

Supplementary Material to Temporally-Evolving Generalised Networks and Their Kernels

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In this Supplementary Material, Section A contains additional mathematical background; Section B contains some additional remarks about the motivations behind the definition on Z_V and Z_E ; Section C explores the reproducing kernel Hilbert space properties of our construction; Section D we state some general results that may be useful to the definition of kernels on arbitrary sets; Section E presents the proofs of the results in the main document; while Section F contains some additional material.

A. Mathematical background

Definition A.1 (Simple, connected graph). Let V a finite set (called *vertices* or *nodes*) and let $E \subseteq V \times V$ a set of connections (called *edges*). Then the pair $G := (V, E)$ is called a *graph* or a *network*. We said that a graph G is *simple* if it is *undirected* (videlicet, whenever $(v_1, v_2) \in E$, then necessarily $(v_2, v_1) \in E$) and if it has no self-loops (namely, for all $v \in V$, $(v, v) \notin E$). For an undirected graph G , two nodes $v_1, v_2 \in V$ are *adjacent* if $(v_1, v_2) \in E$. We write $v_1 \sim v_2$ if v_1 and v_2 are adjacent, $v_1 \not\sim v_2$ if they are not.

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A *path* between two nodes $v \neq w \in V$ is a finite sequence of vertices $(v = v_1, v_2, \dots, v_p = w)$ such that, $\forall i \in \{1, \dots, p-1\}$, $(v_i, v_{i+1}) \in E$. A *connected component* of a graph G is a maximal subset of vertices $V' \subseteq V$ such that, for each pair of nodes $v, w \in V'$, there is a path between v and w . A graph G is *connected* if there is only one connected component, namely if there is a path between each pair of nodes.

Definition A.2 (Moore-Penrose generalised inverse). Let $M \in \mathbb{R}^{n \times n}$ be a matrix. Then its *Moore-Penrose generalised inverse* is the unique matrix $M^+ \in \mathbb{R}^{n \times n}$ such that:

- $MM^+M = M$ and $M^+MM^+ = M^+$,
- $MM^+ = (MM^+)^T$ and $M^+M = (M^+M)^T$.

Definition A.3 (g -embedding, isometric embedding). Let (X, d) be a semi-distance space and $g : D_X^d \rightarrow [0, +\infty)$ a function, where D_X^d denotes the diameter of X . Then (X, d) is said to have a g -embedding into a Hilbert space $(H, \|\cdot\|_H)$, written $(X, d) \xrightarrow{g} H$, if there exists a map $\psi : X \rightarrow H$ such that, for all $x, y \in X$,

$$g(d(x, y)) = \|\psi(x) - \psi(y)\|_H.$$

If g is the identity map, then it is called *isometric embedding*.

B. Additional results and remarks

Lemma B.1. Let L be a $n \times n$ laplacian matrix, and let $\mathbf{x} \in \mathbb{R}^n$ such that $\mathbf{1}_n^\top \mathbf{x} \neq 0$. Let, in addition, $\delta_1, \delta_2 \in [0, 1]$ and $\underline{u}_1, \bar{u}_1, \underline{u}_2, \bar{u}_2 \in \{1, \dots, n\}$. Finally, define $\boldsymbol{\delta}_i$ ($i \in \{1, 2\}$) as in Equation (4.8). Then it holds:

$$(\boldsymbol{\delta}_1 - \boldsymbol{\delta}_2)^\top (L + \mathbf{x}\mathbf{x}^\top)^{-1} (\boldsymbol{\delta}_1 - \boldsymbol{\delta}_2) = (\boldsymbol{\delta}_1 - \boldsymbol{\delta}_2)^\top L^+ (\boldsymbol{\delta}_1 - \boldsymbol{\delta}_2)$$

Proof of Lemma B.1. First, let us show that the thesis is meaningful, that is that $L + \mathbf{x}\mathbf{x}^\top$ is strictly positive definite. Clearly, it is positive semidefinite, as sum of two positive semidefinite matrices. In addition, for $\mathbf{y} \in \mathbb{R}^n \setminus \{\mathbf{0}\}$, we have

$$\mathbf{y}^\top (L + \mathbf{x}\mathbf{x}^\top) \mathbf{y} = \mathbf{y}^\top L \mathbf{y} + \mathbf{y}^\top \mathbf{x}\mathbf{x}^\top \mathbf{y}.$$

Now, if \mathbf{y} does not belong to the kernel of L , that is $L\mathbf{y} \neq 0$, we have that $\mathbf{y}^\top L\mathbf{y}$ is strictly positive. If, instead, $\mathbf{y} \in \ker(L)$, then, by the properties of laplacian matrices stated in Subsection 2.3, $\mathbf{y} = c\mathbf{1}_n$, where $c \in \mathbb{R} \setminus \{0\}$. In such a case we have $\mathbf{y}^\top (L + \mathbf{x}\mathbf{x}^\top) \mathbf{y} = \mathbf{y}^\top L\mathbf{y} + \mathbf{y}^\top \mathbf{x}\mathbf{x}^\top \mathbf{y} = 0 + c^2 (\mathbf{1}_n^\top \mathbf{x})^2 > 0$, since $\mathbf{1}_n^\top \mathbf{x} \neq 0$ by hypothesis.

Now, let us show that the equality holds. In order to express the Moore-Penrose inverse (which coincides with the standard inverse) of the rank-1 update $L + \mathbf{x}\mathbf{x}^\top$, we exploit Theorem 1 of Meyer [1973] with $A := L$ and $\mathbf{c} := \mathbf{d} := \mathbf{x}$. Firstly, let us show that the hypotheses of the theorem are satisfied: we have to prove that $\mathbf{x} \notin R(L)$, where R denotes the range or column space. $R(L)$ is perpendicular to the kernel of L , that is (recall that L is a laplacian matrix) $\ker(L) = \{h\mathbf{1}_n : h \in \mathbb{R}\}$. Now, $\mathbf{x} \in R(L) \iff \mathbf{x} \perp \ker(L) \iff \mathbf{1}_n^\top \mathbf{x} = 0$, yet $\mathbf{1}_n^\top \mathbf{x} \neq 0$ by hypothesis. Therefore $\mathbf{x} \notin R(L)$, *i.e.* we can apply the above-mentioned theorem. In the following computations, we have adopted the notation used by Meyer [1973, Section 2], *i.e.:*

$$\begin{aligned} \mathbf{k} &:= L^- \mathbf{x} & \mathbf{h} &:= \mathbf{x}^\top L^- \\ \mathbf{u} &:= (I_n - LL^-) \mathbf{x} = \frac{1}{n} \mathbf{1}_{n \times n} \mathbf{x} & \mathbf{v} &:= \mathbf{x}^\top (I_n - L^- L) = \frac{1}{n} \mathbf{x}^\top \mathbf{1}_{n \times n} \\ \beta &:= 1 + \mathbf{x}^\top L^- \mathbf{x}. \end{aligned}$$

In addition, we have $\|\mathbf{u}\|^2 = \|\mathbf{v}\|^2 = \mathbf{u}^\top \mathbf{u} = \frac{1}{n^2} \mathbf{1}_n^\top (\mathbf{1}_n^\top \mathbf{x})(\mathbf{1}_n^\top \mathbf{x}) \mathbf{1}_n = \frac{1}{n} (\mathbf{1}_n^\top \mathbf{x})^2 \neq 0$. Let us finally apply Equation (3.1) of Meyer [1973]:

$$\begin{aligned} (L + \mathbf{x}\mathbf{x}^\top)^- &= L^- - \mathbf{k}\mathbf{u}^- - \mathbf{v}^- \mathbf{h} + \beta \mathbf{v}^- \mathbf{u}^- \\ &= L^- - \frac{\mathbf{k}\mathbf{u}^\top}{\|\mathbf{u}\|^2} - \frac{\mathbf{v}^\top \mathbf{h}}{\|\mathbf{v}\|^2} + \beta \frac{\mathbf{v}^\top \mathbf{u}^\top}{\|\mathbf{v}\|^2 \|\mathbf{u}\|^2} \\ &= L^- - \frac{L^- \mathbf{x} \mathbf{1}_n^\top}{\mathbf{1}_n^\top \mathbf{x}} - \frac{\mathbf{1}_n \mathbf{x}^\top L^-}{\mathbf{1}_n^\top \mathbf{x}} + (1 + \mathbf{x}^\top L^- \mathbf{x}) \frac{\mathbf{1}_{n \times n}}{(\mathbf{1}_n^\top \mathbf{x})^2}. \end{aligned}$$

To conclude, it is now sufficient to prove that

$$(\boldsymbol{\delta}_1 - \boldsymbol{\delta}_2)^\top \left((1 + \mathbf{x}^\top L^- \mathbf{x}) \frac{\mathbf{1}_{n \times n}}{(\mathbf{1}_n^\top \mathbf{x})^2} - \frac{L^- \mathbf{x} \mathbf{1}_n^\top}{\mathbf{1}_n^\top \mathbf{x}} - \frac{\mathbf{1}_n \mathbf{x}^\top L^-}{\mathbf{1}_n^\top \mathbf{x}} \right) (\boldsymbol{\delta}_1 - \boldsymbol{\delta}_2) = 0.$$

It is possible to see this by noticing that $\mathbf{1}_n^\top (\boldsymbol{\delta}_1 - \boldsymbol{\delta}_2) = \mathbf{1}_n^\top \boldsymbol{\delta}_1 - \mathbf{1}_n^\top \boldsymbol{\delta}_2 = 1 - 1 = 0$ and similarly $(\boldsymbol{\delta}_1 - \boldsymbol{\delta}_2)^\top \mathbf{1}_n = 0$, therefore each term of the above equation equals 0. \square

A remark about the motivation behind the definitions of the processes Z_V and Z_E follows.

Remark B.1. The *rationale* behind the definitions of Z_V and Z_E is closely related to the desired semi-metric properties. Indeed, the objective in Anderes et al. [2020] is to build an extension to the classical resistance distance and, to achieve such a result, they define the analogous of a Wiener process on the graph. To have an intuition about such a choice, consider the standard Wiener process $(W_t)_t$ on the positive real line \mathbb{R}_0^+ : we have $\text{Cov}(W_t, W_s) = \min(t, s)$ and, as a consequence, $\gamma_W(t, s) := \text{Var}(W_t - W_s) = |t - s|$, *i.e.* the variogram is the Euclidean distance, which, considering the positive real line as a uniform electric resistor, coincides with the effective resistance distance. Perhaps surprisingly, this continues to hold shifting from the positive real line to a graph with Euclidean edges. Clearly, the definition of the Wiener process cannot be applied directly to a graph, which has several differences with \mathbb{R}_0^+ : it is compact and does not have any intrinsic order or sum operation. As a consequence, the Wiener process $(W_t)_t$ needs to be adapted to the new topology and Anderes et al. [2020] defined it via the conditional independence structure offered by the (modified) Laplacian, which entails the topology of the graph. Therefore, they define Z_V on the vertices as the Gaussian random vector with precision matrix L : in such a way, for $v_1 \not\sim v_2 \in V$, $Z_V(v_1)$ and $Z_V(v_2)$ are conditional independent given $Z_V(V \setminus \{v_1, v_2\})$. Furthermore, it has been shown that the inverse laplacian matrix of a resistor graph offers an efficient way to compute all the effective resistance distances between its nodes, as we mentioned in Subsection 2.3. Therefore, since we define Z_E at vertices to be zero and since the linear operation on the inverse laplacian matrix to obtain the effective resistance is actually the variogram, it is natural to define Z_V having precision matrix L .

Once the process is defined on the vertices V , it remains to define it on the edges. The idea is to build, for each edge $e = (v_1, v_2) \in E$, a Brownian bridge linking $Z_V(v_1)$ and $Z_V(v_2)$, thus summing a linear interpolation between $Z_V(v_1)$ and $Z_V(v_2)$, and adding a standard Brownian bridge on $[0, \ell(e)]$.

Clearly, this construction needs to be adapted when we shift from the purely spatial case of Anderes et al. [2020] to the time-evolving setting studied in this paper. Indeed, both Z_V and Z_E need some adaptation to cope with the time-evolving dynamic. Regarding Z_V , the (modified) Laplacian matrix of the equivalent simple graph offers a nice conditional independence structure: while, for a given time t , the conditional independence structure is the same

as there was no time, the links between adjacent time instants of an (order 1) equivalent simple graph provide the same conditional independence structure among times. More specifically Z_V at layer t_1 is independent from Z_V at layer t_3 given Z_V at layer t_2 , for each $t_1 < t_2 < t_3$.

The construction of Z_E extends the original construction by Anderes et al. [2020] as well. On each edge at a given time, its covariance structure is the same, however, we add some correlation (governed by the choice of k_T) between times. This is motivated by the following: imagine that the sampling time of the graph has a scale much smaller than the process on it. Then, for two adjacent time instants, say t and $t + 1$, it is reasonable to assume that the process on a given edge e does not change too much. This is achieved by having a high correlation of the final process (and thus a low variogram of $Z = Z_V + Z_E$). Therefore, a high correlation of Z_E for adjacent time will fix this issue.

C. Reproducing kernel Hilbert space construction

In this section, we provide a constructive definition of the reproducing kernel Hilbert space (RKHS) for the kernel k_Z of the process $Z = Z_V + Z_E$ presented in Proposition 7. We divide the construction in four steps.

Step 1: construction of the RKHS of Z_E on a life λ

Recall from Subsection 4.1 in the main text that $\Lambda := \{\text{lf}(e) : e \in \widetilde{E}\}$ is the set of lives of all the edges of \widetilde{G} . In this step, we characterise the RKHS of the kernel k_E on any $\lambda \in \Lambda$. For the sake of simplicity, we set $n_\lambda := |\lambda|$: the number of edges that share the life λ . Recall that, for a life λ , $k_E|_\lambda : \widetilde{G}|_\lambda \times \widetilde{G}|_\lambda \rightarrow \mathbb{R}$ has the following expression:

$$k_E|_\lambda(u_1, u_2) = \sqrt{\ell(e_1)\ell(e_2)} \cdot k_T(|t(e_1) - t(e_2)|) \cdot (\min(\delta_1, \delta_2) - \delta_2\delta_2).$$

It is patent that such a kernel is the product of a kernel defined on a finite set (λ) and the kernel k_{BB} , defined on $[0, 1]$. As a consequence, following [Berlinet and Thomas-Agnan, 2004, Theorem 13], in order to find the RKHS of $k_E|_\lambda$, it is sufficient to build the tensor Hilbert product between the RKHSs of

$$k_\lambda^{(M)} : \lambda^2 \rightarrow \mathbb{R} \quad k_\lambda^{(M)}(e_1, e_2) := \sqrt{\ell(e_1)\ell(e_2)} \cdot k_T(|t(e_1) - t(e_2)|), \quad (\text{C1})$$

$$k_{BB} : [0, 1]^2 \rightarrow \mathbb{R} \quad k_{BB}(\delta_1, \delta_2) := \min(\delta_1, \delta_2) - \delta_2\delta_2. \quad (\text{C2})$$

Regarding the former, since λ has finite cardinality n_λ , (C1) can be expressed in the following matrix form:

$$k_\lambda^{(M)}(e_1, e_2) := [M_\lambda]_{e_1, e_2},$$

where $M_\lambda \in \mathbb{R}^{n_\lambda \times n_\lambda}$ is defined as

$$[M_\lambda]_{e_1, e_2} := \sqrt{\ell(e_1)\ell(e_2)} \cdot k_T(|t(e_1) - t(e_2)|), \quad e_1, e_2 \in \lambda.$$

By introducing the definitions

$$\begin{aligned} K_T &:= [k_T(|t(e_1) - t(e_2)|)]_{e_1, e_2 \in \lambda} \in \mathbb{R}^{n_\lambda \times n_\lambda} \\ w^\top &:= \left[\sqrt{\ell(e_1)}, \dots, \sqrt{\ell(e_{n_\lambda})} \right] \in \mathbb{R}^{n_\lambda}, \end{aligned}$$

it is possible to compactly write M_λ as

$$M_\lambda = K_T \circ w w^\top = \text{diag}(w) K_T \text{diag}(w),$$

where \circ denotes the Hadamard matrix product. This last expression shows that, if we assume k_T to be a strictly positive definite kernel (and, thus, K_T is strictly positive definite), then M_λ is strictly positive definite as well. This step is crucial in the definition of the RKHS of $k_\lambda^{(M)}$, which is given next.

Remark C.2. The RKHS of $k_\lambda^{(M)}$ is $\mathcal{H}_\lambda^{(M)} := \left(\mathbb{R}^{n_\lambda}, \langle \cdot, \cdot \rangle_\lambda^{(M)} \right)$, where

$$\langle v_1, v_2 \rangle_\lambda^{(M)} := v_1^\top M_\lambda^{-1} v_2.$$

This is proved by noticing that $\langle \cdot, \cdot \rangle_\lambda^{(M)}$ is clearly symmetric, bilinear and positive definite, and that

$$\langle k_\lambda^{(M)}(v_1, \cdot), v_2 \rangle_\lambda^{(M)} = \langle v_1^\top M_\lambda, v_2 \rangle_\lambda^{(M)} = v_1^\top M_\lambda M_\lambda^{-1} v_2 = v_1^\top v_2.$$

Next, we need to characterise the RKHS of the kernel k_{BB} in (C2). By the same argument in the proof of [Anderes et al., 2020, Lemma 3.B], the RKHS of k_{BB} is $\mathcal{H}_{BB} := (\mathcal{F}_{BB}, \langle \cdot, \cdot \rangle_{BB})$, where \mathcal{F}_{BB} is the set of functions $f : [0, 1] \rightarrow \mathbb{R}$ that are absolutely continuous and such that $f' \in L^2([0, 1])$, and

$$\langle f, g \rangle_{BB} := \int_0^1 f'(\delta) g'(\delta) d\delta.$$

Now we have all the ingredients to characterise the RKHS of $k_E|_\lambda$.

Remark C.3. Consider the Hilbert tensor product space $\mathcal{H}_\lambda := \mathcal{H}_\lambda^{(M)} \otimes \mathcal{H}_{BB}$, that is: the completion of the set of functions

$$\begin{aligned} f_\lambda^{(M)} \otimes f_{BB} : \lambda \times [0, 1] &\rightarrow \mathbb{R} \\ (e, \delta) &\mapsto f_\lambda^{(M)}(e) f_{BB}(\delta), \end{aligned}$$

where $f_\lambda^{(M)} \in \mathbb{R}^{n_\lambda}$ and $f_{BB} \in \mathcal{F}_{BB}$. The scalar product of \mathcal{H}_λ is defined on the functions $f_\lambda^{(M)} \otimes f_{BB}$ as:

$$\langle f_\lambda^{(M)} \otimes f_{BB}, g_\lambda^{(M)} \otimes g_{BB} \rangle_{\mathcal{H}_\lambda} := \langle f_\lambda^{(M)}, g_\lambda^{(M)} \rangle_\lambda^{(M)} \cdot \langle f_{BB}, g_{BB} \rangle_{BB},$$

and then extended by linearity. For the sake of completeness, we report an explicit way to build \mathcal{H}_λ . Assume that $\{\eta_i\}_{i=1}^{n_\lambda}$ and $\{\phi_j\}_{j=1}^\infty$ denote two orthonormal bases of $\mathcal{H}_\lambda^{(M)}$ and \mathcal{H}_{BB} respectively, then \mathcal{H}_λ is the space generated by the (orthonormal) basis $\{\eta_i \otimes \phi_j\}_{i,j}$. Therefore, given two generic elements of \mathcal{H}_λ

$$f = \sum_{i,j} b_{ij} \eta_i \otimes \phi_j \quad g = \sum_{i,j} c_{ij} \eta_i \otimes \phi_j,$$

their scalar product is defined as:

$$\begin{aligned} \langle f, g \rangle_{\mathcal{H}_\lambda} &= \left\langle \sum_{i,j} b_{ij} \eta_i \otimes \phi_j, \sum_{i',j'} c_{i',j'} \eta_{i'} \otimes \phi_{j'} \right\rangle_{\mathcal{H}_\lambda} \\ &= \sum_{i,j} \sum_{i',j'} b_{i,j} c_{i',j'} \langle \eta_i \otimes \phi_j, \eta_{i'} \otimes \phi_{j'} \rangle_{\mathcal{H}_\lambda} \\ &= \sum_{i,j} \sum_{i',j'} b_{i,j} c_{i',j'} \langle \eta_i, \eta_{i'} \rangle_\lambda^{(M)} \cdot \langle \phi_j, \phi_{j'} \rangle_{BB} = \sum_{i,j} b_{i,j} c_{i,j}, \end{aligned}$$

where the last step relies on the orthonormality of $\{\eta_i\}_{i=1}^{n_\lambda}$ and $\{\phi_j\}_{j=1}^\infty$.

This concludes the construction of the RKHS of $k_E|_\lambda$.

Step 2: RKHS of k_E on $\tilde{\mathbf{G}}$

Once the RKHSs of k_E have been defined on each life $\lambda \in \Lambda$, it is possible to characterise the RKHS of k_E on the whole set of edges (i.e. on $\tilde{\mathbf{G}}$). Indeed, as k_E is null when computed among points on edges that do not share lives, the RKHS of k_E on $\tilde{\mathbf{G}}$ will be the sheer direct sum of them:

$$\mathcal{H}_\Lambda := \bigoplus_{\lambda \in \Lambda} \mathcal{H}_\lambda.$$

Clearly, the elements of direct sum are the tuples of size $|\Lambda|$ of functions, each belonging to the respective \mathcal{H}_λ . However, there is clearly a bijection between such tuples and the set of functions defined on the union of the lives λ 's. Therefore, \mathcal{H}_Λ can be interpreted as the set of functions $f : \tilde{\mathbf{G}} \rightarrow \mathbb{R}$ such that their restrictions on each life λ belong to the respective \mathcal{H}_λ . In formulae: $\mathcal{H}_\Lambda = (\mathcal{F}_\Lambda, \langle \cdot, \cdot \rangle_\Lambda)$, with:

$$\mathcal{F}_\Lambda := \left\{ f : \tilde{\mathbf{G}} \rightarrow \mathbb{R} : f \text{ is A.C., } f' \in L^2(\tilde{\mathbf{G}}), f(V) = 0 \right\}$$

$$\langle f, g \rangle_\Lambda := \sum_{\lambda \in \Lambda} \langle f|_\lambda, g|_\lambda \rangle_\lambda.$$

By construction (recall, by Berlinet and Thomas-Agnan 2004, Theorem 5, that the direct sum of RKHSs is the RKHS of the sum of the kernels), \mathcal{H}_Λ is the RKHS of the kernel k_E on the whole graph $\tilde{\mathbf{G}}$.

Step 3: RKHS of k_V on $\tilde{\mathbf{G}}$

Since the kernel k_V is exactly the same defined in Anderes et al. [2020], this step is an adaptation. Consider $\mathcal{H}_V := (\mathcal{F}_V, \langle \cdot, \cdot \rangle_V)$, where:

$$\mathcal{F}_V := \left\{ f : \tilde{\mathbf{G}} \rightarrow \mathbb{R} : \forall e \in \tilde{E}, f|_e(u) = (1 - \delta)f(\underline{u}) + \delta f(\bar{u}) \right\},$$

$$\langle f, g \rangle_V := f(V)^\top \mathbf{x} \mathbf{x}^\top g(V) + \sum_{e \in \tilde{E}} \frac{1}{\ell(e)} \int_0^1 f|'_e(\delta) g|'_e(\delta) d\delta$$

$$= f(V)^\top \mathbf{x} \mathbf{x}^\top g(V) + \sum_{e \in \tilde{E}} \frac{(f|_e(1) - f|_e(0)) (g|_e(1) - g|_e(0))}{\ell(e)}.$$

Notice that the sum in the second line is the same quantity indicated by $\int_{\underline{e}}^{\bar{e}} f'_e(t) g'_e(t) dt$ in Anderes et al. [2020]. It is straightforward to show that $\langle \cdot, \cdot \rangle_V$ is a scalar product on \mathcal{F}_V : clearly it is symmetric and bilinear, moreover, for an $f \in \mathcal{F}_V$, we have:

$$\langle f, f \rangle_V = (\mathbf{x}^\top f(V))^2 + \sum_{e \in \tilde{E}} \frac{(f|_e(1) - f|_e(0))^2}{\ell(e)} \geq 0,$$

where $\langle f, f \rangle_V = 0$ if and only if $\mathbf{x}^\top f(V) = 0$ and $\forall e \in \tilde{E}, f|_e(1) = f|_e(0)$. From the latter we get that f is constant at all vertices, that is $f(V) = c\mathbf{1}_n$ for some $c \in \mathbb{R}$, and we conclude thanks to the former:

$$0 = \mathbf{x}^\top f(V) = c \mathbf{x}^\top \mathbf{1}_n,$$

that implies $c = 0$, since $\mathbf{x}^\top \mathbf{1}_n \neq 0$.

Step 4: RKHS of k on $\tilde{\mathbf{G}}$ in the non periodic case

Also this step is quite straightforward, since, being k on $\tilde{\mathbf{G}}$ the sheer sum of k_V and k_E (Equation (4.7)). As a consequence, the RKHS of k_Z will be the direct sum of the RKHSs of k_V and k_E :

$$\mathcal{H} = \mathcal{H}_V \oplus \mathcal{H}_E.$$

Now, analogously to what noticed in Step 2, it is possible to observe that the set of couples $(f_V, f_E) \in \mathcal{H}_V \times \mathcal{H}_E$ is isomorphic to the set \mathcal{F} of functions $f : \tilde{\mathbf{G}} \rightarrow \mathbb{R}$ that are absolutely continuous on every edge and $f|_e'$ belongs to L^2 . Summarising, if we define the two operators $\mathcal{P}_V, \mathcal{P}_\lambda : \mathcal{F} \rightarrow \mathcal{F}$ as follows:

$$\begin{aligned} \mathcal{P}_V(f)(u) &:= (1 - \delta)f(\underline{u}) + \delta f(\bar{u}) \\ \mathcal{P}_\lambda(f)(u) &:= \begin{cases} f(u) - \mathcal{P}_V(f)(u) & \text{if } u \in \lambda \\ 0 & \text{otherwise,} \end{cases} \end{aligned}$$

then it is possible to express the RKHS of k_Z as follows: $\mathcal{H} = (\mathcal{F}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$, where

$$\langle f, g \rangle_{\mathcal{H}} = \langle \mathcal{P}_V f, \mathcal{P}_V g \rangle_V + \sum_{\lambda \in \Lambda} \langle \mathcal{P}_\lambda f, \mathcal{P}_\lambda g \rangle_{\lambda}.$$

Notice that the operators \mathcal{P}_V and \mathcal{P}_λ are the same operators defined in Anderes et al. [2020], where our \mathcal{P}_λ is simply the union of their \mathcal{P}_e , indexed by $e \in \lambda$. Therefore, we obtain that \mathcal{P}_V and \mathcal{P}_E are orthogonal projectors and self-adjoint.

Step 5: RKHS of k on $\tilde{\mathbf{G}}$ in the periodic case

The expression for the kernel k in case of a periodic time-evolving graph, given in Equation (5.10), has an additional term to ensure that the process Z varies at different times, namely $\beta^2 \min(t_1, t_2)$. Being this the kernel of a standard Wiener process multiplied by a constant $\beta > 0$, its RKHS is given by $\mathcal{H}_W := (\mathcal{F}_W, \langle \cdot, \cdot \rangle_W)$, where

$$\begin{aligned} \mathcal{F}_W &:= \{f : \mathbb{R}_0^+ \rightarrow \mathbb{R} : f \text{ is A.C., } f(0) = 0, f' \in L^2(\mathbb{R}_0^+)\} \\ \langle f, g \rangle &:= \frac{1}{\beta^2} \int_0^{+\infty} f'(x)g'(x) dx. \end{aligned}$$

As a consequence, to obtain the RKHS of k in the case of a periodic time-evolving graph, it is sufficient to do the direct sum of \mathcal{H} and \mathcal{H}_W .

D. Definition of isotropic kernels on arbitrary domains

In this brief Section, we state and enrich some crucial results of Anderes et al. [2020] that can be used in a variety of different frameworks. While Theorem 1 provides a straightforward recipe for the definition of kernels as compositions of variograms and completely monotone functions, Proposition D.1 characterises the separation property and the triangle inequality for a variogram. As a sheer application of the former, we obtain the proof of Proposition 8.

Proposition D.1. *Let Z , X and d as in Theorem 1. Then:*

1. *(X, d) is a semi-distance space if and only if, for all $x_1, x_2 \in X$, $Z(x_1) = Z(x_2)$ almost surely implies $x_1 = x_2$;*
2. *d satisfies the triangular inequality if and only if, for all $x_1, x_2, x_3 \in X$, it holds:*

$$\mathbb{C}\text{ov}(Z(x_1) - Z(x_2), Z(x_3) - Z(x_2)) \geq 0.$$

E. Proofs

Proof. of Proposition 1 The proof relies on Lemma B.1. By the proof of Proposition 2, we have:

$$\begin{aligned} \mathbb{V}\text{ar}(Z_V(u_1) - Z_V(u_2)) &= k_{Z_V}(u_1, u_1) + k_{Z_V}(u_2, u_2) - 2k_{Z_V}(u_1, u_2) \\ &= \boldsymbol{\delta}_1^\top (L^*)^{-1} \boldsymbol{\delta}_1 + \boldsymbol{\delta}_2^\top (L^*)^{-1} \boldsymbol{\delta}_2 - 2\boldsymbol{\delta}_1^\top (L^*)^{-1} \boldsymbol{\delta}_2 \\ &= (\boldsymbol{\delta}_1 - \boldsymbol{\delta}_2)^\top (L^*)^{-1} (\boldsymbol{\delta}_1 - \boldsymbol{\delta}_2) \\ &= (\boldsymbol{\delta}_1 - \boldsymbol{\delta}_2)^\top L^+ (\boldsymbol{\delta}_1 - \boldsymbol{\delta}_2), \end{aligned}$$

where the last step follows from Lemma B.1. Notice that the last expression does not depend on \boldsymbol{x} , therefore for all values of \boldsymbol{x} the variogram is the same. This settles the proof. \square

Proof. of Proposition 2

From the definition of Z_V , we have that

$$\begin{aligned} \mathbb{C}\text{ov}(Z_V(u_1), Z_V(u_2)) &= (1 - \delta_1)(1 - \delta_2)L^+[\underline{u}_1, \underline{u}_2] + (1 - \delta_1)\delta_2L^+[\underline{u}_1, \bar{u}_2] \\ &\quad + \delta_1(1 - \delta_2)L^+[\bar{u}_1, \underline{u}_2] + \delta_1\delta_2L^+[\bar{u}_1, \bar{u}_2] \\ &= \boldsymbol{\delta}_1^\top L^+[(\underline{u}_1, \bar{u}_1), (\underline{u}_2, \bar{u}_2)] \boldsymbol{\delta}_2. \end{aligned} \tag{E3}$$

Let us now consider the process Z_E . For the sake of simplicity, here we set $e_1 := (\underline{u}_1, \bar{u}_1)$ and $e_2 := (\underline{u}_2, \bar{u}_2)$. By construction, the covariance between $Z_E(u_1)$ and $Z_E(u_2)$ is null whenever $\text{lf}(e_2) \neq \text{lf}(e_1)$. Furthermore,

$$\text{Cov}(Z_E(u_1), Z_E(u_2)) = \ell(e_1) (\min(\delta_1, \delta_2) - \delta_1 \delta_2)$$

if $e_1 = e_2 \in E_T$ and

$$\text{Cov}(Z_E(u_1), Z_E(u_2)) = \sqrt{\ell(e_1) \ell(e_2)} k_T (|t(\underline{u}_1) - t(\underline{u}_2)|) (\min(\delta_1, \delta_2) - \delta_1 \delta_2)$$

if $e_1, e_2 \in E_S$ and $\text{lf}(e_1) = \text{lf}(e_2)$. By noticing that the covariance expression for former case is actually a special case of the one of the latter (recall that $k_T(0) = 1$), we can summarise the covariance function of Z_E for each couple of points $u_1, u_2 \in \mathbf{G}$ as follows:

$$k_{Z_E}(u_1, u_2) = \mathbb{1}_{\text{lf}(e_1) = \text{lf}(e_2)} \sqrt{\ell(e_1) \ell(e_2)} k_T (|t(\underline{u}_1) - t(\underline{u}_2)|) (\min(\delta_1, \delta_2) - \delta_1 \delta_2). \quad (\text{E4})$$

Notice that the process Z_E is defined on all the vertices V (it is zero) and that the expression (E4) is meaningful even when any of the points u_1 and u_2 belongs to V . Indeed, if, say, $u_1 \in V$, then $\delta_1 \in \{0, 1\}$ regardless of which incident edge (u, v) is taken in the expression $u_1 = (u, v, \delta)$. As a consequence, the last factor in (E4) vanishes and the covariance is therefore null. Finally, notice that, since Z_V and Z_E are independent, the covariance function of Z is simply the sum of (E3) and (E4). \square

Proof. of Proposition 3

Symmetry, non-negativeness and the implication $u_1 = u_2 \implies d(u_1, u_2) = 0$ follow immediately from (4.4). Therefore, we just need to show that $d(u_1, u_2) = 0 \implies u_1 = u_2$. From (4.4), if $d(u_1, u_2) = 0$, then $Z(u_1) = Z(u_2)$ almost surely. As a consequence:

$$Z_V(u_1) - Z_V(u_2) = -Z_E(u_1) + Z_E(u_2).$$

Being Z_V and Z_E independent, necessarily $Z_V(u_1) - Z_V(u_2) = 0$ and $-Z_E(u_1) + Z_E(u_2) = 0$, hence $Z_V(u_1) = Z_V(u_2)$ and $Z_E(u_1) = Z_E(u_2)$ a.s.. Now $Z_V(u_1)$ and $Z_V(u_2)$ are linear combinations of $Z_V(V)$, that is: $Z_V(u_1) = x_1^\top Z_V(V)$ and $Z_V(u_2) = x_2^\top Z_V(V)$ for some $x_1, x_2 \in \mathbb{R}^N$, where $N = |V|$. More specifically,

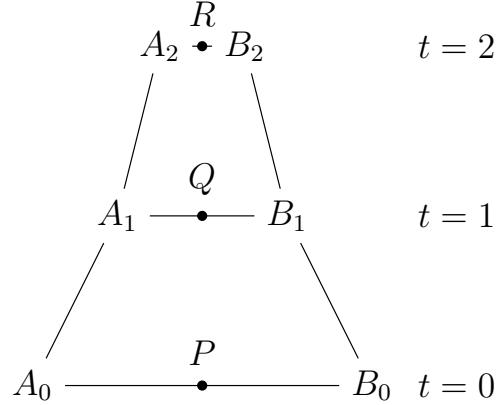


Figure E.1: An example of equivalent simple graph for which the semi-distance defined at (4.9) does not satisfy the triangle inequality. Here the length of the top edge (A_2, B_2) becomes vanishingly small, while length of the bottom edge (A_0, B_0) grows to infinity.

x_1 and x_2 have the following structure (here we assume that the vertices V are ordered, so that \underline{u}_i comes before \bar{u}_i , for $i \in \{1, 2\}$):

$$\begin{cases} x_1^\top = \begin{bmatrix} \mathbf{0}^\top & 1 - \delta_e(u_1) & \mathbf{0}^\top & \delta_e(u_1) & \mathbf{0}^\top \end{bmatrix} \\ x_2^\top = \begin{bmatrix} \mathbf{0}^\top & 1 - \delta_e(u_2) & \mathbf{0}^\top & \delta_e(u_2) & \mathbf{0}^\top \end{bmatrix}, \end{cases}$$

where the $\mathbf{0}$'s represent vectors of zeroes of the appropriate length (possibly zero). Since $Z_V(u_1) = Z_V(u_2)$ a.s., it follows that $(x_1 - x_2)^\top Z_V(V) = 0$ a.s., that is: $x_1 - x_2 = \lambda \mathbf{1}_N$ for some $\lambda \in \mathbb{R}$. Hence,

$$\lambda = \lambda \frac{\mathbf{1}_N^\top \mathbf{1}_N}{N} = \frac{1}{N} \mathbf{1}_N^\top (x_1 - x_2) = \frac{1}{N} (\mathbf{1}_N^\top x_1 - \mathbf{1}_N^\top x_2) = 0.$$

This means that $x_1 = x_2$, that is $u_1 = u_2$. \square

Proof. of Proposition 4 Consider the equivalent simple graph represented in Figure E.1, where all the weights of are 1, exception made for the edges (A_0, B_0) and A_2, B_2 , which have weights ε and $\frac{1}{\varepsilon}$ respectively, for a sufficiently small $\varepsilon > 0$. Considering the vertices in the order $A_0, B_0, A_1, \dots, B_2$, the

Laplacian matrix L is

$$L = \begin{bmatrix} 1+\varepsilon & -\varepsilon & -1 & 0 & 0 & 0 \\ -\varepsilon & 1+\varepsilon & 0 & -1 & 0 & 0 \\ -1 & 0 & 3 & -1 & -1 & 0 \\ 0 & -1 & -1 & 3 & 0 & -1 \\ 0 & 0 & -1 & 0 & 1+\frac{1}{\varepsilon} & -\frac{1}{\varepsilon} \\ 0 & 0 & 0 & -1 & -\frac{1}{\varepsilon} & 1+\frac{1}{\varepsilon} \end{bmatrix}.$$

Let now consider the points $P := (0, A_0, B_0, \frac{1}{2})$, $Q := (1, A_1, B_1, \frac{1}{2})$ and $R := (2, A_2, B_2, \frac{1}{2})$. We will show that, for any $\gamma > 0$, for ε sufficiently small, it holds

$$d(P, Q) + d(Q, R) < d(P, R). \quad (\text{E5})$$

First, let us rewrite and simplify a bit (E5). Notice that here all the δ 's are $\frac{1}{2}$.

$$\begin{aligned} (\text{E5}) &\iff k_Z(P, P) + k_Z(Q, Q) - 2k_Z(P, Q) \\ &\quad + k_Z(Q, Q) + k_Z(R, R) - 2k_Z(Q, R) \\ &\quad < k_Z(P, P) + k_Z(R, R) - 2k_Z(P, R) \\ &\iff k_Z(Q, Q) - k_Z(P, Q) - k_Z(Q, R) < -k_Z(P, R) \\ &\iff \frac{1}{4} \mathbf{1}_2^\top L^+ [(A_1, B_1), (A_1, B_1)] \mathbf{1}_2 + \sqrt{1 \cdot 1} \gamma^0 \cdot \frac{1}{4} \\ &\quad - \frac{1}{4} \mathbf{1}_2^\top L^+ [(A_0, B_0), (A_1, B_1)] \mathbf{1}_2 - \sqrt{\frac{1}{\varepsilon} \cdot 1} \gamma^1 \cdot \frac{1}{4} \\ &\quad - \frac{1}{4} \mathbf{1}_2^\top L^+ [(A_1, B_1), (A_2, B_2)] \mathbf{1}_2 - \sqrt{1 \cdot \varepsilon} \gamma^1 \cdot \frac{1}{4} \\ &< -\frac{1}{4} \mathbf{1}_2^\top L^+ [(A_0, B_0), (A_2, B_2)] \mathbf{1}_2 - \sqrt{\frac{1}{\varepsilon} \cdot \varepsilon} \gamma^2 \cdot \frac{1}{4} \\ &\iff \mathbf{1}_2^\top (L^+ [(A_1, B_1), (A_1, B_1)] + L^+ [(A_0, B_0), (A_2, B_2)]) \mathbf{1}_2 \\ &\quad + \mathbf{1}_2^\top (-L^+ [(A_0, B_0), (A_1, B_1)] - L^+ [(A_1, B_1), (A_2, B_2)]) \mathbf{1}_2 \\ &< -1 + \frac{\gamma}{\sqrt{\varepsilon}} + \gamma \sqrt{\varepsilon} - \gamma^2. \end{aligned} \quad (\text{E6})$$

Notice that the right-hand size of the last inequality (E6) is not limited for any $\gamma > 0$ when $\varepsilon \rightarrow 0^+$. As a consequence, it is sufficient to show that the left-hand size is limited when $\varepsilon \rightarrow 0^+$. Indeed the left-hand side of the last inequality is a sheer signed sum of 16 elements of the matrix L^+ . This sum is surely not greater than

$$16 \max_{i,j \in \{1, \dots, 6\}} |L^+[i, j]| \leq 16 \max_{i \in \{1, \dots, 6\}} |L^+[i, i]|.$$

Now, in our case, the main diagonal of L^+ is given by:

$$\text{diag}(L^+) = \left[\frac{10\varepsilon^2 + 39\varepsilon + 34}{36(\varepsilon^2 + 3\varepsilon + 1)}, \frac{10\varepsilon^2 + 39\varepsilon + 34}{36(\varepsilon^2 + 3\varepsilon + 1)}, \frac{10\varepsilon^2 + 27\varepsilon + 10}{36(\varepsilon^2 + 3\varepsilon + 1)}, \frac{10\varepsilon^2 + 27\varepsilon + 10}{36(\varepsilon^2 + 3\varepsilon + 1)}, \right. \\ \left. \frac{34\varepsilon^2 + 39\varepsilon + 10}{36(\varepsilon^2 + 3\varepsilon + 1)}, \frac{34\varepsilon^2 + 39\varepsilon + 10}{36(\varepsilon^2 + 3\varepsilon + 1)} \right].$$

As all the entries are continuous functions of $\varepsilon \in [0, 1]$, they are limited. Since the maximum of (a finite number of) limited functions on the same domain is limited, the left-hand of (E6) is limited as well. This concludes the proof. \square

Proof. of Proposition 6

The proof is very similar to the one of Proposition 3. Also in this case, we get symmetry, non-negativeness and the implication $u_1 = u_2 \implies d(u_1, u_2) = 0$ immediately from (4.4). Let us show that $d(u_1, u_2) = 0 \implies u_1 = u_2$. From (4.4), if $d(u_1, u_2) = 0$, then $Z(u_1) = Z(u_2)$ almost surely. As a consequence:

$$Z_V(u_1) - Z_V(u_2) = -Z_E(u_1) + Z_E(u_2) - \beta W(t_1) + \beta W(t_2).$$

Since Z_V is independent from Z_E and W , it must be $Z_V(u_1) = Z_V(u_2)$ a.s.. Following the same argument of the proof of Proposition 3, we obtain $(\underline{u}_1, \bar{u}_1, \delta_1) = (\underline{u}_2, \bar{u}_2, \delta_2)$. It remains to be shown that $t_1 = t_2$. Again, using $Z(u_1) = Z(u_2)$, and the independence between W_t and both Z_V and Z_E , we obtain $\beta W(t_1) = \beta W(t_2)$ a.s., that is $t_1 = t_2$. \square

Proof. of Theorem 1

1. Define $\tilde{d} := \sqrt{d}$. Since $d = \tilde{d}^2$ is a variogram, it is conditionally negative semidefinite: as a consequence, by Anderes et al. [2020, Theorem 6], $(X, \tilde{d}) \xrightarrow{id} H$ for some Hilbert space H . Therefore $(X, d) \xrightarrow{\sqrt{\cdot}} H$.
2. Follows immediately from the previous point and Anderes et al. [2020, Corollary 1].
3. If $Z(x_1) = Z(x_2)$ almost surely implies $x_1 = x_2$, then (X, d) is a semi-distance space by Proposition D.1. Thus, by Anderes et al. [2020, Corollary 1], $(x_1, x_2) \mapsto C(d(x_1, x_2))$ is strictly positive definite.

\square

Proof. of Proposition D.1

1. (X, d) is a semi-distance space iff $d(x_1, x_2) = 0$ implies $x_1 = x_2$. But $d(x_1, x_2) = 0$ is equivalent to $Z(x_1) = Z(x_2)$ almost surely.
2. Without loss of generality, we can restrict the proof to a zero-mean process X . Indeed, both the variance and the covariance do not change if we change the mean of their arguments. The proof consists in the following chain of equivalences. Let $x_1, x_2, x_3 \in X$.

$$\begin{aligned}
& d(x_1, x_2) + d(x_2, x_3) \geq d(x_1, x_3) \\
\iff & \mathbb{V}\text{ar}(Z(x_1) - Z(x_2)) + \mathbb{V}\text{ar}(Z(x_2) - Z(x_3)) \geq \mathbb{V}\text{ar}(Z(x_1) - Z(x_3)) \\
\iff & \mathbb{V}\text{ar} Z(x_1) + \mathbb{V}\text{ar} Z(x_2) - 2 \mathbb{C}\text{ov}(Z(x_1), Z(x_2)) \\
& + \mathbb{V}\text{ar} Z(x_2) + \mathbb{V}\text{ar} Z(x_3) - 2 \mathbb{C}\text{ov}(Z(x_2), Z(x_3)) \geq \\
& \mathbb{V}\text{ar} Z(x_1) + \mathbb{V}\text{ar} Z(x_3) - 2 \mathbb{C}\text{ov}(Z(x_1), Z(x_3)) \\
\iff & \mathbb{V}\text{ar} Z(x_2) - \mathbb{C}\text{ov}(Z(x_1), Z(x_2)) - \mathbb{C}\text{ov}(Z(x_2), Z(x_3)) \geq \\
& - \mathbb{C}\text{ov}(Z(x_1), Z(x_3)) \\
\iff & \mathbb{E}(Z^2(x_2) + Z(x_1)Z(x_3) - Z(x_1)Z(x_2) - Z(x_2)Z(x_3)) \geq 0 \\
\iff & \mathbb{E}((Z(x_2) - Z(x_1))(Z(x_2) - Z(x_3))) \geq 0 \\
\iff & \mathbb{C}\text{ov}(Z(x_2) - Z(x_1), Z(x_2) - Z(x_3)) \geq 0
\end{aligned}$$

□

F. Additional plots

The next figure shows some realisations of the process Z_E for an edge at four time steps, for different values of the correlation parameter ϕ , as described in Section 4.1.

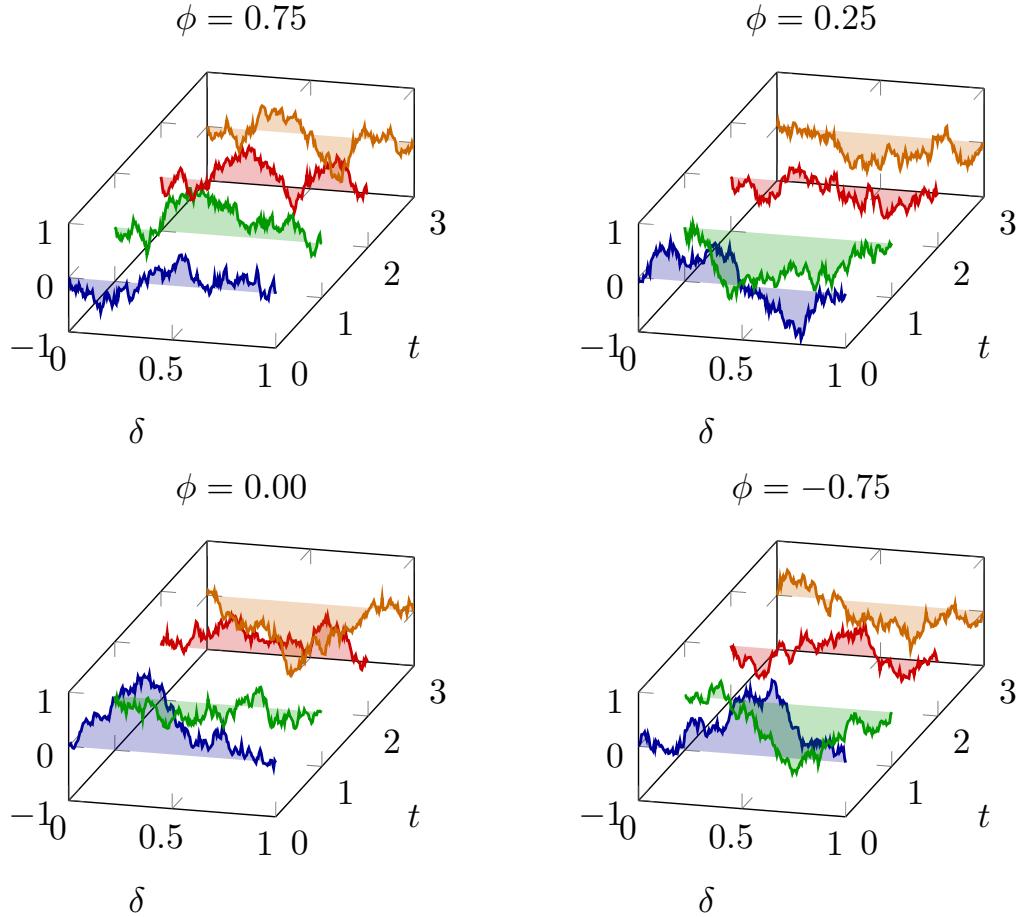
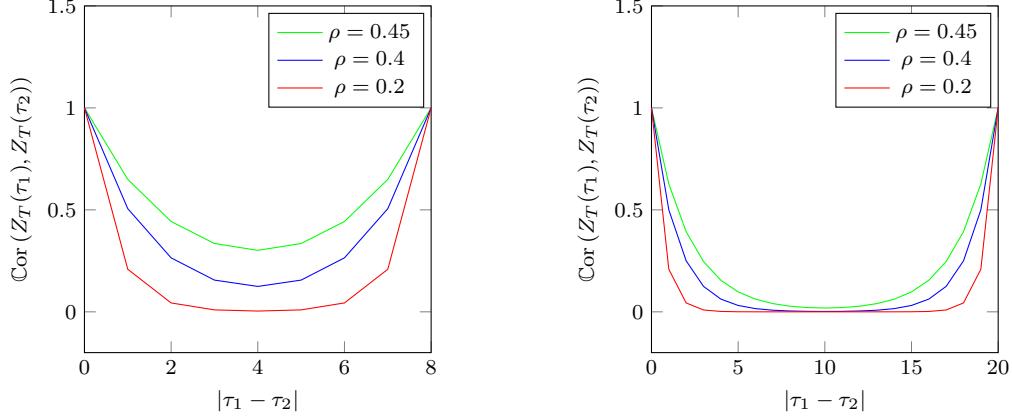


Figure F.1: Draws from the process Z_E on an edge with lifespan $\{0, 1, 2, 3\}$, for several values of the parameter ϕ .

The next Figure show two examples of correlation values σ_{Z_T} , as defined in Subsection 5.1, for some values of the parameter ρ and for two periods ($m = 8, 20$).



The correlations of Z_T for some values of ρ and $m = 8$.

The correlations of Z_T for some values of ρ and $m = 20$.

Figure F.2: Some examples of the correlation functions k_T in the case $\text{ls}(e) = \{0, \dots, m-1\}$.

The next Figure shows some covariance generated by the example presented in Subsection 6.1.

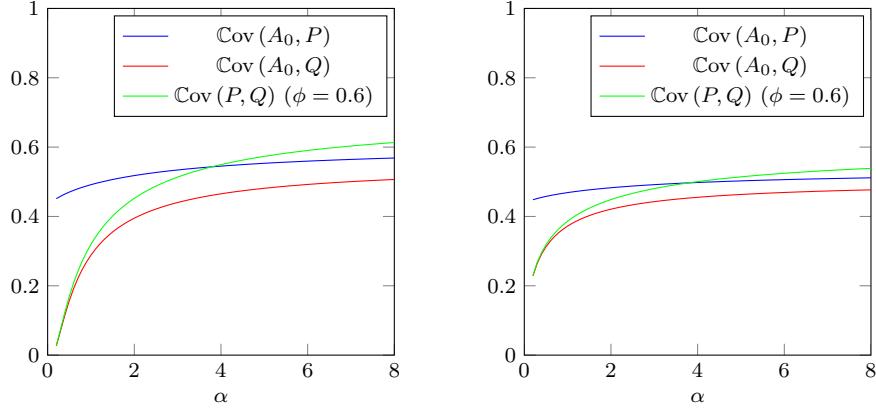


Figure F.3: Covariances generated by the distances in Figure 6 between the points A_0 , P and Q . Left: exponential kernel with parameters $(\alpha = 1, \beta = 1)$ (see Table 1). Right: generalised Cauchy kernel with parameters $(\alpha = 1, \beta = 5, \xi = 0.5)$ (see Table 1).

The next heatmaps provide the estimation of distances and covariances (and their errors) in the worked example presented in Section 7. It is in order to notice the huge difference in terms of accuracy under the two models (the true $\tilde{\mathbf{G}}_1$ and the misspecified static graph $\tilde{\mathbf{G}}_2$).

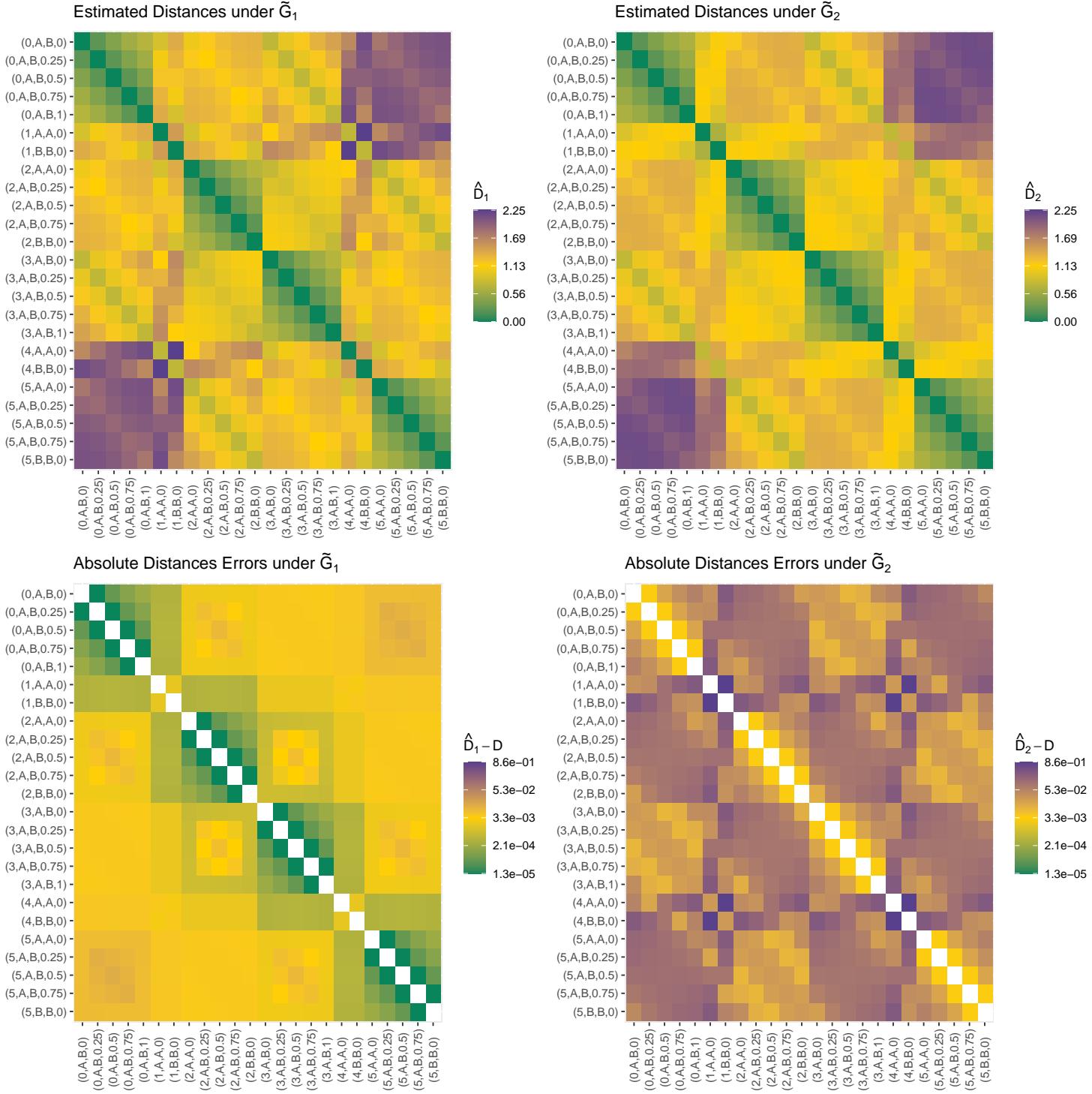


Figure F.4: Estimated distance matrices \hat{D} (top) and distance errors $\hat{D} - D$ (bottom) under the two graphs \tilde{G}_1 (left) and \tilde{G}_2 (right). Each row/column represents a spatio-temporal point, denoted by $(t, e, \bar{e}, \delta_e(u))$, accordingly to Definition 4 in the main text.

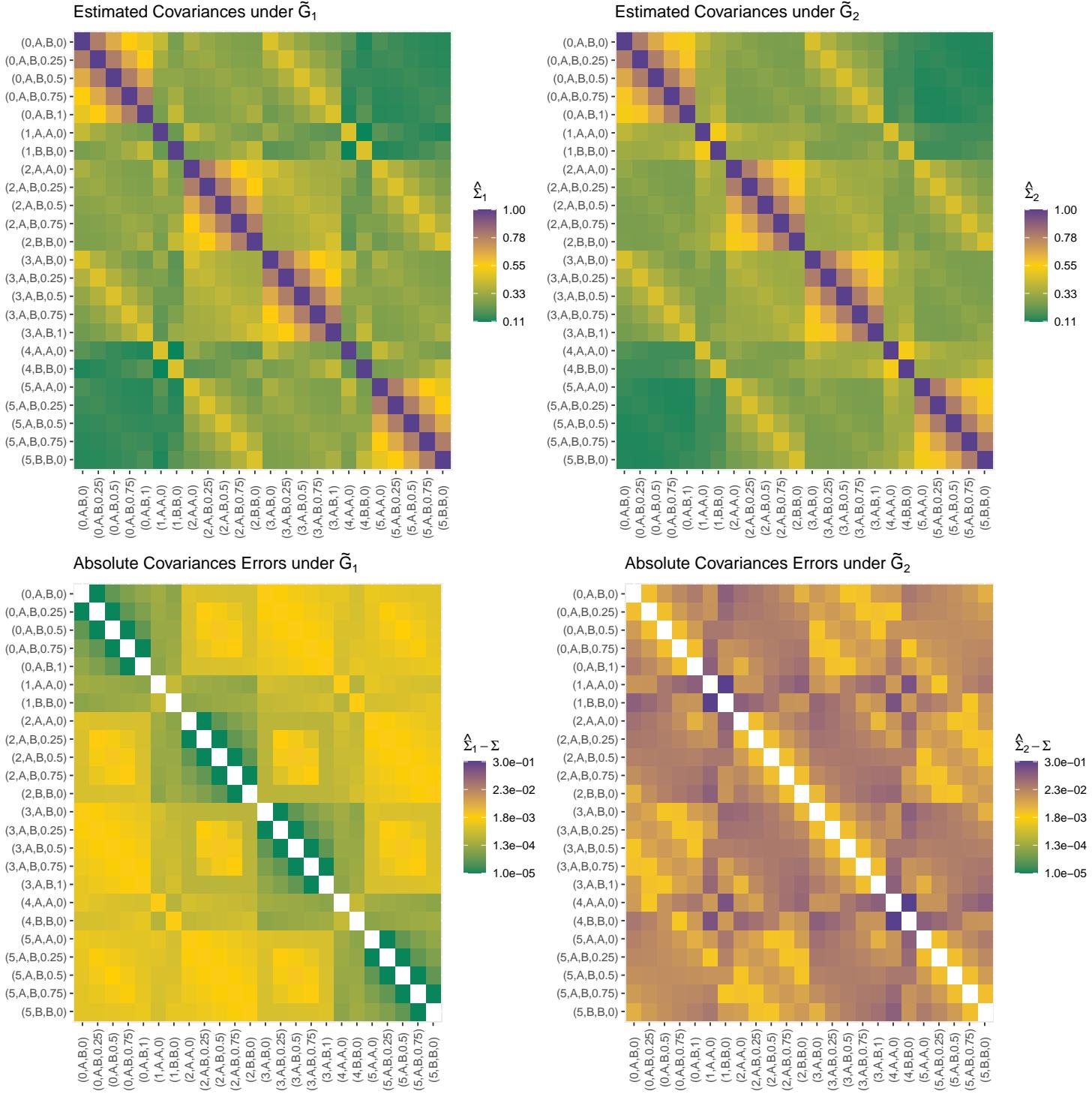


Figure F.5: Estimated covariance matrices $\hat{\Sigma}$ (top) and covariances errors $\hat{\Sigma} - \Sigma$ (bottom) under the two graphs \tilde{G}_1 (left) and \tilde{G}_2 (right). Each row/column represents a spatio-temporal point, denoted by $(t, \underline{e}, \bar{e}, \delta_e(u))$, accordingly to Definition 4 in the main text.

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