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The modified Matérn process

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The behaviour of a stationary random field can be specified through either its covariance or spectrum. In spatial statistics, the Matérn covariance or spectral density is one of the most popular choices due to separation of scale and smoothness effects. We propose a generalization of the Matérn spectral density, generating random processes we term as modified Matérn processes. Our proposal allows for two additional parameters that can loosely be interpreted as arising from a continuous moving average process. The Matérn is a special case under certain parameter restrictions. We illustrate the flexibility of the modified Matérn in an application on an ocean model simulation.

Keywords: Gaussian measure; rational spectral density; Whittle approximation

1 Introduction

Modern spatial statistical applications rely on flexible parametric functions for modelling spatial correlation. For stationary random fields, this second-order structure can be specified through either the covariance function or its spectral density. The Matérn class is probably the most popular parametric choice in use in modern spatial statistics (Stein, 1999). In particular, the Matérn covariance function on $\mathbb{R}^d$ corresponds to a spectral density proportional to

$$f(\boldsymbol{\omega}) = \frac{1}{(a^2 + \|\boldsymbol{\omega}\|^2)^{\nu+d/2}} \tag{1}$$

with $\boldsymbol{\omega} \in \mathbb{R}^d$, and where $a > 0$ is a spatial range parameter and $\nu > 0$ is the smoothness parameter that indexes the Hausdorff or fractal dimension of sample paths of the process (Guttorp & Gneiting, 2006).

In time series, the class of rational spectral densities can be identified with the celebrated autoregressive–moving average processes (Brockwell & Davis, 2009). In the spatial literature, Vecchia (1985) proposed the use of rational spectral densities with integer powers as a flexible class that is the spatial analogue to autoregressive–moving average processes; see also Vecchia (1988) and Jones & Vecchia (1993). Ippoliti et al. (2013) consider rational spectral densities for spatial lattice processes. In this work, we consider a simple rational spectral density that generalizes the Matérn class and works for non-integer valued powers. Note that other extensions of the Matérn class appear in the literature; see, for example, Lim & Teo (2009).

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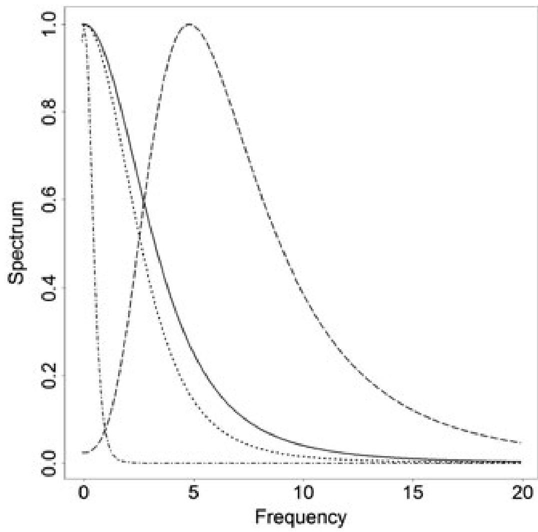

Figure 1. All spectral densities are standardized to have a maximum value of one. The lines correspond to the following: $a = 5, \nu + d/2 = 2$ (solid line, Matérn); $a = 5, \nu + d/2 = 4, b = 7, \xi = 2$ (dotted line); $a = 1, \nu + d/2 = 4, b = 7, \xi = 2$ (dash-dotted line); and $a = 5, \nu + d/2 = 4, b = 1, \xi = 2$ (dashed line).

1.1 The modified Matérn model

In this work, we propose an extension of the Matérn class of covariances that we call the *modified Matérn* class. The modified Matérn model has a spectral density that is proportional to

$$f(\boldsymbol{\omega}) = \frac{(b^2 + \|\boldsymbol{\omega}\|^2)^{\xi}}{(a^2 + \|\boldsymbol{\omega}\|^2)^{\nu + d/2}} \tag{2}$$

where $a, \nu > 0$ and $b \geq 0$ and $\xi < \nu$. The last condition ensures the process has finite variance. If ξ and $\nu + d/2$ are forced to be integer valued, then this is a special case of the models proposed under Vecchia (1985), but we consider arbitrary real values. Note that there may be a non-identifiability problem between ν and ξ if ξ takes on negative values. Forcing $\xi \geq 0$ then reduces to the Matérn class on the boundary $\xi = 0$.

The parameters a and b act as range parameters, while ξ and ν conspire to control the process smoothness. In particular, the process is m times mean square differentiable if and only if $m < \nu - \xi$. One effect of the scale in the numerator is to allow for the mode of the spectrum to fall away from zero. It is easily shown that the maximum of (2) occurs at frequency

$$\|\boldsymbol{\omega}\|^2 = \frac{\xi a^2 - (\nu + d/2) b^2}{\nu + d/2 - \xi}$$

when it is positive and is at zero otherwise. Such behaviour would be desired for processes that exhibit strong periodicities. See Figure 1 for some example spectral densities.

What is the implied covariance function based on (2)? We are not aware of a general closed-form solution, but special cases with integer powers of ξ and ν are available from Proposition 2 of Vecchia (1985). For example, in $d = 2$, Vecchia (1985) shows that a process with spectral density (2) has covariance function

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$$C(\mathbf{h}) = \frac{1}{2\pi}\frac{(-1)^\nu}{\nu!}\frac{\partial^\nu}{\partial(a^2)^\nu}\left((b^2-a^2)^\xi K_0\left(\|\mathbf{h}\|\sqrt{a^2}\right)\right)$$

where $\mathbf{h} \in \mathbb{R}^2$ is a spatial lag and K_0 is a modified Bessel function of the second kind of order zero.

2 Some theory

In spatial statistics, there are two types of asymptotics: fixed domain (or infill) in which the domain is fixed and samples are taken at finer resolutions within a fixed domain; the other type is increasing domain, where samples are taken over an ever increasing area or volume.

If $Z(\mathbf{s})$ is a Gaussian process, the equivalence or orthogonality of Gaussian measures turns out to be a key concept in estimation theory under infill asymptotics. In particular, if two measures $\mathcal{P}_1$ and $\mathcal{P}_2$ are defined on the same measurable space, then we say they are equivalent if they are absolutely continuous with respect to one another. If $\mathcal{P}_1$ and $\mathcal{P}_2$ are equivalent, then $\mathcal{P}_1$ cannot be distinguished from $\mathcal{P}_2$ with probability 1 under $\mathcal{P}_1$, even with infinitely many samples. For more background on Gaussian measures and further results, see Stein (1999).

2.1 Equivalence of implied Gaussian measures

In a landmark paper, Zhang (2004) gave necessary and sufficient conditions on equivalence and orthogonality of Gaussian random measures for Matérn processes and established consistency results of maximum likelihood estimators under infill asymptotics for $d = 1, 2, 3$, while Anderes (2010) extended the results to $d > 4$. We partially extend these results for a special case of the modified Matérn–Gaussian process, although a complete extension is beyond the scope of this paper. In particular, we give sufficient conditions on parameters of a one-dimensional modified Matérn that result in equivalent Gaussian measures with respect to the sample paths of $Z(\mathbf{s})$ on a bounded domain, contained in the following theorem.

The version we examine sets $b = 0$ and $d = 1$, in which case the normalizing constant is available from equation (3.241.4) in Gradshteyn & Ryzhik (2000),

$$f(\omega) = \sigma^2 \frac{2a^{2\nu-2\xi}}{\mathrm{B}(\xi+1/2, \nu-\xi)}\frac{\omega^{2\xi}}{(a^2+\omega^2)^{\nu+1/2}} \tag{3}$$

for $\omega \in \mathbb{R}$ where B is the beta function. In particular, a Gaussian process on $\mathbb{R}$ with spectral density of the form (3) is a modified Matérn process with variance σ^2.

Theorem 1
Let $\mathcal{P}_i$ be probability measures such that under $\mathcal{P}_i$, $Z(s)$ is a stationary Gaussian process on $s \in \mathbb{R}$ with spectral density (3) *and parameters σ_i, a_i, ξ_i and ν_i for $i = 1, 2$. If $\nu_1 - \xi_1 = \nu_2 - \xi_2$ and*

$$\sigma_1^2 a_1^{2(\nu_1-\xi_1)}\frac{\Gamma(\nu_1+1/2)}{\Gamma(\xi_1+1/2)} = \sigma_2^2 a_2^{2(\nu_2-\xi_2)}\frac{\Gamma(\nu_2+1/2)}{\Gamma(\xi_2+1/2)}, \tag{4}$$

then $\mathcal{P}_1$ and $\mathcal{P}_2$ are equivalent on the sample paths of $Z(s)$, $s \in T$ for any bounded subset $T \subset \mathbb{R}$.

The condition that $\nu_1 - \xi_1 = \nu_2 - \xi_2$ is expected as both spectral densities must have the same asymptotic rate of decay at high frequencies. The condition (4) is the modified Matérn generalization of the results of Ying (1991) and

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Zhang (2004): note that when $\xi_1 = \xi_2 = 0$, (4) reduces to the familiar condition $\sigma_1^2 a_1^{2\nu} = \sigma_2^2 a_2^{2\nu}$ where $\nu_1 = \nu_2 = \nu$. Extending Theorem 1 to higher dimensions or $b \neq 0$ relies on finding explicit closed forms for the normalizing constant where we expect the details of the proof become cumbersome.

An interesting special case of Theorem 1 is when $\mathcal{P}_2$ specifies a Matérn covariance, while $\mathcal{P}_1$ is a modified Matérn. In this case, $\xi_2 = 0$ and (4) become

$$\sigma_1^2 a_1^{2(\nu_1 - \xi_1)} \frac{\Gamma(\nu_1 + 1/2)}{\Gamma(\xi_1 + 1/2)} = \sigma_2^2 a_2^{2\nu_2} \frac{\Gamma(\nu_2 + 1/2)}{\sqrt{\pi}}$$

so that there are *non-trivial* versions of the modified Matérn that yield equivalent Gaussian measures to ordinary Matérn models.

3 Examples

As with any stochastic model, it is instructive to show some simulations from the model under different model settings to train the eye. There are many methods to simulate stationary Gaussian random fields, one of the most common being circulant embedding (Wood & Chan, 1994). However, circulant embedding requires knowledge of the covariance function, which is not always available for the modified Matérn. Thus, we generate approximate simulations of a modified Matérn process by discrete sum approximation to the integral spectral representation of a stationary random field (Yaglom, 1987).

Figure 2 shows three simulations of modified Matérn random fields on a 500×500 grid $\{(i/10, j/10)\}_{i,j=1}^{500}$. The figure panels correspond to simulations with

(a) $a = 1, \nu = 0.5, \xi = 0$;
(b) $a = 5, \nu = 2, b = 10, \xi = 1.5$; and
(c) $a = 3, \nu = 2, b = 1, \xi = 1.5$.

Note that the simulation in Figure 2(c) displays behaviour that is apparently somewhat similar to Figure 2(b), but with shorter length scale of correlation; however, Figure 2(c) also contains strong periodicities that are not present in Figure 2(a) or (b). That it is difficult for the eye to detect the periodicities present in Figure 2(c) highlights the importance of using statistical techniques for data analysis.

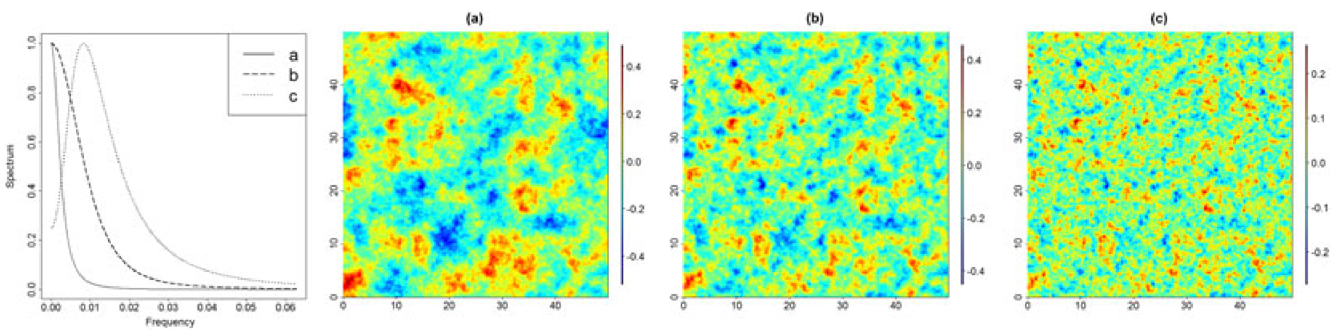

Figure 2. Approximate simulations of modified Matérn random fields.

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3.1 Ocean simulation

We consider a subset of a numerical simulation of an idealized ocean model that was examined by Grooms (2016). The model uses a geostrophic approximation to ocean dynamics that are appropriate for the spatial length scales of mesoscale eddies. Although the physical model is run on a three-dimensional cube, we statistically model the two-dimensional surface field. The physical parameters are set to approximate the behaviour of the ocean in the subtropics. The data are values of the stream function and are on a 32×32 grid at a spacing of 36 km over 20 time points that can be considered uncorrelated realizations of the same random field. The fields are zero-centred using an empirical mean at each spatial location and represent mean zero anomalies.

We model the anomalies as stationary mean zero Gaussian processes that are independent across time with either a Matérn or modified Matérn spectrum. Whittle's (1954) approximation to the likelihood provides a convenient route for maximum likelihood estimation. Using Whittle's approximation, we estimate model parameters by maximum likelihood. Both models include scaling parameters to account for non-trivial variance.

We compare the quality of model fit by the Akaike and Bayesian information criteria; the values are contained in Table I. The modified Matérn is favoured by both criteria, with an estimated improvement in total log-likelihood of 393.1, at the cost of two additional model parameters. Table II contains the maximum likelihood estimates of the spatial parameters under both models. The estimated modified Matérn spectrum has its mode at zero and does not indicate strong periodicities present in the data. Interestingly, estimates from both models imply approximately the same spatial scales, but the implied smoothness under the modified Matérn is 0.8, whereas the Matérn model estimates the process to be much smoother, with a smoothness of 2.9. This discrepancy may be due to the modified Matérn likelihood surface that exhibits long ridges over which changes in parameters do not substantially affect likelihood values. (This can also happen for Matérn processes, Zhang, 2004.)

Table I. Akaike information criterion (AIC) and Bayesian information criterion (BIC) based on the ocean simulation data.

	Matérn	Modified Matérn
AIC	186,768	185,973
BIC	186,782	185,997

Table II. Maximum likelihood-based parameter estimates.

	Matérn	Modified Matérn
a	9.7	22
b	—	30
ν	2.9	18.5
ξ	—	17.7

Note: Scale parameters a and b are in kilometres.

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4 Discussion

We introduced a modified version of the Matérn spectral density for stationary spatial processes. Parameters of the modified model allow for the maximal spectrum to be at a non-zero frequency but contain the Matérn as a special case. We developed some theory that suggests that the equivalence of implied Gaussian measures takes on more complicated forms than that for standard Matérn models and, moreover, that there are non-trivial versions of modified Matérn covariances that yield Gaussian measures that are equivalent to those of Matérn classes. Future research may be devoted to extending the theory to more complicated processes, such as those considered by Vecchia (1985), although we anticipate the proofs becoming technically difficult because of the complicated form of the normalizing constant. Another interesting question is whether certain parameter combinations of the modified Matérn are equivalent to other classes of covariances, such as the generalized Wendland functions (Bevilacqua et al., 2016).

Appendix

This appendix contains the proof of Theorem 1.

Proof of Theorem 1

The proof closely follows that of Theorem 2 of Zhang (2004). First, note that $f_i(\omega)|\omega|^{\alpha_i}$ is bounded away from 0 and ∞ for $\alpha_i = 2\nu_i - 2\xi_i + 1$, $i = 1, 2$ as $|\omega| \to \infty$. It remains to show that

$$\int_c^{\infty} \left(\frac{f_2(u) - f_1(u)}{f_1(u)} \right)^2 \mathrm{d}u < \infty, \tag{A1}$$

for some finite $c > 0$, which is just condition (5) of Zhang (2004). Let

$$c_i = \sigma_i^2 \frac{2a_i^{2\nu_i - 2\xi_i}}{\mathrm{B}(\xi_i + 1/2, \nu_i - \xi_i)}$$

be the normalizing constant, and note that the theorem conditions $\nu_2 - \xi_2 = \nu_1 - \xi_1$ and (4) imply $c_1 = c_2$. Then we have

$$\begin{aligned} \left| \frac{f_2(u)}{f_1(u)} - 1 \right| &= \left| \frac{c_2 u^{2\xi_2} (a_1^2 + u^2)^{\nu_1 + 1/2}}{c_1 u^{2\xi_1} (a_2^2 + u^2)^{\nu_2 + 1/2}} - 1 \right| \\ &\le \frac{1}{u^{2\nu_2 + 1}} \left| \frac{c_2}{c_1} u^{2\xi_2 - 2\xi_1} (a_1^2 + u^2)^{\nu_1 + 1/2} - (a_2^2 + u^2)^{\nu_2 + 1/2} \right| \\ &= \frac{1}{u^{2\nu_2 + 1}} \left| \frac{c_2}{c_1} u^{2\xi_2 - 2\xi_1} u^{2\nu_1 + 1} \left((a_1/u)^2 + 1 \right)^{\nu_1 + 1/2} - u^{2\nu_2 + 1} \left((a_2/u)^2 + 1 \right)^{\nu_2 + 1/2} \right|. \end{aligned}$$

Now, by assumption, $2\xi_2 - 2\xi_1 + 2\nu_1 + 1 = 2\nu_2 + 1$ and $c_1 = c_2$, so this reduces to

$$\begin{aligned} &= \left| \left((a_1/u)^2 + 1 \right)^{\nu_1 + 1/2} - \left((a_2/u)^2 + 1 \right)^{\nu_2 + 1/2} \right| \\ &\le u^{-2} \left| (\nu_1 + 1/2) a_1^2 - (\nu_2 + 1/2) a_2^2 \right| + O\left(u^{-4}\right) \end{aligned}$$

where the last inequality uses $(x+1)^{\alpha} = 1 + \alpha x + O(x^2)$ as $x \to 0$ and $u \to \infty$. Thus, the integral (A1) is finite, so $\mathcal{P}_1$ and $\mathcal{P}_2$ define equivalent measures by Theorem A.1 of Stein (2004). □

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