

# Stochastic adventures 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  $\theta$ , latent fields  $u(s, t)$ , and observations  $y$

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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)

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

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

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

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

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

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

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

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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  $\|f\|^2 = \langle f, f \rangle_{H_{\mathcal{Q}}}$

- $m(\cdot) = \mathbb{E}(u(\cdot) - \mu(\cdot) | \{u(\mathbf{s}_k)\}) \in \tilde{H}_{\mathcal{Q}}$  but  $u(\cdot) - \mu(\cdot) \notin H_{\mathcal{Q}}$ ; the process is less smooth!
- Spatial and spatio-temporal stochastic PDEs generate random field models:

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

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

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# Spatio-temporal separability for functions, covariances, and precisions

- Functional separability for  $s \in \mathcal{D}$  and  $t \in \mathcal{T}$ 
  - Addition:  $w(s, t) = u(s) + v(t)$
  - Multiplication  $w(s, t) = u(s)v(t)$  (degrees of freedom  $|\mathcal{D}| + |\mathcal{T}|$ )
- Covariance separability
  - Addition:  $\mathcal{R}_w[(s, t), (s', t')] = \mathcal{R}_u(s, s') + \mathcal{R}_v(t, t')$
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  - Simple to construct, but with some unrealistic properties
  - Additive combination:  $\sum_k \mathcal{R}_{u_k}(s, s')\mathcal{R}_{v_k}(t, t')$  (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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  - Additive combination:  $\sum_k \mathcal{Q}_{u_k}(\mathbf{s}, \mathbf{s}')\mathcal{Q}_{v_k}(t, t')$  (what is this!?!)

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  $\mathcal{L}_s = \gamma_s^2 - \Delta$ :

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

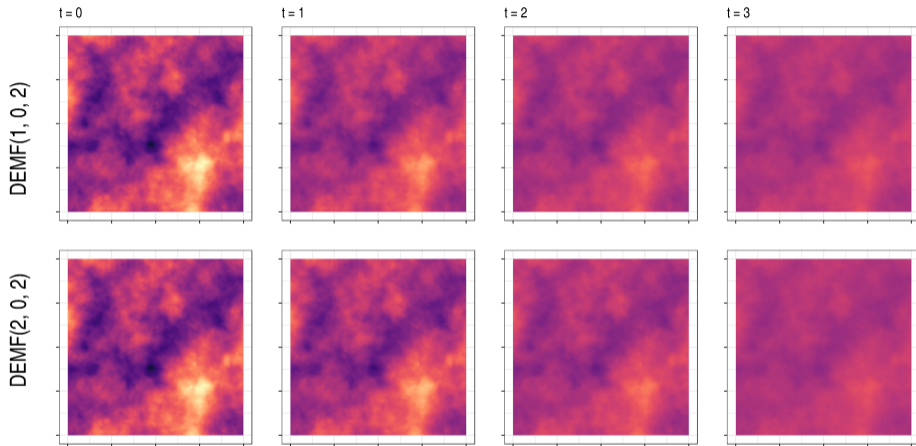
Precision  $Q = \mathcal{L}_s^{\alpha_s}$ , Matérn covariance for  $u(\mathbf{s})$  on  $\mathbb{R}^d$ .

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

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

Precision  $Q = \mathcal{L}_s^{\alpha_s} \left( \kappa^2 - \frac{\partial^2}{\partial t^2} \right)$  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  $(\mathbf{s}, t) \in \mathcal{D} \times \mathcal{T}$ :

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

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  $\alpha_t$  gives precision matrix structure

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

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

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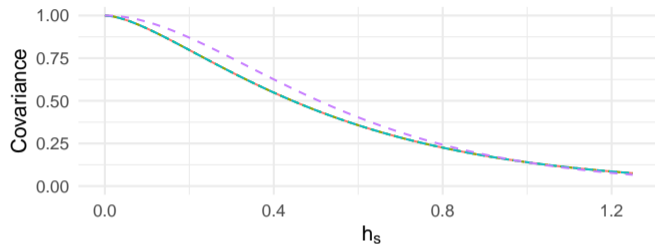
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Non-separable covariances, from spectral inversion;  $\mathbb{R}^2 \times \mathbb{R}$ 

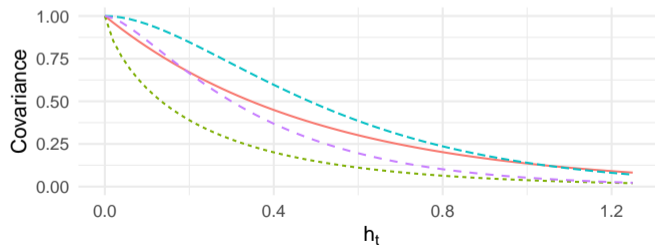
## Model

— A: Separable order 1

⋯ B: Critical diffusion

- - C: Separable order 2

- - D: Iterated diffusion



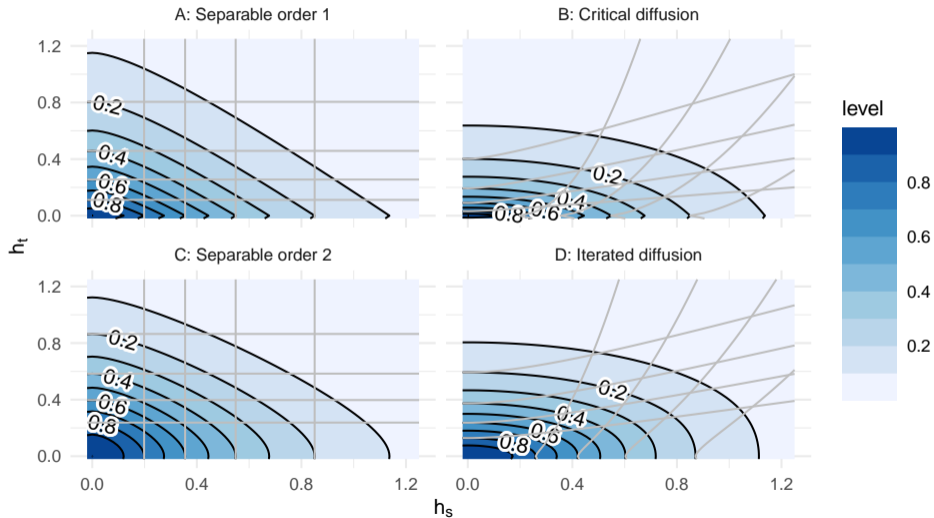
A: DEMF(1,0,1)

B: DEMF(1,2,1)

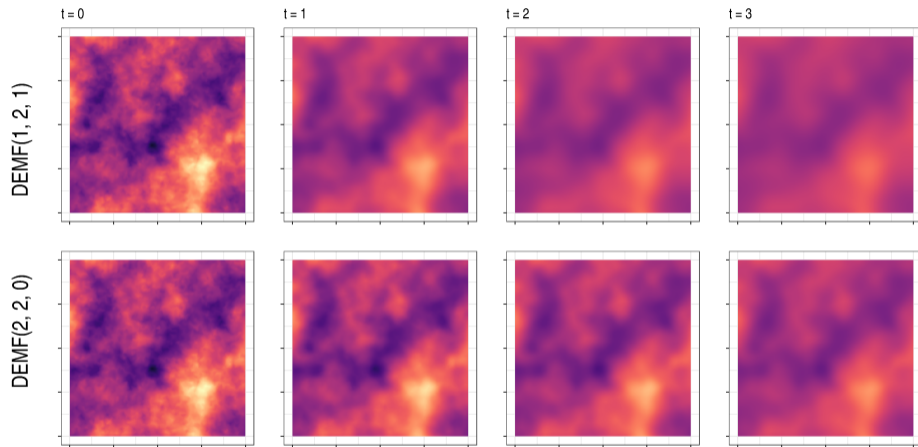
C: DEMF(2,0,1)

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

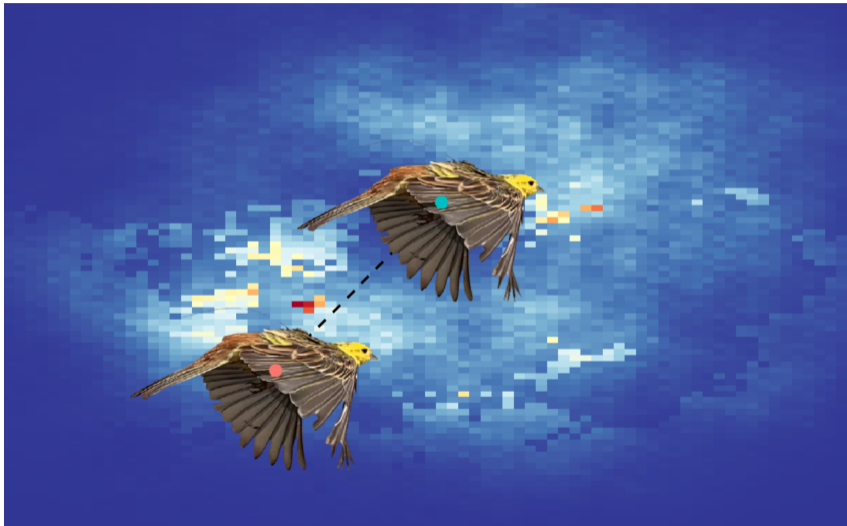
## Further concepts

- 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

## Practical considerations

- Non-separable models are more expensive to fit
- Interpolation/infilling applications show little difference from separable models
- Full temporal predictions are fundamentally different; non-separability can be essential

# 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:

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

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

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

Spatially (or spatio-temporally) varying covariates  $X$ . 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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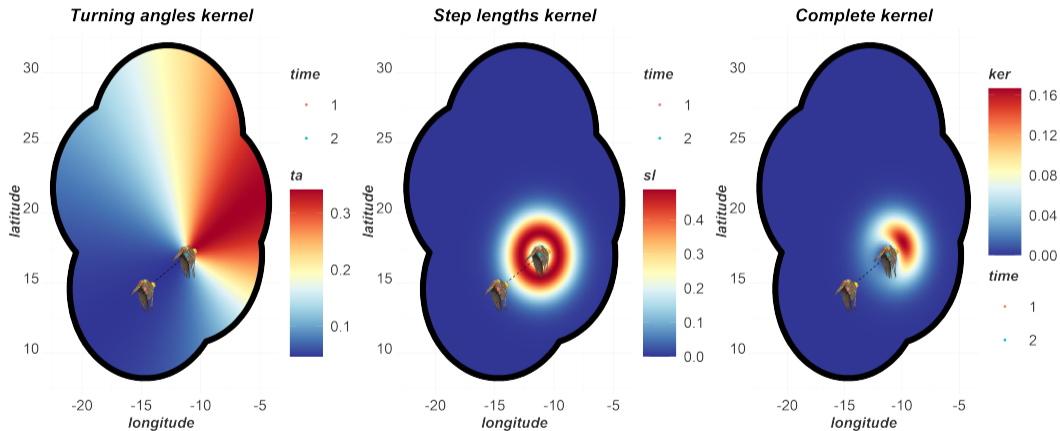
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# Movement kernel

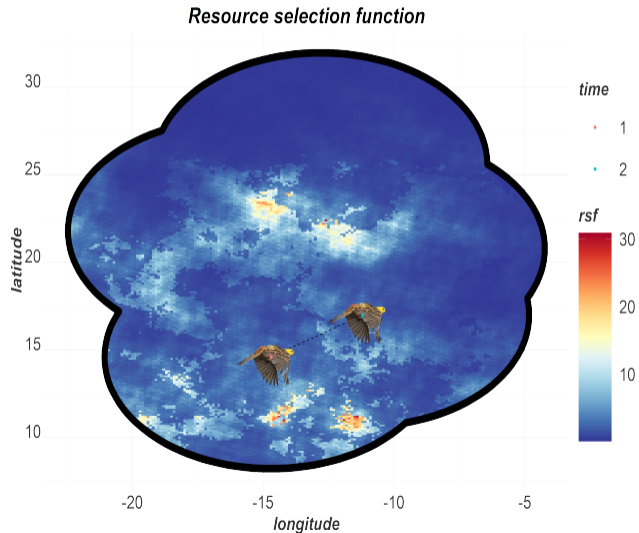
Movement capacity of an animal:





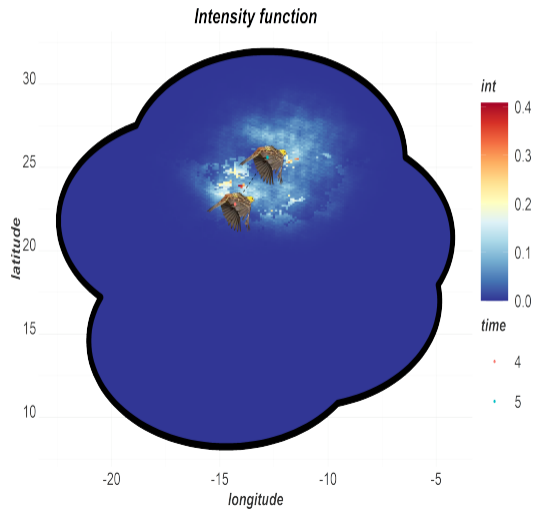
# Resource selection function

Spatial features in the study area:

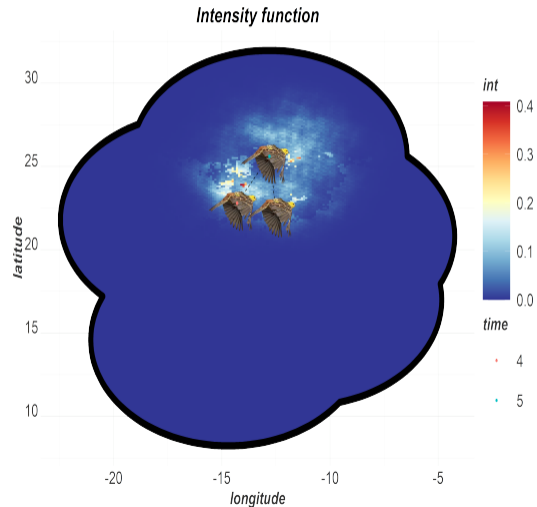


# Combined effect

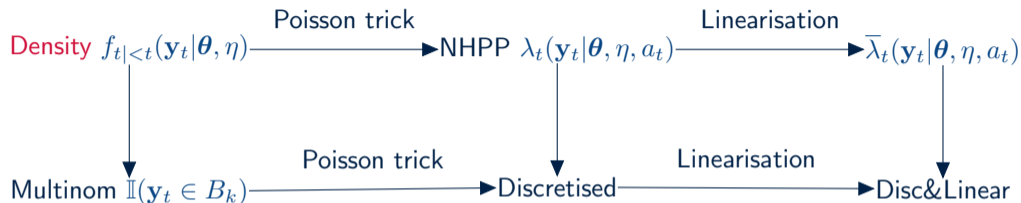
## Intensity function



## Movement decision!



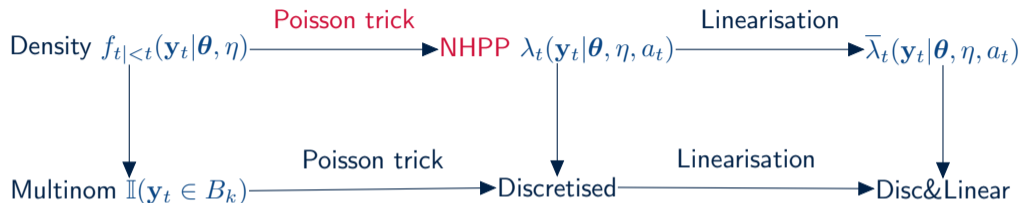
## From movement kernel to discretised point process likelihood



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

Problem: Inconvenient normalisation integral.

## From movement kernel to discretised point process likelihood

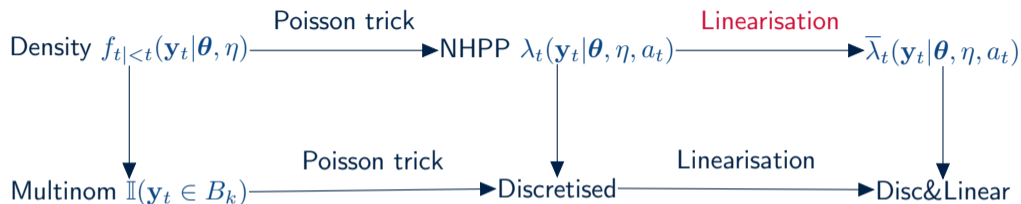


$$\lambda_t(\mathbf{y}_t|\boldsymbol{\theta}, \eta, a_t) = K(\mathbf{y}_t|\mathbf{y}_{<t}, \boldsymbol{\theta}) \exp[\eta(\mathbf{y}_t) + a_t], \quad a_t \sim \text{Unif}(\mathbb{R})$$

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

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  $\boldsymbol{\theta}$ ,  $\beta$ , and  $u(\cdot)$  is unchanged!

## From movement kernel to discretised point process likelihood



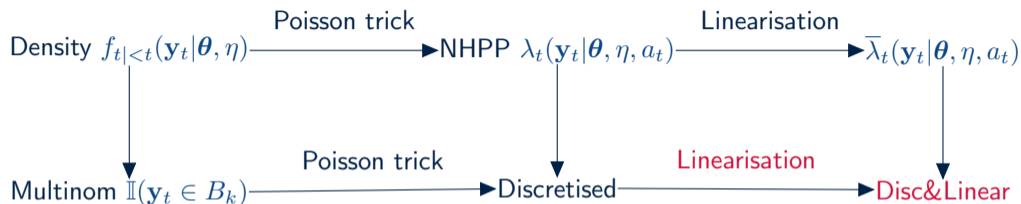
$$\log \bar{\lambda}(\mathbf{y}_t|\boldsymbol{\theta}, \eta, a_t) = \log K(\mathbf{y}_t|\mathbf{y}_{<t}, \boldsymbol{\theta}_0) + \frac{d \log K(\mathbf{y}_t|\mathbf{y}_{<t}, \boldsymbol{\theta})}{d\boldsymbol{\theta}} (\boldsymbol{\theta} - \boldsymbol{\theta}_0) + \eta(\mathbf{y}_t) + a_t$$

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

(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



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

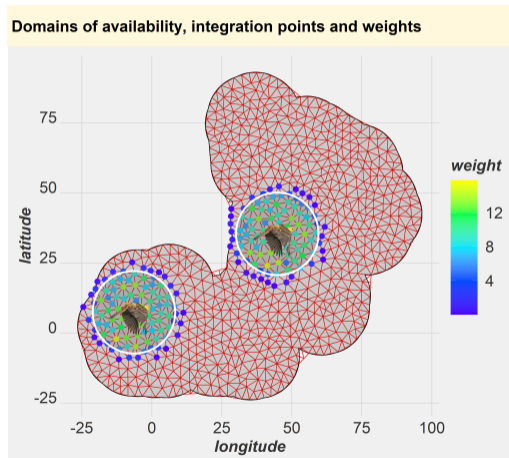
$$l(\{\mathbf{y}_t\}|\boldsymbol{\theta}, \eta, \{a_t\}) \approx - \sum_t \sum_k \bar{\lambda}_t(\mathbf{s}_k|\boldsymbol{\theta}, \eta, a_t) w_k + \sum_t \log \bar{\lambda}_t(\mathbf{y}_t|\boldsymbol{\theta}, \eta, a_t)$$

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  $\lambda$  values.

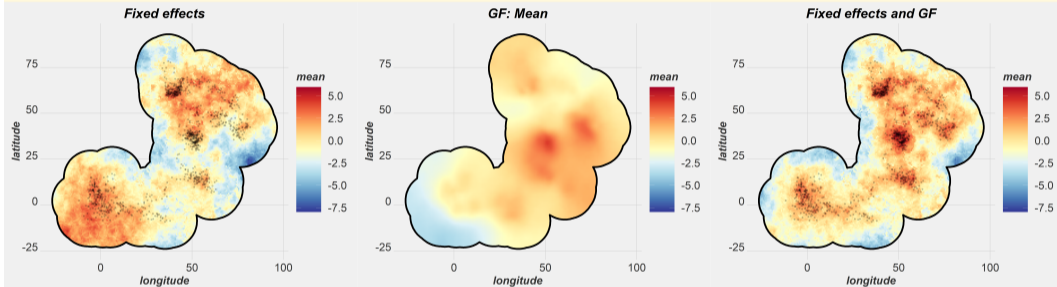
# Mesh, integration points and weights

- 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

## Contributions to the linear predictor

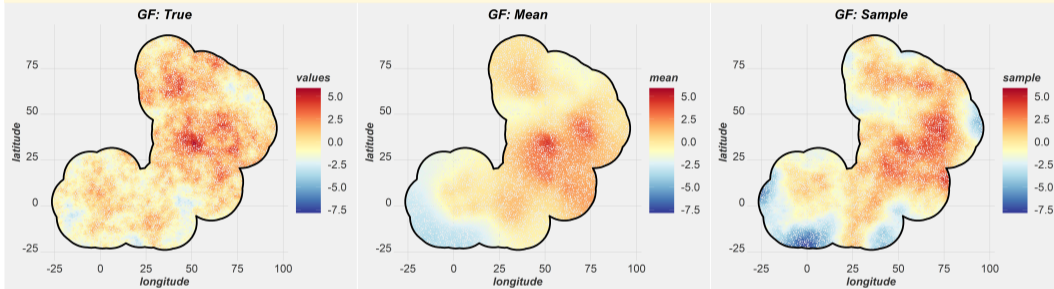


The Gaussian random field (GF) contribution improves the estimated animal density.



# Estimated Gaussian random field (GF)

Comparison of the true GF, the estimated mean and a sample 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>  
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