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Markov Random Geometric Graph (MRGG): A Growth Model for Temporal Dynamic Networks

Yohann De Castro¹ Quentin Duchemin²

Abstract

We introduce Markov Random Geometric Graphs (MRGGs), a growth model for temporal dynamic networks. It is based on a Markovian latent space dynamic: consecutive latent points are sampled on the Euclidean Sphere using an unknown Markov kernel; and two nodes are connected with a probability depending on a unknown function of their latent geodesic distance.

More precisely, at each stamp-time k we add a latent point X_k sampled by jumping from the previous one X_{k-1} in a direction chosen uniformly Y_k and with a length r_k drawn from an unknown distribution called the *latitude function*. The connection probabilities between each pair of nodes are equal to the *envelope function* of the distance between these two latent points. We provide theoretical guarantees for the non-parametric estimation of the latitude and the envelope functions.

We propose an efficient algorithm that achieves those non-parametric estimation tasks based on an ad-hoc Hierarchical Agglomerative Clustering approach. As a by product, we show how MRGGs can be used to detect dependence structure in growing graphs and to solve link prediction problems.

1. Introduction

In Random Geometric Graphs (RGG), nodes are sampled independently in latent space \mathbb{R}^d . Two nodes are connected if their distance is smaller than a threshold. A thorough probabilistic study of RGGs can be found in (Penrose, 2003). RGGs have been widely studied recently due to their ability to provide a powerful modeling tool for networks with

spatial structure. We can mention applications in bioinformatics (Higham et al., 2008) or analysis of social media (Hoff et al., 2002). One main feature is to uncover hidden representation of nodes using latent space and to model interactions by relative positions between latent points.

Furthermore, nodes interactions may evolve with time. In some applications, this evolution is given by the arrival of new nodes as in online collection growth (Lo et al., 2017), online social network growth (Backstrom et al., 2006; Jin et al., 2001), or outbreak modeling (Ugander et al., 2012) for instance. The network is growing as more nodes are entering. Other time evolution modelings have been studied, we refer to (Rossetti and Cazabet, 2018) for a review.

A natural extension of RGG consists in accounting this time evolution. In (Díaz et al., 2008), the expected length of connectivity and dis-connectivity periods of the Dynamic Random Geometric Graph is studied: each node choose at random an angle in $[0, 2\pi)$ and make a constant step size move in that direction. In (Staples, 2009), a random walk model for RGG on the hypercube is studied where at each time step a vertex is either appended or deleted from the graph. Their model falls into the class of Geometric Markovian Random Graphs that are generally defined in (Clementi et al., 2009).

As far as we know, there is no extension of RGG to growth model for temporal dynamic networks. For the first time, in this paper, we consider a Markovian dynamic on the latent space where the new latent point is drawn with respect to the latest latent point and some Markov kernel to be estimated.

Estimation of graphon in RGGs: the Euclidean sphere case Random graphs with latent space can be defined using a *graphon*, see (Lovász, 2012). A graphon is a kernel function that defines edge distribution. In (Tang et al., 2013), Tang and al. prove that spectral method can recover the matrix formed by graphon evaluated at latent points up to an orthogonal transformation, assuming that graphon is a positive definite kernel (PSD). Going further, algorithms have been designed to estimate graphons, as in (Klopp et al., 2017) which provide sharp rates for the Stochastic Block Model (SBM). Recently, the paper (Castro et al., 2020) provides a non-parametric algorithm to estimate RGGs on

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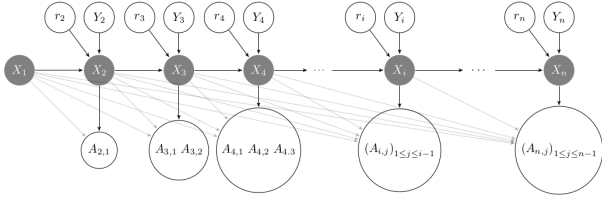


Figure 1. Graphical model of the MRGG model: Markovian dynamics on Euclidean sphere where we jump from X_k onto X_{k+1} . The Y_k encodes direction of jump while r_k encodes its distance, see (2).

Euclidean spheres, without PSD assumption.

We present here RGG on Euclidean sphere. Given n points X_1, X_2, \dots, X_n on the Euclidean sphere \mathbb{S}^{d-1} , we set an edge between nodes i and j (where $i, j \in [n], i \neq j$) with independent probability $p(\langle X_i, X_j \rangle)$. The unknown function $p: [-1, 1] \rightarrow [0, 1]$ is called the *envelope function*. This RGG is a graphon model with a symmetric kernel W given by $W(x, y) = p(\langle x, y \rangle)$. Once the latent points are given, independently draw the random undirected adjacency matrix A by

$$A_{i,j} \sim \mathcal{B}(p(\langle X_i, X_j \rangle)), \quad i < j$$

with Bernoulli r.v. drawn independently (set zero on the diagonal and complete by symmetry), and set

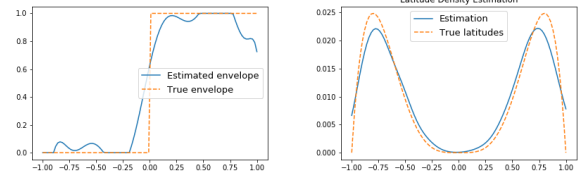
$$T_n := \frac{1}{n} (p(\langle X_i, X_j \rangle))_{i,j \in [n]} \quad \text{and} \quad \hat{T}_n := \frac{1}{n} A, \quad (1)$$

We do not observe the latent point and we have to estimate the envelope p from A only. A standard strategy is to remark that \hat{T}_n is a random perturbation of T_n and to dig into T_n to uncover p .

One important feature of this model is that the interactions between nodes is depicted by a simple object: the envelope function p . The envelope summarises how individuals connect each others given their latent positions. Standard examples (Bubeck et al., 2016) are given by $p_\tau(t) = \mathbb{1}_{\{t \geq \tau\}}$ where one connects two points as soon as their geodesic distance is below some threshold. The non-parametric estimation of p is given by (Castro et al., 2020) where the authors assume that latent points X_i are independently and uniformly distributed on the sphere, which will not be the case in the present paper.

A new growth model: the latent Markovian dynamic

Consider RGGs where latent points are sampled with Markovian jumps, the Graphical Model under consideration can be found in Figure 1. Namely, we sample n points X_1, X_2, \dots, X_n on the Euclidean sphere \mathbb{S}^{d-1} using



(a) Envelope function

(b) Latitude function

Figure 2. Non-parametric estimation of envelope and latitude functions using algorithms of Sections 2 and 3. We built a graph of 1500 nodes sampled on the sphere \mathbb{S}^2 and using envelope and latitude (dot orange curves) defined in Section 5 by (10). The estimated envelope is thresholded to get a function in $[0, 1]$ and the estimated latitude function is normalized with integral 1 (plain blue lines).

a Markovian dynamic. We start by sampling randomly X_1 on \mathbb{S}^{d-1} . Then, for any $i \in \{2, \dots, n\}$, we sample

- a unit vector $Y_i \in \mathbb{S}^{d-1}$ uniformly, orthogonal to X_{i-1} .
- a real $r_i \in [-1, 1]$ encoding the distance between X_{i-1} and X_i , see (3). r_i is sampled from a distribution $f_{\mathcal{L}}: [-1, 1] \rightarrow [0, 1]$, called the *latitude function*.

then X_i is defined by

$$X_i = r_i \times X_{i-1} + \sqrt{1 - r_i^2} \times Y_i. \quad (2)$$

This dynamic can be pictured as follows. Consider that X_{i-1} is the north pole, then chose uniformly a direction (i.e., a longitude) and, in a independent manner, randomly move along the latitudes (the longitude being fixed by the previous step). The geodesic distance γ_i drawn on the latitudes satisfies

$$\gamma_i = \arccos(r_i), \quad (3)$$

where random variable $r_i = \langle X_i, X_{i-1} \rangle$ has density $f_{\mathcal{L}}(r_i)$. The resulting model will be referred to as the Markov Random Geometric Graph (MRGG) and is described with Figure 1.

Temporal Dynamic Networks: MRGG estimation strategy

Seldom growth models exist for temporal dynamic network modeling, see (Rossetti and Cazabet, 2018) for a review. In our model, we add one node at a time making a Markovian jump from the previous latent position. It results in

the observation of $(A_{i,j})_{1 \leq j \leq i-1}$ at time $T = i$,

as pictured in Figure 1. Namely, we observe how a new node connects to the previous ones. For such dynamic, we aim at estimating the model, namely envelope p and

respectively latitude $f_{\mathcal{L}}$. These functions capture in a simple function on $\Omega = [-1, 1]$ the range of interaction of nodes (represented by p) and respectively the dynamic of the jumps in latent space (represented by $f_{\mathcal{L}}$), where, in abscissa Ω , values $r = \langle X_i, X_j \rangle$ near 1 corresponds to close point $X_i \simeq X_j$ while values close to -1 corresponds to antipodal points $X_i \simeq -X_j$. These functions may be non-parametric.

From snapshots of the graph at different time steps, can we recover envelope and latitude functions? This paper proves that it is possible under mild conditions on the Markovian dynamic of the latent points and our approach is summed up with Figure 3.

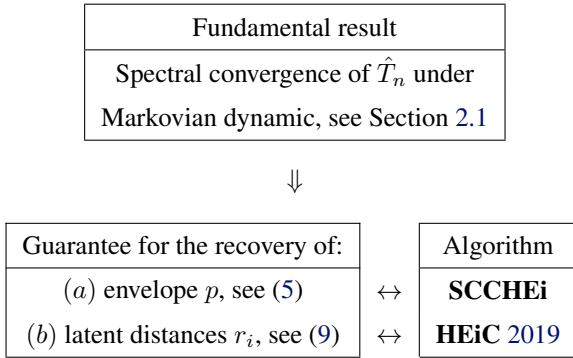


Figure 3. Presentation of our method to recover the envelope and the latitude functions.

Define $\lambda(T_n) := (\lambda_1, \dots, \lambda_n)$ and resp. $\lambda(\hat{T}_n) := (\hat{\lambda}_1, \dots, \hat{\lambda}_n)$ the spectrum of T_n and resp. \hat{T}_n , see (1). Building clusters from $\lambda(\hat{T}_n)$, Algorithm 1 (SCCHEi) estimates the spectrum of envelope p while Algorithm 3 (Araya and De Castro, 2019) (HEiC, see Section E in Appendix) extracts d eigenvectors of \hat{T}_n to uncover the Gram matrix of the latent positions. Both can then be used to estimate the unknown functions of our model (see Figure 2).

Previous works Non-parametric estimation of RGGs on Euclidean sphere has been investigated in (Castro et al., 2020) with i.i.d. latent points. Estimation of latent point relative distances with HEiC Algorithm has been introduced in (Araya and De Castro, 2019) under i.i.d. latent points assumption. Phase transitions on the detection of geometry in RGGs (against Erdős Rényi alternatives) has been investigated in (Bubeck et al., 2016).

For the first time, we introduce latitude function and non-parametric estimations of envelope and latitude using new results on kernel matrices concentration with dependent variables (see Appendix).

Outline Sections 2 and 3 present the estimation method with new theoretical results under Markovian dynamic. These new results are random matrices operator norm control and resp. U-statistics control under Markovian dynamic,

shown in the Appendix at Section G and resp. Section F. The envelope *adaptive* estimate is built from a size constrained clustering (Algorithm 1) tuned by slope heuristic (6), and the latitude function estimate (see Section 3.1) is derived from estimates of latent distances r_i . Sections 5 and 6 investigate synthetic data experiments¹. We propose heuristics to solve link prediction problems and to test for a Markovian dynamic. Our method can handle random graphs with logarithmic growth node degree (i.e., new comer at time $T = n$ connects to $\mathcal{O}(\log n)$ previous nodes), referred to as *relatively sparse* models, see Section 4.

Notations Consider a dimension $d \geq 3$. Denote by $\|\cdot\|_2$ (resp. $\langle \cdot, \cdot \rangle$) the Euclidean norm (resp. inner product) on \mathbb{R}^d . Consider the d -dimensional sphere $\mathbb{S}^{d-1} := \{x \in \mathbb{R}^d : \|x\|_2 = 1\}$ and denote by σ the uniform distribution on \mathbb{S}^{d-1} . For two real valued sequences $(u_n)_{n \in \mathbb{N}}$ and $(v_n)_{n \in \mathbb{N}}$, denote $u_n \underset{n \rightarrow \infty}{=} \mathcal{O}(v_n)$ if there exist $k_1 > 0$ and $n_0 \in \mathbb{N}$ such that $\forall n > n_0, |u_n| \leq k_1 |v_n|$.

Given two sequences x, y of reals—completing finite sequences by zeros—such that $\sum_i x_i^2 + y_i^2 < \infty$, we define the ℓ_2 rearrangement distance $\delta_2(x, y)$ as

$$\delta_2^2(x, y) := \inf_{\pi \in \mathfrak{S}} \sum_i (x_i - y_{\pi(i)})^2,$$

where \mathfrak{S} is the set of permutations with finite support. This distance is useful to compare two spectra.

2. Nonparametric estimation of the envelope function

One can associate with $W(x, y) = p(\langle x, y \rangle)$ the integral operator $\mathbb{T}_W : L^2(\mathbb{S}^{d-1}) \rightarrow L^2(\mathbb{S}^{d-1})$ such that for any $g \in L^2(\mathbb{S}^{d-1})$,

$$\forall x \in \mathbb{S}^{d-1}, (\mathbb{T}_W g)(x) = \int_{\mathbb{S}^{d-1}} g(y) p(\langle x, y \rangle) d\sigma(y),$$

where $d\sigma$ is the Lebesgue measure on \mathbb{S}^{d-1} . The operator \mathbb{T}_W is Hilbert-Schmidt and it has a countable number of bounded eigenvalues λ_k^* with zero as only accumulation point. The eigenfunctions of \mathbb{T}_W have the remarkable property that they do not depend on p (see (Dai, 2013) Lemma 1.2.3): they are given by the real Spherical Harmonics. We denote \mathcal{H}_l the space of real Spherical Harmonics of degree l with dimension d_l and with orthonormal basis $(Y_{l,j})_{j \in [d_l]}$ where

$$d_l := \dim(\mathcal{H}_l) = \begin{cases} 1 & \text{if } l = 0 \\ d & \text{if } l = 1 \\ \binom{l+d-1}{l} - \binom{l+d-3}{l-2} & \text{otherwise.} \end{cases}$$

¹Our code is available at <https://github.com/quentin-duchemin/Markovian-random-geometric-graph.git>

We define also for all $R \in \mathbb{N}$, $\tilde{R} := \sum_{l=0}^R d_l$. We end up with the following spectral decomposition

$$p(\langle x, y \rangle) = \sum_{l \geq 0} p_l^* \sum_{1 \leq j \leq d_l} Y_{l,j}(x) Y_{l,j}(y) = \sum_{k \geq 0} p_k^* c_k G_k^\beta(\langle x, y \rangle) \quad (4)$$

where $\lambda(\mathbb{T}_W) = \{p_0^*, p_1^*, \dots, p_1^*, \dots, p_l^*, \dots, p_l^*, \dots\}$ meaning that each eigenvalue p_l^* has multiplicity d_l ; and G_k^β is the Gegenbauer polynomial of degree k with parameter $\beta := \frac{d-2}{2}$ and $c_k := \frac{2k+d-2}{d-2}$ (see Appendix C). Since p is bounded, one has $p \in L^2((-1, 1), w_\beta)$ where the weight function w_β is defined by $w_\beta(t) := (1-t^2)^{\beta-\frac{1}{2}}$, and it can be decomposed as $p \equiv \sum_{k \geq 0} p_k^* c_k G_k^\beta$ and the Gegenbauer polynomials G_k^β are an orthogonal basis of $w_\beta(t) := (1-t^2)^{\beta-\frac{1}{2}}$.

Weighted Sobolev space The space $Z_{w_\beta}^s((-1, 1))$ with regularity $s > 0$ is defined as the set of functions $g = \sum_{k \geq 0} g_k^* c_k G_k^\beta \in L^2((-1, 1), w_\beta)$ such that

$$\|g\|_{Z_{w_\beta}^s(((-1,1)))}^* := \left[\sum_{l=0}^{\infty} d_l |g_l^*|^2 (1 + (l(l+2\beta))^s) \right]^{1/2} < \infty.$$

2.1. Integral operator spectrum estimation with dependent variables

One key result is a new control of U -statistics with latent Markov variables (see Section F) and it makes use of a Talagrand's concentration inequality for Markov chains (see (Adamczak, 2007)). This article follows the hypothesis made on the Markov chain $(X_i)_{i \geq 1}$ by (Adamczak, 2007). Namely, we referred to as "mild conditions" the assumption that the latitude function $f_{\mathcal{L}}$ is bounded away from zero with $\|f_{\mathcal{L}}\|_{\infty} < \infty$; and the first and the second regeneration times associated with the *split* chain to have sub-exponential tail. Those assumptions are fully described in section F.

Theorem 1 is a theoretical guarantee for a random matrix approximation of the spectrum of integral operator with **dependent** latent variables. Theorem 3 in Appendix G gives explicitly the constants hidden in the big O below which depend on the spectral gap of the Markov chain $(X_i)_{i \geq 1}$.

Theorem 1 *Assume mild conditions on the Markov chain $(X_i)_{i \geq 1}$ and assume the envelope p has regularity $s > 0$. Then, it holds*

$$\begin{aligned} & \mathbb{E} \left[\delta_2^2(\lambda(\mathbb{T}_W), \lambda(T_n)) \vee \delta_2^2(\lambda(\mathbb{T}_W), \lambda^{R_{opt}}(\hat{T}_n)) \right] \\ &= \mathcal{O} \left(\left[\frac{n}{\log^2(n)} \right]^{-\frac{2s}{2s+d-1}} \right), \end{aligned}$$

with $\lambda^{R_{opt}}(\hat{T}_n) = (\hat{\lambda}_1, \dots, \hat{\lambda}_{\tilde{R}_{opt}}, 0, 0, \dots)$ and $R_{opt} = \lfloor (n/\log^2(n))^{\frac{1}{2s+d-1}} \rfloor$ where $\hat{\lambda}_1, \dots, \hat{\lambda}_n$ are the eigenvalues of \hat{T}_n sorted in decreasing order of magnitude.

Remark In Theorem 1 and Theorem 2, note that we recover, up to a log factor, the *minimax rate of non-parametric estimation* of s -regular functions on a space of (Riemannian) dimension $d-1$. Even with i.i.d. latent variables, it is still an open question to know if this rate is the minimax rate of non-parametric estimation of RGGs.

Eq.(4) shows that one could use an approximation of $(p_k^*)_{k \geq 1}$ to estimate the envelope p and Theorem 1 states we can recover $(p_k^*)_{k \geq 1}$ up to a permutation. The problem of finding such a permutation is NP-hard and we introduce in the next section an efficient algorithm to fix this issue.

2.2. Size Constrained Clustering Algorithm

Note the spectrum of \mathbb{T}_W is given by $(p_l^*)_{l \geq 0}$ where p_l^* has multiplicity d_l . In order to recover envelope p , we build clusters from eigenvalues of \hat{T}_n while respecting the dimension d_l of each eigen-space of \mathbb{T}_W . In (Castro et al., 2020), an algorithm is proposed testing all permutations of $\{0, \dots, R\}$ for a given maximal resolution R . To bypass the high computational cost of such approach, we propose an efficient method based on the tree built from *Hierarchical Agglomerative Clustering* (HAC).

In the following, for any $\nu_1, \dots, \nu_n \in \mathbb{R}$, we denote by $\text{HAC}(\{\nu_1, \dots, \nu_n\}, d_c)$ the tree built by a HAC on the real values ν_1, \dots, ν_n using the complete linkage function d_c defined by $\forall A, B \subset \mathbb{R}, d_c(A, B) = \max_{a \in A} \max_{b \in B} \|a-b\|_2$. Algorithm 1 describes our approach.

Algorithm 1 Size Constrained Clustering for Harmonic Eigenvalues (SCCHEi).

Data: Resolution R , matrix $\hat{T}_n = \frac{1}{n} A$, dimensions $(d_k)_{k=0}^R$.

- 1: Let $\hat{\lambda}_1, \dots, \hat{\lambda}_n$ be the eigenvalues of \hat{T}_n sorted in decreasing order of magnitude.
- 2: Set $\mathcal{P} := \{\hat{\lambda}_1, \dots, \hat{\lambda}_{\tilde{R}}\}$ and $\text{dims} = [d_0, d_1, \dots, d_R]$.
- 3: **while** All eigenvalues in \mathcal{P} are not clustered **do**
- 4: $\text{tree} \leftarrow \text{HAC}(\text{nonclustered eigenvalues in } \mathcal{P}, d_c)$
- 5: **for** $d \in \text{dims}$ **do**
- 6: Search for a cluster of size d in tree as close as possible to the root.
- 7: **if** such a cluster \mathcal{C}_d exists **then**
 Update($\text{dims}, \text{tree}, \mathcal{C}_d, d$).
- 8: **end for**
- 9: **for** $d \in \text{dims}$ **do**
- 10: Search for the group \mathcal{C} in tree with a size larger than d and as close as possible to d .
- 11: **if** such a group exists **then** Update($\text{dims}, \text{tree}, \mathcal{C}, d$)
 else Go to line 3.
- 12: **end for**
- 13: **end while**

Return: $\mathcal{C}_{d_0}, \dots, \mathcal{C}_{d_R}, \{\hat{\lambda}_{\tilde{R}+1}, \dots, \hat{\lambda}_n\}$

Algorithm 2 Update($dims, tree, \mathcal{C}, d$).

- 1: Save the subset \mathcal{C}_d consisting of the d eigenvalues in \mathcal{C} with the largest absolute values.
 - 2: Delete from $tree$ all occurrences to eigenvalues in \mathcal{C}_d and delete d from $dims$.
-

2.3. Adaptation: Slope heuristic as model selection of Resolution

A data-driven choice of model size R can be done by *slope heuristic*, see (Arlot, 2019) for a nice review. One main idea of slope heuristic is to penalize the empirical risk by $\kappa \text{pen}(\tilde{R})$ and to calibrate $\kappa > 0$. If the sequence $(\text{pen}(\tilde{R}))_{\tilde{R}}$ is equivalent to the sequence of variances of the population risk of empirical risk minimizer (ERM) as model size \tilde{R} grows, then, penalizing the empirical risk (as done in (6)), one may ultimately uncover an empirical version of the U -shaped curve of the population risk. Hence, minimizing it, one builds a model size \hat{R} that balances between bias (*under-fitting* regime) and variance (*over-fitting* regime). First, note that empirical risk is given by the intra-class variance below.

Definition 1 For any output $(\mathcal{C}_{d_0}, \dots, \mathcal{C}_{d_R}, \Lambda)$ of the Algorithm SCCHEi, the thresholded intra-class variance is defined by

$$\mathcal{I}_R := \frac{1}{n} \left[\sum_{k=0}^R \sum_{\lambda \in \mathcal{C}_{d_k}} \left(\lambda - \frac{1}{d_k} \sum_{\lambda' \in \mathcal{C}_{d_k}} \lambda' \right)^2 + \sum_{\lambda \in \Lambda} \lambda^2 \right],$$

and the estimations $(\hat{p}_k)_{k \geq 0}$ of the eigenvalues $(p_k^*)_{k \geq 0}$ is given by

$$\forall k \in \mathbb{N}, \quad \hat{p}_k = \begin{cases} \frac{1}{d_k} \sum_{\lambda \in \mathcal{C}_{d_k}} \lambda & \text{if } k \in \{0, \dots, \hat{R}\} \\ 0 & \text{otherwise.} \end{cases} \quad (5)$$

Second, as underlined in the proof of Theorem 1 (see Theorem 3 in the Appendix), the estimator's variance of our estimator scales linearly in \tilde{R} .

Hence, we apply Algorithm SCCHEi for R varying from 0 to $R_{\max} := \max\{R \geq 0 : \tilde{R} \leq n\}$ to compute the *thresholded intra-class variance* \mathcal{I}_R (see Definition 1) and given some $\kappa > 0$, we select

$$R(\kappa) \in \arg \min_{R \in \{0, \dots, R_{\max}\}} \left\{ \mathcal{I}_R + \kappa \frac{\tilde{R}}{n} \right\}. \quad (6)$$

The hyper-parameter κ controlling the bias-variance trade-off is set to $2\kappa_0$ where κ_0 is the value of $\kappa > 0$ leading to the “*largest jump*” of the function $\kappa \mapsto R(\kappa)$. Once $\hat{R} := R(2\kappa_0)$ has been computed, we approximate the envelope function p using (5) (see (19) in Appendix for the closed

form). In Appendix D, we describe this slope heuristic on a concrete example and our results can be reproduced using the notebook in the Supplementary Material.

3. Nonparametric estimation of the latitude function

3.1. Our approach to estimate the latitude function in a nutshell

In Theorem 2 (see below), we show that we are able to estimate consistently the pairwise distances encoded by the Gram matrix G^* where

$$G^* := \frac{1}{n} (\langle X_i, X_j \rangle)_{i,j \in [n]}.$$

Taking the diagonal just above the main diagonal (referred to as *superdiagonal*) of \hat{G} - an estimate of the matrix G to be specified - we get estimates of the i.i.d. random variables $(\langle X_i, X_{i-1} \rangle)_{2 \leq i \leq n} = (r_i)_{2 \leq i \leq n}$ sampled from $f_{\mathcal{L}}$. Using $(\hat{r}_i)_{2 \leq i \leq n}$ the superdiagonal of $n\hat{G}$, we can build a kernel density estimator of the latitude function $f_{\mathcal{L}}$. In the following, we describe the algorithm used to build our estimator \hat{G} with theoretical guarantees.

3.2. Spectral gap condition and Gram matrix estimation

The Gegenbauer polynomial of degree one is defined by $G_1^\beta(t) = 2\beta t$, $\forall t \in [-1, 1]$. As a consequence, using the *addition theorem* (see (Dai, 2013, Lem.1.2.3 and Thm.1.2.6)), the Gram matrix G^* is related to the Gegenbauer polynomial of degree one. More precisely, for any $i, j \in [n]$ it holds

$$G_{i,j}^* = \frac{1}{2\beta n} G_1^\beta(\langle X_i, X_j \rangle) = \frac{1}{nd} \sum_{k=1}^d Y_{1,k}(X_i) Y_{1,k}(X_j). \quad (7)$$

Denoting $V^* \in \mathbb{R}^{n \times d}$ the matrix with columns $v_k^* := \frac{1}{\sqrt{n}} (Y_{1,k}(X_1), \dots, Y_{1,k}(X_n))$ for $k \in [d]$, (7) becomes

$$G^* := \frac{1}{d} V^* (V^*)^\top.$$

We will prove that for n large enough there exists a matrix $\hat{V} \in \mathbb{R}^{n \times d}$ where each column is an eigenvector of \hat{T}_n , such that $\hat{G} := \frac{1}{d} \hat{V} \hat{V}^\top$ approximates G^* well, in the sense that the norm $\|G^* - \hat{G}\|_F$ converges to 0. To choose the d eigenvectors of the matrix \hat{T}_n that we will use to build the matrix \hat{V} , we need the following spectral gap condition

$$\Delta^* := \min_{k \in \mathbb{N}, k \neq 1} |p_1^* - p_k^*| > 0. \quad (8)$$

This condition will allow us to apply Davis-Kahan type inequalities.

Now, thanks to Theorem 1, we know that the spectrum of the matrix \hat{T}_n converges towards the spectrum of the integral operator \mathbb{T}_W . Then, based on (7), one can naturally think that extracting the d eigenvectors of the matrix \hat{T}_n related with the eigenvalues that converge towards p_1^* , we can approximate the Gram matrix G^* of the latent positions. Theorem 2 proves that the latter intuition is true with high probability under the spectral gap condition (8). The algorithm HEiC (Araya and De Castro, 2019) (See Section E for a presentation) aims at identifying the above mentioned d eigenvectors of the matrix \hat{T}_n to build our estimate of the Gram matrix G^* .

Theorem 2 *Assume mild conditions on the Markov chain $(X_i)_{i \geq 1}$, assume $\Delta^* > 0$, and assume that graphon W has regularity $s > 0$. We denote $\hat{V} \in \mathbb{R}^{n \times d}$ the d eigenvectors of the matrix \hat{T}_n associated with the eigenvalues returned by the algorithm HEiC and we define $\hat{G} := \frac{1}{d} \hat{V} \hat{V}^\top$. Then for n large enough and for some constant $D > 0$, it holds with probability at least $1 - 5/n^2$,*

$$\|G^* - \hat{G}\|_F \leq D \left(\frac{n}{\log^2(n)} \right)^{\frac{-s}{2s+d-1}}. \quad (9)$$

Based on Theorem 2, we propose a kernel density approach to estimate the latitude function $f_{\mathcal{L}}$ based on the superdiagonal of the matrix \hat{G} , namely $(\hat{r}_i := \hat{G}_{i-1,i})_{i \in \{2, \dots, n\}}$.

In the following, we denote $\hat{f}_{\mathcal{L}}$ this estimator.

4. Relatively Sparse Regime

Although this paper deals with the so-called *dense* regime (i.e. when the expected number of neighbors of each node scales linearly with n), our results may be generalized to the *relatively sparse* model connecting nodes i and j with probability $W(X_i, X_j) = \zeta_n p(\langle X_i, X_j \rangle)$ where $\zeta_n \in (0, 1]$ satisfies $\liminf_n \zeta_n n / \log n \geq Z$ for some universal constant $Z > 0$.

In the relatively sparse model, one can show following the proof of Theorem 1 that the resolution should be chosen as $\hat{R} = \left(\frac{n \zeta_n}{1 + \zeta_n \log^2 n} \right)^{\frac{1}{2s+d-1}}$. Specifying that $\lambda^* = (p_0^*, p_1^*, \dots, p_1^*, p_2^*, \dots)$ and $\hat{T}_n = A/n$, Theorem 1 becomes for a graphon with regularity $s > 0$

$$\mathbb{E} \left[\delta_2^2 \left(\lambda^*, \frac{\lambda(\hat{T}_n)}{\zeta_n} \right) \right] = \mathcal{O} \left(\left(\frac{n \zeta_n}{1 + \zeta_n \log^2 n} \right)^{\frac{-2s}{2s+d-1}} \right).$$

Figure 4 illustrates the estimation of the latitude and the envelope functions in some relatively sparse regimes.

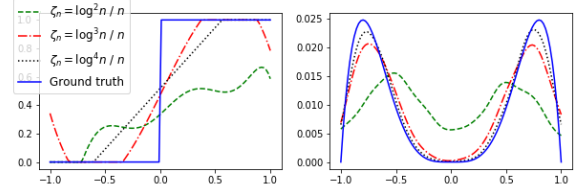


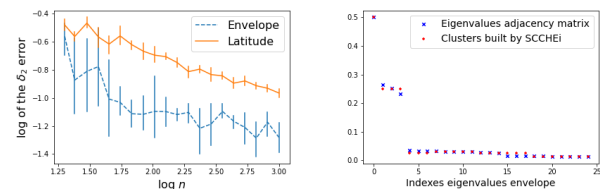
Figure 4. Results of our algorithms for graph of size 2,000 with functions of Eq.(10) and sparsity parameter $\zeta_n = \log^k n/n$, $k \in \{2, 3, 4\}$.

5. Experiments

We test our method using $d = 3$ and considering the following functions

$$p : x \mapsto \mathbb{1}_{x \geq 0}, \quad \text{and} \\ f_{\mathcal{L}} : x \mapsto \begin{cases} \frac{1}{2}g(1-x; 2, 2) & \text{if } x \geq 0 \\ \frac{1}{2}g(1+x; 2, 2) & \text{otherwise} \end{cases}, \quad (10)$$

where $g(\cdot; 2, 2)$ is the density of the beta distribution with parameters $(2, 2)$. Figure 5.(a) presents the δ_2 -error between the spectra of the true envelope (resp. latitude) function and the estimated one when the size of the graph is increasing. In Figure 5.(b), we propose a visualization of the clustering performed by SCCHEi with $n = 1000$ and $R = 4$. Blue crosses represent the \hat{R} eigenvalues of \hat{T}_n with the largest magnitude, which are used to form clusters corresponding to the five-first spherical harmonic spaces. The red circles are the estimated eigenvalues $(\hat{p}_k)_{0 \leq k \leq 4}$ (plotted with multiplicity) defined from the clustering given by our algorithm SCCHEi (see (5)). Those results show that SCCHEi achieves a relevant clustering of the eigenvalues of \hat{T}_n which allows us to recover the envelope function (see Figure 2.(a)).



(a) δ_2 error on envelope and lat-(b) Clustering adjacency eigenvalues ($R = 4$).

Figure 5. Non-parametric estimation of envelope and latitude using algorithms described in Sections 2 and 3. In (a), bars represent standard deviation of δ_2 errors between true and estimated functions.

6. Applications

In this section, we apply the MRGG model to link prediction and hypothesis testing in order to demonstrate the usefulness

of our approach as well as the estimation procedure.

6.1. Markovian Dynamic Testing

As a first application of our model, we propose a hypothesis test to statistically distinguish between an independent sampling the latent positions and a Markovian dynamic. The null is then set to \mathbb{H}_0 : *nodes are independent and uniformly distributed on the sphere* (i.e., *no Markovian dynamic*). Our test is based on estimate $\hat{f}_{\mathcal{L}}$ of latitude and thus the null can be rephrased as \mathbb{H}_0 : $f_{\mathcal{L}} = f_{\mathcal{L}}^0$ where $f_{\mathcal{L}}^0$ is the latitude of uniform law, dynamic is then i.i.d. dynamic. Figure 6 shows the power of a hypothesis test with level 5% (Type I error). One can use any *black-box goodness-of-fit test* comparing $\hat{f}_{\mathcal{L}}$ to $f_{\mathcal{L}}^0$, and we choose χ^2 -test discretizing $(-1, 1)$ in 70 regular intervals. Rejection region is calibrated (i.e.,

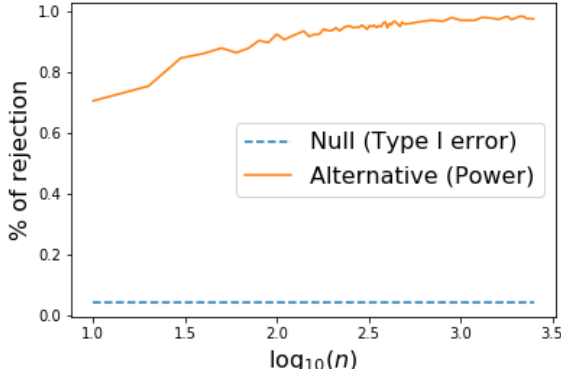


Figure 6. Hypothesis testing.

threshold of the χ^2 -test here) by *Monte Carlo simulations under the null*. It allows us to control Type I error as depicted by dotted blue line. We choose alternative given by Heaviside envelope and latitude $f_{\mathcal{L}}$ of (10). We run our algorithm to estimate latitude from which we sample a batch to compute the χ^2 -test statistic. We see that for graphs of size larger than 1,000, the rejection rate is almost 1 under the alternative (Type II error is almost zero), the test is very powerful.

6.2. Link Prediction

Suppose that we observe a graph with n nodes. Link prediction is the task that consists in estimating the probability of connection between a given node of the graph and the upcoming node.

6.2.1. BAYES LINK PREDICTION

We propose to show the usefulness of our model solving a link prediction problem. Let us recall that we do not estimate the latent positions but only the *pairwise distances* (embedding task is not necessary for our purpose). De-

noting $\text{proj}_{X_n^\perp}(\cdot)$ the orthogonal projection onto the orthogonal complement of $\text{Span}(X_n)$, the decomposition of $\langle X_i, X_{n+1} \rangle$ defined by

$$\langle X_i, X_n \rangle \langle X_n, X_{n+1} \rangle + \sqrt{1 - \langle X_n, X_{n+1} \rangle^2} \times \sqrt{1 - \langle X_i, X_n \rangle^2} \left\langle \frac{\text{proj}_{X_n^\perp}(X_i)}{\|\text{proj}_{X_n^\perp}(X_i)\|_2}, Y_{n+1} \right\rangle, \quad (11)$$

shows that latent distances are enough for link prediction. Indeed, it can be achieved using a *forward step* on our Markovian dynamic, giving the posterior probability (see Definition 2) $\eta_i(\mathbf{D}_{1:n})$ defined by

$$\int_{[-1,1]^2} p(\langle X_i, X_n \rangle r + \sqrt{1-r^2} \sqrt{1-\langle X_i, X_n \rangle^2} u) f_{\mathcal{L}}(r) \frac{dr du}{2}. \quad (12)$$

Definition 2 (Posterior probability function)

The posterior probability function η is defined for any latent pairwise distances $\mathbf{D}_{1:n} = (\langle X_i, X_j \rangle)_{1 \leq i, j \leq n} \in [-1, 1]^{n \times n}$ by

$$\forall i \in [n], \quad \eta_i(\mathbf{D}_{1:n}) = \mathbb{P}(A_{i,n+1} = 1 \mid \mathbf{D}_{1:n}),$$

where $A_{i,n+1} \sim \mathcal{B}(p(\langle X_i, X_{n+1} \rangle))$ is a random variable that equals 1 if there is an edge between nodes i and $n+1$, and is zero otherwise.

We consider a classifier g (see Definition 3) and an algorithm that, given some latent pairwise distances $\mathbf{D}_{1:n}$, estimates $A_{i,n+1}$ by putting an edge between nodes X_i and X_{n+1} if $g_i(\mathbf{D}_{1:n})$ is 1.

Definition 3 A classifier is a function which associates to any pairwise distances $\mathbf{D}_{1:n} = (\langle X_i, X_j \rangle)_{1 \leq i, j \leq n}$, a label $(g_i(\mathbf{D}_{1:n}))_{i \in [n]} \in \{0, 1\}^n$.

The risk of this algorithm is as in *binary classification*,

$$\begin{aligned} \mathcal{R}(g, \mathbf{D}_{1:n}) &:= \frac{1}{n} \sum_{i=1}^n \mathbb{P}(g_i(\mathbf{D}_{1:n}) \neq A_{i,n+1} \mid \mathbf{D}_{1:n}) \\ &= \frac{1}{n} \sum_{i=1}^n \left\{ (1 - \eta_i(\mathbf{D}_{1:n})) \mathbb{1}_{g_i(\mathbf{D}_{1:n})=1} + \eta_i(\mathbf{D}_{1:n}) \mathbb{1}_{g_i(\mathbf{D}_{1:n})=0} \right\}, \end{aligned} \quad (13)$$

where we used the independence between $A_{i,n+1}$ and $g_i(\mathbf{D}_{1:n})$ conditionally on $\sigma(\mathbf{D}_{1:n})$. Pushing further this analogy, we can define the classification error of some classifier g by $L(g) = \mathbb{E}[\mathcal{R}(g, \mathbf{D}_{1:n})]$. Proposition 1 shows that the Bayes estimator - introduced in Definition 4 - is optimal for the risk defined in (13).

Definition 4 (Bayes estimator)

We keep the notations of Definition 2. The Bayes estimator g^* of $(A_{i,n+1})_{1 \leq i \leq n}$ is defined by

$$\forall i \in [n], \quad g_i^*(\mathbf{D}_{1:n}) = \begin{cases} 1 & \text{if } \eta_i(\mathbf{D}_{1:n}) \geq \frac{1}{2} \\ 0 & \text{otherwise.} \end{cases}$$

Proposition 1 (Optimality of the Bayes classifier for the risk \mathcal{R})

We keep the notations of Definitions 2 and 4. For any classifier g , it holds for all $i \in [n]$,

$$\begin{aligned} & \mathbb{P}(g_i(\mathbf{D}_{1:n}) \neq A_{i,n+1} \mid \mathbf{D}_{1:n}) \\ & \quad - \mathbb{P}(g_i^*(\mathbf{D}_{1:n}) \neq A_{i,n+1} \mid \mathbf{D}_{1:n}) \\ & = 2 \left| \eta_i(\mathbf{D}_{1:n}) - \frac{1}{2} \right| \times \mathbb{E} \left\{ \mathbb{1}_{g_i(\mathbf{D}_{1:n}) \neq g_i^*(\mathbf{D}_{1:n})} \mid \mathbf{D}_{1:n} \right\}, \end{aligned}$$

which immediately implies that

$$\mathcal{R}(g, \mathbf{D}_{1:n}) \geq \mathcal{R}(g^*, \mathbf{D}_{1:n}) \text{ and therefore } L(g) \geq L(g^*).$$

6.2.2. HEURISTIC FOR LINK PREDICTION

One natural method to approximate the Bayes classifier from the previous section is to use the *plug-in approach*. This leads to the MRGG classifier introduced in Definition 5.

Definition 5 (The MRGG classifier)

For any n and any $i \in [n]$, we define $\hat{\eta}_i(\mathbf{D}_{1:n})$ as

$$\int \hat{p} \left(\hat{r}_{i,n} r + \sqrt{1-r^2} \sqrt{1-\hat{r}_{i,n}^2} u \right) \hat{f}_{\mathcal{L}}(r) \frac{dr du}{2}, \quad (14)$$

where \hat{p} and $\hat{f}_{\mathcal{L}}$ denote respectively the estimate of the envelope function and the latitude function with our method and where $\hat{r} := n\hat{G}$. The MRGG classifier is defined by

$$\forall i \in [n], \quad g_i^{MRGG}(\mathbf{D}_{1:n}) = \begin{cases} 1 & \text{if } \hat{\eta}_i(\mathbf{D}_{1:n}) \geq \frac{1}{2} \\ 0 & \text{otherwise.} \end{cases}$$

To illustrate our approach we work with a graph of 2,000 nodes with $d = 3$, Heaviside envelope and $f_{\mathcal{L}}(r) = \frac{1}{2} f_{(5,1)}\left(\frac{r+1}{2}\right)$ where $f_{(5,1)}$ is the pdf of the Beta distribution with parameter (5, 1). Figure 7 shows that we are able to recover the probabilities of connection of the nodes already present in the graph with the coming node X_{n+1} . Using the decomposition of $\langle X_i, X_{n+1} \rangle$ given by (11), orange crosses are computed using (12). Green plus are computed similarly replacing p and $f_{\mathcal{L}}$ by their estimations \hat{p} and $\hat{f}_{\mathcal{L}}$ following (14). Blue stars are computed using (12) by replacing $f_{\mathcal{L}}$ by $\frac{w_{\beta}}{\|w_{\beta}\|_1} = \frac{1}{2}$ (since $d = 3$) which amounts to consider that the points are sampled uniformly on the sphere.

In Figure 8, we compare the risk of the *random* classifier - whose guess $g_i(\mathbf{D}_{1:n})$ is a Bernoulli random variable with parameter given by the ratio of edges compared to complete graph - with the risk of the MRGG classifier (see Definition 5). Figure 8 shows that the risk of the MRGG classifier is significantly smaller than the risk of random classifier, it is clearly better than random. Moreover, Figure 8 shows that the MRGG classifier gives similar results compared to the optimal Bayes classifier.

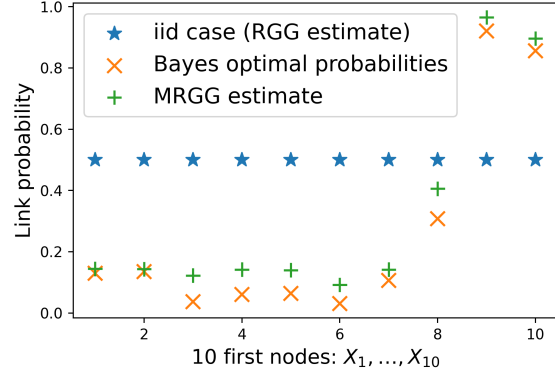


Figure 7. Link predictions between the future node X_{n+1} and the 10 first nodes X_1, \dots, X_{10} .

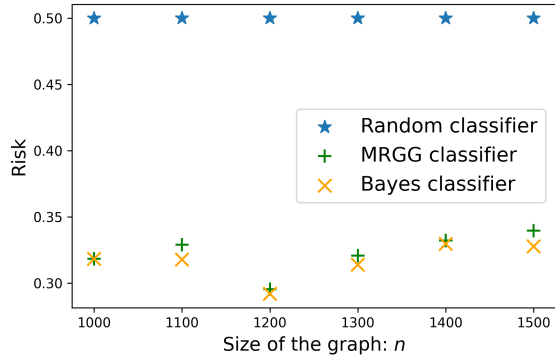


Figure 8. Comparison between the risk (defined in (13)) of the MRGG classifier, the random classifier and the risk of the optimal Bayes classifier.

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Supplementary Material

Markov Random Geometric Graph (MRGG): A Growth Model for Temporal Dynamic Networks

Guidelines for the supplementary material

Sections A to C: Basic definitions and Complements

In Section A we recall basic definitions on Markov chains which are required for Section B where we describe some properties verified by the Markov chain $(X_i)_{i \geq 1}$. Section C provides complementary results on the Harmonic Analysis on \mathbb{S}^{d-1} which will be useful for our proofs.

Sections D to E: Algorithms and Experiments²

Section D describes precisely the slope heuristic used to perform the adaptive selection of the model dimension \tilde{R} . Section E provides a complete description of the HEiC algorithm used to extract d -eigenvectors of the adjacency matrix that will be used to estimate the Gram matrix of the latent positions.

Sections F to H: Proofs of theoretical results

Thereafter, we dig into the most theoretical part of the supplementary material. In Section F, we provide a full description of the assumptions we made on the Markov chain $(X_i)_{i \geq 1}$ and which we have been referring to so far by *mild conditions*. Section F is also dedicated to the presentation of a concentration result for a particular U-statistic of the Markov chain $(X_i)_{i \geq 1}$ that is an essential element of the proof of Theorem 1 which is provided in Section G. Finally, the proof of Theorem 2 can be found in Section H.

A. Definitions for general Markov chains

We consider a state space E and a sigma-algebra Σ on E which is a standard Borel space. We denote by $(X_i)_{i \geq 1}$ a time homogeneous Markov chain on the state space (E, Σ) with transition kernel P .

A.1. Ergodic and reversible Markov chains

Definition 6 (*Roberts and Rosenthal, 2004, section 3.2*) (*ϕ -irreducible Markov chains*)

The Markov chain $(X_i)_{i \geq 1}$ is said ϕ -irreducible if there exists a non-zero σ -finite measure ϕ on E such that for all $A \in \Sigma$ with $\phi(A) > 0$, and for all $x \in E$, there exists a positive integer $n = n(x, A)$ such that $P^n(x, A) > 0$ (where $P^n(x, \cdot)$ denotes the distribution of X_{n+1} conditioned on $X_1 = x$).

Definition 7 (*Roberts and Rosenthal, 2004, section 3.2*) (*Aperiodic Markov chains*)

The Markov chain $(X_i)_{i \geq 1}$ with invariant distribution π is aperiodic if there do not exist $m \geq 2$ and disjoint subsets $A_1, \dots, A_m \subset E$ with $P(x, A_{i+1}) = 1$ for all $x \in A_i$ ($1 \leq i \leq m-1$), and $P(x, A_1) = 1$ for all $x \in A_m$, such that $\pi(A_1) > 0$ (and hence $\pi(A_i) > 0$ for all i).

Definition 8 (*Roberts and Rosenthal, 2004, section 3.4*) (*Geometric ergodicity*)

The Markov chain $(X_i)_{i \geq 1}$ is said geometrically ergodic if there exists an invariant distribution π , $\rho \in (0, 1)$ and $C : E \rightarrow [1, \infty)$ such that

$$\|P^n(x, \cdot) - \pi\|_{TV} \leq C(x)\rho^n, \quad \forall n \geq 0, \pi\text{-a.e } x \in E,$$

where $\|\mu\|_{TV} := \sup_{A \in \Sigma} |\mu(A)|$.

Definition 9 (*Roberts and Rosenthal, 2004, section 3.3*) (*Uniform ergodicity*)

The Markov chain $(X_i)_{i \geq 1}$ is said uniformly ergodic if there exists an invariant distribution π and constants $0 < \rho < 1$ and

²Our code is available at <https://github.com/quentin-duchemin/Markovian-random-geometric-graph.git>

$L > 0$ such that

$$\|P^n(x, \cdot) - \pi\|_{TV} \leq L\rho^n, \quad \forall n \geq 0, \pi\text{-a.e } x \in E,$$

where $\|\mu\|_{TV} := \sup_{A \in \Sigma} |\mu(A)|$.

Remark: A Markov chain geometrically or uniformly ergodic admits a unique invariant distribution and is aperiodic.

Definition 10 A Markov chain is said reversible if there exists a distribution π satisfying

$$\pi(dx)P(x, dy) = \pi(dy)P(y, dx).$$

A.2. Spectral gap

This section is largely inspired from (Fan et al., 2018). Let us consider that the Markov chain $(X_i)_{i \geq 1}$ admits a unique invariant distribution π on \mathbb{S}^{d-1} .

For any real-valued, Σ -measurable function $h : E \rightarrow \mathbb{R}$, we define $\pi(h) := \int h(x)\pi(dx)$. The set

$$\mathcal{L}_2(E, \Sigma, \pi) := \{h : \pi(h^2) < \infty\}$$

is a Hilbert space endowed with the inner product

$$\langle h_1, h_2 \rangle_\pi = \int h_1(x)h_2(x)\pi(dx), \quad \forall h_1, h_2 \in \mathcal{L}_2(E, \Sigma, \pi).$$

The map

$$\|\cdot\|_\pi : h \in \mathcal{L}_2(E, \Sigma, \pi) \mapsto \|h\|_\pi = \sqrt{\langle h, h \rangle_\pi},$$

is a norm on $\mathcal{L}_2(E, \Sigma, \pi)$. $\|\cdot\|_\pi$ naturally allows to define the norm of a linear operator T on $\mathcal{L}_2(E, \Sigma, \pi)$ as

$$N_\pi(T) = \sup\{\|Th\|_\pi : \|h\|_\pi = 1\}.$$

To each transition probability kernel $P(x, B)$ with $x \in E$ and $B \in \Sigma$ invariant with respect to π , we can associate a bounded linear operator $h \mapsto \int h(y)P(\cdot, dy)$ on $\mathcal{L}_2(E, \Sigma, \pi)$. Denoting this operator P , we get

$$Ph(x) = \int h(y)P(x, dy), \quad \forall x \in E, \forall h \in \mathcal{L}_2(E, \Sigma, \pi).$$

Let $\mathcal{L}_2^0(\pi) := \{h \in \mathcal{L}_2(E, \Sigma, \pi) : \pi(h) = 0\}$. We define the absolute spectral gap of a Markov operator.

Definition 11 (Spectral gap) A Markov operator P reversible admits a spectral gap $1 - \lambda$ if

$$\lambda := \sup \left\{ \frac{\|Ph\|_\pi}{\|h\|_\pi} : h \in \mathcal{L}_2^0(\pi), h \neq 0 \right\} < 1.$$

The next result provides a connection between spectral gap and geometric ergodicity for reversible Markov chains.

Proposition 2 (Ferré et al., 2012, section 2.3)

A uniformly ergodic Markov chain admits a spectral gap.

B. Properties of the Markov chain

Let P be the Markov operator of the Markov chain $(X_i)_{i \geq 1}$. By abuse of notation, we will also denote $P(x, \cdot)$ the density of the measure $P(x, dz)$ with respect to $d\sigma$, the uniform measure on \mathbb{S}^{d-1} . For any $x, z \in \mathbb{S}^{d-1}$, we denote $R_x^z \in \mathbb{R}^{d \times d}$ a rotation matrix sending x to z (i.e. $R_x^z x = z$) and keeping $\text{Span}(x, z)^\perp$ fixed. In the following, we denote $e_d := (0, 0, \dots, 0, 1) \in \mathbb{R}^d$.

B.1. Invariant distribution and reversibility for the Markov chain

Reversibility of the Markov chain $(X_i)_{i \geq 1}$.

Lemma 1 For all $x, z \in \mathbb{S}^{d-1}$, $P(x, z) = P(z, x) = P(e_d, R_z^{e_d} x)$.

Proof of Lemma 1.

Using our model described in section 2, we get $X_2 = rX_1 + \sqrt{1-r^2}Y$ where conditionally on X_1 , Y is uniformly sampled on $\mathcal{S}(X_1) := \{q \in \mathbb{S}^{d-1} : \langle q, X_1 \rangle = 0\}$, and where r has density $f_{\mathcal{L}}$ on $[-1, 1]$. Let us consider a gaussian vector $W \sim \mathcal{N}(0, I_d)$. Using the Cochran's theorem and Lemma 2, we know that conditionally on X_1 , the random variable $\frac{W - \langle W, X_1 \rangle X_1}{\|W - \langle W, X_1 \rangle X_1\|_2}$ is distributed uniformly on $\mathcal{S}(X_1)$.

Lemma 2 Let $W \sim \mathcal{N}(0, I_d)$. Then, $\frac{W}{\|W\|_2}$ is distributed uniformly on the sphere \mathbb{S}^{d-1} .

In the following, we denote $\stackrel{\mathcal{L}}{=}$ the equality in distribution sense. We have conditionally on X_1

$$R_{X_1}^{e_d} \frac{W - \langle W, X_1 \rangle X_1}{\|W - \langle W, X_1 \rangle X_1\|_2} = \frac{\hat{W} - \langle \hat{W}, e_d \rangle e_d}{\|\hat{W} - \langle \hat{W}, e_d \rangle e_d\|_2},$$

where $\hat{W} = R_{X_1}^{e_d} W \sim \mathcal{N}(0, I_d)$. Using Cochran's theorem, we know that $\hat{W} - \langle \hat{W}, e_d \rangle e_d$ is a centered normal vector with covariance matrix the orthographic projection matrix onto the space $\text{Span}(e_d)^\perp$, leading to

$$\hat{W} - \langle \hat{W}, e_d \rangle e_d \stackrel{\mathcal{L}}{=} \begin{bmatrix} Y \\ 0 \end{bmatrix},$$

where $Y \sim \mathcal{N}(0, I_{d-1})$. Using Lemma 2, we conclude that conditionally on X_1 , the random variable $\frac{W - \langle W, X_1 \rangle X_1}{\|W - \langle W, X_1 \rangle X_1\|_2}$ is distributed uniformly on $\mathcal{S}(X_1)$ (because the distribution of Y is invariant by rotation).

We deduce that

$$X_2 \stackrel{\mathcal{L}}{=} rX_1 + \sqrt{1-r^2} \frac{W - \langle W, X_1 \rangle X_1}{\|W - \langle W, X_1 \rangle X_1\|_2} \stackrel{\mathcal{L}}{=} rX_1 + \sqrt{1-r^2} \frac{R_{X_2}^{X_1} W' - \langle R_{X_2}^{X_1} W', X_1 \rangle X_1}{\|R_{X_2}^{X_1} W' - \langle R_{X_2}^{X_1} W', X_1 \rangle X_1\|_2},$$

where $W' := R_{X_1}^{X_2} W$. Note that $W' \in \mathbb{R}^d$ is also a standard centered gaussian vector because this distribution is invariant by rotation. Since $\langle R_{X_2}^{X_1} W', X_1 \rangle = \langle W', X_2 \rangle$ and $\|R_{X_2}^{X_1} q\|_2 = \|q\|_2$, $\forall q \in \mathbb{S}^{d-1}$, we deduce that

$$X_2 - rX_1 \stackrel{\mathcal{L}}{=} R_{X_2}^{X_1} \left[\sqrt{1-r^2} \frac{W' - \langle W', X_2 \rangle X_2}{\|W' - \langle W', X_2 \rangle X_2\|_2} \right]. \quad (15)$$

$R_{X_1}^{X_2}$ is the rotation that sends X_1 to X_2 keeping the other dimensions fixed. Let us denote $a_1 := X_1$, $a_2 := \frac{X_2 - rX_1}{\|X_2 - rX_1\|_2}$ and complete the linearly independent family (a_1, a_2) in an orthonormal basis of \mathbb{R}^d given by $a := (a_1, a_2, \dots, a_d)$. Then, the matrix of $R_{X_1}^{X_2}$ in the basis a is

$$\begin{bmatrix} r & -\sqrt{1-r^2} & 0_{d-2}^\top \\ \sqrt{1-r^2} & r & 0_{d-2}^\top \\ 0_{d-2} & 0_{d-2} & I_{d-2} \end{bmatrix}.$$

We deduce that

$$\begin{aligned}
 \left(R_{X_2}^{X_1}\right)^{-1} (X_2 - rX_1) &= R_{X_1}^{X_2} (X_2 - rX_1) \\
 &= \|X_2 - rX_1\|_2 R_{X_1}^{X_2} \left(\frac{X_2 - rX_1}{\|X_2 - rX_1\|_2} \right) \\
 &= \|X_2 - rX_1\|_2 R_{X_1}^{X_2} a_2 \\
 &= \|X_2 - rX_1\|_2 \left[-\sqrt{1-r^2} a_1 + r a_2 \right] \\
 &= -\sqrt{1-r^2} \|X_2 - rX_1\|_2 X_1 + r X_2 - r^2 X_1 \\
 &= -(1-r^2) X_1 + r X_2 - r^2 X_1 \\
 &= -X_1 + r X_2.
 \end{aligned}$$

Going back to (15), we deduce that

$$X_1 \stackrel{\mathcal{L}}{=} rX_2 + \sqrt{1-r^2} \frac{\tilde{W} - \langle \tilde{W}, X_2 \rangle X_2}{\|\tilde{W} - \langle \tilde{W}, X_2 \rangle X_2\|_2}, \quad (16)$$

where $\tilde{W} = -W'$ is also a standard centered gaussian vector in \mathbb{R}^d . Thus, we proved the first equality of Lemma 1. Based on (16) we have,

$$\begin{aligned}
 R_{X_2}^{e_d} X_1 &\stackrel{\mathcal{L}}{=} r R_{X_2}^{e_d} X_2 + \sqrt{1-r^2} \frac{R_{X_2}^{e_d} \tilde{W} - \langle \tilde{W}, X_2 \rangle R_{X_2}^{e_d} X_2}{\|\tilde{W} - \langle \tilde{W}, X_2 \rangle X_2\|_2} \\
 &= r e_d + \sqrt{1-r^2} \frac{R_{X_2}^{e_d} \tilde{W} - \langle R_{X_2}^{e_d} \tilde{W}, e_d \rangle e_d}{\|R_{X_2}^{e_d} \tilde{W} - \langle R_{X_2}^{e_d} \tilde{W}, e_d \rangle e_d\|_2},
 \end{aligned}$$

which proves that $P(e_d, R_{x_2}^{e_d} x_1) = P(x_2, x_1)$ for any $x_1, x_2 \in \mathbb{S}^{d-1}$ because $R_{X_2}^{e_d} \tilde{W}$ is again a standard centered gaussian vector in \mathbb{R}^d .

■

Invariant distribution of the Markov chain.

Proposition 3 *The uniform distribution on the sphere \mathbb{S}^{d-1} is an invariant distribution of the Markov chain $(X_i)_{i \geq 1}$.*

Proof of Proposition 3.

Let us consider $z \in \mathbb{S}^{d-1}$. We denote $d\sigma \equiv d\sigma_d$ the Lebesgue measure on \mathbb{S}^{d-1} and $d\sigma_{d-1}$ the Lebesgue measure on \mathbb{S}^{d-2} . Using (Dai, 2013, Section 1.1), it holds $b_d := \int_{\mathbb{S}^{d-1}} d\sigma = \frac{2\pi^{d/2}}{\Gamma(d/2)}$. We have

$$\begin{aligned}
 &\int_{x \in \mathbb{S}^{d-1}} P(x, z) \frac{d\sigma(x)}{b_d} \\
 &= \int_{x \in \mathbb{S}^{d-1}} P(e_d, R_z^{e_d} x) \frac{d\sigma(x)}{b_d} \quad (\text{Using Lemma 1}) \\
 &= \int_{x \in \mathbb{S}^{d-1}} P(e_d, x) \frac{d\sigma(x)}{b_d} \quad (\text{Using the change of variable } x \mapsto R_z^{e_d} x) \\
 &= \int_0^\pi \int_{\mathbb{S}^{d-2}} P\left(e_d, \begin{bmatrix} \xi \sin \theta \\ \cos \theta \end{bmatrix}\right) (\sin \theta)^{d-2} d\theta \frac{d\sigma_{d-1}(\xi)}{b_d} \quad (\text{Using (Dai, 2013, Eq.(1.5.4) Section 1.5)}) \\
 &= \int_{-1}^1 \int_{\mathbb{S}^{d-2}} P\left(e_d, \begin{bmatrix} \xi \sqrt{1-r^2} \\ r \end{bmatrix}\right) (1-r^2)^{\frac{d-3}{2}} dr \frac{d\sigma_{d-1}(\xi)}{b_d} \\
 &= \int_{-1}^1 f_{\mathcal{L}}(r) dr \times \int_{\mathbb{S}^{d-2}} \frac{1}{b_{d-1}} \frac{d\sigma_{d-1}}{b_d} = \frac{1}{b_d},
 \end{aligned}$$

which proves that the uniform distribution on the sphere is an invariant distribution of the Markov chain.

■

B.2. Ergodicity of the Markov chain

Lemma 3 We consider that $f_{\mathcal{L}}$ is bounded away from zero. Then, the Markov chain $(X_i)_{i \geq 1}$ is π -irreducible and aperiodic.

Lemma 4 We consider that $f_{\mathcal{L}}$ is bounded away from zero. Then the Markov chain $(X_i)_{i \geq 1}$ is uniformly ergodic.

Proof of Lemmas 3 and 4.

Considering for π the uniform distribution on \mathbb{S}^{d-1} , we get that for any $x \in \mathbb{S}^{d-1}$ and any $A \subset \mathbb{S}^{d-1}$ with $\pi(A) > 0$,

$$\begin{aligned}
 P(x, A) &= \int_{z \in A} P(x, z) \frac{d\sigma_d(z)}{b_d} \\
 &= \int_{z \in A} P(e_d, R_x^{e_d} z) \frac{d\sigma_d(z)}{b_d} \quad (\text{Using Lemma 1}) \\
 &= \int_{z \in R_x^{e_d} A} P(e_d, z) \frac{d\sigma_d(z)}{b_d} \\
 & \quad (\text{Using the change of variable } z \mapsto R_x^{e_d} z \text{ with } R_x^{e_d} A = \{R_x^{e_d} a : a \in A\}) \\
 &= \int_{r \in [-1, 1]} \int_{\xi \in \mathbb{S}^{d-2}} f_{\mathcal{L}}(r) \mathbf{1}_{(\xi^\top, r)^\top \in R_x^{e_d} A} dr \frac{d\sigma_{d-1}(\xi)}{b_{d-1} b_d} \\
 &\geq \inf_{s \in [-1, 1]} f_{\mathcal{L}}(s) \int_{r \in [-1, 1]} \int_{\xi \in \mathbb{S}^{d-2}} \mathbf{1}_{(\xi^\top, r)^\top \in R_x^{e_d} A} dr \frac{d\sigma_{d-1}(\xi)}{b_{d-1} b_d} \\
 &\geq \inf_{s \in [-1, 1]} f_{\mathcal{L}}(s) \int_{r \in [-1, 1]} \int_{\xi \in \mathbb{S}^{d-2}} \mathbf{1}_{(\xi^\top, r)^\top \in R_x^{e_d} A} (1-r^2)^{\frac{d-3}{2}} dr \frac{d\sigma_{d-1}(\xi)}{b_{d-1} b_d} \\
 &= \frac{1}{b_{d-1}} \inf_{s \in [-1, 1]} f_{\mathcal{L}}(s) \pi(R_x^{e_d} A) = \frac{1}{b_{d-1}} \inf_{s \in [-1, 1]} f_{\mathcal{L}}(s) \pi(A), \tag{17}
 \end{aligned}$$

since π is invariant by rotation and $f_{\mathcal{L}}$ is bounded away from zero. We also used that $\int_{-1}^1 (1-r^2)^{\frac{d-3}{2}} = \frac{b_d}{b_{d-1}}$. This result means that the whole space \mathbb{S}^{d-1} is a small set. Hence, the Markov chain is uniformly ergodic (see (Meyn and Tweedie, 1993, Theorem 16.0.2)) and thus aperiodic and π -irreducible.

■

Remark: Thanks to Proposition 2 and Lemma 4, we know that the Markov chain has a spectral gap. In the following subsection, we show that this spectral gap is equal to 1.

B.3. Computation of the spectral gap of the Markov chain

Keeping notations of Appendix A, let us consider $h \in \mathcal{L}_2^0(\sigma)$ such that $\|h\|_\sigma = 1$. Then

$$\begin{aligned}
 \|Ph\|_\sigma^2 &= \int_{x \in \mathbb{S}^{d-1}} \left(\int_{y \in \mathbb{S}^{d-1}} P(x, dy) h(y) \right)^2 d\sigma(x) \\
 &= \int_{x \in \mathbb{S}^{d-1}} \left(\int_{y \in \mathbb{S}^{d-1}} P(x, y) h(y) d\sigma(y) \right)^2 d\sigma(x) \\
 &= \int_{x \in \mathbb{S}^{d-1}} \left(\int_{y \in \mathbb{S}^{d-1}} P(e_d, R_y^{e_d} x) h(y) d\sigma(y) \right)^2 d\sigma(x) \quad (\text{Using Lemma 1}) \\
 &= \int_{x \in \mathbb{S}^{d-1}} \left(\int_{y \in \mathbb{S}^{d-1}} P(e_d, x) h(y) d\sigma(y) \right)^2 d\sigma(x) \quad (\text{Using the rotational invariance of } \sigma) \\
 &= \int_{x \in \mathbb{S}^{d-1}} P(e_d, x)^2 \left(\int_{y \in \mathbb{S}^{d-1}} h(y) d\sigma(y) \right)^2 d\sigma(x) \\
 &= 0,
 \end{aligned}$$

where the last equality comes from $h \in \mathcal{L}_2^0(\sigma)$. Hence, the Markov chain $(X_i)_{i \geq 1}$ has 1 for spectral gap.

C. Complement on Harmonic Analysis on the sphere

This section completes the brief introduction to Harmonic Analysis on the sphere \mathbb{S}^{d-1} provided in Section 2. We will need in our proof the following result which states that fixing one variable and integrating with respect to the other one with the uniform measure on \mathbb{S}^{d-1} gives $\|W - W_R\|_2^2$.

Lemma 5 For any $x \in \mathbb{S}^{d-1}$,

$$\mathbb{E}_{X \sim \pi}[(W - W_R)^2(x, X)] = \|W - W_R\|_2^2,$$

where π is the uniform measure on the \mathbb{S}^{d-1} .

Proof of Lemma 5.

$$\begin{aligned} \mathbb{E}_{X \sim \pi}[(W - W_R)^2(x, X)] &= \int_y (W - W_R)^2(x, y) \pi(dy) \\ &= \int_y \left(\sum_{r>R} p_r^* \sum_{l=1}^{d_r} Y_{r,l}(x) Y_{r,l}(y) \right)^2 \pi(dy) \\ &= \int_y \sum_{r_1, r_2 > R} p_{r_1}^* p_{r_2}^* \sum_{l_1=1}^{d_{r_1}} \sum_{l_2=1}^{d_{r_2}} Y_{r_1, l_1}(x) Y_{r_1, l_1}(y) Y_{r_2, l_2}(x) Y_{r_2, l_2}(y) \pi(dy) \\ &= \sum_{r_1, r_2 > R} p_{r_1}^* p_{r_2}^* \sum_{l_1=1}^{d_{r_1}} \sum_{l_2=1}^{d_{r_2}} Y_{r_1, l_1}(x) Y_{r_2, l_2}(x) \int_y Y_{r_1, l_1}(y) Y_{r_2, l_2}(y) \pi(dy). \end{aligned}$$

Since $\int_y Y_{r,l}(y) Y_{r',l'} \pi(dy)$ is 1 if $r = r'$ and $l = l'$ and 0 otherwise, we have that

$$\begin{aligned} \mathbb{E}_{X \sim \pi}[(W - W_R)^2(x, X)] &= \sum_{r>R} (p_r^*)^2 \sum_{l=1}^{d_r} Y_{r,l}(x)^2 \\ &= \sum_{r>R} (p_r^*)^2 d_r \quad (\text{Using (Dai, 2013, Eq.(1.2.9))}) \\ &= \|W - W_R\|_2^2. \end{aligned}$$

■

Let us consider $\beta := \frac{d-2}{2}$ and the weight function $w_\beta(t) := (1-t^2)^{\beta-\frac{1}{2}}$. As highlighted in section 2, any envelope function $p \in L^2([-1, 1], w_\beta)$ can be decomposed as $p \equiv \sum_{k=0}^R p_k^* c_k G_k^\beta$ where G_l^β is the Gegenbauer polynomial of degree l with parameter β and where $c_k := \frac{2k+d-2}{d-2}$. The Gegenbauer polynomials are orthonormal polynomials on $[-1, 1]$ associated with the weight function w_β .

The eigenvalues $(p_k^*)_{k \geq 0}$ of the envelope function can be computed numerically through the formula

$$\forall l \geq 0, \quad p_l^* = \left(\frac{c_l b_d}{d_l} \right) \int_{-1}^1 p(t) G_l^\beta(t) w_\beta(t) dt, \quad (18)$$

where $b_d := \frac{\Gamma(\frac{d}{2})}{\Gamma(\frac{1}{2})\Gamma(\frac{d-1}{2})}$ with Γ the Gamma function. Hence, it is possible to recover the envelope function p thanks to the identity

$$p = \sum_{l \geq 0} \sqrt{d_l} p_l^* \frac{G_l^\beta}{\|G_l^\beta\|_{L^2([-1,1], w_\beta)}} = \sum_{l \geq 0} p_l^* c_l G_l^\beta. \quad (19)$$

For $R \geq 0$, let us define $\tilde{R} = \sum_{k=0}^R d_k$ which corresponds to the dimension of the space of Spherical Harmonics with degree at most R . We introduce the truncated graphon W_R which is obtained from W by keeping only the \tilde{R} first eigenvalues, that is

$$\forall x, y \in \mathbb{S}^{d-1}, \quad W_R(x, y) := \sum_{k=0}^R p_k^* \sum_{l=1}^{d_k} Y_{k,l}(x) Y_{k,l}(y).$$

Similarly, we denote for all $t \in [0, 1]$, $p_R(t) = \sum_{k=0}^R p_k^* c_k G_k^\beta(t)$.

D. Slope heuristic

We propose a detailed analysis of the slope heuristic described in section 2.2 on the simulated data presented in section 6.2.2. We recall that $R(\kappa)$ represents the optimal value of R to minimize the bias-variance decomposition defined by (6) for a given hyperparameter κ . Figure 9 shows the evolution of $\tilde{R}(\kappa)$ with respect to κ which is sampled on a logscale. $\tilde{R}(\kappa)$ is the dimension of the space of Spherical Harmonics with degree at most $\tilde{R}(\kappa)$. Our slope heuristic consists in choosing the value κ_0 leading to the larger jump of the function $\kappa \mapsto \tilde{R}(\kappa)$. In our case, Figure 9 shows that $\kappa_0 = 10^{-3.9}$. As described in Section 2.2, the resolution level \hat{R} selected to cluster the eigenvalues of the matrix \hat{T}_n is given by $R(2\kappa_0)$.

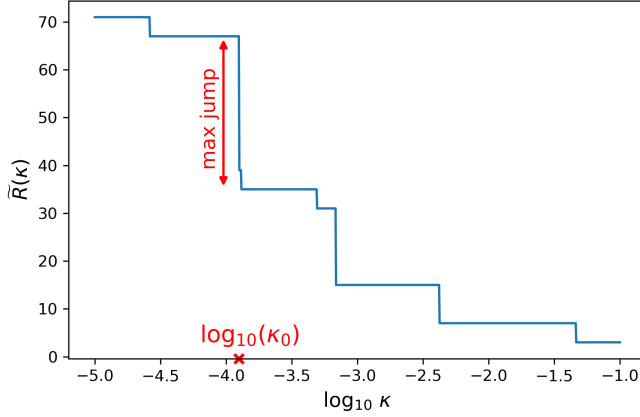


Figure 9. We sample the parameter κ on a logscale between 10^{-5} and 10^{-1} and we compute the corresponding $R(\kappa)$ defined in (6). We plot the values of $\tilde{R}(\kappa)$ with respect to κ . The larger jump allows us to define κ_0 .

E. Reminder on Harmonic EigenCluster(HEiC)

Before presenting the algorithm HEiC, let us define for a given set of indices $i_1, \dots, i_d \in [n]$

$$\text{Gap}_1(\hat{T}_n; i_1, \dots, i_d) := \min_{i \notin \{i_1, \dots, i_d\}} \max_{j \in \{i_1, \dots, i_d\}} |\hat{\lambda}_i - \hat{\lambda}_j|.$$

Algorithm 3 Harmonic EigenCluster(HEiC) algorithm.

Data: Adjacency matrix A . Dimension d .

- 1: $(\hat{\lambda}_1^{\text{sort}}, \dots, \hat{\lambda}_n^{\text{sort}}) \leftarrow$ eigenvalues of \hat{T}_n sorted in decreasing order.
- 2: $\Lambda_1 \leftarrow \{\hat{\lambda}_1^{\text{sort}}, \dots, \hat{\lambda}_d^{\text{sort}}\}$.
- 3: Initialize $i = 2$ and $\text{gap} = \text{Gap}_1(\hat{T}_n; 1, 2, \dots, d)$.
- 4: **while** $i \leq n - d + 1$ **do**
- 5: **if** $\text{Gap}_1(\hat{T}_n; i, i + 1, \dots, i + d - 1) > \text{gap}$ **then**
- 6: $\Lambda_1 \leftarrow \{\hat{\lambda}_i^{\text{sort}}, \dots, \hat{\lambda}_{i+d-1}^{\text{sort}}\}$
- 7: **end if**
- 8: $i = i + 1$
- 9: **end while**

Return: Λ_1, gap .

F. Concentration inequality for U-statistics with Markov chains

In this section, we present a recent concentration inequality for a U-statistic of the Markov chain $(X_i)_{i \geq 1}$ from (Duchemin et al., 2020) which is a key result to prove Theorem 1. In the first subsection, we remind the assumptions made on the Markovian dynamic, namely Assumption A.

F.1. Assumptions and notations for the Markov chain

Assumption A The latitude function $f_{\mathcal{L}}$ is such that $\|f_{\mathcal{L}}\|_{\infty} < \infty$ and $\inf_{r \in [-1, 1]} f_{\mathcal{L}}(r) > 0$.

Assumption A guarantees that there exist $\delta_m, \delta_M > 0$ such that

$$\forall x \in \mathbb{S}^{d-1}, \forall A \in \mathcal{B}(\mathbb{S}^{d-1}), \quad \delta_m \nu(A) \leq P(x, A) \leq \delta_M \nu(A),$$

for some probability measure ν (e.g. the uniform measure on the sphere π). We refer to (17) for the left inequality while the right inequality is straightforward. Hence **Assumption A** implies in particular that the whole state space \mathbb{S}^{d-1} is a *small set*. This has the important consequence that the Markov chain $(X_i)_{i \geq 1}$ is **uniformly ergodic** (see (Dorea and Pereira, 2006, section 1)), with associated constants $L > 0$ and $0 < \rho < 1$ (see Definition 9).

F.2. Concentration inequality of U-statistic for Markov chain

One key result to prove Theorem 1 is the concentration of the following U-statistic

$$U_{stat}(n) = \sum_{1 \leq i < j \leq n} [(W - W_R)^2(X_i, X_j) - \|W - W_R\|_2^2].$$

Note that $\|W - W_R\|_2^2$ corresponds to the expectation of the kernel $(W - W_R)^2(\cdot, \cdot)$ under the uniform distribution on \mathbb{S}^{d-1} which is known to be the unique invariant distribution π of the Markov chain $(X_i)_{i \geq 1}$ (see Appendix B). More precisely, for any $x \in \mathbb{S}^{d-1}$, it holds

$$\|W - W_R\|_2^2 = \mathbb{E}_{X \sim \pi}[(W - W_R)^2(x, X)] = \mathbb{E}_{(X, X') \sim \pi \otimes \pi}[(W - W_R)^2(X, X')],$$

see Lemma 5 for a proof. Applying (Duchemin et al., 2020, Theorem 2) in our framework leads to the following result.

Lemma 6 *Let us consider $\gamma \in (0, 1)$ satisfying $\log(e \log(n)/\gamma) \leq n$. Then it holds with probability at least $1 - \gamma$,*

$$U_{stat}(n) \leq M \frac{\|p - p_R\|_\infty^2 \log n}{n} \log(e \log(n)/\gamma),$$

where $M > 0$ only depends on constants related to the Markov chain $(X_i)_{i \geq 1}$.

G. Proof of Theorem 1

The proof of Theorem 1 mainly lies in the following result which is proved in Appendix G.1. Coupling the convergence of the spectrum of the matrix of probability T_n with a concentration result on the spectral norm of random matrices with independent entries (see (Bandeira and van Handel, 2016)), we show the convergence in metric δ_2 of the spectrum of \hat{T}_n towards the spectrum of the integral operator \mathbb{T}_W .

Theorem 3 *Let us consider $\gamma \in (0, 1)$ satisfying $\log(e \log(n)/\gamma) \leq n/(13\tilde{R})$. Then it holds with probability at least $1 - \gamma$,*

$$\begin{aligned} & \delta_2(\lambda(\mathbb{T}_W), \lambda(T_n)) \\ & \leq 2\|p - p_R\|_2 + 8\sqrt{\frac{\tilde{R}}{n} \ln(e/\gamma)} + M\|p - p_R\|_\infty \sqrt{\frac{\log n}{n} (\log(e \log(n)/\gamma))^{1/2}}, \end{aligned}$$

where $M > 0$ only depends on constants related to the Markov chain $(X_i)_{i \geq 1}$ (see Lemma 6).

First part of the proof for Theorem 1 We start by establishing the convergence rate for $\delta_2(\lambda(\mathbb{T}_W), \lambda(T_n))$. We keep notations of Theorem 3. Let us consider $\gamma \in (0, 1)$ satisfying $\log(e \log(n)/\gamma) \leq n/(13\tilde{R})$, and assume that $p \in Z_{w_\beta}^s((-1, 1))$ with $s > 0$.

Let us define the event

$$\begin{aligned} \Omega(\gamma) := & \left\{ \delta_2(\lambda(\mathbb{T}_W), \lambda(T_n)) \leq 2\|p - p_R\|_2 + 8\sqrt{\frac{\tilde{R}}{n} \ln(e/\gamma)} \right. \\ & \left. + M\|p - p_R\|_\infty \sqrt{\frac{\log n}{n} (\log(e \log(n)/\gamma))^{1/2}} \right\}. \end{aligned}$$

Using Theorem 3, it holds $\mathbb{P}(\Omega(\gamma)) \geq 1 - \gamma$. Remarking further that

$$\delta_2(\lambda(\mathbb{T}_W), \lambda(T_n)) \leq \delta_2(\lambda(\mathbb{T}_W), 0) + \delta_2(0, \lambda(T_n)) \leq \|p\|_2 + \sqrt{n} \leq \sqrt{2} + \sqrt{n},$$

we have

$$\begin{aligned} & \mathbb{E}[\delta_2^2(\lambda(\mathbb{T}_W), \lambda(T_n))] \\ &= \mathbb{E}[\delta_2^2(\lambda(\mathbb{T}_W), \lambda(T_n)) \mathbb{1}_{\Omega(\gamma)}] + (1 + \sqrt{2})^2 n \mathbb{P}(\Omega(\gamma)^c) \\ &\leq c \|p - p_R\|_2^2 + c \frac{\tilde{R}}{n} \log(e/\gamma) + c \|p - p_R\|_\infty^2 \frac{\log n}{n} \log(e \log(n)/\gamma) \\ &\quad + (1 + \sqrt{2})^2 n \gamma, \end{aligned}$$

where $c > 0$ is a constant that does not depend on R , d or n .

Since

$$\|p - p_R\|_2^2 = \sum_{k>R} (p_k^*)^2 d_k \frac{(1 + k(k + 2\beta))^s}{(1 + k(k + 2\beta))^s} \leq C(p, s, d) R^{-2s}, \quad (20)$$

and since

$$\tilde{R} = O(R^{d-1}), \quad (21)$$

we have choosing $\gamma = 1/n^2$

$$\mathbb{E}[\delta_2^2(\lambda(\mathbb{T}_W), \lambda(T_n))] \leq D' \left[R^{-2s} + R^{d-1} \frac{\log(n)}{n} + \|p - p_R\|_\infty^2 \frac{\log^2(n)}{n} \right], \quad (22)$$

where $D' > 0$ is a constant independent of n and R .

Let us show that choosing $R = \lfloor (n/\log^2(n))^{\frac{1}{2s+d-1}} \rfloor$ concludes the proof.

Since $\|G_k^\beta\|_\infty = G_k^\beta(1) = d_k/c_k$, we get that

$$\|p_R\|_\infty \leq \sum_{k=0}^R |p_k^*| c_k G_k^\beta(1) = \sum_{k=0}^R |p_k^*| d_k \leq \sqrt{\tilde{R}} \|p_R\|_2,$$

and using (28), we deduce that

$$\|p - p_R\|_\infty \leq \|p\|_\infty + \|p_R\|_\infty \leq 1 + \sqrt{2\tilde{R}}. \quad (23)$$

Hence, (22) becomes

$$\mathbb{E}[\delta_2^2(\lambda(\mathbb{T}_W), \lambda(T_n))] \leq D'' \left[R^{-2s} + R^{d-1} \frac{\log(n)}{n} + \tilde{R} \frac{\log^2(n)}{n} \right],$$

where D'' is a constant that does not depend on n or R .

Choosing $R = \lfloor (n/\log^2(n))^{\frac{1}{2s+d-1}} \rfloor$ and using (21) we get

$$\begin{aligned} & \mathbb{E}[\delta_2^2(\lambda(\mathbb{T}_W), \lambda(T_n))] \\ &\leq D'' \left[\left(\frac{n}{\log^2(n)} \right)^{\frac{-2s}{2s+d-1}} + 2 \left(\frac{n}{\log^2(n)} \right)^{\frac{d-1}{2s+d-1}} \frac{\log^2(n)}{n} \right] \\ &\leq 3D'' \left(\frac{n}{\log^2(n)} \right)^{\frac{-2s}{2s+d-1}}. \end{aligned}$$

Second part of the proof for Theorem 1 Let us recall that in the statement of Theorem 1, $\lambda^{R_{opt}}(\hat{T}_n)$ is the sequence of the \tilde{R}_{opt} first eigenvalues (sorted in decreasing absolute values) of the matrix \hat{T}_n where R_{opt} is the value of the parameter R leading to the optimal bias-variance trade off, namely

$$\lambda^{R_{opt}}(\hat{T}_n) = (\hat{\lambda}_1, \dots, \hat{\lambda}_{\tilde{R}_{opt}}, 0, 0, \dots).$$

From the computations of the first part of the proof, we know that $R_{opt} = \lfloor (n/\log^2(n))^{\frac{1}{2s+d-1}} \rfloor$. That corresponds to the situation where we choose optimally R and it is in practice possible to approximate this best model dimension using e.g. the slope heuristic. Therefore, $\delta_2(\lambda(\mathbb{T}_W), \lambda^{R_{opt}}(\hat{T}_n))$ is the quantity of interest since it represents the distance between the eigenvalues used to build our estimates $(\hat{p}_k)_k$ and the true spectrum of the envelope function p . Since $\tilde{R} = \mathcal{O}(R^{d-1})$ for all integer $R \geq 0$, we have $\tilde{R}_{opt} = \mathcal{O}\left((n/\log^2(n))^{\frac{d-1}{2s+d-1}}\right)$. We deduce that for n large enough $2\tilde{R}_{opt} \leq n$ and using (Castro et al., 2020, Proposition 15) we obtain

$$\begin{aligned} & \delta_2(\lambda^{R_{opt}}(\hat{T}_n), \lambda(\mathbb{T}_{W_{R_{opt}}})) \\ & \leq \delta_2(\lambda(T_n), \lambda(\mathbb{T}_{W_{R_{opt}}})) + \sqrt{2\tilde{R}_{opt}} \|\hat{T}_n - T_n\| \\ & \leq \delta_2(\lambda(T_n), \lambda(\mathbb{T}_W)) + \delta_2(\lambda(\mathbb{T}_W), \lambda(\mathbb{T}_{W_{R_{opt}}})) + \sqrt{2\tilde{R}_{opt}} \|\hat{T}_n - T_n\|, \end{aligned} \quad (24)$$

where $\lambda(\mathbb{T}_{W_{R_{opt}}}) = (\lambda_1^*, \dots, \lambda_{\tilde{R}_{opt}}^*, 0, 0, \dots)$. Let us consider $\gamma \in (0, 1)$. Using Theorem 3, we know that with probability at least $1 - \gamma$ it holds for n large enough

$$\begin{aligned} & \delta_2(\lambda(T_n), \lambda(\mathbb{T}_W)) \\ & \leq 2\|p - p_{R_{opt}}\|_2 + 8\sqrt{\frac{\tilde{R}_{opt}}{n} \ln(e/\gamma)} + M\|p - p_{R_{opt}}\|_\infty \sqrt{\frac{\log n}{n}} (\log(e \log(n)/\gamma))^{1/2}. \end{aligned}$$

Using (20), (23) and the fact that $\tilde{R} = \mathcal{O}(R^{d-1})$, it holds with probability at least $1 - 1/n^2$,

$$\begin{aligned} \delta_2^2(\lambda(T_n), \lambda(\mathbb{T}_W)) & \leq c \left[R_{opt}^{-2s} + R_{opt}^{d-1} \frac{\log n}{n} + M R_{opt}^{d-1} \frac{\log^2 n}{n} \right] \\ & \leq (M')^2 (n/\log^2 n)^{\frac{-2s}{2s+d-1}}, \end{aligned}$$

where $c > 0$ is a numerical constant and $M' > 0$ depends on constants related to the Markov chain $(X_i)_{i \geq 1}$ (see Theorem 3 for details). Moreover,

$$\delta_2^2(\lambda(\mathbb{T}_W), \lambda(\mathbb{T}_{W_{R_{opt}}})) = \|p - p_{R_{opt}}\|_2^2 \leq C(p, s, d) R_{opt}^{-2s} = \mathcal{O}\left((n/\log^2 n)^{\frac{-2s}{2s+d-1}}\right), \quad (25)$$

where we used (20). Finally, using the concentration of spectral norm for random matrices with independent entries from (Bandeira and van Handel, 2016), there exists a universal constant $C_0 > 0$ such that conditionally on $(X_i)_{i \geq 1}$, it holds with probability at least $1 - 1/n^2$,

$$\|T_n - \hat{T}_n\| \leq \frac{3}{\sqrt{2n}} + C_0 \frac{\sqrt{\log(n^3)}}{n}.$$

Using again $\tilde{R} = \mathcal{O}(R^{d-1})$, this implies that for n large enough, it holds conditionally on $(X_i)_{i \geq 1}$ with probability at least $1 - 1/n^2$,

$$\sqrt{2\tilde{R}_{opt}} \|T_n - \hat{T}_n\| \leq D (n/\log^2 n)^{\frac{-s}{2s+d-1}},$$

where $D > 0$ is a numerical constant.

From (24), we deduce that $\mathbb{P}(\Omega) \geq 1 - 2/n^2$ where the event Ω is defined by

$$\Omega = \left\{ \delta_2^2(\lambda^{R_{opt}}(\hat{T}_n), \lambda(\mathbb{T}_{W_{R_{opt}}})) \leq \left(C(p, s, d)^{1/2} + D + M' \right)^2 (n/\log^2 n)^{\frac{-2s}{2s+d-1}} \right\}.$$

Remarking finally,

$$\delta_2 \left(\lambda^{R_{opt}}(\hat{T}_n), \lambda(\mathbb{T}_{W_{R_{opt}}}) \right) \leq \delta_2 \left(\lambda(\mathbb{T}_{W_{R_{opt}}}), 0 \right) + \delta_2 \left(0, \lambda(\hat{T}_n) \right) \leq \|p\|_2 + \sqrt{n} \leq \sqrt{2} + \sqrt{n},$$

we obtain

$$\begin{aligned} & \mathbb{E} \left[\delta_2^2 \left(\lambda^{R_{opt}}(\hat{T}_n), \lambda(\mathbb{T}_{W_{R_{opt}}}) \right) \right] \\ & \leq \mathbb{E} \left[\delta_2^2 \left(\lambda^{R_{opt}}(\hat{T}_n), \lambda(\mathbb{T}_{W_{R_{opt}}}) \right) \mid \Omega \right] + \mathbb{P}(\Omega^c)(\sqrt{2} + \sqrt{n})^2 \\ & \leq \left(C(p, s, d)^{1/2} + D + M' \right)^2 (n / \log^2 n)^{\frac{-2s}{2s+d-1}} + 2 \frac{(\sqrt{2} + \sqrt{n})^2}{n^2} \\ & = \mathcal{O} \left((n / \log^2 n)^{\frac{-2s}{2s+d-1}} \right). \end{aligned} \tag{26}$$

Using the triangle inequality, (25) and (27) leads to

$$\begin{aligned} \mathbb{E} \left[\delta_2^2 \left(\lambda^{R_{opt}}(\hat{T}_n), \lambda(\mathbb{T}_W) \right) \right] & \leq 3\mathbb{E} \left[\delta_2^2 \left(\lambda^{R_{opt}}(\hat{T}_n), \lambda(\mathbb{T}_{W_{R_{opt}}}) \right) \right] + 3\delta_2^2 \left(\lambda(\mathbb{T}_{W_{R_{opt}}}), \lambda(\mathbb{T}_W) \right) \\ & = \mathcal{O} \left((n / \log^2 n)^{\frac{-2s}{2s+d-1}} \right), \end{aligned}$$

which concludes the proof of Theorem 1.

■

G.1. Proof of Theorem 3

We follow the same sketch of proof as in (Castro et al., 2020).

Let $R \geq 1$ and define,

$$\begin{aligned} \Phi_{k,l} &= \frac{1}{\sqrt{n}} [Y_{k,l}(X_1), \dots, Y_{k,l}(X_n)] \in \mathbb{R}^n, \\ E_{R,n} &= \left(\langle \Phi_{k,l}, \Phi_{k',l'} \rangle - \delta_{(k,l),(k',l')} \right)_{(k,k') \in [R], l \in \{1, \dots, d_k\}, l' \in \{1, \dots, d_{k'}\}} \in \mathbb{R}^{\tilde{R} \times \tilde{R}}, \\ X_{R,n} &= [\Phi_{0,1}, \Phi_{1,1}, \Phi_{1,2}, \dots, \Phi_{R,d_R}] \in \mathbb{R}^{n \times \tilde{R}}, \\ A_{R,n} &= (X_{R,n}^\top X_{R,n})^{1/2} \text{ with } A_{R,n}^2 = Id_{\tilde{R}} + E_{R,n}, \\ K_R &= \text{Diag}(\lambda_1(\mathbb{T}_W), \dots, \lambda_{\tilde{R}}(\mathbb{T}_W)), \\ T_{R,n} &= \sum_{k=0}^R p_k^* \sum_{l=1}^{d_k} \Phi_{k,l} (\Phi_{k,l})^\top = X_{R,n} K_R X_{R,n}^\top \in \mathbb{R}^{n \times n}, \\ \tilde{T}_{R,n} &= ((1 - \delta_{i,j}) T_{R,n})_{i,j \in [n]} \in \mathbb{R}^{n \times n}, \\ T_{R,n}^* &= A_{R,n} K_R A_{R,n}^\top \in \mathbb{R}^{\tilde{R} \times \tilde{R}}, \\ W_R(x, y) &= \sum_{k=0}^R p_k^* \sum_{l=1}^{d_k} Y_{k,l}(x) Y_{k,l}(y). \end{aligned}$$

It holds

$$\delta_2(\lambda(\mathbb{T}_W), \lambda(\mathbb{T}_{W_R})) = \left(\sum_{k>R} d_k (p_k^*)^2 \right)^{1/2}.$$

We point out the equality between spectra of the operator \mathbb{T}_{W_R} and the matrix K_R . Using the SVD decomposition of $X_{R,n}$, one can also easily prove that $\lambda(T_{R,n}) = \lambda(T_{R,n}^*)$. We deduce that

$$\delta_2(\lambda(\mathbb{T}_{W_R}), \lambda(T_{R,n})) = \delta_2(\lambda(K_R), \lambda(T_{R,n}^*)) \leq \|T_{R,n}^* - K_R\|_F = \|A_{R,n} K_R A_{R,n} - K_R\|_F,$$

with the Hoffman-Wielandt inequality. Using equation (4.8) at ((Koltchinskii and Giné, 2000) p.127) gives

$$\delta_2(\lambda(\mathbb{T}_{W_R}), \lambda(T_{R,n})) \leq \sqrt{2} \|K_R\|_F \|E_{R,n}\| = \sqrt{2} \|W_R\|_2 \|E_{R,n}\|.$$

Using again the Hoffman-Wielandt inequality we get

$$\delta_2(\lambda(T_{R,n}), \lambda(\tilde{T}_{R,n})) \leq \|\tilde{T}_{R,n} - T_{R,n}\|_F = \left[\frac{1}{n^2} \sum_{i=1}^n W_R(X_i, X_i)^2 \right]^{1/2},$$

and

$$\delta_2(\lambda(\tilde{T}_{R,n}), \lambda(T_n)) \leq \|\tilde{T}_{R,n} - T_n\|_F = \left[\frac{1}{n^2} \sum_{i \neq j} (W - W_R)^2(X_i, X_j) \right]^{1/2}.$$

Now, we invoke Lemmas 7, 8 and 6 to conclude the proof. Proofs of those lemmas are provided in Appendix G.2, G.3 and F respectively.

Lemma 7 *Let us consider $\gamma > 0$ and assume that $13\tilde{R} \ln(e/\gamma) \leq n$. Then it holds with probability at least $1 - \gamma$*

$$\|E_{R,n}\| \leq 4\sqrt{\frac{\tilde{R}}{n} \ln(2/\gamma)}.$$

Lemma 8 *Let $R \geq 1$. We have*

$$\frac{1}{n^2} \sum_{i=1}^n W_R(X_i, X_i)^2 = \frac{1}{n} \left(\sum_{k=0}^R p_k^* d_k \right)^2.$$

For any $\gamma \in (0, 1)$ with $\log(e \log(n)/\gamma) \leq (n/(13\tilde{R}))$, it holds with probability at least $1 - \gamma$,

$$\begin{aligned} & \delta_2(\lambda(\mathbb{T}_W), \lambda(T_n)) \\ & \leq \delta_2(\lambda(\mathbb{T}_W), \lambda(\mathbb{T}_{W_R})) + \delta_2(\lambda(\mathbb{T}_{W_R}), \lambda(T_{R,n})) + \delta_2(\lambda(T_{R,n}), \lambda(\tilde{T}_{R,n})) \\ & \quad + \delta_2(\lambda(\tilde{T}_{R,n}), \lambda(T_n)) \\ & \leq 4\sqrt{\frac{\tilde{R}}{n} \ln(2/\gamma)} + \sqrt{2} \left(\sum_{k=0}^R d_k (p_k^*)^2 \right)^{1/2} + \frac{1}{\sqrt{n}} \left| \sum_{k=0}^R p_k^* d_k \right| + 2\|p - p_R\|_2 \\ & \quad + M\|p - p_R\|_\infty \sqrt{\frac{\log n}{n}} (\log(e \log(n)/\gamma))^{1/2}, \end{aligned}$$

where $M > 0$ depends only on constants related to the Markov chain $(X_i)_{i \geq 1}$.

Now remark that

$$\left| \sum_{k=0}^R p_k^* d_k \right| \leq \left(\sum_{k=0}^R d_k \right)^{1/2} \left(\sum_{k=0}^R d_k (p_k^*)^2 \right)^{1/2} = \sqrt{\tilde{R}} \|p_R\|_2,$$

and that

$$\|p_R\|_2^2 \leq \|p\|_2^2 \leq 2, \tag{28}$$

because p_R is the orthogonal projection of p , and $\|p\| \leq 1$.

We deduce that

$$\delta_2(\lambda(\mathbb{T}_W), \lambda(T_n))$$

$$\begin{aligned}
 &\leq 2\|p - p_R\|_2 + 4\sqrt{\frac{\tilde{R}}{n} \ln(2/\gamma)} + \sqrt{\frac{2\tilde{R}}{n}} \\
 &\quad + M\|p - p_R\|_\infty \sqrt{\frac{\log n}{n}} (\log(e \log(n)/\gamma))^{1/2} \\
 &\leq 2\|p - p_R\|_2 + 8\sqrt{\frac{\tilde{R}}{n} \ln(e/\gamma)} \\
 &\quad + M\|p - p_R\|_\infty \sqrt{\frac{\log n}{n}} (\log(e \log(n)/\gamma))^{1/2}. \tag{29}
 \end{aligned}$$

■

G.2. Proof of Lemma 7

Observe that $nE_{R,n} = \sum_{i=1}^n (Z_i Z_i^\top - Id_{\tilde{R}})$ where for all $i \in [n]$, $Z_i \in \mathbb{R}^{\tilde{R}}$ is defined by

$$Z_i := Z(X_i) := (Y_{0,1}(X_i), Y_{1,1}(X_i), Y_{1,2}(X_i), \dots, Y_{1,d_1}(X_i), \dots, Y_{R,1}(X_i), \dots, Y_{R,d_R}(X_i)).$$

By definition of the spectral norm for a hermitian matrix,

$$\left\| \frac{1}{n} \sum_{i=1}^n Z_i Z_i^\top - Id_{\tilde{R}} \right\| = \max_{x, \|x\|=1} \left| x^\top \left(\frac{1}{n} \sum_{i=1}^n Z_i Z_i^\top \right) x - 1 \right|.$$

We use a covering set argument based on the following Lemma.

Lemma 9 (see (Gilles, 1989))

Let us consider an integer $D \geq 2$. For any $\epsilon_0 > 0$, there exists a set $Q \subset \mathbb{S}^{D-1}$ of cardinality at most $(1 + 2/\epsilon_0)^D$ such that

$$\forall \alpha \in \mathbb{S}^{D-1}, \quad \exists q \in Q, \quad \|\alpha - q\|_2 \leq \epsilon_0.$$

We consider Q the set given by Lemma 9 with $D = d$ and $\epsilon_0 \in (0, 1/2)$. Let us define $x_0 \in \mathbb{S}^{d-1}$ such that $|x_0^\top E_{R,n} x_0| = \|E_{R,n}\|$ and $q_0 \in Q$ such that $\|x_0 - q_0\|_2 \leq \epsilon_0$. Then,

$$\begin{aligned}
 |x_0^\top E_{R,n} x_0| - |q_0^\top E_{R,n} q_0| &\leq |x_0^\top E_{R,n} x_0 - q_0^\top E_{R,n} q_0| \text{ (by triangle inequality)} \\
 &= |x_0^\top E_{R,n} (x_0 - q_0) - (q_0 - x_0)^\top E_{R,n} q_0| \\
 &\leq \|x_0\|_2 \|E_{R,n}\| \|x_0 - q_0\|_2 + \|q_0 - x_0\|_2 \|E_{R,n}\| \|q_0\|_2 \\
 &\leq 2\epsilon_0 \|E_{R,n}\|.
 \end{aligned}$$

which leads to

$$|x_0^\top E_{R,n} x_0| = \|E_{R,n}\| \leq |q_0^\top E_{R,n} q_0| + 2\epsilon_0 \|E_{R,n}\|.$$

Hence,

$$\|E_{R,n}\| \leq \frac{1}{1 - 2\epsilon_0} \max_{q \in Q} |q^\top E_{R,n} q|.$$

We introduce for any $q \in Q$ the function

$$F_q : x = (x_1, \dots, x_n) \mapsto \frac{1}{n} \sum_{i=1}^n q^\top (Z_i Z_i^\top - 1) q := \frac{1}{n} \sum_{i=1}^n f_q(x_i),$$

where $f_q(x) = q^\top (Z(x)Z(x)^\top - 1) q$.

Let us consider $t > 0$. We want to apply Bernstein's inequality for Markov chains from (Jiang et al., 2018, Theorem 1.1). We remark that $\mathbb{E}_\pi[f_q(X)] = 0$ and that $\|f_q\|_\infty \leq \tilde{R} - 1$. For all $m \in [\tilde{R}]$, we denote $\phi_m = Y_{r,l}$ with $r \in \{0, \dots, R\}$

and $l \in [d_r]$ such that $m = l + \sum_{i=0}^r d_i - 1$. Then, for any $x \in \mathbb{S}^{d-1}$, and for all $k, l \in [\tilde{R}]$, $((Z(x)^\top Z(x))^2)_{k,l} = \sum_{m=1}^{\tilde{R}} \phi_l(x) \phi_m(x)^2 \phi_k(x) = \tilde{R} \phi_l(x) \phi_k(x) = \tilde{R} (Z(x)Z(x)^\top)_{k,l}$ where we used (Dai, 2013, Eq.(1.2.9)). We deduce that

$$\begin{aligned} \mathbb{E}_\pi [f_q(X)^2] &= \mathbb{E}_\pi [q^\top Z(X)Z(X)^\top q q^\top Z(x)Z(x)^\top q] - 2\mathbb{E}_\pi [q^\top Z(X)Z(X)^\top q] + 1 \\ &= \mathbb{E}_\pi [q^\top \underbrace{(Z(X)Z(X)^\top)^2}_{=\tilde{R} \cdot Z(X)Z(X)^\top} q] - 2q^\top \underbrace{\mathbb{E}_\pi [Z(X)Z(X)^\top]}_{=\text{Id}} q + 1 \\ &= \tilde{R} \cdot q^\top \mathbb{E}_\pi [Z(X)Z(X)^\top] q - 1 \\ &= \tilde{R} - 1. \end{aligned}$$

Using that the Markov chain $(X_i)_{i \geq 1}$ has a spectral gap equals to 1 (see Appendix B.3), we get from (Jiang et al., 2018, Eq. (1.6)) that

$$\mathbb{P}(|F_q(X)| \geq t) = \mathbb{P}(|q^\top E_{R,n} q| \geq t) \leq 2 \exp\left(\frac{-nt^2}{4(\tilde{R}-1) + 10(\tilde{R}-1)t}\right),$$

which leads to

$$\mathbb{P}\left(\max_{q \in Q} |q^\top E_{R,n} q| \geq t\right) \leq \mathbb{P}\left(\bigcup_{q \in Q} |q^\top E_{R,n} q| \geq t\right) \leq 2 \exp\left(\frac{-nt^2/(\tilde{R}-1)}{4+10t}\right) (1+2/\epsilon_0)^{\tilde{R}}.$$

Choosing $\epsilon_0 = 2 \left(\exp\left(\frac{nt^2/2}{(\tilde{R}-1)\tilde{R}(4+10t)}\right) - 1\right)^{-1}$ in order to satisfy $(1+2/\epsilon_0)^{\tilde{R}} = \exp(nt^2(\tilde{R}-1)^{-1}(4+10t)^{-1}/2)$, we get

$$\mathbb{P}\left(\max_{q \in Q} |q^\top E_{R,n} q| \geq t\right) \leq 2 \exp\left(\frac{-nt^2}{(\tilde{R}-1)(8+20t)}\right).$$

We deduce that if $\frac{25}{2} \ln(2/\alpha) \tilde{R} \leq n$, it holds with probability at least $1 - \alpha$,

$$\max_{q \in Q} |q^\top E_{R,n} q| \leq 16 \sqrt{\frac{\tilde{R}}{n} \ln(2/\alpha)}.$$

Assuming that $200 \ln(7) \tilde{R}^3 \ln(2/\alpha) \leq n^3$ in order to have $1/(1-2\epsilon_0) \leq 4$, it holds with probability at least $1 - \alpha$

$$\|E_{R,n}\| \leq \frac{1}{1-2\epsilon_0} \max_{q \in Q} |q^\top E_{R,n} q| \leq 4 \sqrt{\frac{\tilde{R}}{n} \ln(2/\alpha)}.$$

■

G.3. Proof of Lemma 8

Reminding that for all $x \in \mathbb{S}^{d-1}$ and for all $k \geq 0$, $\sum_{l=1}^{d_k} Y_{k,l}(x)^2 = d_k$ (see Corollary 1.2.7 from (Dai, 2013)), we get

$$\begin{aligned} \frac{1}{n^2} \sum_{i=1}^n W_R(X_i, X_i)^2 &= \frac{1}{n^2} \sum_{i=1}^n \left(\sum_{k=0}^R p_k^* \sum_{l=1}^{d_k} Y_{k,l}(X_i)^2 \right)^2 \\ &= \frac{1}{n^2} \sum_{i=1}^n \left(\sum_{k=0}^R p_k^* d_k \right)^2 \\ &= \frac{1}{n} \left(\sum_{k=0}^R p_k^* d_k \right)^2. \end{aligned}$$

■

H. Proof of Theorem 2

Proposition 4 is the counterpart of Proposition 1 in (Araya and De Castro, 2019) in our dependent framework. This result is the cornerstone of Theorem 2 and is proved in Appendix H.1.

Proposition 4 *We assume that $\Delta^* > 0$. Let us consider $\gamma > 0$ and define the event*

$$\mathcal{E} := \left\{ \delta_2(\lambda(T_n), \lambda(\mathbb{T}_W)) \vee \frac{2^{\frac{9}{2}} \sqrt{d}}{\Delta^*} \|T_n - \hat{T}_n\| \leq \frac{\Delta^*}{4} \right\}.$$

Then for n large enough,

$$\mathbb{P}(\mathcal{E}) \geq 1 - \gamma/2.$$

Moreover, on the event \mathcal{E} , there exists one and only one set Λ_1 , consisting of d eigenvalues of \hat{T}_n , whose diameter is smaller than $\Delta^*/2$ and whose distance to the rest of the spectrum of \hat{T}_n is at least $\Delta^*/2$. Furthermore, on the event \mathcal{E} , the algorithm HEiC returns the matrix $\hat{G} = \frac{1}{d} \hat{V} \hat{V}^\top$, where \hat{V} has by columns the eigenvectors corresponding to the eigenvalues in Λ_1 .

In the following, we work on the event \mathcal{E} . Let us consider $\gamma \in (0, 1)$.

We choose $R = (n/\log^2 n)^{\frac{1}{2s+d-1}}$. Reminding that W_R is the rank R approximation of W , the Gram matrix associated with the kernel W_R is

$$T_{R,n} = \sum_{k=0}^R p_k^* \sum_{l=1}^{d_k} \Phi_{k,l} (\Phi_{k,l})^\top = X_{R,n} K_R X_{R,n}^\top \in \mathbb{R}^{n \times n}$$

where

$$\begin{aligned} \Phi_{k,l} &= \frac{1}{\sqrt{n}} [Y_{k,l}(X_1), \dots, Y_{k,l}(X_n)] \in \mathbb{R}^n, \\ X_{R,n} &= [\Phi_{0,1}, \Phi_{1,1}, \Phi_{1,2}, \dots, \Phi_{R,d_R}] \in \mathbb{R}^{n \times \tilde{R}} \text{ and} \\ K_R &= \text{Diag}(\lambda_1(\mathbb{T}_W), \dots, \lambda_{\tilde{R}}(\mathbb{T}_W)). \end{aligned}$$

Let us denote now \tilde{V} (resp. \tilde{V}_R) the orthonormal matrix formed by the eigenvectors of the matrix T_n (resp. $T_{R,n}$). We have the following eigenvalue decompositions

$$T_n = \tilde{V} \Lambda \tilde{V}^\top \text{ and } T_{R,n} = \tilde{V}_R \Lambda_R \tilde{V}_R^\top,$$

where $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$ are the eigenvalues of the matrix T_n and where

$\Lambda_R = (p_0^*, p_1^*, \dots, p_1^*, \dots, p_R^*, \dots, p_R^*, 0, \dots, 0) \in \mathbb{R}^n$ where each p_k^* has multiplicity d_k . Then, we note by $V \in \mathbb{R}^{n \times d}$ (resp. V_R) the matrix formed by the columns $1, \dots, d$ of the matrix \tilde{V} (resp. \tilde{V}_R). The matrix $V^* \in \mathbb{R}^{n \times d}$ is the orthonormal matrix with i -th column $\frac{1}{\sqrt{n}} (Y_{1,1}(X_i), \dots, Y_{1,d}(X_i))$. The matrices G^* , G , G_R and G_{proj}^* are defined as follows

$$\begin{aligned} G^* &:= \frac{1}{c_1} V^* (V^*)^\top \\ G &:= \frac{1}{c_1} V V^\top \\ G_R &:= \frac{1}{c_1} V_R V_R^\top \\ G_{proj}^* &:= V^* ((V^*)^\top V^*)^{-1} (V^*)^\top. \end{aligned}$$

G_{proj}^* is the projection matrix for the columns span of the matrix V^* . Using the triangle inequality we have

$$\|G^* - G\|_F \leq \|G^* - G_{proj}^*\|_F + \|G_{proj}^* - G_R\|_F + \|G_R - G\|_F.$$

Step 1: Bounding $\|G - G_R\|_F$. Since the columns of the matrices V and V_R correspond respectively to the eigenvectors of the matrices T_n and $T_{R,n}$, applying the Davis Kahan sinus Theta Theorem (see Theorem 4) gives that there exists $O \in \mathbb{R}^{d \times d}$ such that

$$\|VO - V_R\|_F \leq \frac{2^{3/2}\|T_n - T_{R,n}\|_F}{\Delta},$$

where $\Delta := \min_{k \in \{0,2,3,\dots,R\}} |p_1^* - p_k^*| \geq \Delta^* = \min_{k \in \mathbb{N}, k \neq 1} |p_1^* - p_k^*|$. Using Lemma 10 and $c_1 = \frac{d}{d-2}$, we get that

$$\|G - G_R\|_F = \frac{d-2}{d} \|VO(VO)^\top - V_R V_R^\top\|_F \leq 2\|VO - V_R\|_F.$$

Hence, using the proof of Theorem 1, we get that with probability at least $1 - 1/n^2$,

$$\|G - G_R\|_F \leq 2\|VO - V_R\|_F \leq \frac{C}{\Delta^*} \left(\frac{n}{\log^2 n} \right)^{-\frac{s}{2s+d-1}},$$

where $C > 0$ is a constant.

Step 2: Bounding $\|G^* - G_{proj}^*\|_F$. To bound $\|G^* - G_{proj}^*\|_F$, we apply first Lemma 11 with $B = V^*$. This leads to

$$\|G^* - G_{proj}^*\|_F \leq \|\text{Id}_d - (V^*)^\top V^*\|_F \leq \sqrt{d} \|\text{Id}_d - (V^*)^\top V^*\|.$$

Using a proof rigorously analogous to the proof of Lemma 7, it holds with probability at least $1 - \gamma$ and for n large enough,

$$\|\text{Id}_d - (V^*)^\top V^*\| \leq 4\sqrt{\frac{d \log(e/\gamma)}{n}}.$$

We get by choosing $\gamma = 1/n^2$ that it holds with probability at least $1 - 1/n^2$,

$$\|\text{Id}_d - (V^*)^\top V^*\| \leq C' \sqrt{\frac{d \log(n)}{n}},$$

where $C' > 0$ is a universal constant.

Step 3: Bounding $\|G_{proj}^* - G_R\|_F$. We proceed exactly like in (Araya and De Castro, 2019) but we provide here the proof for completeness. Since G_{proj}^* and G_R are projectors we have, using for example (Bhatia, 1996, p.202),

$$\|G_{proj}^* - G_R\|_F = 2\|G_{proj}^* G_R^\perp\|_F. \quad (30)$$

We use Theorem 5 with $E = G_{proj}^*$, $F = G_R^\perp$, $B = T_{R,n}$ and $A = T_{R,n} + H$ where

$$H = \tilde{X}_{R,n} K_R \tilde{X}_{R,n}^\top - X_{R,n} K_R X_{R,n},$$

where the columns of the matrix $\tilde{X}_{R,n}$ are obtained using a Gram-Schmidt orthonormalization process on the columns of $X_{R,n}$. Hence there exists a matrix L such that $\tilde{X}_{R,n} = X_{R,n}(L^{-1})^\top$. This matrix L is such that a Cholesky decomposition of $X_{R,n}^\top X_{R,n}$ reads as LL^\top .

A and B are symmetric matrices thus we can apply Theorem 5. On the event \mathcal{E} , we can take $S_1 = (\lambda_1 - \frac{\Delta^*}{8}, \lambda_1 + \frac{\Delta^*}{8})$ and $S_2 = \mathbb{R} \setminus (\lambda_1 - \frac{7\Delta^*}{8}, \lambda_1 + \frac{7\Delta^*}{8})$. By Theorem 5 we get

$$\|G_{proj}^* G_R^\perp\|_F \leq \frac{\|A - B\|_F}{\Delta^*} = \frac{\|H\|_F}{\Delta^*}. \quad (31)$$

We only need to bound $\|H\|_F$.

$$\begin{aligned} \|H\|_F &\leq \|L^{-\top} K_R L^{-1} - K_R\|_F \|X_{R,n}^\top X_{R,n}\| \\ &\leq \|K_R\|_F \|L^{-1} L^{-\top} - \text{Id}_R\| \|X_{R,n}^\top X_{R,n}\|, \end{aligned} \quad (32)$$

where the last inequality comes from Lemma 12. From the previous remarks on the matrix L , we directly get

$$\|L^{-1}L^{-\top} - \text{Id}_{\tilde{R}}\| = \|(X_{R,n}^\top X_{R,n})^{-1} - \text{Id}_{\tilde{R}}\|.$$

Using the notations of the proof of Theorem 3 which is provided in Appendix G.1, we get

$$\|L^{-1}L^{-\top} - \text{Id}_{\tilde{R}}\| \|X_{R,n}^\top X_{R,n}\| = \|X_{R,n}^\top X_{R,n} - \text{Id}_{\tilde{R}}\| = \|E_{R,n}\|.$$

Noticing further that $\|K_R\|_F^2 \leq \sum_{k \geq 0} (p_k^*)^2 d_k = \|p\|_2^2 \leq 2$ (because $|p| \leq 1$), (32) becomes

$$\|H\|_F \leq \sqrt{2} \|E_{R,n}\|. \quad (33)$$

Using Lemma 7, it holds with probability at least $1 - \gamma$ and for n large enough,

$$\|E_{R,n}\| \leq 4 \sqrt{\frac{\tilde{R}}{n} \ln(2/\gamma)}. \quad (34)$$

Since $\tilde{R} = \mathcal{O}(R^{d-1})$ and $R = \mathcal{O}\left((n/\log^2 n)^{\frac{1}{2s+d-1}}\right)$, we obtain using (30), (31), (33) and (34) that with probability at least $1 - 1/n^2$ it holds

$$\|G_{proj}^* - G_R\|_F = 2 \|G_{proj}^* G_R^\perp\|_F \leq \frac{C_d}{\Delta^*} \left(\frac{n}{\log^2(n)}\right)^{\frac{-s}{2s+d-1}},$$

where $C_d > 0$ is a constant that may depend on d and on constants related to the Markov chain $(X_i)_{i \geq 1}$.

Conclusion. We proved that on the event \mathcal{E} , it holds with probability at least $1 - 3/n^2$,

$$\|G^* - G\|_F \leq D_1 \left(\frac{n}{\log^2(n)}\right)^{\frac{-s}{2s+d-1}},$$

where $D_1 > 0$ is a constant that depends on Δ^* , d and on constants related to the Markov chain $(X_i)_{i \geq 1}$. Moreover, Eq. (38) from the proof of Proposition 4 gives that on the event \mathcal{E} , we have

$$\|G - \hat{G}\|_F = \frac{d-2}{d} \|VV^\top - \hat{V}\hat{V}^\top\|_F \leq \frac{2^{\frac{9}{2}} \sqrt{d} \|T_n - \hat{T}_n\|}{3\Delta^*}.$$

Using the concentration result from (Bandeira and van Handel, 2016) on spectral norm of centered random matrix with independent entries we get that there exists some constant $D_2 > 0$ such that with probability at least $1 - 1/n^2$ it holds

$$\|G - \hat{G}\|_F \leq D_2 \frac{\sqrt{\log n}}{n}.$$

Using again Proposition 4, we know that for n large enough, $\mathbb{P}(\mathcal{E}) \geq 1 - 1/n^2$. We conclude that for n large enough, it holds with probability at least $1 - 5/n^2$,

$$\|G^* - \hat{G}\|_F \leq D_3 \left(\frac{n}{\log^2(n)}\right)^{\frac{-s}{2s+d-1}},$$

for some constant $D_3 > 0$ that depends on Δ^* , d and on constants related to the Markov chain $(X_i)_{i \geq 1}$ (see Theorem 3 for details).

■

H.1. Proof of Proposition 4

First part of the proof Let us consider $\gamma > 0$.

Using the concentration of spectral norm for random matrices with independent entries from (Bandeira and van Handel, 2016), there exists a universal constant C_0 such that

$$\mathbb{P} \left(\|T_n - \hat{T}_n\| \leq \frac{3\sqrt{2D_0}}{n} + C_0 \frac{\sqrt{\log n/\gamma}}{n} \right) \leq \gamma,$$

where denoting $Y = T_n - \hat{T}_n$, we define $D_0 := \max_{1 \leq i \leq n} \sum_{j=1}^n Y_{i,j} (1 - Y_{i,j})$. We deduce that for n large enough, it holds with probability at least $1 - \gamma/4$,

$$\|T_n - \hat{T}_n\| \leq \frac{(\Delta^*)^2}{2^{\frac{13}{2}} \sqrt{d}}. \quad (35)$$

Using now Theorem 1, it holds with probability at least $1 - \gamma/4$ for n large enough

$$\delta_2(\lambda(T_n), \lambda(\mathbb{T}_W)) \leq C \left(\frac{\log^2 n}{n} \right)^{\frac{s}{2s+d-1}} \leq \frac{\Delta^*}{8}. \quad (36)$$

Putting together (35) and (36), we deduce that for n large enough,

$$\mathbb{P}(\mathcal{E}) \geq 1 - \gamma/2.$$

Second part of the proof In the following, we work on the event \mathcal{E} . Since $\Delta^* > 0$ by assumption, we get that $p_1^* = \lambda_1^* = \dots = \lambda_d^*$ is the only eigenvalue of \mathbb{T}_W with multiplicity d . Indeed, all eigenvalue p_k^* with $k > d$ has multiplicity $d_k > d$ and p_0^* has multiplicity 1. Moreover, from (36), we have that there exists a unique set of d eigenvalues of T_n , denoted $\lambda_{i_1}, \lambda_{i_2}, \dots, \lambda_{i_d}$, such that they are at a distance least $3\Delta^*/4$ away from the other eigenvalues, i.e.

$$\Delta := \min_{\nu_1 \in \lambda(T_n) \setminus \{\lambda_{i_1}, \lambda_{i_2}, \dots, \lambda_{i_d}\}} \max_{\nu_2 \in \{\lambda_{i_1}, \lambda_{i_2}, \dots, \lambda_{i_d}\}} |\nu_1 - \nu_2| \geq \frac{3\Delta^*}{4}. \quad (37)$$

Let us form the matrix $V \in \mathbb{R}^{n \times d}$ where the k -th column is the eigenvector of T_n associated with the eigenvalue λ_{i_k} . We denote further $G := VV^\top/d$. Let $\hat{V} \in \mathbb{R}^{n \times d}$ be the matrix with columns corresponding to the eigenvectors associated to eigenvalues $\hat{\lambda}_{i_1}, \hat{\lambda}_{i_2}, \dots, \hat{\lambda}_{i_d}$ of \hat{T}_n and $\hat{G} := \hat{V}\hat{V}^\top/d$. Using Theorem 4 there exists some orthonormal matrix $O \in \mathbb{R}^{d \times d}$ such that

$$\|VO - \hat{V}\|_F \leq \frac{2^{\frac{3}{2}} \min\{\sqrt{d}\|T_n - \hat{T}_n\|, \|T_n - \hat{T}_n\|_F\}}{\Delta}.$$

Denoting $\lambda_{i_1}^{sort} \geq \lambda_{i_2}^{sort} \geq \dots \geq \lambda_{i_d}^{sort}$ (resp. $\hat{\lambda}_{i_1}^{sort} \geq \hat{\lambda}_{i_2}^{sort} \geq \dots \geq \hat{\lambda}_{i_d}^{sort}$) the sorted version of the eigenvalues $\lambda_{i_1}, \lambda_{i_2}, \dots, \lambda_{i_d}$ (resp. $\hat{\lambda}_{i_1}, \hat{\lambda}_{i_2}, \dots, \hat{\lambda}_{i_d}$), we have

$$\begin{aligned} & \left[\sum_{k=1}^d \left(\lambda_{i_k}^{sort} - \hat{\lambda}_{i_k}^{sort} \right)^2 \right]^{1/2} \\ & \leq \|VV^\top - \hat{V}\hat{V}^\top\|_F \quad (\text{Hoffman-Wielandt inequality (Bhatia, 1996, Thm VI.4.1)}) \\ & \leq 2\|VO - \hat{V}\|_F \quad (\text{Using Lemma 10}) \\ & \leq \frac{2^{\frac{3}{2}} \min\{\sqrt{d}\|T_n - \hat{T}_n\|, \|T_n - \hat{T}_n\|_F\}}{\Delta} \\ & \leq \frac{2^{\frac{3}{2}} \min\{\sqrt{d}\|T_n - \hat{T}_n\|, \|T_n - \hat{T}_n\|_F\}}{3\Delta^*} \quad (\text{Using (37)}) \\ & \leq \Delta^*/8. \quad (\text{Using (35)}) \end{aligned} \quad (38)$$

Using the triangle inequality, we get that

$$\hat{\Delta} := \min_{\nu_1 \in \lambda(\hat{T}_n) \setminus \{\hat{\lambda}_{i_1}, \hat{\lambda}_{i_2}, \dots, \hat{\lambda}_{i_d}\}} \max_{\nu_2 \in \{\hat{\lambda}_{i_1}, \hat{\lambda}_{i_2}, \dots, \hat{\lambda}_{i_d}\}} |\nu_1 - \nu_2| \geq \frac{\Delta^*}{2}. \quad (39)$$

We proved that on the event \mathcal{E} , the eigenvalues in $\Lambda_1 := \{\hat{\lambda}_{i_1}, \dots, \hat{\lambda}_{i_d}\}$ are at distance at least $\Delta^*/2$ from the other eigenvalues of \hat{T}_n (see (39)) and are at distance at most $\Delta^*/8$ of the eigenvalues $\lambda_{i_1}, \dots, \lambda_{i_d}$ of T_n . We could have done this analysis for different eigenvalues. Let us consider some $k \geq 0$. Eq. (36) shows that on the event \mathcal{E} , there exists a set of d_k eigenvalues of T_n which concentrate around p_k^* and such that it has diameter at most $\Delta^*/4$. Weyl's inequality (see (Bhatia, 1996, p.63)) proves that there exist d_k eigenvalues of \hat{T}_n that are at distance at most $\Delta^*/4$ from p_k^* . If we consider now a subset $L \neq \Lambda_1$ of d eigenvalues of \hat{T}_n , then the previous analysis shows that there exists some eigenvalue $\hat{\lambda}$ of \hat{T}_n which is not in L and that is at distance at most $\Delta^*/4$ from one eigenvalue in L . Using (37), we deduce that Algorithm (HEiC) returns $\hat{G} = \hat{V}\hat{V}^\top/d$ where the columns of \hat{V} correspond to the eigenvectors of \hat{T}_n associated to the eigenvalues in Λ_1 .

■

H.2. Useful results

Lemma 10 *Let A, B be two matrices in $\mathbb{R}^{n \times d}$ then*

$$\|AA^\top - BB^\top\|_F \leq (\|A\| + \|B\|)\|A - B\|_F.$$

If $A^\top A = B^\top B = \text{Id}$ then

$$\|AA^\top - BB^\top\|_F \leq 2\|A - B\|_F.$$

Proof of Lemma 10.

$$\begin{aligned} \|AA^\top - BB^\top\|_F &= \|(A - B)A^\top + B(A^\top - B^\top)\|_F \\ &\leq \|A(A - B)^\top\|_F + \|(B - A)B^\top\|_F \\ &\leq \|(A \otimes \text{Id}_n) \text{vec}(A - B)\|_2 + \|(\text{Id}_d \otimes B) \text{vec}(A - B)^\top\|_2 \\ &\leq (\|A \otimes \text{Id}_n\| + \|\text{Id}_d \otimes B\|) \|A - B\|_F \\ &= (\|A\| + \|B\|)\|A - B\|_F, \end{aligned}$$

where $\text{vec}(\cdot)$ represent the vectorization of a matrix that its transformation into a column vector and \otimes is the notation for the Kronecker product between two matrices.

■

Theorem 4 (Davis-Kahan Theorem) *Let Σ and $\hat{\Sigma}$ be two symmetric $\mathbb{R}^{n \times n}$ matrices with eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ and $\hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \dots \geq \hat{\lambda}_n$ respectively. For $1 \leq r \leq s \leq n$ fixed, we assume that $\min\{\lambda_{r-1} - \lambda_r, \lambda_s - \lambda_{s+1}\} > 0$ where $\lambda_0 := \infty$ and $\lambda_{n+1} = -\infty$. Let $d = s - r + 1$ and V and \hat{V} two matrices in $\mathbb{R}^{n \times d}$ with columns $(v_r, v_{r+1}, \dots, v_s)$ and $(\hat{v}_r, \hat{v}_{r+1}, \dots, \hat{v}_s)$ respectively, such that $\Sigma v_j = \lambda_j v_j$ and $\hat{\Sigma} \hat{v}_j = \lambda_j \hat{v}_j$. Then there exists an orthogonal matrix \hat{O} in $\mathbb{R}^{d \times d}$ such that*

$$\|\hat{V}\hat{O} - V\|_F \leq \frac{2^{3/2} \min\{\sqrt{d}\|\Sigma - \hat{\Sigma}\|, \|\Sigma - \hat{\Sigma}\|_F\}}{\min\{\lambda_{r-1} - \lambda_r, \lambda_s - \lambda_{s+1}\}}.$$

Lemma 11 *Let B be a $n \times d$ matrix with full column rank. Then we have*

$$\|BB^\top - B(B^\top B)^{-1}B^\top\|_F = \|\text{Id}_d - B^\top B\|_F.$$

Proof of Lemma 11. Using the cyclic property of the trace, we have

$$\begin{aligned} \|BB^\top - B(B^\top B)^{-1}B^\top\|_F^2 &= \|B(\text{Id}_d - (B^\top B)^{-1})B^\top\|_F^2 \\ &= \text{Tr}(B(\text{Id}_d - (B^\top B)^{-1})B^\top B(\text{Id}_d - (B^\top B)^{-1})B^\top) \\ &= \text{Tr}(B^\top B(\text{Id}_d - (B^\top B)^{-1})B^\top B(\text{Id}_d - (B^\top B)^{-1})) \\ &= \text{Tr}((B^\top B - \text{Id}_d)(B^\top B - \text{Id}_d)) \\ &= \|\text{Id}_d - B^\top B\|_F^2. \end{aligned}$$

■

Theorem 5 (see (Bhatia, 1996, ThmVII.3.4)) Let A and B be two normal operators and S_1 and S_2 two sets separated by a strip of size δ . Let E be the orthogonal projection matrix of the eigenspaces of A with eigenvalues inside S_1 and F be the orthogonal projection matrix of the eigenspaces of B with eigenvalues inside S_2 . Then

$$\|EF\|_F \leq \frac{1}{\delta} \|E(A - B)F\|_F \leq \frac{1}{\delta} \|A - B\|_F.$$

Lemma 12 (Ostrowski's inequality) Let $A \in \mathbb{R}^{n \times n}$ be a Hermitian matrix and $S \in \mathbb{R}^{d \times n}$ be a general matrix then

$$\|SAS^\top - A\|_F \leq \|A\|_F \times \|S^\top S - \text{Id}_n\|.$$

I. Proofs for Bayes Link Prediction.

I.1. Proof of Proposition 1.

Notice that for any $i \in [n]$,

$$\mathbb{P}(g_i(\mathbf{D}_{1:n}) \neq A_{i,n+1}) = \mathbb{E}[\mathbb{1}_{g_i(\mathbf{D}_{1:n}) \neq A_{i,n+1}}] = \mathbb{E}\mathbb{E}[\mathbb{1}_{g_i(\mathbf{D}_{1:n}) \neq A_{i,n+1}} \mid \mathbf{D}_{1:n}],$$

and that

$$\begin{aligned} \mathbb{E}[\mathbb{1}_{g_i(\mathbf{D}_{1:n}) \neq A_{i,n+1}} \mid \mathbf{D}_{1:n}] &= \mathbb{E}[\mathbb{1}_{g_i(\mathbf{D}_{1:n})=1} \mathbb{1}_{A_{i,n+1}=0} \mid \mathbf{D}_{1:n}] + \mathbb{E}[\mathbb{1}_{g_i(\mathbf{D}_{1:n})=0} \mathbb{1}_{A_{i,n+1}=1} \mid \mathbf{D}_{1:n}] \\ &= \eta_i(\mathbf{D}_{1:n}) \mathbb{1}_{g_i(\mathbf{D}_{1:n})=0} + (1 - \eta_i(\mathbf{D}_{1:n})) \mathbb{1}_{g_i(\mathbf{D}_{1:n})=1}, \end{aligned}$$

which leads to

$$\mathbb{P}(g_i(\mathbf{D}_{1:n}) \neq A_{i,n+1}) = \mathbb{E}[\eta_i(\mathbf{D}_{1:n}) \mathbb{1}_{g_i(\mathbf{D}_{1:n})=0} + (1 - \eta_i(\mathbf{D}_{1:n})) \mathbb{1}_{g_i(\mathbf{D}_{1:n})=1}]. \quad (40)$$

By definition of the Bayes classifier g^* , we have for any $i \in [n]$,

$$\begin{aligned} \mathbb{P}(g_i^*(\mathbf{D}_{1:n}) \neq A_{i,n+1}) &= \mathbb{E}[\eta_i(\mathbf{D}_{1:n}) \mathbb{1}_{\eta_i(\mathbf{D}_{1:n}) < \frac{1}{2}} + (1 - \eta_i(\mathbf{D}_{1:n})) \mathbb{1}_{\eta_i(\mathbf{D}_{1:n}) \geq \frac{1}{2}}] \\ &= \mathbb{E}[\min\{\eta_i(\mathbf{D}_{1:n}), 1 - \eta_i(\mathbf{D}_{1:n})\} (\mathbb{1}_{\eta_i(\mathbf{D}_{1:n}) \geq \frac{1}{2}} + \mathbb{1}_{\eta_i(\mathbf{D}_{1:n}) < \frac{1}{2}})] \\ &= \mathbb{E}[\min\{\eta_i(\mathbf{D}_{1:n}), 1 - \eta_i(\mathbf{D}_{1:n})\}] \end{aligned}$$

Given another classifier g , we have for any $i \in [n]$,

$$\begin{aligned} &\mathbb{P}(g_i(\mathbf{D}_{1:n}) \neq A_{i,n+1}) - \mathbb{P}(g_i^*(\mathbf{D}_{1:n}) \neq A_{i,n+1}) \\ &= \mathbb{E} \left[\eta_i(\mathbf{D}_{1:n}) \mathbb{1}_{g_i(\mathbf{D}_{1:n})=0} + (1 - \eta_i(\mathbf{D}_{1:n})) \mathbb{1}_{g_i(\mathbf{D}_{1:n})=1} \right. \\ &\quad \left. - (\eta_i(\mathbf{D}_{1:n}) \mathbb{1}_{g_i^*(\mathbf{D}_{1:n})=0} + (1 - \eta_i(\mathbf{D}_{1:n})) \mathbb{1}_{g_i^*(\mathbf{D}_{1:n})=1}) \right] \\ &= \mathbb{E}[\eta_i(\mathbf{D}_{1:n}) (\mathbb{1}_{g_i(\mathbf{D}_{1:n})=0} - \mathbb{1}_{g_i^*(\mathbf{D}_{1:n})=0}) + (1 - \eta_i(\mathbf{D}_{1:n})) (\mathbb{1}_{g_i(\mathbf{D}_{1:n})=1} - \mathbb{1}_{g_i^*(\mathbf{D}_{1:n})=1})] \\ &= \mathbb{E}[(2\eta_i(\mathbf{D}_{1:n}) - 1) (\mathbb{1}_{g_i^*(\mathbf{D}_{1:n})=1} - \mathbb{1}_{g_i(\mathbf{D}_{1:n})=1})], \end{aligned}$$

where we used that $g(\mathbf{D}_{1:n})$ takes only the values 0 and 1, so that $\mathbb{1}_{g_i(\mathbf{D}_{1:n})=0} - \mathbb{1}_{g_i^*(\mathbf{D}_{1:n})=0} = (\mathbb{1}_{g_i^*(\mathbf{D}_{1:n})=1} - \mathbb{1}_{g_i(\mathbf{D}_{1:n})=1})$. Since

$$\begin{aligned} \mathbb{1}_{g_i^*(\mathbf{D}_{1:n})=1} - \mathbb{1}_{g_i(\mathbf{D}_{1:n})=1} &= \begin{cases} 1 & \text{if } g_i^*(\mathbf{D}_{1:n}) = 1 \text{ and } g_i(\mathbf{D}_{1:n}) = 0 \\ 0 & \text{if } g_i^*(\mathbf{D}_{1:n}) = g_i(\mathbf{D}_{1:n}) \\ -1 & \text{if } g_i^*(\mathbf{D}_{1:n}) = 0 \text{ and } g_i(\mathbf{D}_{1:n}) = 1 \end{cases} \\ &= \mathbb{1}_{g_i^*(\mathbf{D}_{1:n}) \neq g_i(\mathbf{D}_{1:n})} \text{sgn}(\eta_i(\mathbf{D}_{1:n}) - 1/2), \end{aligned}$$

we deduce that

$$\mathbb{P}(g_i(\mathbf{D}_{1:n}) \neq A_{i,n+1}) - \mathbb{P}(g_i^*(\mathbf{D}_{1:n}) \neq A_{i,n+1}) = 2\mathbb{E} \left[\left| \eta_i(\mathbf{D}_{1:n}) - \frac{1}{2} \right| \times \mathbb{1}_{g_i(\mathbf{D}_{1:n}) \neq g_i^*(\mathbf{D}_{1:n})} \right],$$

which concludes the proof.