Stochastic adventures in space and time

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THE UNIVERSITY *of* EDINBURGH

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THE STORY BEGINS HERE...
AN ADVENTURE IN SPACE AND TIME
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Context: spatial and spatio-temporal modelling and estimation

Problem examples:

- Reconstructing past temperatures from weather stations, satellite, and ship measurements
- Estimating the abundance of dolphins, from ship observations
- Tracking electrical signals across the heart
- Estimating the habitats and movement of birds, from GPS measurements

Modelling and estimation tools:

- Additive models (GAMM/GLM/GLMM/LGM/etc)
- Stochastic processes, specifically Gaussian, dynamical and static
- Bayesian methods (MCMC, INLA, variational Bayes)
- Software for special cases, and for general models

Focus today:

- Gaussian process dynamics, and
- movement modelling, with
- general model specifications for parameters $\boldsymbol{\theta}$, latent fields $u(\mathbf{s}, t)$, and observations $\boldsymbol{y}$

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Direct Bayesian inference:
The inner core of the Integrated Nested Laplace Approximation method

- Latent Gaussian model structure (Bayesian GAMs with Gaussian process components)

$$\boldsymbol{\theta} \sim p(\boldsymbol{\theta}) \quad \text{(precision parameters)} \qquad \eta(\mathbf{s},t) = \sum_{k=1}^{n} \psi_k(\mathbf{s},t) u_k \quad \text{(predictor)}$$

$$\boldsymbol{u}|\boldsymbol{\theta} \sim \mathsf{N}[\boldsymbol{\mu}_u, \boldsymbol{Q}_u^{-1}] \quad \text{(latent field)} \qquad \boldsymbol{y}|\boldsymbol{\theta},\boldsymbol{u} \sim p(\boldsymbol{y}|\boldsymbol{\theta},\eta) \quad \text{(observations)}$$

- Conditional log-posterior mode ($\boldsymbol{\mu}_{u|y}$) and Hessian ($\boldsymbol{Q}_{u|y}$), for each $\boldsymbol{\theta}$, by iteration:

$$\boldsymbol{g}_y^* = -\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{u}} \log p(\boldsymbol{y}|\boldsymbol{\theta},\eta)\Big|_{\boldsymbol{u}=\boldsymbol{u}^*}$$

$$\boldsymbol{H}_y^* = -\frac{\mathrm{d}^2}{\mathrm{d}\boldsymbol{u}\mathrm{d}\boldsymbol{u}^\top} \log p(\boldsymbol{y}|\boldsymbol{\theta},\eta)\Big|_{\boldsymbol{u}=\boldsymbol{u}^*}$$

$$\boldsymbol{Q}_{u|y} = \boldsymbol{Q}_u + \boldsymbol{H}_y^*$$

$$\boldsymbol{Q}_{u|y}(\boldsymbol{\mu}_{u|y} - \boldsymbol{\mu}_u) = \boldsymbol{H}_u^*(\boldsymbol{u}^* - \boldsymbol{\mu}_u) - \boldsymbol{g}_y^*$$

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The eternal quest for spatial dependence models

- Gaussian random field: $u(\mathbf{s})$, $\mathbf{s} \in \mathcal{D}$ (subset of $\mathbb{R}^d$ or a manifold)
- Moment characterisation:
  - Expectation $\mu(\mathbf{s}) = \mathbb{E}[u(\mathbf{s})]$
  - Covariance $\mathcal{R}(\mathbf{s}, \mathbf{s}') = \mathbb{C}[u(\mathbf{s}), u(\mathbf{s}')]$, symmetric positive definite function.
- Precision operator; inverse covariance: $\mathcal{Q} = \mathcal{R}^{-1}$

  In practice, easier conditions for valid models
- Reproducing Kernel Hilbert Space (RKHS) $H_\mathcal{Q}$: Inner product

$$\langle f, g \rangle_{H_\mathcal{Q}} = \langle f, \mathcal{Q} g \rangle_\mathcal{D}$$

  and squared norm $\|f\|^2 = \langle f, f \rangle_{H_\mathcal{Q}}$
- $m(\cdot) = \mathbb{E}(u(\cdot) - \mu(\cdot) | \{u(\mathbf{s}_k)\}) \in H_\mathcal{Q}$ but $u(\cdot) - \mu(\cdot) \notin H_\mathcal{Q}$; the process is less smooth!
- Spatial and spatio-temporal stochastic PDEs generate random field models:

$$\mathcal{L} u(\mathbf{s}) \,\mathrm{d}\mathbf{s} = \mathrm{d}\mathcal{W}(\mathbf{s})$$

$$\mathcal{Q}_u = \mathcal{L}^* \mathcal{L}$$

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Spatio-temporal separability for functions, covariances, and precisions

- Functional separability for $\mathbf{s} \in \mathcal{D}$ and $t \in \mathcal{T}$
  - Addition: $w(\mathbf{s}, t) = u(\mathbf{s}) + v(t)$
  - Multiplication $w(\mathbf{s}, t) = u(\mathbf{s})v(t)$ (degrees of freedom $|\mathcal{D}| + |\mathcal{T}|$)
- Covariance separability
  - Addition: $\mathcal{R}_w[(\mathbf{s}, t), (\mathbf{s}', t')] = \mathcal{R}_u(\mathbf{s}, \mathbf{s}') + \mathcal{R}_v(t, t')$
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  - Simple to construct, but with some unrealistic properties
  - Additive combination: $\sum_k \mathcal{R}_{u_k}(\mathbf{s}, \mathbf{s}')\mathcal{R}_{v_k}(t, t')$ (sum of cov-product-separable processes)
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Question 1: Are there interpretable process constructions that lead to this structure?
Question 2: Is the "separable" vs "non-separable" dichotomy sufficient?

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Question 1: Are there interpretable process constructions that lead to this structure? Yes!

Question 2: Is the "separable" vs "non-separable" dichotomy sufficient? No!

From temporal random walks to spatio-temporal diffusion

- Spatial Whittle-Matérn models with $\mathcal{L}_s = \gamma_s^2 - \Delta$:

$$\mathcal{L}_s^{\alpha_s/2} u(\mathbf{s})\,\mathrm{d}\mathbf{s} = \mathrm{d}\mathcal{W}(\mathbf{s}) \quad \text{(spatial white noise)}$$

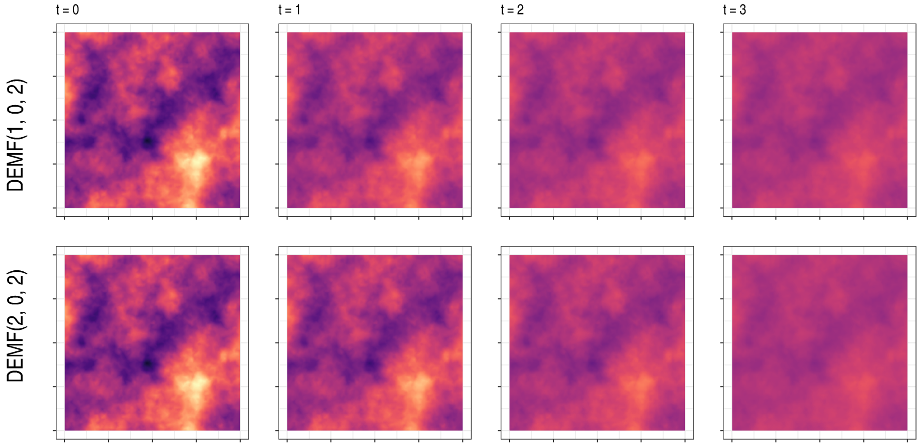
  Precision $\mathcal{Q} = \mathcal{L}_s^{\alpha_s}$, Matérn covariance for $u(\mathbf{s})$ on $\mathbb{R}^d$.

- Separable space-time model (separable vector Ornstein-Uhlenbeck/AR(1) process):

$$\mathcal{L}_s^{\alpha_s/2} \left(\frac{\partial}{\partial t} + \kappa \right) u(\mathbf{s}, t)\,\mathrm{d}\mathbf{s}\,\mathrm{d}t = \mathrm{d}\mathcal{W}(\mathbf{s}, t) \quad \text{(spatio-temporal white noise)}$$

  Precision $\mathcal{Q} = \mathcal{L}_s^{\alpha_s} \left(\kappa^2 - \frac{\partial^2}{\partial t^2} \right)$ for $u(\mathbf{s}, t)$, covariance is a product of a temporal Matérn kernel and the spatial covariance.

Prediction



Conditional expectations into the future decay pointwise towards zero; no spatial dynamics.

Diffusion extension of Matérn fields (DEMF)

- Non-separable space-time DEMF$(\alpha_t, \alpha_s, \alpha_e)$ model for $(\mathbf{s}, t) \in \mathcal{D} \times \mathcal{T}$:

$$\gamma_e \mathcal{L}_s^{\alpha_e/2} \left(\gamma_t \frac{\partial}{\partial t} + \mathcal{L}_s^{\alpha_s/2} \right)^{\alpha_t} u(\mathbf{s}, t) \, \mathrm{d}\mathbf{s} \, \mathrm{d}t \overset{d}{=} \gamma_e \mathcal{L}_s^{\alpha_e/2} \left(-\gamma_t^2 \frac{\partial^2}{\partial t^2} + \mathcal{L}_s^{\alpha_s} \right)^{\alpha_t/2} u(\mathbf{s}, t) \, \mathrm{d}\mathbf{s} \, \mathrm{d}t = \mathrm{d}\mathcal{W}(\mathbf{s}, t),$$

  where $\gamma_e, \gamma_t > 0$, and $\alpha_t > 0$, $\alpha_s, \alpha_e \geq 0$.
- In the stationary case, the resulting field has Matérn covariance for every time point
- The spatial smoothness is $\nu_s = \alpha_s(\alpha_t - 1/2) + \alpha_e - d/2$
- The temporal smoothness is $\nu_t = \min(\alpha_t - 1/2, \, \nu_s/\alpha_s)$.
- Non-separability parameter: $\beta_s = 1 - \frac{\alpha_e}{\nu_s + d/2} \in [0, 1]$
- Tensor product basis discretisation for integer α_t gives precision matrix structure

$$\boldsymbol{Q} = \gamma_e^2 \sum_{k=0}^{2\alpha_t} \gamma_t^k \boldsymbol{J}_{\alpha_t, k/2} \otimes \boldsymbol{K}_{\alpha_s(\alpha_t - k/2) + \alpha_e}$$

  where $\boldsymbol{J}_{\cdot,\cdot}$ are purely temporal and $\boldsymbol{K}_{\cdot}$ are purely spatial.
  This is what we were looking for!

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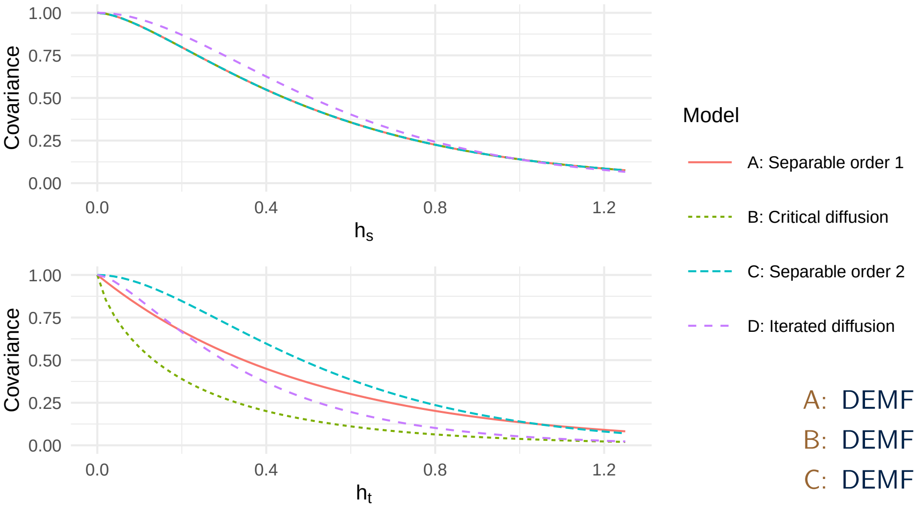
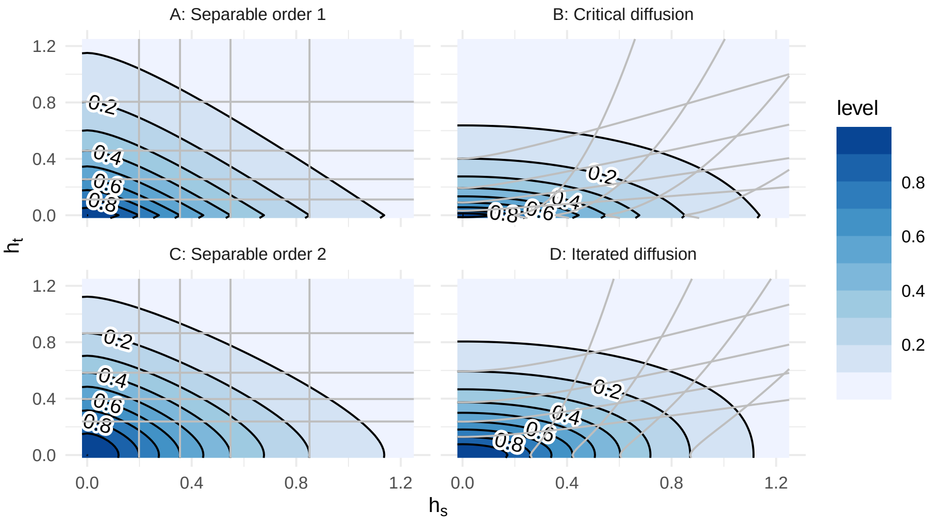
Non-separable covariances, from spectral inversion; $\mathbb{R}^2 \times \mathbb{R}$

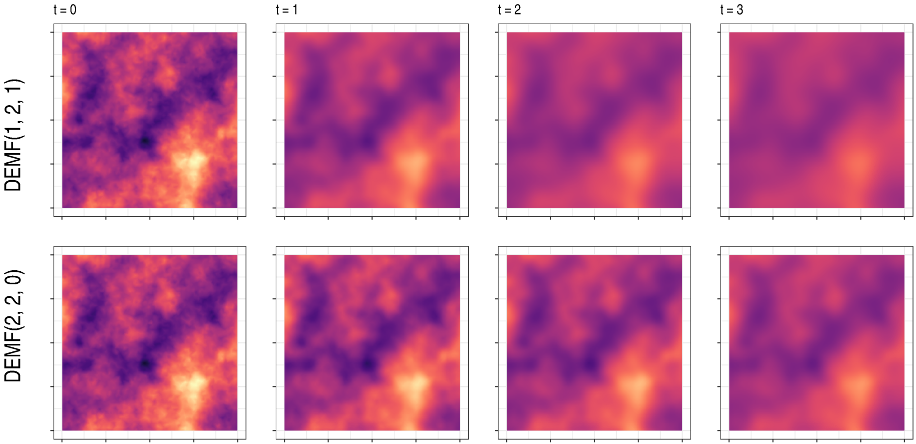


A: DEMF(1,0,1)
B: DEMF(1,2,1)
C: DEMF(2,0,1)
D: DEMF(2,2,0)

Non-separable covariances, from spectral inversion; $\mathbb{R}^2 \times \mathbb{R}$



Prediction



Conditional expectations into the future diffuse across space; some spatial dynamics.

Summary of separability concepts

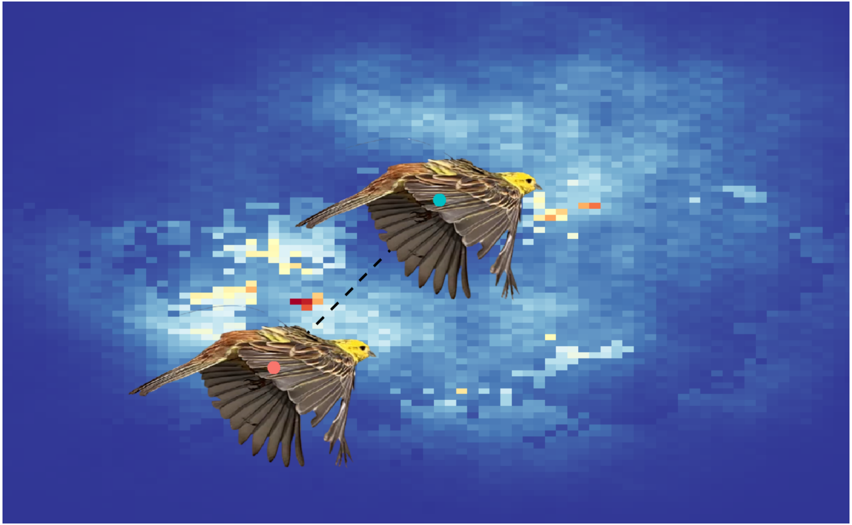
Basics:

- Functions, covariance, precision
- Additive, multiplicative, additive multiplication combinations
- Non-separability needed for realistic dynamics

Further concepts

- Non-stationarity; separable and non-separable
- Asymmetry; transport/advection terms in the space-time operator
- Manifold domains; easy in practice and most of the theory; some theory more difficult

Animal movement



Step selection analysis with telemetry data

Goal: Understand sequential movement decisions

- The general movement capacity of an animal. Expressed by a movement kernel:

$$K(\mathbf{y}_t|\mathbf{y}_{t-1},\mathbf{y}_{t-2},\boldsymbol{\theta}) = K_{\text{length}}(\mathbf{y}_t|\mathbf{y}_{t-1},\boldsymbol{\theta})K_{\text{angle}}(\mathbf{y}_t|\mathbf{y}_{t-1},\mathbf{y}_{t-2},\boldsymbol{\theta}), \quad \mathbf{y}_\cdot \in \mathcal{D} \subset \mathbb{R}^2$$

- Selection behaviour of the animal. Modelled by a resource selection function (RSF):

$$\xi(\mathbf{s}) = \exp[\eta(\mathbf{s})] = \exp[\beta_1 X_1(\mathbf{s}) + \ldots + \beta_p X_p(\mathbf{s}) + u(\mathbf{s})], \quad \mathbf{s} \in \mathcal{D}$$

  Spatially (or spatio-temporally) varying covariates $X_\cdot$ and a residual random field $u(\mathbf{s})$.
- Combined normalised conditional observation density function:

$$f_{t|<t}(\mathbf{y}_t|\boldsymbol{\theta},\eta) = \frac{K(\mathbf{y}_t|\mathbf{y}_{<t},\boldsymbol{\theta})\exp[\eta(\mathbf{y}_t)]}{\int_{\mathcal{D}} K(\mathbf{s}|\mathbf{y}_{<t},\boldsymbol{\theta})\exp[\eta(\mathbf{s})]\,\mathrm{d}\mathbf{s}}$$

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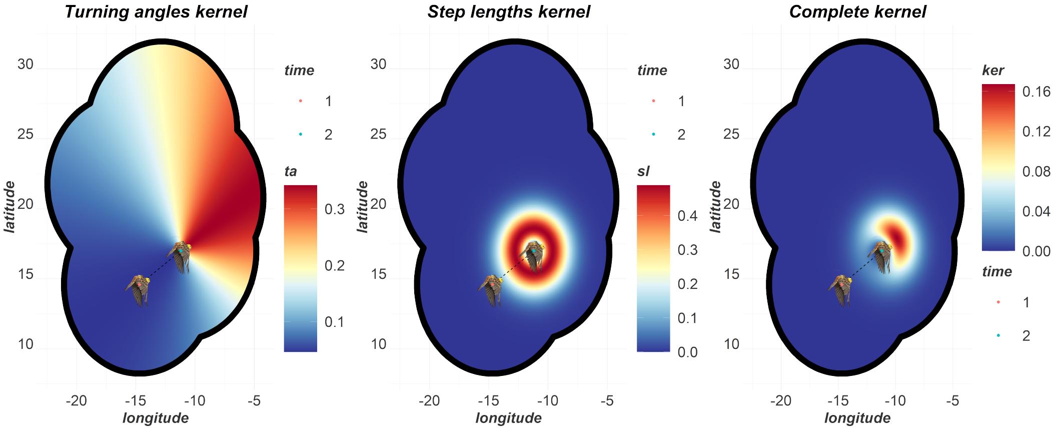
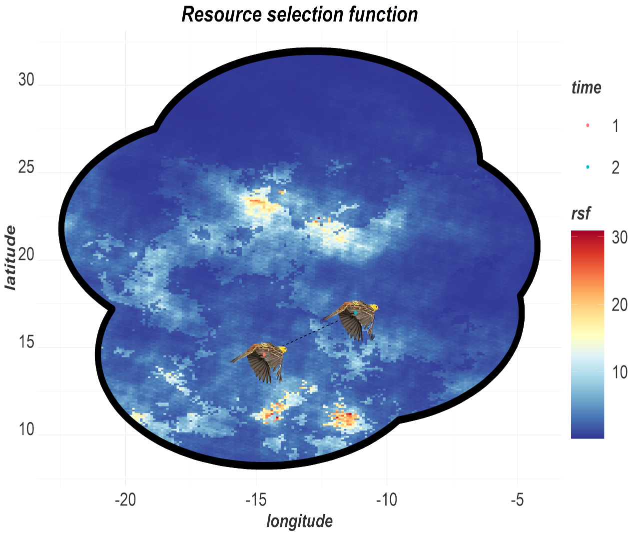
Movement kernel

Movement capacity of an animal:



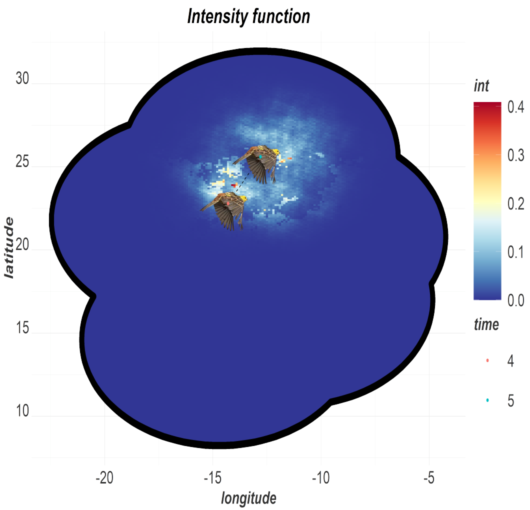
Resource selection function

Spatial features in the study area:

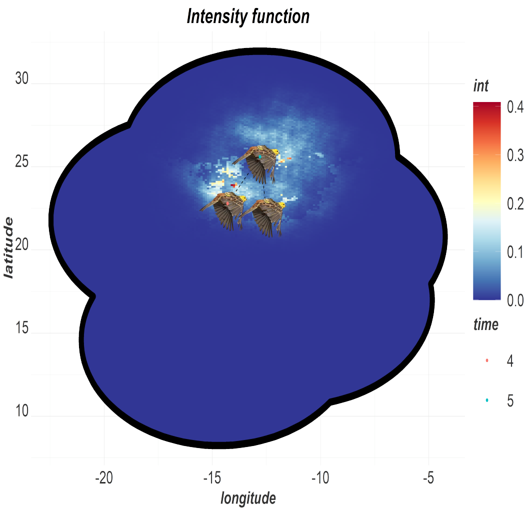


Combined effect

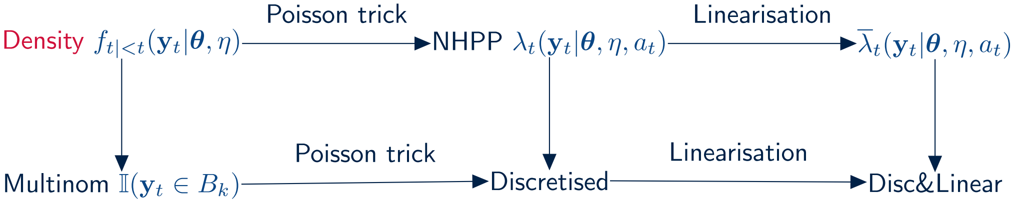
Intensity function



Movement decision!



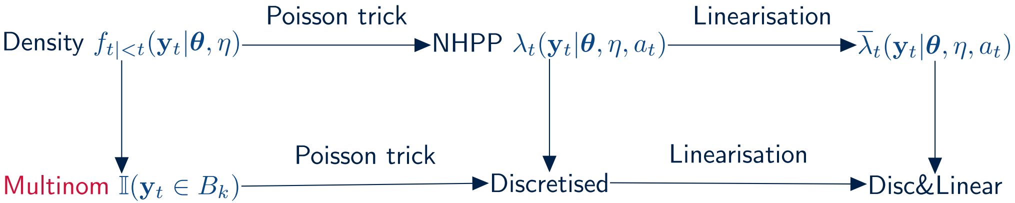
From movement kernel to discretised point process likelihood



$$
f_{t|<t}(\mathbf{y}_t|\boldsymbol{\theta},\eta) = \frac{K(\mathbf{y}_t|\mathbf{y}_{<t},\boldsymbol{\theta})\exp[\eta(\mathbf{y}_t)]}{\int_{\mathcal{D}} K(\mathbf{s}|\mathbf{y}_{<t},\boldsymbol{\theta})\exp[\eta(\mathbf{s})]\,\mathrm{d}\mathbf{s}}
$$

Problem: Inconvenient normalisation integral.

From movement kernel to discretised point process likelihood



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$$

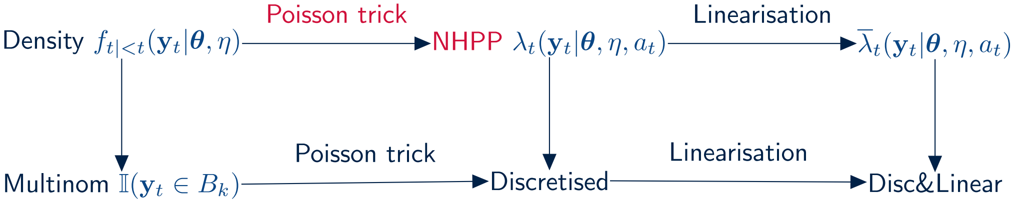
Previous approach: Subdivide space into disjoint sets B_k, with $\mathcal{D}=\cup_{k=1}^N B_k$.

$$
\mathbf{z}_t=[\mathbb{I}(\mathbf{y}_t\in B_1),\dots,\mathbb{I}(\mathbf{y}_t\in B_N)]\sim\text{Multinomial}\left(1,\{p_k,k=1,\dots,N\}\right)
$$

$$
p_k=\mathbb{P}(\mathbf{y}_t\in B_k|\mathbf{y}_{<t},\boldsymbol{\theta},\eta)=\int_{B_k}f_{t|<t}(\mathbf{s}|\boldsymbol{\theta},\eta)\,\mathrm{ds}
$$

(No improvement: multiple integrals)

From movement kernel to discretised point process likelihood

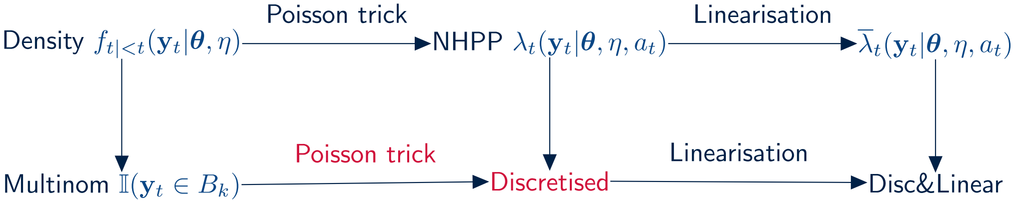


$$\lambda_t(\mathbf{y}_t|\boldsymbol{\theta},\eta,a_t) = K(\mathbf{y}_t|\mathbf{y}_{<t},\boldsymbol{\theta})\exp[\eta(\mathbf{y}_t)+a_t], \quad a_t \sim \text{Unif}(\mathbb{R})$$

$$l(\{\mathbf{y}_t\}|\boldsymbol{\theta},\eta,\{a_t\}) = -\sum_t \int_{\mathcal{D}} \lambda_t(\mathbf{s}|\boldsymbol{\theta},\eta,a_t)\,\mathrm{d}\mathbf{s} + \sum_t \log\lambda_t(\mathbf{y}_t|\boldsymbol{\theta},\eta,a_t)$$

Non-homogeneous Poisson point process with a single point observation for each t.
a_t replaces the explicit density normalisation by *estimating* it.
The posterior distribution for $\boldsymbol{\theta}$, $\beta_\cdot$, and $u(\cdot)$ is unchanged!

From movement kernel to discretised point process likelihood



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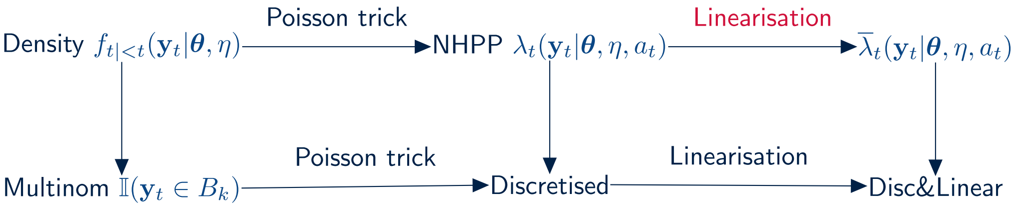
$$l(\{\mathbf{y}_t\}|\boldsymbol{\theta},\eta,\{a_t\}) \approx -\sum_t\sum_k \lambda_t(\mathbf{s}_k|\boldsymbol{\theta},\eta,a_t)w_k + \sum_t \log\lambda_t(\mathbf{y}_t|\boldsymbol{\theta},\eta,a_t)$$

Integration points and weigths $(\mathbf{s}_k, w_k)$, adapted to the spatial model resolution.

From movement kernel to discretised point process likelihood

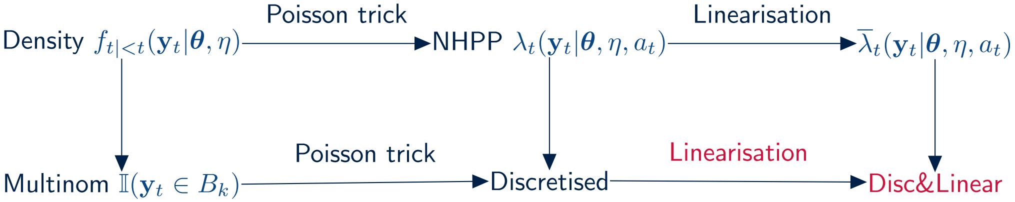


$$\log\overline{\lambda}(\mathbf{y}_t|\boldsymbol{\theta},\eta,a_t)=\log K(\mathbf{y}_t|\mathbf{y}_{<t},\boldsymbol{\theta}_0)+\frac{\mathrm{d}\log K(\mathbf{y}_t|\mathbf{y}_{<t},\boldsymbol{\theta})}{\mathrm{d}\boldsymbol{\theta}}(\boldsymbol{\theta}-\boldsymbol{\theta}_0)+\eta(\mathbf{y}_t)+a_t$$

$$l(\{\mathbf{y}_t\}|\boldsymbol{\theta},\eta,\{a_t\})=-\sum_t\int_{\mathcal{D}}\overline{\lambda}_t(\mathbf{s}|\boldsymbol{\theta},\eta,a_t)\,\mathrm{d}\mathbf{s}+\sum_t\log\overline{\lambda}_t(\mathbf{y}_t|\boldsymbol{\theta},\eta,a_t)$$

(Iterative) linearisation to a log-linear point process intensity allows more general movement kernel parameterisation.
(Preliminary theory: posterior approximation related to Fischer scoring)

From movement kernel to discretised point process likelihood



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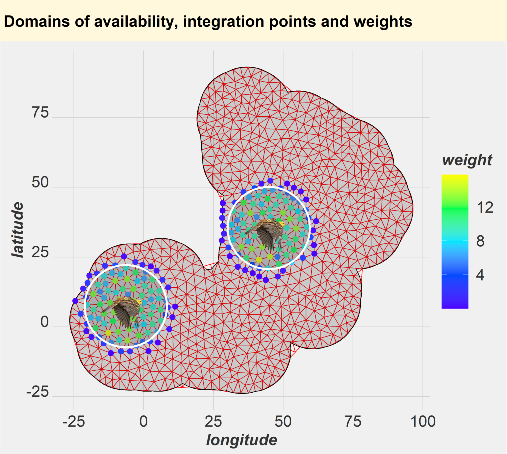
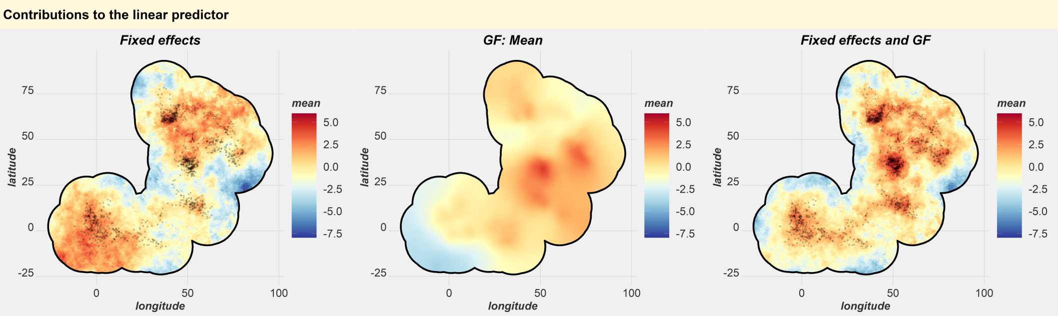
This is *almost* a log-linear Poisson count log-likelihood;
In $-E\lambda+y\log(E\lambda)$, R-INLA allows us to specify the two terms separately, without pairing them up with equal E and λ values.

Mesh, integration points and weights

- Restricted domain of availability at each time point: Disk with radius (at least) equal to the maximum observed step length
- Integration points: At mesh nodes to ensure stability
- Deterministic integration: Previous Monte Carlo strategies are inefficient and unstable

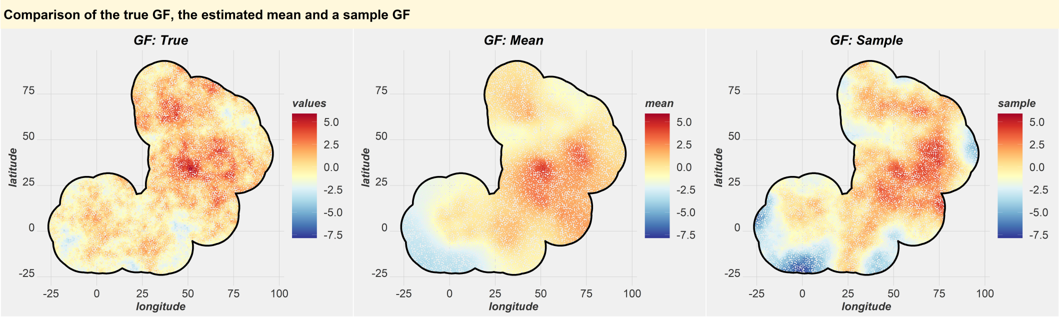


Estimated log-intensity function



The Gaussian random field (GF) contribution improves the estimated animal density.

Estimated Gaussian random field (GF)



Posterior samples can be used to quantify uncertainty of the fields and linear/nonlinear functionals of the fields.

Note: Recall that conditional means are fundamentally smoother than conditional realisations!

Summary

- (Relatively) simple stochastic PDEs provide useful building blocks
- Computational methods need to handle hierarchical structures, not just additive noise.
- The Poisson trick & iterative linearisation allows `inlabru` to estimate new model classes
- The SPDE approach for Gaussian and non-Gaussian fields: 10 years and still running (Lindgren et al, 2022, Spatial Statistics)
  https://arxiv.org/abs/2111.01084
  https://doi.org/10.1016/j.spasta.2022.100599
- A diffusion-based spatio-temporal extension of Gaussian Matérn fields (Lindgren et al)
  https://arxiv.org/abs/2006.04917
- Accounting for unobserved spatial variation in step selection analyses of animal movement via spatial random effects (Guillen et al)
  https://www.biorxiv.org/content/10.1101/2023.01.17.524368v1
- `inlabru` documentation and examples:
  https://inlabru-org.github.io/inlabru/

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