Appendix B – Stochastic partial differential equation approximation to Gaussian random fields

As a maximum likelihood implementation of the spatial Gompertz model, we use a stochastic partial differential equation (SPDE) approximation to a Gaussian random field (Lindgren et al. 2011), as previously implemented and tested in the integrated nested Laplace approximation (INLA) software (Rue et al. 2009). This approach approximates a Gaussian random field using a Gaussian Markov random field whose pairwise correlations follow the Matérn class. This approximation yields the following equivalence:

$$\mathbf{Q} = \tau^2(\kappa^4\mathbf{C} + 2\kappa^2\mathbf{G}_1 + \mathbf{G}_2) \tag{B.1}$$

where **Q** is the precision matrix of Gaussian Markov random field approximation, κ and τ are parameters in the Matérn approximation (when specifying Matérn smoothness parameter $\nu=1$), and **C**, $\mathbf{G}_1$, and $\mathbf{G}_2$ are sparce matrices representing a piecewise linear basis function for the approximation (see Lindgren et al. 2010, Lindgren and Rue 2013 for details). **C**, $\mathbf{G}_1$, and $\mathbf{G}_2$ are calculated using the R-INLA software (Lindgren and Rue 2013) in two steps. First, nodes for a finite element analysis "mesh" are calculated using R-INLA, where this mesh defines a piecewise linear (i.e., triangular in 2-dimensional space) approximation to **C**, $\mathbf{G}_1$, and $\mathbf{G}_2$ between nodes. This mesh has K nodes, where nodes are included at each of I stations as well as additional locations, and the number of additional locations can be predefined to control the tradeoff between precision and computational complexity of the SPDE approximation. R-INLA then calculates values for **C**, $\mathbf{G}_1$, and $\mathbf{G}_2$ at each node. These three sparce matrices are then extracted from R-INLA, and used in Template Model Builder (TMB, Kristensen et al. 2013) in subsequent steps of the maximum likelihood estimation.

Maximum likelihood estimation proceeds by defining $\mathbf{\Omega}^{(k)}$ and $\mathbf{\Psi}_t^{(k)}$, i.e., random fields defined at each node in the SPDE approximation. These follow a multivariate normal distribution.

$$\begin{aligned} \mathbf{\Omega} &\sim MVN\left(\alpha\mathbf{1},\Sigma_{\Omega}\right) \\ \mathbf{\Psi} &\sim MVN\left(0,\Sigma_{\mathrm{E}}\otimes\Sigma_{\psi}\right) \end{aligned} \tag{B.2}$$

where:

$$\begin{aligned} \mathbf{\Sigma}_{\Omega} &= \left(\tau_{\Omega}^2(\kappa_{\Omega}^4\mathbf{C}+2\kappa_{\Omega}^2\mathbf{G}_1+\mathbf{G}_2)\right)^{-1} \\ \mathbf{\Sigma}_{\mathrm{E}} &= \left(\tau_{\mathrm{E}}^2(\kappa_{\mathrm{E}}^4\mathbf{C}+2\kappa_{\mathrm{E}}^2\mathbf{G}_1+\mathbf{G}_2)\right)^{-1} \end{aligned} \tag{B.3}$$

and $\mathbf{\Sigma}_{\psi}$ is as defined in Eq. 2c (in the present application, we assume that $\kappa_{\Omega} = \kappa_{\mathrm{E}}$, although future applications could explore the consequences of relaxing this assumption). $\mathbf{\Omega}^{(k)}$ and $\mathbf{\Psi}_t^{(k)}$ at knots that correspond to stations with data are then used to calculate the conditional probability of available data.

The computational cost of this SPDE approximation is $O(n^{3/2})$, while the cost of inverting the original Gaussian random field is $O(n^3)$, so this approximation is expected to gain in importance as the number of stations for available data increases. Following an emprical hierarchical modelling strategy (*sensu* Cressie and Wikle 2011), $\mathbf{\Omega}^{(k)}$ and $\mathbf{\Psi}_t^{(k)}$ are integrated across while calculating the marginal likelihood of κ, τ_{Ω}, τ_{E}, α, and any other hyperparameters of interest. We then use the delta-method to back-calculate the value of interpretable parameters, i.e., the distance at which the correlation has fallen to approximately 13% of its maximum (the spatial "range" λ):

$$\lambda = \frac{\sqrt{8\nu}}{\kappa} \tag{B.4}$$

and the marginal variance σ^2 of the random field:

$$\sigma^2 = \frac{\Gamma(\nu)}{\Gamma(\nu + 0.5d)(4\pi)^{d/2}\kappa^{2\nu}\tau^2} \quad \text{(B.5)}$$

where Γ is the gamma function, d is the dimension (i.e., 2 in the 2-dimensional spatial model), $\nu=1$ as assumed in the Matérn approximation, and κ and τ are the estimated parameters.

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