New Classes of Nonseparable Space-Time Covariance Functions

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June 24, 2014

Outline

- Introduction
- Matérn Family of covariance functions
- Separable Modeling
- Nonseparable modeling
- Application and Numerical Studies
- Discussion

Notation, Stationarity

- p-dimensional multivariate random field $\mathbf{Z}(\mathbf{x}) = \{Z_1(\mathbf{x}), \ldots, Z_p(\mathbf{x})\}^{\mathrm{T}}$ defined on a spatial region $\mathcal{D} \subset \mathbb{R}^d$, $d \geq 1$
- A multivariate random field is second-order stationary (or just stationary) if the marginal and cross-covariance functions depend only on the separation vector $\mathbf{h} = \mathbf{x}_1 - \mathbf{x}_2$

$$C_{ij} : \mathbb{R}^d \to \mathbb{R};\, C_{ij}(\mathbf{h}) := \mathrm{cov}\{Z_i(\mathbf{x}_1), Z_j(\mathbf{x}_2)\}, \mathbf{h} \in \mathbb{R}^d$$

  - stationarity can be thought of as an invariance property under the translation of coordinates

Isotropy

- A multivariate random field is isotropic if it is stationary and invariant under rotations and reflections,

$$C_{ij} : \mathbb{R}_+ \cup \{0\} \to \mathbb{R}; C_{ij}(||\mathbf{h}||) := \mathrm{cov}\{Z_i(\mathbf{x}_1), Z_j(\mathbf{x}_2)\}, \mathbf{h} \in \mathbb{R}^d$$

- Isotropy or even stationarity are not always realistic, especially for large spatial regions, but sometimes are satisfactory working assumptions and serve as basic elements of more sophisticated anisotropic and nonstationary models

Spatial Matérn

- Matérn family: correlation function (named after the Swedish forestry statistician Bertil Matérn)

$$M(\mathbf{h}|\nu,\alpha) := \frac{1}{2^{\nu-1}\Gamma(\nu)}(\alpha||\mathbf{h}||)^{\nu} B_{\nu}(\alpha||\mathbf{h}||), \mathbf{h} \in \mathbb{R}^{d}$$

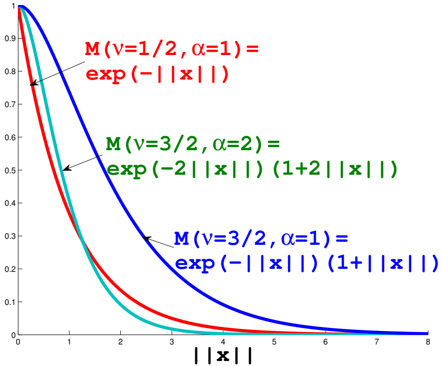
  - B_ν, modified Bessel function of the second kind
  - $\nu > 0$, smoothness and $\alpha > 0$, scale parameters
- for $\nu =$ odd integer/2 has a closed form expression
  - $\nu = 1/2$, $M(\mathbf{h}|1/2,\alpha) = \exp(-\alpha||\mathbf{h}||)$
- In the numerical analysis literature this kernel is also called the Sobolev kernel

Spatial Matérn

- Mean Square Differentiability here is defined as an $\mathcal{L}^2$ limit
  - e.g. an isotropic process is mean squared continuous if $\mathrm{E}\{Z(\mathbf{s}+\mathbf{h}) - Z(\mathbf{s})\}^2 \rightarrow 0$, as $||h|| \rightarrow 0$
  - Z is m times mean square differentiable if and only if $C^{(2m)}(0)$ exists and finite
  - Z is m times mean squares differentiable if and only if $\nu > m$

Spatial Matérn

- Covariance functions for various level of $\nu > 0$(smoothness) and $\alpha > 0$(scale) parameters
  - bigger ν, the smoother C around 0
  - increasing as function of ν,
    $M(\mathbf{h}|\nu = 1/2, \alpha = 1) < M(\mathbf{h}|\nu = 3/2, \alpha = 1)$
  - decreasing as function of α,
    $M(\mathbf{h}|\nu = 3/2, \alpha = 1) > M(\mathbf{h}|\nu = 3/2, \alpha = 2)$



Univariate and Multivariate Matérn Family

- In the pure spatial setting: Matérn family (Matérn, 1960) has found widespread interest in recent years (Stein (1999), Guttorp and Gneiting (2006) for a historical account of this model)
- Multivariate Matérn : Marginal Spatial and cross -covariance as a function of Spatial lag are from Matérn (Gneiting et al. JASA (2011), Apanasovich et al. JASA (2012))
  - special case of multivariate space-time process was considered in Apanasovich et al. Biometrika (2010)

Positive Defitness

- The cross-covariance functions $C_{ij}(\mathbf{x}_1 - \mathbf{x}_2)$ $i, j = \overline{1, p}, \mathbf{x}_1, \mathbf{x}_2 \in \mathcal{D}$
  - must form $np \times np$ non-negative definite matrix for any positive integer n and points $\mathbf{x}_1, \ldots, \mathbf{x}_n$ in D
- $\{\mathbf{K}(\mathbf{h})\}_{ij} = C_{ij}(\mathbf{h})$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \mathbf{K}(\mathbf{0}) & \mathbf{K}(\mathbf{x}_1 - \mathbf{x}_2) & \cdots & \mathbf{K}(\mathbf{x}_1 - \mathbf{x}_n) \\ \mathbf{K}(\mathbf{x}_2 - \mathbf{x}_1) & \mathbf{K}(\mathbf{0}) & \cdots & \mathbf{K}(\mathbf{x}_2 - \mathbf{x}_n) \\ \vdots & \vdots & \ldots & \vdots \\ \mathbf{K}(\mathbf{x}_n - \mathbf{x}_1) & \mathbf{K}(\mathbf{x}_n - \mathbf{x}_2) & \cdots & \mathbf{K}(\mathbf{0}) \end{pmatrix}$$

$$\text{var}(\mathbf{a}^T\mathbf{Z}) = \mathbf{a}^T\boldsymbol{\Sigma}\mathbf{a} \geq 0, \forall \mathbf{a} \in \mathbb{R}^{np}, \forall \mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathcal{D}, \forall n \in \mathcal{I}$$

Positive Defitness

- Define the cross-spectral densities as $f_{ij} : \mathbb{R}^d \to \mathbb{R}$ as

$$f_{ij}(\boldsymbol{\omega}) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \exp(-\iota \mathbf{h}^T \boldsymbol{\omega}) C_{ij}(\mathbf{h}) d\mathbf{h}, \quad \boldsymbol{\omega} \in \mathbb{R}^d$$

  - $\iota = \sqrt{-1}$
- Cramer's Theorem (slightly modefied) A necessary and sufficient condition for $\mathbf{K}(\cdot)$ to be a valid (i.e., nonnegative definite), stationary matrix-valued covariance function is for the matrix function $\{f_{ij}(\boldsymbol{\omega})\}_{i,j=1}^{p}$ to be nonnegative definite for any $\boldsymbol{\omega}$ (Cramer 1940).

Separable Multivariate RF

- Separable forms: Mardia and Goodall (1993).

$$K_{ij}(\mathbf{x}_1 - \mathbf{x}_2) = \sigma_{ij} K(\mathbf{x}_1 - \mathbf{x}_2), \quad i, j = 1, \cdots, p$$

  - $\Sigma = \{\sigma_{ij}\}$ is a positive definite matrix
  - $K(\cdot)$ is a valid correlation function
  - Problem: same form of correlation for all is and cross-correlations for all $\{i, j\}$s
    - E.g. $K_{ij}(\mathbf{x}_1 - \mathbf{x}_2) = \sigma_{ij} \exp(-\alpha||\mathbf{x}_1 - \mathbf{x}_2||)$ (same α)

Nonseparable Multivariate RF

- It is a challenging task
  - Fit marginal covariances, different α_{ii}, $i = 1, \cdots, p$

$$K_{ii}(\mathbf{x}_1, \mathbf{x}_2) := \exp(-\alpha_{ii}||\mathbf{x}_1 - \mathbf{x}_2||), \alpha_{ii} > 0$$

  - Evidence for spatial cross-correlation
    - How about

$$K_{ij}(\mathbf{x}_1, \mathbf{x}_2) := \exp(-\alpha_{ij}||\mathbf{x}_1 - \mathbf{x}_2||), \alpha_{ij} > 0, (\alpha_{ij} = \alpha_{ji})$$

    - WRONG! will NOT be a valid cross covariance unless $\alpha_{ij} = \alpha$ for any $i, j = \bar{1, p}$ (back to separability).
    - Solution $K_{ij}(\mathbf{x}_1, \mathbf{x}_2) := \gamma(\alpha_{ij}) \exp(-\alpha_{ij}||\mathbf{x}_1 - \mathbf{x}_2||)$ for some carefully chosen $\gamma(\cdot)$

Linear model of coregionalization: Wackernagel (2003)

- Linear model of coregionalization: Wackernagel (2003)

$$\mathbf{Z}(\mathbf{x}) = A\mathbf{w}(\mathbf{x}),$$

  - components of $\mathbf{w}(\mathbf{x}) \in \mathbb{R}^p$ are iid spatial processes,
  - A is $p \times p$ full rank such that

$$K_{ij}(\mathbf{x}_1 - \mathbf{x}_2) = \sum_{k=1}^{p} \rho_k(\mathbf{x}_1 - \mathbf{x}_2) A_{ik} A_{jk}$$

Linear model of coregionalization: Wackernagel (2003)

- The LMC can additionally be built from a conditional perspective (Royle and Berliner 1999; Gelfand et al. 2004)
- $$Z_j(\mathbf{x}) = \sum_{i=1}^{j-1} \alpha_i Z_i(\mathbf{x}) + \sigma_j w_j(\mathbf{x})$$
- Drawbacks (In My Humble Frequentist Opinion)
  - with a large number of processes, the number of parameters can quickly become large
  - smoothness of any component of the multivariate random field is restricted to that of the roughest underlying univariate process.

Covariance convolution

- A variant of a result of Gaspari et al. (2006) and theorem 1 of Majumdar and Gelfand (2007)
  - Suppose that $c_1, ..., c_p$ are real-valued functions on $\mathbb{R}^d$ which are both integrable and square-integrable.

$$C_{ij}(\mathbf{h}) = (c_i \star c_j)(\mathbf{h}), \qquad \text{for } i, j = 1, \cdots, p$$

    - $\star$ denotes the convolution operator
- Drawbacks
  - Although some closed-form expressions exist, this method usually requires Monte Carlo integration
  - The models for which the closed form expressions exist are somewhat rigit

Covariance convolution: Matérn

- Recall

$$K_{ij}(\mathbf{h}) = (c_i \star c_j)(\mathbf{h}), \qquad \text{for } i,j = 1,\cdots,p$$

- From Gneiting, Kleiber, Schlather(2012)
  - c_i are being suitably normalized Matérn functions with common scale $\alpha > 0$ and smoothness $\nu_i/2 - d/4$
  - Hence, recall $M(\cdot|\cdot)$ is a univariate Matérn

$$K_{ij}(\mathbf{h}) = \gamma(\nu_i, \nu_j) M\{\mathbf{h}|(\nu_i + \nu_j)/2, \alpha\}$$

$$\gamma(\nu_i, \nu_j) = \frac{\{\Gamma(\nu_i + d/2)\}^{1/2}}{\{\Gamma(\nu_i)\}^{1/2}} \frac{\{\Gamma(\nu_j + d/2)\}^{1/2}}{\{\Gamma(\nu_j)\}^{1/2}} \frac{\Gamma\{(\nu_i + \nu_j)/2\}}{\Gamma\{(\nu_i + \nu_j + d)/2}$$

Based on Latent dimensions

- The key idea is to represent i-th vector's component ($i = 1, \cdots, p$ for p dimensional random field) as a point in a k-dimensional space ($1 \leq k \leq p$), $\xi_i = (\xi_{i1}, \cdots, \xi_{ik})^T$; and include it INSIDE the covariance function

$$K_{ij}(\mathbf{x}_1, \mathbf{x}_2) = \tilde{K}\{(\mathbf{x}_1, \xi_i), (\mathbf{x}_2, \xi_j)\}$$

- Similar to multidimensional scaling with latent measures of dissimilarities between vector's components
- Apanasovich, T. V., and Genton, M. G. (2010), "Cross-covariance functions for multivariate random fields based on latent dimensions," Biometrika, 97, 15-30.

Based on Latent dimensions: Matérn

- The idea of using Latent Dimensions is very general
- A special case that is discussed in the paper in relationship to Matérn is
  - $-\alpha_{ij}^2$ form a conditionally nonnegative definite matrices

$$K_{ij}(\mathbf{h}) = \gamma(\alpha_{ij})M\{\mathbf{h}|\nu, 1/\alpha_{ij}\}$$
$$\gamma(\alpha_{ij}) = 1/\alpha_{ij}^d$$

Mixture Representation

- There a well-known closure properties for matrix-valued covariance functions (Reisert and Burkhardt 2001) to use for sufficient conditions for validity.
  - Suppose that for all $r \in L \subset \mathbb{R}^l$, $C_r : \mathbb{R}^d \to \mathbb{R}$ is a (univariate) correlation function, while $\mathbf{D}_r \in \mathbb{R}^{p \times p}$ is symmetric and nonnegative definite. Suppose furthermore that for all $\mathbf{h} \in \mathbb{R}^d$ the product $\mathbf{D}_r C_r(\mathbf{h})$ is componentwise integrable with respect to the positive measure F on L. Then

$$\mathbf{C}(\mathbf{h}) = \int_L \mathbf{D}_r C_r(\mathbf{h}) dF(r)$$

- Drawback: it is hard to come up with all the elements

Mixture Representation: Matérn

- From Gneiting, Kleiber, Schlather(2012) : only for byvariate

Multivariate GRF and SPDE approach: Matérn

- By Hu, Simpson, Lindgren, Rue
- The advantage: there is no explicit dependency on the theory of positive definite matrix
- Next talk. Stay tuned!

Sufficient/Cramer : Matérn

- Recall cross-spectral densities are

$$f_{ij}(\boldsymbol{\omega}) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \exp(-\iota \mathbf{h}^T \boldsymbol{\omega}) C_{ij}(\mathbf{h}) d\mathbf{h}, \quad \boldsymbol{\omega} \in \mathbb{R}^d$$

  - $\iota = \sqrt{-1}$
- Need to show that $\{f_{ij}(\boldsymbol{\omega})\}_{i,j=1}^{p}$ is nonnegative definite for any $\boldsymbol{\omega}$
- From Apanasovich, Genton, Sun (2012) JASA "A Valid Matérn Class of Cross-Covariance Functions for Multivariate Random Fields with any Number of Components"

Main Result

- The flexible multivariate Matérn model
  1. Marginal parameters: ν_{ii}, α_{ii}, σ_{ii};
  2. Somewhat flexible cross-covariance parameters: σ_{ij};
  3. Extra parameters $\nu_{ij} = \nu_{ji}$, $\alpha_{ij} = \alpha_{ji}$, $i \neq j$ with some constraints which involve nontrivial functions of ν_{ii}, ν_{jj}, α_{ii}, α_{jj} and σ_{ij}
- Recall: Gneiting, Kleiber, Schlather(2012) for $p \geq 3$
  1. Marginal parameters: ν_{ii}, $\alpha_{ii} = \alpha$, σ_{ii};
  2. Less flexible cross-covariance parameters: σ_{ij};
  3. Other parameters for cross-covariances $\nu_{ij} = (\nu_{ii} + \nu_{jj})/2$, $\alpha_{ij} = \alpha$, $i \neq j$

Main Result

- **Theorem** The flexible multivariate Matérn model provides a valid structure if there exists $\Delta_A \geq 0$, such that
  1. $\nu_{ij} - (\nu_{ii} + \nu_{jj})/2 = \Delta_A(1 - A_{ij})$, $i, j = 1, \cdots, p$, where $0 \leq A_{ij}$ form a valid correlation matrix;
  2. $-\alpha_{ij}^2$ $i, j = 1, \cdots, p$, form a conditional nonnegative definite matrix;
  3. $\sigma_{ij}\alpha_{ij}^{2\Delta_A+\nu_{ii}+\nu_{jj}} \frac{\Gamma(\nu_{ij}+d/2)}{\Gamma\{(\nu_{ii}+\nu_{jj})/2+d/2\}\Gamma(\nu_{ij})}$ $i, j = 1, \cdots, p$, form a nonnegative definite matrix

Parameterization

- marginal parameters: α_{ii}, ν_{ii}, σ_{ii}
- cross -covariance parameters
  - $\nu_{ij} = (\nu_{ii} + \nu_{jj})/2 + \Delta_B(1 - R_{A,ij})$, $\Delta_A > 0$, R_A is a valid correlation matrix with nonnegative entries $i, j = 1, \cdots, p$
  - $\alpha_{ij}^2 = (\alpha_{ii}^2 + \alpha_{jj}^2)/2 + \Delta_B(1 - R_{B,ij})$, $\Delta_B > 0$, R_B is a valid correlation matrix with nonnegative entries $i, j = 1, \cdots, p$
  - $\rho_{ij} = R_{V,ij}\gamma(\alpha_{ii}, \alpha_{jj}, \alpha_{ij}, \nu_{ii}, \nu_{jj}, \nu_{ij})$, $\gamma(\cdot)$ is a well defied function (see the paper), R_V is a valid correlation matrix
- Hence to model cross-covariance parameters, one need to choose parameterization for correlation matrixes
  - In case of a small number of variables, p, one can use equicorrelated R_Ls, so that $R_{L,ij} = \rho_L$, $i \neq j$, $L \in \{A, B, V\}$
  - latent dimention $R_{L,ij} = \exp(-||\xi_{L,i} - \xi_{L,j}||)$, for vectors $\xi_{L,i} \in \mathbb{R}^k$, $1 \leq k \leq p$, under constraints discussed in Apanasovich and Genton (2010).

Special Case

- The least flexible parametrization

$\nu_{ij} = \frac{\nu_{ii}+\nu_{jj}}{2}, \alpha_{ij} = \left(\frac{\alpha_{ii}^2+\alpha_{jj}^2}{2}\right)^{1/2}$, $\sigma_{ij} = (\sigma_{ii}\sigma_{jj})^{1/2}\rho_{ij}$ with

$$\rho_{ij} = \frac{\alpha_{ii}^{\nu_{ii}}\alpha_{jj}^{\nu_{jj}}}{\alpha_{ij}^{2\nu_{ij}}} \frac{\Gamma(\nu_{ij})}{\Gamma^{1/2}(\nu_{ii})\Gamma^{1/2}(\nu_{jj})} R_{ij}$$

where R_{ij} is a valid correlation matrix

  - Marginal parameters: ν_{ii} α_{ii} σ_{ii}
  - No extra parameters to model ν_{ij}, α_{ij}
  - Extra parameters involved in cross-covariances: R_{ij}

Simulations

- we conducted simulation studies for the cases $p = 2, 3$.
- The simulation scenarios are motivated by a meteorological dataset discussed by Gneiting et al. (2012). It consists of temperature and pressure observations, as well as forecasts, at 157 locations in the North American Pacific Northwest. In our simulation studies, we use these same 157 locations and generate a bivariate or trivariate spatial Gaussian random field with multivariate Matérn cross-covariance structure

Simulations

Table 1: Summary statistics of parameter estimation of the bivariate ($p = 2$) Matérn model over 1,000 replicates.

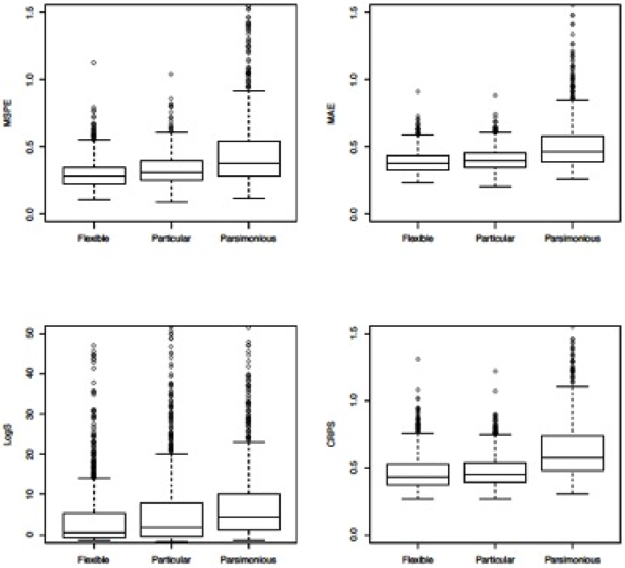
Parameter	True	Min	Q_1	Median	Mean	Q_3	Max
α_{11}	0.02	0.0095	0.0193	0.0217	0.0225	0.0248	0.0511
α_{22}	0.01	0.0041	0.0099	0.0124	0.0133	0.0153	0.1139
α_{12}	0.0158	0.0074	0.0165	0.0186	0.0194	0.0215	0.0826
ν_{11}	1.6	1.1580	1.5670	1.7060	1.7600	1.8730	4.2040
ν_{22}	0.6	0.4082	0.6018	0.6760	0.7508	0.7737	2.8400
ν_{12}	1.3	0.9209	1.2220	1.3590	1.5330	1.6490	4.3800
σ_{11}	1	0.6035	0.9381	1.0520	1.0530	1.1600	1.6190
σ_{22}	1	0.5942	0.9575	1.0500	1.0510	1.1380	1.6350
σ_{12}	−0.497	−0.9921	−0.5352	−0.4425	−0.4352	−0.3403	0.0000

Table 2: Summary statistics of parameter estimation of the trivariate ($p = 3$) Matérn model over 1,000 replicates.

Simulations

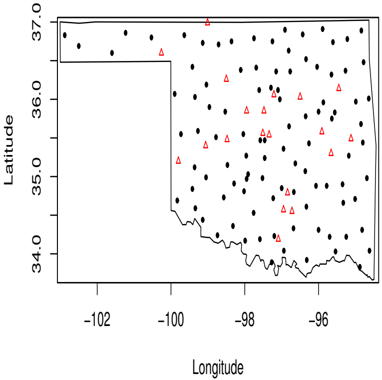
Parameter	True	Min	Q_1	Median	Mean	Q_3	Max
α_{11}	0.01	0.0035	0.0095	0.0111	0.0115	0.0130	0.0237
α_{22}	0.02	0.0076	0.0188	0.0236	0.0273	0.0300	0.2659
α_{33}	0.03	0.0013	0.0288	0.0326	0.0691	0.0722	0.8220
α_{12}	0.0205	0.0093	0.0185	0.0222	0.0252	0.0269	0.1943
α_{13}	0.0263	0.0071	0.0254	0.0363	0.0626	0.0614	0.8220
α_{23}	0.0282	0.0138	0.0303	0.0404	0.0668	0.0648	0.8220
ν_{11}	1.2	0.9953	1.1800	1.2560	1.2770	1.3480	1.9090
ν_{22}	0.6	0.3552	0.5915	0.6938	0.9028	0.8264	7.3200
ν_{33}	0.3	0.0515	0.3235	0.3677	1.2800	0.8636	7.3100
ν_{12}	1.093	0.8709	1.0690	1.1300	1.1790	1.2080	5.2270
ν_{13}	1.092	0.8449	1.0850	1.1490	1.3090	1.2510	6.3270
ν_{23}	0.990	0.5943	0.8659	1.1740	1.2450	1.3390	5.2270
σ_{11}	1	0.3354	0.7560	0.9158	0.9460	1.0990	3.2600
σ_{22}	1	0.5932	0.8726	0.9770	0.9812	1.0680	1.4650
σ_{33}	1	0.2341	0.8059	0.9265	0.9126	1.0290	1.4900
σ_{12}	−0.286	−0.7036	−0.3306	−0.2565	−0.2583	−0.1916	0.0000
σ_{13}	−0.181	−0.4858	−0.2692	−0.1715	−0.1711	−0.0518	0.0000
σ_{23}	0.274	0.0000	0.1103	0.2313	0.2916	0.3669	0.5199

Simulations



Wind speed/Temperature/Pressure

- Meteorological dataset: at 120 locations in Oklahoma
- 100 locations for model fitting; 20 locations to evaluate the wind speed prediction performance.
- Fit a random field after removing a quadratic trend of longitude, latitude and elevation



Results: Trivariate Spatial Field

- Estimates of parameters for our flexible trivariate Matérn model

$\hat{\nu}_{11}$	$\hat{\nu}_{22}$	$\hat{\nu}_{33}$	$\hat{\nu}_{12}$	$\hat{\nu}_{13}$	$\hat{\nu}_{23}$
0.77	1.32	1.97	1.05	1.37	1.64

$1/\hat{\alpha}_{11}$	$1/\hat{\alpha}_{22}$	$1/\hat{\alpha}_{33}$	$1/\hat{\alpha}_{12}$	$1/\hat{\alpha}_{13}$	$1/\hat{\alpha}_{23}$
14.5	20.0	11.0	15.6	11.9	13.0

Results: Trivariate Spatial Field

- Marginal correlation and cross-correlation fits: solid curves=flexible, and dashed=parsimonious

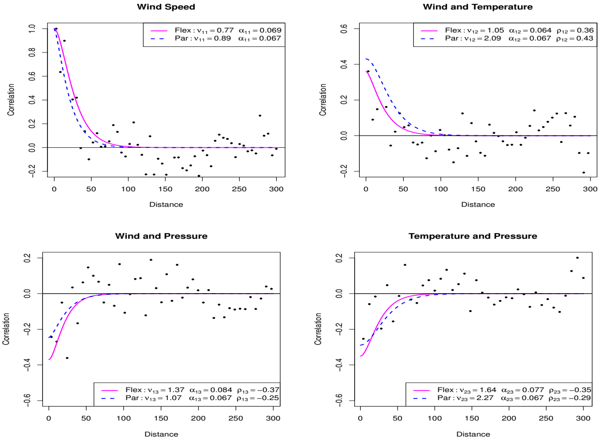


Figure : Marginal correlation and cross-correlation fits for wind speed, temperature, and pressure: solid curves for the flexible trivariate Matérn

Results: Trivariate Spatial Field

Model	#Para	Loglik
5. Flexible Matérn ($\Delta_{A,ij}$,$\Delta_{B,ij}$)	$+8$	$-34,359.6$
4. $\nu_{ij} = (\nu_{ii} + \nu_{jj})/2 + \Delta_A$, $\alpha^2_{ij} = (\alpha^2_{ii} + \alpha^2_{jj})/2 + \Delta_B$	$+4$	$-35,125.6$
3. $\nu_{ij} = (\nu_{ii} + \nu_{jj})/2 + \Delta_A$, $\alpha^2_{ij} = (\alpha^2_{ii} + \alpha^2_{jj})/2$	$+3$	$-35,615.9$
2. $\nu_{ij} = (\nu_{ii} + \nu_{jj})/2$, $\alpha^2_{ij} = (\alpha^2_{ii} + \alpha^2_{jj})/2 + \Delta_B$	$+3$	$-36,193.3$
1. Parsimonious:$\nu_{ij} = (\nu_{ii} + \nu_{jj})/2$, $\alpha_{ij} = \alpha$	0	$-36,572.3$

Cokriging Trivariate Spatial Field

- temperature and pressure at all 120 locations, wind speed at 100, predict the wind speed at 20
- Different predictive scores for wind speed

Model	MSPE	MAE	LogS	CRPS
Flexible	17.5	3.3	4.0	4.4
Parsimonious	24.8	3.8	4.4	5.3

- Prediction errors for the flexible (magenta) and parsimonious (blue) for each of the 20 left-out locations