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Rejoinder

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We are grateful to the discussants for providing very valuable and insightful comments. Next, we present our views on some of the comments of the discussants and provide further discussion.

We thank Bevilacqua, Hering and Porcu (hereafter, BHP) for bringing attention to the fundamental problem of comparing multivariate models. Until now, almost all comparisons between models have been relegated to empirical performance on specific datasets, whether it be performance on cokriging or particular scoring rules. BHP introduce two theoretical approaches to comparing the flexibility of multivariate frameworks: (A) assessing the size of allowable co-located cross-correlation between processes, and (B) a measure of difference in allowed spatial (cross)-correlation at differing distances.

Regarding (A), BHP claim the bivariate Matérn is less flexible than the LMC in that there are nontrivial restrictions on the cross-correlation coefficient for the bivariate Matérn that are not present for the LMC. We emphasize, however, that the bivariate Matérn restrictions are a *characterizing* feature of the covariance class—no LMC construction can allow for marginal and cross exact Matérn behavior while allowing for unrestricted choice of co-located cross-correlation. Rather, it is a physical restriction on the covariance class, not a flexibility restriction.

Most spatial modelers include a nugget effect in the statistical model, $Y_i(\mathbf{s}) = Z_i(\mathbf{s}) + \varepsilon_i(\mathbf{s})$, where $Z_i(\mathbf{s})$ is endowed with a multivariate model, and $\varepsilon_i(\mathbf{s})$ is a white noise process that is uncorrelated with $Z_i(\mathbf{s})$. If $\varepsilon_i(\mathbf{s})$ is nontrivial with variance τ_i^2 , then the restrictions on the cross-correlation coefficient can be relaxed, the amount depending on the magnitude of the nugget effect and sample size. To see this, let p = 2 and write the covariance matrix for two unit variance processes at n = 1 locations $\{Z_1(\mathbf{s}_1), \ldots, Z_1(\mathbf{s}_n), Z_2(\mathbf{s}_1), \ldots, Z_2(\mathbf{s}_n)\}^T$ as

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 $B \odot \Sigma$, where $\Sigma = \{C_{ij}(\mathbf{s}_k, \mathbf{s}_\ell)\}_{i,j=1;k,\ell=1}^{2;n}$ and B = $(B_{ij})_{i,j=1}^2$ consists of four $n \times n$ block matrices. For simplicity, assume $\tau_1 = \tau_2$, so that $B_{12} = B_{21}$ are matrices populated by a constant ρ_0 and $B_{11} = B_{22}$ are matrices of ones with diagonal $1 + \tau^2$. Note that the case $\rho_0 = 1$ results in $B \odot \Sigma$ having the specified multivariate dependence; if $\rho_0 > 1$, then the two processes can have larger cross-correlation than allowed by the specified model. The cases where $\rho_0 > 1$ are valid when $B_{12} = B_{11}^{1/2} K B_{22}^{1/2}$, where *K* is a contraction matrix (i.e., a matrix whose singular values are bounded by unity); this follows from Proposition 1 of Kleiber and Genton (2013). This is one feasible way to relax the restrictions that are suggested by BHP's (A) criterion. We view BHP's (B) as an alternative interesting route to comparing models, although it is still unclear what improvements a modeler would expect to gain for various magnitudes of the (B) criterion.

Cressie et al. focus on three main aspects: the importance of modeling the nugget effect (which yields additional potential difficulties in the multivariate context), the pseudo cross-variogram and alternative approaches to building multivariate structures.

We focused our efforts on reviewing multivariate covariance functions, not multivariate modeling, a byproduct of which is that we left little discussion to the issue of modeling the nugget effect. For instance, the underlying latent smooth process W of Cressie et al. [(2015), equation (4)] still requires specification of the multivariate structure, regardless of whether a nugget effect will or will not ultimately be included. Nonetheless, these authors bring up an important point in that, especially for multivariate processes, some variables may be measured by the same instrument, in which case it may be expected that measurement errors are correlated across variables at individual locations. Disentangling microscale variability of the process from measurement error is indeed a difficult prospect; Sang, Jun and Huang (2011) used a full-scale approximation for multivariate processes that explicitly breaks up large scale, small scale and measurement error variability.

Cressie et al. champion a traditional geostatistical approach to estimation, using a weighted least squares distance from empirical pseudo cross-variograms to estimate parameters of a parametric class of crosscovariance functions. Although this is a feasible route to estimation, interpretation of the pseudo cross-variogram remains unclear, unless the process is stationary and the variables are standardized, so that the pseudo cross-variogram can be rewritten $Var\{Z_1(s +$ $\mathbf{h})/\sigma_1 - Z_2(\mathbf{s})/\sigma_2$, where σ_i is the standard deviation of the ith process. This seems a particularly important consideration if the scales of the two processes differ by orders of magnitude. A more modern approach to estimation (albeit one that requires more modeling assumptions) is to adopt a maximum likelihood or Bayesian framework. Even if the processes are not strictly Gaussian, say, these other approaches can still be used for estimation if the deviation from Gaussianity is not too great.

We agree with Cressie et al. that the conditional approach to estimation has utility in certain situations when there is clear directional dependence between variables. However, if many (say, greater than four) processes are considered simultaneously, we echo Cressie et al.'s caution: "when more variables are involved, the order may not always be obvious but, if the goal is to construct valid covariance and cross-covariance functions, the different orderings can be viewed as enlarging the space of valid models." On the other hand, the factor process approach seems promising. Given the difficulties basis decomposition approaches experience in the univariate setting (Finley et al., 2009, Stein, 2014), we expect similar issues to arise in the multivariate setting. Thus, we suggest a multiresolution approach, decomposing differing scales of support into various resolutions of basis functions (Nychka et al., 2002, 2015).

Finally, Cressie et al. bring up some important issues in validating and comparing statistical models that we view as sensible guidelines for future authors working in this field. Indeed, direct likelihood comparisons may be muddled by the varying numbers of parameters between models, and BHP have introduced some tools apart from the usual information criteria to compare multivariate models.

We are pleased that Simpson, Lindgren and Rue (hereafter, SLR) decided to expand on our very brief mention of the spectral representation of the cross-covariance matrix function, which for simplicity was restricted to the symmetric case in our review. Although we did address the topic of asymmetric cross-covariance functions in Section 5.1, SLR now provided

information about the spectral representation in the asymmetric setting and further discussed the spectral representation of multivariate Gaussian random fields themselves. SLR also argued that this path leads naturally to non-Gaussian or nonstationary multivariate random fields, and they further made the link with physics-constrained cross-covariance models.

Although SLR advocated the SPDE approach as a computationally efficient reformulation of univariate and multivariate Gaussian random fields, there are also limitations that can only be exacerbated in the multivariate setting. For example, the smoothness parameter of the Matérn covariance function is restricted to certain values. Moreover, this methodology requires a strong background in numerical analysis techniques which is not common among statisticians. Thus, we view the multivariate kernel convolution approach as a compromise where physics-based information can be incorporated, without confronting the numerous difficulties in implementing a SPDE framework. Nevertheless, the route of SPDEs offers many interesting and challenging avenues for future research.

SLR end their discussion with an important point about the inflation of the number of parameters in cross-covariance models as the number of variables increases. This is indeed a challenging issue when applying likelihood methods and various authors have resorted to composite likelihood approaches, although more investigations in this area are warranted. Finally, the problem of parameter identifiability under infill asymptotics in the multivariate setting is mentioned and we see no reason for this effect to disappear in this context.

The discussion of Zhang and Cai (hereafter, ZC) centers on trying to understand why and when cokriging does not always outperform kriging. This is a very relevant topic given the numerical results provided in our two data analyses. To address this topic, ZC start by deriving sufficient conditions for the equivalence of Gaussian measures for a bivariate Matérn cross-covariance model with common length scale and smoothness parameters, but allowing for different marginal variances. Using ZC's notation, an example of two bivariate Gaussian measures that satisfy their sufficient conditions is given by $\nu = 1$, $\sigma_{11,1} = \sigma_{22,1} = 1$, $\sigma_{11,2} = \sigma_{22,2} = 2$, $\sigma_{12,1} = 1/2$, $\sigma_{12,2} = 1$, $\alpha_1 = 2$, and $\alpha_2 = 1$.

The example provided by ZC where cokriging is equivalent to kriging falls into the category of autokrigeability (Wackernagel, 2003, page 149). A variable is autokrigeable with respect to a set of variables

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if the kriging of this variable is equivalent to the cokriging. A trivial case is when all variables are uncorrelated. Another case, as illustrated by ZC, is when the cross-covariance function is separable (also called intrinsically correlated in geostatistics). Generalizations of the concept of autokrigeability to various simplifications of large cokriging systems by means of screen effects were investigated by Subramanyam and Pandalai (2008); see also Furrer and Genton (2011) for related methods to handle highly multivariate spatial data.

ZC conclude by investigating a situation where the auxiliary variable is observed at more locations than the predicted variable, leading to the cokriging predictor being more efficient than the kriging predictor as a function of the co-located correlation coefficient, r, in a separable exponential cross-covariance function setting. Interestingly, their formula (9) shows that the mean squared prediction error of the cokriging predictor can be reduced to at most 1/2 of that of the kriging predictor in this particular case. We conjecture that the factor 1/2 could be further reduced by either adding more observation points in O or by adding more variables $Y_3(\mathbf{s}), \ldots, Y_p(\mathbf{s})$ in a similar cross-covariance function framework.

Finally, one last issue that remains is the availability of statistical software for implementing, simulating and estimating multivariate models. Indeed, the choice of a particular model to use in any application requires fair expertise in spatial statistics, and we expect these models to become more mainstream as welldocumented software becomes more available. There are some promising packages available currently that end users should be aware of, all of which are available in R. Whereas RandomFields contains a large number of multivariate models and can perform high resolution simulation of these (Schlather et al., 2014), spBayes is geared toward Bayesian analyses of hierarchical multivariate models (Finley, Banerjee and Gelfand, 2015), and gstat contains some variogrambased estimation routines for the linear model of coregionalization (Pebesma, 2004).

REFERENCES

- CRESSIE, N., BURDEN, S., DAVIS, W., KRIVITSKY, P. N., MOKHTARIAN, P., SUESSE, T. and ZAMMIT-MANGION, A. (2015). Capturing multivariate spatial dependence: Model, estimate and then predict. *Statist. Sci.* 30 170–175.
- FINLEY, A. O., BANERJEE, S. and GELFAND, A. E. (2015). SpBayes for large univariate and multivariate point-referenced spatio-temporal data models. *J. Stat. Softw.* **63** 1–28.
- FINLEY, A. O., SANG, H., BANERJEE, S. and GELFAND, A. E. (2009). Improving the performance of predictive process modeling for large datasets. *Comput. Statist. Data Anal.* 53 2873– 2884. MR2667597
- FURRER, R. and GENTON, M. G. (2011). Aggregation-cokriging for highly multivariate spatial data. *Biometrika* 98 615–631. MR2836410
- KLEIBER, W. and GENTON, M. G. (2013). Spatially varying cross-correlation coefficients in the presence of nugget effects. *Biometrika* 100 213–220. MR3034334
- NYCHKA, D., WIKLE, C. and ROYLE, J. A. (2002). Multiresolution models for nonstationary spatial covariance functions. *Stat. Model.* **2** 315–331. MR1951588
- NYCHKA, D., BANDYOPADHYAY, S., HAMMERLING, D., LIND-GREN, F. and SAIN, S. (2015). A multi-resolution Gaussian process model for the analysis of large spatial data sets. *J. Comput. Graph. Statist.* To appear.
- PEBESMA, E. J. (2004). Multivariable geostatistics in S: The gstat package. *Comput. Geosci.* **30** 683–691.
- SANG, H., JUN, M. and HUANG, J. Z. (2011). Covariance approximation for large multivariate spatial data sets with an application to multiple climate model errors. *Ann. Appl. Stat.* 5 2519–2548. MR2907125
- SCHLATHER, M., MALINOWSKI, A., OESTING, M., BOECKER, D., STROKORB, K., ENGELKE, S., MARTINI, J., BALLANI, F., MENCK, P. J., GROSS, S., OBER, U., BURMEISTER, K., MANITZ, J., RIBEIRO, P., SINGLETON, R. and PFAFF, B. (2014). RandomFields: Simulation and Analysis of Random Fields, R package version 3.0.44. Available at http://CRAN.R-project.org/package=RandomFields.
- STEIN, M. L. (2014). Limitations on low rank approximations for covariance matrices of spatial data. *Spatial Statistics* **8** 1–19.
- SUBRAMANYAM, A. and PANDALAI, H. S. (2008). Data configurations and the cokriging system: Simplification by screen effects. *Math. Geosci.* **40** 425–443. MR2401515
- WACKERNAGEL, H. (2003). *Multivariate Geostatistics*: An Introduction with Applications, 3rd ed. Springer, Berlin.