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On the Flexibility of Multivariate Covariance Models: Comment on the Paper by Genton and Kleiber

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INTRODUCTION

We congratulate the authors for their considerable effort to collect and synthesize all of the information contained in this review paper. Given the breadth of models, we were particularly inspired by the idea of how a practitioner would choose among them. We define some general criteria of flexibility that should be considered when choosing between different multivariate covariance models, and we apply these criteria in the comparison between the bivariate linear model of coregionalization (LMC) and the bivariate multivariate Matérn.

Which Model Is the Most Flexible?

Since most of the contributions listed by the authors refer to parametric models of multivariate covariances, we seek to answer the question, "which parametric model is more flexible?" We propose to define flexibility with respect to the following:

(A) the colocated correlation coefficient, and
(B) the strength of spatial dependence. For instance, how different can the scales of the cross-covariances and the marginal covariances between the two models be.

As far as (A) is concerned, ideally the colocated correlation coefficient should be defined over the interval $[-1, 1]$. Let us consider models of the type

$$\mathbf{C}(\mathbf{h}) = [\sigma_i \sigma_j \rho_{ij} R(\mathbf{h}; \boldsymbol{\theta}_{ij})]_{i,j=1}^{2}, \qquad \mathbf{h} \in \mathbb{R}^d, \tag{1}$$

with $R(\cdot)$ being a parametric univariate correlation model in $\mathbb{R}^d$ and $\boldsymbol{\theta}_{ij} \in A \subset \mathbb{R}^q$ being parameter vectors. Here $\sigma_i^2 > 0$, $i = 1, 2$ are the marginal variances, and ρ_{12} is the colocated parameter describing the correlation between the components of the bivariate random field at $\mathbf{h} = 0$. The bivariate Matérn [2] and Wendland [1] models are special cases of equation (1).

For the bivariate Matérn case, the validity bound for ρ_{12} is given in Theorem 3 of [2], and in general it depends on the smoothness parameters, $\boldsymbol{\nu} = (\nu_{11}, \nu_{22}, \nu_{12})'$, and the scale parameters, $\boldsymbol{\alpha} = (\alpha_{11}, \alpha_{22}, \alpha_{12})'$. For instance, assuming a constant smoothness parameter, and $\alpha_{12} < \min(\alpha_{11}, \alpha_{22})$, a necessary and sufficient condition for the validity of the bivariate Matérn becomes $|\rho_{12}| \le \frac{\alpha_{12}^2}{\alpha_{22}\alpha_{11}} \le 1$. In the case where the scale and smoothness parameters are pairwise equal (i.e., the separable case), then $|\rho_{12}| \le 1$, and there are no restrictions on the colocated parameter. These features are also present in the bivariate Wendland construction in [1], where the elements of the matrix-valued covariance are parameterized in the same way as the bivariate Matérn. As the difference between the parameters α_{11} and α_{22} increases, the bound on ρ_{12} becomes tighter, as shown in Figure 1.

The linear model of coregionalization (LMC) does not necessarily share this limitation on the colocated correlation coefficient. In order to illustrate this, we start with a simple example: for the following, we write $R(\cdot) := C(\cdot)/C(0)$, for C some univariate covariance function in $\mathbb{R}^d$. Then, the bivariate LMC correlation model $\mathbf{R}(\mathbf{h}) = [R_{ij}(\mathbf{h})]_{i,j=1}^{2}$, $\mathbf{h} \in \mathbb{R}^d$, can be written as

$$R_{11}(\mathbf{h}) = a_{11}^2 R_1(\mathbf{h}) + a_{12}^2 R_2(\mathbf{h}),$$
$$R_{22}(\mathbf{h}) = a_{21}^2 R_1(\mathbf{h}) + a_{22}^2 R_2(\mathbf{h}), \quad \text{and}$$
$$R_{12}(\mathbf{h}) = a_{11}a_{21} R_1(\mathbf{h}) + a_{12}a_{22} R_2(\mathbf{h}).$$

The 2×2 matrix $\mathbf{A} = \{a_{ij}\}$ has rank 2. Here we focus, without loss of generality, only on positive cor-

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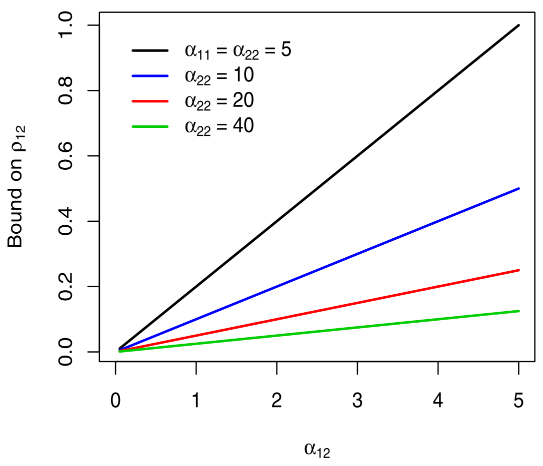

FIG. 1. *The upper bound on ρ_{12} as a function of α_{12} for various values of α_{11} and α_{22}. Note that for the colored lines, $\alpha_{11} = 5$.*

relations between the components, and, in order to do that, we consider $a_{ij} > 0$ for $i, j = 1, 2$. Let us now consider the special case $a_{12} = a_{21}$. Since $R_{ii}(\mathbf{0})$ must be identically equal to one, we get, as necessary conditions, that $a_{11}^2 + a_{12}^2 = 1 = a_{22}^2 + a_{12}^2$, which in turn implies that necessarily $a_{11} = a_{22} =: a$. Then the previous system of equations can be rewritten as

$$R_{11}(\mathbf{h}) = a^2 R_1(\mathbf{h}) + (1 - a^2) R_2(\mathbf{h}),$$
$$R_{22}(\mathbf{h}) = (1 - a^2) R_1(\mathbf{h}) + a^2 R_2(\mathbf{h}), \quad \text{and}$$
$$R_{12}(\mathbf{h}) = a\sqrt{1 - a^2}\big(R_1(\mathbf{h}) + R_2(\mathbf{h})\big).$$

In this case the colocated correlation coefficient is identically equal to $\rho_{12} := R_{12}(\mathbf{0}) = 2a\sqrt{1 - a^2} \in [0, 1]$ since $a \in [0, 1]$. Thus, the LMC seems to be more flexible than the bivariate Matérn with respect to issue (A) since its colocated correlation coefficient is free to vary through the maximum extent of its possible range, regardless of the form of the marginal covariances.

Issue (B) is clearly more critical to address, since it is not directly interpretable from the parameterization. In particular, it would be nice to have models that allow for different levels of strength of spatial correlation, which is directly related to the scales. Clearly, the conditions on the bivariate Matérn as well as those on the bivariate Wendland indicate that we have an ill-posed problem because the colocated correlation coefficient's upper bound is related to the scales. Thus, we analyze issue (B) for a fixed value of ρ_{12}. In particular, we try to address the question: "which model allows for bigger differences with respect to the strength of spatial correlation for a given colocated correlation coefficient?" We introduce here two multivariate measures that once again we illustrate for the bivariate case for ease of exposition.

[(B.1)] Since we are dealing with isotropic models, we shall write $R(t)$ instead of $R(\|\mathbf{h}\|)$ for $\mathbf{h} \in \mathbb{R}^d$. For a given multivariate covariance model x, we define

$$(2) \quad \mathcal{D}^x_{i,j,k} := \max_t \big|R_{ii}(t) - R_{kj}(t)\big|, \quad t := \|\mathbf{h}\| > 0,$$

where $k \in \{i, j\}$. When $k = j \neq i$, $\mathcal{D}^x_{i,j,j} = \mathcal{D}^x_{j,i,i}$ is a measure of the maximum difference between the correlation of the ith and jth components; while for $k = i$, $\mathcal{D}^x_{i,j,i} = \mathcal{D}^x_{i,i,j}$ reflects the maximum difference between the cross correlation R_{ij} and the correlation of the ith component. According to this criterion, for two given models x and y, with a common (fixed) colocated correlation coefficient $\rho^x_{12} = \rho^y_{12}$, if $\mathcal{D}^x_{i,k,j} < \mathcal{D}^y_{i,k,j}$, then model y is preferable.

The computation of the indicator above can be tedious, depending on the functional forms of the involved marginal and cross correlations. For instance, for the bivariate Matérn model, obtained when fixing the parameters ν_{11}, ν_{22} and ν_{12} to be identically equal to 0.5, the general form of the bivariate correlation function can be written as $0 \le t \mapsto R_{ij}(t) = \rho_{ij} e^{-t\alpha_{ij}}$, $\alpha_{ij} > 0$, $\rho_{ii} = 1$. In this case, inspection of equation (2) directly relates to finding the stationary solution of the problem

$$G(a, b, \rho) := \max_{t \ge 0} \big|f(t, a, b, \rho)\big|,$$

where $f(t, a, b, \rho) = \mathrm{e}^{-at} - \rho \mathrm{e}^{-bt}$, with $a, b > 0$, and ρ could be a function of a and b but is fixed here and belongs to the interval $[-1, 1]$. The case $\rho < 0$ is trivial since the maximum is attained at $t = 0$, so we focus on the case $\rho > 0$. The problem has the following solutions:

$$(3) \quad G(a, b, \rho) = \begin{cases} \max\big(-f(t^*, a, b, \rho), 1 - \rho\big), \\ \quad \text{if } b < a, \\ f(t^*, a, b, \rho), \\ \quad \text{if } b > a, \log \rho + \log(b/a) > 0, \\ 1 - \rho, \\ \quad \text{if } b > a, \log \rho + \log(b/a) < 0, \end{cases}$$

where $t^* = \frac{\log \rho + \log(b/a)}{b - a}$. For $b = a$, $G(a, b, \rho) = 1 - \rho$. For the bivariate exponential model, we can compute

$$\mathcal{D}^{\mathrm{Exp}}_{1,2,2} = G(\alpha_{11}, \alpha_{22}, 1)$$
$$= \begin{cases} 0, & \alpha_{11} = \alpha_{22}, \\ -f\left(\dfrac{\log(\alpha_{22}/\alpha_{11})}{\alpha_{22} - \alpha_{11}}, \alpha_{11}, \alpha_{22}, 1\right), & \text{if } \alpha_{22} < \alpha_{11}, \\ f\left(\dfrac{\log(\alpha_{22}/\alpha_{11})}{\alpha_{22} - \alpha_{11}}, \alpha_{11}, \alpha_{22}, 1\right), & \text{if } \alpha_{22} > \alpha_{11}. \end{cases}$$

Similarly, $\mathcal{D}^{\mathrm{Exp}}_{1,2,1}$ and $\mathcal{D}^{\mathrm{Exp}}_{2,2,1}$ can be computed using equation (3) as $G(\alpha_{11}, \alpha_{12}, \rho_{12})$ and $G(\alpha_{22}, \alpha_{12}, \rho_{12})$. Note that $\mathcal{D}^{\mathrm{Exp}}_{1,2,2}$ does not depend on the colocated correlation coefficient and that, for this example, $0 \le \mathcal{D}^{\mathrm{Exp}}_{1,2,2} \le 1$, and, similarly, we have $0 \le \mathcal{D}^{\mathrm{Exp}}_{1,2,1} \le 1$.

Let us now analyze a special case of the LMC model as illustrated through issue (A), supposing that $R_1(t) = \exp(-\alpha t)$ and $R_2(t) = \exp(-\beta t)$, for α and β positive. Direct inspection shows that in this case $\mathcal{D}^{\mathrm{LMC}}_{1,2,2} = k|2a^2 - 1|$, where $k = G(\alpha, \beta, 1)$. Now, we note that $\rho_{12} = 2a\sqrt{1-a^2}$ for $0 < a < 1$ and, as shown before, ρ_{12} can belong to any value inside the interval [0, 1]. Since $a = [\frac{1 \pm \sqrt{1-\rho_{12}^2}}{2}]^{0.5}$, then $\mathcal{D}^{\mathrm{LMC}}_{1,2,2} = k\sqrt{1-\rho_{12}^2} \le \sqrt{1-\rho_{12}^2}$, with equality if and only if $\rho_{12} = 0$. Similarly, it can be shown that $\mathcal{D}^{\mathrm{LMC}}_{1,2,1} \le 1 - \rho_{12}$ and $\mathcal{D}^{\mathrm{LMC}}_{2,2,1} \le 1 - \rho_{12}$.

Comparing the index between the bivariate LMC and exponential model, when $\rho_{12} \to 1$, then $\mathcal{D}^{\mathrm{LMC}}_{1,2,2} < \mathcal{D}^{\mathrm{Exp}}_{1,2,2}$. Thus, it seems that more flexibility is offered by the bivariate exponential at least for the marginal correlations R_{11} and R_{22}.

[(B.2)] As a second indicator for a given multivariate covariance model x, we propose

$$\widetilde{\mathcal{D}}^{x}_{i,k,j} := \left| \int_0^\infty \big(R_{ii}(t) - R_{kj}(t)\big)\,\mathrm{d}t \right|. \tag{4}$$

For instance, let us consider the case of the radial part of a bivariate Matérn model, so that

$$R_{ij}(t) = \rho_{ij}(\alpha_{ij}t)^{\nu_{ij}}\mathcal{K}_{\nu_{ij}}(\alpha_{ij}t), \qquad t \ge 0,$$

for which direct inspection shows that

$$\widetilde{\mathcal{D}}^{\mathrm{Mat}}_{1,1,2} = \left| \sqrt{\pi}\left(\frac{\Gamma(\nu_{11} + (1/2))}{\alpha_{11}\Gamma(\nu_{11})} - \frac{\rho_{12}\Gamma(\nu_{12} + (1/2))}{\alpha_{12}\Gamma(\nu_{12})} \right) \right|.$$

Observe that in a bivariate exponential model, we easily get $\widetilde{\mathcal{D}}^{\mathrm{Exp}}_{1,1,2} = |\alpha_{11}^{-1} - \rho_{12}\alpha_{12}^{-1}|$, and $\widetilde{\mathcal{D}}^{\mathrm{Exp}}_{1,2,2} = |\alpha_{11}^{-1} - \alpha_{22}^{-1}|$ does not depend on the colocated correlation coefficient (as in the previous index). For the LMC model we easily get that $\widetilde{\mathcal{D}}^{\mathrm{LMC}}_{1,2,2} = \sqrt{1-\rho_{12}^2}|\alpha^{-1} - \beta^{-1}|$ for the exponentials as assumed earlier. As with the first index when $\rho_{12} \to 1$, $\widetilde{\mathcal{D}}^{\mathrm{LMC}}_{1,2,2} < \widetilde{\mathcal{D}}^{\mathrm{Exp}}_{1,2,2}$. Again the bivariate exponential model seems to be more flexible with respect to LMC, at least when comparing the marginal correlations R_{11} and R_{22}.

CONCLUSION

Comparing multivariate covariance models from a flexibility point of view is an important issue, since it can be helpful when choosing between the set of parametric models described in this review paper. In this discussion we have proposed two possible criteria in order to define the flexibility of a multivariate covariance model. Using the criteria proposed, we compare the flexibility of the LMC with the multivariate Matérn in the bivariate case. There is a clear trade-off between the two models. In particular, the LMC is more flexible in terms of the allowable interval for the colocated correlation coefficient, which varies freely over the interval $[-1, 1]$. Instead, the bivariate Matérn has restrictions on the permissible range of the colocated correlation for given spatial scales and smoothness parameters. On the other hand, the two indices highlight that if the colocated correlation is the same for the two models, the bivariate Matérn has more flexibility as the colocated correlation tends to 1.

In conclusion, we believe that more work should be done in order to compare multivariate models from a flexibility viewpoint. In this discussion, we have offered some instruments that might be useful in this direction.

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