1}^{n_2} \frac{\left(\left\{\mathbf{v}_{\rho_1}\right\}_i \otimes \left\{\mathbf{v}_{\rho_2}\right\}_j\right)^2}{\left(\left\{\lambda_{\rho_1}\right\}_i + \left\{\lambda_{\rho_2}\right\}_j\right)^{\nu+1}}$$

Marginal Standard Deviations

```r
dim1 <- 50; dim2 <- 50
rho1 <- 0.5; rho2 <- 0.3
nu <- 2
Q1 <- make_AR_prec_matrix(dim1, rho1)
Q2 <- make_AR_prec_matrix(dim2, rho2)
I1 <- Matrix::Diagonal(dim1)
I2 <- Matrix::Diagonal(dim2)

Q <- temp <- kronecker(Q1, I2) + kronecker(I1, Q2)
for (i in seq_len(nu)) Q <- Q %*% temp
```

```r
msd <- function(Q1, Q2) {
  E1 <- eigen(Q1)
  E2 <- eigen(Q2)
  marginal_sd_eigen(
    E1$values, E1$vectors, dim1,
    E2$values, E2$vectors, dim2,
    nu
  ) |>
  sort()
}
```

```r
bench::mark(
  "solve" = solve(Q) |> diag() |> sqrt() |> sort(),
  "inla.qinv" = inla.qinv(Q) |> diag() |> sqrt() |> sort(),
  "marginal_sd_eigen" = msd(Q1, Q2),
  iterations = 10, filter_gc = FALSE
)
```

```
# A tibble: 3 x 6
  expression             min   median `itr/sec` mem_alloc `gc/sec`
  <bch:expr>        <bch:tm> <bch:tm>     <dbl> <bch:byt>    <dbl>
1 solve                1.26s    1.27s     0.781   78.17MB    0.781
2 inla.qinv          377.1ms 384.86ms     2.49     4.35MB    0
3 marginal_sd_eigen   3.47ms   3.54ms   262.     649.35KB    0
```