Multivariate Gaussian Random Fields with SPDEs

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Outline

- ☞ The Matérn covariance function and SPDEs
- ☞ Multivariate GRFs with SPDEs
- ☞ Multivariate GRFs with oscillating covariance functions
- ☞ Sampling the multivariate GRFs
- ☞ Fast inference approach
- ☞ Results with simulated datasets and real datasets
- ☞ Conclusion and Discussion

Multivariate Gaussian random fields are needed in real world

Why we need *Multivariate* random fields?

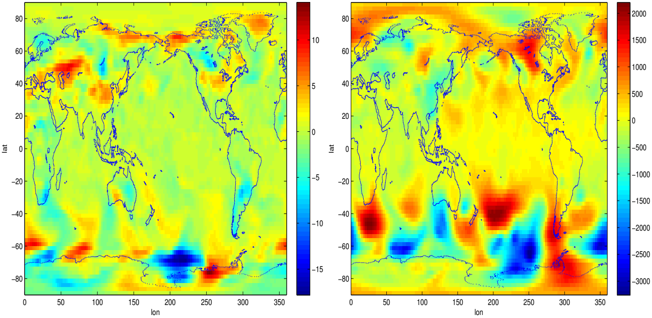
☞ Used to model the correlated datasets;

☞ Capture the spatial dependence structures;

☞ Helpful to predict the other fields;

☞ Big area and a lot of issues needed to be solved.

Multivariate Gaussian random fields are needed in real world



Motivation

Why systems of SPDEs for *Multivariate* GRFs ???

- ☞ Automatically fulfill the non-negative definite constrain;
- ☞ The precision matrix Q is sparse;
- ☞ The parameters in the (systems of) SPDEs are interpretable;
- ☞ Fast infernece can be achieved;
- ☞ Can be extended in various of ways.

Matérn covariance function

The Matérn covariance function is isotropic and has the form

$$\mathrm{Cov}\,(x(0), x(\boldsymbol{h})) = \sigma^2 M(\mathbf{h}|\nu, \kappa) = \frac{\sigma^2 2^{1-\nu}}{\Gamma(\nu)} (\kappa\|\mathbf{h}\|)^\nu K_\nu(\kappa\|\mathbf{h}\|),$$

- ☞ $\|\mathbf{h}\|$ denotes the Euclidean distance;
- ☞ $\nu > 0$ is the smoothness parameter;
- ☞ $\kappa > 0$ is the scaling parameter;
- ☞ σ^2 is the marginal variance;
- ☞ K_ν is the modified Bessel function of second kind.

Link to SPDE

The important relationship is that a Gaussian Field $x(\mathbf{s})$ with the Matérn covariance function is a stationary solution to the linear fractional SPDE (Lindgren et al, 2011)

$$(\kappa^2 - \Delta)^{\alpha/2} x(\mathbf{s}) = \mathcal{W}(\mathbf{s}), \quad \alpha = \nu + d/2, \quad \nu > 0$$

- ☞ $(\kappa^2 - \Delta)^{\alpha/2}$ is a pseudo-differential operator,
- ☞ $\mathcal{W}(\mathbf{s})$ is standard spatial Gaussian white noise
- ☞ Δ is the Laplacian

The Matérn covariance function, restrictive ???

- ☞ At the first glance, modelling with the Matérn covariance function seems quite restrictive,
- ☞ But actually it is not since it covers the most important and mostly used covariance models in spatial statistics.
- ☞ Stein (1999), on Page 14, recommend with "Use the Matérn model".

Multivariate Gaussian random field

A multivariate GRF is a collection of continuously indexed multivariate normal random vectors

$$\mathbf{x}(\mathbf{s}) \sim MVN(\mathbf{0}, \mathbf{\Sigma}(\mathbf{s})),$$

where, $\mathbf{\Sigma}(\mathbf{s})$ is a non-negative definite matrix which depends on the points $\mathbf{s} \in \mathbb{R}^d$.

Multivariate SPDE model

Define system of SPDEs

$$\begin{pmatrix} \mathcal{L}_{11} & \mathcal{L}_{12} & \dots & \mathcal{L}_{1p} \\ \mathcal{L}_{21} & \mathcal{L}_{22} & \dots & \mathcal{L}_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{L}_{p1} & \mathcal{L}_{p2} & \dots & \mathcal{L}_{pp} \end{pmatrix} \begin{pmatrix} x_1(\mathbf{s}) \\ x_2(\mathbf{s}) \\ \vdots \\ x_p(\mathbf{s}) \end{pmatrix} = \begin{pmatrix} \varepsilon_1(\mathbf{s}) \\ \varepsilon_2(\mathbf{s}) \\ \vdots \\ \varepsilon_p(\mathbf{s}) \end{pmatrix}.$$

- ☞ $\mathcal{L}_{ij} = b_{ij}(\kappa_{ij}^2 - \Delta)^{\alpha_{ij}/2}$ are differential operators;
- ☞ ε_i are independent but not necessarily identically distributed noise processes;
- ☞ Currently, we can only take integer valued α_{ij}.

Solve the SPDEs

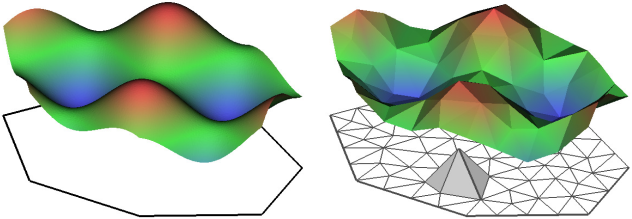
The idea is taken from finite element analysis. The solution of the SPDE could be represented by

$$x(\mathbf{s}) = \sum_{i=1}^{n} \psi_i(\mathbf{s})\omega_i,$$

- ☞ $\psi_i(\mathbf{s})$ is some chosen basis-function;
- ☞ ω_i is some Gaussian distributed weights;
- ☞ n is the number of the vertices in the triangulation.

Piece-wise linear basis function

We choose the piece-wise linear basis function.



The Precision matrix

Denote Q_{α_i} as the precision matrix for the Gaussian weights ω_i for $\alpha_i = 1, 2, 3, \cdots$ as a function of κ_{ij}

$$\begin{cases} \mathbf{Q}_{1,\kappa_{ij}^2} & = \mathbf{K}_{\kappa_{ij}^2} \\ \mathbf{Q}_{2,\kappa_{ij}^2} & = \mathbf{K}_{\kappa_{ij}^2}^T \mathbf{C}^{-1} \mathbf{K}_{\kappa_{ij}^2} \\ \mathbf{Q}_{\alpha,\kappa_{ij}^2} & = \mathbf{K}_{\kappa_{ij}^2}^T \mathbf{C}^{-1} \mathbf{Q}_{\alpha-2,\kappa_{ij}^2} \mathbf{C}^{-1} \mathbf{K}_{\kappa_{ij}^2}, \text{ for } \alpha = 3, 4, \cdots . \end{cases}$$

- ☞ $\langle \cdot, \cdot \rangle$ denote the inner product;
- ☞ $C_{ij} = \langle \psi_i, \psi_j \rangle$, $G_{ij} = \langle \nabla\psi_i, \nabla\psi_j \rangle$, $\mathbf{K}_{\kappa_{ij}^2} = \kappa_{ij}^2 C_{ij} + G_{ij}$.

GMRF approximation

$C_{ij} = \langle \psi_i, \psi_j \rangle$ is replaced by $\tilde{C}_{ii} = \langle \psi_i, 1 \rangle$.

- ☞ $\tilde{C}_{ii}$ is a diagonal matrix;
- ☞ diagonal matrix $\tilde{C}_{ii}$ yields a Markov approximation;
- ☞ difference is negligible.

Covariance-based model

Gneinting et al. (2010) "Matérn Cross-Covariance Functions for Multivariate Random Fields":

$$\mathbf{C}(\mathbf{h}) = \begin{pmatrix} C_{11}(\mathbf{h}) & C_{12}(\mathbf{h}) & \cdots & C_{1p}(\mathbf{h}) \\ C_{21}(\mathbf{h}) & C_{22}(\mathbf{h}) & \cdots & C_{2p}(\mathbf{h}) \\ \vdots & \vdots & \ddots & \vdots \\ C_{p1}(\mathbf{h}) & C_{p2}(\mathbf{h}) & \cdots & C_{pp}(\mathbf{h}) \end{pmatrix},$$

- ☞ $C_{ii}(\mathbf{h}) = \sigma_{ii} M(\mathbf{h}|\nu_{ii}, a_{ii})$ is the marginal covariance function;
- ☞ $C_{ij}(\mathbf{h}) = \rho_{ij}\sigma_i\sigma_j M(\mathbf{h}|\nu_{ij}, a_{ij})$ is the cross-covariance function.

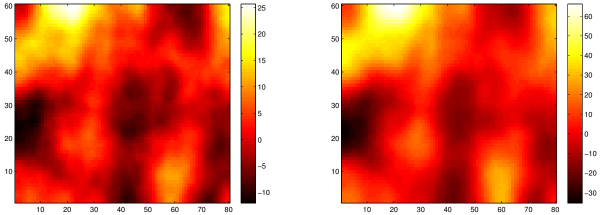
Model matching

- The models based on the SPDEs approach and the covariance-based approach are compared by matching the corresponding elements of the spectral matrix.

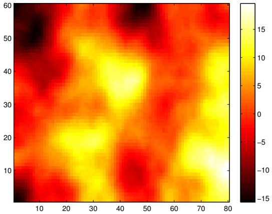
- Under the assumption that $a_{11} = a_{21} = a_{22}$ and $\nu_{11} = \nu_{21} = \nu_{22}$, the models constructed by using SPDEs approach and the covariance-based approach becomes equivalent when

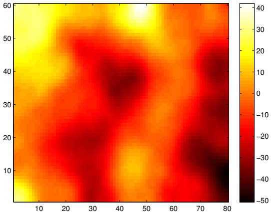
$$
\begin{aligned}
-\frac{b_{22}}{b_{21}} &= \frac{\sigma_1}{\rho\sigma_2}, \\
\frac{b_{22}^2}{b_{11}^2 + b_{21}^2} &= \frac{\sigma_{11}}{\sigma_{22}}.
\end{aligned}
$$

Sampling the positively correlated bivariate GRFs

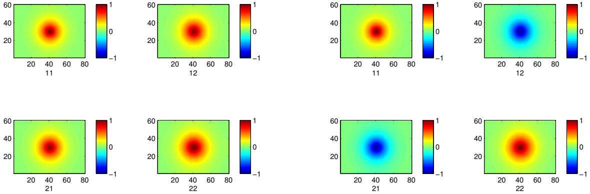


Sampling the negatively correlated bivariate GRFs





The correlation functions



Example and application

It can be shown that the logarithm of posterior distribution of $\boldsymbol{\theta}$ is

$$\begin{aligned}\log(\pi(\boldsymbol{\theta}|\mathbf{y})) = \text{Const} + \log(\pi(\boldsymbol{\theta})) + \frac{1}{2}\log(|\mathbf{Q}(\boldsymbol{\theta})|) \\ -\frac{1}{2}\log(|\mathbf{Q}_c(\boldsymbol{\theta})|) + \frac{1}{2}\boldsymbol{\mu}_c(\boldsymbol{\theta})^T\mathbf{Q}_c(\boldsymbol{\theta})\boldsymbol{\mu}_c(\boldsymbol{\theta}).\end{aligned}$$

Triangular system of SPDEs

The triangular system of SPDEs is commonly used:

$$\begin{pmatrix} \mathcal{L}_{11} & 0 & \dots & 0 \\ \mathcal{L}_{21} & \mathcal{L}_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{L}_{p1} & \mathcal{L}_{p2} & \dots & \mathcal{L}_{pp} \end{pmatrix} \begin{pmatrix} x_1(\mathbf{s}) \\ x_2(\mathbf{s}) \\ \vdots \\ x_p(\mathbf{s}) \end{pmatrix} = \begin{pmatrix} \varepsilon_1(\mathbf{s}) \\ \varepsilon_2(\mathbf{s}) \\ \vdots \\ \varepsilon_p(\mathbf{s}) \end{pmatrix}.$$

- ☞ Can be solved sequentially;
- ☞ Much faster and robust;
- ☞ Possible to model high dimensional multivariate GRFs.

Results from simulated data

Table : Inference with simulated dataset 1

Parameters	True value	Estimated	Standard deviations
κ_{11}	0.3	0.295	0.019
κ_{21}	0.5	0.471	0.044
κ_{22}	0.4	0.380	0.020
b_{11}	1	1.009	0.069
b_{21}	1	1.032	0.064
b_{22}	1	0.997	0.059

Statistical inference with real data example

- ☞ Show how to use the SPDEs approach for constructing the *multivariate* GRFs in real application;
- ☞ The same meteorological dataset used by Gneiting et al. (2010) was chosen and analyzed;
- ☞ It contains the following data: pressure errors (in Pascal), temperature errors (in Kelvin), measured against longitude and latitude;
- ☞ This meteorological dataset contains one observation at 157 locations in the north American Pacific Northwest;
- ☞ Valid on 18th, December of 2003 at 16:00 local time.

The system of SPDEs

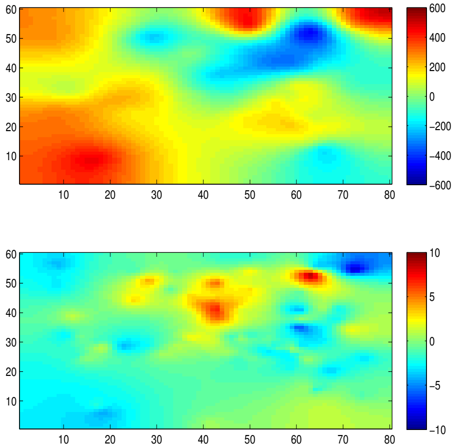
- The system of SPDEs has been used for this dataset can be written down explicitly as

$$
\begin{aligned}
&b_{11}(\kappa_{11}^2 - \Delta)^{\alpha_{11}/2} x_1(\mathbf{s}) = \varepsilon_1(\mathbf{s}),\\
&b_{22}(\kappa_{22}^2 - \Delta)^{\alpha_{22}/2} x_2(\mathbf{s}) + b_{21}(\kappa_{21}^2 - \Delta)^{\alpha_{21}/2} x_1(\mathbf{s}) = \varepsilon_2(\mathbf{s}).
\end{aligned}
$$

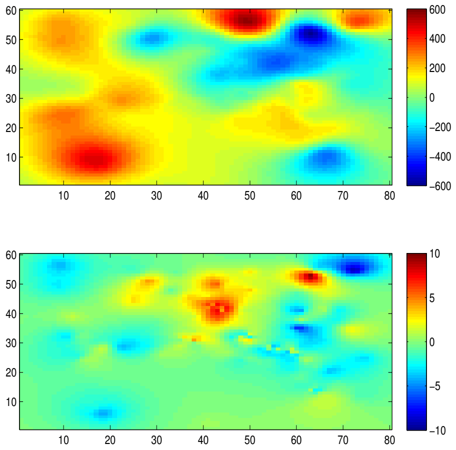
- The noise processes are from SPDEs

$$
\begin{aligned}
(\kappa_{n_1}^2 - \Delta)^{\alpha_{n_1}/2} \varepsilon_1(\mathbf{s}) &= \mathcal{W}_1(\mathbf{s}),\\
(\kappa_{n_2}^2 - \Delta)^{\alpha_{n_1}/2} \varepsilon_2(\mathbf{s}) &= \mathcal{W}_2(\mathbf{s}).
\end{aligned}
$$

The re-construct bivariate fields from SPDEs approach



The re-construct bivariate fields from Gneiting et al. (2010) approach



The predictive performance

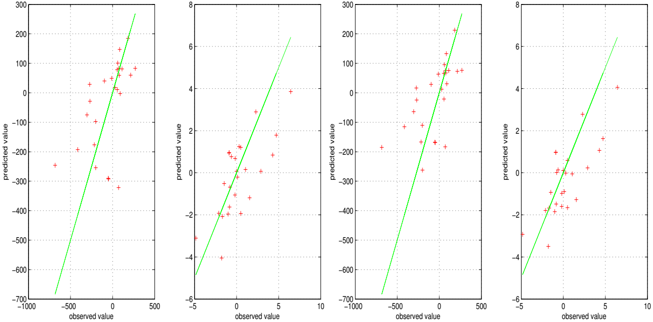


Figure : the covariance-based approach (left) and the predictive performances of SPDEs approach (right)

The predictive performance

Table : predictive errors for the SPDEs approach and the covariance-based models

Models	relative errors	
	pressure field	temperature field
Covariance-based model	0.821	0.716
SPDEs approach	0.777	0.690

Now we go even further!

Construct the multivariate GRFs with oscillating covariance functions. Two approaches can be considered.

- Re-parametrization the systems of the SPDEs,
- Using the noise process with oscillating covariance function.

Question: Why oscillating covariance functions

- Some random fields could have the oscillating covariance structure, such as the pressure on the globe;
- Using the SPDE approach, it is not hard to do that.
- Didn't find many literatures doing this in spatial statistics. (Am I Wrong?)

Systems of SPDEs with oscillating noise processes

$$\begin{pmatrix} \mathcal{L}_{11} & \mathcal{L}_{12} & \dots & \mathcal{L}_{1p} \\ \mathcal{L}_{21} & \mathcal{L}_{22} & \dots & \mathcal{L}_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{L}_{p1} & \mathcal{L}_{p2} & \dots & \mathcal{L}_{pp} \end{pmatrix} \begin{pmatrix} x_1(\mathbf{s}) \\ x_2(\mathbf{s}) \\ \vdots \\ x_p(\mathbf{s}) \end{pmatrix} = \begin{pmatrix} \varepsilon_1(\mathbf{s}) \\ \varepsilon_2(\mathbf{s}) \\ \vdots \\ \varepsilon_p(\mathbf{s}) \end{pmatrix}.$$

- ☞ $\mathcal{L}_{ij} = b_{ij}(\kappa_{ij}^2 - \Delta)^{\alpha_{ij}/2}$ are differential operators;
- ☞ ε_i are independent but not necessarily identically distributed noise processes;
- ☞ Some ε_i can have oscillating covariance functions

Triangular system of SPDEs

☞ We recommend the lower triangular operator matrix

$$\begin{pmatrix} \mathcal{L}_{11} & & & \\ \mathcal{L}_{21} & \mathcal{L}_{22} & & \\ \vdots & \vdots & \ddots & \\ \mathcal{L}_{p1} & \mathcal{L}_{p2} & \dots & \mathcal{L}_{pp} \end{pmatrix} \begin{pmatrix} x_1(\mathbf{s}) \\ x_2(\mathbf{s}) \\ \vdots \\ x_p(\mathbf{s}) \end{pmatrix} = \begin{pmatrix} \varepsilon_1(\mathbf{s}) \\ \varepsilon_2(\mathbf{s}) \\ \vdots \\ \varepsilon_p(\mathbf{s}). \end{pmatrix}.$$

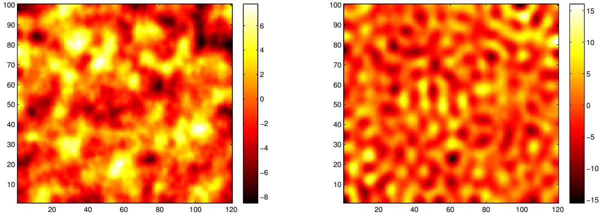
☞ Many advantages: less parameters, fast inference, easy interpreting, and easy locating the position of the oscillating fields.

Triangular system of SPDEs

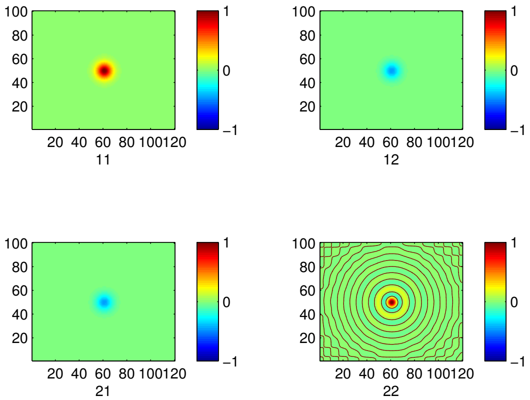
If only the noise process $\varepsilon_i(\mathbf{s})$ has oscillating covariance function, then

- ☞ All random fields $x_j(\mathbf{s}), j < i$ will have non-oscillating covariance functions;
- ☞ Random fields $x_j(\mathbf{s}), j = i$ will be sure to have oscillating covariance function;
- ☞ Random fields $x_j(\mathbf{s}), j > i$ could possibly have oscillating covariance functions;

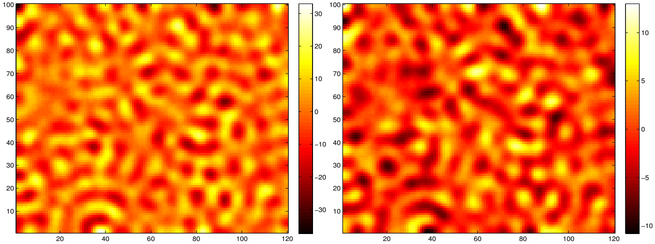
systems of SPDEs with oscillating noise processes



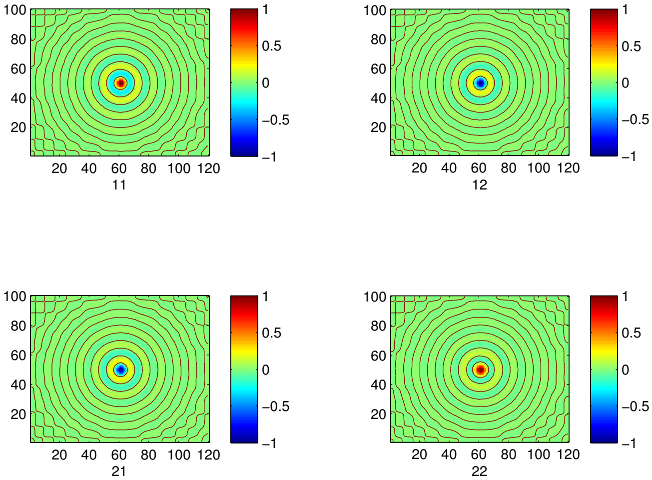
The correlation function



systems of SPDEs with oscillating noise processes



The correlation function



Results from simulated data 1

Table : Inference for the simulated dataset 1

Parameters	True values	Estimates	Standard deviations
b_{11}	0.5	0.495	0.013
b_{21}	0.25	0.248	0.017
b_{22}	1	1.027	0.032
h_{11}	0.25	0.248	0.010
h_{22}	0.36	0.355	0.029
κ_{n_2}	0.6	0.601	0.004
ω	0.95	0.953	0.092

This is with the case only the second random field is oscillating and the first fields is a Matérn random field.

Results from simulated data 2

Table : Inference for the simulated dataset 2

Parameters	True values	Estimates	Standard deviations
b_{11}	0.5	0.497	0.014
b_{21}	0.25	0.234	0.012
b_{22}	1	0.964	0.029
h_{11}	0.25	0.269	0.024
h_{22}	0.36	0.339	0.022
κ_{n_1}	0.5	0.496	0.005
κ_{n_2}	0.6	0.636	0.049
ω	0.95	0.956	0.113

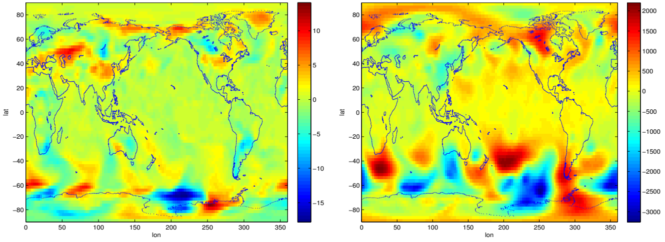
This is with the case both the random fields are with oscillating covariance functions.

Practical settings for inference

- ☞ $\kappa_{11} = \kappa_{n_1}$ and $\kappa_{22} = \kappa_{n_2}$;
- ☞ Model selection: fix α_{ij} and α_{n_i} at different values;
- ☞ Multivariate GRFs with oscillating covariance functions:
  - ✔ Fewer noise processes with oscillating covariance functions when possible;
  - ✔ Pre-analysis for the location the oscillating random fields.

Inference with real dataset

This dataset is from the ERA 40 database, and this dataset contains the temperature and pressure data on the whole globe on 4th of September, 2002.



(a) (b)

Figure : Real dataset from ERA 40 database with temperature (a) and pressure (b)

Estimated bivariate random fields: 2D

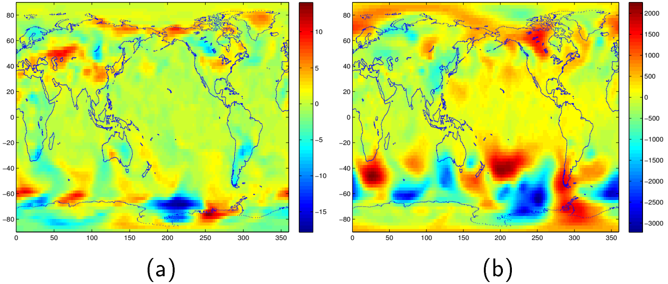


Figure : Estimated conditional mean of bivariate random fields for temperature (a) and pressure (b)

Prediction

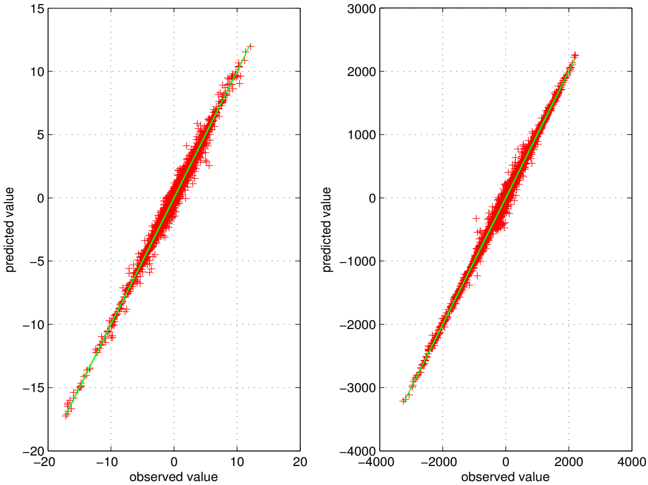


Figure : Prediction for the bivariate random fields at another 5000 data points for temperature (left) and pressure (right)

Conclusion, discussion and future work

- ☞ Illustrated the possibility of construction the *multivariate* GRFs with the system of SPDEs;
- ☞ the GRFs constructed by the system of SPDEs fulfill the "non-negative definite " constrain;
- ☞ The precision matrix for the GMRFs are sparse and hence fast inferences are feasible even for large datasets;
- ☞ Demonstrate the connection between the covariance-based models and SPDE-based models;
- ☞ Looking for real datasets for good applications!!!