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:

\[ Q = \tau^2(\kappa^4C + 2\kappa^2G_1 + G_2) \]  

(B.1)

where \( Q \) is the precision matrix of Gaussian Markov random field approximation, \( \kappa \) and \( \tau \) are parameters in the Matérn approximation (when specifying Matérn smoothness parameter \( v=1 \)), and \( C, G_1, \) and \( G_2 \) are sparse matrices representing a piecewise linear basis function for the approximation (see Lindgren et al. 2010, Lindgren and Rue 2013 for details). \( C, G_1, \) and \( G_2 \) 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 \( C, G_1, \) and \( G_2 \) 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 \( C, G_1, \) and \( G_2 \) at each node. These three sparse 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 $\Omega^{(k)}$ and $\Psi^{(k)}$, i.e., random fields defined at each node in the SPDE approximation. These follow a multivariate normal distribution.

$$\Omega \sim MVN(\alpha I, \Sigma_\Omega)$$
$$\Psi \sim MVN(0, \Sigma_E \otimes \Sigma_\nu)$$  

(B.2)

where:

$$\Sigma_\Omega = \left( \tau_\Omega^2 (\kappa_\Omega^4 C + 2\kappa_\Omega^2 G_1 + G_2) \right)^{-1}$$

$$\Sigma_E = \left( \tau_E^2 (\kappa_E^4 C + 2\kappa_E^2 G_1 + G_2) \right)^{-1}$$  

(B.3)

and $\Sigma_\nu$ is as defined in Eq. 2c (in the present application, we assume that $\kappa_\Omega = \kappa_E$, although future applications could explore the consequences of relaxing this assumption). $\Omega^{(k)}$ and $\Psi^{(k)}$ 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 empirical hierarchical modelling strategy (sensu Cressie and Wikle 2011), $\Omega^{(k)}$ and $\Psi^{(k)}$ are integrated across while calculating the marginal likelihood of $\kappa$, $\tau_\Omega$, $\tau_E$, $\alpha$, 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” $\lambda$):

$$\lambda = \frac{\sqrt{8\nu}}{\kappa}$$  

(B.4)

and the marginal variance $\sigma^2$ of the random field:
\[
\sigma^2 = \frac{\Gamma(\nu)}{\Gamma(\nu + 0.5d)(4\pi)^{d/2} \kappa^{2\nu} \tau^2}
\]

(B.5)

where \(\Gamma\) 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 \(\kappa\) and \(\tau\) are the estimated parameters.
LITERATURE CITED


