Spatial Extremes: A R package for Modelling Spatial Extremes

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Appendix A

Density and Gradient **Computations**

A.1The Smith Characterisation

The Smith characterisation of a max-stable process is given by:

$$\Pr[Z_1 \le z_1, Z_2 \le z_2] = \exp\left[-\frac{1}{z_1}\Phi\left(\frac{a}{2} + \frac{1}{a}\log\frac{z_2}{z_1}\right) - \frac{1}{z_2}\Phi\left(\frac{a}{2} + \frac{1}{a}\log\frac{z_1}{z_2}\right)\right] \tag{A.1}$$

where Φ is the standard normal cumulative distribution function and, for two location #1 and #2

$$a^2 = \Delta x^T \Sigma^{-1} \Delta x$$
 and $\Sigma = \begin{bmatrix} cov_{11} & cov_{12} \\ cov_{12} & cov_{22} \end{bmatrix}$

where Δx is the distance vector between location #1 and location #2.

A.1.1Useful quantities

Computation of the density as well as the gradient of the density is not difficult but "heavy" though. For computation facilities and to help readers, we define:

$$c_1 = \frac{a}{2} + \frac{1}{a} \log \frac{z_2}{z_1}$$
 and $c_2 = \frac{a}{2} + \frac{1}{a} \log \frac{z_1}{z_2}$ (A.2)

From these definitions, we note that $c_1 + c_2 = a$.

A.1.2 Density computation

From (A.1), we note the standard normal distribution appears. Consequently, we need to compute its derivatives in c_1 and c_2 .

$$\frac{\partial c_1}{\partial z_1} = \frac{1}{a} \left(-\frac{z_2}{z_1^2} \frac{z_1}{z_2} \right) = -\frac{1}{az_1} \qquad \frac{\partial c_1}{\partial z_2} = \frac{1}{a} \frac{1}{z_1} \frac{z_1}{z_2} = \frac{1}{az_2} \qquad (A.3)$$

$$\frac{\partial c_2}{\partial z_1} = -\frac{\partial c_1}{\partial z_1} = \frac{1}{az_1} \qquad \frac{\partial c_2}{\partial z_2} = -\frac{\partial c_1}{\partial z_2} = -\frac{1}{az_2} \qquad (A.4)$$

$$\frac{\partial c_2}{\partial z_1} = -\frac{\partial c_1}{\partial z_1} = \frac{1}{az_1} \qquad \qquad \frac{\partial c_2}{\partial z_2} = -\frac{\partial c_1}{\partial z_2} = -\frac{1}{az_2}$$
 (A.4)

As the normal distribution appears in the Smith characterisation, the following quantities will

be useful:

$$\frac{\partial \Phi(c_1)}{\partial z_1} = \frac{\partial \Phi(c_1)}{\partial c_1} \frac{\partial c_1}{\partial z_1} = -\frac{\varphi(c_1)}{az_1} \qquad \qquad \frac{\partial \Phi(c_1)}{\partial z_2} = \frac{\partial \Phi(c_1)}{\partial c_1} \frac{\partial c_1}{\partial z_2} = \frac{\varphi(c_1)}{az_2}$$
(A.5)

$$\frac{\partial \Phi(c_1)}{\partial z_1} = \frac{\partial \Phi(c_1)}{\partial c_1} \frac{\partial c_1}{\partial z_1} = -\frac{\varphi(c_1)}{az_1} \qquad \frac{\partial \Phi(c_1)}{\partial z_2} = \frac{\partial \Phi(c_1)}{\partial c_1} \frac{\partial c_1}{\partial z_2} = \frac{\varphi(c_1)}{az_2} \qquad (A.5)$$

$$\frac{\partial \Phi(c_2)}{\partial z_1} = \frac{\partial \Phi(c_2)}{\partial c_2} \frac{\partial c_2}{\partial z_1} = \frac{\varphi(c_2)}{az_1} \qquad \frac{\partial \Phi(c_2)}{\partial z_2} = \frac{\partial \Phi(c_2)}{\partial c_2} \frac{\partial c_2}{\partial z_2} = -\frac{\varphi(c_2)}{az_2} \qquad (A.6)$$

$$\frac{\partial \varphi(c_1)}{\partial z_1} = \frac{\partial \varphi(c_1)}{\partial c_1} \frac{\partial c_1}{\partial z_1} = \frac{c_1 \varphi(c_1)}{az_1} \qquad \frac{\partial \varphi(c_1)}{\partial z_2} = \frac{\partial \varphi(c_1)}{\partial c_1} \frac{\partial c_1}{\partial z_2} = -\frac{c_1 \varphi(c_1)}{az_2} \qquad (A.7)$$

$$\frac{\partial \varphi(c_2)}{\partial z_1} = \frac{\partial \varphi(c_2)}{\partial c_2} \frac{\partial c_2}{\partial z_1} = -\frac{c_2 \varphi(c_2)}{az_1} \qquad \frac{\partial \varphi(c_2)}{\partial z_2} = \frac{\partial \varphi(c_2)}{\partial c_2} \frac{\partial c_2}{\partial z_2} = \frac{c_2 \varphi(c_2)}{az_2} \qquad (A.8)$$

$$\frac{\partial \varphi(c_1)}{\partial z_1} = \frac{\partial \varphi(c_1)}{\partial c_1} \frac{\partial c_1}{\partial z_1} = \frac{c_1 \varphi(c_1)}{a z_1} \qquad \qquad \frac{\partial \varphi(c_1)}{z_2} = \frac{\partial \varphi(c_1)}{\partial c_1} \frac{\partial c_1}{\partial z_2} = -\frac{c_1 \varphi(c_1)}{a z_2} \qquad (A.7)$$

$$\frac{\partial \varphi(c_2)}{\partial z_1} = \frac{\partial \varphi(c_2)}{\partial c_2} \frac{\partial c_2}{\partial z_1} = -\frac{c_2 \varphi(c_2)}{a z_1} \qquad \qquad \frac{\partial \varphi(c_2)}{\partial z_2} = \frac{\partial \varphi(c_2)}{\partial c_2} \frac{\partial c_2}{\partial z_2} = \frac{c_2 \varphi(c_2)}{a z_2}$$
(A.8)

Define

$$A = \frac{1}{z_1} \Phi(c_1)$$
 and $B = \frac{1}{z_2} \Phi(c_2)$ (A.9)

Consequently, $F(z_1, z_2) = exp(-A - B)$ and

$$\frac{\partial F}{\partial z_1}(z_1, z_2) = -\left(\frac{\partial A}{\partial z_1} + \frac{\partial B}{\partial z_1}\right) F(z_1, z_2) \qquad \frac{\partial F}{\partial z_2}(z_1, z_2) = -\left(\frac{\partial A}{\partial z_2} + \frac{\partial B}{\partial z_2}\right) F(z_1, z_2) \tag{A.10}$$

By noting that

$$\frac{\partial A}{\partial z_1} = -\frac{\Phi(c_1)}{z_1^2} + \frac{1}{z_1} \left(-\frac{\varphi(c_1)}{az_1} \right) = -\frac{\Phi(c_1)}{z_1^2} - \frac{\varphi(c_1)}{az_1^2}$$
(A.11)

$$\frac{\partial B}{\partial z_1} = \frac{1}{z_2} \frac{\varphi(c_2)}{az_1} = \frac{\varphi(c_2)}{az_1 z_2} \tag{A.12}$$

$$\frac{\partial A}{\partial z_2} = \frac{1}{z_1} \frac{\varphi(c_1)}{az_2} = \frac{\varphi(c_1)}{az_1 z_2} \tag{A.13}$$

$$\frac{\partial B}{\partial z_2} = -\frac{\Phi(c_2)}{z_2^2} + \frac{1}{z_2} \left(-\frac{\varphi(c_2)}{az_2} \right) = -\frac{\Phi(c_2)}{z_2^2} - \frac{\varphi(c_2)}{az_2^2}$$
 (A.14)

and

$$\frac{\partial^2 A}{\partial z_2 \partial z_1} = \frac{\partial}{\partial z_2} \left(-\frac{\Phi(c_1)}{z_1^2} - \frac{\varphi(c_1)}{az_1^2} \right) = -\frac{\varphi(c_1)}{az_1^2 z_2} + \frac{c_1 \varphi(c_1)}{a^2 z_1^2 z_2} = -\frac{c_2 \varphi(c_1)}{a^2 z_1^2 z_2}$$
(A.15)

$$\frac{\partial^2 B}{\partial z_2 \partial z_1} = \frac{\partial}{\partial z_2} \frac{\varphi(c_2)}{a z_1 z_2} = -\frac{c_1 \varphi(c_2)}{a^2 z_1 z_2^2} \tag{A.16}$$

So that,

$$\frac{\partial F}{\partial z_1}(z_1, z_2) = \left(\frac{\Phi(c_1)}{z_1^2} + \frac{\varphi(c_1)}{az_1^2} - \frac{\varphi(c_2)}{az_1 z_2}\right) F(z_1, z_2) \tag{A.17}$$

$$\frac{\partial F}{\partial z_2}(z_1, z_2) = \left(\frac{\Phi(c_2)}{z_2^2} + \frac{\varphi(c_2)}{az_2^2} - \frac{\varphi(c_1)}{az_1 z_2}\right) F(z_1, z_2) \tag{A.18}$$

Finally,

$$\frac{\partial^2 F}{\partial z_2 \partial z_1}(z_1, z_2) = -\left(\frac{\partial^2 A}{\partial z_2 \partial z_1} + \frac{\partial^2 B}{\partial z_2 \partial z_1}\right) F(z_1, z_2) - \left(\frac{\partial A}{\partial z_1} + \frac{\partial B}{\partial z_1}\right) \frac{\partial F}{\partial z_2}(z_1, z_2) \tag{A.19}$$

Thus, it leads to the following relation:

$$\frac{f(z_1, z_2)}{F(z_1, z_2)} = \frac{c_2 \varphi(c_1)}{a^2 z_1^2 z_2} + \frac{c_1 \varphi(c_2)}{a^2 z_1 z_2^2} + \left(\frac{\Phi(c_1)}{z_1^2} + \frac{\varphi(c_1)}{a z_1^2} - \frac{\varphi(c_2)}{a z_1 z_2}\right) \left(\frac{\Phi(c_2)}{z_2^2} + \frac{\varphi(c_2)}{a z_2^2} - \frac{\varphi(c_1)}{a z_1 z_2}\right) \quad (A.20)$$

A.1.3 Gradient computation

The gradient of the density must be known as we fit our model using pairwise likelihood rather than the "full" likelihood. Consequently, our model is "mispecified" and we need to compute standard errors using a **sandwich estimator**. Let $\hat{\theta}$ be the maximum pairwise likelihood estimate; then:

$$\hat{\theta} \sim \mathcal{N} \left(\theta, H^{-1} J H^{-1} \right)$$

where H is the Fisher information matrix and J the gradient of the log pairwise likelihood. Let us recall that the log pairwise likelihood is defined by:

$$\ell_{pair}(\mathbf{x}, \Sigma^{-1}) = \sum_{k=1}^{n_{obs}} \sum_{i=1}^{n_{site}-1} \sum_{j=i+1}^{n_{site}} \log f(x_k^{(i)}, x_k^{(j)})$$

where n_{obs} is the number of observations, $\mathbf{x}_k = (x_k^{(1)}, \dots, x_k^{(n_{site})})$ is the k-th observation vector, n_{site} is the number of site within the region and f is the bivariate density.

Consequently, the gradient of the log pairwise density is given by:

$$\nabla f_{pair}(\mathbf{x}, \Sigma^{-1}) = \sum_{i=1}^{n_{site}-1} \sum_{j=i+1}^{n_{site}} \nabla \log f(x_k^{(i)}, x_k^{(j)})$$

Define:

$$A = -\frac{\Phi(c1)}{z_1} - \frac{\Phi(c2)}{z_2}$$

$$B = \frac{\Phi(c_2)}{z_2^2} + \frac{\varphi(c_2)}{az_2^2} - \frac{\varphi(c_1)}{az_1z_2}$$

$$C = \frac{\Phi(c_1)}{z_1^2} + \frac{\varphi(c_1)}{az_1^2} - \frac{\varphi(c_2)}{az_1z_2}$$

$$D = \frac{c_2\varphi(c_1)}{a^2z_1^2z_2} + \frac{c_1\varphi(c_2)}{a^2z_1z_2^2}$$

so that.

$$\log f(x_k^{(i)}, x_k^{(j)}) = A + \log(BC + D)$$

As the logarithm of the bivariate density f is only a function of the Mahalanobis distance a, the gradient is given through the following relation¹:

$$\nabla \log f(x_k^{(i)}, x_k^{(j)}) = \frac{\partial}{\partial a} \log f(x_k^{(i)}, x_k^{(j)}) \left(\frac{\partial a}{\partial cov11}, \frac{\partial a}{\partial cov12}, \frac{\partial a}{\partial cov22} \right)^T$$

For clarity purposes, we first compute the following quantities:

$$\frac{\partial c_1}{\partial a} = \frac{1}{2} - \frac{1}{a^2} \log \frac{z_2}{z_1} = \frac{c_2}{a} \qquad \qquad \frac{\partial c_2}{\partial a} = \frac{c_1}{a}$$

$$\frac{\partial \Phi(c_1)}{\partial a} = \frac{\partial \Phi(c_1)}{\partial c_1} \frac{\partial c_1}{\partial a} = \frac{c_2 \varphi(c_1)}{a} \qquad \qquad \frac{\partial \Phi(c_2)}{\partial a} = \frac{c_1 \varphi(c_2)}{a}$$

$$\frac{\partial \varphi(c_1)}{\partial a} = \frac{\partial \varphi(c_1)}{\partial c_1} \frac{\partial c_1}{\partial a} = -\frac{c_1 c_2 \varphi(c_1)}{a} \qquad \qquad \frac{\partial \varphi(c_2)}{\partial a} = -\frac{c_1 c_2 \varphi(c_2)}{a}$$

$$\frac{\partial c_2 \varphi(c_1)}{\partial a} = \frac{c_1 (1 - c_2^2) \varphi(c_1)}{a} \qquad \qquad \frac{\partial c_1 \varphi(c_2)}{\partial a} = \frac{(1 - c_1^2) c_2 \varphi(c_2)}{a}$$

¹algebra operators are defined component-wise.

Consequently, we have:

$$\begin{array}{lll} dA & = & \displaystyle \frac{\partial A}{\partial a} = -\frac{1}{z_1} \frac{c_2 \varphi(c_1)}{a} - \frac{1}{z_2} \frac{c_1 \varphi(c_2)}{a} = -\frac{c_2 \varphi(c_1)}{az_1} - \frac{c_1 \varphi(c_2)}{az_2} \\ dC & = & \displaystyle \frac{\partial C}{\partial a} = \frac{1}{z_1^2} \frac{c_2 \varphi(c_1)}{a} + \frac{1}{z_1^2} \frac{-\frac{c_1 c_2 \varphi(c_1)}{a} a - \varphi(c_1)}{a^2} - \frac{1}{z_1 z_2} \frac{-\frac{c_1 c_2 \varphi(c_2)}{a} a - \varphi(c_2)}{a^2} \\ & = & \displaystyle \frac{c_2 \varphi(c_1)}{az_1^2} - \frac{(1 + c_1 c_2) \varphi(c_1)}{a^2 z_1^2} + \frac{(1 + c_1 c_2) \varphi(c_2)}{a^2 z_1 z_2} \\ & = & \displaystyle \frac{[c_2 (a - c_1) - 1] \, \varphi(c_1)}{a^2 z_1^2} + \frac{(1 + c_1 c_2) \varphi(c_2)}{a^2 z_1 z_2} \\ & = & \displaystyle \frac{(c_2^2 - 1) \varphi(c_1)}{a^2 z_1^2} + \frac{(1 + c_1 c_2) \varphi(c_2)}{a^2 z_1 z_2} \\ dB & = & \displaystyle \frac{\partial B}{\partial a} = \frac{(c_1^2 - 1) \varphi(c_2)}{a^2 z_2^2} + \frac{(1 + c_1 c_2) \varphi(c_1)}{a^2 z_1 z_2} \\ dD & = & \displaystyle \frac{\partial D}{\partial a} = \frac{1}{z_1^2 z_2} \frac{c_1 (1 - c_2^2) \varphi(c_1)}{a} a^2 - 2ac_2 \varphi(c_1)}{a^4} + \frac{1}{z_1 z_2^2} \frac{(1 - c_1^2) c_2 \varphi(c_2)}{a} a^2 - 2ac_1 \varphi(c_2)}{a^4} \\ & = & \displaystyle \frac{(c_1 - 2c_2 - c_1 c_2^2) \varphi(c_1)}{a^3 z_1^2 z_2} + \frac{(c_2 - 2c_1 - c_1^2 c_2) \varphi(c_2)}{a^3 z_1 z_2^2} \end{array}$$

Finally,

$$\nabla \log f(x_k^{(i)}, x_k^{(j)}) = \left[dA + \frac{(CdB + BdC + dD)}{BC + D} \right] \left(\frac{\partial a}{\partial cov11}, \frac{\partial a}{\partial cov12}, \frac{\partial a}{\partial cov22} \right)^T$$

A.2 The Schlather Characterisation

The Schlather characterisation of a max-stable process is given by:

$$\Pr[Z_1 \le z_1, Z_2 \le z_2] = \exp\left[-\frac{1}{2}\left(\frac{1}{z_1} + \frac{1}{z_2}\right)\left(1 + \sqrt{1 - 2(\rho(h) + 1)\frac{z_1 z_2}{(z_1 + z_2)^2}}\right)\right]$$
(A.21)

where h is the distance between location #1 and location #2 and $\rho(h)$ is a valid correlation function such as $-1 \le rho(h) \le 1$.

A.2.1 Density computation

Computation of the density as well as the gradient of the density is not difficult but "heavy" though.

By noting that,

$$\frac{\partial^2}{\partial z_1 \partial z_2} \exp(V(z_1, z_2)) = \left[\frac{\partial^2}{\partial z_1 \partial z_2} V(z_1, z_2) + \left(\frac{\partial}{\partial z_1} V(z_1, z_2) \right) \left(\frac{\partial}{\partial z_2} V(z_1, z_2) \right) \right] \exp(V(z_1, z_2))$$

where $V(z_1, z_2)$ is any function in C^2 .

Consequently, to compute the (bivariate) density, we only need to compute the partial derivatives and the mixed partial derivatives. For our case, it turns out to be:

$$V(z_1, z_2) = -\frac{1}{2} \left(\frac{1}{z_1} + \frac{1}{z_2} \right) \left(1 + \sqrt{1 - 2(\rho(h) + 1) \frac{z_1 z_2}{(z_1 + z_2)^2}} \right)$$

$$\frac{\partial}{\partial z_1}V(z_1,z_2) = -\frac{\rho(h)z_1 - c1 - z_2}{2c_1z_1^2} \quad \frac{\partial}{\partial z_2}V(z_1,z_2) = -\frac{\rho(h)z_2 - c1 - z_1}{2c_1z_2^2} \quad \frac{\partial^2}{\partial z_1\partial z_2}V(z_1,z_2) = \frac{1 - \rho(h)^2}{2c_1^2}$$

where

$$c_1 = \sqrt{z_1^2 + z_2^2 - 2z_1z_2\rho(h)}$$

Lastly,

$$f(z_1, z_2) = \left[\frac{1 - \rho(h)^2}{2c_1^3} + \left(-\frac{\rho(h)z_1 - c_1 - z_2}{2c_1 z_1^2} \right) \left(-\frac{\rho(h)z_2 - c_1 - z_1}{2c_1 z_2^2} \right) \right] \exp(V(z_1, z_2)) \quad (A.22)$$

A.2.2 Gradient computation

From equation (A.22), we have:

$$\log f(z_1, z_2) = A \log(B + CD)$$

where

$$A = V(z_1, z_2) \quad B = \frac{1 - \rho(h)^2}{2c_1^3} \quad C = -\frac{\rho(h)z_1 - c1 - z_2}{2c_1z_1^2} \quad D = -\frac{\rho(h)z_2 - c1 - z_1}{2c_1z_2^2}$$

As the bivariate density is only a function of the covariance function $\rho(h)$, we have:

$$\nabla \log f(z_1, z_2) = \frac{\partial}{\partial \rho(h)} \log f(z_1, z_2) \left(\nabla \rho(h)\right)^T$$

where $\nabla \rho(h)$ is the vector of the partial derivatives of the covariance function $\rho(h)$ with respect to its parameters.

$$\begin{split} dA &= \frac{\partial A}{\partial \rho(h)} = \frac{1}{2c_1} \\ dB &= \frac{\partial B}{\partial \rho(h)} = -\frac{\rho(h)}{c_1^3} + \frac{3(1-\rho(h))z_1z_2}{c_1^5} \\ dC &= \frac{\partial C}{\partial \rho(h)} = -\frac{z_1 - z_2\rho(h)}{2c_1^3} \\ dD &= \frac{\partial D}{\partial \rho(h)} = -\frac{z_2 - z_1\rho(h)}{2c_1^3} \end{split}$$

So that,

$$\nabla \log f(z_1, z_2) = \left[dA + \frac{(CdB + BdC + dD)}{BC + D} \right] (\nabla \rho(h))^T$$