Causal Spatial Models

Multivariate models constructed using a conditional approach

— joint work with Noel Cressie —

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Section 1

Introduction

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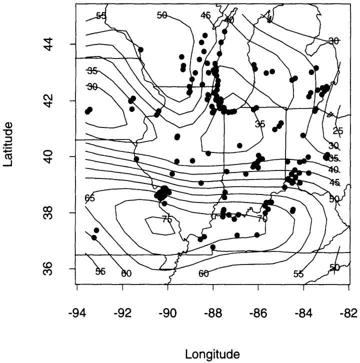
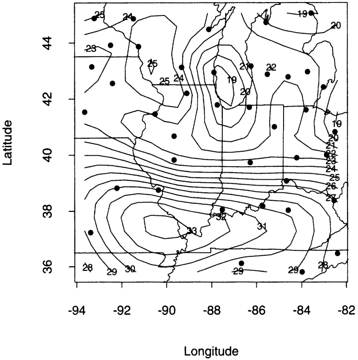
- **Univariate** spatial model.
- **Multivariate** spatial model.
  - Two or more interacting spatial variables.
  - Improve prediction on one of the variates by observing the others: **Cokriging**.
  - Determine which variate caused the observed phenomenon: **Source separation**.

Royle and Berliner (1999), Midwestern USA.

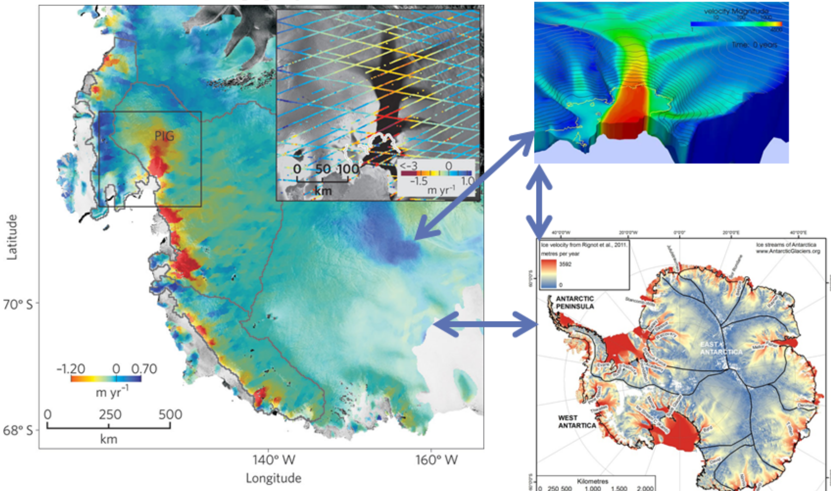




Example 2: Antarctica Mass Balance

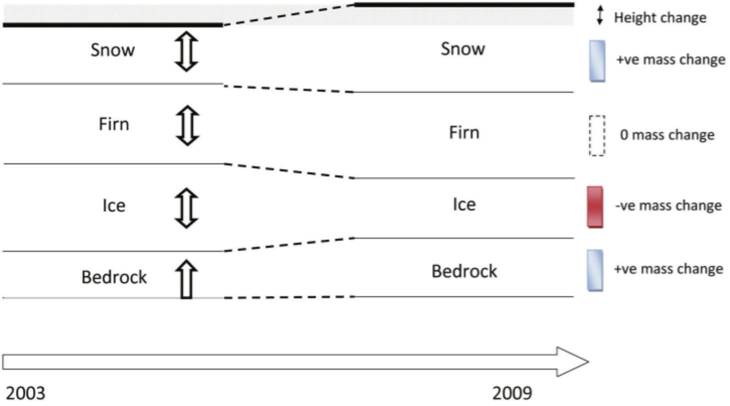
ICESAT data (elevation change per year)

Elmer/Ice (LGGE) model



Example 2: Antarctica Mass Balance

- Zammit-Mangion et al. (2014, 2015b,a), Antarctica.



The challenge

- **Modelling**: Given a bivariate process $(Y_1(\cdot), Y_2(\cdot))$, what is a valid *cross-covariance function matrix* (CCFM)

$$\begin{pmatrix} C_{11}(\cdot,\cdot) & C_{12}(\cdot,\cdot) \\ C_{21}(\cdot,\cdot) & C_{22}(\cdot,\cdot) \end{pmatrix}, \tag{1}$$

  such that **any** covariance matrix derived from it is positive-definite?

- **Computational**: Sometimes we struggle with univariate models – how do our algorithms scale to multivariate models?

- **Linear model of co-regionalisation** (LMC, Wackernagel, 1995): Define

$$Y_1(\cdot) = a_{11}\widetilde{Y}_1(\cdot) + a_{12}\widetilde{Y}_2(\cdot), \quad (2)$$
$$Y_2(\cdot) = a_{21}\widetilde{Y}_1(\cdot) + a_{22}\widetilde{Y}_2(\cdot), \quad (3)$$

where, independently,

$$\widetilde{Y}_1(\cdot) \sim \mathcal{N}(\mu_1(\cdot), C_1(\cdot,\cdot)), \quad (4)$$
$$\widetilde{Y}_2(\cdot) \sim \mathcal{N}(\mu_2(\cdot), C_2(\cdot,\cdot)). \quad (5)$$

- $C_{ij}(\cdot,\cdot) = a_{i1}a_{j1}C_1(\cdot,\cdot) + a_{i2}a_{j2}C_2(\cdot,\cdot)$.
- CCFM is positive-definite for any $\{a_{ij} : i,j = 1,\dots,2\}$.

- **Bivariate parsimonious Matérn model** (Gneiting et al., 2010): Let $C^o(\cdot)$ be a stationary, isotropic covariance function. Define

$$C^o_{ij}(\cdot) \equiv \beta_{ij} M(\cdot; \nu_{ij}, \kappa_{ij}), \tag{6}$$

  where $M(\cdot)$ is a Matérn covariance function. Let $\kappa_{ii} = \kappa_{ij} = \kappa$ and set $\nu_{ij} = (\nu_{ii} + \nu_{jj})/2$. Then if $(\beta_{ij} : i, j = 1, 2)$ is positive-definite, the CCFM is positive-definite.

- **Bivariate full Matérn model**: Relaxes assumptions on smoothness and scales, but finding valid parameters is much more involved.

Current approaches (limitations)

- Stuck with homogeneous models (e.g., convolution methods).
- Stuck with fixed scales (parsimonious Matérn).
- Stuck with Matérn models (e.g., full Matérn models).
- **Stuck with symmetry (e.g., LMC)**.

Asymmetry

- $Y_1(\cdot)$: precipitation at present.
- $Y_2(\cdot)$: precipitation in 5 minutes time.

Section 2

Causal spatial models

Specification:

$$E\left(Y_2(\mathbf{s}) \mid Y_1(\cdot)\right) = \int_D b(\mathbf{s},\mathbf{v})\,Y_1(\mathbf{v})\,\mathrm{d}\mathbf{v}; \quad \mathbf{s} \in D, \tag{7}$$

$$\mathrm{cov}\left(Y_2(\mathbf{s}), Y_2(\mathbf{u}) \mid Y_1(\cdot)\right) = C_{2|1}(\mathbf{s},\mathbf{u}); \quad \mathbf{s},\mathbf{u} \in \mathbb{R}^d. \tag{8}$$

Building blocks:

- $C_{11}(\cdot,\cdot)$,
- $C_{2|1}(\cdot,\cdot)$,
- $b(\cdot,\cdot)$ (interaction function).

- CCFM is easy to find:

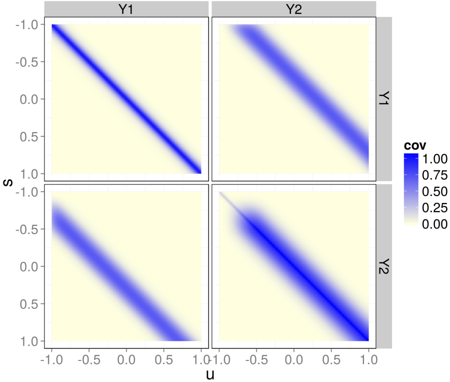
$$\begin{bmatrix} C_{11}(\mathbf{s},\mathbf{u}) & \int_D C_{11}(\mathbf{s},\mathbf{v})b(\mathbf{u},\mathbf{v})\mathrm{d}\mathbf{v} \\ \int_D b(\mathbf{s},\mathbf{v})C_{11}(\mathbf{v},\mathbf{u})\mathrm{d}\mathbf{v} & C_{22}(\mathbf{s},\mathbf{u}) \end{bmatrix}; \tag{9}$$

$$C_{22}(\mathbf{s},\mathbf{u}) = C_{2|1}(\mathbf{s},\mathbf{u}) + \int_D \int_D b(\mathbf{s},\mathbf{v})C_{11}(\mathbf{v},\mathbf{w})b(\mathbf{w},\mathbf{u})\mathrm{d}\mathbf{v}\mathrm{d}\mathbf{w}, \tag{10}$$

and is always valid (we will outline the proof soon).

- Asymmetry (i.e., $C_{12}(\mathbf{s},\mathbf{u}) \neq C_{21}(\mathbf{s},\mathbf{u})$) is guaranteed if $b(\cdot,\cdot)$ is not symmetric.

- Assume $b^o(\cdot) = b(\cdot, \cdot)$ and that it is off-centre.
- $\mathbf{s}, \mathbf{u} \in \{-1, -0.9, \ldots, 1\}$.



Properties of causal spatial models

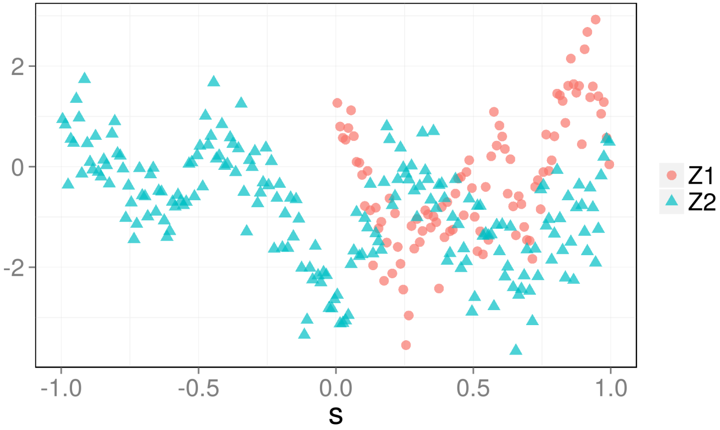
- Heterogeneity, since $C_{11}(\cdot,\cdot)$, $C_{2|1}(\cdot,\cdot)$ need not be homogeneous and $b(\mathbf{s},\mathbf{u})$ need not be symmetric.
- We are not restricted to Matérn fields. The bivariate parsimonious Matérn field is a **special case**.
- $Y_2(\cdot)$ can be arbitrarily smoother than $Y_1(\cdot)$ **and** have a different scale.

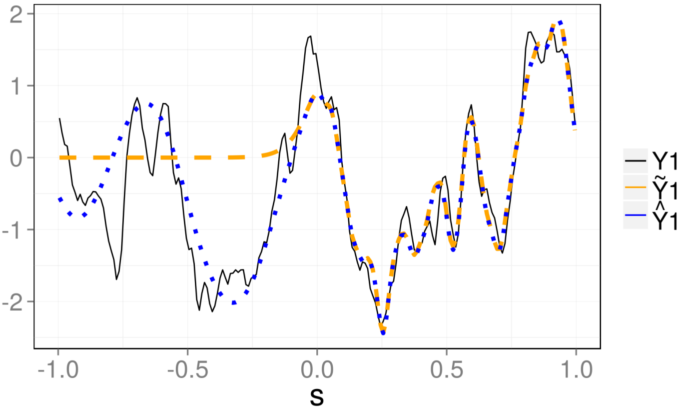
- Assume all parameters are known and $Y_1(\cdot)$ is only partially observed.

- Use simple cokriging **or** simple kriging to estimate $Y_1(\cdot)$:

$$
\begin{aligned}
\hat{Y}_1(\mathbf{s}_0) &\equiv E(Y_1(\mathbf{s}_0) \mid \mathbf{Z}_1, \mathbf{Z}_2) \quad && \text{simple cokriging predictor,} \\
\widetilde{Y}_1(\mathbf{s}_0) &\equiv E(Y_1(\mathbf{s}_0) \mid \mathbf{Z}_1) \quad && \text{simple kriging predictor.}
\end{aligned}
$$

Example

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Is the bivariate model always valid?

- If $C_{11}(\mathbf{s},\mathbf{u})$ and $C_{2|1}(\mathbf{s},\mathbf{u})$ are positive-definite, then $C_{22}(\cdot,\cdot)$ is positive-definite (recall quadratic form).
- $C_{12}(\mathbf{s},\mathbf{u}) = C_{21}(\mathbf{u},\mathbf{s})$.
- CCFM is positive-definite if, for any n_1, n_2 such that $n_1 + n_2 > 0$, any locations $\{\mathbf{s}_{1k}\}, \{\mathbf{s}_{2l}\}$ and any real numbers $\{a_{1k}\}, \{a_{2l}\}$,

$$\begin{aligned}
&\mathrm{var}\left(\sum_{k=1}^{n_1} a_{1k} Y_1^0(\mathbf{s}_{1k}) + \sum_{l=1}^{n_2} a_{2l} Y_2^0(\mathbf{s}_{2l})\right) \\
&= \sum_{k=1}^{n_1}\sum_{k'=1}^{n_1} a_{1k}a_{1k'} C_{11}^0(\mathbf{s}_{1k},\mathbf{s}_{1k'}) + \sum_{l=1}^{n_2}\sum_{l'=1}^{n_2} a_{2l}a_{2l'} C_{22}^0(\mathbf{s}_{2l},\mathbf{s}_{2l'}) \\
&+ \sum_{k=1}^{n_1}\sum_{l'=1}^{n_2} a_{1k}a_{2l'} C_{12}^0(\mathbf{s}_{1k},\mathbf{s}_{2l'}) + \sum_{l=1}^{n_2}\sum_{k'=1}^{n_1} a_{2l}a_{1k'} C_{21}^0(\mathbf{s}_{2l},\mathbf{s}_{1k'}) \;\geq 0.
\end{aligned}$$

- It can be shown that

$$\mathrm{var}\left(\sum_{k=1}^{n_1} a_{1k}Y_1^0(\mathbf{s}_{1k}) + \sum_{l=1}^{n_2} a_{2l}Y_2^0(\mathbf{s}_{2l})\right)$$

$$= \sum_{l=1}^{n_2}\sum_{l'=1}^{n_2} a_{2l}a_{2l'}C_{2|1}(\mathbf{s}_{2l},\mathbf{s}_{2l'}) + \int_D\int_D a(\mathbf{s})a(\mathbf{u})C_{11}(\mathbf{s},\mathbf{u})\,\mathrm{d}\mathbf{s}\mathrm{d}\mathbf{u},$$

where

$$a(\mathbf{s}) \equiv \sum_{k=1}^{n_1} a_{1k}\delta(\mathbf{s}-\mathbf{s}_{1k}) + \sum_{l=1}^{n_2} a_{2l}b(\mathbf{s}_{2l},\mathbf{s}); \quad \mathbf{s}\in\mathbb{R}^d.$$

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- $[Y_1(\cdot), \ldots, Y_p(\cdot)]$ can be decomposed as,

$$[Y_p(\cdot) \mid Y_{p-1}(\cdot), Y_{p-2}(\cdot), \ldots, Y_1(\cdot)] \ldots [Y_1(\cdot)].$$

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$$[Y_p(\cdot) \mid Y_{p-1}(\cdot), Y_{p-2}(\cdot), \ldots, Y_1(\cdot)] \ldots [Y_1(\cdot)].$$

- The conditional expectation is

$$E(Y_q(\mathbf{s}) \mid \{Y_r(\cdot) : r = 1, \ldots, (q-1)\}) \equiv \sum_{r=1}^{q-1} \int_D b_{qr}(\mathbf{s}, \mathbf{v}) Y_r(\mathbf{v}) \mathrm{d}\mathbf{v};$$
$$\mathbf{s} \in D.$$

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- The conditional covariance is

$$\mathrm{cov}(Y_q(\mathbf{s}), Y_q(\mathbf{u}) \mid \{Y_r(\cdot) : r = 1, \ldots, (q-1)\}) \equiv C_{q|(r<q)}(\mathbf{s}, \mathbf{u}); \quad \mathbf{s}, \mathbf{u} \in \mathbb{R}^d,$$

where $\{b_{qr}(\cdot, \cdot) : r = 1, \ldots, (q-1); \; q = 2, \ldots, p\}$ are integrable.

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We need to show that the p-variate process is well defined. The proof is by induction:

- We know that the bivariate process is well defined.
- Assume that the $(p-1)$-variate process is well defined.
- Show that the p-variate process is well defined.

$$\mathrm{var}\left(\sum_{q=1}^{p}\sum_{m=1}^{n_q} a_{qm}Y_q(\mathbf{s}_{qm})\right) = \sum_{m=1}^{n_p}\sum_{m'=1}^{n_p} a_{pm}a_{pm'}C_{p|(q<p)}(\mathbf{s}_{pm},\mathbf{s}_{pm'}) + \sum_{q=1}^{p-1}\sum_{r=1}^{p-1}\int_D\int_D a_q(\mathbf{s})a_r(\mathbf{u})C_{qr}(\mathbf{s},\mathbf{u})\mathrm{d}\mathbf{s}\mathrm{d}\mathbf{u},$$

where

$$a_q(\mathbf{s}) \equiv \left(\sum_{k=1}^{n_q} a_{qk}\delta(\mathbf{s}-\mathbf{s}_{qk}) + \sum_{m=1}^{n_p} a_{pm}b_{pq}(\mathbf{s}_{pm},\mathbf{s})\right).$$

The following can all be shown to be special cases of causal spatial models:

- The parsimonious Matérn model of Gneiting et al. (2010),
- The full Matérn model of Gneiting et al. (2010),
- The linear model of coregionalisation, used for example by Wackernagel (1995),
- The moving average model of Ver Hoef and Barry (1998).

- No restriction on graphical structure. It could be undirected, directed, or a chain graph (Lauritzen, 1996).
- Computationally-efficient algorithms available for some structures.

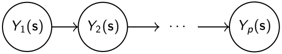
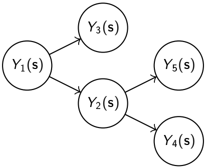


Figure : Ordered nodes



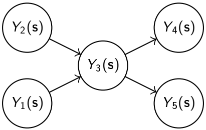


Figure : Trees and polytrees

Model flexibility

$C_{11}(\cdot,\cdot)$	
$C_{21}(\cdot,\cdot)$	$C_{22}(\cdot,\cdot)$

Figure : Bivariate system: Need to specify three marginal/cross-covariance functions.

Available building blocks: Three functions, $C_{11}(\cdot,\cdot)$, $C_{2|1}(\cdot,\cdot)$, $b(\cdot,\cdot)$.

Model flexibility

$C_{11}(\cdot,\cdot)$		
$C_{21}(\cdot,\cdot)$	$C_{22}(\cdot,\cdot)$	
$C_{31}(\cdot,\cdot)$	$C_{32}(\cdot,\cdot)$	$C_{33}(\cdot,\cdot)$

Figure : Trivariate system: Need to specify six marginal/cross-covariance functions.

Available building blocks: Six functions, $C_{11}(\cdot,\cdot)$, $C_{2|1}(\cdot,\cdot)$, $C_{3|1,2}(\cdot,\cdot)$, $b_{21}(\cdot,\cdot)$, $b_{31}(\cdot,\cdot)$, $b_{32}(\cdot,\cdot)$.

Min-max temperatures in Colorado, USA

- Minimum and maximum temperatures taken on September 19, 2004 in the state of Colorado, USA.
- 94 measurement stations (collocated measurements); residuals are obtained by subtraction of statewide mean.
- Maximum-temperature residual later in the afternoon ($Y_2(\cdot)$) highly dependent on minimum-temperature residual in the early morning hours ($Y_1(\cdot)$).
- Fit three models and compare using DIC:

$$\begin{aligned}
&\text{Model 1:} \quad b_o(\mathbf{h}) \equiv 0, \\
&\text{Model 2:} \quad b_o(\mathbf{h}) \equiv A\delta(\mathbf{h}), \\
&\text{Model 3:} \quad b_o(\mathbf{h}) \equiv \begin{cases} A\{1 - (\|\mathbf{h} - \boldsymbol{\Delta}\|/r)^2\}^2, & \|\mathbf{h} - \boldsymbol{\Delta}\| \leq r \\ 0, & \text{otherwise.} \end{cases}
\end{aligned}$$

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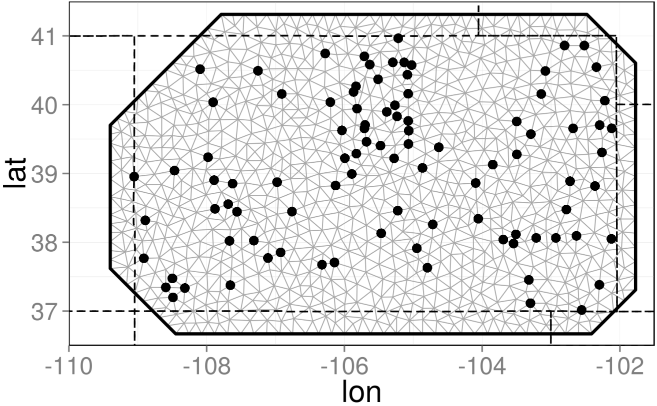
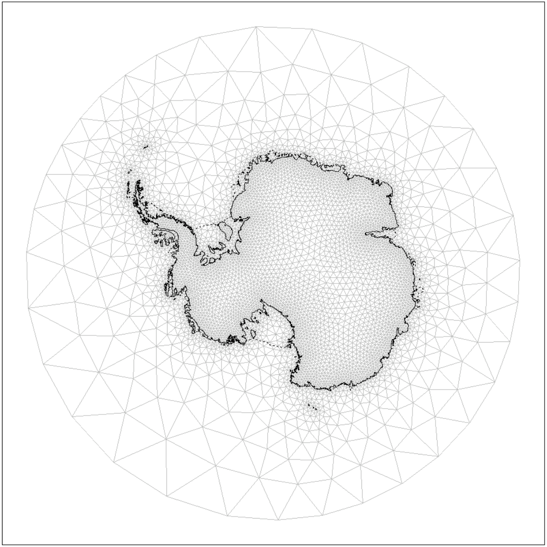
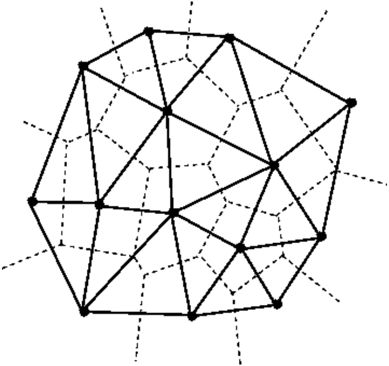
- Consider a discretisation of $Y_1(\cdot)$ and $Y_2(\cdot)$, $\mathbf{Y}_1$ and $\mathbf{Y}_2$ respectively, and let $\mathbf{Y} \equiv (\mathbf{Y}_1, \mathbf{Y}_2)'$, $\mathbf{Z} \equiv (\mathbf{Z}_1, \mathbf{Z}_2)'$.



Why use finite elements?





$$E\left(Y_2(\mathbf{s}) \mid Y_1(\cdot)\right) = \int_D b(\mathbf{s}, \mathbf{v}) Y_1(\mathbf{v})\, \mathrm{d}\mathbf{v}; \quad \mathbf{s} \in D.$$

$$E(Y_2(\mathbf{s}_l) \mid Y_1(\cdot)) \simeq \sum_{k=1}^{n} \eta_k b(\mathbf{s}_l, \mathbf{v}_k) Y_1(\mathbf{v}_k),$$

where $\{\eta_k\}$ are the tessellation areas.

- Observation model:

$$\begin{pmatrix} \mathbf{Z}_1 \\ \mathbf{Z}_2 \end{pmatrix} \Bigg| \begin{pmatrix} \mathbf{Y}_1 \\ \mathbf{Y}_2 \end{pmatrix}, \boldsymbol{\theta} \sim \mathcal{N}\left(\begin{pmatrix} \mathbf{D}\mathbf{Y}_1 \\ \mathbf{D}\mathbf{Y}_2 \end{pmatrix}, \sigma_\varepsilon^2 \begin{pmatrix} \mathbf{I} & \rho_\varepsilon \mathbf{I} \\ \rho_\varepsilon \mathbf{I} & \mathbf{I} \end{pmatrix} \right),$$

where $\mathbf{D}$ is an incidence matrix and $\boldsymbol{\theta}$ includes σ_ε^2 and ρ_ε.

- Process model:

$$\begin{pmatrix} \mathbf{Y}_1 \\ \mathbf{Y}_2 \end{pmatrix} \Bigg| \boldsymbol{\theta} \sim \mathcal{N}\left(\begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}, \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{11}\mathbf{B}' \\ \mathbf{B}\boldsymbol{\Sigma}_{11} & \mathbf{B}\boldsymbol{\Sigma}_{11}\mathbf{B}' + \boldsymbol{\Sigma}_{2|1} \end{pmatrix} \right),$$

where $\boldsymbol{\Sigma}_{11}, \boldsymbol{\Sigma}_{2|1}$ and $\mathbf{B}$ depend on parameters in $\boldsymbol{\theta}$.

We have many unknown parameters!

- Assume that $C_{11}(\cdot)$ and $C_{2|1}(\cdot)$ are Matérn covariance functions with smoothness parameter $\nu = 3/2$.

Parameter	Model 1	Model 2	Model 3
σ_ε^2	x	x	x
ρ_ε	x	x	x
σ_{11}^2	x	x	x
$\sigma_{2\|1}^2$	x	x	x
κ_{11}	0.98 [0.76, 1.22]	1 [0.8, 1.26]	1.03 [0.83, 1.25]
$\kappa_{2\|1}$	0.76 [0.56, 1]	0.62 [0.46, 0.81]	3.65 [1.16, 6.72]
A		x	x
r			x
Δ_1			x
Δ_2			x
DIC	992.45	985.17	982.45

Median fields

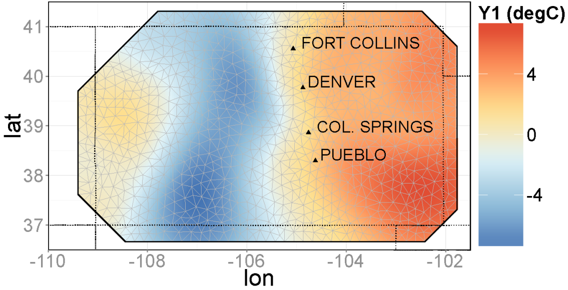


Figure : Interpolated map in degrees Celsius (degC) of $E(\mathbf{Y}_1 \mid \mathbf{Z}_1, \mathbf{Z}_2)$.

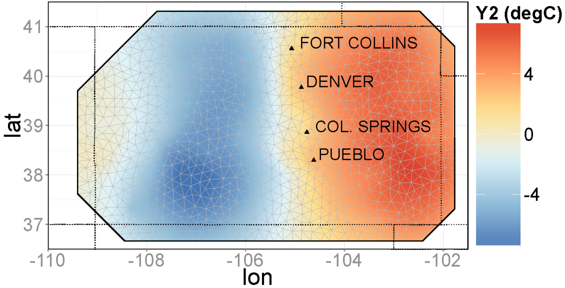


Figure : Interpolated map in degrees Celsius (degC) of $E(\mathbf{Y}_2 \mid \mathbf{Z}_1, \mathbf{Z}_2)$.

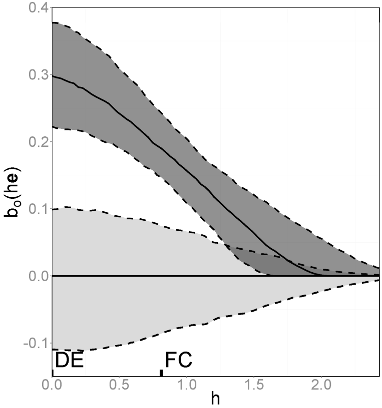


Figure : Prior (light grey) and posterior (dark grey) median (solid line) and inter-quartile ranges (enclosed by dashed lines) of the interaction function $b_o(\cdot)$ of Model 3, along a unit vector **e** originating at Denver (DE) in the direction of Fort Collins (FC)

Section 3

Atmospheric trace-gas inversion in the UK and Ireland

Atmospheric trace-gas inversion

- $Y_1(\mathbf{s})$ is methane emissions per unit area – this is approximately temporally invariant.
- $Y_{2,t}(\mathbf{s})$ is methane mole fraction and is spatio-temporally varying.
- **Aim:** Infer the (spatial) emissions from observation of (spatio-temporal) mole fraction.

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- The interaction function is obtained from a Lagrangian particle dispersion simulator (Met Office's NAME).

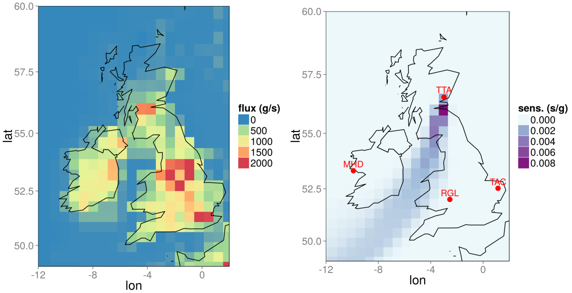
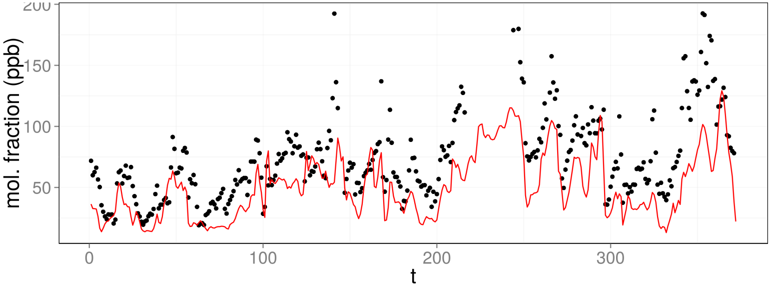


Figure : Emissions map obtained from the NAEI for January 2014 (left panel) and the interaction function $b_t(\mathbf{s}, \cdot)$ obtained from the Met Office's NAME with $\mathbf{s}$ set to the coordinates of the Angus measurement station (TTA), Scotland (right panel).



- The inversion is an ill-posed problem: We need to estimate a (spatial) emissions field from measurements that aggregate spatio-temporally.

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- Let $Y_1(\mathbf{s})$ be a lognormal spatial process, that is, $\widetilde{Y}_1(\cdot) \equiv \log Y_1(\cdot)$ is a Gaussian process.
- Let $E(\widetilde{Y}_1(\mathbf{s})) \equiv \widetilde{\mu}_1(\mathbf{s};\boldsymbol{\vartheta})$ and $\mathrm{cov}(\widetilde{Y}_1(\mathbf{s}), \widetilde{Y}_1(\mathbf{u})) \equiv \widetilde{C}_{11}(\mathbf{s},\mathbf{u};\boldsymbol{\vartheta})$.

$$\begin{aligned} \mu_1(\mathbf{s};\boldsymbol{\vartheta}) &\equiv E(Y_1(\mathbf{s})) \\ &\equiv \exp(\widetilde{\mu}_1(\mathbf{s};\boldsymbol{\vartheta}) + (1/2)\widetilde{C}_{11}(\mathbf{s},\mathbf{s};\boldsymbol{\vartheta})); \quad \mathbf{s} \in D, \end{aligned}$$

$$\begin{aligned} C_{11}(\mathbf{s},\mathbf{u};\boldsymbol{\vartheta}) &\equiv \mathrm{cov}(Y_1(\mathbf{s}), Y_1(\mathbf{u})) \\ &\equiv \mu_1(\mathbf{s};\boldsymbol{\vartheta})\mu_1(\mathbf{u};\boldsymbol{\vartheta})[\exp(\widetilde{C}_{11}(\mathbf{s},\mathbf{u};\boldsymbol{\vartheta})) - 1]; \quad \mathbf{s},\mathbf{u} \in D. \end{aligned}$$

Lognormal bivariate model

- We have a causal **spatio-temporal** bivariate model:

$$E\left(Y_{2,t}(\mathbf{s}) \mid Y_1(\cdot)\right) = \int_D b_t(\mathbf{s},\mathbf{v})Y_1(\mathbf{v})\,\mathrm{d}\mathbf{v}; \quad \mathbf{s} \in D,$$
$$\operatorname{cov}\left(Y_{2,t}(\mathbf{s}), Y_{2,t'}(\mathbf{u}) \mid Y_1(\cdot)\right) = C_{2|1,t,t'}(\mathbf{s},\mathbf{u}); \quad \mathbf{s},\mathbf{u} \in \mathbb{R}^d,$$

with the mole-fraction covariance:

$$C_{22,t,t'}(\mathbf{s},\mathbf{u}) = C_{2|1,t,t'}(\mathbf{s},\mathbf{u}) + \int_D \int_D b_t(\mathbf{s},\mathbf{v})C_{11}(\mathbf{v},\mathbf{w})b_{t'}(\mathbf{w},\mathbf{u})\mathrm{d}\mathbf{v}\mathrm{d}\mathbf{w}.$$

- The conditional covariance $C_{2|1,t,t'}$ is used to account for simulator discrepancy (boundary conditions, model discretisation, linearisation, etc.).

$$\mathbf{Y}_t(\cdot) \sim \mathrm{Dist}\left(\begin{pmatrix}\mu_1(\cdot)\\ \mu_{2,t}(\cdot)\end{pmatrix}, \begin{pmatrix}C_{11}(\cdot,\cdot) & C_{12,t'}(\cdot,\cdot)\\ C_{21,t}(\cdot,\cdot) & C_{22,t,t'}(\cdot,\cdot)\end{pmatrix}\right), \quad t, t' \in \mathbb{R}^+.$$

- What to choose for $C_{2|1,t,t'}(\mathbf{s},\mathbf{u})$?
- *Strategy 1*: If $\dim(\mathbf{Z}_{2,t}) < 10$, say, then use standard spatio-temporal covariance functions, which yield (dense) covariance matrices, and evaluate $Y_{2,t}(\cdot)$ only where we take observations.
- *Strategy 2*: If $\dim(\mathbf{Z}_{2,t}) \gg 10$, then we need to use sequential estimation methods, dimensionality reduction and/or **matrix sparsity**.

- The discrepancy is a separable spatio-temporal Gaussian process with

$$C_{2|1,t,t'}(\mathbf{s},\mathbf{u}) = \sigma^2_{2|1}\rho_s(\mathbf{s},\mathbf{u};d)\rho_t(t,t';a),$$
$$\rho_s(\mathbf{s},\mathbf{u};d) \equiv \exp(\|\mathbf{s}-\mathbf{u}\|/d); \quad d>0,$$
$$\rho_t(t,t';a) \equiv a^{|t-t'|}; \quad |a|<1,$$

- Then $\boldsymbol{\Sigma}_{2|1} = \sigma^2_{2|1}\widetilde{\boldsymbol{\Sigma}}_{2|1,t} \otimes \widetilde{\boldsymbol{\Sigma}}_{2|1,s}$.
- $\mathbf{B}$ is obtained by concatenating $\{\mathbf{B}_t : t = 1,2,\dots\}$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{11}\mathbf{B}' \\ \mathbf{B}\boldsymbol{\Sigma}_{11} & \mathbf{B}\boldsymbol{\Sigma}_{11}\mathbf{B}' + \boldsymbol{\Sigma}_{2|1} \end{pmatrix}.$$

.

- $\mathbf{B}$ is dense: Sparse covariance matrices are not of any use.

Model 2

$$\boldsymbol{\Sigma}^{-1} = \begin{pmatrix} \mathbf{B}'\mathbf{Q}_{2|1}\mathbf{B} + \mathbf{Q}_{11} & -\mathbf{B}'\mathbf{Q}_{2|1} \\ -\mathbf{Q}_{2|1}\mathbf{B} & \mathbf{Q}_{2|1} \end{pmatrix}.$$

- Large benefit by making sure the (very large) matrix $\mathbf{Q}_{2|1}$ is sparse.

$$\Sigma^{-1} = \begin{pmatrix} \mathbf{B}'\mathbf{Q}_{2|1}\mathbf{B} + \mathbf{Q}_{11} & -\mathbf{B}'\mathbf{Q}_{2|1} \\ -\mathbf{Q}_{2|1}\mathbf{B} & \mathbf{Q}_{2|1} \end{pmatrix}.$$

- Large benefit by making sure the (very large) matrix $\mathbf{Q}_{2|1}$ is sparse.
- We define

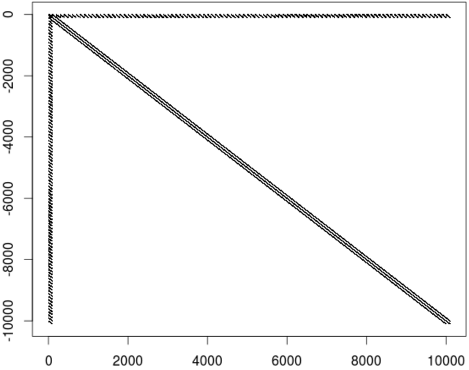
$$\mathbf{Q}_{2|1} \equiv \sigma_{2|1}^{-2}\widetilde{\mathbf{Q}}_{2|1,t} \otimes \widetilde{\mathbf{Q}}_{2|1,s} \quad ,$$

where

$$\widetilde{\mathbf{Q}}_{2|1,t} \equiv \begin{pmatrix} 1 & -a & 0 & & & & 0 \\ -a & (1+a^2) & -a & & & & 0 \\ & & & \ddots & & & \\ 0 & & & & -a & (1+a^2) & -a \\ 0 & & & & 0 & -a & 1 \end{pmatrix}.$$

and we get $\mathbf{Q}_{2|1,s}$ from an intrinsic Gaussian Markov random field specification.

$$\Sigma^{-1} = \begin{pmatrix} \mathbf{B}'\mathbf{Q}_{2|1}\mathbf{B} + \mathbf{Q}_{11} & -\mathbf{B}'\mathbf{Q}_{2|1} \\ -\mathbf{Q}_{2|1}\mathbf{B} & \mathbf{Q}_{2|1} \end{pmatrix}.$$



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- $b_t(\mathbf{s}, \mathbf{u})$ is assumed known from NAME.
- We can obtain reasonable estimates of the parameters appearing in $C_{11}(\mathbf{s}, \mathbf{u})$ from inventories (range, marginal variance, and nugget).
- We have no idea what the parameters appearing in $C_{2|1}(\mathbf{s}, \mathbf{u})$ are. These need to be estimated.

- This is an ill-posed problem: MCMC chains where both the parameters and the fields are unknown will not mix well.

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- We know the first two moments – use a **Laplace-approximated-EM** to estimate the parameters, then fix the parameters and use MCMC for inferring the fields.
- This is known as an empirical hierarchical model (EHM; Cressie and Wikle, 2011).
- We can compute all the (horrible) gradients analytically, use an MCMC method that takes advantage of these. This is known as Hamiltonian Monte Carlo (HMC).

HMC

- Use Hamiltonian dynamics to propose the next state in an MCMC chain (Duane et al., 1987).
- Need knowledge of gradient to simulate dynamics.
- Suitable when variables are highly correlated a posteriori (ill-posed problem).
- Dynamics are simulated using standard methods (Euler or leapfrog method).
- One-step updates = Langevin method.
- HMC chains are ergodic and reversible (Neal, 2011).

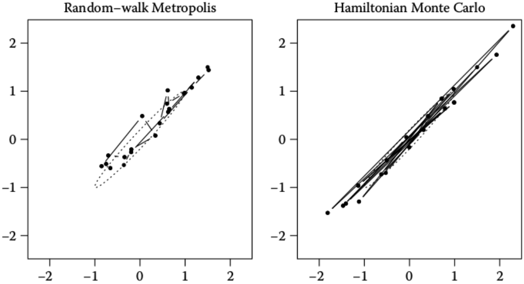
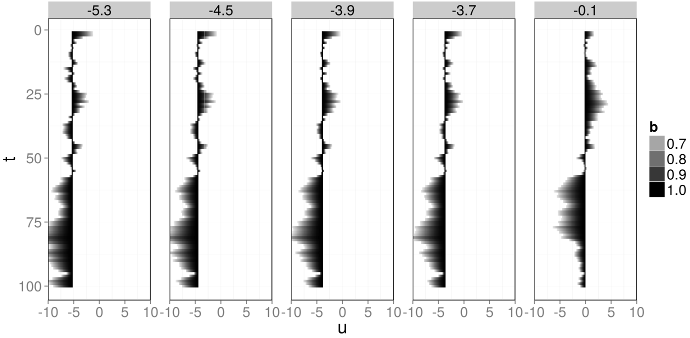


FIGURE 5.4
Twenty iterations of the random-walk Metropolis method (with 20 updates per iteration) and of the Hamiltonian Monte Carlo method (with 20 leapfrog steps per trajectory) for a two-dimensional Gaussian distribution with marginal standard deviations of one and correlation 0.98. Only the two position coordinates are plotted, with ellipses drawn one standard deviation away from the mean.

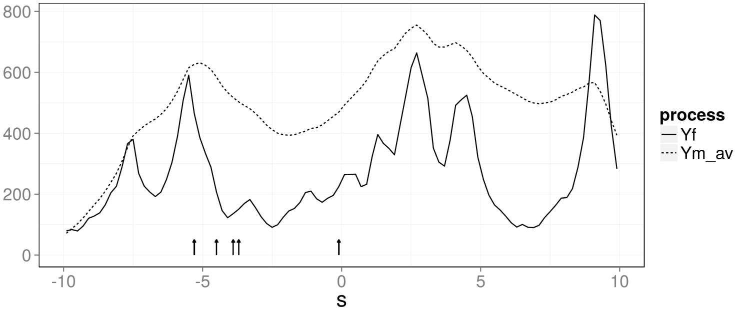
- Figure taken from Neal (2011).

1. Assume the properties of the lognormal flux spatial process (i.e., $\widetilde{C}_{11}$ and $\widetilde{\mu}_1$ are known), and simulate a realisation.
2. Simulate a spatio-temporal interaction function (assumed known).
3. Simulate mole fraction observations at a few locations (Model 1) and at many (1000) locations (Model 2).
4. Infer the flux $Y_1(\mathbf{s})$ from the data in both cases.

- Simulated interaction function.



- Flux and time-averaged mole-fraction field.



Simulation study

- Laplace-EM proved relatively straightforward to implement.
- Convergence with Model 1 $\simeq$ 80 iterations.
- Convergence with Model 2 $\simeq$ 5 iterations (much more data).
- Convergence may be hard to achieve when mode is close to zero and tails are heavy (gradient descents with varying tolerance for convergence).
- "Bouncing method" needs to be implemented for the HMC chain to respect positivity constraint (Neal, 2011).

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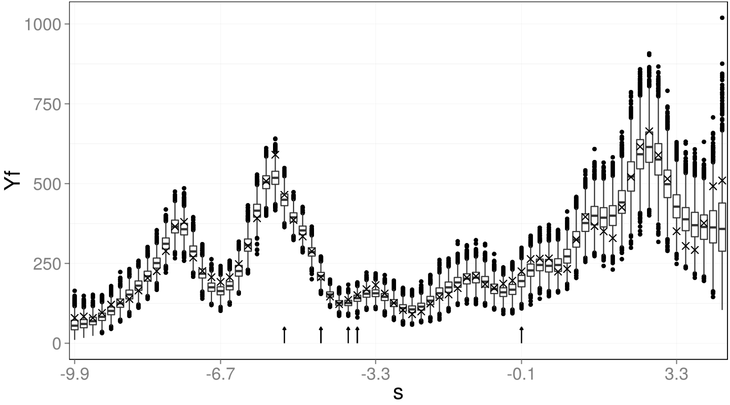
- Inference on flux field for Model 1 using HMC (10,000 samples).



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- Why include the HMC if we have a Laplace-EM?

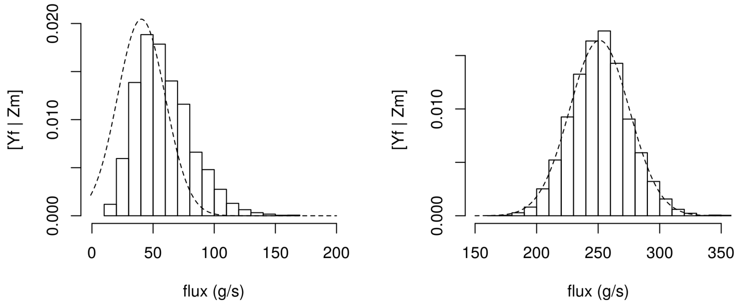


Figure : Laplace approximation (dashed line) and a histogram of the empirical posterior distribution from the MCMC samples (solid line) for methane emissions at $s = -9.9$ (left panel) and $s = -8.1$ (right panel).

UK and Ireland emissions

- Extract spatial properties from the emissions inventory.

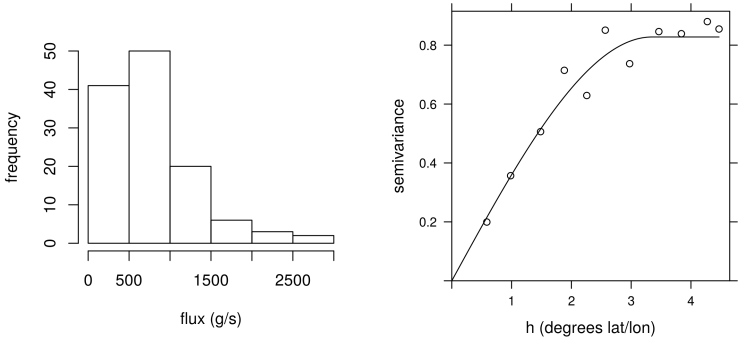
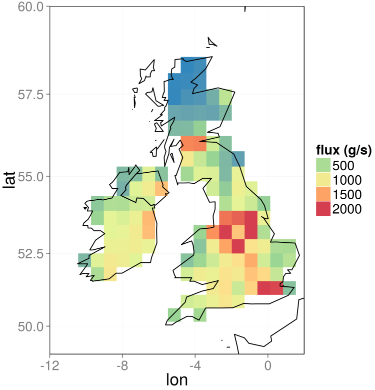


Figure : Histogram of NAEI fluxes in the UK and Ireland following regridding (left panel) and the empirical (open circles) and fitted (solid line) semi-variogram as a function of lag distance in degrees lat/lon.

UK and Ireland emissions

- We used Model 1 since we only have 4 stations.
- Laplace-EM converged in $\simeq$ 30 iterations.
- Simulator discrepancy is not negligible:
  1. $\hat{\sigma}_{2|1} \simeq 20$ ppb,
  2. $\hat{d} \simeq 200$ km,
  3. $\hat{a} \simeq 0.94$ ($1/e$ rate of 32 h).



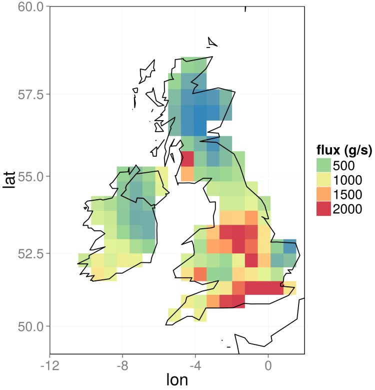


Figure : NAEI (left panel) and 95 percentile (right panel) methane emissions in the UK and Ireland, obtained using the Laplace-EM/HMC approach. Emissions in the white grid cells were treated as background emissions and used to correct the observations.

Section 4

Conclusions

Conclusions

- Bivariate and multivariate models often appear in environmental studies. Usually, one or more of these are 'explained away' prior to commencing the analysis.
- Causal models allow for a (very) flexible model class through interaction functions that can be arbitrarily complex.
- Computation is key: For large, non-Gaussian systems, approximate message passing + variational techniques are probably needed (Cseke et al., 2014).
- Slides and reproducible code available at `https://github.com/andrewzm/bicon`.
- Thanks for Anita Ganesan and Matthew Rigby (University of Bristol) for help with the application case study.

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