Bivariate spatio-temporal statistical models for atmospheric trace gas inversions

– joint work with Noel Cressie, Anita Ganesan and Matt Rigby –

Andrew Zammit-Mangion

National Institute for Applied Statistics Research Australia
University of Wollongong

Introduction

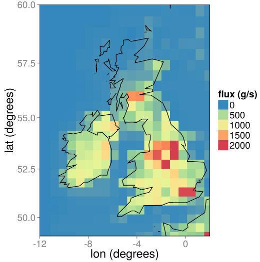
- **Univariate** spatial/spatio-temporal model.
- **Multivariate** spatial/spatio-temporal model.
  - Two or more interacting variables.
  - Improve prediction on one of the variates by observing the others: **Cokriging**.
  - Determine which variate caused the observed phenomenon: **Source separation**, Zammit-Mangion et al. (2014, 2015a,b), Antarctica.

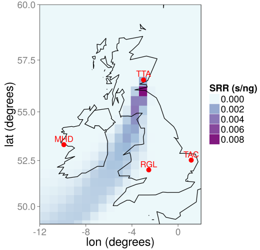
NIASRA NATIONAL INSTITUTE FOR APPLIED STATISTICS RESEARCH AUSTRALIA

- $Y_1(\mathbf{s}) \equiv Y_f(\mathbf{s})$ is methane flux per unit area – we assume this is temporally invariant over a period of one month.
- $Y_{2,t}(\mathbf{s}) \equiv Y_{m,t}(\mathbf{s})$ is methane mole fraction (in ppm) and is spatio-temporally varying due to varying weather patterns etc.
- **Aim:** Infer the (spatial) emissions from observation of (spatio-temporal) mole fraction.

What is available?

- Methane emissions inventories, (e.g., the National Atmospheric Emissions Inventory (NAEI)).
- A Lagrangian Particle Dispersion Model (LPDM) is used to trace particles backwards in time and thus establish the flux-mole-fraction interaction function (SRR), $b_t(\mathbf{s}, \mathbf{u})$.
- The LPDM we use is the Met Office's National Atmospheric Modelling Environment (NAME).
- Data available at four measuring stations averaged over 2 h time periods.





Challenges / current state-of-the-art

- Not use the inventory as a prior (try a spatially invariant prior).
- Not assume Gaussianity of the flux field.
- Not assume independence of flux at the locations of interest.
- Not assume that the LPDM is perfect.

NIASRA
NATIONAL INSTITUTE FOR APPLIED STATISTICS RESEARCH AUSTRALIA

- Observation model:

$$Z_{m,t}(\mathbf{s}) = Y_{m,t}(\mathbf{s}) + \varepsilon_{m,t}(\mathbf{s}); \quad \mathbf{s} \in D^O_{m,t}; \quad t \in \mathcal{T}. \tag{1}$$

- Mole-fraction process model:

$$Y_{m,t}(\mathbf{s}) = \int_D b_t(\mathbf{s},\mathbf{u}) Y_f(\mathbf{u}) \mathrm{d}\mathbf{u} + \zeta_t(\mathbf{s}); \quad \mathbf{s} \in D; \quad t \in \mathcal{T}. \tag{2}$$

- Flux process model:

$$Y_f(\mathbf{s}) \sim \mathcal{LGP}(\widetilde{\mu}_f(\mathbf{s};\boldsymbol{\vartheta}), \widetilde{C}_{ff}(\mathbf{s},\mathbf{u};\boldsymbol{\vartheta})); \quad \mathbf{s},\mathbf{u} \in D. \tag{3}$$

- Let $Y_f(\mathbf{s}) \equiv \exp(\widetilde{Y_f}(\mathbf{s}))$ be a lognormal spatial process.

Bivariate lognormal spatial model for the flux field

- Let $Y_f(\mathbf{s}) \equiv \exp(\widetilde{Y_f}(\mathbf{s}))$ be a lognormal spatial process.
- Then, if $E(\widetilde{Y}_f(\mathbf{s})) \equiv \widetilde{\mu}_f(\mathbf{s};\boldsymbol{\vartheta})$ and $\mathrm{cov}(\widetilde{Y}_f(\mathbf{s}), \widetilde{Y}_f(\mathbf{u})) \equiv \widetilde{C}_{ff}(\mathbf{s},\mathbf{u};\boldsymbol{\vartheta})$.

$$
\begin{aligned}
\mu_f(\mathbf{s};\boldsymbol{\vartheta}) &\equiv E(Y_f(\mathbf{s})) \\
&= \exp(\widetilde{\mu}_f(\mathbf{s};\boldsymbol{\vartheta}) + (1/2)\widetilde{C}_{ff}(\mathbf{s},\mathbf{s};\boldsymbol{\vartheta})); \quad \mathbf{s} \in D,
\end{aligned}
$$

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

Lognormal bivariate model

- We have a spatio-temporal bivariate model:

$$\begin{aligned} E\left(Y_{m,t}(\mathbf{s}) \mid Y_f(\cdot)\right) &= \int_D b_t(\mathbf{s},\mathbf{v})\, Y_f(\mathbf{v})\, \mathrm{d}\mathbf{v}; \quad \mathbf{s} \in D, \\ \operatorname{cov}\left(Y_{m,t}(\mathbf{s}), Y_{m,t'}(\mathbf{u}) \mid Y_f(\cdot)\right) &= C_{m|f,t,t'}(\mathbf{s},\mathbf{u}); \quad \mathbf{s},\mathbf{u} \in \mathbb{R}^d, \end{aligned}$$

Lognormal bivariate model

NIASRA NATIONAL INSTITUTE FOR APPLIED STATISTICS RESEARCH AUSTRALIA

- We have a spatio-temporal bivariate model:

$$E\left(Y_{m,t}(\mathbf{s}) \mid Y_f(\cdot)\right) = \int_D b_t(\mathbf{s},\mathbf{v}) Y_f(\mathbf{v})\,\mathrm{d}\mathbf{v}; \quad \mathbf{s} \in D,$$

$$\mathrm{cov}\left(Y_{m,t}(\mathbf{s}), Y_{m,t'}(\mathbf{u}) \mid Y_f(\cdot)\right) = C_{m|f,t,t'}(\mathbf{s},\mathbf{u}); \quad \mathbf{s},\mathbf{u} \in \mathbb{R}^d,$$

with the mole-fraction covariance:

$$C_{mm,t,t'}(\mathbf{s},\mathbf{u}) = C_{m|f,t,t'}(\mathbf{s},\mathbf{u}) + \int_D \int_D b_t(\mathbf{s},\mathbf{v}) C_{ff}(\mathbf{v},\mathbf{w}) b_{t'}(\mathbf{w},\mathbf{u})\mathrm{d}\mathbf{v}\mathrm{d}\mathbf{w}.$$

Expectations and covariances

$$\mathbf{Y}_t(\cdot) \sim \mathrm{Dist}\left(\begin{pmatrix}\mu_f(\cdot)\\ \mu_{m,t}(\cdot)\end{pmatrix}, \begin{pmatrix}C_{ff}(\cdot,\cdot) & C_{fm,t'}(\cdot,\cdot)\\ C_{mf,t}(\cdot,\cdot) & C_{mm,t,t'}(\cdot,\cdot)\end{pmatrix}\right), \quad t, t' \in \mathbb{R}^+.$$

- Is the cross-covariance function matrix (CCFM) nonnegative-definite?

Expectations and covariances

$$\mathbf{Y}_t(\cdot) \sim \mathrm{Dist}\left(\begin{pmatrix}\mu_f(\cdot)\\ \mu_{m,t}(\cdot)\end{pmatrix}, \begin{pmatrix} C_{ff}(\cdot,\cdot) & C_{fm,t'}(\cdot,\cdot)\\ C_{mf,t}(\cdot,\cdot) & C_{mm,t,t'}(\cdot,\cdot)\end{pmatrix}\right), \quad t, t' \in \mathbb{R}^+.$$

- Is the cross-covariance function matrix (CCFM) nonnegative-definite?
- Consider two spatial processes $Y_1^0(\mathbf{s})$, $Y_2^0(\mathbf{s})$ and interaction function $b(\mathbf{s}, \mathbf{u})$. The CCFM is nonnegative-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 $\{a_{1k}\}, \{a_{2l}\}$,

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

Is the bivariate model always valid?

- 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

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

- For details and proof for p-variate processes see Cressie and Zammit-Mangion (`http://arxiv.org/abs/1504.01865`).

NIASRA
NATIONAL INSTITUTE FOR APPLIED STATISTICS RESEARCH AUSTRALIA

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

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

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

$$
\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{ff} & \boldsymbol{\Sigma}_{ff}\mathbf{B}' \\ \mathbf{B}\boldsymbol{\Sigma}_{ff} & \mathbf{B}\boldsymbol{\Sigma}_{ff}\mathbf{B}' + \boldsymbol{\Sigma}_{m|f} \end{pmatrix}.
$$

.

Inference

- Interaction function (transport model) $b_t(\mathbf{s}, \mathbf{u})$ is assumed known from NAME.

- We can obtain reasonable estimates of the parameters appearing in $C_{ff}(\mathbf{s}, \mathbf{u})$ from inventories (range, marginal variance, and nugget).

- We have no idea what the parameters appearing in $C_{m|f}(\mathbf{s}, \mathbf{u})$ are. We estimate these using an approximate EM algorithm. Flux prediction is done using Hamiltonian Monte Carlo (HMC).

UK and Ireland emissions

- We set the prior-flux expectation to be spatially constant.
- Laplace-EM converged in $\simeq$ 30 iterations.
- Simulator discrepancy is not negligible:
  1. $\hat{\sigma}_{2|1} \simeq 26$ ppb, (observation error $\simeq 10$ ppb)
  2. $\hat{d} \simeq 200$ km,
  3. $\hat{a} \simeq 0.97$ ($1/e$ rate of 66 h).

Posterior distribution of mole fractions

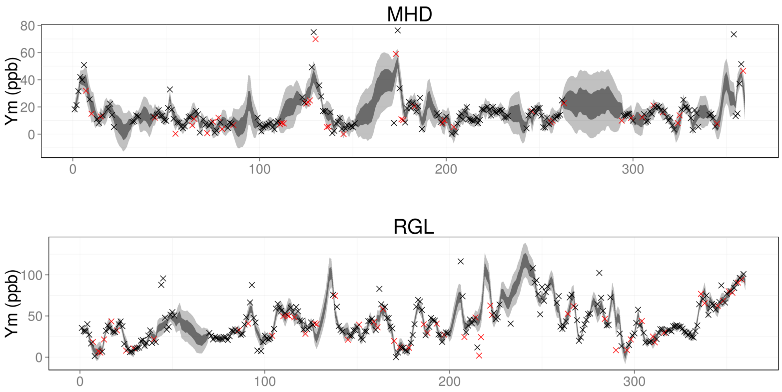


Figure : Distributions of mole fraction due to UK and Ireland land-based emissions at two measurement stations between 1 January 2014 02:00 and 31 January 2014 22:00. The red crosses denote the observations used for validation, whilst the black crosses denote those used for training.

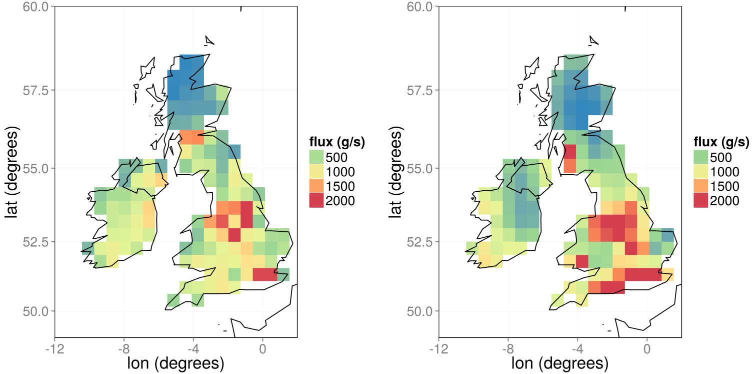


Figure : Emissions inventory (left panel) and 95 percentile (right panel) methane emissions in the UK and Ireland, obtained using the Laplace-EM/HMC approach. Emissions in the white grid cells were assumed known and used to correct the observations.

Conclusions

- Bivariate and multivariate models often appear in environmental studies. Usually, one or more of these are 'explained away' prior to commencing the analysis.
- Such 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 available from `https://github.com/andrewzm/bicon`.

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

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. 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.

Zammit-Mangion, A., Rougier, J. C., 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.