Multivariate Non Gaussian random fields

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joint work with David Bolin
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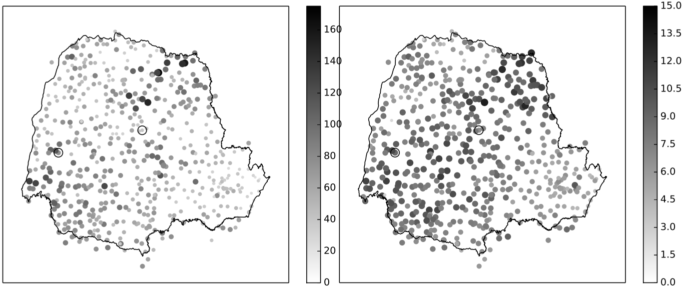
LUND UNIVERSITY

Multivariate geostatistical models



- Standard model:

$$\mathbf{Y}_i = \mathbf{x}(\mathbf{s}_i) + \boldsymbol{\varepsilon}_i,$$

where $\mathbf{Y} = (Y_1, Y_2)$ is data, $\mathbf{x}(s) = (x_1(s), x_2(s))$ is a multivariate random field, and $\boldsymbol{\varepsilon}$ is measurement noise.

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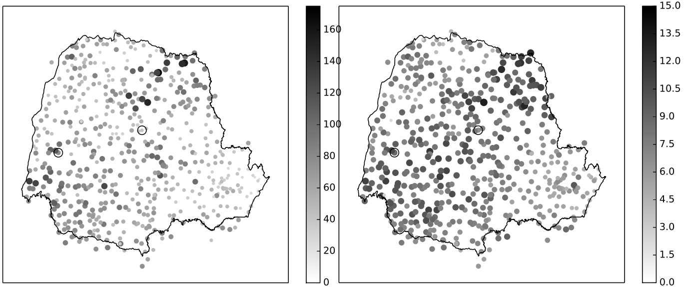

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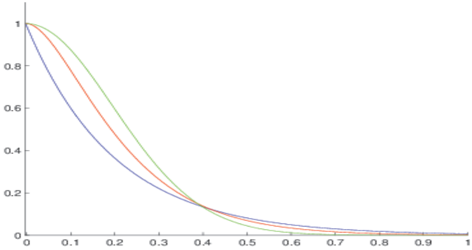
  where $\mathbf{Y} = (Y_1, Y_2)$ is data, $\mathbf{x}(s) = (x_1(s), x_2(s))$ is a multivariate random field, and $\boldsymbol{\varepsilon}$ is measurement noise.
- Computationally demanding, also hard to find valid models.

Univariate Gaussian random field

A Gaussian random field $X(\mathbf{s})$, is uniquely determined by

- $\boldsymbol{\mu}(\mathbf{s}) = \mathsf{E}[X(\mathbf{s})]$
- It covariance function $c(\mathbf{s}_1, \mathbf{s}_2) = \mathbb{C}[X(\mathbf{s}_1), X(\mathbf{s}_2)]$.

The Gaussian Matérn fields



The most popular covariance model in spatial statistics:

$$c(\mathbf{s},\mathbf{t}) \propto (\kappa\|\mathbf{s}-\mathbf{t}\|)^{\nu} K_{\nu}(\kappa\|\mathbf{s}-\mathbf{t}\|)$$

where K_ν is a modified Bessel function of the second kind

- $\nu > 0$ controls smoothness of the process
- $\kappa > 0$ controls the covariance range.

The SPDE connection

Whittle (1963) noted that a Gaussian Matérn fields are stationary (zero mean) solutions to the SPDE

$$(\kappa^2 - \Delta)^{\frac{\alpha}{2}} x(\mathbf{s}) = \dot{\mathcal{W}},$$

where $\dot{\mathcal{W}}$ is Gaussian white noise, $\alpha = \nu + d/2$, and $\mathbf{s} \in \mathbb{R}^d$.

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- Construct computationally efficient GMRF approximations of Gaussian Matérn fields.
- We will later replace $\dot{\mathcal{W}}$ to generate Non Gaussain random field.

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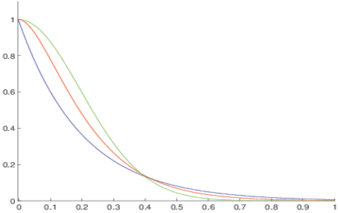
- $\boldsymbol{\mu}(\mathbf{s}) = \mathsf{E}[X(\mathbf{s})]$, which we shall with loss of generality ignore.
- It covariance function $c_{ij}(\mathbf{s}_1, \mathbf{s}_2) = \mathbb{C}[X_i(\mathbf{s}_1), X_j(\mathbf{s}_2)]$.
- The issue is to create a function $c_{ij}(\mathbf{s}_1, \mathbf{s}_2)$ such that it is always positive definite.

The multivariate Matérn model



$$M\left(\mathbf{h} \mid \kappa, \nu\right) = \frac{1}{2^{\nu-1}\Gamma(\nu)} \left(\kappa\|\mathbf{h}\|\right)^{\nu} K_{\nu}\left(\kappa\|\mathbf{h}\|\right)$$

- A multivariate Matérn field is a Gaussian field $\mathbf{x}(\mathbf{s})$, with $c_{ij}(\mathbf{t},\mathbf{s}) = \sigma_i\sigma_j\rho_{ij}M\left(\mathbf{t}-\mathbf{s} \mid \kappa_{ij}, \nu_{ij}\right)$.

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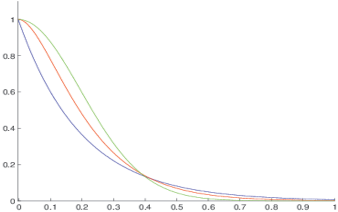

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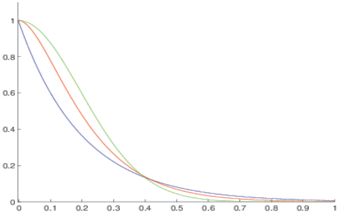

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- Not all parameter values are allowed. Gneiting et al. (2012) and Apanasovich et al. (2012).
- One simple choice is the so-called parsimonious Matérn model, which has $\kappa_{ij} \equiv \kappa, \nu_{ii} = \nu_i$, and $\nu_{ij} = (\nu_i + \nu_j)/2$ for $i \neq j$.

Multivariate SPDE-based models

- Hu et al. (2013) and later Hu and Steinsland (2016) proposed using systems of the form

$$\begin{bmatrix} \mathcal{K}_{11} & \mathcal{K}_{12} & \cdots & \mathcal{K}_{1p} \\ \mathcal{K}_{21} & \mathcal{K}_{22} & \cdots & \mathcal{K}_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{K}_{p1} & \mathcal{K}_{p2} & \cdots & \mathcal{K}_{pp} \end{bmatrix} \begin{bmatrix} x_1(s) \\ x_2(s) \\ \vdots \\ x_p(s) \end{bmatrix} = \begin{bmatrix} \dot{\mathcal{W}}_1 \\ \dot{\mathcal{W}}_2 \\ \vdots \\ \dot{\mathcal{W}}_p \end{bmatrix}$$

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- They focused on the triangular system of SPDEs

$$\begin{bmatrix} \mathcal{L}_{11} & \mathcal{L}_{12} \\ & \mathcal{L}_{22} \end{bmatrix} \begin{bmatrix} x_1(\mathbf{s}) \\ x_2(\mathbf{s}) \end{bmatrix} = \begin{bmatrix} \dot{\mathcal{W}}_1(\mathbf{s}) \\ \dot{\mathcal{W}}_2(\mathbf{s}) \end{bmatrix}.$$

  where $\mathcal{L}_{ij} = \tau_i(\kappa_{ij}^2 - \Delta)^{\frac{\alpha_{ij}}{2}}$.

Multivariate SPDE-based models

- We can informally invert the operator matrix to obtain

$$\begin{bmatrix} x_1(s) \\ x_2(s) \end{bmatrix} = \begin{bmatrix} \mathcal{L}_{11}^{-1} & -\mathcal{L}_{11}^{-1}\mathcal{L}_{12}\mathcal{L}_{22}^{-1} \\ & \mathcal{L}_{22}^{-1} \end{bmatrix} \begin{bmatrix} \dot{\mathcal{W}}_1 \\ \dot{\mathcal{W}}_2 \end{bmatrix}.$$

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- The marginal distribution of x_2 is completely determined by the operator $\mathcal{L}_{22}$ whereas x_1 is affected by all operators.
- Thus, x_2 is marginally a Gaussian Matérn field whereas x_1 has a more complicated covariance structure.

Multivariate SPDE-based models

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- The full SPDE-system is too general.
- Suppose we have a d-dimensional system and we wan't to ensure that all the marginal covariances are Matérn. Is this possible?

It turns out to be possible:

Definition (Multivariate Matérn SPDE field)

We define a p-variate Multivariate Matérn SPDE field as

$$\mathbf{D}\begin{bmatrix}\mathcal{L}_1 & & & & \\ & \mathcal{L}_2 & & & \\ & & \ddots & & \\ & & & \mathcal{L}_{p-1} & \\ & & & & \mathcal{L}_p\end{bmatrix}\begin{bmatrix}x_1(\mathbf{s}) \\ x_2(\mathbf{s}) \\ \vdots \\ x_{p-1}(\mathbf{s}) \\ x_p(\mathbf{s})\end{bmatrix} = \begin{bmatrix}\dot{\mathcal{W}}_1(\mathbf{s}) \\ \dot{\mathcal{W}}_2(\mathbf{s}) \\ \vdots \\ \dot{\mathcal{W}}_{p-1}(\mathbf{s}) \\ \dot{\mathcal{W}}_p(\mathbf{s})\end{bmatrix}.$$

where $\dot{\mathcal{W}}_i(\mathbf{s})$ are mutually independent white noise processes, $\mathcal{L}_i = \tau_i(\kappa_i^2 - \Delta)^{\frac{\alpha_i}{2}}$, and $\mathbf{D}$ is a $p \times p$ invertible matrix.

Proposition

A multivariate Matérn-SPDE field, $\mathbf{x}(\mathbf{s})$, has the covariance function

$$\operatorname{Cov}(x_i(s), x_j(t)) = \begin{cases} \frac{\Gamma(\nu_i)\sum_{j=1}^{p} R_{ii}^2}{\Gamma(\alpha_i)(4\pi)^{d/2}\kappa_i^{2\nu_i}} M\left(\|\mathbf{s}-\mathbf{t}\| \mid \kappa_i,\, \nu_i\right) & i = j, \\ \mathcal{F}^{-1}(S_{ij})(\|\mathbf{s}-\mathbf{t}\|) & i \neq j, \end{cases}$$

where R_{il} are the elements of the matrix $\mathbf{R} = \mathbf{D}^{-1}$ and

$$S_{ij}(\mathbf{k}) = \frac{\sum_{l=1}^{2} R_{il}R_{jl}}{(2\pi)^d} \frac{1}{(\kappa_i^2 + \|\mathbf{k}\|^2)^{\frac{\alpha_i}{2}}(\kappa_j^2 + \|\mathbf{k}\|^2)^{\frac{\alpha_j}{2}}}. \quad (1)$$

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- Our aim is to construct a class of multivariate fields that
  - have Matérn covariances and flexible marginals.
  - are easy to estimate using likelihood-based methods.

Sketch of generation of Non-Gaussian random fields

We working with

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- After discretization

$$\mathbf{K}\begin{bmatrix}\mathbf{X}_1\\ \mathbf{X}_2\end{bmatrix} = \begin{bmatrix}\mathbf{Z}_1\\ \mathbf{Z}_2\end{bmatrix},$$

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- We can generate Non-Gaussian random field by replacing $\mathbf{Z}_i$ with $diag(\sqrt{\mathbf{V}_i})\mathbf{Z}_i$, where $\mathbf{V}_i$ is non negative random vector.

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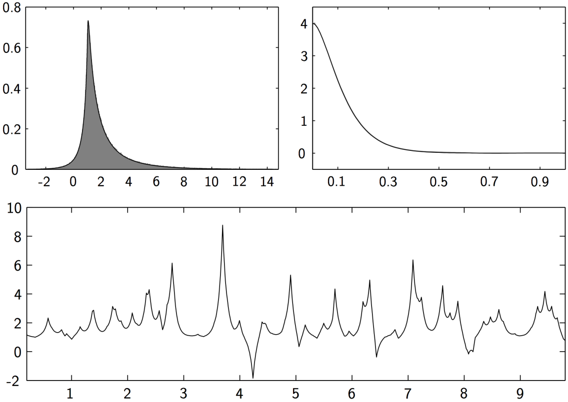
- Basically, a prior on the variance of the field. If repeated measurement mixed-effect model.

Type-G_4

An other version we consider is Type-G_4

- Used in a univariate setting in Bolin (2014) and Wallin and Bolin(2015).



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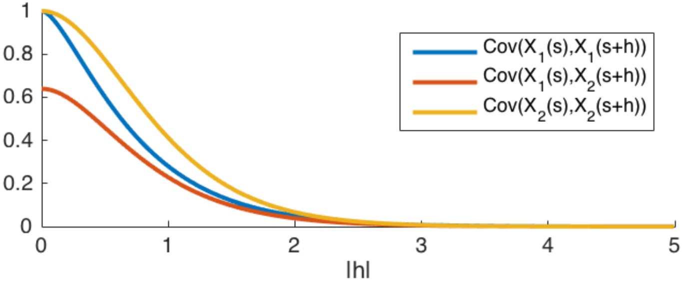
  where $Z_k \sim N(0,1)$ and E_k non negative variable, and $\mathbf{s}_k$ is uniformly distributed over the area.
- For instance, if $\mathbf{V}_i \sim IG(\nu_i, \mathbf{h}\nu_i)$ then we get NIG fields.

Example: Bivariate NIG Matérn fields

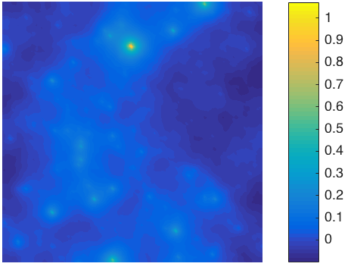


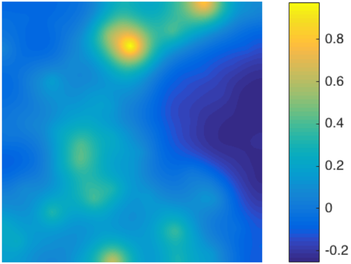
Covariance functions for the solution to the bivariate SPDE

$$\begin{bmatrix} \sqrt{1.81} & -0.9 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \tau_1(\kappa_1^2 - \Delta)^{\frac{\alpha_1}{2}} & \\ & \tau_2(\kappa_2^2 - \Delta)^{\frac{\alpha_2}{2}} \end{bmatrix} \begin{bmatrix} x_1(\mathbf{s}) \\ x_2(\mathbf{s}) \end{bmatrix} = \begin{bmatrix} \dot{\mathcal{N}}_1(\mathbf{s}) \\ \dot{\mathcal{N}}_2(\mathbf{s}) \end{bmatrix}.$$

with $\kappa_1 = 2, \kappa_2 = 3$, $\alpha_1 = 2$ and $\alpha_2 = 4$.

Example simulations





Example of simulations (x_1 left, x_2 right) from a bivariate SPDE

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Parameterization

- $\mathcal{K} = \mathbf{D}_1 \operatorname{diag}(\mathcal{L}_1, \ldots, \mathcal{L}_p)$ and $\mathcal{K} = \mathbf{D}_2 \operatorname{diag}(\mathcal{L}_1, \ldots, \mathcal{L}_p)$ are equivalent if $\mathbf{Q}\mathbf{D}_1 = \mathbf{D}_2$. Where $\mathbf{Q}$ is a orthonormal matrix.

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$$\mathbf{Q} = \begin{bmatrix} cos(\theta) & -sin(\theta) \\ sin(\theta) & cos(\theta) \end{bmatrix}$$

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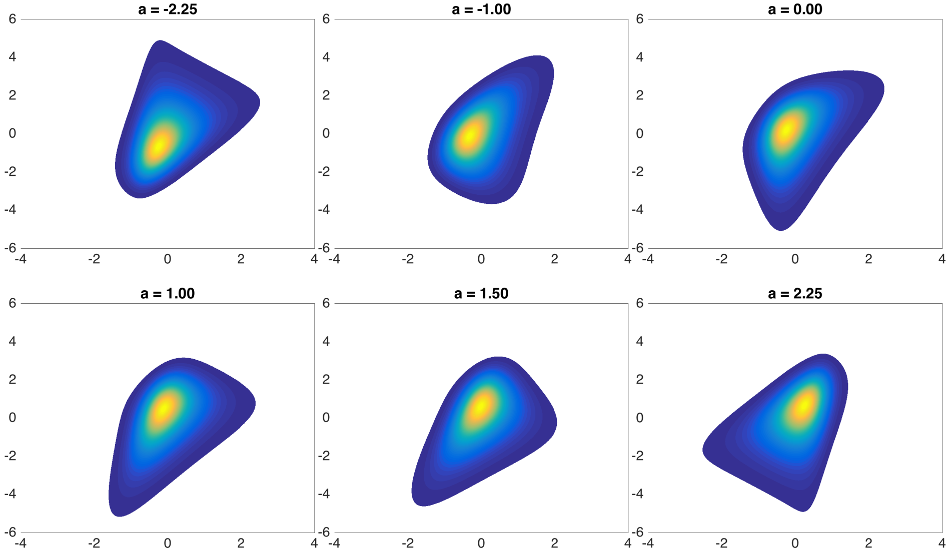
- $\mathcal{K} = \mathbf{D}_1 \operatorname{diag}(\mathcal{L}_1, \ldots, \mathcal{L}_p)$ and $\mathcal{K} = \mathbf{D}_2 \operatorname{diag}(\mathcal{L}_1, \ldots, \mathcal{L}_p)$ are equivalent if $\mathbf{QD}_1 = \mathbf{D}_2$. Where $\mathbf{Q}$ is a orthonormal matrix.
- In $p = 2$

$$\mathbf{Q} = \begin{bmatrix} cos(\theta) & -sin(\theta) \\ sin(\theta) & cos(\theta) \end{bmatrix}$$

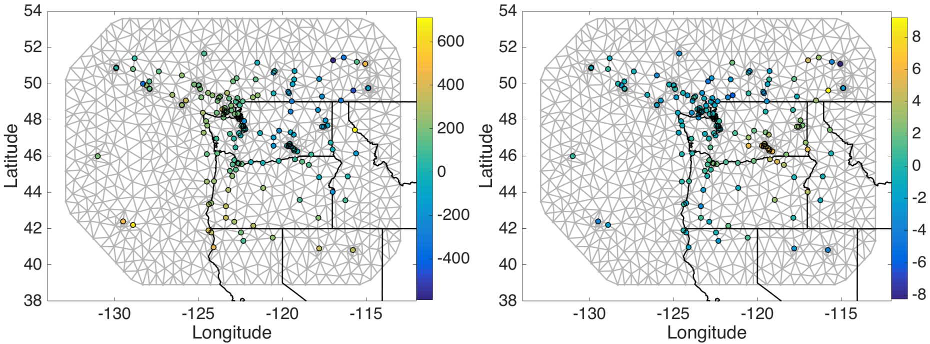
- θ is not identifiable for Gaussian models, but it is for the type-G$_4$ fields.

A general class of bivariate Matérn models



For NIG noise, θ determines bivariate marginals.

Bivariate pressure and temperature data



- 157 observations of pressure (left) and temperature (right) in the North American Pacific Northwest
- The mesh we will use for the SPDE models is also shown.
- Data from Gneiting et al. (2012)

Models for the data

The bivariate observations $\mathbf{y}_i = (y_{P,i}, y_{T,i})^T$ are modeled as

$$\mathbf{y}_i = \mathbf{x}(\mathbf{s}_i) + \boldsymbol{\varepsilon}_i,$$

where $\boldsymbol{\varepsilon}_i$ are independent Gaussian noise, and $\mathbf{x}(\mathbf{s}) = (x_P(\mathbf{s}), x_T(\mathbf{s}))^T$.

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- SPDE models with Gaussian noise for both components, or with Gaussian noise for temperature and NIG noise for pressure.

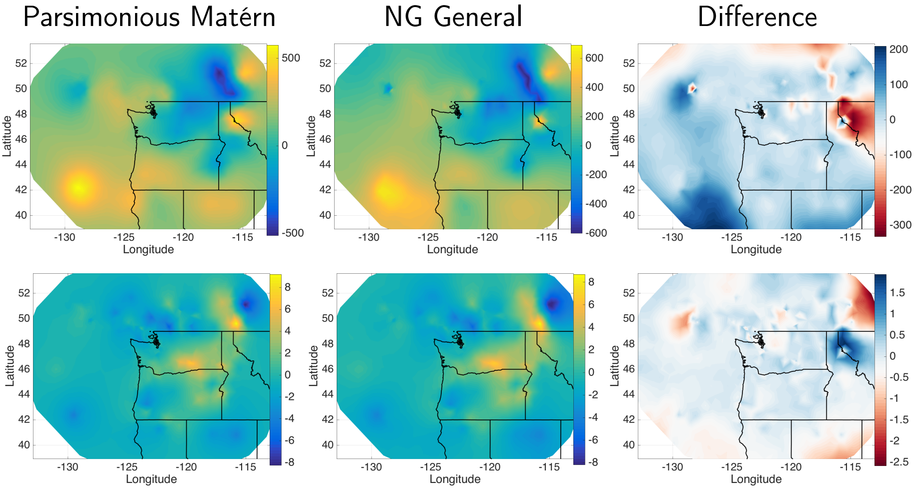
Model comparisons

Model	Number of parameters	Pressure (Pascal)		Temperature (degrees Celcius)	
		MAE	CRPS	MAE	CRPS
Independent	10	40.585	26.546	0.956	0.598
Parsimonious	10	39.068	27.682	0.921	0.576
GG Diagonal	8	38.624	31.711	0.917	0.594
GG Upper	9	38.856	31.829	0.915	0.580
NG Diagonal	10	37.404	26.231	0.917	0.594
NG Upper	11	38.333	25.823	0.917	0.576
NG Lower	11	**37.280**	25.859	**0.898**	0.557
NG General	12	37.928	**25.510**	0.911	**0.555**

Results for leave-one-out crossvalidation, where

- Values are median values of the 157 locations.
- GG denotes Gaussian and NG denotes non-Gaussian SPDEs.

Kriging estimates: pressure (top) and temperature (bottom)



References

For references and further details, see

- Bolin, D. (2014). Spatial Matérn fields driven by non-Gaussian noise. *Scand. J. Statist.*, 41:3, 557-579.
- Wallin, J. and Bolin, D. (2015). Geostatistical Modeling Using Non-Gaussian Matérn Fields. *Scand. J. Statist.*, 42:3, 872-890
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Thanks for your attention!