

Nested covariance functions on graphs with Euclidean edges cross time*

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Abstract: Covariance functions over generalized networks have been explored to a very limited extent. We consider nested spatial or space-time covariance models, where *space* is a generalized network, and where *time* can be linear (the real line) or circular. We show sufficient conditions allowing preservation of positive semidefiniteness when at least one of the weights involved in the linear combination is negative. Several examples illustrate our findings. In particular, we show nested constructions for Euclidean trees with a finite number of leaves involving basic covariance functions with different scale parameters or different compact supports. We also provide criteria that allow one to build space-time models through half spectral modeling on graphs cross linear or circular time.

Keywords and phrases: Covariance functions, Euclidean trees, generalized networks, graphs with Euclidean edges, circular time, linear time.

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1. Introduction

1.1. Context

This paper deals with the design of covariance functions associated with random fields with index set a generalized (or a linear) network, as well as generalized networks cross time, where time is either the real line or the circle. Defining covariance functions over a linear or a generalized network is a nontrivial task. The *tour de force* by Anderes et al. (2020) provides sufficient conditions for candidate functions, defined on the positive real line, that can be composed with special metrics, to be positive semidefinite (hence, valid covariance functions) over these spaces. Related works in this direction can be found in Monestiez et al. (2005); Bailly et al. (2006); de Fouquet and Bernard-Michel (2006); Ver Hoef et al. (2006) and Peterson et al. (2007).

1.2. Quasi-metric, semi-metric and metric spaces

Generalized network as in Anderes et al. (2020) are actually a special case of quasi-metric spaces (Menegatto et al., 2020). A quasi-metric space is a pair (X, σ) where X is a nonempty set and σ is a quasi-distance, that is, a function $\sigma : X \times X \rightarrow [0, \infty)$ satisfying $\sigma(x, x') = \sigma(x', x)$ and $\sigma(x, x) = 0$ for $x, x' \in X$. The quasi-metric space becomes semi-metric if, additionally, σ satisfies the triangle inequality. If $\sigma(x, x')$ is strictly positive when $x \neq x'$, then X is a metric space. We denote D_X^σ the diameter set of X , that is

$$D_X^\sigma = \{\sigma(x, x'), x, x' \in X\}.$$

Normed spaces and inner product spaces are typical examples of quasi-metric spaces with quasi-distance given by $\sigma(x, x') = \|x - x'\|$, $x, x' \in X$, with $\|\cdot\|$ denoting the related norm.

1.3. Linear graphs, graphs with Euclidean edges, and Euclidean trees

A network (or equivalently, a graph), \mathcal{G} , is a pair $(\mathcal{V}, \mathcal{E})$, where \mathcal{V} is a collection of nodes (called vertices in graph theory) and \mathcal{E} denotes a collection of edges. \mathcal{G} is planar if it can be drawn on the plane in such a way that different edges only possibly intersect with each other at one of their vertices, *i.e.*, there is no edge crossing. It is linear if, in addition, the edges are line segments.

Anderes et al. (2020) propose graphs with Euclidean edges as a generalization of linear networks. That is, they consider graphs where each edge is associated with an abstract set that is in bijective correspondence with a segment of the real line. This allows one to associate each edge with a Cartesian coordinate system to measure distances between any two points located over the edge. Specifically, a graph with Euclidean edges is a triple $(\mathcal{G}, \mathcal{V}, \{\varphi_e\}_{e \in \mathcal{E}})$ such that:

- a. $(\mathcal{V}, \mathcal{E})$ is a finite simple connected graph, meaning that the vertex set \mathcal{V} is finite, the graph has no repeated edges or edge which joins a vertex to itself, and every pair of vertices is connected by a path.
- b. Each edge $e \in \mathcal{E}$ is associated with an abstract set, denoted with the same symbol e , where the vertex set \mathcal{V} and all the edge sets $e \in \mathcal{E}$ are mutually disjoint.
- c. For each edge $e \in \mathcal{E}$ and every pair of vertices $(u, v) \in \mathcal{V} \times \mathcal{V}$ that is connected by e , the mapping φ_e is a bijection that applies to e, u and v as follows: φ_e maps e into an open interval $(\underline{e}, \bar{e}) \subset \mathbb{R}$, and φ_e maps $\{u, v\}$ into $\{\underline{e}, \bar{e}\}$.
- d. Denote with $d_G(u, v) : \mathcal{V} \times \mathcal{V} \rightarrow [0, \infty)$ the standard shortest-path weighted graph metric on the vertices of $(\mathcal{V}, \mathcal{E})$ with edge weights given by $\bar{e} - \underline{e}$ for every $e \in \mathcal{E}$. Then, $d_G(u, v) = \bar{e} - \underline{e}$ for all $u, v \in \mathcal{V}$ and for each $e \in \mathcal{E}$.

The graph \mathcal{G} endowed with a quasi-distance becomes a quasi-metric space. Anderes et al. (2020) propose two alternative metrics. The geodesic distance, d_G , is the shortest path merging any pair of points over \mathcal{G} . The resistance metric, d_R , is defined as the variance of the increments – *i.e.*, a variogram – of a special class of random processes (see Anderes et al., 2020, for a detailed *essay*). Depending on the characteristics of the graph \mathcal{G} , one metric might be used or not to build positive definite functions. When the metrics d_R and d_G can be equivalently used, we use the notation d_* ; this notation slightly deviates from that of Anderes et al. (2020) and Tang and Zimmerman (2020).

Finally, we call Euclidean tree any tree-like graph (which is planar). Vertices of a Euclidean tree that are connected to one edge only are called leaves.

Figure 1 provides some examples of a linear graph, graphs with Euclidean edges and a Euclidean tree. Other illustrations can be found in Anderes et al. (2020) as well as in Tang and Zimmerman (2020). As noted in Tang and Zimmerman (2020), an arbitrary point x belongs to \mathcal{G} when $x \in \mathcal{V} \cup \bigcup_{e \in \mathcal{E}} e$. As in their paper, we assume that the topological structure of \mathcal{G} does not evolve over time.

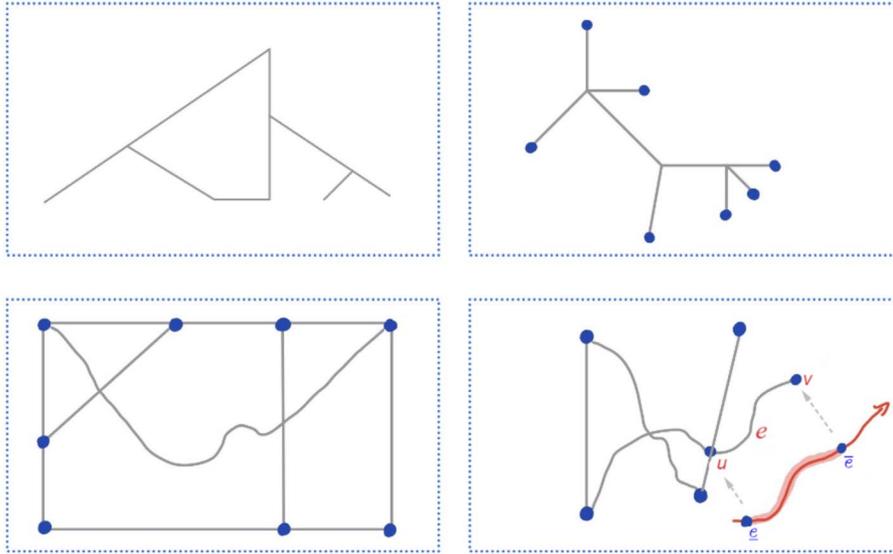


FIG 1. Up-Left: an example of linear network; Up-Right: A Euclidean tree with 7 leaves (blue dots), which may represent a stream network; Bottom-Left: A graph with Euclidean edges that may represent a road traffic network; crosses between edges with no vertices represent bridges or tunnels. Bottom-Right: another graph with Euclidean edges; the bijection mapping the vertices u and v into \underline{e} and \bar{e} and the edge e into the open interval (\underline{e}, \bar{e}) gives an Euclidean system with orientation and a way to measure distances.

1.4. Nested covariance models

Nested covariance models are linear combinations of basic covariance functions. They have an old history that can be traced back to geostatistics (Matheron, 1971; Journel and Huijbregts, 1978; Wackernagel, 2003; Gregori et al., 2008; Chilès and Delfiner, 2012).

Since covariance functions form a convex cone that is closed under elementary algebraic operations, a linear combination of covariance functions results in a new covariance function, provided the weights are all nonnegative. As discussed by Gregori et al. (2008), restricting all the weights to be nonnegative can represent a serious limitation. A constructive criticism about this fact is provided by Peron et al. (2018): admissible nested models with negative weights have important consequences to several branches of applied sciences. Discussion on the importance of negative weights in nested models stems from turbulence theory (Yakhot et al., 1989), but also classical statistical inference (Bonat and Jørgensen, 2016), where some nontrivial extensions of GLM to multivariate covariance functions require at least one weight in the linear combination to be negative. The idea of modeling a function of the covariance matrix by a linear structure goes back to Pourahmadi (1999, 2011) and Pan and Mackenzie (2003), among others (see Bonat and Jørgensen, 2016, for a thorough review).

A third consequence of nested models with only nonnegative weights is their implications in terms of statistical inference and testing, since, for instance, the *zero-value* for a specific weight lies on the boundary of the parameter space. Some criticism about this fact is expressed in Bevilacqua et al. (2012).

Nested covariance models have been already proposed over planar surfaces (Gregori et al., 2008) and over spheres (Peron et al., 2018). Covariance functions over generalized network are recent, and apparently the literature has not devoted attention to the problem of nested covariance models for these spaces, or over generalized networks cross time.

1.5. State of the art. Our contribution

Spatial and space-time nested covariance models have already received attention for simple examples of quasi-metric spaces. For $(X, \sigma) = (\mathbb{R}^n, \|\cdot\|^2)$, with n a positive integer and $\|\cdot\|$ denoting the Euclidean norm, and for $(Y, \sigma) = (\mathbb{R}, |\cdot|)$, the problem of covariance models over the product space $X \times Y$ has been addressed by Gregori et al. (2008) and Mateu et al. (2008). For $(X, \sigma) = (\mathbb{S}^n, \theta)$, with \mathbb{S}^n denoting the unit radius n -dimensional sphere embedded in \mathbb{R}^{n+1} , and θ the geodesic distance on the sphere, and for $(Y, \sigma') = (\mathbb{R}, |\cdot|)$, the problem has been tackled by Peron et al. (2018). For all these contributions, the solution to the problem is based on Fourier inversion and on spectral representations of the covariance functions over their related spaces.

This paper considers the following cases:

- a.** $(X, \sigma) = (\mathcal{G}, d_*)$, with \mathcal{G} either a graph with Euclidean edges, or a Euclidean tree with a given number of leaves;
- b.** $(X, \sigma) = (\mathcal{G}, d_*)$ as in **a.** above, and $(Y, \sigma) = (\mathbb{R}, |\cdot|)$, or $(Y, \sigma') = (\mathbb{S}^1, \theta)$.

What makes problems **a.** and **b.** challenging is that no spectral representation is available for covariance functions over generalized networks (Anderes et al., 2020). Hence, different mathematical techniques are needed in comparison with earlier contributions in the literature.

The outline of the paper is as follows. Section 2 provides background material. Section 3 challenges spatial nested models where the space is either a graph with Euclidean edges or a Euclidean tree with a finite number of leaves. The generalization of this approach to space-time models is then provided in Section 4. Conclusions follow in Section 5, while technical proofs are deferred to Appendix 5 to avoid mathematical burden.

2. Background material

2.1. Covariance functions over quasi-metric spaces

We consider a real-valued random field $\{Z(x, y) : (x, y) \in X \times Y\}$, where (X, σ) and (Y, σ') are quasi-metric spaces. In particular, we shall consider two cases: $(Y, \sigma') = (\mathbb{R}, |\cdot|)$ or $(Y, \sigma') = (\mathbb{S}^1, \theta)$, where θ is the geodesic distance over the

circle. Throughout the paper, we shall specify whether (X, σ) is equal to (\mathcal{G}, d_G) or (\mathcal{G}, d_R) , where d_G and d_R have been previously defined.

The choice of the metric is crucial to determine valid covariance functions as explained below. When the reference space Y is the unit sphere \mathbb{S}^n embedded in \mathbb{R}^{n+1} , then \mathbb{S}^n equipped with the geodesic distance θ is a quasi-metric space as well. In this case, we can express the geodesic distance θ as the arccosine of the dot product between any pair of points located over the sphere.

We suppose Z to be real-valued, weakly stationary, with zero mean and with covariance function that is pairwise isotropic. That is,

$$\mathbb{E}(Z(x, y)Z(x', y')) = K(\sigma(x, x'), \sigma'(y, y')), \quad (x, y), (x', y') \in X \times Y, \quad (2.1)$$

where the mapping K is defined over $D_X^\sigma \times D_Y^{\sigma'}$ and is real-valued. The mapping $K(\sigma, \sigma')$ is positive semidefinite over $X \times Y$, *i.e.*:

$$\sum_{k=1}^{\ell} \sum_{h=1}^{\ell} a_k K(\sigma(x_k, x_h), \sigma'(y_k, y_h)) a_h \geq 0,$$

for all finite system $\{a_k\}_{k=1}^{\ell} \subset \mathbb{R}$ and points $\{(x_k, y_k)\}_{k=1}^{\ell} \subset X \times Y$. Most of the literature on space-time covariance functions is concerned with $(X, \sigma) = (\mathbb{R}^n, \|\cdot\|)$, with $\|\cdot\|$ denoting the Euclidean distance, and $(Y, \sigma') = (\mathbb{R}, |\cdot|)$. In this case, $D_{\mathbb{R}^n}^{\|\cdot\|} = [0, \infty)$. A thorough account for this setting is provided in the review by Porcu et al. (2021).

More recent literature considers space, X , as the unit sphere \mathbb{S}^n embedded in \mathbb{R}^{n+1} , with the quasi metric $\sigma(x, x') = \theta(x, x')$ and θ denoting the geodesic distance on the sphere. In this case, $D_{\mathbb{S}^n}^\theta = [0, \pi]$. The reader is referred to Porcu et al. (2016), Berg and Porcu (2017) and Porcu et al. (2021), with the references therein. Porcu et al. (2016) consider the case $(X, \sigma) = (\mathbb{S}^n, \theta)$ and $(Y, \sigma') = (\mathbb{S}^1, \theta)$, so that time is treated as circular.

It is useful to note that, if $K(\sigma, \sigma')$ is a pairwise isotropic covariance for the product space $X \times Y$ then the functions $K(\sigma(\cdot, \cdot), 0)$ and $K(0, \sigma'(\cdot, \cdot))$ are isotropic covariance functions on $X \times X$ and $Y \times Y$, respectively.

Remark 1. Throughout, we shall equivalently use the following notation: either we say that $K(\sigma, \sigma')$ is positive semidefinite over the product space $X \times Y$, where (X, σ) and (Y, σ') are quasi-metric spaces, or we shall use the notation $K(\sigma(\cdot, \cdot), \sigma'(\cdot, \cdot))$ is positive semidefinite over $(X \times Y) \times (X \times Y)$.

2.2. Auxiliary background material

A function $f : [0, \infty) \rightarrow \mathbb{R}$ is completely monotonic if $f(0) > 0$, f is infinitely differentiable over $(0, \infty)$ and $(-1)^m f^{(m)}(x) \geq 0$ for $x \geq 0$ and for all $m \in \mathbb{N}$. Here, $f^{(m)}$ denotes the m th derivative of f , and we use the abuse of notation $f^{(0)}$ for f . By Bernstein's theorem (Bernstein, 1929), f is completely monotonic if and only if

$$f(t) = \int_{[0, \infty)} e^{-\xi t} \mu(d\xi), \quad t \geq 0, \quad (2.2)$$

where μ is a positive and bounded measure.

Let m be a fixed positive integer. We consider the class of continuous mappings $f : [0, \infty) \rightarrow \mathbb{R}$ such that $f(0) = 1$ and such that f can be uniquely written as

$$f(t) = \int_{[0, \infty)} \omega_m(\xi t) \mu(d\xi), \quad t \geq 0, \quad (2.3)$$

where μ is a positive and bounded measure, and where

$$\omega_m(t) = \frac{\Gamma(m/2)}{\Gamma((m-1)/2) \sqrt{\pi}} \int_1^\infty \Omega_m(\sqrt{vt}) v^{-m/2} (v-1)^{(m-3)/2} dv, \quad t \geq 0,$$

with $\Omega_m(t) = \Gamma(m/2) (2/t)^{(m-2)/2} J_{(m-2)/2}(t)$ and J_ν the Bessel function of the first kind of order ν .

Anderes et al. (2020) show that:

1. For a completely monotonic function $f : [0, \infty) \rightarrow \mathbb{R}$, the composition $f(d_R(\cdot, \cdot))$ is positive semidefinite on $\mathcal{G} \times \mathcal{G}$, with \mathcal{G} a graph with Euclidean edges, where d_R is the resistance metric.
2. If a function f admits the representation (2.3), then the mapping $(x, y) \mapsto f(d_*(x, y))$ is positive semidefinite over $\mathcal{G} \times \mathcal{G}$, for \mathcal{G} a Euclidean tree with $\lceil m/2 \rceil$ leaves, with $\lceil \cdot \rceil$ denoting the ceiling function.
3. A sufficient condition for a candidate function f to admit the scale mixture representation (2.3) is that $f^{(2\lceil m/2 \rceil - 2)}$ is convex on the positive real line, with $\lim_{t \rightarrow \infty} f(t) = 0$.

Remark 2. Let $f : [0, \infty) \rightarrow \mathbb{R}$. To build a function $f(\sigma(\cdot, \cdot))$, we should use the notation $f_{D_X^\sigma}$ to denote the restriction of f to D_X^σ . Furthermore, such a function is positive semidefinite on $X \times X$ if $K(\sigma, 0) := f(\sigma)$ is positive semidefinite on X . Throughout, such a notation will not be adopted unless it becomes necessary from the context.

3. Nested models over the space \mathcal{G}

We explain our strategy and will then specialize for the cases where \mathcal{G} is either a graph with Euclidean edges, or a Euclidean tree with a given number of leaves. Let φ_k , $k = 1, \dots, N$, be a collection of continuous functions, defined on the positive real line, such that the function $(x, x') \mapsto \varphi_k(\sigma(x, x'))$ is positive semidefinite over the quasi-metric space $X \times X$ with quasi-metric σ , for $k = 1, \dots, N$. Define the mapping $\varphi : [0, \infty) \rightarrow \mathbb{R}$ through the identity

$$\varphi(t) = \sum_{k=1}^N c_k \varphi_k(t), \quad t \geq 0, \quad (3.1)$$

where c_1, \dots, c_N is a finite collection of real constants. We are going to provide conditions on the constant c_N , assuming that c_1, \dots, c_{N-1} are fixed and non-negative, such that the function $\varphi(d_*(\cdot, \cdot))$ is positive semidefinite over $\mathcal{G} \times \mathcal{G}$, with \mathcal{G} a graph with Euclidean edges, \mathcal{G} , or over a Euclidean tree with a given number of leaves.

3.1. Graphs with Euclidean edges

For this case, we start by invoking Theorem 1 in Anderes et al. (2020): if φ_k is completely monotonic on the positive real line with $\varphi_k(0) < \infty$, then the function $\varphi_k(d_R(\cdot, \cdot))$ is positive semidefinite over $\mathcal{G} \times \mathcal{G}$. Hence, a direct application of Equation (2.2) in concert with (3.1) provides the identity

$$\varphi(t) = \int_0^\infty e^{-\xi t} \mu(d\xi), \quad t \geq 0,$$

where $\mu(d\xi) := \sum_k c_k \mu_k(d\xi)$ and μ_k is the measure associated with φ_k as per (2.2). Accordingly, the problem is to find the range for c_1, \dots, c_N such that μ is positive and bounded. Obviously, this is always true when $c_k \geq 0$ for all $k = 1, \dots, N$. For what follows, we always assume $c_k \geq 0$ for $k = 1, \dots, N - 1$, and evaluate a (hopefully negative) lower bound for c_N such that φ provides a positive semidefinite function.

Some examples of completely monotonic functions follow.

a. The **Matérn family**. The Matérn function, \mathcal{M}_ν , is defined as (Matérn, 1986)

$$\mathcal{M}_\nu(t) = \frac{2^{1-\nu}}{\Gamma(\nu)} t^\nu \mathcal{K}_\nu(t), \quad t \geq 0, \tag{3.2}$$

where \mathcal{K}_ν is a modified Bessel function of the second kind. $\mathcal{M}_\nu(\cdot)$ is completely monotonic for $0 < \nu \leq \frac{1}{2}$, and $\mathcal{M}_\nu(\sqrt{\cdot})$ is completely monotonic for any positive ν .

b. The **Cauchy family**. Another useful example comes by considering the function

$$\mathcal{C}_\beta(t) = (1 + t)^{-\beta}, \quad t \geq 0,$$

which is completely monotonic for $\beta > 0$.

Below we provide sufficient conditions for the model (3.1) to be positive semidefinite over graphs with Euclidean edges when the functions φ_k belong to either the Matérn or Cauchy families.

Theorem 3. *Let \mathcal{G} be a graph with Euclidean edges. Let φ be as in Equation (3.1) with $\varphi_k(\cdot) = \mathcal{M}_{\nu_k}(\sqrt{\cdot}/\sqrt{b_k})$, $k = 1, \dots, N$, $\nu_k > 0$ and $b_k > 0$. If $c_1, \dots, c_{N-1} \geq 0$ and*

$$c_N \geq - \sum_{k \in A_1} c_k \left(\frac{b_N}{b_k}\right)^{\nu_N} - \sum_{k \in A_2} c_k \frac{\Gamma(\nu_N)}{\Gamma(\nu_k)} \frac{(4b_N)^{\nu_N}}{(4b_k)^{\nu_k}} \left(\frac{e\left(\frac{1}{b_N} - \frac{1}{b_k}\right)}{4(\nu_N - \nu_k)}\right)^{\nu_N - \nu_k}, \tag{3.3}$$

with e standing for Euler’s number, $A_1 = \{k \in \{1, \dots, N - 1\} : \nu_k = \nu_N \text{ and } b_k \geq b_N\}$ and $A_2 = \{k \in \{1, \dots, N - 1\} : \nu_k < \nu_N \text{ and } b_k > b_N\}$, then $\varphi(d_R(\cdot, \cdot))$ is positive semidefinite over $\mathcal{G} \times \mathcal{G}$.

A direct application of Theorem 3 shows the following. The upper bound of the weight c can largely exceed 1, as shown in Figure 2 for a few particular cases.

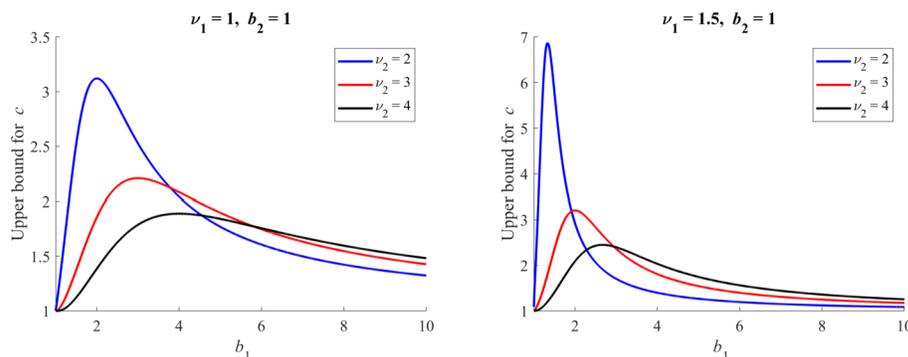


FIG 2. Upper bound for c as a function of b_1 , for $\nu_1 = 1$ (left) or $\nu_1 = 1.5$ (right), $b_2 = 1$ and $\nu_2 = 2, 3$ and 4 .

Corollary 4. Let \mathcal{G} be a graph with Euclidean edges. Let φ be as in Equation (3.1) with $N = 2$, $c_1 := c \geq 0$ and $c_2 = 1 - c$, $\varphi_k(\cdot) = \mathcal{M}_{\nu_k}(\sqrt{\cdot}/\sqrt{b_k})$, $k = 1, 2$, $\nu_k > 0$ and $b_k > 0$. If

$$c \leq \left(1 - \left(\frac{b_2}{b_1} \right)^{\nu_2} \mathbb{I}_{A_1} - \frac{\Gamma(\nu_2) (4b_2)^{\nu_2}}{\Gamma(\nu_1) (4b_1)^{\nu_1}} \left(\frac{e \left(\frac{1}{b_2} - \frac{1}{b_1} \right)}{4(\nu_2 - \nu_1)} \right)^{\nu_2 - \nu_1} \mathbb{I}_{A_2} \right)^{-1},$$

where \mathbb{I}_A is the indicator function of the set A , and A_1 and A_2 are defined as in Theorem 3, then $\varphi(d_R(\cdot, \cdot))$ is positive semidefinite over $\mathcal{G} \times \mathcal{G}$.

Theorem 5. Let \mathcal{G} be a graph with Euclidean edges. Let φ be as in Equation (3.1) with $\varphi_k(\cdot) = \mathcal{C}_{\beta_k}(\cdot/b_k)$, $k = 1, \dots, N$, $\beta_k > 0$ and $b_k > 0$. If $c_1, \dots, c_{N-1} \geq 0$ and

$$c_N \geq - \sum_{k \in A_1} c_k \left(\frac{b_k}{b_N} \right)^{\beta_N} - \sum_{k \in A_2} c_k \frac{b_k^{\beta_k}}{b_N^{\beta_N}} \frac{\Gamma(\beta_N)}{\Gamma(\beta_k)} \left(\frac{\beta_k - \beta_N}{e(b_k - b_N)} \right)^{\beta_k - \beta_N}, \quad (3.4)$$

with $A_1 = \{k \in \{1, \dots, N-1\} : \beta_k = \beta_N \text{ and } b_k \leq b_N\}$ and $A_2 = \{k \in \{1, \dots, N-1\} : \beta_k < \beta_N \text{ and } b_k < b_N\}$, then $\varphi(d_R(\cdot, \cdot))$ is positive semidefinite over $\mathcal{G} \times \mathcal{G}$.

The following come as a direct application of Theorem 5, the proof of which is omitted. Figure 3 provides some examples of upper bounds for the weight c .

Corollary 6. Let \mathcal{G} be a graph with Euclidean edges. Let φ be as in Equation (3.1) with $N = 2$, $c_1 := c \geq 0$ and $c_2 = 1 - c$, with $\varphi_k(\cdot) = \mathcal{C}_{\beta_k}(\cdot/b_k)$, $k = 1, \dots, N$, $\beta_k > 0$ and $b_k > 0$. If

$$c \leq \left(1 - \left(\frac{b_1}{b_2} \right)^{\beta_2} \mathbb{I}_{A_1} - \frac{b_1^{\beta_1}}{b_2^{\beta_2}} \frac{\Gamma(\beta_2)}{\Gamma(\beta_1)} \left(\frac{\beta_1 - \beta_2}{e(b_1 - b_2)} \right)^{\beta_1 - \beta_2} \mathbb{I}_{A_2} \right)^{-1},$$

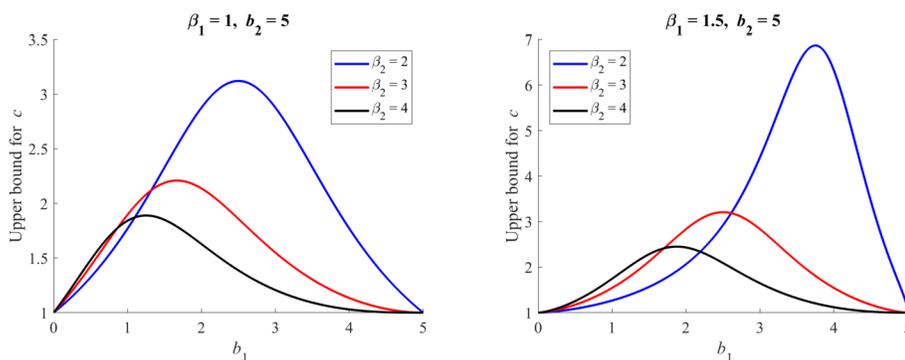


FIG 3. Upper bound for c as a function of b_1 , for $\beta_1 = 1$ (left) or $\beta_1 = 1.5$ (right), $b_2 = 5$ and $\beta_2 = 2, 3$ and 4 .

with A_1 and A_2 as in Theorem 5, then $\varphi(d_R(\cdot, \cdot))$ is positive semidefinite over $\mathcal{G} \times \mathcal{G}$.

3.2. Euclidean trees

Below we describe a class of functions that turns out to be useful for our purposes.

The **Askey family** of functions (Askey, 1973) is defined by

$$\psi_\nu(t) := (1 - t)_+^\nu, \quad \nu > 0, \tag{3.5}$$

The function $\psi_\nu(\|\cdot\|/b)$ is compactly supported over a ball of \mathbb{R}^n , with radius $b > 0$.

Arguments in Zastavnyi (2002) show that ψ_ν admits the integral representation (2.3) for a given positive integer m , provided $\nu \geq 2m - 1$. We can now state our next result.

Theorem 7. *Let \mathcal{G} be a Euclidean tree with $\lceil m/2 \rceil$ leaves, $m \geq 3$. Let φ be the class of functions defined through Equation (3.1), with $\varphi_k(\cdot) = \psi_{\nu+m_k+1}(\cdot/b_k)$, $b_k > 0$, $m_k > 0$ and $\nu \geq 2m - 1$. If $c_1, \dots, c_{N-1} \geq 0$, then $\varphi(d_*(\cdot, \cdot))$ is positive semidefinite over $\mathcal{G} \times \mathcal{G}$ provided*

$$c_N \geq - \sum_{k \in A_1} c_k \frac{b_N^{\nu+1} B(\nu+1, m_N+1)}{b_k^{\nu+1} B(\nu+1, m_k+1)} - \sum_{k \in A_2} c_k \frac{b_N^{\nu+1+m_N} B(\nu+1, m_N+1)}{b_k^{\nu+1+m_k} B(\nu+1, m_k+1)} \frac{m_k^{m_k}}{m_N^{m_N}} \left(\frac{b_k - b_N}{m_k - m_N} \right)^{m_k - m_N}, \tag{3.6}$$

where B denotes the beta function, $A_1 = \{k \in \{1, \dots, N-1\} : b_k \geq b_N \text{ and } m_k \leq m_N\}$ and $A_2 = \{k \in \{1, \dots, N-1\} : b_k > b_N \text{ and } m_k > m_N\}$.

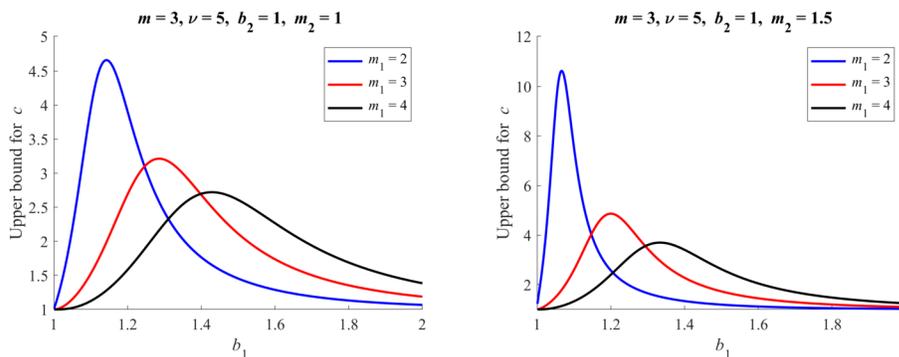


FIG 4. Upper bound for c as a function of b_1 , for $m = 3$, $\nu = 5$, $b_2 = 1$, $m_2 = 1$, (left) or $m_2 = 1.5$ (right), and $m_1 = 2, 3$ or 4 .

In the same spirit of Theorems 3 and 5, the following is provided as a direct inspection from Theorem 7. The upper bound for the weight c can be much greater than 1, as illustrated in Figure 4 for two particular cases.

Corollary 8. Let \mathcal{G} be a Euclidean tree with $\lceil m/2 \rceil$ leaves, $m \geq 3$. Let φ be as in Equation (3.1) with $N = 2$, $c_1 := c \geq 0$ and $c_2 = 1 - c$, with $\varphi_k(\cdot) = \psi_{\nu+m_k+1}(\cdot/b_k)$, $b_k > 0$, $m_k > 0$ and $\nu \geq 2m - 1$. If

$$c \leq \left(1 - \frac{b_2^{\nu+1} B(\nu+1, m_2+1)}{b_1^{\nu+1} B(\nu+1, m_1+1)} \mathbb{I}_{A_1} - \frac{b_2^{\nu+1+m_2} B(\nu+1, m_2+1) m_1^{m_1}}{b_1^{\nu+1+m_1} B(\nu+1, m_1+1) m_2^{m_2}} \left(\frac{b_1 - b_2}{m_1 - m_2} \right)^{m_1 - m_2} \mathbb{I}_{A_2} \right)^{-1},$$

with A_1 and A_2 as in Theorem 7, then $\varphi(d_*(\cdot, \cdot))$ is positive semidefinite over $\mathcal{G} \times \mathcal{G}$.

Another promising avenue is provided by the following theorem.

Theorem 9. Let \mathcal{G} be a Euclidean tree with $\lceil m/2 \rceil$ leaves, $m \geq 3$. Let φ be the class of functions defined through Equation (3.1), with $\varphi_k(\cdot)$ such that the mapping $\vartheta_k(t) := \varphi_k^{(2\lceil m/2 \rceil - 2)}(t)$ is convex on the positive real line, with $\lim_{t \rightarrow \infty} \vartheta_k(t) = 0$ and $\vartheta_N^{(i)}$ being nonzero for $i = 1, 2$. Then, $\varphi(d_*(\cdot, \cdot))$ is positive semidefinite over $\mathcal{G} \times \mathcal{G}$ provided c_1, \dots, c_{N-1} are nonnegative and

$$-\sum_{k=1}^{N-1} c_k \sup_{t \geq 0} \frac{\vartheta_k^{(2)}(t)}{\vartheta_N^{(2)}(t)} \leq c_N \leq -\sum_{k=1}^{N-1} c_k \inf_{t \geq 0} \frac{\vartheta_k^{(1)}(t)}{\vartheta_N^{(1)}(t)}.$$

4. Nested models over the space \mathcal{G} cross linear or circular time

We start by explaining the general strategy, and then provide case-by-case solutions depending on the quasi-metric spaces involved in the calculations.

Let $\varphi_k, f_k, k = 1, \dots, N$, be two collections of continuous functions defined on the positive real line, such that the functions $(x, x') \mapsto \varphi_k(\sigma(x, x'))$ and $(y, y') \mapsto f_k(\sigma'(y, y'))$ are, respectively, positive semidefinite over $X \times X$ and over $Y \times Y$, where (X, σ) and (Y, σ') are quasi-metric spaces, for $k = 1, \dots, N$. We let

$$\Psi(t, u) = \sum_{k=1}^N c_k \varphi_k(t) f_k(u), \quad t, u \geq 0, \tag{4.1}$$

where c_1, \dots, c_N is a finite collection of real constants. Finding conditions for $\Psi(\sigma, \sigma')$ to be positive semidefinite on $X \times Y$ is not an obvious task.

Below we provide spectral representations for the case when (Y, σ') is either $(\mathbb{R}, |\cdot|)$ or (\mathbb{S}^1, θ) . These will turn to be useful for the subsequent findings.

Theorem 10. *Let $(X, \sigma) = (\mathcal{G}, d_*)$, with \mathcal{G} a graph with Euclidean edges.*

- A. *Let $(Y, \sigma') = (\mathbb{R}, |\cdot|)$ and $\Psi : D_{\mathcal{G}}^{d_*} \times [0, \infty) \rightarrow \mathbb{R}$ be such that Ψ is continuous, bounded, and integrable. Then, $\Psi(d_*, |\cdot|)$ is positive semidefinite on $\mathcal{G} \times \mathbb{R}$ if and only if the mapping $\Psi_\tau(d_*)$, defined as*

$$\Psi_\tau(d_*) = \frac{1}{2\pi} \int_0^\infty \cos(\tau|u|) \Psi(d_*, |u|) du, \tag{4.2}$$

is positive semidefinite on \mathcal{G} for almost all $\tau \geq 0$ (w.r.t. Lebesgue measure).

- B. *Let $(Y, \sigma') = (\mathbb{S}^1, \theta)$ and $\Psi : D_{\mathcal{G}}^{d_*} \times [0, \pi] \rightarrow \mathbb{R}$ be such that Ψ is continuous and bounded. Then, $\Psi(d_*, \theta)$ is positive semidefinite on $\mathcal{G} \times \mathbb{S}^1$ if and only if*

$$\Psi(d_*, \theta) = \sum_{k=0}^\infty \Psi_k(d_*) \cos(k\theta), \tag{4.3}$$

where the sequence $\{\Psi_k(\cdot)\}_{k=0}^\infty$ of continuous functions Ψ_k is such that $\Psi_k(d_(\cdot, \cdot))$ is positive semidefinite over $\mathcal{G} \times \mathcal{G}$ for all $k = 0, 1, \dots$, and additionally $\sum_{k=0}^\infty \Psi_k(0) < \infty$.*

4.1. Graphs with Euclidean edges cross time

In this section, \mathcal{G} will be always a graph with Euclidean edges with metric d_R . We start from Equation (4.1) and call \hat{f}_k the Fourier transform of $f_k(|\cdot|)$, $k = 1, \dots, N$. We suppose $f_k(|\cdot|)$ to be absolutely integrable on the real line, so that \hat{f}_k is well defined. Additionally, we suppose \hat{f}_N to be strictly positive. Using point A. in Theorem 10 we find that $\Psi(d_R, |\cdot|)$ is positive semidefinite $\mathcal{G} \times \mathbb{R}$ if and only if the mapping Ψ_τ as in (4.2) is positive semidefinite on \mathcal{G} a.e. $\tau \geq 0$. We now assume φ_k to be completely monotonic on the positive real line, with associated measure μ_k as per (2.2). A direct inspection shows that

$$\Psi_\tau(t) = \int_0^\infty e^{-\xi t} \mu(d\xi; \tau), \quad t \geq 0,$$

where

$$\mu(d\xi; \tau) := \sum_{k=1}^N c_k \mu_k(d\xi) \hat{f}_k(\tau). \quad (4.4)$$

Clearly, μ is nonnegative and bounded if and only if

$$c_N \geq - \sum_{k=1}^{N-1} c_k \left(\inf_{\xi \geq 0} \frac{\mu_k(d\xi)}{\mu_N(d\xi)} \right) \left(\inf_{\tau \geq 0} \frac{\hat{f}_k(\tau)}{\hat{f}_N(\tau)} \right). \quad (4.5)$$

When $(Y, \sigma') = (\mathbb{S}^1, \theta)$ we invoke Schoenberg's theorem (Schoenberg, 1942) and write

$$f_k(\theta) = \sum_{h=0}^{\infty} \lambda_{h,k} \cos(h\theta),$$

where for every $k = 1, \dots, N$, the sequence $\{\lambda_{h,k}\}_{h=0}^{\infty}$ have nonnegative and summable coefficients. We can now resort to Theorem 10, part B., so that, after some algebra,

$$K(d_R, \theta) = \sum_{h=0}^{\infty} \cos(h\theta) K_h(d_R),$$

with

$$K_h(d_R) = \sum_{k=1}^N c_k \lambda_{h,k} \varphi_k(d_R).$$

To show that $K(d_R, \theta)$ is positive semidefinite on $\mathcal{G} \times \mathbb{S}^1$, we need to show that $\{K_h(d_R(\cdot, \cdot))\}_{h=0}^{\infty}$ is a sequence of positive semidefinite functions over $\mathcal{G} \times \mathcal{G}$ with the additional requirement that $\sum_{h=0}^{\infty} K_h(0) < \infty$. A direct inspection shows

$$K_h(d_R) = \int_0^{\infty} e^{-\xi d_R} \Delta_h(d\xi),$$

with

$$\Delta_h(d\xi) = \sum_{k=1}^N c_k \lambda_{h,k} \mu_k(d\xi),$$

and clearly verifying its positiveness amounts to similar conditions than those found in Section 3. A relevant comment is that each sequence $\{\lambda_{h,k}\}_{h=0}^{\infty}$ is a convergent sequence of nonnegative coefficients (Schoenberg, 1942), for $k = 1, \dots, N$. Further, the measures μ_k are finite. Hence, the series

$$\sum_{h=0}^{\infty} K_h(0) = \sum_{k=1}^N \left(c_k \mu_k(\mathbb{R}_+ \cup \{0\}) \sum_{h=0}^{\infty} \lambda_{h,k} \right)$$

is convergent.

Some examples follow. We state those formally for an easier reading.

Theorem 11. *Let \mathcal{G} be a graph with Euclidean edges.*

A. *Let Ψ be as in Equation (4.1) with $\varphi_k(\cdot) = \mathcal{M}_{\nu_k}(\sqrt{\cdot}/\sqrt{b_k})$, $k = 1, \dots, N$, $\nu_k > 0$ and $b_k > 0$. Let $f_k(\cdot) = \mathcal{M}_{\eta_k}(\cdot/a_k)$ with $a_k > 0$ and $\eta_k > 0$. If $c_1, \dots, c_{N-1} \geq 0$ and*

$$c_N \geq - \sum_{k \in A_1} c_k \left(\frac{b_N}{b_k} \right)^{\nu_N} \frac{\Gamma(\eta_k + \frac{1}{2})\Gamma(\eta_N)a_k}{\Gamma(\eta_k)\Gamma(\eta_N + \frac{1}{2})a_N} \kappa(a_k, a_N, \eta_k, \eta_N) - \sum_{k \in A_2} c_k \frac{\Gamma(\nu_N)}{\Gamma(\nu_k)} \frac{b_N^{\nu_N}}{b_k^{\nu_k}} \frac{\Gamma(\eta_k + \frac{1}{2})\Gamma(\eta_N)a_k}{\Gamma(\eta_k)\Gamma(\eta_N + \frac{1}{2})a_N} \kappa(a_k, a_N, \eta_k, \eta_N) \left(\frac{e}{\nu_N - \nu_k} - \frac{e}{b_N - b_k} \right)^{\nu_N - \nu_k}, \tag{4.6}$$

with $A_1 = \{k \in \{1, \dots, N-1\} : \nu_k = \nu_N, b_k \geq b_N \text{ and } \eta_N \geq \eta_k\}$, $A_2 = \{k \in \{1, \dots, N-1\} : \nu_k < \nu_N, b_k > b_N \text{ and } \eta_N \geq \eta_k\}$ and $\kappa(a_k, a_N, \eta_k, \eta_N)$ defined as

$$\kappa(a_k, a_N, \eta_k, \eta_N) = \begin{cases} 1 & \text{if } \frac{(1+2\eta_N)a_k^2}{(1+2\eta_k)a_N^2} \geq 1 \\ \left(\frac{a_k}{a_N}\right)^{2\eta_N+1} & \text{if } \frac{a_k}{a_N} < 1; \eta_k = \eta_N \\ \left(1 + \frac{\tau_0^2}{a_N^2}\right)^{\eta_N + \frac{1}{2}} \left(1 + \frac{\tau_0^2}{a_k^2}\right)^{-\eta_k - \frac{1}{2}} & \text{otherwise,} \end{cases} \tag{4.7}$$

then $\varphi(d_R(\cdot, \cdot), |\cdot|)$ is positive semidefinite over $\mathcal{G} \times \mathcal{G} \times \mathbb{R}$.

B. *Let Ψ be as in Equation (4.1) with $\varphi_k(\cdot) = \mathcal{C}_{\beta_k}(\cdot/b_k)$, $k = 1, \dots, N$, $\nu_k > 0$ and $b_k > 0$. Let $f_k(\cdot) = \mathcal{M}_{\eta_k}(\cdot/a_k)$ with $a_k > 0$ and $\eta_k > 0$. If $c_1, \dots, c_{N-1} \geq 0$ and*

$$c_N \geq - \sum_{k \in A_1} c_k \left(\frac{b_k}{b_N} \right)^{\beta_N} \frac{\Gamma(\eta_k + \frac{1}{2})\Gamma(\eta_N)a_k}{\Gamma(\eta_k)\Gamma(\eta_N + \frac{1}{2})a_N} \kappa(a_k, a_N, \eta_k, \eta_N) - \sum_{k \in A_2} c_k \frac{b_k^{\beta_k}\Gamma(\beta_N)\Gamma(\eta_k + \frac{1}{2})\Gamma(\eta_N)a_k}{b_N^{\beta_N}\Gamma(\beta_k)\Gamma(\eta_k)\Gamma(\eta_N + \frac{1}{2})a_N} \kappa(a_k, a_N, \eta_k, \eta_N) \left(\frac{\beta_k - \beta_N}{e(b_k - b_N)} \right)^{\beta_k - \beta_N}, \tag{4.8}$$

with $A_1 = \{k \in \{1, \dots, N-1\} : \beta_k = \beta_N, b_k \leq b_N \text{ and } \eta_N \geq \eta_k\}$, $A_2 = \{k \in \{1, \dots, N-1\} : \beta_k < \beta_N, b_k < b_N \text{ and } \eta_N \geq \eta_k\}$ and $\kappa(a_k, a_N, \eta_k, \eta_N)$ defined in (4.7), then $\varphi(d_R(\cdot, \cdot), \theta(\cdot, \cdot))$ is positive semidefinite over $(\mathcal{G} \times \mathbb{S}^1) \times (\mathcal{G} \times \mathbb{S}^1)$.

The following result is a direct consequence of Theorem 11.

Corollary 12. *Let \mathcal{G} be a graph with Euclidean edges.*

A. *Let Ψ be as in Equation (4.1) with $N = 2$, $c_1 := c \geq 0$ and $c_2 = 1 - c$, with $\varphi_k(\cdot) = \mathcal{M}_{\nu_k}(\sqrt{\cdot}/\sqrt{b_k})$, $k = 1, 2$, $\nu_k > 0$ and $b_k > 0$. Let $f_k(\cdot) = \mathcal{M}_{\eta_k}(\cdot/a_k)$*

with $a_k > 0$ and $\eta_k > 0$. If

$$c \leq \left(1 - \left(\frac{b_2}{b_1} \right)^{\nu_2} \frac{\Gamma(\eta_1 + \frac{1}{2})\Gamma(\eta_2)a_1}{\Gamma(\eta_1)\Gamma(\eta_2 + \frac{1}{2})a_2} \kappa(a_1, a_2, \eta_1, \eta_2) \mathbb{I}_{A_1} - \frac{\Gamma(\nu_2)}{\Gamma(\nu_1)} \frac{b_2^{\nu_2}}{b_1^{\nu_1}} \frac{\Gamma(\eta_1 + \frac{1}{2})\Gamma(\eta_2)a_1}{\Gamma(\eta_1)\Gamma(\eta_2 + \frac{1}{2})a_2} \kappa(a_1, a_2, \eta_1, \eta_2) \left(\frac{e \left(\frac{1}{b_2} - \frac{1}{b_1} \right)}{\nu_2 - \nu_1} \right)^{\nu_2 - \nu_1} \mathbb{I}_{A_2} \right)^{-1}, \quad (4.9)$$

where A_1 and A_2 are specified through A. in Theorem 11 and κ is the function defined at (4.7), then $\varphi(d_R(\cdot, \cdot), |\cdot|)$ is positive semidefinite over $\mathcal{G} \times \mathcal{G} \times \mathbb{R}$.

B. Let Ψ be as in Equation (4.1), with $N = 2$, $c_1 := c \geq 0$ and $c_2 = 1 - c$, with $\varphi_k(\cdot) = \mathcal{C}_{\beta_k}(\cdot/b_k)$, $k = 1, 2$, $\nu_k > 0$ and $b_k > 0$. Let $f_k(\cdot) = \mathcal{M}_{\eta_k}(\cdot/a_k)$ with $a_k > 0$ and $\eta_k > 0$. If

$$c \leq \left(1 - \left(\frac{b_1}{b_2} \right)^{\beta_2} \frac{\Gamma(\eta_1 + \frac{1}{2})\Gamma(\eta_2)a_1}{\Gamma(\eta_1)\Gamma(\eta_2 + \frac{1}{2})a_2} \kappa(a_1, a_2, \eta_1, \eta_2) \mathbb{I}_{A_1} - \frac{b_1^{\beta_1}}{b_2^{\beta_2}} \frac{\Gamma(\beta_2)}{\Gamma(\beta_1)} \frac{\Gamma(\eta_1 + \frac{1}{2})\Gamma(\eta_2)a_1}{\Gamma(\eta_1)\Gamma(\eta_2 + \frac{1}{2})a_2} \kappa(a_1, a_2, \eta_1, \eta_2) \left(\frac{\beta_1 - \beta_2}{e(b_1 - b_2)} \right)^{\beta_1 - \beta_2} \mathbb{I}_{A_2} \right)^{-1}, \quad (4.10)$$

with A_1 and A_2 as in B. of Theorem 11, and κ as defined in (4.7), then $\varphi(d_R(\cdot, \cdot), \theta(\cdot, \cdot))$ is positive semidefinite over $(\mathcal{G} \times \mathbb{S}^1) \times (\mathcal{G} \times \mathbb{S}^1)$.

4.2. Examples with circular time

Example 1. We consider the functions

$$\theta \mapsto f_k(\theta) = \frac{1}{a_k^2} (a_k - \theta)_+, \quad 0 < a_k \leq \pi,$$

for which we can directly compute the cosine expansion as

$$f_k(\theta) = \sum_{h=0}^{\infty} \lambda_{h,k} \cos(h\theta),$$

with $\lambda_{0,k} = 1/(2\pi)$ and

$$\lambda_{h,k} = \frac{2}{\pi} \frac{1 - \cos(ha_k)}{h^2 a_k^2}, \quad h = 1, \dots$$

To verify conditions for positive semidefiniteness of the model (4.1) under this setting, we need to check conditions on c_N , for $c_1, \dots, c_{N-1} \geq 0$, such that the measures

$$\Delta_0(d\xi) = \frac{1}{2\pi} \sum_{k=1}^N c_k \mu_k(d\xi), \quad \xi \geq 0$$

and

$$\Delta_h(d\xi) = \frac{2}{\pi} \sum_{k=1}^N c_k \frac{1 - \cos(ha_k)}{h^2 a_k^2} \mu_k(d\xi), \quad \xi \geq 0, \quad h = 1, 2, \dots$$

are nonnegative. Here, μ_k are the measures associated with the completely monotonic functions φ_k . The nonnegativeness of Δ_h for $h > 0$ is automatically fulfilled if a_N is a multiple of 2π , in which case one only has to ensure the nonnegativeness of Δ_0 ; this leads to

$$c_N \geq - \sum_{k=1}^{N-1} c_k \left(\inf_{\xi \geq 0} \frac{\mu_k(d\xi)}{\mu_N(d\xi)} \right).$$

Considering now the case when a_N is not a multiple of 2π , some simple algebra provides the following sufficient condition to ensure the nonnegativeness of Δ_h for $h = 0, 1, \dots$:

$$c_N \geq \max \left\{ - \sum_{k=1}^{N-1} c_k \left(\inf_{\xi \geq 0} \frac{\mu_k(d\xi)}{\mu_N(d\xi)} \right), - \sum_{k=1}^{N-1} c_k \frac{a_N^2}{a_k^2} \left(\inf_{h \in \{1, \dots, \infty\}} \frac{1 - \cos(ha_k)}{1 - \cos(ha_N)} \right) \left(\inf_{\xi \geq 0} \frac{\mu_k(d\xi)}{\mu_N(d\xi)} \right) \right\}.$$

The infimum of $\frac{1 - \cos(ha_k)}{1 - \cos(ha_N)}$ is greater than zero if one assumes that a_N is a multiple of a_k , *i.e.*, $a_N = Pa_k$ with $P \in \mathbb{N} \setminus \{0\}$. In such a case:

$$\frac{1 - \cos(ha_k)}{1 - \cos(ha_N)} = \left(\frac{\sin(ha_k/2)}{\sin(ha_N/2)} \right)^2 \geq \frac{1}{P^2},$$

where the last inequality is due to the fact that, for any real x such that $\sin x$ is different from zero,

$$\left| \frac{\sin(Px)}{\sin(x)} \right| = \left| \frac{e^{iPx} \sin(Px)}{e^{ix} \sin(x)} \right| = \left| \frac{1 - e^{2iPx}}{1 - e^{2ix}} \right| = \left| \sum_{p=0}^{P-1} e^{2ipx} \right| \leq \sum_{p=0}^{P-1} |e^{2ipx}| = P,$$

with i denoting the imaginary unit. Under the condition that a_N is not a multiple of 2π , one therefore obtains the following sufficient condition for the model (4.1) to be positive semidefinite:

$$c_N \geq \max \left\{ - \sum_{k=1}^{N-1} c_k \left(\inf_{\xi \geq 0} \frac{\mu_k(d\xi)}{\mu_N(d\xi)} \right), - \sum_{k \in A} c_k \left(\inf_{\xi \geq 0} \frac{\mu_k(d\xi)}{\mu_N(d\xi)} \right) \right\} \\ = - \sum_{k \in A} c_k \left(\inf_{\xi \geq 0} \frac{\mu_k(d\xi)}{\mu_N(d\xi)} \right),$$

with $A = \{k \in \{1, \dots, N - 1\} : a_N/a_k \in \mathbb{N} \setminus \{0\}\}$. The infimum of μ_k/μ_N can be determined in a closed-form expression if the functions φ_k , $k = 1, \dots, N$,

belong to the Matérn or Cauchy families, as previously exposed in Theorems 3 and 5, respectively.

Example 2. By Lemma 2 in Gneiting (2013), the function

$$\theta \mapsto f_k(\theta) = \left(1 + \frac{\theta}{2a_k}\right) \left(1 - \frac{\theta}{a_k}\right)_+^2, \quad a_k \geq \pi,$$

is positive semidefinite on \mathbb{S}^1 , having the cosine expansion

$$f_k(\theta) = \sum_{h=0}^{\infty} \lambda_{h,k} \cos(h\theta),$$

with

$$\begin{cases} \lambda_{0,k} = \frac{1}{8a_k^3}(8a_k^3 - 6\pi a_k^2 + \pi^3), \\ \lambda_{2h,k} = \frac{3\pi}{4h^2 a_k^3}, & h = 1, 2, \dots, \\ \lambda_{2h+1,k} = \frac{3}{\pi a_k^3(2h+1)^4} ((2a_k^2 - \pi^2)(2h+1)^2 + 4), & h = 0, 1, \dots \end{cases}$$

As before we need to check conditions on c_N , given $c_1, \dots, c_{N-1} \geq 0$, such that the measures

$$\Delta_0(d\xi) = \sum_{k=1}^N c_k \frac{1}{8a_k^3} (8a_k^3 - 6\pi a_k^2 + \pi^3) \mu_k(d\xi), \quad \xi \geq 0,$$

$$\Delta_{2h}(d\xi) = \sum_{k=1}^N c_k \frac{3\pi}{4h^2 a_k^3} \mu_k(d\xi), \quad \xi \geq 0, \quad h = 1, 2, \dots,$$

$$\Delta_{2h+1}(d\xi) = \sum_{k=1}^N c_k \frac{3((2a_k^2 - \pi^2)(2h+1)^2 + 4)}{\pi a_k^3(2h+1)^4} \mu_k(d\xi), \quad \xi \geq 0, \quad h = 0, 1, \dots,$$

are nonnegative.

It is not difficult to see that, if $\pi \leq a_N \leq a_k$, then

$$\frac{(2a_k^2 - \pi^2)(2h+1)^2 + 4}{(2a_N^2 - \pi^2)(2h+1)^2 + 4} \geq 1, \quad h = 0, 1, \dots,$$

and

$$\frac{(8a_k^3 - 6\pi a_k^2 + \pi^3)}{(8a_N^3 - 6\pi a_N^2 + \pi^3)} \geq 1.$$

Therefore, if we assume $\pi \leq a_N$, we obtain the following sufficient condition for the model (4.1) to be positive semidefinite:

$$c_N \geq - \sum_{k \in A} c_k \frac{a_N^3}{a_k^3} \left(\inf_{\xi \geq 0} \frac{\mu_k(d\xi)}{\mu_N(d\xi)} \right).$$

with $A = \{k \in \{1, \dots, N-1\} : a_N \leq a_k\}$.

5. Concluding remarks

This paper has provided a simple and practical solution to the problem of modeling the spatial correlation of random fields observed over linear and generalized networks. An increasing number of applications to both statistics and machine learning witnesses the importance of studying random fields in such spaces for modeling data located on transportation, telecommunication, social, biological and ecological networks (e.g., road networks; railways; power lines; computer, machine and sensor networks; fruit trees; streams, rivers and drainage networks), and the reader is referred to Monestiez et al. (1989); Audergon et al. (1993); Cressie and Majure (1997); Bruno et al. (2001); Gardner et al. (2003); Monestiez et al. (2005); Bailly et al. (2006); Cressie et al. (2006); de Fouquet and Bernard-Michel (2006); Ver Hoef et al. (2006); Polus-Lefebvre et al. (2008); Garreta et al. (2010); Peterson and Ver Hoef (2010); Ver Hoef and Peterson (2010); Perry and Wolfe (2013); Peterson et al. (2013); Alsheikh et al. (2014); Deng et al. (2014); Georgopoulos and Hasler (2014); Isaak et al. (2014); Baddeley et al. (2017); Hamilton et al. (2017); Xiao et al. (2017).

The present research might provide the starting point for extensions to frameworks that have not been studied. For instance, multivariate random fields over nonlinear networks are, to the knowledge of the authors, completely unexplored. Also, it is unclear how to incorporate nonstationarity into the second order structure for a random field over a nonlinear network. In particular, the approach proposed by Paciorek and Schervish (2006) might not be adapted to the case of nonlinear networks.

Another interesting problem is how to simulate random fields over graphs with Euclidean edges. Simulating a random process on the plane and retaining those realizations inside the graph is certainly not a good idea, as such a restriction would result in a very unrealistic process for a graph with Euclidean edges. The ingenious approach provided by Anderes et al. (2020) to construct a Brownian bridge over graphs is a promising avenue in this direction.

Proofs

Proof of Theorem 3

We give a constructive proof. We start by noting that (Gradshteyn and Ryzhik, 2007, formula 3.471.9)

$$\mathcal{M}_{\nu_k} \left(\frac{\sqrt{t}}{\sqrt{b_k}} \right) = \int_0^\infty \frac{e^{-\xi t}}{\Gamma(\nu_k)} \left(\frac{1}{4b_k} \right)^{\nu_k} \xi^{-1-\nu_k} e^{-\frac{1}{4\xi b_k}} d\xi, \quad t \geq 0.$$

Hence, we need to show under which conditions on c_N , for $c_1, \dots, c_{N-1} \geq 0$,

$$\sum_k^N c_k \frac{1}{\Gamma(\nu_k)} \left(\frac{1}{4b_k} \right)^{\nu_k} \xi^{-1-\nu_k} e^{-\frac{1}{4\xi b_k}} \geq 0,$$

for all $\xi \geq 0$. A sufficient condition for this to happen is

$$c_N \geq - \sum_{k=1}^{N-1} c_k \frac{\Gamma(\nu_N)}{\Gamma(\nu_k)} \frac{(4b_N)^{\nu_N}}{(4b_k)^{\nu_k}} \inf_{\xi \geq 0} \left\{ \xi^{\nu_N - \nu_k} e^{-\frac{1}{4\xi} \left(\frac{1}{b_k} - \frac{1}{b_N} \right)} \right\}.$$

We now notice that the function

$$\xi \mapsto f(\xi; \nu, a) := \xi^\nu \exp\left(-\frac{a}{4\xi}\right), \quad \xi \geq 0,$$

is always nonnegative. Its infimum is equal to 1 if $a \leq 0$ and $\nu = 0$, and to 0 if $a > 0$, or $a = 0$ and $\nu \neq 0$, or $a < 0$ and $\nu < 0$. Otherwise, if $a < 0$ and $\nu > 0$, the infimum is reached at $\xi_0 = -a/(4\nu)$ and is equal to $(-\frac{ae}{4\nu})^\nu$. This provides the desired conditions and completes the proof. \square

Proof of Theorem 5

The proof is similar to that in Theorem 3. We start by noting that (Gradshteyn and Ryzhik, 2007, formula 3.381.4)

$$\mathcal{C}_{\beta_k} \left(\frac{t}{b_k} \right) = \int_0^\infty e^{-\xi t} \frac{b_k^{\beta_k}}{\Gamma(\beta_k)} \xi^{\beta_k - 1} e^{-b_k \xi} d\xi, \quad t \geq 0.$$

By using similar arguments and after some elementary algebra, we get that a sufficient condition for positive semidefiniteness becomes

$$c_N \geq - \sum_{k=1}^{N-1} c_k \frac{b_k^{\beta_k}}{b_N^{\beta_N}} \frac{\Gamma(\beta_N)}{\Gamma(\beta_k)} \inf_{\xi \geq 0} \left\{ \xi^{\beta_k - \beta_N} e^{-\xi(b_k - b_N)} \right\}.$$

We now consider the function

$$\xi \mapsto g(\xi; \beta, b) := \xi^\beta \exp(-b\xi), \quad \xi \geq 0,$$

which is always nonnegative. Its infimum is equal to 1 if $b \leq 0$ and $\beta = 0$, and to 0 if $b > 0$ or $b = 0$ and $\beta \neq 0$, or $b < 0$ and $\beta > 0$. Otherwise, if $b < 0$ and $\beta < 0$, the infimum is reached at $\xi_0 = \beta/b$ and is equal to $e^{-\beta(\beta/b)^\beta}$. This provides the desired conditions and completes the proof. \square

Proof of Theorem 7

Again, we provide a proof of the constructive type. Let \mathcal{G} be a Euclidean tree with $\lceil m/2 \rceil$ leaves, $m \geq 3$. Let φ be the class of functions defined through Equation (3.1), with $\varphi_k(\cdot) = \psi_{\nu+m_k+1}(\cdot/b_k)$, with $b_k > 0$, $m_k > 0$ and $\nu \geq 2m - 1$. Theorem 1 in Daley et al. (2015) shows that, for $t \geq 0$,

$$\left(1 - \frac{t}{b_k}\right)_+^{\nu+m_k+1} = \frac{1}{b_k^{\nu+1} B(\nu+1, m_k+1)} \int_0^\infty \left(1 - \frac{t}{\xi}\right)_+^\nu \xi^\nu \left(1 - \frac{\xi}{b_k}\right)_+^{m_k} d\xi.$$

A direct inspection in concert with some algebra show that the nested model is valid provided

$$\sum_{k=1}^N \frac{c_k (b_k - \xi)_+^{m_k}}{b_k^{\nu+1+m_k} B(\nu + 1, m_k + 1)}$$

is nonnegative for any $\xi \geq 0$. This condition always holds for $\xi \geq b_N$, insofar as c_1, \dots, c_{N-1} are assumed to be positive and the N -th summand is zero when ξ is greater than or equal to b_N . Accordingly, the nested model is valid if

$$c_N \geq - \sum_{k=1}^{N-1} c_k \frac{b_N^{\nu+1+m_N} B(\nu + 1, m_N + 1)}{b_k^{\nu+1+m_k} B(\nu + 1, m_k + 1)} \inf_{\xi \in [0, b_N[} \frac{(b_k - \xi)_+^{m_k}}{(b_N - \xi)^{m_N}}.$$

If $b_k < b_N$, then the infimum of $(b_k - \xi)_+^{m_k} / (b_N - \xi)^{m_N}$ is reached at $\xi = b_k$ and is equal to 0. If $b_k = b_N$ and $m_k > m_N$, the infimum is also zero and is reached at $\xi = b_N$. If $b_k \geq b_N$ and $m_k \leq m_N$, the infimum is reached at $\xi = 0$ and is equal to $b_k^{m_k} / b_N^{m_N}$. Finally, if $b_k > b_N$ and $m_k > m_N$, the infimum is reached at $\xi = (m_k b_N - m_N b_k) / (m_k - m_N)$ and is equal to $\frac{m_k^{m_k}}{m_N^{m_N}} \left(\frac{b_k - b_N}{m_k - m_N} \right)^{m_k - m_N}$. The proof is completed. \square

Proof of Theorem 9

The proof comes straight by noting that a sufficient condition for positive semidefiniteness is that the weighted sum

$$\vartheta(t) = \sum_{k=1}^N c_k \vartheta_k(t), \quad t \geq 0$$

is convex on the positive real line and that $\lim_{t \rightarrow \infty} \vartheta(t) = 0$ (Anderes et al., 2020, theorem 5). All these requirements can be verified by direct inspection. Since ϑ_k is convex by assumption for all $k = 1, \dots, N$, inspecting for convexity of ϑ amounts to solve the inequalities

$$c_N \leq - \sum_{k=1}^{N-1} c_k \frac{\vartheta_k^{(1)}(t)}{\vartheta_N^{(1)}(t)},$$

and

$$c_N \geq - \sum_{k=1}^{N-1} c_k \frac{\vartheta_k^{(2)}(t)}{\vartheta_N^{(2)}(t)}.$$

Upon simplification, we get the result. \square

Proof of Theorem 10

Part B. is a direct application of Theorem 3.3 in Berg and Porcu (2017). To prove part A., we start by the necessary condition. Let $\Psi(d_*(\cdot, \cdot), |\cdot - \cdot|)$ be

positive semidefinite over $(\mathcal{G} \times \mathbb{R}) \times (\mathcal{G} \times \mathbb{R})$. Then, the function

$$\tilde{\Psi}(d_*, |u|) := \Psi(d_*, |u|) \cos(|u|), \quad u \in \mathbb{R},$$

is positive semidefinite over $\mathcal{G} \times \mathbb{R}$ as a direct application of Schur's product theorem. Since positive semidefinite functions are closed under rescaling, we have that

$$K_\tau(d_*, |u|) := \tilde{\Psi}(d_*, \tau|u|), \quad \tau \geq 0,$$

is positive semidefinite over $\mathcal{G} \times \mathbb{R}$ for every τ .

We now adapt Lemma 3.4 in Berg and Porcu (2017) to the product space $\mathcal{G} \times \mathbb{R}$: for a Radon measure $d\mu : \mathcal{G} \times \mathbb{R}$, we have

$$\int_{\mathcal{G} \times \mathbb{R}} \int_{\mathcal{G} \times \mathbb{R}} K_\tau(d_*(x, x'), |u - u'|) d\lambda(x, u) d\lambda(x', u') \geq 0, \quad \forall \tau \geq 0.$$

We now specialize the assertion to the tensor product measure

$$d\lambda(x, u) = \sigma(dx) \otimes \mu(du), \quad (s, u) \in \mathcal{G} \times \mathbb{R},$$

where we use the abuse of notation μ for the Lebesgue measure over the real line, and where σ is a Radon measure. A direct application of Fubini's theorem shows that

$$\int_{\mathcal{G} \times \mathcal{G}} \left(\int_{\mathbb{R} \times \mathbb{R}} K_\tau(d_*(x, x'), |u - u'|) \mu(du) \mu(du') \right) \sigma(dx) \sigma(dx') \geq 0, \quad \forall \tau \geq 0.$$

This proves that the function

$$d_* \mapsto \int_{\mathbb{R} \times \mathbb{R}} K_\tau(d_*, |u - u'|) \mu(du) \mu(du'),$$

is positive semidefinite over \mathcal{G} . This completes the necessary part. The sufficient part is trivial. The proof is completed. \square

Proof of Theorem 11

We consider the function

$$f_k(u) := \mathcal{M}_{\eta_k} \left(\frac{|u|}{a_k} \right), \quad u \in \mathbb{R},$$

with $\nu_k > 0$ and $a_k > 0$, $k = 1, \dots, N$. The symmetric Fourier transform of f_k , denoted \hat{f}_k , admits expression (Lantuéjoul, 2002)

$$\hat{f}_k(\tau) = \frac{\Gamma(\eta_k + \frac{1}{2}) a_k}{\Gamma(\eta_k)} \left(1 + \frac{\tau^2}{a_k^2} \right)^{-\eta_k - \frac{1}{2}}, \quad \tau \in \mathbb{R}.$$

Hence, getting the admissibility condition (4.5) is equivalent to attain

$$\inf_{\tau \geq 0} \frac{\left(1 + \frac{\tau^2}{a_N^2}\right)^{\eta_N + \frac{1}{2}}}{\left(1 + \frac{\tau^2}{a_k^2}\right)^{\eta_k + \frac{1}{2}}}.$$

If $\eta_N < \eta_k$, the infimum is zero, as the ratio tends to zero as τ tends to infinity. If $\eta_N \geq \eta_k$, the infimum is reached at $\tau_0 = \sqrt{\frac{a_N^2(1+2\eta_k) - a_k^2(1+2\eta_N)}{2(\eta_N - \eta_k)}}$ when $(1 + 2\eta_N) a_k^2 < (1 + 2\eta_k) a_N^2$ and at $\tau_0 = 0$ otherwise, the infimum being $\kappa(a_k, a_N, \eta_k, \eta_N)$ as defined in (4.7). The rest of the proof comes straight, and we omit it.

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