Causal Spatial Models

Multivariate models constructed using a conditional approach
— joint work with Noel Cressie —

Andrew Zammit-Mangion

National Institute of Applied Statistics Research Australia
University of Wollongong

Goulburn Fellows Research Meeting
18 March, 2015

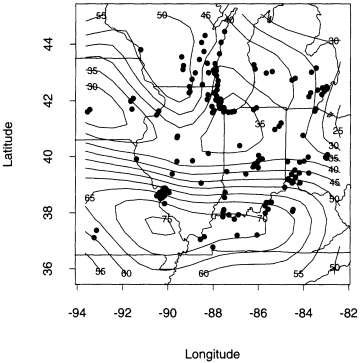
Section 1

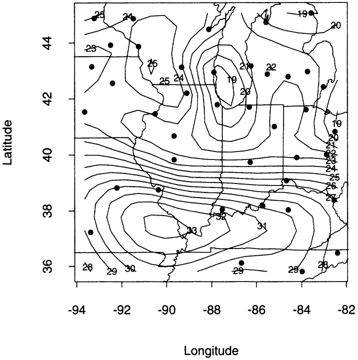
Introduction

- **Univariate** spatial models

- **Multivariate** spatial models.
    - 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**.

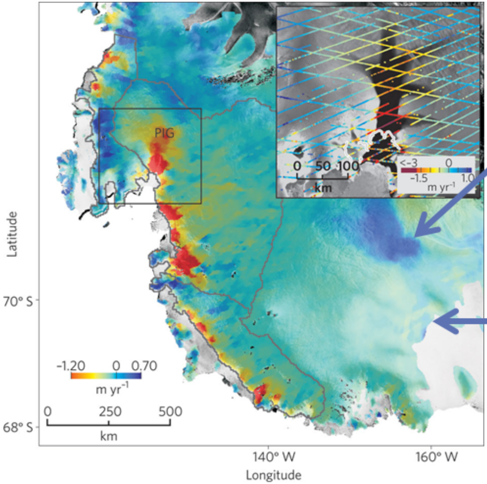
Royle and Berliner (1999), Midwestern USA.



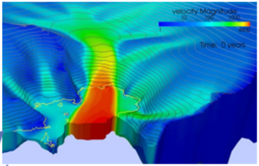


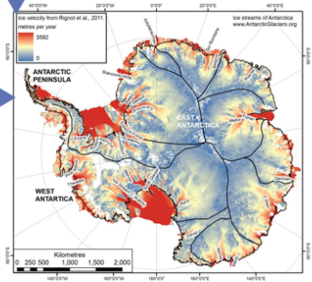
NIASRA
NATIONAL INSTITUTE FOR APPLIED STATISTICS RESEARCH AUSTRALIA

ICESAT data (elevation change per year)

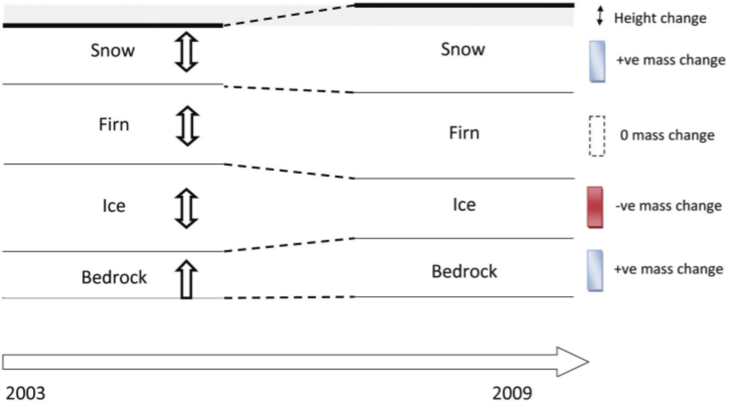


Elmer/Ice (LGGE) model





Example 2: Antarctica Mass Balance



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

- **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 we scale up?

NIASRA NATIONAL INSTITUTE FOR APPLIED STATISTICS RESEARCH AUSTRALIA

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

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

where

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

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

- **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. If we 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.

- 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)**.

- $Y_1(\cdot)$: 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:

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

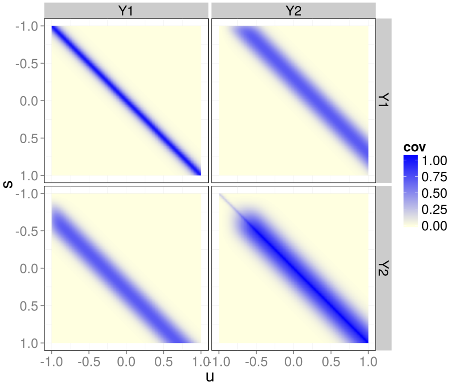
$$C_{22}(\mathbf{s},\mathbf{u}) = C_{2|1}(\mathbf{s},\mathbf{u}) + \int_D \int_D b(\mathbf{s},\mathbf{v})C_{11}(\mathbf{v},\mathbf{w})b(\mathbf{w},\mathbf{u})\mathrm{d}\mathbf{v}\mathrm{d}\mathbf{w}, \tag{10}$$

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

- Asymmetry is guaranteed if $b(\cdot,\cdot)$ is not symmetric.

Properties of causal spatial models

- 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.

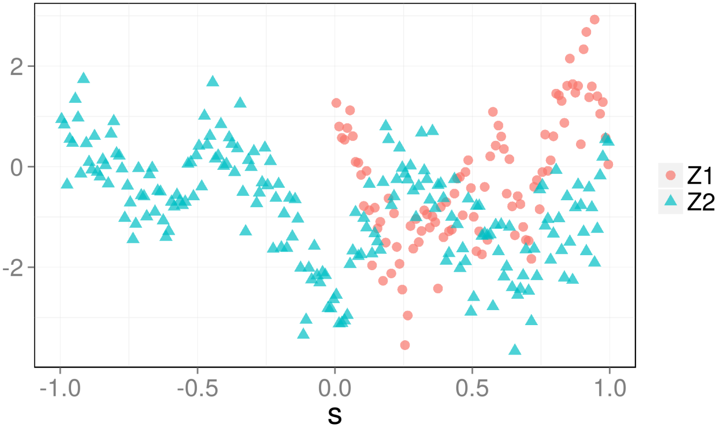
Example

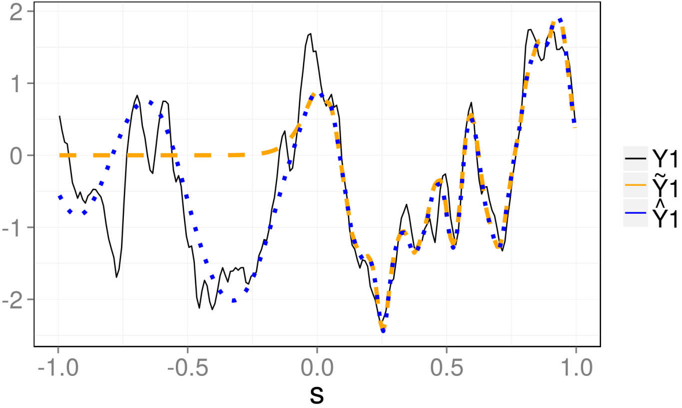
- Assume all parameters are known and $Y_1(\cdot)$ is only partially observed.

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

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

Example




2
1
0
-1
-2
-1.0
-0.5
0.0
0.5
1.0
s
Y1
$\tilde{Y}1$
$\hat{Y}1$

- 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 $n_1 + n_2 > 0$, locations $\{\mathbf{s}_{1k}\}, \{\mathbf{s}_{2l}\}$ and any real numbers $\{a_{1k}\}, \{a_{2l}\}$,

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

NIASRA NATIONAL INSTITUTE FOR APPLIED STATISTICS RESEARCH AUSTRALIA

- 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

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

NIASRA
NATIONAL INSTITUTE FOR APPLIED STATISTICS RESEARCH AUSTRALIA

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

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

- The conditional expectation is

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

- 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.

We need to show that the p-variate process is well defined. Proof 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.

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

where

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

Generalisations

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

- The parsimonious Matern model of Gneiting et al. (2010),
- The full Matern model of Gneiting et al. (2010),
- The linear model of coregionalsiation Wackernagel (1995),
- The moving average model of Ver Hoef and Barry (1998).

Graphical structure

- No restriction on graphical structure.
- Computationally-efficient algorithms available for some structures.

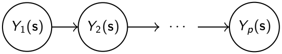


Figure : Chains

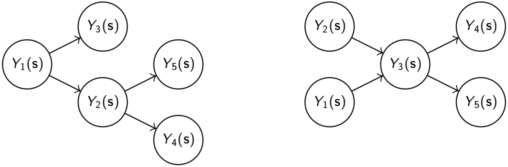


Figure : Trees and polytrees

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: $C_{11}(\cdot,\cdot)$, $C_{2|1}(\cdot,\cdot)$, $b(\cdot,\cdot)$.

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

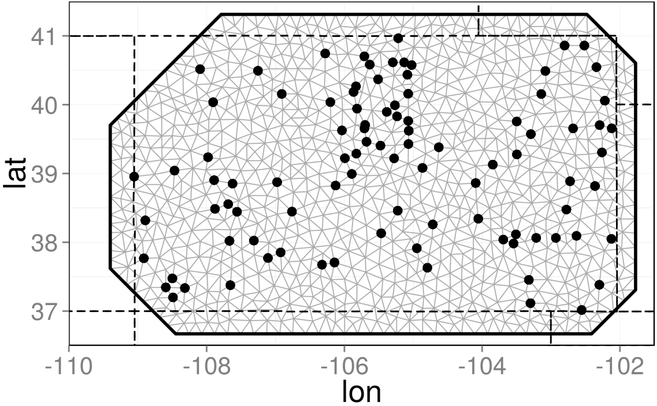
Illustrative example: Min-max temperatures in Colorado, USA

- Minimum and maximum temperatures taken on September 19, 2004.
- 94 measurement stations (collocated measurements).
- Maximum temperature residual later in the afternoon ($Y_2(\cdot)$) highly dependent on minimum temperature residual (from state-wide mean) in the early morning hours ($Y_1(\cdot)$).
- Fit three models and compare using DIC:

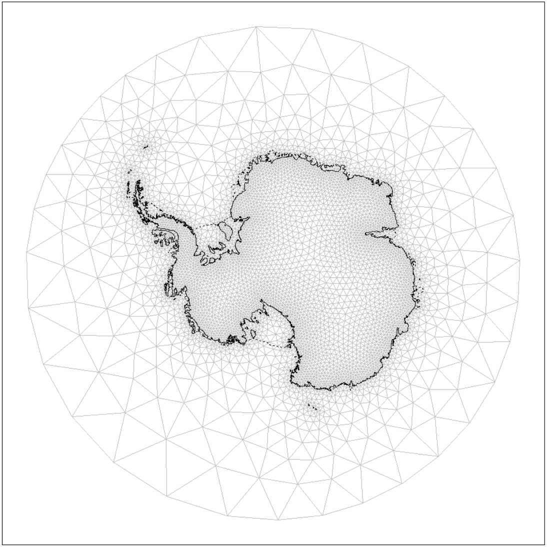
$$
\begin{aligned}
\text{Model 1:} \quad & b_o(\mathbf{h}) \equiv 0, \\
\text{Model 2:} \quad & b_o(\mathbf{h}) \equiv A\delta(\mathbf{h}), \\
\text{Model 3:} \quad & b_o(\mathbf{h}) \equiv \begin{cases} A\{1 - (\|\mathbf{h} - \boldsymbol{\Delta}\|/r)^2\}^2, & \|\mathbf{h} - \boldsymbol{\Delta}\| \leq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

Discretisations

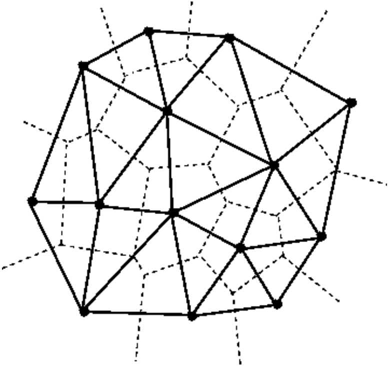
- Consider a discretisation of $Y_1(\cdot)$ and $Y_2(\cdot)$, $\mathbf{Y}_1$ and $\mathbf{Y}_2$ respectively, and let $\mathbf{Y} \equiv (\mathbf{Y}_1, \mathbf{Y}_2)'$, $\mathbf{Z} \equiv (\mathbf{Z}_1, \mathbf{Z}_2)'$.



Why use finite elements?



Numerical integrations



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

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

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

- Observation model:

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

where $\mathbf{D}$ is an incidence matrix.

- Process model:

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

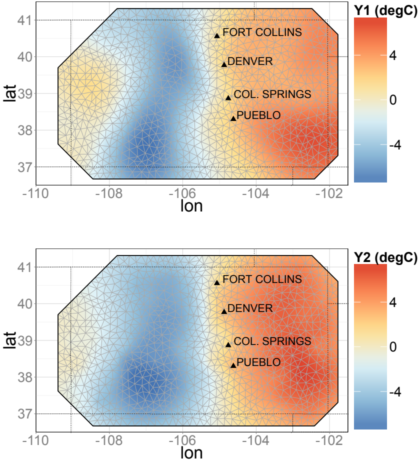
where $\boldsymbol{\Sigma}_{11},\boldsymbol{\Sigma}_{2|1}$ and $\mathbf{B}$ depend on $\boldsymbol{\theta}$.

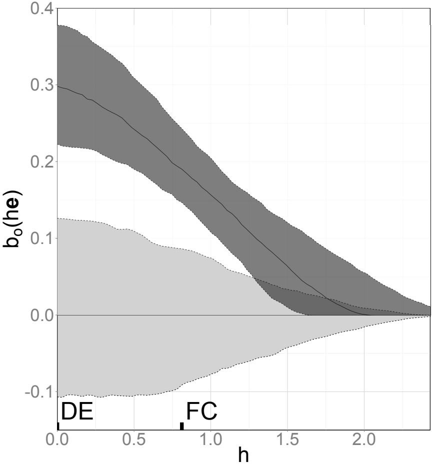
We have many unknown parameters!

- Assume that $C_{11}(\cdot)$ and $C_{2|1}(\cdot)$ areMatérn 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
$\sigma_{2\mid 1}^2$	x	x	x
κ_{11}	0.98 [0.76, 1.22]	1 [0.8, 1.26]	1.03 [0.83, 1.25]
$\kappa_{2\mid 1}$	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

Interaction function





Section 3

Atmospheric trace-gas inversion in the UK and Ireland

- $Y_1(\mathbf{s})$ 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.

NIASRA NATIONAL INSTITUTE FOR APPLIED STATISTICS RESEARCH AUSTRALIA

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

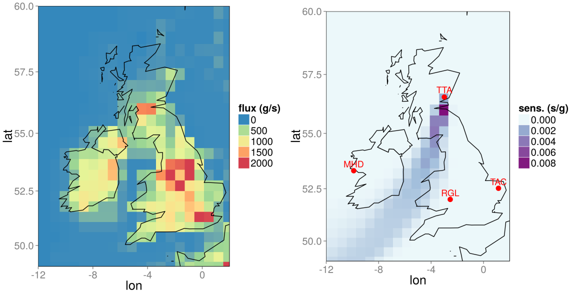
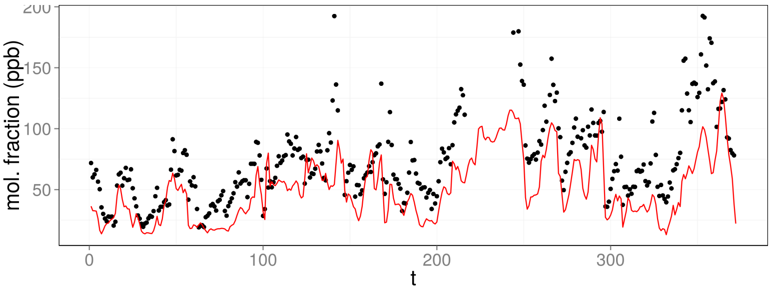


Figure : Emissions map obtained from the NAEI for January 2014 (left panel) and the sensitivity function $b_t(\mathbf{s}, \cdot)$ obtained from the Met Office's NAME with $\mathbf{s}$ set to the coordinates of the Angus measurement station (TTA), Scotland (right panel).



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

NIASRA NATIONAL INSTITUTE FOR APPLIED STATISTICS RESEARCH AUSTRALIA

- 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 $\mathrm{cov}(\widetilde{Y}_1(\mathbf{s}), \widetilde{Y}_1(\mathbf{u})) \equiv \widetilde{C}_{11}(\mathbf{s},\mathbf{u};\boldsymbol{\vartheta})$.

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

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

NIASRA NATIONAL INSTITUTE FOR APPLIED STATISTICS RESEARCH AUSTRALIA

- Now we have a causal **spatio-temporal** bivariate model:

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

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.).

$$\mathbf{Y}_{\cdot}(\cdot) \sim \mathrm{Dist}\left(\begin{pmatrix}\mu_1(\cdot)\\ \mu_{2,\cdot}(\cdot)\end{pmatrix}, \begin{pmatrix} C_{11}(\cdot,\cdot) & C_{12,\cdot}(\cdot,\cdot)\\ C_{21,\cdot}(\cdot,\cdot) & C_{22,\cdot,\cdot}(\cdot,\cdot)\end{pmatrix}\right),$$

- What to choose for $C_{2|1,t,t'}(\mathbf{s},\mathbf{u})$?
- *Strategy 1*: If $\dim(\mathbf{Z}_{2,t}) < 10$, 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 Guassian process with

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

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

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

.

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

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

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

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

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

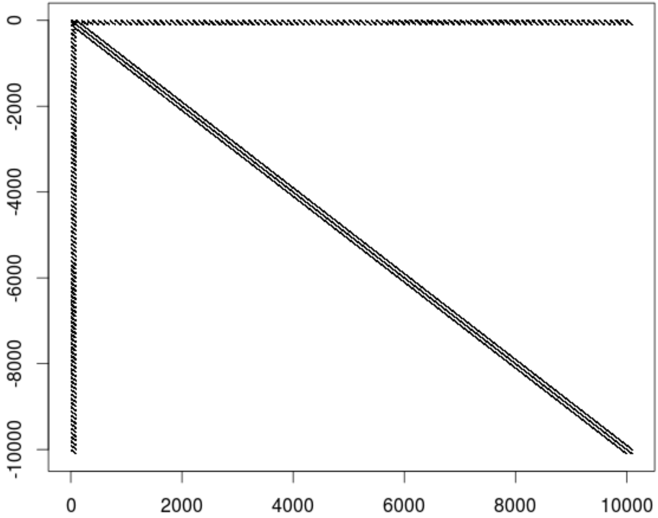
$$\mathbf{Q}_{2|1} \equiv \sigma_{2|1}^{-2}\widetilde{\mathbf{Q}}_{2|1,t} \otimes \widetilde{\mathbf{Q}}_{2|1,s},$$

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 GMRF specification.

Σ^{-1} is sparse



NIASRA
NATIONAL INSTITUTE FOR APPLIED STATISTICS RESEARCH AUSTRALIA

- $b_t(\mathbf{s}, \mathbf{u})$ 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.

Computational strategy

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

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

Computational strategy

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

- This is an ill-posed problem: MCMC chains where both the parameters and the fields are unknown will not mix well.
- 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 which takes advantage of these (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).

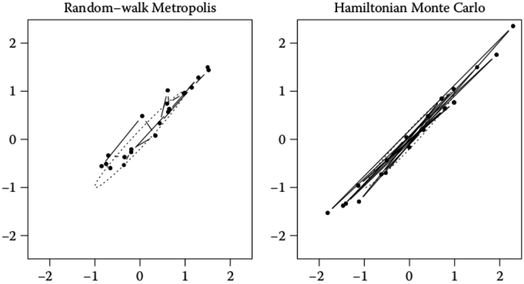
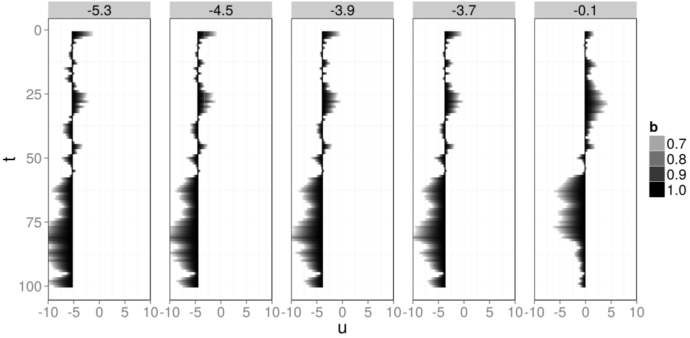


FIGURE 5.4
Twenty iterations of the random-walk Metropolis method (with 20 updates per iteration) and of the Hamiltonian Monte Carlo method (with 20 leapfrog steps per trajectory) for a two-dimensional Gaussian distribution with marginal standard deviations of one and correlation 0.98. Only the two position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

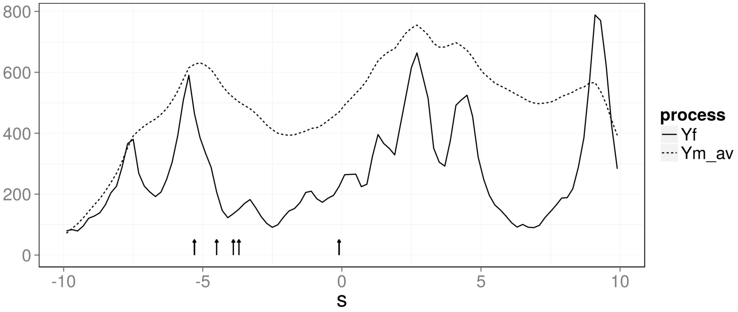
- Figure taken from Neal (2011).

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 (Model 1) a few locations and (Model 2) many 1000 locations.
4. Infer the flux $Y_1(\mathbf{s})$ from the data in both cases.

- Simulated interaction function



- Flux and time-averaged mole fraction field.

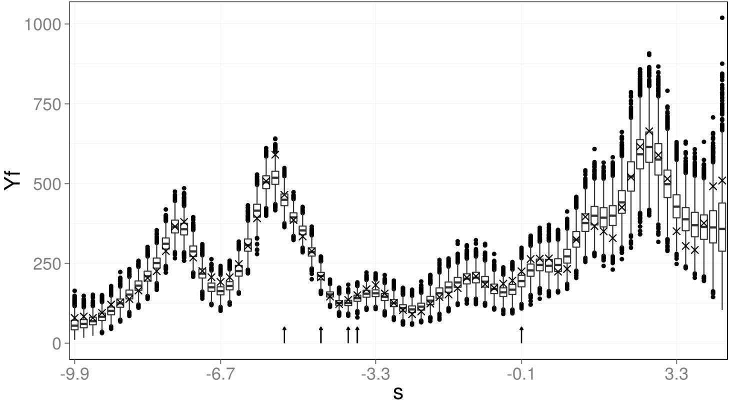


Simulation study

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

NIASRA
NATIONAL INSTITUTE FOR APPLIED STATISTICS RESEARCH AUSTRALIA

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



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

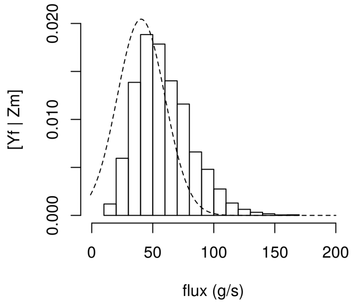


Figure : Laplace approximation (dashed line) and a histogram of the empirical posterior distribution from the MCMC samples (solid line) for methane emissions at $s = -9.9$ (left panel) and $s = -8.1$ (right panel).

- Extract spatial properties from the emissions inventory.

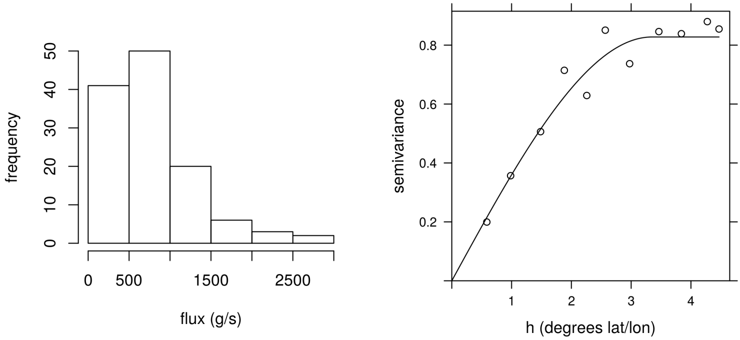


Figure : Histogram of NAEI fluxes in the UK and Ireland following regridding (left panel) and the empirical (open circles) and fitted (solid line) variogram as a function of lag distance in degrees lat/lon.

UK and Ireland emissions

- 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).

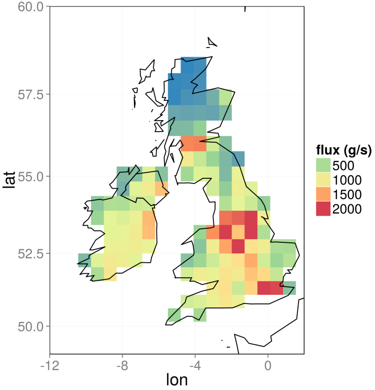


Figure : NAEI (left panel) and 95 percentile (right panel) methane emissions in the UK and Ireland, obtained using the Laplace-EM/HMC approach. Emissions in the white grid cells were treated as background emissions and used to correct the observations.

Section 4

Conclusion

Conclusion

NIASRA
NATIONAL INSTITUTE FOR APPLIED STATISTICS RESEARCH AUSTRALIA

- Bivariate and multivariate models appear in several 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 which can be arbitrarily complex.
- Computation is key: For large, non-Gaussian systems approximate message passing + variational techniques 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.

Cressie, N. and Wikle, C. K. (2011). *Statistics for Spatio-Temporal Data*. John Wiley and Sons, Hoboken, NJ.

Cseke, B., Mangion, A. Z., Sanguinetti, G., and Heskes, T. (2014). Sparse approximations in spatio-temporal point-process models. *arXiv preprint arXiv:1305.4152*.

Duane, S., Kennedy, A. D., Pendleton, B. J., and Roweth, D. (1987). Hybrid Monte Carlo. *Physics Letters B*, 195:216–222.

Gneiting, T., Kleiber, W., and Schlather, M. (2010). Matérn cross-covariance functions for multivariate random fields. *Journal of the American Statistical Association*, 105:1167–1177.

Neal, R. (2011). MCMC using Hamiltonian dynamics. In Brooks, S., Gelman, A., Jones, G. L., and Meng, X.-L., editors, *Handbook of Markov Chain Monte Carlo*. Chapman & Hall/CRC Press, Boca Raton, FL.

Royle, J. A. and Berliner, L. M. (1999). A hierarchical approach to multivariate spatial modeling and prediction. *Journal of Agricultural, Biological, and Environmental Statistics*, 4:29–56.

Ver Hoef, J. M. and Barry, R. P. (1998). Constructing and fitting models for cokriging and multivariable spatial prediction. *Journal of Statistical Planning and Inference*, 69:275–294.

Wackernagel, H. (1995). *Multivariate Geostatistics*. Springer, Berlin, DE.

Zammit-Mangion, A., Bamber, J. L., Schoen, N. W., and Rougier, J. C. (2015a). A data-driven approach for assessing ice-sheet mass balance in space and time. *Annals of Glaciology, in press*.

Zammit-Mangion, A., Rougier, J., Schoen, N., Lindgren, F., and Bamber, J. (2015b). Multivariate spatio-temporal modelling for assessing Antarctica's present-day contribution to sea-level rise. *Environmetrics*, :doi: 10.1002/env.2323, in press.

Zammit-Mangion, A., Rougier, J. C., Bamber, J. L., and Schoen, N. W. (2014). Resolving the Antarctic contribution to sea-level rise: a hierarchical modelling framework. *Environmetrics*, 25:245–264.