THE COMPLETION OF COVARIANCE KERNELS

BY KARTIK G. WAGHMARE AND VICTOR M. PANARETOS

We consider the problem of positive-semidefinite continuation: extending a partially specified covariance kernel from a subdomain \( \Omega \) of a rectangular domain \( I \times I \) to a covariance kernel on the entire domain \( I \times I \). For a broad class of domains \( \Omega \) called serrated domains, we are able to present a complete theory. Namely, we demonstrate that a canonical completion always exists and can be explicitly constructed. We characterise all possible completions as suitable perturbations of the canonical completion, and determine necessary and sufficient conditions for a unique completion to exist. We interpret the canonical completion via the graphical model structure it induces on the associated Gaussian process. Furthermore, we show how the estimation of the canonical completion reduces to the solution of a system of linear statistical inverse problems in the space of Hilbert-Schmidt operators, and derive rates of convergence. We conclude by providing extensions of our theory to more general forms of domains, and by demonstrating how our results can be used to construct covariance estimators from sample path fragments of the associated stochastic process. Our results are illustrated numerically by way of a simulation study and a real example.

CONTENTS

1 Introduction .......................................................... 1
2 Background and Notation .......................................... 3
3 The Canonical Completion ......................................... 5
4 Canonicity and Graphical Models ............................... 8
5 Necessary and Sufficient Conditions for Unique Completion 10
6 Characterisation of All Completions ............................ 11
7 Estimation of the Canonical Completion ....................... 14
  7.1 Definition of the Estimator ................................ 15
  7.2 Rate of Convergence ........................................ 16
8 Beyond Serrated Domains ....................................... 17
9 Covariance Estimation from Sample Path Fragments ......... 19
10 Simulation Study .................................................. 21
  10.1 General Simulation Study ................................ 21
  10.2 Estimator Performance versus \( m \) ...................... 22
  10.3 Comparative Simulations ................................. 23
11 Illustrative Data Analysis ....................................... 24
References ............................................................ 24

1. Introduction. Consider a bivariate function \( K_\Omega : \Omega \to \mathbb{R} \) where \( \Omega \) is a subset of \( I \times I \) for some bounded interval \( I \subset \mathbb{R} \). An extension of \( K_\Omega \) to a covariance kernel on \( I \) is called a completion. Under appropriate conditions on \( \Omega \) and \( K_\Omega \), we would like to answer the following questions: Does a completion always exist? Is there a canonical completion and can we construct it explicitly? Can we characterise the set of all completions? Can we give
necessary and sufficient conditions for a unique completion to exist? Is a unique completion necessarily canonical?

Such questions are arguably very natural from a mathematical point of view, with connections to the trigonometric moment problem and the continuation of characteristic functions, via Bochner’s theorem. They are well understood for covariance matrices and for stationary/isotropic kernels. It appears that the study of positive-definite completions was initiated by Carathéodory [4], who showed that every positive-definite function on a subset \( \{ j \in \mathbb{Z} : |j| \leq n \} \) of \( \mathbb{Z} \) extends to a positive-definite function on \( \mathbb{Z} \). A continuous analogue of this result was proved by Krein in [21] for continuous positive-definite functions on a symmetric interval of the real line, and the problem of uniqueness as well as that of description of all extensions in case of non-uniqueness was considered in the same context by Krein & Langer [22].

The case of positive-definite completions of banded matrices was considered by Gohberg & Dym [12]. The general case was treated by Grone et al. [16]. Many of these results have been further extended to matrices with operator entries in Gohberg, Kaashoek & Woerdeman [14] and Paulsen [25]. An extensive survey concerning the importance of positive-definite functions and kernels can be found in Stewart [31].

Our interest is to obtain a theory for the case where \( I \) is an interval and \( K_\Omega \) is not constrained to satisfy invariance properties such as stationarity. Besides the intrinsically mathematical motivation for developing such extensions, we are motivated by the problem of covariance estimation from sample path fragments. Namely, estimating the covariance of a (potentially non-stationary) second-order process \( X = \{ X_t : t \in I \} \) on the basis of i.i.d. sample paths \( \{ X_j \} \) censored outside subintervals \( \{ I_j \} \), i.e. on the basis of fragments \( X_j|I_j \), drawn from \( X_{I_j} = \{ X_t : t \in I_j \} \) for a collection of subintervals \( \{ I_j \} \) of \( I \). Because of the fragmented nature of the observations, one is only able to estimate a restriction \( K_\Omega \) of \( K \) to a symmetric region, say \( \Omega \subset I \times I \) centered around the diagonal. Nevertheless, one needs an estimator of the full covariance \( K \), as this is necessary for further statistical analysis – tasks like dimension reduction, regression, testing, and classification require the complete covariance.

The problem thus reduces to ascertaining how and under what conditions one can estimate \( K \) from an estimate \( K_\Omega \) of \( K_\Omega \). This problem arises in a range of contexts, as documented in the references in the next paragraph. For instance, in longitudinal studies where a continuously varying random quantity (e.g. bone mineral density or systolic blood pressure) is measured on each study subject over a short time interval (see Section 11 for a presentation and analysis of such an example), or in the modeling of hourly electricity pricing, where price functions are only partially observed.

Kraus [20] originally introduced and studied a simpler version of this problem, where some samples were observable over the entire domain, hence resulting in reduced rather than no information outside \( \Omega \). Delaigle & Hall [7] were the first to attack the genuinely fragmented problem, by imposing a (discrete) Markov assumption. Though their approach also yielded a completion, it was more focussed on predicting the missing segments. Similarly, Kneip & Leibl [19] focussed on how to optimally reconstruct the missing segments using linear prediction. The problem has been recently revisited with a firm focus on the identifiability and estimation of the complete covariance itself, see Descary & Panaretos [10], Delaigle et al. [8] and Lin et al. [23]. At a high level, they all proceed by (differently) penalized least squares fitting of a finite-rank tensor product expansion over the region \( \Omega \), which is then used to extrapolate the covariance beyond \( \Omega \). While there are substantial differences in their set up and technique, common to all three approaches is the pursuit of sufficient conditions on the process \( X \) for identifiability to hold, i.e. for a uniquely existing completion. Imposing such
conditions \textit{a priori} ensures that extrapolation is sensible. Starting with a strong condition in [10] (namely, analyticity), these sufficient conditions have progressively been weakened, albeit not to the point of attaining conditions that are also necessary.

We shall pursue a different approach to the problem, which we believe sheds more insight, and ultimately leads to necessary and sufficient conditions for uniqueness. Rather than start by focussing on uniqueness, we will aim at a comprehensive description of the set of all valid completions from a broad class of domains $\Omega$ called \textit{serrated domains}. Specifically, we will exhibit that a \textit{canonical completion} can always be explicitly and uniquely constructed (Section 3). Canonicity will be clearly interpreted by means of a graphical model structure on the associated Gaussian process (Section 4). We will then obtain necessary and sufficient conditions for a unique completion to exist, and discuss how these relate to the problem of identifiability (Section 5). Furthermore, we will constructively characterise the set of completions as suitable perturbations of the canonical completion (i.e. show how any other valid completion can be built using the canonical completion; see Section 6) and parametrize this set in terms of contractions between certain $L^2$ spaces (Theorem 6.3). As for the statistical side of the question related to fragments, since a canonical solution always exists uniquely, and is equivalent to the unique completion when uniqueness holds, it is always an identifiable and interpretable target of estimation. We thus consider how to estimate it based on an estimator of the observed partial covariance, say $\hat{K}_\Omega$, and provide rates of convergence in Section 7.

We then show how our results can be adapted to more general domains $\Omega$ in Section 8. This allows us to give a treatment of the statistical problem of covariance estimation from sample path fragments in Section 9. The finite sample performance of our statistical methodology is investigated by means of an extensive simulation study (Section 10) and a data analysis (Section 11). The proofs of our results are collected in the Supplementary Material.

Our general perspective is inspired by the work of Grone et al. [16] and Dym & Gohberg [12] on matrices. Our methods, however, are very different, because algebraic tools such as determinants and matrix factorizations that are elemental to those works are unavailable in the kernel case. Instead, we generalize the concept of canonical extension [12] (or determinant-maximizing completion [16]) to a general kernel version by demonstrating and exploiting its intimate connection to Reproducing Kernel Hilbert Spaces (RKHS) and graphical models for random processes (Theorem 4.3). An apparent consequence is that our necessary and sufficient conditions for a partial covariance to complete uniquely (Theorem 5.1) seem to be novel even in the context of matrices.

2. Background and Notation. To set the context of the problem, we delineate the functions $K_\Omega$ that are admissible as partial covariances, and the types of domains $\Omega$ under consideration. Recall that $K : I \times I \to \mathbb{R}$ is a covariance kernel on $I$ if

1. $K(s, t) = K(t, s)$ for $s, t \in I$, and
2. $\sum_{i,j=1}^{n} \alpha_i \alpha_j K(t_i, t_j) \geq 0$ for $n \geq 1$, $\{t_i\}_{i=1}^{n} \subset I$ and $\{\alpha_i\}_{i=1}^{n} \subset \mathbb{R}$.

We shall denote the set of covariances on $I$ by $\mathcal{C}$. We shall say that $\Omega \subset I \times I$ is a \textit{symmetric domain} if $(s, t) \in \Omega$ if $(t, s) \in \Omega$ for $s, t \in I$ and $\{(t, t) : t \in I\} \subset \Omega$. Since a covariance is always defined over square domains, it is natural to define partial covariances as follows:

**Definition 2.1 (Partial Covariance).** Let $I$ be a set and $\Omega \subset I \times I$ be a symmetric domain. A function $K_\Omega : \Omega \to \mathbb{R}$ is called a partial covariance on $\Omega$ if for every $J \subset I$ such that $J \times J \subset \Omega$, the restriction $K_J = K_\Omega|_{J \times J}$ is a covariance on $J$.

In the above definition, the set $J$ need not be an interval.
Remark 2.2 (On Notation). Whenever we write $K_J$ for some $J \subset I$, we will always understand that this refers to the restriction $K_I|_{J \times J}$ of the partial covariance $K_I$ to the square $J \times J \subseteq \Omega$.

A completion of the partial covariance $K_I$ will be a function $K : I \times I \to \mathbb{R}$ such that

$$K \in \mathcal{C}$$

and $K|_{\Omega} = K_{\Omega}$.

The set of all possible completions of $K_I$ will be denoted by

$$\mathcal{C}(K_{\Omega}) = \{ K \in \mathcal{C} : K|_{\Omega} = K_{\Omega} \}.$$  

Note that our definition of partial covariance does not a priori assume that $K_{\Omega}$ arises as the restriction of a covariance $K$ on $I$. Rather, it defines $K_{\Omega}$ intrinsically on $\Omega$. In this sense, our setting is more general than the functional fragment setting. Consequently, $\mathcal{C}(K_{\Omega})$ is not automatically non-empty. Notice however that if $K_1, K_2 \in \mathcal{C}(K_{\Omega})$ then $\alpha K_1 + (1 - \alpha)K_2 \in \mathcal{C}(K_{\Omega})$ for every $\alpha \in (0, 1)$. $\mathcal{C}(K_{\Omega})$ is thus convex. It is also bounded so as $\sup_{t \in I} |K(t, t)| < \infty$ because for every $K \in \mathcal{C}(K_{\Omega})$ we have $|K(s, t)| \leq \sqrt{K(s, s)}K(t, t) \leq \sup_{t \in I} |K(t, t)|$. It follows from convexity that $\mathcal{C}(K_{\Omega})$ can either be an empty set, a singleton or have an (uncountably) infinite number of elements. Finally, the elements of $\mathcal{C}(K_{\Omega})$ inherit the regularity properties of $K_{\Omega}$. In particular, if $K_{\Omega} \in C^{k,k}(\Omega)$, then $K \in C^{k,k}(I \times I)$, where $C^{k,k}(\Delta)$ for a domain $\Delta \subset I \times I$ denotes the set of functions $F : \Delta \to \mathbb{R}$ such that the partial derivatives $\partial^i_x \partial^j_y F(x, y)$ and $\partial^i_x \partial^j_y F(x, y)$ exist for $0 \leq i, j \leq k$. This is a direct consequence of the fact that the process $X$ is $k$-differentiable in quadratic mean if and only its covariance’s partial derivatives $\partial^i_x \partial^j_y K$ and $\partial^i_x \partial^j_y K$ exist for $0 \leq i, j \leq k$ at the diagonal $\{ (x, x) : x \in I \}$ (see [24] or [29]). Indeed, if $K_{\Omega} \in C^{k,k}(\Omega)$, then the corresponding process $X$ is $k$-differentiable in quadratic mean and hence $K \in C^{k,k}(I \times I)$.

In some cases, we will need to work with the covariance operators associated with the corresponding covariance kernels. For a measure $\mu$ on the Borel sets of $I$, and $S \subseteq I$ we define the Hilbert space $L^2(S)$ to be the set of all $f : S \to \mathbb{R}$ such that $\int_S f^2(x) \mu(dx) < \infty$ with associated inner product

$$\langle f, g \rangle_2 = \int_S f(x)g(x)\mu(dx), \quad f, g \in L^2(S).$$

Since continuity of $K_{\Omega}$ implies continuity of any completion thereof, any completion $K$ induces a Hilbert-Schmidt integral operator $K : L^2(I) \to L^2(I)$ given by

$$Kf(x) = \int_I K(x, y)f(y)\mu(dy), \quad \mu - \text{a.e.},$$

i.e. an operator with $K$ as its integral kernel. Similarly, any restriction $K|_{S \times S}$ on a square domain induces an integral operator $K|_S : L^2(S) \to L^2(S)$ by way of

$$K|_S g(x) = \int_S K(x, y)g(y)\mu(dy), \quad \mu|_S - \text{a.e.}$$

The operator norm $\| \cdot \|_\infty$ and Hilbert-Schmidt norm $\| \cdot \|_2$ of an operator $K : L^2(S_1) \to L^2(S_2)$, $S_1, S_2 \subseteq I$, with continuous kernel $K : S_1 \times S_2 \to \mathbb{R}$ will be defined via

$$\|K\|_\infty = \sup_{f \in L^2(S_1) \setminus \{0\}} \frac{\int_{S_2} \left( \int_{S_1} K(u, v)f(v)\mu(du) \right)^2 \mu(du)}{\int_{S_1} f^2(u)\mu(du)}$$

and

$$\|K\|_2 = \int_{S_1} \int_{S_2} K^2(u, v)\mu(du)\mu(dv).$$
The positive root of an operator $A$ will be denoted by $|A| = (A^*A)^{1/2}$. We denote the space of Hilbert-Schmidt operators from $L^2(S_1)$ to $L^2(S_2)$ as $S_2(S_1, S_2)$. The image of a subset $S_1 \subseteq L^2(S_1)$ via the operator $K : L^2(S_1) \to L^2(S_2)$ will be simply denoted as $K S_1 = \{ K f : f \in S_1 \}$. We shall use the same convention for operator multiplication, for example, we denote $K S_2(S_3, S_1) = \{ K A : A \in S_2(S_3, S_1) \}$.

Given a Hilbert-Schmidt operator $K : L^2(S_1) \to L^2(S_1)$ with integral kernel $K : S_1 \times S_1 \to \mathbb{R}$, we define the Reproducing Kernel Hilbert Space (RKHS) of $K$ (equivalently of $K$) as the Hilbert space $\mathcal{H}(K) = K^{1/2} L^2(S_1)$, endowed with the inner product

$$\langle f, g \rangle_{\mathcal{H}(K)} := \langle K^{-1/2} f, K^{-1/2} g \rangle_{L^2(S_1)}, \quad f, g \in \mathcal{H}(K).$$

As for the types of symmetric domains $\Omega$ under consideration, our main focus will be on serrated domains:

**Definition 2.3 (Serrated Domain).** Let $I \subset \mathbb{R}$ be a bounded interval. A domain $\Omega \subseteq I \times I$ is called serrated if it can be written as a union $\Omega = \bigcup_j (I_j \times I_j)$ for $\{I_j\}$ a finite cover of $I$ comprised of subintervals $I_j \subseteq I$.

Informally, a serrated domain consists of a collection of squares of varying sizes, strung symmetrically along the diagonal in a manner that covers it (see Figure 1). When restricting attention to matrices or stationary kernels, serrated domains reduce to the types of domains on which the problem has been previously studied. In the functional fragments problem, the observation of a finite collection of path fragments $X_j|_{I_j}$ leads to partial covariance information on the serrated domain $\Omega = \bigcup_j (I_j \times I_j)$. By taking sequences of covers consisting of progressively more squares, serrated domains can approximate a very rich class of symmetric domains that we call nearly serrated (see Figure 1 and Definition 8.1 for a rigorous definition). In the next sections, we develop an essentially complete theory of completion for serrated domains. Then, Section 8 demonstrates how our results on serrated domains can be used to obtain results for nearly serrated domains.

3. The Canonical Completion. Recall that the set of completions $\mathcal{C}(K_\Omega)$ of a partial covariance $K_\Omega$ can be empty, a singleton, or uncountably infinite. We will now show that for $\Omega$ a serrated domain, $\mathcal{C}(K_\Omega)$ is never empty. We will do so by explicitly constructing a completion $K_*$, that will be subsequently argued to be canonical.

It is instructive to commence with the 2-serrated case, i.e. when $\Omega = (I_1 \times I_1) \cup (I_2 \times I_2)$ for two intervals $\{I_1, I_2\}$ such that $I_1 \cup I_2 = I$, depicted in Figure 2 (left). Define a function $K_* : I \times I \to \mathbb{R}$ as follows:

$$K_*(s, t) = \begin{cases} K_\Omega(s, t), & (s, t) \in \Omega \\ \langle K_\Omega(s, \cdot), K_\Omega(\cdot, t) \rangle_{\mathcal{H}(K_{I_1 \cap I_2})}, & (s, t) \notin \Omega. \end{cases}$$
Here, $K_{I_1 \cap I_2} = K_{\Omega}|_{(I_1 \cap I_2)^2}$ is the restriction of the partial covariance $K_{\Omega}$ to the square $(I_1 \cap I_2) \times (I_1 \cap I_2)$ and $\mathcal{H}(K_{I_1 \cap I_2})$ is the RKHS of $K_{I_1 \cap I_2}$. It is implicit in the notation $(K_{\Omega}(s, \cdot), K_{\Omega}(\cdot, t))_{2\mathcal{H}(K_{I_1 \cap I_2})}$ that the domain of $K_{\Omega}(s, \cdot)$ and $K_{\Omega}(\cdot, t)$ is automatically restricted to $I_1 \cap I_2$ within that inner product, as depicted in Figure 2 (right).

**Remark 3.1.** The reproducing kernel inner product in Equation 2 can be seen as the infinite-dimensional equivalent of matrix multiplication formulas appearing in maximum entropy matrix completion [17] and low rank matrix completion [11].

Our first result is now:

**Theorem 3.2 (Canonical Completion from a 2-Serrated Domain).** Given any partial covariance $K_{\Omega}$ on a 2-serrated domain $\Omega \subseteq I \times I$, the function $K_* : I \times I \to \mathbb{R}$ defined in (2) is a well-defined covariance that constitutes a valid completion, i.e.

$$K_* \in \mathcal{C}(K_{\Omega}).$$

In particular, if $K_{\Omega}$ admits a unique completion, then this must equal $K_*$. 

The second part of the theorem hints at why we refer to the completion $K_*$ as the canonical completion of $K_{\Omega}$. We will provide a more definitive reason in Section 4, but first we will use the formula from the 2-serrated case in order to extend our result to a general serrated domain.

**Fig 2:** A two serrated domain (left) and a heuristic illustration of the formula for $K_*$. 

We will do this iteratively. Intuitively, if we have a general serrated domain generated by a cover of $m$ subintervals $\{I_1, ..., I_m\}$, we can apply the 2-serrated formula to any pair of successive squares $\{I_p^2, I_{p+1}^2\}$, to reduce to the problem to one of completion from a serrated domain generated the reduced set of $m-1$ subintervals $\{I_1, ..., I_{p-1}, I_p \cup I_{p+1}, I_{p+2}, ..., I_m\}$ (see Figure 3). Repeating the same prescription, we can eventually complete $K_\Omega$ to a covariance on $I$. To be more precise, let $\Omega = \bigcup_{j=1}^m (I_j \times I_j)$ be an $m$-serrated domain and for notational ease assume that the indices of the $\{I_j\}$ correspond to their natural partial ordering as intervals. Define the intersection of any two successive squares as

$$J_p = (I_p \times I_p) \cap (I_{p+1} \times I_{p+1})$$

and the corresponding restriction of $K_{\Omega}$ as $K_{J_p} = K_{\Omega}|_{J_p \times J_p}$. Next define the square of the union of the intervals $\{I_1, ..., I_p\}$ as

$$U_p = (I_1 \cup ... \cup I_p) \times (I_1 \cup ... \cup I_p).$$
Finally, define the serrated domain generated by the cover \( \{ \bigcup_{j=1}^{p} I_j, I_p+1, \ldots, I_m \} \) as

\[
\Omega_p = U_p \bigcup \{ \bigcup_{j=p+1}^{m} (I_j \times I_j) \}
\]

noting that \( \Omega_1 = \Omega \).

The following algorithm uses the formula from the 2-serrated case to extend \( K_\Omega \) to a partial covariance on \( \Omega_2 \), then \( \Omega_3 \), and so on, until completion to covariance on \( I^2 = \Omega_m \):

**Algorithm 1:** \( m \)-Serrated Completion by Successive 2-Serrated Completions

1. Initialise with the partial covariance \( K_1 = K_\Omega \) on \( \Omega_1 = \Omega \).

2. For \( p \in \{1, \ldots, m-1\} \) define the partial covariance \( K_{p+1} \) on \( \Omega_{p+1} \) as

\[
K_{p+1}(s,t) = \begin{cases} K_p(s,t), & (s,t) \in \Omega_p \\ \langle K_p(s,\cdot), K_p(\cdot,t) \rangle_{\mathcal{G}(K_{Jp})}, & (s,t) \in \Omega_{p+1} \setminus \Omega_p. \end{cases}
\]

3. Output the covariance \( K_\ast = K_m \) on \( I \times I = \Omega_m \).

Of course, there is nothing special about the application of the iterative completion in ascending order. We could have set up our notation and algorithm using a descending order starting with \( \{ I^2_{p+1}, I^2_{m-1} \} \), or indeed using an arbitrary order, starting from any pair of successive squares \( \{ I^2_p, I^2_{p+1} \} \) and moving up and down to neighbouring squares. Our second result shows that, no matter the chosen order, the algorithm will output the same valid completion \( K_\ast \in \mathcal{C}(K_\Omega) \):

**Theorem 3.3 (Canonical Completion from a General Serrated Domain).** The recursive application of the 2-serrated formula as described in Algorithm (1) to a partial covariance \( K_\Omega \) on a serrated domain \( \Omega \) yields the same valid completion \( K_\ast \in \mathcal{C}(K_\Omega) \), irrespective of the order it is applied in. In particular, if \( K_\Omega \) admits a unique completion, then this must equal \( K_\ast \).

Notice that Theorems 3.2 and 3.3 make no assumption on \( K_\Omega \) except that it be a partial covariance. In particular, \( K_\Omega \) need not be continuous or even bounded.
Example 3.4 (Brownian Motion). As an example, consider the following partial covariance on a 2-serrated subdomain of \([0, 1]^2\):

\[
K_\Omega(s, t) = s \wedge t, \quad (s, t) \in \Omega = \left(\left[0, \frac{2}{3}\right] \times \left[0, \frac{2}{3}\right]\right) \cup \left(\left[\frac{1}{3}, 1\right] \times \left[\frac{1}{3}, 1\right]\right).
\]

Clearly, this can be completed to the covariance of standard Brownian motion on \([0, 1]^2\),

\[
K(s, t) = s \wedge t, \quad (s, t) \in [0, 1]^2.
\]

To see what our completion algorithm yields, we note that the restriction \(K_{[1/3, 2/3]}\) yields the RKHS inner product

\[
(f, g)_{\mathcal{H}(K_{[1/3, 2/3]})} = \frac{1}{(1/3)} \int_{1/3}^{2/3} f'(u)g'(u)du.
\]

Thus, for \(s \in (2/3, 1]\) and \(t \in [0, 1/3)\),

\[
K_s(s, t) = \frac{1}{(1/3)} \int_{1/3}^{2/3} \frac{\partial}{\partial u}K_\Omega(s, u)\frac{\partial}{\partial u}K_\Omega(u, t)du = t = s \wedge t, \quad \text{since } t < s.
\]

Iterating, we can directly see that the extension of a partial covariance that has the form \(s \wedge t\) on an arbitrary domain by means of Algorithm 1 will also yield the covariance of Brownian motion.

The example illustrates that Algorithm 1 yields the “right” answer in an important special case. The next section demonstrates that this is no accident, and that the completions given in Theorems 3.2 and 3.3 are indeed canonical in a strong sense.

4. Canonicity and Graphical Models. We will now interpret the canonical completion via the conditional independence structure it induces on the associated Gaussian process. Recall that an undirected graph \(G\) on a set \(I\) is an ordered pair \(G = (I, \Omega)\) where \(I\) is called the vertex set and \(\Omega \subseteq I \times I\) is the edge set such that \((s, t) \in \Omega\) if and only if \((t, s) \in \Omega\). We shall often refer to the graph \((I, \Omega)\) as \(\Omega\). Notice that if \(I\) is an interval of the real line, then a symmetric domain \(\Omega\) induces an uncountable graph on \(I\) with \(\Omega\) serving as the edge set.

We shall say that \(S \subseteq I\) separates \(s, t \in I\) with respect to the graph \((I, \Omega)\) if every path from \(s\) to \(t\) comprised of edges in \(\Omega\) is intercepted by \(S\), that is, for every \(\{t_i\}_{i=1}^{r} \subseteq I\) with \(r \geq 1\) such that \(t_1 = s\), \((t_i, t_{i+1}) \in \Omega\) for \(1 \leq i < r\) and \(t_r = t\), we have that \(t_j \in S\) for some \(1 < j < r\).

A graph \((I, \Omega)\) induces a conditional independence structure on a Gaussian process \(X_I := \{X_t : t \in I\}\) much in the same way as in the finite dimensional case.

Definition 4.1 (Graphical Models on Gaussian Processes). The Gaussian process \(X = \{X_t : t \in I\}\) is said to form an undirected graphical model over the graph \(\Omega \subseteq I \times I\), if for every \(s \in I\) separated by \(J \subset I\), we have

\[
\text{Cov}(X_s, X_t | X_J) = \mathbb{E}[(X_s - \mathbb{E}[X_s | X_J])(X_t - \mathbb{E}[X_t | X_J]) | X_J] = 0 \quad \text{a.s.}
\]

Equation (3) implies that \(\mathbb{E}[X_s X_t | X_J] = \mathbb{E}[X_s | X_J] \mathbb{E}[X_t | X_J]\) almost surely. Taking the expectation gives

\[
\mathbb{E}[X_s X_t] = \mathbb{E}[\mathbb{E}[X_s | X_J] \mathbb{E}[X_t | X_J]],
\]
i.e. the covariance of $X_s$ and $X_t$ coincides with that of their best predictors given $X_J$ when $J$ separates $s$ and $t$. Notice that from (4), it follows that
\[
\mathbb{E} \left[ \mathbb{E} [X_s | X_J] \mathbb{E} [X_t | X_J] \right] = \mathbb{E} \left[ \mathbb{E} \left[ \mathbb{E} [X_s | X_J] | X_J \right] \mathbb{E} [X_t | X_J] \right] = \mathbb{E} [X_s \mathbb{E} [X_t | X_J]]
\]
and thus, $\mathbb{E} \left[ (X_t - \mathbb{E} [X_t | X_J]) X_s \right] = 0$ which implies that $\mathbb{E} [X_t | X_J] = \mathbb{E} [X_t | X_J, X_s]$. Similar reasoning yields,
\[
\mathbb{E} [f(X_t) | X_J, X_s] = \mathbb{E} [f(X_t) | X_J]
\]
which is reminiscent of Markov processes, where
\[
\mathbb{E} [f(X_t) | \{X_u : u \leq v \}] = \mathbb{E} [f(X_t) | X_v]
\]
Indeed, the undirected graphical model structure induced by $\Omega$ is a natural generalization of the Markov property, but with a notion of separation stemming from the graph structure rather than simple time ordering. In the terminology of Markov random fields, Definition 4.1 is equivalent to the global Markov property with respect to $\Omega$.

Theorem 4.2. Let $K_\Omega$ be a partial covariance on a serrated domain $\Omega \subset I$. The canonical completion $K_*$ is the only completion of $K_\Omega$ such that the associated Gaussian process \{ $X_t : t \in I$ \} forms an undirected graphical model with respect to the graph $G = ([0,1], \Omega)$.

Said differently, $K_*$ is the only completion of $K_\Omega$ that possesses the global Markov property with respect to the edge set $\Omega$. Intuitively, the canonical completion is the unique completion to rely exclusively on correlations intrinsic to the “observed” set $\Omega$: it propagates the “observable” correlations of $K_\Omega$ to the rest of $I$ via the Markov property, without introducing any extrinsic “unobserved” correlations. By contrast, any other completion will introduce correlations extrinsic to those observed via $K_\Omega$. This last statement is considerably refined in Section 6, where we characterise all possible completions as perturbations of the canonical completion.

In closing this section, we give a result going in the opposite direction: namely we show that a Gaussian process admits a graphical model structure w.r.t. a serrated $\Omega$ if and only if it has a covariance that satisfies the defining equations (2) of a canonical completion. This is a result that is of interest in its own right, since it characterises the set of all Gaussian process graphical models compatible with $\Omega$. In doing so, it provides an arguably more convenient way of expressing conditional independence relations in a Gaussian process than, say, cross-covariance operators defined by Baker [3]. To state it rigorously, define the set of covariances
\[
\mathcal{G}_\Omega = \left\{ K \in \mathcal{C} : K(s,t) = \langle K(s, \cdot), K(\cdot, t) \rangle_{\mathcal{C}(K_J)} \text{ for all } J \subset I \text{ separating } s,t \in I \text{ in } \Omega \right\}.
\]
We can now state:

Theorem 4.3. Let $\{X_t : t \in I\}$ be a Gaussian process with covariance $K$. Then, $X$ forms an undirected graphical model with respect to a serrated $\Omega$ if and only if $K \in \mathcal{G}_\Omega$.

There is actually no reason to restrict attention to Gaussian processes, and we did this solely for interpretability: for a Gaussian process, the condition $K \in \mathcal{G}_\Omega$ can be interpreted in terms of conditional independence. But we can more generally define a second-order graphical model as long as we focus solely on conditional uncorrelatedness rather than conditional independence – just take Definition 4.1 and drop the word “Gaussian”, while replacing “graphical model” by “second order graphical model”.

5. Necessary and Sufficient Conditions for Unique Completion. We will now state necessary and sufficient conditions guaranteeing unique completion from a serrated domain \( \Omega \subset I \). And we will argue that identifiability can occur even without enforcing the existence of a unique extension. For this, we need some additional notation. Given \( A \subset B \subset \Omega \), let \( K_B/K_A \) be the Schur complement of \( K_B \) with respect to \( K_A \).

\[
(K_B/K_A)(s,t) = K_B(s,t) - \langle K_B(s,\cdot), K_B(\cdot,t) \rangle_{\mathcal{H}(K_A)}
\]

i.e. the covariance of the residuals \( \{X_t - \Pi(X_t|X_A) : t \in B \setminus A \} \), where \( \Pi(W|Z) \) is the best linear predictor of \( W \) given \( Z \). We now have:

**Theorem 5.1** (Unique Completion from a Serrated Domain). Let \( K_\Omega \) be a partial covariance kernel on a serrated domain \( \Omega = \bigcup_{p=1}^{m} I_p \times I_p \subset I \) corresponding to \( m \) intervals \( \{I_p\}_{p=1}^{m} \) covering \( I \). The following two statements are equivalent:

(I) \( K_\Omega \) admits a unique completion on \( I \), i.e. \( \mathcal{C}(K_\Omega) \) is a singleton.

(II) there exists an \( r \in \{1, \ldots, m\} \), such that

\[
K_{I_p}/K_{I_p \cap I_{p+1}} = 0, \text{ for } 1 \leq p < r \quad \text{and} \quad K_{I_{q-1}}/K_{I_0 \cap I_{q+1}} = 0, \text{ for } r \leq q < m.
\]

Condition (II) is strictly weaker than any of the sufficient conditions that have previously been stated in the literature on functional fragments (e.g. [8, Theorem 1] and [10, Proposition 2]). Consequently, none of those conditions is necessary in the context of a serrated domain (for a discussion of more general domains, see Section 8). Furthermore, an appealing feature of (II) is that it is checkable at the level of \( K_\Omega \) in a concrete manner by constructing a finite number of Schur complements (in fact the number is linear in \( m \)).

Theorem 5.1 elucidates just how restrictive it is to a priori assume that a unique completion exists. When the Schur complements involved in (II) vanish, one can start with the associated process \( \{X_t : t \in I_r\} \) restricted to \( I_r \), and iteratively perfectly predict each segment \( \{X_t : t \in I_j\} \) by means of best linear prediction. Consequently, the entire process \( \{X_t : t \in I\} \) is generated as the image of its restriction \( \{X_t : t \in I_r\} \) via a deterministic linear operator. Indeed which interval(s) \( \{I_j\}_{j=1}^{m} \) generate(s) the process can be discovered by checking the equations given in (II).

Note, however, that being able to identify \( K \) from \( K_{|\Omega} \) does not require assuming that \( K_{|\Omega} \) completes uniquely – all we need is a way to select one element from \( \mathcal{C}(K_{|\Omega}) \). For example, to obtain identifiability, it would be much less restrictive to assume the admittance of a (second order) graphical model with respect to \((I, \Omega)\). The set of covariances \( \mathcal{G}_\Omega \) corresponding to such processes is potentially very large, and encompasses highly “non-deterministic” dependence structures. Assuming that \( K \in \mathcal{G}_\Omega \) will then yield identifiability given \( K_{|\Omega} \) via Theorem 4.2, which can be re-interpreted in this notation as stating

\[
\mathcal{C}(K_{|\Omega}) \cap \mathcal{G}_\Omega = \{K_\ast\}
\]

Since a unique completion is automatically canonical, it must also lie in \( \mathcal{G}_\Omega \). Therefore, the assumption \( K \in \mathcal{G}_\Omega \) is strictly weaker than the uniqueness assumption, while still guaranteeing identifiability. As noted earlier, in the last paragraph of Section 4, one can easily define a “second-order graphical model” structure with conditional uncorrelatedness replacing conditional independence, so imposing the assumption \( K \in \mathcal{G}_\Omega \) in no way entails assuming Gaussianity. The family \( \mathcal{G}_\Omega \) can also be thought of as a covariance selection model of the kind first proposed by Dempster [9] for multivariate normal distributions, so that imposing the condition \( K \in \mathcal{G}_\Omega \) amounts to doing continuous-domain parameter reduction.
Fig 4: Illustration of Theorem 6.1. The 2-serrated domain $\Omega$ is shaded in grey, and the central square is $(I_1 \cap I_2)^2$. The set $\mathcal{C}(K_{\Omega})$ is spanned as $K_\star + C$, where $C$ ranges over cross-covariances supported on the union of the two squares shaded in red, and compatible with the covariances $K_{I_1 \setminus I_1 \cap I_2}$ and $K_{I_2 \setminus I_1 \cap I_2}$ (outlined in red).

6. Characterisation of All Completions. We will now show how the elements of $\mathcal{C}(K_{\Omega})$ can be spanned by suitable perturbations of the canonical completion, when $\Omega$ is serrated. Again, it is instructive to commence with the the 2-serrated case (see the left plot in Figure 2, p. 6).

**Theorem 6.1 (Characterisation of Completions in the 2-Serrated Case).** Let $\Omega = (I_1 \times I_1) \cup (I_2 \times I_2)$ be a 2-serrated subdomain in $I \times I$. The function $K : I \times I \to \mathbb{R}$ is a completion of $K_{\Omega} : \Omega \to \mathbb{R}$ if and only if

$$K = K_\star + C$$

where $C : (I_1 \cup I_2)^2 \to \mathbb{R}$ satisfies $C(s, t) = 0$ for $(s, t) \in I_1^2 \cup I_2^2$ and is otherwise such that the function $L : [(I_1 \setminus I_2) \cup (I_2 \setminus I_1)]^2 \to \mathbb{R}$ given by

$$L|_{(I_1 \setminus I_2)^2} = K_{I_1} / K_{I_1 \cap I_2}, \quad L|_{(I_1 \setminus I_2) \times (I_2 \setminus I_1)} = C|_{(I_1 \setminus I_2) \times (I_2 \setminus I_1)},$$

$$L|_{(I_2 \setminus I_1)^2} = K_{I_2} / K_{I_1 \cap I_2}, \quad L|_{(I_2 \setminus I_1) \times (I_1 \setminus I_2)} = C|_{(I_2 \setminus I_1) \times (I_1 \setminus I_2)}$$

is a covariance.

Said differently, in the 2-serrated case $\Omega = (I_1 \times I_1) \cup (I_2 \times I_2)$ one has

$$K \in \mathcal{C}(K_{\Omega}) \iff K = K_\star + C$$

where $K_\star$ is the canonical completion and $C$ is a valid perturbation. The set of all valid perturbations $C$ is given by the cross-covariances $C|_{(I_1 \setminus I_2) \times (I_2 \setminus I_1)}$ (with $C|_{(I_2 \setminus I_1) \times (I_1 \setminus I_2)}$ determined by symmetry, i.e. $C(s, t) = C(t, s)$) corresponding to all possible couplings $(Y_t, W_t)$ of the Gaussian processes

$$\{Y_t : t \in I_1 \setminus I_2\}, \quad Y \sim N(0, K_{I_1} / K_{I_1 \cap I_2})$$

$$\{W_t : t \in I_2 \setminus I_1\}, \quad W \sim N(0, K_{I_2} / K_{I_1 \cap I_2})$$

over the indicated region, and are zero elsewhere.
Selecting valid perturbations \( C \) is straightforward: it basically amounts to the functional analogue of “assigning a correlation to two variances”. At the same time, notice that any non-zero perturbation \( C \) introduces arbitrary correlations that were never observed (i.e. are entirely extrinsic to the partial covariance \( K_\Omega \)). This observation crystallises some of the remarks made in the closing of Section 4, i.e. that the canonical completion is unique in not introducing any arbitrary correlations extrinsic to \( K_\Omega \).

We will now re-interpret the last result through the lens of operator theory – this perspective will allow a fruitful extension of our characterisation to general serrated domains. First, we note that if \( K_\Omega \) is continuous on \( \Omega \), then so are all elements of \( \mathcal{C}(K_\Omega) \) on \( I \) and \( L \) is also continuous on \( [(I_1 \setminus I_2) \cup (I_2 \setminus I_1)]^2 \) (for the latter, see Remark 2.9 in Section 2 in the Supplementary Material). As a result, we can think of \( L \) as the kernel of a covariance operator. Let

\[
L_1 : L^2(I_1 \setminus I_2) \to L^2(I_1 \setminus I_2) \quad \text{and} \quad L_2 : L^2(I_2 \setminus I_1) \to L^2(I_2 \setminus I_1)
\]
denote the integral operators induced by the covariance kernels

\[
L|(I_1 \setminus I_2) \times (I_1 \setminus I_2) = K_{I_1}/K_{I_1 \setminus I_2} \quad \text{and} \quad L|(I_2 \setminus I_1) \times (I_2 \setminus I_1) = K_{I_2}/K_{I_1 \setminus I_2}.
\]

Moreover, let

\[
L_{12} : L^2(I_2 \setminus I_1) \to L^2(I_1 \setminus I_2)
\]
denote the integral operator corresponding to the kernel

\[
L|(I_2 \setminus I_1) \times (I_1 \setminus I_2).
\]

Finally, define

\[
L : L^2(I_1 \setminus I_2) \times L^2(I_2 \setminus I_1) \to L^2(I_1 \setminus I_2) \times L^2(I_2 \setminus I_1)
\]
to be a linear operator defined via its action:

\[
L(f, g) = (L_1 f + L_{12} g, L_{12}^* f + L_2 g).
\]

Clearly, \( L \) is a completion if and only if \( L \) is positive semidefinite. Notice that \( L_1 \) and \( L_2 \) are trace-class and positive semidefinite, and as a result \( L \) is trace-class if it is positive-semidefinite. Now, \( L \) is positive semidefinite if and only if there is Gaussian measure \( \mu_{12} \) on the Hilbert space \( L^2(I_1 \setminus I_2) \times L^2(I_2 \setminus I_1) \) with zero mean and covariance operator \( L \) which has two Gaussian measures \( \mu_1 \) and \( \mu_2 \) with zero mean and covariance operators \( L_1 \) and \( L_2 \) as marginals. According to Baker [3, Theorem 2], the possible values of \( L \) are precisely the ones given when setting

\[
L_{12} = L_1^{1/2} \Psi L_2^{1/2}
\]
for \( \Psi : L^2(I_1 \setminus I_2) \to L^2(I_2 \setminus I_1) \) a bounded linear map with operator norm \( \| \Psi \|_\infty \leq 1 \). In summary, if \( K_\Omega \) is continuous, Theorem 6.1 can be re-interpreted at the level of operators. Namely, in block notation, the operator \( K \) has a kernel in \( \mathcal{C}(K_\Omega) \) if and only if

\[
(7) \quad Kf = K_\omega f + \begin{pmatrix}
0 & 0 & (L_1^{1/2} \Psi L_2^{1/2})^* \\
0 & 0 & 0 \\
L_1^{1/2} \Psi L_2^{1/2} & 0 & 0
\end{pmatrix}
\begin{pmatrix}
f|_{I_1 \setminus I_2} \\
f|_{I_1 \setminus I_2} \\
f|_{I_2 \setminus I_1}
\end{pmatrix},
\]

Here \( K_\omega \) is the operator with the canonical completion \( K_\omega \) as its kernel, and as \( \Psi \) ranges over the ball \( \| \Psi \|_\infty \leq 1 \), the expression above generates all possible operator completions. Choosing \( \Psi = 0 \) obviously yields the canonical completion. Note that the operator \( C \) in
Equation (7) is precisely the operator corresponding to the (cross-covariance) integral kernel $C$ as described earlier.

We will use this operator perspective to obtain a characterisation in the general case, where $\Omega = \bigcup_{j=1}^{m} (I_j \times I_j)$ is an $m$-serrated domain. This will require some additional notation to avoid excessively cumbersome expressions. For $1 \leq p < m$ define the following sets:

$$J_p = I_p \setminus I_{p+1}, \quad D_p = I_{p+1} \setminus I_p, \quad S_p = \left[ \bigcup_{j=1}^{p} I_j \right] \setminus I_{p+1}, \quad R_p = D_p \times S_p, \quad R'_p = S_p \times D_p.$$ 

See Figure 5 for a visual interpretation.

Let $K$ be a covariance on $I$ with associated operator $K$. For every $1 \leq j \leq m$, let $K_j : L^2(I_I) \rightarrow L^2(I_I)$ be the Hilbert-Schmidt operator induced by the integral kernel $K_{I_j} = K_{I_I \times I_I}$. And for $1 \leq p < m$, let $J_p \in S_2(J_p, J_p)$ and $R_p \in S_2(D_p, S_p)$ be Hilbert-Schmidt operators induced by the integral kernels $K_{I_p} = K_{I_I \times I_p}$ and $K_{R_p} = K_{S_p \times D_p}$, respectively.

We will now show that $K$ can always be written in a sort of “block notation”, i.e. in terms of $\{K_j\}_j$, $\{J_p\}_p$ and $\{R_p\}_p$. This will allow us to generalise the type of expression Equation (7) to the $m$-serrated case.

**LEMMA 6.2.** Given any $f \in L^2(I)$ and continuous kernel $K : I \times I \rightarrow \mathbb{R}$ with associated operator $K$, the mapping $f \mapsto Kf$ can be represented blockwise as

$$Kf(t) = \sum_{j : t \in I_j} K_j f|_{I_j}(t) + \sum_{p : t \in S_p} R_p f|_{D_p}(t) + \sum_{p : t \in D_p} R'_p f|_{S_p}(t) - \sum_{p : t \in J_p} J_p f|_{J_p}(t) \text{ a.e.}$$

Consequently, in order to characterize any integral operator corresponding to a completion of $K_\Omega$, it suffices to characterize the operators $\{R_p\}_p$. These are the only “missing pieces”, as the rest is known from $K_\Omega$ (see Figure 5).

To this end, for $1 \leq p < m$, we define $D_p \in S_2(J_p, D_p)$ and $S_p \in S_2(S_p, J_p)$ to be the Hilbert-Schmidt operators induced by the integral kernels $K_{D_p \times J_p}$ and $K_{J_p \times S_p}$, respectively (with $K_\ast$ the canonical completion, as always).

Now we have all the ingredients to characterise all completions from a serrated domain:
THEOREM 6.3 (Characterisation of Completions from a General Serrated Domain). Let $K_\Omega$ be a continuous partial covariance on a serrated domain $\Omega$ of $m$ intervals. Then $K : I \times I \to \mathbb{R}$ with $K|_I = K_\Omega$ is a completion of $K_\Omega$ if and only if the integral operator $K$ corresponding to $K$ is of the form

$$
Kf(t) = \sum_{j,t \in I_j} K_{j}(f_I)(t) + \sum_{p,t \in S_p} R_{p}(f_p)(t) + \sum_{p,t \in D_p} R^\ast_{p}(f_p)(t) - \sum_{p,t \in J_p} J_{p}(f_I)(t) \text{ a.e.}
$$

where for $1 \leq p < m$,

$$
R_p = \left[ J_p^{-1/2}S_p^\ast \right]^\ast \left[ J_p^{-1/2}D_p \right] + U_p^{1/2}\Psi_p V_p^{1/2}
$$

with

$$
U_p = K_{S_p} - \left[ J_p^{-1/2}S_p^\ast \right]^\ast \left[ J_p^{-1/2}S_p^\ast \right], \quad V_p = K_{D_p} - \left[ J_p^{-1/2}D_p^\ast \right]^\ast \left[ J_p^{-1/2}D_p^\ast \right]
$$

and $\Psi_p : L^2(D_p) \to L^2(S_p)$ is a bounded linear map with $\|\Psi_p\| \leq 1$.

The only degrees of freedom in Equation (9) stem from the $m$ contractions $\{\Psi_p\}_{p=1}^m$. All other operators involved in Equation (9) (and in the right hand side of Equation (8)) are uniquely defined via $K_\Omega$ (or equivalently via $K_\ast$). Allowing these to range over the unit balls

$$
\|\Psi_p\| \leq 1, \quad \Psi_p : L^2(D_p) \to L^2(S_p), \quad p = 1, \ldots, m
$$

we trace out the set $\mathcal{C}(K_\Omega)$ and get an idea of what the different possibilities of the actual covariance may look like. Substituting $\Psi_p = 0$ for all $1 \leq p < m$ returns the integral operator corresponding to the canonical completion $K_\ast$ of $K_\Omega$. Since all other elements of Equation (9) are fully determined by $K_\Omega$, it is clear that the choice of $\{\Psi_p\}$ is arbitrary, and any non-zero choice will introduce information extrinsic to observed correlation patterns – extending the intuition build in the 2-serrated case relating to the canonicity of $K_\ast$.

Theorem 6.3 also complements Theorem 3.3, in that it expresses the canonical completion as the solution of a system of equations rather than the output of an algorithm. This manner of specification is slightly weaker, in that it assumes continuity of $K_\Omega$, whereas Theorem 3.3 makes no such assumption. On the other hand, it provides a characterisation of the canonical solution in a form that lends itself for the problem of estimation, treated in the next Section.

7. Estimation of the Canonical Completion. In this section, we consider the problem of estimation of the canonical completion $K_\ast$ when we only have access to an estimator of the partial covariance $K_\Omega$. From a purely analytical sense, we are studying the stability of the canonical completion $K_\ast$ of $K_\Omega$ with respect to perturbations of the partial covariance $K_\Omega$. From the statistical point of view, this relates to the problem that arises in the context of covariance recovery from functional fragments: when we observe fragments $X_j|_{I_j}$ of i.i.d. realisations of a second-order process $\{X_t : t \in I\}$ for a collection $\{I_j\}$ of subintervals $I_j \subset I$ covering $I$. Because of the fragmented nature of the observations, we only have covariance information on the serrated domain $\Omega = \cup_j I_j \times I_j$, or equivalently we only can identify the partial covariance $K_\Omega$ corresponding to the restriction of $\text{Cov}\{X_s, X_t\} = K(s, t)$ to the serrated domain $\Omega$.

In this context, we posit that it makes good sense to choose the canonical completion $K_\ast$ as the target of estimation. This is because the canonical completion is always an identifiable and interpretable object:

1. When a unique completion exists, it must be the canonical one. So choosing the canonical completion allows us to adapt to uniqueness.
2. When multiple completions exist, the canonical completion remains identifiable, and is least presumptuous – it relies solely on the available data.

Targeting the canonical completion without any attempt to enforce uniqueness is qualitatively very different from previous approaches to covariance recovery from fragmented paths. Those approaches imposed uniqueness by way of assumptions (indeed assumptions implying very rigid consequences, as demonstrated in Section 5). Once uniqueness is a priori guaranteed, any estimator \(\hat{K}\) whose restriction \(\hat{K}_Ω\) is consistent for \(K_Ω\) will be valid – so, for instance, one can safely extrapolate an estimator \(\hat{K}_Ω\) of \(K_Ω\) by means of a basis expansion or matrix completion. But when uniqueness fails to hold, such “extrapolation” estimators are liable to yielding arbitrary completions, indeed completions that likely will not even converge asymptotically, but rather oscillate in some open neighbourhood of \(C(K_Ω)\).

On the other hand, the adaptivity (to uniqueness) and stability/interpretability (under non-uniqueness) of the canonical completion comes at a price: to be able to target the canonical completion \(K_⋆\) we need an estimator that is not merely consistent for \(K_Ω\) on \(Ω\), but one that (asymptotically) also satisfies the system of equations in Theorem 6.3 (with \(Ψ_p\) identically zero). This has consequences on the rates of convergence, which can no longer be as fast as the rates of estimating the partial covariance \(K_Ω\).

Fig 6: Illustration of the problem of covariance recovery from fragments: (from the left) fully observed sample paths of a process on the unit interval \(I = [0, 1]\); the region \(I^2\) on which the covariance can be estimated in the fully observed case; partially observed versions of the same sample paths; and, the region on which the covariance can be estimated from the sample paths of the corresponding colour.

7.1. Definition of the Estimator. Courtesy of Theorem 6.3, the specification of \(K_⋆\) reduces to that the solution the following system of linear equations:

\[
\begin{align*}
J_p^{1/2}X_p &= S_p^* \\
J_p^{1/2}Y_p &= D_p
\end{align*}
\]  

(10)

Notice that the operator \(J_p^{1/2}\) is compact because \(J_p\) is. It follows that the canonical completion \(K_⋆\) does not depend continuously on the partial covariance \(K_Ω\). In practice we only have access to an estimator \(\hat{K}_Ω\) of \(K_Ω\). Therefore, the operator of the inverse problem, i.e. \(J_p^{1/2}\), as well as the data of the inverse problem, in the form of \(D_p\) and \(S_p\), are inexactly specified.

We will thus define our estimator as the solution of a regularized empirical version of the system. Let \(\hat{K}_Ω\) be an estimator of \(K_Ω\). Let \(\hat{K}_Ω, \hat{D}_p\) and \(\hat{J}_p\) be the Hilbert-Schmidt operators with the kernels \(\hat{K}_Ω|_{I_p \times I_p}, \hat{K}_Ω|_{J_p \times D_p}\) and \(\hat{K}_Ω|_{J_p \times J_p}\), respectively.
Finally, motivated by the definition

\[ \mathbf{R}_p = \left[ \mathbf{J}_p^{-1/2} \mathbf{S}_p \right]^* \left[ \mathbf{J}_p^{-1/2} \mathbf{D}_p \right] \]

and using a truncated inverse of \( \hat{\mathbf{J}}_p \), we define the regularised empirical version of \( \mathbf{R}_p \) as

\[ \hat{\mathbf{R}}_p = \sum_{k=1}^{N_p} \frac{1}{\hat{\lambda}_{p,k}} \cdot \hat{\mathbf{S}}_p \hat{e}_{p,k} \otimes \hat{\mathbf{D}}_p \hat{e}_{p,k} \]

where \( \hat{\lambda}_{p,k} \) and \( \hat{e}_{p,k} \) denote the \( k \)th eigenvalue and eigenfunction of \( \hat{\mathbf{J}}_p \), \( N_p \) is the truncation or regularization parameter, and \( \hat{\mathbf{S}}_p \) has kernel \( \hat{K}_s|_{S_p \times J_p} \). Notice that the definition is recursive:

- \( \hat{\mathbf{R}}_p \) depends on \( \hat{\mathbf{S}}_p \) and thus on \( \hat{\mathbf{R}}_i \) for \( i < p \).
- \( \hat{\mathbf{S}}_1 \) is fully determined by \( \hat{K}_\Omega \), and \( \hat{\mathbf{S}}_{p+1} \) is fully determined by \( \hat{K}_\Omega \) and \( \hat{\mathbf{R}}_p \).

In particular, though the kernel of \( \hat{\mathbf{S}}_p \) can a posteriori be seen to equal \( \hat{K}_s|_{S_p \times J_p} \), this does not mean that it depends a priori on \( \hat{K}_s \) (i.e. there is no vicious circle in the definition).

We can now define our estimator \( \hat{K}_s : I \times I \to \mathbb{R} \) of \( K_s \) to be the the integral kernel of the Hilbert-Schmidt operator \( K_s : L^2(I) \to L^2(I) \) defined via the action

\[ \hat{K}_s f(t) = \sum_{j \in I} \hat{K}_j f|_{I_j}(t) + \sum_{p \in S_p} \hat{\mathbf{R}}_p f|_{D_p}(t) + \sum_{p \in D_p} \hat{\mathbf{R}}_p f|_{S_p}(t) - \sum_{p \in S_p} \hat{\mathbf{J}}_p f|_{J_p}(t). \]

Equivalently, we can define \( \hat{K}_s \in L^2(I \times I) \) recursively as follows: \( \hat{K}_s|_I = \hat{K}_\Omega \) and \( \hat{K}_s|_{R_p} \) is the kernel associated with the Hilbert-Schmidt operator \( \hat{\mathbf{R}}_p \) defined recursively via (11).

**7.2. Rate of Convergence.** We will now characterize the rate of convergence of \( \hat{K}_s \) to \( K_s \) in terms of the spectral properties of the partial covariance \( K_\Omega \), and the rate of convergence of the partial covariance estimator \( \hat{K}_\Omega \) we have used as a basis, to the partial covariance \( K_\Omega \) itself. Concerning the spectral properties of \( K_\Omega \), let \( \{\lambda_{p,k}\}_{k=1}^{\infty} \) be the eigenvalues of \( \mathbf{J}_p \) and define \( A_{p,k} \) as:

\[ A_{p,k} = \left\| \sum_{j=k+1}^{\infty} \mathbf{S}_p e_{p,k} \otimes \mathbf{D}_p^* e_{p,k} \lambda_{p,k} \right\|_2^2 \]

where \( \{e_{p,k}\}_{k=1}^{\infty} \) are the eigenfunctions of \( \mathbf{J}_p \). Notice that \( A_{p,0} \) is simply the Hilbert-Schmidt norm of \( \mathbf{R}_p \) and \( A_{p,k} \) represents the error in approximating \( \mathbf{R}_p \) by using a rank-\( k \) truncated inverse of \( \mathbf{J}_p^{-1/2} \) instead of \( \mathbf{J}_p^{1/2} \) in the expression

\[ \mathbf{R}_p = \left[ \mathbf{J}_p^{-1/2} \mathbf{S}_p^* \right]^* \left[ \mathbf{J}_p^{-1/2} \mathbf{D}_p \right]. \]

Consequently, \( A_{p,k} \) must necessarily converge to 0 as \( k \to \infty \). The following result gives the rate of convergence for the case when the eigenvalues and approximation errors decay at a polynomial rate.

**THEOREM 7.1 (Consistency and Rate of Convergence).** Let \( K_\Omega \) be a partial covariance on a serrated domain \( \Omega \) of \( m \) intervals and \( \hat{K}_\Omega \) be an estimator thereof. Let \( \hat{K} \) be defined as in Equation (12). Assume that for every \( 1 \leq p < m \), we have \( \lambda_{p,k} \sim k^{-\alpha} \) and \( A_{p,k} \sim k^{-\beta} \). If the error in the estimation of \( K_\Omega \) satisfies

\[ \| \hat{K}_\Omega - K_\Omega \|_{L^2(\Omega)} = O_p(1/n^{\delta}) \]
where \( n \) is the number of fragments, then the error in the estimation of the canonical completion satisfies, for every \( \varepsilon > 0 \),

\[
\| \hat{K}_* - K_* \|_{L^2(I \times I)} = O_p\left(\frac{1}{n^{\gamma_{m-1} - \varepsilon}}\right)
\]

provided the truncation parameters \( N = (N_p)_{p=1}^{m-1} \) scale according to the rule

\[
N_p \sim n^\gamma_p
\]

where \( \gamma_{m-1} = \frac{\beta}{\beta + 2\alpha + 3/2} \left[ \frac{\beta}{\beta + \alpha + 1/2} \right]^{m-2} \).

**Remark 7.2 (Plug-in Interpretation).** The theorem can be seen as a plug-in rate of convergence theorem. We plug-in the “baseline” rate of convergence of \( \hat{K}_\Omega \to K_\Omega \), and get a rate for \( \hat{K}_* \to K_* \). Note that the tuning of the truncation parameters also depends on the baseline rate of convergence. Baseline rates are readily available for sparse, dense, and complete observation regimes.

Notice that the rate of convergence \( \gamma_{m-1} \) strictly decreases as a function of the number of intervals \( m \), but can get arbitrarily close to 1 for a large enough rate of decay of approximation errors \( \beta \). Moreover, an increase in the rate of decay of eigenvalues \( \alpha \) is accompanied by a decrease in the rate of convergence. If \( K_\Omega \) is \( r \)-times differentiable then the same applies to the kernels \( \hat{K}_\Omega \big|_{J_p \times J_p} \) of \( J_p \) implying \( \lambda_{p,k} \) is \( o(1/n^{r+1}) \) for every \( 1 \leq p < m \) and thus \( \alpha = r + 1 \). Thus, all other things being equal, an increase in the smoothness of \( K_\Omega \) also tends to decrease the rate of convergence—which is not surprising from an inverse problems perspective.

**8. Beyond Serrated Domains.** Our theory has thus far concentrated on domains that are **serrated** in the sense of Definition 2.3. We now turn our attention to a much larger class of domains, namely domains that can be approximated to an arbitrary level of precision by serrated domains. Recall that for subsets \( X \) and \( Y \) of a metric space \((M,d)\), the Hausdorff distance between is defined as

\[
d_H(X,Y) = \left[ \sup_{x \in X} \inf_{y \in Y} d(x,y) \right] \vee \left[ \sup_{y \in Y} \inf_{x \in X} d(x,y) \right].
\]

We define the class of **nearly serrated domains** as the Hausdorff “closure” of the set of serrated subdomains of \( I \times I \):

**Definition 8.1 (Nearly Serrated Domain).** We say that \( \tilde{\Omega} \subset I \times I \) is a nearly serrated domain if for every \( \varepsilon > 0 \), there exist serrated domains \( \Omega_* \) and \( \Omega^\varepsilon \) such that \( \Omega_* \subset \tilde{\Omega} \subset \Omega^\varepsilon \) and \( d_H(\Omega, \Omega_*), d_H(\Omega, \Omega^\varepsilon) < \varepsilon \), where \( d_H \) is the Hausdorff metric induced by the Euclidean metric on \( I \times I \subset \mathbb{R}^2 \).

Notice that every serrated domain is nearly serrated according to the above definition. Of particular importance is the case when \( \Omega \) is a strip of width \( w > 0 \) around the diagonal, that is, \( \Omega = \{(s,t) \in I \times I : |s-t| \leq w/\sqrt{2}\} \). This occurs asymptotically in the problem of covariance recovery from fragments, when each sample path is observable which over “uniformly distributed” intervals of constant length \( w/\sqrt{2} \).

It should be clear from Figure 7 that we cannot exploit Equation 2 to recover the canonical completion of a partial covariance on a nearly serrated but not serrated domain, as we did for serrated domains previously. This is because for such domains there are points \((s,t)\) for which the cross-covariances \( K_\Omega(s, \cdot) \) and \( K_\Omega(\cdot, t) \) are not available, nor can they be
Fig 7: Left: Illustration of a nearly serrated domain (in green) as enveloped by two serrated domains (in light and dark grey). Right: a point \((s, t)\) escaping the scope of Equation (2).

iteratively calculated from the part of the covariance that is known. Thus one cannot evaluate their inner product \(\langle K_\Omega(s, \cdot), K_\Omega(\cdot, t) \rangle \) as required in Equation 2. It was precisely because the domain was serrated that that we were able to recover the value of the canonical completion over successively larger regions as we did in Algorithm (1).

Additionally, since we cannot apply Algorithm 1, it is unclear what it means for a completion of a partial covariance \(K_\Omega\) on a nearly serrated domain to be canonical. Here we must lean on our graphical models interpretation to define the canonical completion. We shall say that a covariance \(K\) is a canonical completion of \(K_\Omega\) if it is a completion i.e. \(K|_\Omega = K_\Omega\) and \(K \in G_\Omega\) as defined in Section 4.

Our focus will, therefore, be to obtain results pertaining to uniqueness/canonicity of completions from nearly serrated domains \(\tilde{\Omega}\) by means of serrated subdomains \(\Omega \subset \tilde{\Omega}\) or super-domains \(\Omega \subset \tilde{\Omega}\). Our first result gives a sufficient condition for unique completion from a nearly serrated domain:

**Theorem 8.2 (Checking Uniqueness via Serrated Subdomains).** Let \(K_{\tilde{\Omega}}\) be a partial covariance on a nearly serrated domain \(\tilde{\Omega}\) and let \(\Omega \subset \tilde{\Omega}\) be a serrated domain. If the restriction \(K_{\tilde{\Omega}}|_\Omega\) admits a unique completion, then so does \(K_{\tilde{\Omega}}\).

Theorem 8.2, via our necessary and sufficient conditions for uniqueness on serrated domains (Theorem 5.1), yields sufficient conditions for unique completion from a banded domain that are strictly weaker than any previously known set of sufficient conditions.

In the serrated case, a unique completion is necessarily canonical. A natural question is whether this remains the case for nearly serrated domains. The answer is in the affirmative:

**Theorem 8.3 (Unique Completions are Canonical).** If the partial covariance \(K_{\tilde{\Omega}}\) on a nearly serrated domain \(\tilde{\Omega}\) has a unique completion on \(I \times I\), this completion is canonical.

Theorem 8.3 shows that targeting canonical completions remains a sensible strategy in the context of nearly serrated domains – they remain interpretable and yield the “correct answer” in the presence of uniqueness. That is, of course, if we know how to construct them. Our last result pertains to this matter:
Theorem 8.4 (Construction of Canonical Completions). A covariance \( K \) on \( I \) can be recovered as the canonical completion of its restriction \( K|_{\Omega} \) on a serrated domain \( \Omega \) if and only if it is the canonical completion of a partial covariance on some nearly serrated domain \( \tilde{\Omega} \subset \Omega \).

In particular, if a unique completion of \( K|_{\tilde{\Omega}} \) exists then it equals the canonical completion of \( K|_{\Omega} \) for a (in fact any) serrated \( \Omega \supset \tilde{\Omega} \). Alternatively, if the process \( X \) with covariance \( K \) forms a second-order graphical model with respect to the nearly serrated \( \tilde{\Omega} \), then \( K \) can be obtained by means of Algorithm 1 applied to \( K|_{\Omega} \) for any \( \Omega \supset \tilde{\Omega} \). This is possible because if \( \tilde{\Omega} \subset \Omega \), then every separator of \( \Omega \) also separates \( \tilde{\Omega} \). As a result, if the “separation equation” is satisfied by \( (s,t) \in (\tilde{\Omega})^c \) for separators of \( \tilde{\Omega} \), then it is also satisfied for separators of \( \Omega \). Thus \( \Omega \subset \tilde{\Omega} \) implies \( G_{\Omega} \subset G_{\tilde{\Omega}} \).

9. Covariance Estimation from Sample Path Fragments. We now elucidate how one can make combined use of our results from Section 7 and Section 8, in order to address the problem of covariance estimation from sample path fragments in a general context. Let \( X \) be a second-order process on the unit interval \( I \) with the covariance \( \hat{K} \). Suppose that for \( n \) intervals \( I_i \subset I \) we observe \( n \) sample path fragments \( X_i = X|_{I_i} \), where \( X_i \sim X \) independently. Now define the domain

\[
\Omega_\infty = \limsup_{k \to \infty} (I_k \times I_k),
\]

as the set of pairs \( (x, y) \in I \times I \) such that \( I_i \ni (x, y) \) infinitely often. The sequence \( \{X_i\}_{i=1}^n \) enables us to consistently estimate the restriction \( \hat{K}_{\Omega} := K|_{\Omega} \) of \( K \) on any \( \Omega \subset \Omega_\infty \). Call such a consistent estimator \( \hat{K}_{\Omega} \).

However, we wish to estimate the complete \( K \), not merely its restrictions to \( \Omega \subset \Omega_\infty \). This requires \( K \) to be identifiable from \( \Omega_\infty \). One means to securing identifiability is to impose unique extendability, i.e. assume that \( \mathcal{E}(K|_{\Omega}) = \{K\} \) for some \( \Omega \) whose elements are covered infinitely often by the sequence of rectangles \( I_k \times I_k \) (i.e. we have the inclusion\(^1\) \( \Omega \subset \Omega_\infty \)). But uniqueness was seen to be overly restrictive (see Theorem 5.1). We therefore wish to avoid this route to identifiability. Instead, following the development in Section 4 we will secure identifiability by assuming that the underlying process \( X \) is globally Markov with respect to some domain \( \Omega \) (i.e. \( K \in G_{\Omega} \)) whose elements are covered infinitely often by the sequence the rectangles \( I_k \times I_k \) (i.e. \( \Omega \subset \Omega_\infty \)). This is a substantially weaker assumption (due to Theorem 8.3), and arguably much more intuitive.

Proceeding thus, let \( \Omega \subset \Omega_\infty \) be some nearly serrated domain with respect to which \( X \) is global Markov. By Theorem 4.3, the true covariance \( K \) is the canonical completion from \( \Omega \), and by Theorem 8.4, it is also the canonical completion from any serrated domain containing \( \Omega \). Thus we can identify \( K \) directly from \( \hat{K}_{\Omega} \) as the canonical completion of \( K_{\Omega_m} \) for some \( m \)-serrated \( \Omega_m \) (with some \( m < \infty \)) satisfying \( \Omega \subseteq \Omega_m \subseteq \Omega_\infty \). The inclusions will always be possible for some \( m < \infty \) provided the boundaries \( \partial \Omega \) and \( \partial \Omega_\infty \) are everywhere distinct (i.e. \( ||u - v|| > 0 \) for all \( u \in \partial \Omega \) and \( v \in \partial \Omega_\infty \)).

Now we distinguish two cases:

(i) \( \Omega_\infty \) is serrated. If intervals \( \{I_j\}_{j=1}^n \) are sampled from a finite cover of \( I \), then \( \Omega_\infty \) will be a serrated domain. This represents a fixed domain setting, in that for all sufficiently large \( n \) the observation domain becomes almost surely fixed.

---

\(^1\)Note that in general the inclusion \( \Omega_\infty \subset \Omega \) is to be taken as strict. The “critical” equality case would be rather exceptional, because \( \Omega_\infty \) is defined by the censoring mechanism, whereas the \( \Omega \) is a population quantity. Stipulating that the structure of \( X \) varies with or is tailored to the censoring mechanism would be contrived.
(ii) \( \Omega_\infty \) is nearly serrated. If the intervals \( \{I_j\}_{j=1}^n \) are sampled from an infinite cover of \( I \), then \( \Omega_\infty \) will be a nearly serrated domain. This represents a variable domain setting, as our observation domain will continue evolving as \( n \) grows.

Fig 8: The regions \( \Omega \) (red), \( \Omega_m \) (gray), and \( \Omega_\infty \) (blue).

In case (i), we are squarely within the context of Section 7 and can use \( \hat{K}_\Omega \) to directly define the estimator \( K \) used in Equation 12.

In case (ii), we choose and fix an \( m \)-serrated approximation of the observable region \( \Omega_m \subset \Omega \). We then construct the estimator \( \hat{K} \) in Equation 12 based on \( \hat{K}_{\Omega_m} \). So long as \( \Omega_m \) contains \( \Omega \) and \( m \) is held fixed, the estimator thus constructed will converge to \( K \) as per Theorem 7.1. A good choice of \( \Omega_m \) involves a trade-off between covering a large subregion of \( \Omega_\infty \) (to use as much of the observable domain as possible) and keeping \( m \) small (to limit the number of inverse problems solved). This approach is illustrated through a data analysis in Section 11, and its performance is investigated via extensive simulations in Section 10 (with special focus on the effect of the choice of \( m \)).

**Remark 9.1 (On \( m \) vs \( n \) – Practical Considerations).** From a practical point of view, the choice of a serrated approximation \( \Omega_m \) to \( \Omega_\infty \) does not entail any significant loss. In practice, \( \Omega_\infty \) is in fact unknown, and the de facto domain of observation is the \( n \)-serrated domain \( \bigcup_{j=1}^n (I_j \times I_j) \). Nevertheless, statistical considerations suggest that we should not use the full observation domain, namely:

1. The domain \( \bigcup_{j=1}^n (I_j \times I_j) \) generally “overfits” \( \Omega = \lim \sup_j (I_j \times I_j) \). Regions of \( I \times I \) that are more densely populated by observations are better proxies for \( \Omega_\infty \) (meaning regions comprised of pairs \((x, y) \in I \times I\) such that \( \# \{k \leq n : \{x, y\} \subset I_k \} \) is large). This suggests choosing \( \Omega_m \) with \( m \) distinctly smaller than \( n \).
2. When the fragments are observed discretely and smoothing is used to construct \( \hat{K}_{\Omega_m} \), we still use data in the the region \( \bigcup_{j=1}^n (I_j \times I_j) \setminus \Omega_m \) as part of the local averaging, even though we desist from estimating outside \( \Omega_m \). Hence we do not necessarily discard information, but rather focus on a smaller region on which we can estimate more efficiently: because this region is more densely populated by observations and furthermore because we avoid boundary effects.

**Remark 9.2 (On \( m \) vs \( n \) – Asymptotic Considerations).** As argued earlier, \( m \) need not grow with \( n \) for consistent estimation. We can nevertheless ask at what rate one might choose
to let \( m \) grow with \( n \), in the spirit of trading off more error due to a higher number of inverse problems to solve in exchange for more data. Theorem 7.1 can partially inform heuristics on this. Suppose that the error \( \hat{K}_n \) is \( n^{-\alpha} \)-consistent for \( K_\Omega \), \( \alpha \in (0, 1) \) – which is certainly the case under complete observation. Take \( \gamma_{m-1} = O(\eta^m) \) where \( \eta \in (0, 1) \). Plugging these into Theorem 7.1 would suggest that

\[
\| \hat{K}_n - K_\Omega \|_{L^2(I \times I)} \lesssim n^{-\alpha(m)} = \exp[-\alpha \eta^m \log n] \to 1
\]

This would indicate that \( m \) should not grow any faster than \( O(\log \log n) \), effectively leading to \( m \) being practically constant: the increase in ill-posedness overwhelms any gain by adding more data.

### 10. Simulation Study.

We consider three covariances:

\[
K_1(s, t) = \sum_{j=1}^{4} \frac{\phi_j(s) \phi_j(t)}{2^{j-1}}, \quad K_2(s, t) = s \wedge t, \quad K_3(s, t) = 10 \text{ste}^{-10|s-t|^2}
\]

where \( \phi_1(t) = 1, \phi_2(t) = \sqrt{3}(2t - 1), \phi_3(t) = \sqrt{5}(6t^2 - 6t + 1) \) and \( \phi_4(t) = \sqrt{\pi}(20t^3 - 30t^2 + 12t - 1) \). The first covariance is both finite-rank and analytic, the second is infinite-rank and non-analytic and the third is infinite-rank and analytic. For the first and the third covariance, every restriction to a serrated domain admits a unique completion (due to analyticity), which is not the case for the second covariance (by Lemma 2.6 in the Supplementary Material). Define the domains \( \Omega_j \) as follows:

\[
\Omega_1 = [0, 3/5]^2 \cup [2/5, 1]^2 \\
\Omega_2 = \Omega_1 \cup [1/5, 4/5]^2 \\
\Omega_3 = \Omega_2 \cup [1/10, 7/10]^2 \cup [3/10, 9/10]^2 \\
\Omega_4 = \Omega_3 \cup [1/20, 13/20]^2 \cup [3/20, 15/20]^2 \cup [5/20, 17/20]^2 \cup [7/20, 19/20]^2 \\
\Omega_5 = \Omega_4 \cup [1/40, 25/40]^2 \cup [3/40, 27/40]^2 \cup [5/40, 29/40]^2 \cup [7/40, 31/40]^2 \\
\quad \cup [9/40, 33/40]^2 \cup [11/40, 35/40]^2 \cup [13/40, 37/40]^2 \cup [15/40, 39/40]^2.
\]

The number of intervals \( m \) for the domains is 2, 3, 5, 9 and 17, respectively. The variable domain simulations of [8] roughly correspond to an implicit choice of \( m = 17 \) (i.e. \( \Omega_5 \)).

The computations have been implemented in the \texttt{R} programming language [27] with the exception of those involving the estimator proposed in [8] which was implemented in MATLAB. The implementation of our estimator in \texttt{R} can be found in the covcomp package [33].

#### 10.1. General Simulation Study.

For the covariances \( K = K_1, K_2 \) and \( K_3 \), we study the performance of our Estimator (12) for the domains \( \Omega_2 \) (\( m = 3 \)) and \( \Omega_4 \) (\( m = 9 \)), and the number of fragments \( n = 100 \) and 500, for two different sampling regimes:

(a) **Regularly Observed Fragments.** We simulate \( n \) fragments corresponding to \( \Omega \) over a regular grid of size 100 over the unit interval. And, we estimate the covariance over \( \Omega \) using the pairwise empirical covariance estimator given by: for \( s, t \) such that \( n(s, t) = \#\{j : s, t \in U_j\} \geq 10 \),

\[
\hat{K}_\Omega(s, t) = \frac{1}{n(s, t)} \sum_{j : s, t \in U_j} X_j(s) X_j(t)
\]

where \( U_j \subset I \) denotes the support of the fragment \( X_j \).
(b) *Sparsely Observed Fragments*. We generate $n$ fragments as before in (a) but retain only \( \sim 6 \) points for every fragment chosen randomly and discard the rest. We estimate the covariance over \( \Omega \) by locally linear kernel smoothing. For \( K_1 \) and \( K_2 \), this is achieved using the fdapace package [6] in \( \mathbb{R} \) under the default parameters. For \( K_2 \), the same method is unsuitable due to non-differentiability at the diagonal, and so we use the reflected triangle estimator proposed in [18] instead.

Using the estimate of \( K_\Omega \), we construct the completion using the method described in Section 7. We do this 100 times for every combination of covariance, domain and number of samples. We calculate the median and mean absolute deviation for the error in the form of integrated squared error in estimating \( K \). For infinite rank covariances exhibiting fast eigenvalue decay, such as \( K_2 \) and \( K_3 \), small values of \( N_p \) such as 2 or 3 work well. Accordingly, we choose \( N_p = 2 \) for them. This choice also seems to work slightly better in practice.

The results are summarised in Table 1. Naturally, the error in the estimation of \( K_\Omega \) and \( K_\ast \) tends to decrease as \( N \) increases in all cases. The error in estimating \( K_\Omega \) tends to increase as \( m \) increases, even relative to the norm of \( K_\Omega \). The same applies to the error in estimating \( K_\ast \) in the case of regular observations, however for sparse observations there does not seem to be a clear relationship.

10.2. *Estimator Performance versus m*. We now turn to studying the dependence of the error of estimating \( K_\ast \) on the number of intervals \( m \) corresponding to \( \Omega \). To this end, we generate \( n = 100 \) fragments of the covariances \( K = K_1, K_2 \) and \( K_3 \) corresponding to the domains \( \Omega \in \{ \Omega_j \}_{j=1}^5 \) over a grid of length 100, estimate the partial covariance on the corresponding domain using the pairwise empirical covariance estimator as defined by Equation 13 and apply the completion algorithm. We then compute the ratio of relative errors (RRE) defined as the ratio of the median ISE in estimating \( K_\Omega \) to that of \( K_\Omega \) both relative to the norms of the respective quantities they are estimating. In other words,

\[
\text{RRE} = \frac{\int_{\Omega_r} |\hat{K}_\ast - K|^2 / \int_{\Omega_r} |K|^2}{\int_{\Omega} |\hat{K}_\Omega - K_\Omega|^2 / \int_{\Omega} |K|^2}.
\]

The results have been summarized as boxplots in Figure 9. We observe that the median RRE does not vary much in response the number of intervals \( m \) for any of the covariance scenarios as we move from smaller values such as \( m = 2,3 \) to larger values such as \( m = 17 \). The most noticeable effect appears to be in the finite rank case, where the interquantile range of the RRE increases with \( m \), even if the median is relatively stable. Importantly, we observe that the increase in error (across scenarios) is nowhere so large so as to affect the utility of the estimation procedure and the empirical performance appears more optimistic than what predicted by Theorem 7.1.
Comparative Simulations. In order to benchmark the performance of our estimator $\hat{K}^*$, we compare to that of the estimator $\hat{K}_p$ proposed in [8]. For different choices of $K$, $m$, and $n$ we generate fragments on a regular grid of size 50 on the unit interval. We then estimate the covariance on $\Omega$ using locally linear kernel smoothing and then apply the completion procedure. We do this 100 times and calculate the median and mean absolute deviation of the integrated squared error. We do the same for the estimator $\hat{K}_p$. The results are summarized by Table 2. As can be expected, neither estimator dominates, and performance varies according to scenario. The scenarios involving $K_1$ and $K_3$ feature covariances that are analytic and exactly or effectively low rank. As expected, $\hat{K}_p$ has better performance here, since these two settings admit unique extension and their infinite smoothness combined with their low (effective) rank is ideally suited for truncated series extrapolation. That being said, the performance of $\hat{K}^*$ remains competitive, with errors of similar magnitude in these two

---

### Table 1

Results of General Simulation Study

| Parameters | Regular Observations | Sparse Observations | Squared Norms |
|------------|----------------------|---------------------|---------------|
|            | $f_{\Omega} | \hat{K}_\Omega - K\Omega |^2$ | $f_{\Omega} | \hat{K}_\Omega - K\Omega |^2$ | $f_{\Omega} | \hat{K}_\Omega - K\Omega |^2$ | $\hat{K}^*_p | K\Omega |^2$ | $\hat{K}^*_p | K\Omega |^2$ |
| $K_1$      |                     |                     |               |
| 3          | 0.0901 ± 0.0604     | 0.0318 ± 0.0325     | 0.1395 ± 0.0823 | 0.1489 ± 0.1630 | 1.3080 ± 0.0381 |
| 3          | 0.0152 ± 0.0099     | 0.0100 ± 0.0112     | 0.0397 ± 0.0182 | 0.0930 ± 0.1136 | 1.3080 ± 0.0381 |
| 3          | 0.1781 ± 0.1159     | 0.1980 ± 0.1947     | 0.1729 ± 0.0893 | 0.0749 ± 0.0713 | 1.3225 ± 0.0236 |
| 3          | 0.0301 ± 0.0197     | 0.0482 ± 0.0465     | 0.0567 ± 0.0310 | 0.0664 ± 0.0633 | 1.3225 ± 0.0236 |

*values computed for $n = 200$. 

---

Fig 9: Boxplot of Ratio of Relative Errors (RRE) vs. the number of intervals $m$ for $K_1$ (left), $K_2$ (middle) and $K_3$ (right).
Table 2
Results of Comparative Simulation Study

| Parameters | Our estimator $\hat{K}_*$ | The estimator $\hat{K}_p$ |
|------------|--------------------------|--------------------------|
| $K$ | $m$ | $N$ | $\|K_{\Omega} - K_0\|^2$ | $\|K_{\Omega} - K_0\|^2$ | $\|K_{\Omega} - K_p\|^2$ | $\|K_{\Omega} - K_p\|^2$ |
| $K_1$ | 3 | 100 | 0.0779 ±0.0541 | 0.0984 ±0.1080 | 0.0614 ±0.0402 | 0.0742 ±0.0407 |
| | 3 | 500 | 0.0157 ±0.0103 | 0.0288 ±0.0295 | 0.0146 ±0.0086 | 0.0145 ±0.0099 |
| | 9 | 100 | 0.1250 ±0.0773 | 0.1400 ±0.1450 | 0.0982 ±0.0479 | 0.1115 ±0.0721 |
| | 9 | 500 | 0.0279 ±0.0204 | 0.0622 ±0.0760 | 0.0225 ±0.0123 | 0.0224 ±0.0143 |
| $K_2$ | 3 | 100 | 0.0058 ±0.0053 | 0.0007 ±0.0005 | 0.0049 ±0.0041 | 0.0055 ±0.0049 |
| | 3 | 500 | 0.0016 ±0.0014 | 0.0001 ±0.0001 | 0.0009 ±0.0006 | 0.0010 ±0.0008 |
| | 9 | 100 | 0.0129 ±0.0073 | 0.0012 ±0.0007 | 0.0081 ±0.0065 | 0.0059 ±0.0052 |
| | 9 | 500 | 0.0029 ±0.0020 | 0.0003 ±0.0002 | 0.0020 ±0.0017 | 0.0012 ±0.0009 |
| $K_3$ | 3 | 100 | 0.0232 ±0.0202 | 0.0057 ±0.0059 | 0.0023 ±0.0018 | 0.0025 ±0.0022 |
| | 3 | 500 | 0.0053 ±0.0039 | 0.0009 ±0.0008 | 0.0006 ±0.0004 | 0.0006 ±0.0004 |
| | 9 | 100 | 0.0340 ±0.0254 | 0.0064 ±0.0054 | 0.0050 ±0.0035 | 0.0044 ±0.0034 |
| | 9 | 500 | 0.0058 ±0.0037 | 0.0013 ±0.0010 | 0.0010 ±0.0009 | 0.0008 ±0.0005 |

scenarios. On the other hand, $\hat{K}_*$ outperforms $\hat{K}_p$ by an order of magnitude in scenario $K_2$, which is a low regularity scenario without a unique completion. One would summarise that $\hat{K}_*$ behaves like a “robust” estimator: competitively in “easy” scenarios, but substantially better otherwise. Another overarching observation (in line with intuition and theoretical results) is that the performance of $\hat{K}_*$ is tied to the performance of the estimator of $K_{\Omega}$ – in some cases (see e.g. scenario $K_3$), the larger errors relative to $\hat{K}_p$ might have more to do with the quality of estimation on $\Omega$ itself, than the with completion procedure.

11. Illustrative Data Analysis. Following [8], we apply our method to the spine bone mineral density (BMD) data described in [2]. We consider measurements of 117 females taken between the ages of 9.5 and 21 years. The measurements for every subject are taken over a short period of time, comprising in each case an interval far shorter than the age-range interval. Hence, the measurements on each subject constitute independent sparsely observed fragments, see Figure 10 (left) and yield information only on a partial covariance. Nevertheless, if we wish to conduct further analyses such as classification, regression, prediction, or even dimension reduction, we need access to a complete covariance.

We plot all those pairs of ages for which we have measurements on the same subject, see Figure 10 (right). Based on the plot, we infer that the covariance can be estimated reasonably well over the serrated domain $\Omega$ (colored in red) corresponding to the intervals [9.5, 13.5], [11.5, 15.5], [13.5, 17.5], [15, 19.5] and [17, 21]. We then estimate the covariance on $\Omega$ using locally linear kernel smoothing through the fdapace package and use the completion algorithm to estimate the covariance over the entire region, see Figure 11.

Acknowledgements

We are thankful to the reviewers for their very constructive feedback.

REFERENCES

[1] Artjomenko, A. P., 1941. Hermitian positive functions and positive functionals. (Russian). Dissertation, Odessa State University. Published in Teor. Funkcii, Funkcional. Anal. i Prilozen. 41, (1983) 1–16; 42 (1984), 1–21.
Fig 10: (left) Sparsely observed spine BMD curves for 117 females (right) Scatter plot of pairs of ages for which simultaneous observations are available.

Fig 11: Completed covariance of the BMD data.

[2] Bachrach, L.K., Hastie, T., Wang, M.C., Narasimhan, B. and Marcus, R., 1999. Bone mineral acquisition in healthy Asian, Hispanic, black, and Caucasian youth: a longitudinal study. The Journal of Clinical Endocrinology & Metabolism, 84(12), pp.4702-4712.

[3] Baker, C.R., 1973. Joint measures and cross-covariance operators. Transactions of the American Mathematical Society, 186, pp.273-289.

[4] Carathéodory, C., 1907. Über den Variabilitätsbereich der Koeffizienten von Potenzreihen, die gegebene Werte nicht annehmen. Math. Ann. 64, 95–115.

[5] Calderón, A. and Pepinsky, R, 1952. On the phases of Fourier coefficients for positive real periodic functions. Computing Methods and the Phase Problem in X-Ray Crystal Analysis, published by The X-Ray Crystal Analysis Laboratory, Department of Physics, The Pennsylvania State College, 339–348.

[6] Carroll, C., Gajardo, A., Chen, Y., Dai, X., Fan, J., Hadjipantelis, P. Z., Han, K., Ji, H., Mueller, H.-G., and Wang, J.-L., 2021. fdapace: Functional Data Analysis and Empirical Dynamics. R package version 0.5.6. https://CRAN.R-project.org/package=fdapace.

[7] Delaigle, A. and Hall, P., 2016. Approximating fragmented functional data by segments of Markov chains. Biometrika, 103(4), pp.779-799.

[8] Delaigle, A., Hall, P., Huang, W. and Kneip, A., 2020. Estimating the covariance of fragmented and other related types of functional data. Journal of the American Statistical Association, pp.1-19.
[9] Dempster, A.P., 1972. Covariance selection. Biometrics, pp.157-175.
[10] Descary, M.H. and Panaretos, V.M., 2019. Recovering covariance from functional fragments. Biometrika, 106(1), pp.145-160.
[11] Descary, M.H. and Panaretos, V.M., 2019. Functional data analysis by matrix completion. The Annals of Statistics, 47(1), pp.1-38.
[12] Dym, H. and Gohberg, I., 1981. Extensions of band matrices with band inverses. Linear algebra and its applications, 36, pp.1-24.
[13] Gneiting, T. and Sasvári, Z., 1999. The Characterization Problem for Isotropic Covariance Functions Math. Geology 31(1), 105–111.
[14] Gohberg, I., Kaashoek, M.A. and Woerdeman, H.J., 1989. The band method for positive and contractive extension problems. Journal of operator theory, pp.109-155.
[15] Hanke, M., 2017. A Taste of Inverse Problems: Basic Theory and Examples. Society for Industrial and Applied Mathematics.
[16] Grone, R., Johnson, C.R., Sá, E.M. and Wolkowicz, H., 1984. Positive definite completions of partial Hermitian matrices. Linear algebra and its applications, 58, pp.109-124.
[17] Johnson, C.R., 1990. Matrix theory and applications (Vol. 40). American Mathematical Society.
[18] Jouzdani, N.M. and Panaretos, V.M., 2021. Functional Data Analysis with Rough Sampled Paths?. arXiv preprint arXiv:2105.12035.
[19] Kneip, A. and Liebl, D., 2020. On the optimal reconstruction of partially observed functional data. Annals of Statistics, 48(3), pp.1692-1717.
[20] Kraus, D., 2015. Components and completion of partially observed functional data. Journal of the Royal Statistical Society: Series B: Statistical Methodology, pp.777-801.
[21] Krein, M.G., 1940. Sur le probleme du prolongement des fonctions hermitiennes positives et continues. In CR (Doklady) Acad. Sci. URSS (NS) (Vol. 26, No. 1, pp. 17-22).
[22] Krein, M.G. and Langer, H., 2014. Continuation of Hermitian positive definite functions and related questions. Integral Equations and Operator Theory, 78(1), pp.1-69.
[23] Lin, Z., Wang, J.L. and Zhong, Q., 2021. Basis expansions for functional snippets. Biometrika, 108(3), pp.709-726.
[24] Loève, M., 2017. Probability theory, 3rd ed. Dover Publications.
[25] Paulsen, V.I., Power, S.C. and Smith, R.R., 1989. Schur products and matrix completions. Journal of functional analysis, 85(1), pp.151-178.
[26] Paulsen, V.I. and Raghupathi, M., 2016. An introduction to the theory of reproducing kernel Hilbert spaces (Vol. 152). Cambridge University Press.
[27] R Core Team, 2019. R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria. https://www.R-project.org/.
[28] Rudin, W., 1963. The extension problem for positive-definite functions. Illinois J. Math. 7, 532–539.
[29] Saitoh, S. and Sawano, Y., 2016. Theory of reproducing kernels and applications. Singapore: Springer Singapore.
[30] Sasvári, Z., 2005. The extension problem for positive definite functions. A short historical survey. In Operator Theory and Indefinite Inner Product Spaces (pp. 365-379). Birkhäuser Basel.
[31] Stewart, J., 1976. Positive definite functions and generalizations, an historical survey. The Rocky Mountain Journal of Mathematics, 6(3), pp.409-434.
[32] Tikhonov, A.N., Goncharsky, A.V., Stepanov, V.V. and Yagola, A.G., 2013. Numerical methods for the solution of ill-posed problems (Vol. 328). Springer Science & Business Media.
[33] Waghmare, K., 2022. covcomp: Covariance Completion. R package. https://github.com/kgwstat/covcomp.