The diffusion-based extension of the Matérn field to space-time

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Abstract

The Matérn field is the most well known family of covariance functions used for Gaussian processes in spatial models. We build upon the original research of Whittle (1953, 1964) and develop the diffusion-based extension of the Matérn field to space-time (DEMF). We argue that this diffusion-based extension is the natural extension of these processes, due to the strong physical interpretation. The corresponding non-separable spatio-temporal Gaussian process is a spatio-temporal analogue of the Matérn field, with range parameters in space and time, smoothness parameters in space and time, and a separability parameter. We provide a sparse representation based on finite element methods that is well suited for statistical inference.

1 Introduction

1.1 Modelling spatio-temporal data

Statistical models for spatio-temporal data is a rich area of study, with applications ranging from environmental data (Cameletti et al., 2013), to climate data (Wood et al., 2004), to resource and risk models (e.g., of wildfires, Serra et al. (2014)), to disease modeling (Bhatt et al., 2015; Moraga, 2019), and analyses in ecology (Yuan et al., 2017; Zuur et al., 2017). These models use spatio-temporal random effects, defined as (Gaussian) spatio-temporal stochastic processes indexed by a set of hyperparameters, and rely on a large body of theoretical and methodological literature, see Stein (2012), Gelfand et al. (2010), Cressie and Wikle (2015), and references therein.

At best, this theory is carefully studied when the spatio-temporal model is constructed, so that the model with the most appropriate assumptions can be used. In practice, however, users of statistical software often choose a model based on convenience. If there are available code examples, the choices made in these will often be carried forward into future analyses. For example, users of R-INLA (Rue et al., 2009, 2017) construct space-time models through Kronecker products of a spatial Matérn model, and order 1 or 2 autoregressive models in time, following the code examples in Krainski et al. (2019). This paper is aimed at improving the general practice of space-time data analysis, by providing a new family of spatio-temporal stochastic processes for use as random effects in statistical software.

We will mainly discuss spatio-temporal stochastic processes $u(s,t)$ that are stationary and spatially isotropic, i.e., the covariance function can be written as $\text{Cov}(u(s_1,t_1),u(s_2,t_2)) = C(h_s, h_t)$, where $h_s = ||s_1 - s_2||$ and $h_t = |t_1 - t_2|$. We consider these stochastic processes in the context

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of hierarchical models, as a latent model component, observed through some measurement process, with no direct measurements of the stochastic process itself.

Take the example

$$\eta(s, t) = X \beta + f_1(z_1) + f_2(z_2) + \ldots + f_k(z_k) + u(s, t), \tag{1}$$

where $\eta$ is the predictor, connected to the response $y$ through some likelihood or loss function (Bissiri et al., 2016). We use spatio-temporal covariates $X(s, t)$ and $z_j(s, t)$. Further, $X \beta$ are the intercept(s), factors, and fixed effects, $f_j(z_j)$ are model components over covariates $z_j$, where $z_j$ is not limited to be one-dimensional. Typical examples are splines explaining the effect of altitude or distance to coastline. Further, $u(s, t)$ is the spatio-temporal stochastic process we discuss in this paper, which we will refer to as the spatio-temporal model component whenever we are considering it as part of a hierarchical model. The $f_j$ terms can also include a temporal trend, a spatial reference level, and time-varying or space-varying regressions; possibly partially confounded with the spatio-temporal model component.

This common view of a stochastic process as a model component impacts the methodological considerations we make. The predictor is also a spatio-temporal stochastic process, with a covariance function that can be deduced from the assumptions on the model components. Properties we discover of the covariance function of the predictor does not imply that the spatio-temporal model component $u$ has the same properties. Hence, we usually have little information about the covariance structure of the spatio-temporal model component, except that it should be physically realistic, and should mimic the dependency structure in models of physical processes.

The stochastic process $u$ is separable when $C(h_s, h_t) = C_s(h_s)C_t(h_t)$, for some spatial and temporal covariance functions $C_s$ and $C_t$. Users of software for spatio-temporal modelling most often use separable models (see, e.g., Bakka et al. (2018); Krainski et al. (2019)). However, this is not because this is a desired property, but because it is easy to construct and readily available in statistical software. We note that there are many good arguments for why models should not be assumed separable, see Stein (2005), Cressie and Huang (1999), Fonseca and Steel (2011), Rodrigues and Diggle (2010), Gneiting (2002), Sigrist et al. (2015), Wikle (2015), and our Section 1.4.

1.2 The Matérn family of covariance functions

The most well known family of covariance functions for spatial data is the Matérn covariance,

$$C_M(h_s) = \frac{\sigma^2}{2^{\nu-1} \Gamma(\nu)} (\kappa h_s)^\nu K_\nu (\kappa h_s), \tag{2}$$

where $\nu > 0$ is the smoothness parameter, $\kappa > 0$ is the scale parameter, $K_\nu$ is the bessel function of the second kind of order $\nu$, and $\Gamma$ is the Gamma function. The Matérn field is usually attributed to Matérn (1960), it was presented early in Handcock and Stein (1993), and the book by Stein (2012, Ch 1) states “use the Matérn covariance”. Guttorp and Gneiting (2006) provides a historical account of the Matérn covariance, showing the connections to various areas in physics.

In this paper we extend the Matérn covariance function to a family of spatio-temporal covariance functions. We construct a family of spatio-temporal processes which when restricted to space gives the Matérn field, and which inherits the main attributes of the Matérn field. The Matérn field allows one to choose how differentiable the stochastic process should be, and thereby how differentiable the covariance function should be at 0, through $\nu$. The scale parameter has several forms in different papers, we refer to the range parameter $r = \sqrt{8\nu}/\kappa$ in Lindgren et al. (2011). Together, these two parameters allow us to precisely manipulate the concept of “wiggliness”, both in terms of differentiability and in terms of correlation range. The effect of the correlation range is often interpreted as “smoothness”, as a longer range results in a visually increased smoothness, however, in this paper smoothness will only refer to differentiability.
1.3 Different views of the Matérn field motivate different extensions

Here we present four equivalent mathematical representations, or views, of the Matérn field. Together with studying the (power) spectrum, these views improve our understanding of how to define, analyse, and compute with the Matérn field. Crucially, different views also motivate different extensions of the Matérn field to space-time.

The first view is through the covariance function. The Matérn field was not defined because its covariance function has a natural expression. The Bessel function used therein is, for some parameters, just an integral which cannot be represented by standard functions, that has been defined to have a name. A similar problem occurs for example when Stein (2005) proposes a new family of non-separable spatio-temporal covariance functions, the covariance function itself cannot be computed explicitly, and has to be computed numerically.

The second view is through the stochastic partial differential equation (SPDE). Let $L$ be a pseudo-differential operator, and define stochastic process $u$ as a solution to the SPDE

$$Lu = W,$$

(3)

where $W$ is Gaussian white noise. The process $u$ is a Matérn field if the operator is chosen as

$$L_M = (\kappa^2 - \Delta)^{\alpha/2},$$

(4)

where $\kappa > 0, \alpha > 0$ are constants, and $\Delta = d^2/dx^2 + d^2/dy^2$ is the Laplacian, see Whittle (1954, 1963), Lindgren et al. (2011), and Bolin and Kirchner (2019).

The third view is through the precision operator. We get the precision operator $Q$ by using the pseudo-differential operator $L$ twice, giving us $Q = LL$. The precision operator is the continuous version of the precision matrix, similar to how the covariance function is the continuous version of the covariance matrix. The precision operator of the Matérn field is a simple and natural operator, and leads us to using Bessel functions when we compute the covariance function. For the theory behind the SPDE view, see Kelbert et al. (2005) and Prévôt and Röckner (2007).

As an example on the spatial domain $s \in \mathbb{R}^2$, consider a precision operator which is a polynomial in the Laplacian,

$$Q = p(-\Delta),$$

for example (4) with $\alpha \in \mathbb{N}$. Informally, we get the Fourier transform of the precision operator by replacing derivatives with wave-numbers, and this results in a polynomial

$$F(Q) = p(w^2).$$

This function in the frequency domain is the reciprocal of the spectrum, illustrating why many common spectrums are the reciprocal of an even polynomial. Rozanov (1977) showed that the stochastic process is Markov if and only if the spectral density is the reciprocal of a polynomial, see Simpson et al. (2012).

The fourth view is through the Greens function. The kernel of the Matérn field is the Greens function of the differential operator $L_M$ (Bolin, 2014). The kernel can be used to define valid covariance functions, see, e.g., Fuentes (2002), Higdon (2002), and Rodrigues and Diggle (2010).

The modeling approaches stemming from these four views can be thought of as implicit and explicit. In implicit approaches, the properties one is after is not part of the definition of the stochastic process itself. For example, when one defines the covariance function, one cannot immediately see the properties of interest of the resulting family. Typically for implicit approaches, after deriving the properties of the stochastic process, and finding issues with these properties, one looks for new families iteratively. In explicit, or constructive, approaches one aims for a structure, and constructs, e.g., an SPDE or a kernel with that structure encoded. Derived properties are then additional consequences stemming from the explicitly encoded structures. In this paper we follow the explicit approach to construct a stochastic process based on diffusion processes. Other properties, e.g. that the stochastic process is non-separable, is then merely a consequence of our explicit construction.
1.4 Generalising the Whittle covariance to space-time

We use the term Whittle covariance function for the Matérn covariance function with smoothness \( \nu = 2 - d/2 \) where \( d \) is the dimension, and we mainly consider \( d = 2, \nu = 1 \), similar to Sigrist et al. (2015, Sec 2.2). Whittle (1954, 1963) presented this covariance function based on arguments on how to construct physically reasonable models of reality. We now rephrase some of these arguments, and we will later build on these to construct an extension to space-time.

Whittle (1954) discusses the “simplest non-degenerate [autoregressive] scheme” in two dimensions, and how the continuous version of this scheme is described in the SPDE view through

\[
L_W = \kappa^2 - \Delta. \tag{5}
\]

From this, he computes the (Matérn) covariance function for the stochastic process with operator \( L_W \), \( C_W(h_s) = C_M(h_s; \nu = 1) \). Further, he states (page 448),

The correlation function (...) is of interest in that it may be regarded as the ‘elementary’ correlation in two dimensions, similar to the exponential \( e^{-\alpha |x|} \) in one dimension.

A common extension of the Whittle covariance to space-time is to use it as the spatial component in a separable model. Jones and Zhang (1997) discuss how separable covariance functions can be understood through differential operators, written as

\[
L = L_sL_t, \tag{6}
\]

where \( L_s \) is a purely spatial operator and \( L_t \) is a purely temporal operator. In agreement with Jones and Zhang (1997), we note that these operators are almost never encountered when modeling physical reality, hence, separable models are not physically realistic models for the spatio-temporal process.

For our spatio-temporal extension, the development of the Whittle covariance is particularly relevant. Whittle (1963) considers a stochastic process

\[
\frac{\partial u}{\partial t} + \alpha u = \frac{1}{2} \Delta u + \mathcal{E}, \tag{7}
\]

for \( u(s,t) \), where \( \mathcal{E}(s,t) \) is some noise process. Considering this as a “stationary process in space alone”, and assuming \( \mathcal{E} \) to be a white noise process, he motivates the construction of the Whittle covariance function based on its physical realism as a diffusion process.

The diffusion process is one of the most fundamental and common models for physical processes, in everything from the heat equation to spread of disease, as it is a mathematical representation of the conservation of “mass” (mass, energy, individuals, particles). We refer to appendix A.1 for more details on the physical interpretation of the diffusion equation.

We claim that the most appropriate generalisation of the Whittle covariance function to space-time is simply to use the space-time equation Whittle himself employed in his motivation of the Whittle covariance function. Hence, equation (7) is the centre-point of our proposed generalisation in Section 2.

1.5 From the Whittle process to the Matérn field

We present arguments for using the entire family of Matérn covariance functions in spatial applications, not just the Whittle covariance, hence moving from \( \nu = 2 - d/2 \) to arbitrary \( \nu > 0 \). Historically, Whittle (1954) criticized arbitrary fractional powers of the operator \( L_W \),

[...] the exponential function has no divine right in two dimensions, while the example of the last section indicated that a \( K_1 \) function fitted the observations better than did an exponential.
He proceeds to note that what we now refer to as the Matérn covariance with $\nu = 1/2$ is the exponential covariance function, but that this, in 2 dimensions, is represented by $L = L_{W}^{3/4}$. The operator $L_{W}^{3/4}$ does not give a Markovian stochastic process (Rozanov, 1977), and this is related to the non-locality of the operator.

Physical processes are usually understood to exist in 3 spatial dimensions, even if we often model them in 2 dimensions. If we construct a Whittle function in $\mathbb{R}^3$, then $\nu = 2 - 3/2 = 1/2$ results in an exponential covariance. If, next, we take a 2-dimensional section of this covariance function, we end up with one that has exponential covariance in $\mathbb{R}^2$. This counters Whittle’s argument that the exponential covariance function is not appropriate in $\mathbb{R}^2$.

For general values of $\nu$, we note that the spatio-temporal model component is not modeling a single process, but a variety of unmeasured and unspecified processes. We assume that these are diffusion processes, as the diffusion equation is the basic equation for most physical processes (Appendix A.1). The operators we consider are linear, $L(u_1 + cu_2) = L(u_1) + cL(u_2)$, which means that if each of these unspecified processes follow the same diffusion equation, with the same range parameter, then the the sum of all these unspecified processes, the spatio-temporal model component, also does. However, in many cases it is not appropriate to assume that they all have the same range parameter. A Matérn field in $\mathbb{R}^2$ with fractional $\nu$ can be interpreted as a sum of Matérn fields with integer $\nu$’s but different correlation ranges. This can be seen both in the approximations to fractional operators (Bolin et al., 2018; Bolin and Kirchner, 2019) and, in one dimension, in approximating fractional Gaussian noise by a sum of autoregressive models (Serbye et al., 2019).

In total, these arguments force us to consider the entire family of Matérn covariance functions as reasonable models for the spatial marginal of the spatio-temporal model component. Hence, the space-time extension should also allow for fractional $\nu$, both in space and in time.

1.6 SPDE generalisations of Whittle and Matérn

Several papers have been using the SPDE view to suggest models for spatio-temporal stochastic processes, that are also generalisations of the Whittle covariance, by generalising the operator in (5). Jones and Zhang (1997) propose

$$\frac{\partial}{\partial t} + (\kappa^2 - \Delta)^\alpha u(s, t) = \mathcal{E}(s, t),$$

(8)

where $\mathcal{E}$ is Gaussian white noise (white in space and in time). They present this as a generalisation of Whittle’s equation, and although their aim is similar in spirit to the aim of this paper, the stochastic diffusion (7) is not in their family.

Lindgren et al. (2011) (Section 3.5) suggest using

$$\frac{\partial}{\partial t} + \kappa^2 + m \cdot \nabla - \nabla \cdot \mathbf{H} \nabla u(s, t) = \mathcal{E}(s, t),$$

(9)

where $\mathbf{H}$ is a constant diffusion matrix. Lindgren et al. (2011) state that there needs to be a spatially smooth innovation process $\mathcal{E}(s, t)$, see also Sigrist et al. (2015, Sec 2.2) which takes the place of the forcing in the deterministic diffusion equation. Physically, this is because it is believed that mechanisms for introducing new mass (or, particles) into the system, through innovation noise, are usually spatially smooth. Additionally, without this assumption the model does not have a pointwise meaning.

Stein (2005) defines a family of space-time covariance functions with good properties through the spectrum

$$S(w_s, w_t) = \{c_1(a_1^2 + \|w_s\|^2)^{\alpha_1} + c_2(a_2^2 + |w_t|^2)^{\alpha_2}\}^{-\nu}$$

(10)

where $c_1 > 0, c_2 > 0, a_1, a_2$ are scale parameters, $a_1^2 + a_2^2 > 0$, $\alpha_1$, $\alpha_2$ and $\nu$ are smoothness parameters, here on a two-dimensional spatial and one-dimensional temporal domain, and $2/\alpha_1 + 1/\alpha_2 < 2\nu$ is
required for the stochastic process to be well defined. Stein’s model can be stated as an SPDE with the differential operator

\[ L_{\text{Stein}} = \left( c_1(a_1^2 - \nabla^2)^{\alpha_1} + c_2 \left( a_2^2 - \frac{\partial^2}{\partial t^2} \right)^{\alpha_2} \right)^{\nu/2}, \]

see Krainski (2018) and Vergara et al. (2018).

The Stein family generalises the family by Jones and Zhang (1997), but neither family contains the stochastic diffusion process (7), that was motivated by Whittle. We can attempt to recover the stochastic diffusion process, in the Stein family, by \( \nu = 2, \alpha_2 = 1/2, \) and \( \alpha_1 = 1, \) but this is prohibited by the requirement that \( 2/\alpha_1 + 1/\alpha_2 < 2\nu. \) Another approach to recovering this equation would be to use \( \nu = 4, \) by interpreting this as \( \nu = 2 \) iterated twice, with the first iteration giving us a smoothed innovation process, and the second iteration representing the stochastic diffusion equation. This would lead to an innovation process that is smooth in time, which is clearly not desirable; we would then be able to predict future innovation noise from past innovation noise.

Other related approaches, that are less similar to the current work than those we have discussed here, are Fuentes et al. (2008), and Liu et al. (2019). Storvik et al. (2002) construct covariance functions by evolving a spatial covariance function discretely in time, by, for each time step, convolving the stochastic process at the previous step and adding innovation noise.

1.7 Plan of this paper

In this paper we introduce a new family of stochastic processes to be used as space-time model components, in Section 2. We interpret the scale and smoothness parameters, for the spatial and temporal dimensions, in Section 3. We show that there is a subfamily of Markovian diffusion processes which are non-separable due to their diffusive nature. Additionally, we have a subfamily which overlaps with a Stein subfamily, including the models by Jones and Zhang (1997), and a subfamily of separable models. We elicit priors in Section 4.

Computational issues are challenging for these models. We present a sparse representation in Section 5 and an implementation in R-INLA (Rue et al., 2009) in Supplementary Materials, which allows us to construct models with different likelihoods and several random effects. We discuss two applications in Section 6, a forecasting example that illustrates clearly the difference between separable models and non-separable diffusion-based models, and an application to a global temperature dataset.

2 The DEMF family of spatio-temporal stochastic processes

In this section we define the diffusion-based extension of the Matérn field (DEMF) family of spatio-temporal stochastic processes. The main property we aim for is that the process should have a spatial Matérn covariance when considered for a fixed time point, i.e. the spatial marginalisations of the process are Gaussian Matérn fields. This property allows us to consider the new family of models an extension of the spatial Matérn field.

Consider again the Matérn operator, \( L = \gamma_2^2 - \Delta \) and introduce the precision operator \( Q(\gamma_0, \gamma_\epsilon, \alpha_\epsilon) = \gamma_2^2 L^{\alpha_\epsilon} \) the precision operator for the Matérn field, see Whittle (1954) and Lindgren et al. (2011). As an alternative to the space-time white noise \( \mathcal{E} \) used in (8), we introduce \( \mathcal{E}_Q \) as Gaussian noise that is white in time but correlated, with precision operator \( Q, \) in space. The process \( u(s, t) \) in

\[ \frac{\partial}{\partial t} u(s, t) = \mathcal{E}_Q(s, t), \]

for \( t > 0, \) can thought of as a Q-Wiener process \( \mathcal{E}_Q(t) \) (Da Prato and Zabczyk 2014). Alternatively,

\[ \left( \frac{\partial}{\partial t} + \kappa \right) u(s, t) = \mathcal{E}_Q(s, t) \]
results in a model with a separable covariance function where the temporal covariance is exponential and the spatial covariance is Matérn. This is what we call the Kronecker product of Matérn and the Ornstein-Uhlenbeck processes. We aim to produce a space-time model with diffusive behaviour. For this, we need to replace the time derivative in (13) with an operator containing both a time derivative and the diffusion operator, hence we propose

\[
\left( \gamma_t \frac{d}{dt} + L \right) u(s, t) = \mathcal{E}_Q(s, t). \tag{14}
\]

The use of \( L \) on both sides of this equation is what causes the spatial marginalisation of the process to be Matérn fields, as will be shown in Section 3. Equation (14) can be generalised, while still preserving the required properties, to

\[
\left( \gamma_t \frac{d}{dt} + L^{\alpha_t/2} \right)^{\alpha_t} u(s, t) = \mathcal{E}_Q(s, t). \tag{15}
\]

In total, the model has non-negative smoothness parameters \((\alpha_t, \alpha_s, \alpha_e)\) and non-negative scale parameters \((\gamma_t, \gamma_s, \gamma_e)\). This equation defines the new family of spatio-temporal models introduced in this paper, written \(\text{DEMF}(\alpha_t, \alpha_s, \alpha_e)\).

### 3 Parameter interpretations and model properties

In this section we discuss marginal spatial and temporal properties of \(\text{DEMF}(\alpha_t, \alpha_s, \alpha_e)\). In order to simplify the exposition, we focus on the case when the spatial domain is \(\mathbb{R}^2\) and the temporal domain is \(\mathbb{R}\). In this case, the space-time spectrum of the solution \(u(s, t)\) to (15) is

\[
S_u(\omega_s, \omega_t) = \frac{1}{(2\pi)^3 \gamma_e^2 \gamma_t^2 \omega_t^2 + (\gamma_s^2 + \|\omega_s\|^2) \alpha_e} \Omega(\gamma_s^2 + \|\omega_s\|^2)^{\alpha_e} \text{e}^{-\nu \|\omega_s\|^2 \sigma^2}, \quad \omega_t \in \mathbb{R}, \omega_s \in \mathbb{R}^2. \tag{16}
\]

Next, we show that the spatial marginal of \(u(s, t)\) is a Matérn field, given that the smoothness parameters are chosen appropriately. To formulate this requirement, define \(\alpha = \alpha_e + \alpha_s (\alpha_t - 1/2)\).

**Proposition 3.1.** Assume \(\alpha_t, \alpha_s, \alpha_e\) satisfy \(\alpha > 1\). Then the solution \(u(s, t)\) to (15) has marginal spatial covariance function

\[
C(u(t, s_1), u(t, s_2)) = \frac{\sigma^2}{\Gamma(\nu_s)^2} (\gamma_s \|s_1 - s_2\|)^{\nu_s} K_{\nu_s}(\gamma_s \|s_1 - s_2\|),
\]

where \(\nu_s = \alpha - 1\) and

\[
\sigma^2 = \frac{\Gamma(\alpha - 1/2) \Gamma(\alpha - 1)}{\Gamma(\alpha) \Gamma(\alpha) 8\pi^{3/2} \gamma_e^2 \gamma_t^2 \gamma_s^2 (\alpha - 1)}. \tag{17}
\]

**Proof.** See appendix [A.2.1].

The mean square differentiability of the process is determined by the decay rate of its spectrum. If \(S(\omega_t) \sim \omega_t^{-\gamma}\) for large \(\omega_t\), then the process is \(\nu\) times mean square differentiable if \(2\nu < \gamma - 1\) [Stein, 2005]. We use this in the following proposition to derive the temporal smoothness of the process. Let \(F_1(a, b, c, z)\) denote the hypergeometric function.

**Proposition 3.2.** Assume \(\alpha_t, \alpha_s, \alpha_e\) satisfy \(\alpha > 1\). The marginal temporal spectrum of the solution \(u(s, t)\) to (15) is

\[
S_t(\omega_t) \propto F_1 \left( \alpha_t, \frac{\alpha_e - 1}{\alpha_s} + \alpha_t, \frac{\alpha_e - 1}{\alpha_s} + \alpha_t + 1; -\gamma_t^2 s_t^2, \omega_t^2 \right),
\]

and the temporal smoothness is

\[
\nu_t = \min \left[ \alpha_t - \frac{1}{2}, \frac{\nu_s}{\alpha_s} \right].
\]
Table 1: Summary of the smoothness properties of the solution $u(s,t)$ for different values of the parameters $\alpha_t$, $\alpha_s$, $\alpha_e$, together with some examples. Here $\nu_t$ and $\nu_s$, respectively denotes the temporal and spatial smoothness of the process. DEMF is the new family of models we introduce, and the example models will be denoted by e.g. DEMF(1, 0, 2). The three example models are the same as what we study in Figures 1 and 2. The type we refer to as fully nonseparable is the subfamily of the family in (11). The example denoted “Diffusion” is the stochastic process analogue of the physical diffusion equation (7), and is the main model in sections 5 and 6.

| $\alpha_t$ | $\alpha_s$ | $\alpha_e$ | Type | $\nu_t$ | $\nu_s$ |
|------------|------------|------------|------|--------|--------|
| $\alpha_t$ | $\alpha_s$ | $\alpha_e$ | DEMF($\alpha_t$, $\alpha_s$, $\alpha_e$) | $\min\left[\alpha_t - \frac{1}{2} \frac{\alpha_s}{\alpha_t}, \alpha_e + \alpha_s(\alpha_t - 1/2) - 1\right]$ | $\alpha_e - 1$ |
| $\alpha_t$ | 0          | $\alpha_e$ | Separable | $\alpha_t - \frac{1}{2} \frac{\alpha_s}{\alpha_t}$ | $\alpha_s(\alpha_t - 1/2) - 1$ |
| $\alpha_t$ | $\alpha_s$ | 0          | Fully nonseparable | $\alpha_t - \frac{1}{2} - \frac{1}{\alpha_s}$ | $\alpha_s(\alpha_t - 1/2) - 1$ |

1 0 2 Separable 1/2 1
1 2 1 Diffusion 1/2 1
3/2 2 0 Fully nonseparable 1/2 1

Proof. See appendix A.2.2.

For integer values of the smoothness parameters, the hypergeometric function can be expressed using elementary functions. When $\alpha_s = 2$ and $\alpha_t = 2$, we obtain

$$S_u(\omega_t) \propto \int_0^{\infty} \frac{1}{(\omega_t^2 + (1 + u)^2)^2} du = \frac{\arctan(\omega_t)}{2\omega_t^3} - \frac{1}{2\omega_t^2(\omega_t^2 + 1)}, \quad (18)$$

showing that the marginal temporal covariance is not a Matérn covariance. However, similarly to the Matérn covariance, we can control its smoothness and range.

In the separable case, the temporal covariance function is a Matérn covariance function with smoothness parameter given by $\alpha_t$.

**Corollary 3.3.** Assume that $\alpha_s = 0$, $\alpha_t > 1/2$, and $\alpha_e > 1$. Then the solution $u(s,t)$ to (15) has a separable space-time covariance function where the spatial covariance is given by Proposition 3.1 and the marginal temporal covariance function is

$$C(u(t_1, s), u(t_2, s)) = \frac{\sigma^2}{\Gamma(\nu_t)2^{\nu_t-1}(\gamma_t^{-1}|t_1 - t_2|)^\nu_t K_{\nu_t}(\gamma_t^{-1}|t_1 - t_2|)},$$

where $\nu_t = \alpha_t - 1/2$ and $\sigma^2$ given by (17).

Proof. See appendix A.2.3.

We summarise the general smoothness results, as well as some important special cases, in Table 1. The restriction on permissible values of the $\alpha$’s can be written as $\nu_s > 0$. For temporal smoothness, we note that the process is separable or $\alpha_t > 1/2$, $\nu_s > 0$ guarantees $\nu_t > 0$. For integer values for the $\alpha$’s, we note that $\alpha_e = 0$ does not allow for ($\alpha_t = 1, \alpha_s = 1$), ($\alpha_t = 1, \alpha_s = 2$), or smaller, while $\alpha_e = 1$ does not allow $\alpha_t = 0$ nor $\alpha_s = 0$, while $\alpha_e = 2$ allows for any values for $\alpha_t, \alpha_s$, for the process to be well defined.

An interesting case is $\alpha_e = 0$, which we refer to as the fully non-separable models. Here, the model has a spectral density which is a subfamily of the Stein family, and the requirement $\alpha > 1$ corresponds to the restriction $\alpha_s(\alpha_t - 1/2) > 1$ on the relation between $\alpha_s$ and $\alpha_t$. 

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For fixed marginal smoothness parameters \( \nu_t \) and \( \nu_s \), the \( \alpha_s \) parameter controls the type of non-separability, which can take values in the interval \([0, \nu_s/\nu_t]\). To simplify interpretability of the parameters, we introduce a separability parameter
\[
\beta_s = \alpha_s \frac{\nu_t}{\nu_s} \in [0, 1],
\]
so \( \beta_s = 0 \) gives a separable model, and \( \beta_s = 1 \) gives the “maximally non-separable” model.

To improve the interpretability of the scale parameters, we define \( \sigma, r_s, r_t \),
\[
c_1 = \frac{\Gamma(\alpha_t - 1/2)\Gamma(\alpha - 1)}{\Gamma(\alpha)\Gamma(\alpha)4\sqrt{\pi}},
\]
\[
\sigma = \gamma_e^{-1} c_1^{1/2} \gamma_t^{-1/2} \gamma_s^{-(\alpha-1)},
\]
\[
r_s = \gamma_s^{-1} \sqrt{8 \nu_s},
\]
\[
r_t = \gamma_t \sqrt{8(\alpha_t - 1/2)\gamma_s^{-\alpha_s}},
\]
where \( r_s \) is the correlation range as in [Lindgren et al. (2011)](https://doi.org/10.1007/s11222-011-9257-5), giving approximately correlation of 0.13 at \( r_s \) distance in space (keeping time fixed). Similarly, \( r_t \) is the temporal correlation range for the separable model, and an approximate correlation range when the model is not separable.

### 3.1 Examples

We now illustrate the behaviour of the DEMF models, and the interpretation of the parameters, through the three specific examples in Table 1. The parameters in the three examples are chosen so that \( \nu_t = 1/2 \) and \( \nu_s = 1 \). These examples have been standardised to have \( \sigma = 1 \), \( r_s = 1 \), and \( r_t \) is near 1. The non-separable examples have to be adjusted on the temporal scale compared to the separable example; the separable example uses \( r_t = 1 \), but the DEMF(1,2,1) example uses \( r_t = 1.9 \), and the DEMF(3/2, 2, 0) example uses \( r_t = 1.8 \).

In Figure 1 we show the spatio-temporal covariance function for these three models, and in Figure 2 we show the marginal covariances. There is a clear difference between the three spatio-temporal covariances, even though the marginal spatial covariances are identical, and the marginal temporal covariances are very similar. The marginal covariances confirm the interpretation of the interpretable parameters \( \sigma, r_s, r_t \). Note that \( \sigma, r_s \) and \( r_t \) do not influence the shape of the covariance functions.

### 4 Penalized complexity priors

In this section we use the interpretable parameters to define penalized complexity priors (Simpson et al. [2017](https://doi.org/10.1093/biomet/asx014)). We first fix \( r_t \), and construct a prior for the other hyper-parameters based on the marginal spatial structure. Here, we use the penalized complexity priors developed by Fuglstad et al. (2017),
\[
\sigma \sim \exp(\lambda_e)
\]
\[
1/r_s \sim \exp(\lambda_s)
\]
where the \( \lambda_e \) and \( \lambda_s \) are found by eliciting prior information about a quantile, see Fuglstad et al. (2017) and the Appendix of Bakka et al. (2019).

The prior for \( r_t \) we define conditionally on \( \sigma \) and \( r_s \). In the separable case \( (\alpha_s = 0) \) we suggest the prior
\[
1/\sqrt{r_t} \sim \exp(\lambda_t),
\]
Figure 1: Three examples of space-time covariance functions, where the parameters in the three cases are chosen so that \( \nu_t = 1/2 \) and \( \nu_s = 3/2 \). Model 1 is separable, model 2 and 3 are non-separable. The other model parameters are chosen so that the field has variance 1, the same spatial range, and approximately the same temporal range for each model, as seen in Figure 2.

because that is the PC prior for the marginal temporal model (Fuglstad et al., 2017). We use this prior also in the non-separable case, due to the similarity between the separable and non-separable marginal temporal covariance functions shown in Figure 2. The slight changes in the interpretation of \( r_t \) between different models is not of sufficient magnitude to warrant a more complex prior formula.

5 GMRF representation

In this section we represent the continuously indexed random process DEMF(1,2,1) by a discretely indexed Gaussian Markov random field (GMRF), to enable fast inference. Specifically, we give a GMRF representation of the process \( u(s,t) \) in (14), on the domain \( \Omega \times [a,b] \) where \( \Omega \subset \mathbb{R}^2 \) is a polygonal domain, \( a,b \in \mathbb{R} \). For the spatial domain, we use the Neumann boundary condition

\[
\frac{\partial u}{\partial n} = 0, \quad \text{on } \partial \Omega,
\]

where \( n \) is the normal vector to the boundary. Here, we assume that the domain is extended away from the region of interest, as in [Lindgren et al., 2011, Appendix A4]. For the temporal boundary, we ensure that the stochastic process is stationary in time,

\[
C(u(s_1,t_1), u(s_2,t_2)) = C(u(s_1,t_1 + d), u(s_2,t_2 + d))
\]

whenever \( t_1, t_2, t_1 + d, t_2 + d \) are in the domain.

5.1 Spatio-temporal GMRF representation

Let \( \Phi_t = \{ \phi_1(t), \ldots, \phi_N(t) \} \) denote piecewise linear temporal basis functions over a regular grid. Let \( \Psi_s = \{ \psi_1(s), \ldots, \psi_N(s) \} \) denote a set of piecewise linear spatial basis functions obtained by a triangulation of the spatial domain. We approximate the process \( u(s,t) \) in (14), with boundary conditions as in (26) and (27), in the Kronecker basis \( \Psi_s \otimes \Phi_t \). This approximation can be written as

\[
\hat{u}(s,t) = \sum_{i,j} u_{i,j} \psi_i(s) \phi_j(t)
\]
where the coefficient vector is \( \mathbf{u} = ((u_{i,j}))_j = (u_{1,1}, u_{2,1}, \ldots) \). For \( \alpha_t = 1, \alpha_s = 2, \alpha_e = 1 \), \( \mathbf{u} \) is a Gaussian vector with mean zero and precision matrix \( Q_\mathbf{u} \), with

\[
\gamma_e^{-2} Q_\mathbf{u} = M_0 \otimes Q_3 + 2\gamma_t M_1 \otimes Q_2 + \gamma_t^2 M_2 \otimes Q_1.
\] (29)

See Appendix A.3 for a detailed derivation. The derivation relies on semi-discretisation, where the space-time process can be written as coefficients for spatial eigenfunctions propagated in time through independent one-dimensional stationary processes.

5.2 Computational considerations

In order to use these models in practice, we need to understand their computational complexity. The neighborhood structure of the GMRF approximation of the corresponding separable model DEMF(1,0,2) is easy to understand. The spatial model has a second order neighbourhood structure, the temporal model has a first order neighbourhood structure, and the kronecker product fills out the square, giving \( 5^2 \cdot 3 - 1 = 74 \) neighbours in space-time. The neighbourhood structure of the non-separable model DEMF(1,2,1) can be seen from (29). Ignoring the boundary we get 84 neighbours in space-time.

The two neighbourhood structures are similar enough that we expect the separable and the non-separable spatio-temporal model component to incur a similar computational cost when used as part of a latent Gaussian model, which typically do not exploit the Kronecker product structure, see Rue et al. (2009) and Bakka et al. (2018). For settings where the Kronecker product structure is an essential part of computational efficiency, one could look for an approximation to a separable representation (Genton, 2007).

6 Applications

6.1 Separable vs non-separable forecasting

One of the clearest practical differences between the separable model DEMF(1,0,2) and the non-separable diffusion model DEMF(1,2,1) is seen in forecasting. We simulate a spatial dataset representing “today” (year 1), from the Matérn model and we add 1 percent nugget effect. We condition
on this dataset to predict into the future, for year 2 and year 3. Note that this conditioning is without any model misspecification due to the separable and non-separable models having the same spatial marginals. The parameters are set to $r_s = 2.5, r_t = 4, \sigma = 1$, and $r_t$ in the non-separable model is multiplied with 1.8 as in Section 3.1.

Figure 3 compares the predictions from these two models. Year 1 is very similar between the two fits, due to the informative simulation. For year 2 and 3, we note how the non-separable model diffuses the point prediction. The point prediction at a location next year depends heavily on the values in the local region for the previous year. This diffusive behaviour is beneficial for many practical applications, and was part of the theoretical motivation of Whittle (1954, 1963), and a major motivation for developing the DEMF family. Inference is computed using a computationally efficient GMRF procedure in van Niekerk et al. (2019). A code example producing similar figures, using the full R-INLA interface, can be found in the supplementary materials.

6.2 Global temperature dataset

*Version notes: This application will be included in the journal version.*

7 Discussion

In this paper we developed a natural spatio-temporal extension of the Matérn field, natural in the sense that it uses a stochastic version of the physical diffusion equation, also used by Whittle (1954, 1963). We named the new family DEMF, for Diffusion-based Extension of the Matérn Field, and showed that this family has good properties. The spatial marginals give exactly the Matérn field, the family contains Markovian diffusion processes with strong physical interpretation, we can control the smoothness in space and in time, the type of non-separability, and interpret all the parameters.

In the DEMF family, we focused on DEMF(1,2,1), because this is the closest stochastic process analogue to the diffusion equation (see (7) and Appendix A.1), hence a natural choice for the spatio-temporal model component. The non-separable DEMF(1,2,1) has the same smoothness in space and in time as the separable DEMF(1,0,2), which is a Kronecker product of Matérn in space and auto-regressive in time. With the GMRF representation presented herein the computational costs of the two models are similar. Together with interpretable parameters, this makes the non-separable model as practically accessible as the separable model. In the supplementary materials we provide an implementation with examples in R-INLA. This implementation includes model specification in R, which can be extracted and used in other statistical software, e.g. MGCV (Wood, 2011) and TMB (Kristensen et al., 2016).

The proposed model is non-separable, but this was not the goal from the outset, rather, it is a consequence of following what we deem to be a natural extension of the Matérn model. This gives another argument for using non-separable models, namely that a model explicitly constructed to represent a physical process can be non-separable. More importantly, this paper sheds light on which types of non-separable models that are desirable. Although there are strong arguments in the literature against using a separable model, the space of non-separable models is vastly larger than the space of separable models, hence we need to consider which types of non-separable models are more, and which are less, appropriate than the separable alternatives.

The DEMF family contains several important subfamilies; 1) Separable models, 2) Markov models, 3) a subfamily of the Stein (2005) family. This provides a rich outset for studying the practical and methodological impacts these assumptions have. For example, one can consider a separable model as a limiting case of non-separable diffusion models. In this paper we only consider stationary fields, which are also spatially isotropic, but we note that non-stationarity can be obtained in a natural way by making $L = L(s,t)$, as discussed by Lindgren et al. (2011). We also leave the implementation of other integer and non-integer $\alpha$’s for future work.
Figure 3: Predictions from DEMF(1,0,2) and DEMF(1,2,1) when conditioned on a spatially dense dataset in year 1, but no data in year 2 or 3. The temporal correlation range has been set to 4 in the separable model.
8 Supplementary materials

We provide alternative code for the first application which uses the full INLA interface at https://haakonbakkagit.github.io/btopic132.html. We provide a code example with real data at https://haakonbakkagit.github.io/btopic133.html however, this is only a code example meant to run quickly, and not an adequate analysis of the data in question.

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### Appendix

#### A.1 Diffusion - a fundamental property of nature

Diffusion processes are fundamental when modeling space-time processes in nature, in everything from climate and weather models, to geophysics, and to population and disease models. One of the most used of all physical models is the deterministic diffusion equation, which is built around the assumption of a system preserving “particles”, e.g. mass, energy or heat, commonly written as

\[
\frac{\partial u(s, t)}{\partial t} = \nabla \cdot D(s) \nabla u(s, t). \tag{30}
\]

Here, \(u(s, t)\) is the number of particles per unit area and time, \(\partial\) denotes partial derivative, \(\nabla \cdot = [\partial/\partial x, \partial/\partial y]\) is the divergence operator, \(D(s)\) is any known function (bounded and somewhat regular), and \(\nabla = [\partial/\partial x, \partial/\partial y]\) is the gradient operator. The physical intuition behind the diffusion equation is that a system seeks equilibrium, if there are more particles in one area than in the neighbouring area, the units will naturally flow from the more populated to the less populated area. For example, the units of heat energy in your coffee cup flow into the air, because your coffee is warmer than the air, making the coffee colder as you read this, and the air slightly warmer. In this example \(D\) describes how easily heat is transferred across space. We will consider only constant \(D\) in this paper, and add the standard forcing \(g\) representing new particles entering the system,

\[
\frac{\partial u(s, t)}{\partial t} - D \Delta u(s, t) = g(s, t), \tag{31}
\]

where \(\Delta = \nabla \cdot \nabla\) is the Laplace operator. We use a diffusion equation with random forcing \(g\); informally \(g\) is replaced by an innovation process \(W\).
A stochastic understanding of deterministic diffusion comes from Brownian motion. The simplest model for Brownian motion tracks a specific particle, as it moves randomly through space, over time. If we have an infinitely large collection of these particles, and instead of tracking the individuals, we zoom out and keep track of how many particles are in each spatial cell, tracking the density \( u(s, t) \) over time, the equation that describes this density is the diffusion equation (Øksendal [2013]).

### A.2 Proofs

#### A.2.1 Proof of Proposition 3.1

Integrating out \( \omega_t \) from (16) we have the spatial marginal spectral density

\[
S_u (\omega_s) = \frac{1}{(2\pi)^2 \gamma_t^2 (\gamma_s^2 + ||\omega_s||^2)^{\alpha_s}} \int \frac{1}{2\pi (\omega_t^2 + (\gamma_s^2 + ||\omega_s||^2)\gamma_t^2)^{\alpha_t}} d\omega_t
\]

\[
= \frac{1}{(2\pi)^2 \gamma_t^2 (\gamma_s^2 + ||\omega_s||^2)^{\alpha_s}} \frac{1}{\Gamma(\alpha_t - 1/2)} \Gamma(\alpha_t) (4\pi (\gamma_s^2 + ||\omega_s||^2)\gamma_t^{2\alpha_t})^{1/2} \frac{\gamma_t^2}{\Gamma(\alpha_t - 1/2)} \frac{8\pi^{5/2} \gamma_t^2 \gamma_s^2}{\Gamma(\alpha_t)}
\]

This shows that we must choose the parameters so that \( \alpha > 1 \) in order to have an integrable spectral density, and a field with pointwise meaning. Under this assumption, we recognize this as the spectral density corresponding to a spatial Matérn covariance function with range parameter \( \gamma_s \), smoothness parameter \( \nu_s = \alpha - 1 \), and marginal variance \( \sigma^2 \).

#### A.2.2 Proof of Proposition 3.2

Let \( B(x, y) \) be the beta function,

\[
B(x, y) = \int_0^1 t^{x-1} (1-t)^{y-1} \; dt.
\]

The marginal temporal spectrum is

\[
S_u (\omega_t) \propto \int \frac{1}{R^2} \frac{\gamma_t^2 \omega_t^2 + (\gamma_s^2 + ||\omega_s||^2)^{\alpha_s}}{\omega_t^2 + (\gamma_s^2 + ||\omega_s||^2)^{\alpha_s}} d\omega_t
\]

\[
\propto \int_0^\infty r \left[ \frac{\gamma_t^2 \omega_t^2 + (r^2 + \gamma_s^2)^{\alpha_s}}{\gamma_t^2 + r^2 + \gamma_s^2} \right]^{-\alpha_t} (\gamma_s^2 + ||\omega_s||^2)^{\alpha_s} dr
\]

\[
\propto \int_0^\infty (1 + u)^{-\alpha_t} (\omega_t^2 + (1 + u)^{\alpha_s})^{-\alpha_t} du
\]

\[
\propto \int_0^\infty (1 + x)^{-\frac{\alpha_t - 1}{\alpha_s}} (-1)(\omega_t^2 + 1 + x)^{-\alpha_t} dx
\]

\[
\propto B \left( \frac{\alpha_t - 1}{\alpha_s} + x, 1 \right) \left. \frac{2 F_1 (\alpha_t, \frac{\alpha_t - 1}{\alpha_s} + x, \frac{\alpha_t - 1}{\alpha_s} + \alpha_t + 1, -\omega_t^2) \right|_x^\infty
\]

because \( \frac{\alpha_t - 1}{\alpha_s} + x = \frac{\nu_t}{\nu_s} + \frac{1}{2} > 0 \). Now, assuming that \( a - b \) is not an integer, the hypergeometric function \( _2F_1 (a, b, c, z) \) for large values values of \( z \) behaves like

\[
_2F_1 (a, b, c, z) \sim c_1 z^{-a} + c_2 z^{-b} + O(z^{-a-1}) + O(z^{-b-1})
\]

as \( z \to \infty \). If \( a - b \) is an integer we have to multiply \( z^{-a} \) or \( z^{-b} \) with \( \log(z) \) [Erdélyi (1953) volume 1, section 2.3.2, page 76]. This extra logarithmic factor will not make a difference for the final smoothness. Thus, we may write

\[
S_t (\omega_t) \sim \omega_t^{-2\alpha_t} + \omega_t^{-2\frac{\alpha_t - 1}{\alpha_s} + \alpha_t} = \omega_t^{-2\alpha_t + \frac{1}{\alpha_s} \min(0, \alpha_t - 1)}
\]
Now, if \( S_t(\omega_t) \sim \omega_t^{-\gamma} \) for large \( \omega_t \), then the process is \( \nu \) times mean square differentiable if \( \gamma - 1 > 2\nu \). Thus, in our case the process is

\[
\nu_t = \frac{2(\alpha_t + \frac{1}{\alpha_s} \min(0, \alpha_e - 1)) - 1}{2} = \alpha_t + \frac{1}{\alpha_s} \min(0, \alpha_e - 1) - \frac{1}{2}
\]

times differentiable, which completes the proof. Equivalently,

\[
\nu_t = \min \left[ \alpha_t - \frac{1}{2}, \frac{1}{\alpha_s} \right].
\]

A.2.3 Proof of Corollary 3.3

The marginal temporal spectrum for \( \alpha_s = 0 \) is

\[
S_u(\omega_t) = (2\pi)^{-3} \gamma_e^{-2} \int_{R^2} [\gamma_t^2 \omega_t^2 + 1]^{-\alpha_t} (\gamma_s^2 + ||\omega_s||^2)^{-\alpha_e} d\omega_s
\]

\[
= (2\pi)^{-3} \gamma_e^{-2} 4\pi \int_0^\infty r[\gamma_t^2 \omega_t^2 + 1]^{-\alpha_t} (\gamma_s^2 + r^2)^{-\alpha_e} dr
\]

\[
= \frac{1}{2\pi^2 \gamma_e^2 \gamma_s^{(\alpha_e-1)}} \int_0^\infty r(1 + r)^{-\alpha_t} (\tilde{\omega}_t^2 + 1)^{-\alpha_e} dr, \tag{33}
\]

where \( \tilde{\omega}_t = \omega_t \gamma_t \). The evaluation of this integral results in the spectral function for the Matérn with \( \nu_t = \alpha_t - 1/2 \).

A.3 Details on the finite element representation

A.3.1 Temporal GMRF representation with boundary condition

We first present precision matrices for stationary autoregressive order 2 (AR2) processes, and then show how this can be used to give a stationary GMRF representation of the Ornstein-Uhlenbeck (OU) process.

**Lemma A.1.** Let \( Q \) be a quint-diagonal (symmetric) precision matrix. Let the diagonal element be denoted \( q_0 \), and the off-diagonals \( q_1, q_2 \), except for in the first two and last two rows and columns. Define the constants

\[
b_+ = \sqrt{q_0 + 2q_1 + 2q_2}
\]

\[
b_- = \sqrt{q_0 - 2q_1 + 2q_2},
\]

\[
b_s = b_+ + b_-,
\]

and the derived constants

\[
a_0 = \frac{1}{4} \left( b_s + \sqrt{b_s^2 - 16q_2} \right)
\]

\[
a_1 = \frac{b_+ - b_-}{2}
\]

\[
a_2 = \frac{1}{4} \left( b_s - \sqrt{b_s^2 - 16q_2} \right).
\]

Assume that \( Q \) has the following entries in the first and last two rows and columns,

\[
Q_{0,0} = Q_{N,N} = a_0^2
\]

\[
Q_{1,1} = Q_{N-1,N-1} = a_0^2 + a_1^2
\]

\[
Q_{0,1} = Q_{N,N-1} = a_1 a_0
\]

\[
Q_{1,0} = Q_{N-1,N} = a_1 a_0.
\]
and that all other elements are zero. Then, \( Q \) is the precision matrix for the stationary AR2 process with evolution

\[
a_0 u_t + a_1 u_{t-1} + a_2 u_{t-2} = z_t \sim N(0,1).
\]

Additionally,

\[
q_0 = a_2^2 + a_1^2 + a_0^2 \\
q_1 = a_1(a_0 + a_2) \\
q_2 = a_0a_2.
\]

**Proof.** Straight forward computations.

Let \( \Phi_t = \{\phi_1(t), ..., \phi_{N_t}(t)\} \) be a set of piecewise linear basis functions in time, on a regular grid, and consider precision matrices on the coefficients for a linear combination of these basis functions. We want to represent the OU process

\[
\kappa z + \frac{d}{dt}z = b^{-1/2}\epsilon,
\]

as a GMRF, where \( \epsilon \) is white noise. However, we instead represent the equivalent stochastic process

\[
\left(\kappa^2 - \frac{d^2}{dt^2}\right)^{1/2} z = b^{-1/2}\epsilon.
\]

These two stationary processes are equivalent in the sense that they have the same covariance function. Let \( M_0 = (\langle \phi_i, \phi_j \rangle)_{i,j} \), \( M_2 = (\langle \nabla \phi_i, \nabla \phi_j \rangle)_{i,j} \). Assuming Neumann boundary conditions and (35), the precision matrix is

\[
R = b(\kappa^2 M_0 + M_2),
\]

see [Lindgren et al. 2011] (Sec 2.3). This matrix does not represent a stationary process. However, it is quint-diagonal, and can be corrected to give a stationary GMRF by adding

\[
b\kappa \sqrt{1 + 0.25h^2\kappa^2} \approx b\kappa,
\]

to the first and the last entries of the matrix \( R \), per the previous lemma. Here, \( h \) is the step-size in the mesh, and we assume that \( h\kappa \) is small. Let \( M_1 \) be a matrix of zeroes, except the first and last elements which are \( 1/2 \). We then have a stationary GMRF representation of the OU process with precision matrix

\[
R = b(\kappa^2 M_0 + 2\kappa M_1 + M_2).
\]

**A.3.2 Spatial GMRF representation with boundary condition**

Let \( \Psi_s = \{\psi_1(s), ..., \psi_{N_s}(s)\} \) denote a set of piecewise linear spatial basis functions obtained by a triangulation of the spatial domain. Define the mass matrix \( C \) with elements \( C_{ij} = \langle \psi_i, \psi_j \rangle \) and the stiffness matrix \( G \) with elements \( G_{ij} = \langle \nabla \psi_i, \nabla \psi_j \rangle \). For integer values of \( \alpha \), we represent the precision operator \( L^\alpha \), with Neumann boundary conditions, as a GMRF with precision matrix

\[
Q_1(\gamma_s) = K_{\gamma_s} = \gamma_e^2[\gamma_s^2C + G] \\
Q_2(\gamma_s) = K_{\gamma_s} C^{-1} K_{\gamma_s} = \gamma_e^4[\gamma_s^2C + 2\gamma_s^2G + G(2)] \\
Q_\alpha(\gamma_s) = K_{\gamma_s} C^{-1} Q_{\alpha-2}(\gamma_s) C^{-1} K_{\gamma_s} \text{ for } \alpha = 3, 4, ..., 
\]

see [Lindgren et al. 2011] (Sec 2.3).
A.3.3 Derivation of equation \([29]\)

Define the semi-discrete solution \(\hat{u}(t) = \sum_{i=1}^{N_t} \phi_i(s)u_i(t)\), where the vector valued stochastic process \(u_i(t) = (u_1(t), \ldots, u_{N_s}(t))\) obtained by solving

\[
\left\{ \begin{array}{l}
\langle \psi_i, \left(\gamma_t \frac{d}{dt} + L^{\alpha_s/2}\right) u(.,t) \rangle \Omega \\
\end{array} \right\}, i = 1, \ldots, N_s
\]

\(\hat{u}(t) \Leftrightarrow \left\{ \langle \psi_i, \mathcal{E}\gamma_2 L_\alpha(.,t) \rangle \Omega, i = 1, \ldots, N_s \right\}. \quad (42)
\]

The right-hand side of this equation is a vector-valued white noise process \(\mathcal{E}_i(\cdot)\), with covariance measure \(\text{Cov}(\mathcal{E}_i(t_2) - \mathcal{E}_i(t_1), \mathcal{E}_j(t_2) - \mathcal{E}_j(t_1)) = |t_1 - t_2|CQ_{\alpha_s}^{-1}(\gamma_e, \gamma_s)C^T\) on any interval \([t_1, t_2]\). Now, assume that \(\alpha_t = 1\) and \(\alpha_s = 2\), so \(42\) gives

\[
C\gamma_t \frac{d}{dt} u(t) + \gamma_s^2 C u(t) + Gu(t) = C\mathcal{E}_{Q_1}. \quad (43)
\]

Define the eigenvector matrix \(V\) and the eigenvalue (diagonal) matrix \(\Lambda\) of solving the generalised eigenvalue problem \(G V = C V \Lambda\). Note that both \(G\) and \(C\) are symmetric positive definite, so we can assume that \(V^T C V = I\) in the generalised eigenvalue problem. Define \(u_i(t) = V z(t)\), to get

\[
C\gamma_t \frac{d}{dt} V z(t) + \gamma_s^2 V z(t) + C V \Lambda z(t) = C\mathcal{E}_{Q_1}. \quad (44)
\]

Next, we multiply by \(C^{-1} V^{-1}\) from the left to get

\[
\gamma_t \frac{d}{dt} z(t) + \gamma_s^2 z(t) + \Lambda z(t) = V^{-1} \mathcal{E}_{Q_1} \quad (45)
\]

where the precision matrix of \(V^{-1} \mathcal{E}_{Q_1}\) is \(Q_s\). For a fixed \(t\),

\[
\gamma_e^{-2} Q_s = \gamma_s^2 V^T C V + V^T G V = \gamma_s^2 I + V^T C V \Lambda = \gamma_s^2 I + \Lambda, \quad (46)
\]

which is a diagonal matrix, where we index the diagonal elements as \(a_j = (\gamma_s^2 + \lambda_j)\). This leads to independent stationary OU processes

\[
\frac{d}{dt} z_j(t) + \frac{\gamma_s^2}{\gamma_t} z_j(t) + \frac{\lambda_j}{\gamma_t} z_j(t) = \gamma_t^{-1} a_j^{-1/2} \epsilon_j \quad (47)
\]

where \(\epsilon_j\) are independent white noise processes. Using \(38\) with \(\kappa = (\gamma_s^2 + \lambda_j)/\gamma_t\),

\[
\gamma_e^{-2} Q_{z_j} = (\gamma_s^2 + \lambda_j)^2 M_0 + 2\gamma_t (\gamma_s^2 + \lambda_j)^2 + \gamma_s^2 (\gamma_s^2 + \lambda_j)^2 M_2. \quad (48)
\]

Because the processes are independent, we get the precision matrix for the space-time coefficient vector \(z\),

\[
\gamma_e^{-2} Q_z = M_0 \otimes (\gamma_s^2 I + \Lambda)^2 + 2\gamma_t M_1 \otimes (\gamma_s^2 I + \Lambda)^2 + \gamma_t^2 M_2 \otimes (\gamma_s^2 I + \Lambda). \quad (49)
\]

Transforming back to \(u = V z\) we get precision matrix

\[
\gamma_e^{-2} Q_u = M_0 \otimes V^{-T}(\gamma_s^2 I + \Lambda)^2 V^{-1} + 2\gamma_t M_1 \otimes V^{-T}(\gamma_s^2 I + \Lambda)^2 V^{-1} \quad (50)
\]

\[
+ \gamma_t^2 M_2 \otimes V^{-T}(\gamma_s^2 I + \Lambda)V^{-1} \quad (51)
\]

for the vector of space-time coefficients \((u_{i,j})_{i,j}\). We use that

\[
V^{-1} C^{-1} G = \Lambda V^{-1}
\]

and thus

\[
V^{-1}(\gamma_s^2 I + C^{-1} G) = (\gamma_s^2 I + \Lambda)V^{-1} \quad (52)
\]
repeatedly, and get

$$\gamma_e^{-2} Q_u = \gamma_e^2 [M_0 \otimes V^{-\top} V^{-1}(\gamma_s^2 I + C^{-1} G)^3 + 2\gamma_t M_1 \otimes V^{-\top} V^{-1}(\gamma_s^2 I + C^{-1} G)^2$$

$$+ \gamma_l^2 M_2 \otimes V^{-\top} V^{-1}(\gamma_s^2 I + C^{-1} G)].$$

Finally,

$$\gamma_e^{-2} Q_u = M_0 \otimes C(\gamma_s^2 I + C^{-1} G)^3 + 2\gamma_t M_1 \otimes C(\gamma_s^2 I + C^{-1} G)^2 + \gamma_l^2 M_2 \otimes C(\gamma_s^2 I + C^{-1} G).$$

This can be re-written as

$$\gamma_e^{-2} Q_u = M_0 \otimes Q_3(\gamma_s) + 2\gamma_t M_1 \otimes Q_2(\gamma_s) + \gamma_l^2 M_2 \otimes Q_1(\gamma_s)).$$