

A Conditional Approach to Multivariate Spatial Modelling

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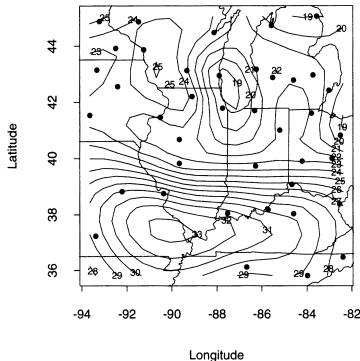
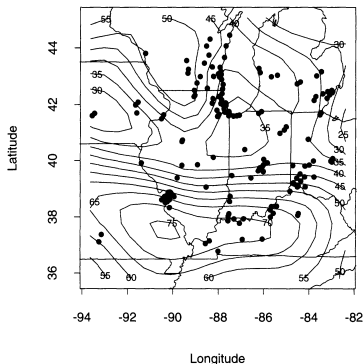


- **Univariate** spatial model
 - “Marginal” behaviour of a single spatial variable
 - Optimally predict at all spatial locations: **Kriging**
- **Multivariate** spatial model
 - Two or more interacting spatial variables
 - Optimally predict one of the variables by using the observations on all variables: **Cokriging**
 - Determine which variable caused the observed phenomenon: **Source separation**

Example: Ozone and Max Temperature

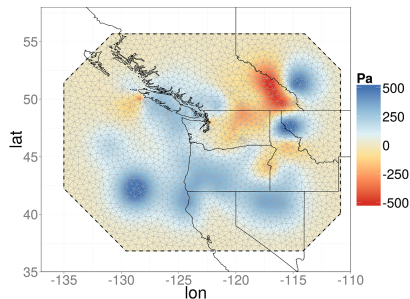
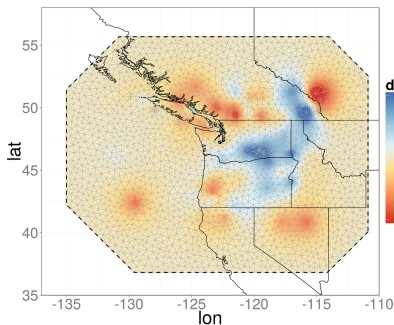


Royle and Berliner (1999), Midwestern USA, centred on Illinois, Lake Michigan, and Chicago (Left panel: Tropospheric ozone concentrations in ppb. Right panel: Maximum temperature in degC)





Gneiting et al. (2010), North American Pacific Northwest (Left panel: Forecast temperature errors. Right panel: Forecast pressure errors)



- **Statistical Modelling**: Given a bivariate process $(Y_1(\cdot), Y_2(\cdot))$, we say that the *cross-covariance function matrix* (**CCFM**),

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

is **nonnegative-definite (nnd)** if **any** covariance matrix derived from it is nnd. In the CCFM,

$$C_{ij}(\mathbf{s}, \mathbf{u}) \equiv \text{cov}(Y_i(\mathbf{s}), Y_j(\mathbf{u})); \mathbf{s}, \mathbf{u} \in \mathbb{R}^d.$$

- **Computational**: Sometimes we have computational difficulty with kriging (univariate models) – how do such algorithms scale to multivariate modelling and **multivariate spatial prediction** (including cokriging)?

- **Linear model of co-regionalisation**, or LMC (Journel and Huijbregts, 1978; Wackernagel, 1995): Define

$$Y_1(\cdot) \equiv a_{11} \tilde{Y}_1(\cdot) + a_{12} \tilde{Y}_2(\cdot),$$

$$Y_2(\cdot) \equiv a_{21} \tilde{Y}_1(\cdot) + a_{22} \tilde{Y}_2(\cdot),$$

where, independently,

$$\tilde{Y}_1(\cdot) \sim \mathcal{N}(\mu_1(\cdot), C_1(\cdot, \cdot)),$$

$$\tilde{Y}_2(\cdot) \sim \mathcal{N}(\mu_2(\cdot), C_2(\cdot, \cdot)).$$

The CCFM is nnd for any $\{a_{ij} : i, j = 1, 2\}$, and

$$C_{ij}(\cdot, \cdot) = a_{i1}a_{j1}C_1(\cdot, \cdot) + a_{i2}a_{j2}C_2(\cdot, \cdot).$$

Hence, $C_{ij}(\mathbf{s}, \mathbf{u}) = C_{ji}(\mathbf{s}, \mathbf{u}) = C_{ij}(\mathbf{u}, \mathbf{s})$. This **symmetry constraint** can be inappropriate.

Multivariate Matérn models can be built from the assumption that $\{C_{ij}(\mathbf{h}) : \mathbf{h} \in \mathbb{R}^d\}$ are each proportional to a **univariate Matérn correlation function**; that is,

$$C_{ij}(\mathbf{h}) \propto 2^{1-\nu_{ij}} \Gamma(\nu_{ij})^{-1} (\kappa_{ij} \|\mathbf{h}\|)^{\nu_{ij}} K_{\nu_{ij}}(\kappa_{ij} \|\mathbf{h}\|),$$

where $\{\nu_{ij}\}$ are smoothness parameters, and $\{\kappa_{ij}\}$ are spatial-scale parameters. The proportionality constants are given by a covariance matrix $\{\tau_{ij}\}$. Restrictions on parameters are needed to obtain a CCFM that is nnd.

Consider now the **bivariate Matérn** models:

Gneiting et al. (2010) defined bivariate Matérn models, however they satisfy the symmetry constraint, $C_{ij}(\mathbf{s}, \mathbf{u}) = C_{ji}(\mathbf{s}, \mathbf{u})$.

- **Bivariate parsimonious Matérn model:** Suppose that $\nu_{ij} \equiv (\nu_i + \nu_j)/2$ and $\kappa_{ij} \equiv \kappa; i, j = 1, 2$. In \mathbb{R}^2 , the CCFM is nnd iff

$$\frac{\tau_{12}^2}{\tau_{11}\tau_{22}} \leq \frac{\nu_1\nu_2}{((\nu_1 + \nu_2)/2)^2}.$$

- **Bivariate full Matérn model:** Here assumptions on smoothness and spatial-scale parameters are relaxed, but finding the parameters for which the CCFM is nnd is much more involved.



Often one process ($Y_1(\cdot)$) “lags” the other ($Y_2(\cdot)$). If this is the case, we should not use models that have the symmetry constraint.

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

The **symmetry constraint**, $C_{12}(\mathbf{s}, \mathbf{u}) = C_{21}(\mathbf{s}, \mathbf{u})$, is **inappropriate** here.



- An easy way to introduce asymmetry is to consider $Y_1(\cdot)$ and $Y_2(\cdot)$ modelled with the symmetry constraint, and then **shift** one of the processes by Δ (e.g., fit the model $Y_1(\cdot)$ and $Y_2(\cdot - \Delta)$).
References: Ver Hoef and Cressie (1993); Christensen and Amemiya (2001, 2002); Li and Zhang (2011)
- Another approach is to introduce latent dimensions. Then asymmetry in the full-dimensional space implies asymmetry in the original space.
Reference: Apanasovich and Genton (2010)



This approach is valid regardless of whether $Y_1(\cdot)$ is the baseline process or whether $Y_2(\cdot)$ is. It is often obvious which one lags and which one leads. Here we choose $Y_1(\cdot)$ as the baseline (i.e., $Y_1(\cdot)$ lags) with covariance function $C_{11}(\cdot, \cdot)$. Write:

$$E(Y_2(\mathbf{s}) \mid Y_1(\cdot)) = \int_D b(\mathbf{s}, \mathbf{v}) Y_1(\mathbf{v}) d\mathbf{v}; \quad \mathbf{s} \in D,$$
$$\text{cov}(Y_2(\mathbf{s}), Y_2(\mathbf{u}) \mid Y_1(\cdot)) = C_{2|1}(\mathbf{s}, \mathbf{u}); \quad \mathbf{s}, \mathbf{u} \in \mathbb{R}^d.$$

Building blocks:

- $C_{11}(\cdot, \cdot)$ (**univariate** covariance); nnd function
- $C_{2|1}(\cdot, \cdot)$ (**univariate** covariance); nnd function
- $b(\cdot, \cdot)$ (**interaction** function); any integrable function

- The CCFM is easy to find:

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

where

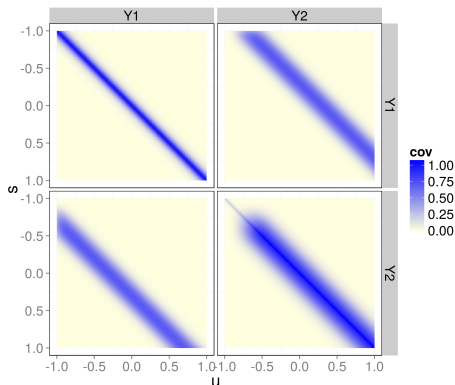
$$C_{22}(\mathbf{s}, \mathbf{u}) = C_{2|1}(\mathbf{s}, \mathbf{u}) + \int_D \int_D b(\mathbf{s}, \mathbf{v}) C_{11}(\mathbf{v}, \mathbf{w}) b(\mathbf{w}, \mathbf{u}) d\mathbf{v} d\mathbf{w},$$

and it is **always nnd** (the proof is given later).

- **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 (i.e., $b(\mathbf{s}, \mathbf{u}) \neq b(\mathbf{u}, \mathbf{s})$, for some \mathbf{s}, \mathbf{u}).

A small example of asymmetry in \mathbb{R}^1 :

- Define $b^o(s - u) \equiv b(s, u)$ that is off-centre (i.e., not symmetric about 0).
- $s, u \in \{-1, -0.9, \dots, 0.9, 1\}$.
- From the figure, $C_{22}(\cdot, \cdot)$ has edge effects and $C_{12}(s, u) \neq C_{21}(s, u)$; see the figure below.



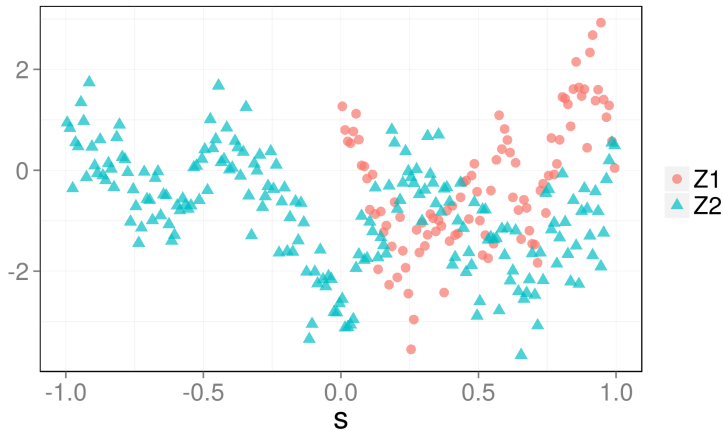
A conditional approach to multivariate spatial modelling:

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

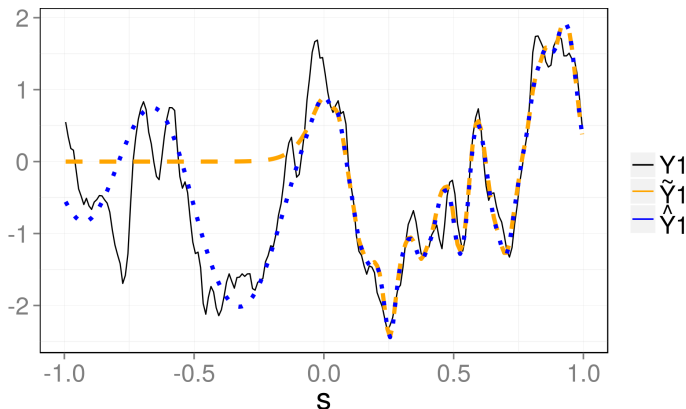
In this simple example, $d = 1$ (i.e., \mathbb{R}^1) and $D = \{-1, -0.9, \dots, 0.9, 1\}$.

- For simplicity, assume all parameters are known. Assume $Y_1(\cdot)$ is only partially observed and with measurement error.
- $Z_j(s) = Y_j(s) + \varepsilon_j(s)$, for all **observation locations** s , where $\{\varepsilon_j(\cdot)\}$ are independent white-noise components.
- Use both **simple cokriging** and **simple kriging** to estimate $Y_1(\cdot)$:

$$\begin{aligned}\hat{Y}_1(s_0) &\equiv E(Y_1(s_0) \mid \mathbf{Z}_1, \mathbf{Z}_2) && \text{simple cokriging predictor,} \\ \tilde{Y}_1(s_0) &\equiv E(Y_1(s_0) \mid \mathbf{Z}_1) && \text{simple kriging predictor.}\end{aligned}$$



Observations on the first spatial variable are non-existent in the left-hand half of D , but **cokriging based on all observations** captures the spatial variability over all of D .





- $C_{11}(\cdot, \cdot)$ and $C_{2|1}(\cdot, \cdot)$ are nnd. Then $C_{22}(\cdot, \cdot)$ is nnd (recall its expression as a quadratic form).
- $C_{12}(\mathbf{s}, \mathbf{u}) = C_{21}(\mathbf{u}, \mathbf{s})$; this is **not** symmetry, and it trivially holds for all \mathbf{s}, \mathbf{u} .
- We now show that **CCFM is nnd**. That is, 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 $\{a_{1k}\}, \{a_{2l}\}$, we show that

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



- It is straightforward to show that

$$\begin{aligned}
 & \text{var} \left(\sum_{k=1}^{n_1} a_{1k} Y_1(\mathbf{s}_{1k}) + \sum_{l=1}^{n_2} a_{2l} Y_2(\mathbf{s}_{2l}) \right) \\
 &= \sum_{l=1}^{n_2} \sum_{l'=1}^{n_2} a_{2l} a_{2l'} C_{2|1}(\mathbf{s}_{2l}, \mathbf{s}_{2l'}) + \int_D \int_D a(\mathbf{s}) a(\mathbf{u}) C_{11}(\mathbf{s}, \mathbf{u}) d\mathbf{s} d\mathbf{u},
 \end{aligned}$$

where for $\delta(\cdot)$ the Dirac delta function,

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

Since $C_{11}(\cdot, \cdot)$ and $C_{2|1}(\cdot, \cdot)$ are nnd by assumption, the right-hand side is ≥ 0 .



- For $p \geq 2$, $[Y_1(\cdot), \dots, Y_p(\cdot)]$ can be decomposed as,

$$[Y_1(\cdot)][Y_2(\cdot)|Y_1(\cdot)] \dots [Y_p(\cdot) | Y_{p-1}(\cdot), Y_{p-2}(\cdot), \dots, Y_1(\cdot)].$$

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- Assume the conditional expectation for the q -th term is, for $\mathbf{s} \in D$,

$$E(Y_q(\mathbf{s}) | \{Y_r(\cdot) : r = 1, \dots, q-1\}) \equiv \sum_{r=1}^{q-1} \int_D b_{qr}(\mathbf{s}, \mathbf{v}) Y_r(\mathbf{v}) d\mathbf{v},$$

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

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

- Assume the conditional covariance for the q -th term is, for $\mathbf{s}, \mathbf{u} \in \mathbb{R}^d$,

$$\text{cov}(Y_q(\mathbf{s}), Y_q(\mathbf{u}) | \{Y_r(\cdot) : r = 1, \dots, (q-1)\}) \equiv C_{q|(r < q)}(\mathbf{s}, \mathbf{u}).$$

We show that the p -variate process is well defined, by induction:

- For nnd C_{11} and $C_{2|1}$, the bivariate process is valid.
- Assume that the $(p-1)$ -variate process is valid.
- Show that the p -variate process is valid. For any n 's, s 's, and a 's,

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

where for $\delta(\cdot)$ the Dirac delta function and for $\mathbf{s} \in \mathbb{R}^d$,

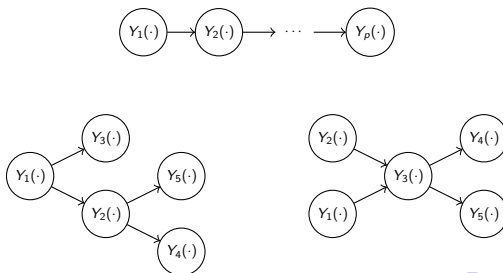
$$a_q(\mathbf{s}) \equiv \left(\sum_{k=1}^{n_q} a_{qk} \delta(\mathbf{s} - \mathbf{s}_{qk}) + \sum_{m=1}^{n_p} a_{pm} b_{pq}(\mathbf{s}_{pm}, \mathbf{s}) \right).$$

The following families of multivariate spatial processes contain classes that are special cases of models defined by the conditional approach:

- The parsimonious 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).
- The shifted models of Ver Hoef and Cressie, Christensen and Amemiya, and Li and Zhang (see earlier slide: Bivariate spatial models with asymmetry).

- Directed acyclic graphs on the variables define a partial order that specifies which conditional covariances, $\{C_{q|}(r < q)\}$, appear in the model.
- Computationally efficient algorithms are available for directed acyclic graphs.

Examples include:





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

Bivariate system: We need to specify **three** marginal/cross-covariance functions. Recall that $C_{12}(\mathbf{s}, \mathbf{u}) = C_{21}(\mathbf{u}, \mathbf{s})$, which is not asymmetry.

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

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

Trivariate system: Need to specify **six** marginal/cross-covariance functions.
Recall that $C_{ij}(\mathbf{s}, \mathbf{u}) = C_{ji}(\mathbf{u}, \mathbf{s})$.

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

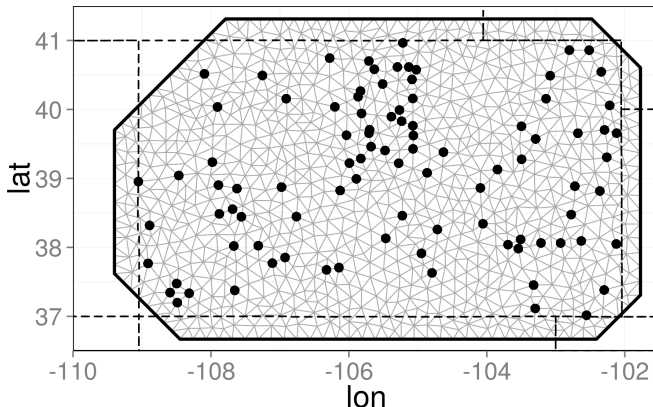
- Dataset: Minimum and maximum temperatures taken on September 19, 2004 in the state of Colorado, USA.
- Data come from 94 measurement stations (collocated measurements); our data are residuals \mathbf{Z}_1 (min. temp.) and \mathbf{Z}_2 (max. temp.) obtained by subtraction of the respective statewide means.
- The maximum-temperature residual process, occurring later in the afternoon ($Y_2(\cdot)$), is highly dependent on the minimum-temperature residual process, occurring in the early-morning hours ($Y_1(\cdot)$).
- We fit three models and compare them using DIC:

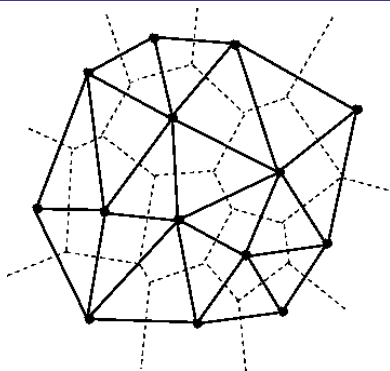
Model 1: $b_o(\mathbf{h}) \equiv 0$ (i.e., independence)

Model 2: $b_o(\mathbf{h}) \equiv A\delta(\mathbf{h})$ (i.e., pointwise dependence)

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

- Consider a discretisation of $Y_1(\cdot)$ and $Y_2(\cdot)$; call the resulting n -dimensional ($n = 968$) vectors \mathbf{Y}_1 and \mathbf{Y}_2 respectively, and define $\mathbf{Y} \equiv (\mathbf{Y}_1', \mathbf{Y}_2')'$. The 188-dimensional data vector is $\mathbf{Z} \equiv (\mathbf{Z}_1', \mathbf{Z}_2')'$ at 94 locations:





Approximate $E(Y_2(\mathbf{s}) \mid Y_1(\cdot)) = \int_D b(\mathbf{s}, \mathbf{v}) Y_1(\mathbf{v}) d\mathbf{v}; \mathbf{s} \in D$, by

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

where $\{A_k : k = 1, \dots, 968\}$ are the polygonal-tessellation areas.

- Data model:

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

where \mathbf{D} is a 94×968 incidence matrix and $\boldsymbol{\theta}$ includes σ_ε^2 and ρ_ε .

- Process model:

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

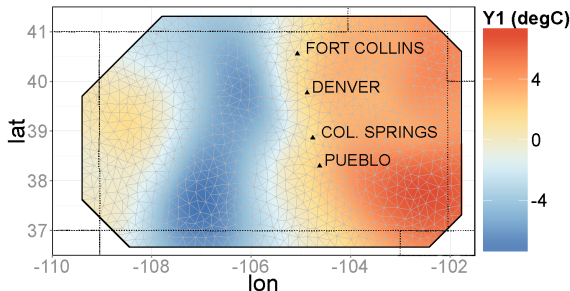
where \mathbf{B} (**interaction matrix**), $\boldsymbol{\Sigma}_{11}$ (**marginal covariance matrix**), and $\boldsymbol{\Sigma}_{2|1}$ (**conditional covariance matrix**) are 968×968 matrices that depend on parameters included in $\boldsymbol{\theta}$.

- Parameter model: see <https://github.com/andrewzm/bicon>

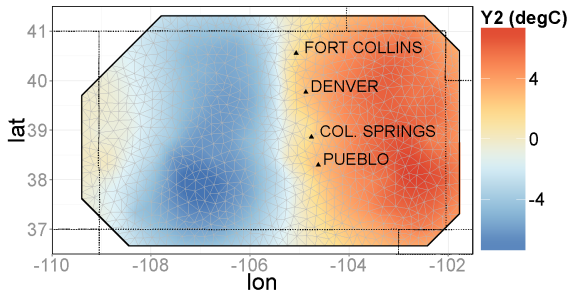
We have many unknown parameters!

Assume $C_{11}(\cdot)$ and $C_{2|1}(\cdot)$ are equally smooth Matérn covariance functions with parameters $(\nu_{11} = 1.5, \kappa_{11}, \sigma_{11}^2)$ and $(\nu_{2|1} = 1.5, \kappa_{2|1}, \sigma_{2|1}^2)$, respectively. Here we show our (Bayesian) inference on the **scale parameters** only.

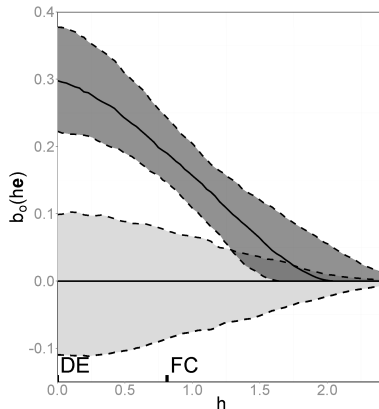
Parameter	Model 1	Model 2	Model 3
σ_ε^2	x	x	x
ρ_ε	x	x	x
σ_{11}^2	x	x	x
$\sigma_{2 1}^2$	x	x	x
κ_{11}	0.98 (0.76, 1.22)	1 (0.8, 1.26)	1.03 (0.83, 1.25)
$\kappa_{2 1}$	0.76 (0.56, 1)	0.62 (0.46, 0.81)	3.65 (1.16, 6.72)
A		x	x
r			x
Δ_1			x
Δ_2			x
<i>DIC</i>	992.45	985.17	982.45



Interpolated map of predicted (residual) **minimum temperature**, $E(Y_1 | Z_1, Z_2)$, in degrees Celsius (degC).



Interpolated map of predicted (residual) **maximum temperature**, $E(Y_2 | Z_1, Z_2)$, in degrees Celsius (degC).



Prior (light grey) and posterior (dark grey) median (solid line) and interquartile ranges (enclosed by dashed lines) of $b_o(\cdot)$ from Model 3, along a unit vector \mathbf{e} originating at Denver (DE) in the direction of Fort Collins (FC).



- **Bivariate and multivariate spatial models** often appear in environmental studies. For convenience, one or more of these variables are often “explained away” prior to commencing a univariate spatial analysis. We wish to avoid this by providing a methodology for building flexible (e.g., no symmetry constraint) multivariate spatial models whose CCFMs are nnd.
- The **conditional approach** allows for a (very) flexible model class through the use of integrable **interaction functions** that can be arbitrarily complex.
- For large, non-Gaussian systems, computational efficiency is key.
- Slides and reproducible code available at <https://github.com/andrewzm/bicon>.

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