Supplement of Geosci. Model Dev., 9, 2407–2414, 2016
http://www.geosci-model-dev.net/9/2407/2016/
doi:10.5194/gmd-9-2407-2016-supplement

Geoscientific Model Development
Open Access

Supplement of

A new test statistic for climate models that includes field and spatial dependencies using Gaussian Markov random fields

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Mathematical details to find Q for a 2×2 lattice.

Consider $\mathbf{x} \sim N(\mathbf{0}_{4\times1}, \mathbf{Q}_{4\times4})$, a vector of measurements on a 2×2 lattice, as represented in Figure 1 of the main manuscript. Assume a neighborhood structure between the four elements of $\mathbf{x}$. In Figure 2 of the main manuscript, the neighbors for each element of $\mathbf{x}$ are defined graphically. Given this structure, one can write expressions for the conditional means that reflect how information at each grid point might be related to its neighbors. Therefore,

$$E(x_1|x_2, x_3, x_4) = \beta_{12}x_2 + \beta_{13}x_3, \tag{1}$$

$$E(x_2|x_1, x_3, x_4) = \beta_{21}x_1 + \beta_{24}x_4, \tag{2}$$

$$E(x_3|x_1, x_2, x_4) = \beta_{31}x_1 + \beta_{34}x_4, \tag{3}$$

$$E(x_4|x_1, x_2, x_3) = \beta_{42}x_2 + \beta_{43}x_3. \tag{4}$$

These expressions are used to find a relationship between the β coefficients and the elements of $\mathbf{Q}$. Since $\mathbf{x} \sim N(\mathbf{0}_{4\times1}, \mathbf{Q}_{4\times4})$, the joint probability distribution of $\mathbf{x}$ is given by,

$$\begin{aligned} f(x_1, x_2, x_3, x_4) \propto \;\; & exp(-\tfrac{1}{2}(Q_{11}x_1^2 + Q_{22}x_2^2 + Q_{33}x_3^2 + Q_{44}x_4^2 + 2Q_{12}x_1x_2 + 2Q_{13}x_1x_3 + 2Q_{14}x_1x_4 \\ & +2Q_{23}x_2x_3 + 2Q_{24}x_2x_4 + 2Q_{34}x_3x_4)). \end{aligned}$$

Using this joint probability distribution, we derive the full conditional of x_1 given x_2, x_3, x_4,

$$f(x_1|x_2, x_3, x_4) \propto exp\left\{-\frac{1}{2}Q_{11}\left(x_1^2 - 2x_1\left(-\frac{Q_{12}}{Q_{11}}x_2 - \frac{Q_{13}}{Q_{11}}x_3 - \frac{Q_{14}}{Q_{11}}x_4\right)\right)\right\}. \tag{5}$$

This expression can be re-written as

$$f(x_1|x_2, x_3, x_4) \propto exp\left\{-\frac{1}{2}Q_{11}\left(x_1 - \left(-\frac{Q_{12}}{Q_{11}}x_2 - \frac{Q_{13}}{Q_{11}}x_3 - \frac{Q_{14}}{Q_{11}}x_4\right)\right)^2\right\}. \tag{6}$$

From matching (6) to the expression of a univariate normal distribution,

$$E(x_1|x_2, x_3, x_4) = -\frac{Q_{12}}{Q_{11}}x_2 - \frac{Q_{13}}{Q_{11}}x_3 - \frac{Q_{14}}{Q_{11}}x_4, \tag{7}$$

and

$$Prec(x_1|x_2, x_3, x_4) = Q_{11}. \tag{8}$$

By comparing equations (1) and (7), we obtain

$$\beta_{12} = -\frac{Q_{12}}{Q_{11}}, \qquad \beta_{13} = -\frac{Q_{13}}{Q_{11}}, \qquad \beta_{14} = -\frac{Q_{14}}{Q_{11}} = 0.$$

Considering the full conditionals for x_2, x_3 and x_4 and its conditional expectations respectively, yield similar relationships between the β coefficients and the elements of $\mathbf{Q}$:

$$\beta_{21} = -\frac{Q_{21}}{Q_{22}}, \qquad \beta_{23} = -\frac{Q_{23}}{Q_{22}} = 0, \qquad \beta_{24} = -\frac{Q_{24}}{Q_{44}}$$

$$\beta_{31} = -\frac{Q_{31}}{Q_{33}}, \qquad \beta_{32} = -\frac{Q_{32}}{Q_{33}} = 0, \qquad \beta_{34} = -\frac{Q_{34}}{Q_{33}}$$

$$\beta_{41} = -\frac{Q_{41}}{Q_{44}} = 0, \qquad \beta_{42} = -\frac{Q_{42}}{Q_{44}}, \qquad \beta_{43} = -\frac{Q_{43}}{Q_{44}}.$$

These relationships hold for an n dimensional distribution as established in Rue and Held [1]. If the conditional means and precisions can be written as

$$E(x_i|x_{-i}) = \mu_i + \sum_{j \neq i} \beta_{ij}(x_j - \mu_j) \quad \text{and} \tag{9}$$

$$Prec(x_i|x_{-i}) = k_i > 0, \tag{10}$$

then $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ follows a multivariate normal distribution with mean $\boldsymbol{\mu} = (\mu_1, \mu_2, \ldots, \mu_n)$ and precision matrix $\mathbf{Q}$ of entries Q_{ij}, where

$$Q_{ij} = \begin{cases} -k_i\beta_{ij} & i \neq j \\ k_i & i = j \end{cases} \tag{11}$$

provided $k_i\beta_{ij} = k_j\beta_{ji}$, $i \neq j$.

If we let $Prec(x_i|x_{-i}) = 2$ $(i = 1, 2, 3, 4)$, $\beta_{12} = \beta_{13} = \beta_{21} = \beta_{24} = \beta_{31} = \beta_{34} = \beta_{42} = \beta_{43} = 1/2$ and $\beta_{14} = \beta_{23} = \beta_{32} = \beta_{41} = 0$ using equations (9)-(11), $\mathbf{x} = (x_1, x_2, x_3, x_4)$ follows a multivariate normal distribution with mean $\mu = (0, 0, 0, 0)^T$ and precision matrix

$$\mathbf{Q} = \begin{pmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & 0 & -1 \\ -1 & 0 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{pmatrix}.$$

Generalizing Q to deal with multiple fields.

The generalization of $\mathbf{Q}$ to handle multiple fields is illustrated by a case with two fields, $\mathbf{x}$ and $\mathbf{y}$ which represent the difference between a model and observations for these fields. These observations are assumed to be on a 2×2 lattice, as shown in Figure 1.

Firstly $\mathbf{x}$ and $\mathbf{y}$ are combined into one vector $\mathbf{v}$ so that $\mathbf{v} = (v_1, v_2, v_3, v_4, v_5, v_6, v_7, v_8)^T = (x_1, x_2, x_3, x_4, y_1, y_2, y_3, y_4)^T$. The covariance among these observations can be represented by a 2×2 matrix between the field 1, $\mathbf{x}$, and the field 2, $\mathbf{y}$,

$$\mathbf{S} = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{pmatrix},$$

where $Var(\mathbf{x}) = \sigma_{11}$, $Var(\mathbf{y}) = \sigma_{22}$, and $Cov(\mathbf{x}, \mathbf{y}) = \sigma_{12}$. Recalling that the correlation between fields 1 and 2 is defined as: $\rho = \frac{\sigma_{12}}{\sqrt{\sigma_{11}\sigma_{22}}}$, it is easy to verify that the inverse of $\mathbf{S}$ is

Field One

X_1	X_2
X_3	X_4

Field Two

Y_1	Y_2
Y_3	Y_4

Figure 1: Two fields with observations $\mathbf{x}$, $\mathbf{y}$ defined on a 2×2 lattice.

$$\mathbf{S}^{-1} = \begin{pmatrix} \frac{1}{\sigma_{11}(1-\rho^2)} & \frac{-\rho}{(1-\rho^2)\sqrt{\sigma_{11}\sigma_{22}}} \\ \frac{-\rho}{(1-\rho^2)\sqrt{\sigma_{11}\sigma_{22}}} & \frac{1}{\sigma_{11}(1-\rho^2)} \end{pmatrix}.$$

Defining $\mathbf{Q}^*$ as $\mathbf{S}^{-1} \otimes \mathbf{Q}$, the Kronecker product of $\mathbf{S}^{-1}$ and $\mathbf{Q}$, then,

$$\mathbf{Q}^* = \mathbf{S}^{-1} \otimes \mathbf{Q} = \begin{pmatrix} \frac{1}{\sigma_{11}(1-\rho^2)}\mathbf{Q} & \frac{-\rho}{(1-\rho^2)\sqrt{\sigma_{11}\sigma_{22}}}\mathbf{Q} \\ \frac{-\rho}{(1-\rho^2)\sqrt{\sigma_{11}\sigma_{22}}}\mathbf{Q} & \frac{1}{\sigma_{11}(1-\rho^2)}\mathbf{Q} \end{pmatrix}.$$

To see what type of relationships are imposed by $\mathbf{Q}^*$ on the elements of $\mathbf{v}$, consider the first element $v_1 = x_1$. Also notice that the first row of $\mathbf{Q}^*$ is,

$$\begin{pmatrix} \frac{2}{\sigma_{11}(1-\rho^2)} & \frac{-1}{(1-\rho^2)\sigma_{11}} & \frac{-1}{(1-\rho^2)\sigma_{11}} & 0 & \frac{-2\rho}{\sqrt{\sigma_{11}\sigma_{22}}(1-\rho^2)} & \frac{\rho}{\sqrt{\sigma_{11}\sigma_{22}}(1-\rho^2)} & \frac{\rho}{\sqrt{\sigma_{11}\sigma_{22}}(1-\rho^2)} & 0 \end{pmatrix}. \tag{12}$$

Using equations (9)-(11), it can be easily checked that the value for $\beta_{12} = \frac{-Q^*_{12}}{Q^*_{11}} = \frac{1}{2}$. The other β values can be determined in a similar fashion. Using these β coefficients, the equations for the conditional mean and precision of $v_1 = x_1$ given the rest of the elements of $\mathbf{v}$ are

$$E(v_1|\mathbf{v_{-1}}) = \frac{1}{2}x_2 + \frac{1}{2}x_3 + \frac{\rho\sigma_{11}}{\sqrt{\sigma_{11}\sigma_{22}}}y_1 - \frac{\rho\sigma_{11}}{2\sqrt{\sigma_{11}\sigma_{22}}}y_2 - \frac{\rho\sigma_{11}}{2\sqrt{\sigma_{11}\sigma_{22}}}y_3 \tag{13}$$

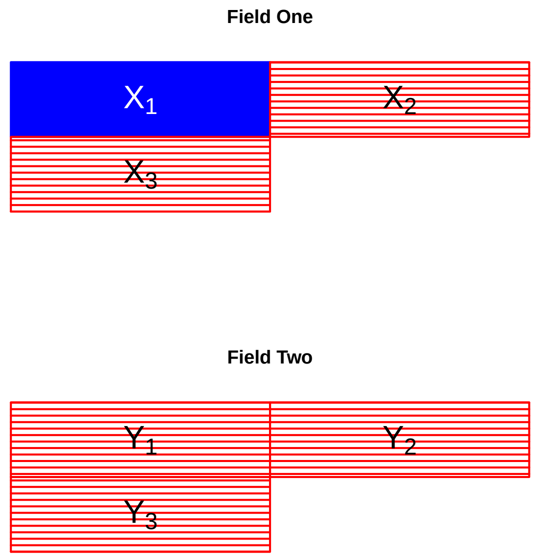

Figure 2: Neighbors of x_1 for a 2×2 lattice and two fields $\mathbf{x}$ and $\mathbf{y}$.

and

$$Prec(v_1|\mathbf{v_{-1}}) = \frac{1}{\sigma_{11}(1-\rho^2)}. \tag{14}$$

The expression for the conditional mean can be rewritten in terms of the slope b of the linear regression between $\mathbf{x}$ and $\mathbf{y}$, $b = \frac{\rho\sqrt{\sigma_{11}}}{\sqrt{\sigma_{22}}}$, with ρ equal to their correlation,

$$E(v_1|\mathbf{v_{-1}}) = \frac{1}{2}x_2 + \frac{1}{2}x_3 + by_1 - \frac{b}{2}y_2 - \frac{b}{2}y_3. \tag{15}$$

Equation (15) implies that the neighbors of x_1 are x_2, x_3, y_1, y_2 and y_3. Figure 2 shows a graphical display of all neighbors of x_1 in the context of the two fields $\mathbf{x}$, $\mathbf{y}$ and a 2×2 lattice.

Interpretation of S matrix

Reviewers raised the question about the physical interpretation of the correlation matrix $\mathbf{R}$, corresponding to the $\mathbf{S}$ matrix of 2-year JJA seasonal mean variances and covariances. We noted that it is difficult to ascribe a particular interpretation to these numbers since taking a spatial average may result in a small correlation from fields that have large but opposing correlations. Figure 3 shows maps of the grid point correlations between JJA mean 2m air temperature (TREFHT), sea level pressure (PSL), and precipitation (PRECT) with sea level pressure (PSL). What is clear between all these figures is that there is a lot of structure to all these maps. The sign of the correlation is regionally dependent. This is the case for 2m air temperature (TREFHT) and precipitation (PRECT) which has a near zero correlation within the correlation matrix **R** but have regionally very high correlations. Figure 4 shows that the 'witch hat' test of the GMRF-based estimate of covariances between these two fields show that GMRFs are doing a reasonable job.

References Cited

[1] Rue, H. and Held, L.: Gaussian Markov random fields, vol. 104, Chapman & Hall/CRC, 2005.

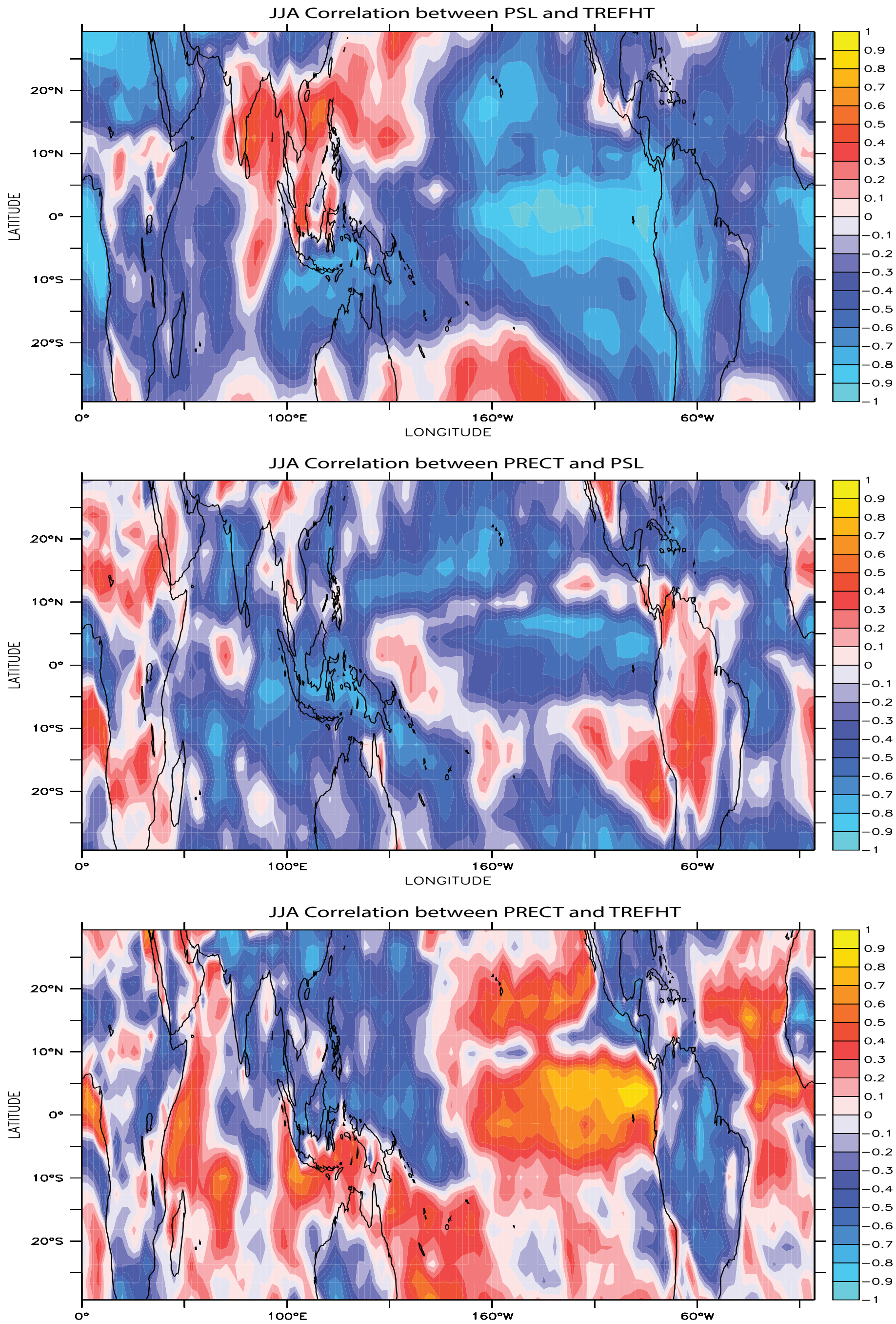

Figure 3: JJA correlations between 2m air temperature (TREFHT), sea level pressure (PSL), and precipitation (PRECT).

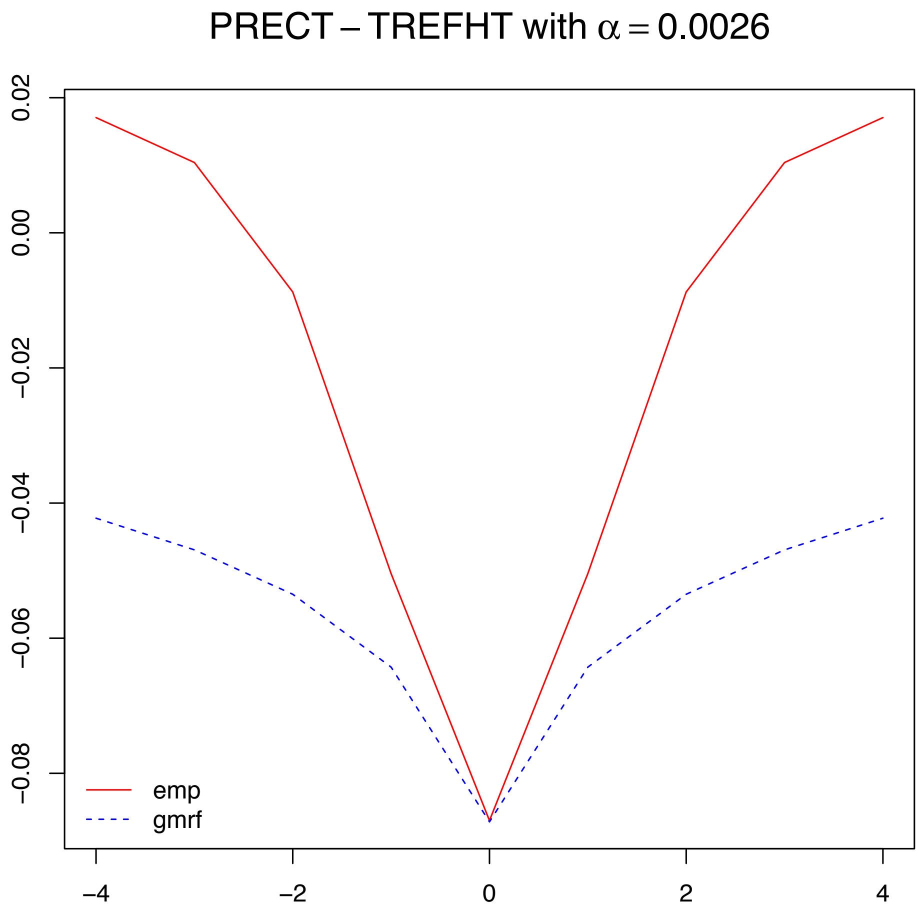

Figure 4: ‘Witch hat’ graphs testing GMRF approximations to empirical estimates of covariances between TREFHT and PRECT.