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# Supplementary material: On the estimation of persistence intensity functions and linear representations of persistence diagrams

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24 **Notation.** We use boldface small letters like  $\mathbf{u}, \mathbf{x}, \boldsymbol{\omega}$  to denote points in  $\mathbb{R}^2$  and sub-scripted letters  
 25 like  $x_1, x_2$  to denote their entries. Boldface capital letters like  $\mathbf{X}, \mathbf{Y}$  would be used to denote points  
 26 on a Riemann manifold. For any positive integer  $n$ , the symbol  $[n]$  refers to the set of all positive  
 27 integers no larger than  $n$ . For any set  $S$ , the symbol  $2^S$  represents the power set of  $S$ , which contains  
 28 all subsets of  $S$  as its elements. The set of all non-negative real numbers would be denoted as  $\mathbb{R}_{\geq 0}$ .  
 29 For any function  $f$  with domain  $\mathcal{A}$ , the infinity norm of  $f$  is denoted as  $\|f\|_{\infty} := \sup_{x \in \mathcal{A}} |f(x)|$ .

## 30 A Background: The persistence diagram

31 In this section, we give a brief introduction to the persistence diagram. We refer readers to [CD19]  
 32 for a detailed description. Consider a random point cloud  $\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_N) \in \mathcal{M}^N$  where  
 33  $\mathcal{M}$  is a Riemann manifold; and a *filtering function*  $\varphi : 2^{[N]} \times \mathcal{M}^N \rightarrow \mathbb{R}$ , which satisfies

$$\varphi(J, \mathbf{X}) \leq \varphi(J', \mathbf{X}), \quad \forall J \subset J' \in 2^{[N]}, \mathbf{X} \in \mathcal{M}^N.$$

34 A simplicial complex given  $\mathbf{X}$  and  $\varphi$  at level  $\alpha$  is defined as

$$K_{\alpha}(\mathbf{X}, \varphi) = \{J \subset 2^{[N]} \mid \varphi(J, \mathbf{X}) \leq \alpha\}.$$

35 Two common examples are the *Cech complex*, where  $\varphi(J, \mathbf{X})$  equals the radius of the circumscribed  
 36 ball of  $\mathbf{X}[J]$ ; and the *Vietoris-Rips complex*, where  $\varphi[J, \mathbf{X}]$  is chosen as the maximum distance  
 37 between points in  $\mathbf{X}[J]$ .

38 Throughout the paper, we assume that the filtering function  $\varphi$  takes its value in  $[0, L]$ . For all values  
 39  $\alpha \in [0, L]$ , the sequence of simplicial complexes  $\{K_{\alpha}(\mathbf{X}, \varphi)\}_{\alpha \in [0, L]}$  forms a *filtration* denoted as  
 40  $\mathcal{F}(\mathbf{X}, \varphi)$ , where  $K_{\alpha}(\mathbf{X}, \varphi) \subseteq K_{\alpha'}(\mathbf{X}, \varphi)$  whenever  $\alpha \leq \alpha'$ .

41 *Persistent homology* is a method for computing topological features of a simplicial complex, and can  
 42 be represented by the *persistence diagram*. In the filtration  $\mathcal{F}(\mathbf{X}, \varphi)$ , for any persistent homology  
 43 that begins to appear at level  $b$  and disappears at level  $d$ , we say that the homology is *born* at  $b$  and  
 44 *dies* at  $d$ . With  $\Omega$  defined as in (1), the persistence diagram of the point cloud  $\mathbf{X}$  is a multiset on  $\Omega$   
 45 that summarizes the birth and death times of all persistent homologies in the filtration  $\mathcal{F}(\mathbf{X}, \varphi)$ :

$$\text{Dgm}(\mathbf{X}, \varphi) = \{(b_i, d_i) : \text{the } i\text{-th persistent homology in } \mathcal{F}(\mathbf{X}, \varphi) \\ \text{that is born at } b_i \text{ and dies at } d_i\}.$$

## 46 B Supportive theoretical results

### 47 B.1 Validation of Assumption 3.3

48 In this part, we provide some common data-generating mechanisms where Assumption 3.3 can be  
 49 validated.

50 **Theorem B.1** *Let  $q, d$  be two positive integers and  $q > d$ . Let  $\kappa$  be a density on  $[0, 1]^d$  such that*  
 51  *$0 < \inf \kappa \leq \sup \kappa < \infty$ . Suppose that  $\mathbf{X}_N$  be either a binomial process with parameters  $N$  and  $\kappa$*   
 52 *or a Poisson process of intensity  $N\kappa$  in the cube  $[0, 1]^d$ . Denote  $p(\mathbf{u})$  as the intensity function for the*  
 53  *$k$ -dimensional expected persistent measure induced by the Vietoris-Rips filtration. Then when  $N$  is*  
 54 *sufficiently large, for  $\mathbf{u} \in \Omega$ , there exists a polynomial function  $\text{poly}(\cdot)$ , such that*

$$p(\mathbf{u}) \leq \text{poly}(N, d) \sup \kappa,$$

55 *and  $\bar{p}(\mathbf{u})$  can be correspondingly bounded.*

56 **Theorem B.2** *Let  $q, d$  be two positive integers and  $q > d$ . Let  $\kappa$  be a density on  $[0, 1]^{d \times N}$*   
 57 *such that  $0 < \inf \kappa < \sup \kappa < \infty$ . Suppose that  $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_N \in [0, 1]^d$  and that*  
 58  *$\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_N) \sim \kappa$ . Denote  $\tilde{p}(\mathbf{u})$  as the persistence density induced by the Vietoris-Rips*  
 59 *filtration of  $\mathbf{X}$ . Then there exists a polynomial function  $(\cdot)$ , such that*

$$\tilde{p}(\mathbf{u}) \leq \text{poly}(N, d) \sup \kappa.$$

### 60 B.2 Clarification of Assumptions

61 In this part, we provide the details in the smoothness assumption of the persistence intensity and  
 62 density functions, and the regularization assumptions of the kernel function.

63 **Hölder smoothness.** Recall from Assumption 3.2 that we assume the persistence intensity function  
64  $p(\cdot)$  and the persistence density function  $\tilde{p}(\cdot)$  are Hölder smooth. A function  $f : \Omega \rightarrow \mathbb{R}_{\geq 0}$  is  
65  $s$ -th order Hölder smooth with parameter  $L_f$  if it is at least  $(s - 1)$ -differentiable and that for any  
66  $\mathbf{x}, \mathbf{x}' \in \Omega$ ,

$$\left| f(\mathbf{x}') - f(\mathbf{x}) - \sum_{t=1}^{s-1} \frac{1}{t!} \sum_{t_1+t_2=t} \frac{d^t f(\mathbf{x})}{dx_1^{t_1} dx_2^{t_2}} (x'_1 - x_1)^{t_1} (x'_2 - x_2)^{t_2} \right| \leq L_f \|\mathbf{x}' - \mathbf{x}\|_2^s. \quad (1)$$

67 **Assumptions regarding the kernel function.** Throughout the paper, we assume the kernel func-  
68 tion  $K(\cdot)$  satisfies some properties that are commonly used in non-parametric statistics [GN21].  
69 Specifically, we make the following assumption.

70 **Assumption B.3** *The kernel function  $K : \mathbb{R}^2 \rightarrow \mathbb{R}$  satisfies the following conditions:*

- 71 (a)  $K(\mathbf{x}) = 0$  for all  $\mathbf{x}$  with  $\|\mathbf{x}\|_2 > 1$ ;
- 72 (b)  $\|K\|_\infty := \sup_{\mathbf{x}} |K(\mathbf{x})| < \infty$ ;
- 73 (c)  $\int_{\mathbb{R}^2} K(\mathbf{x}) d\mathbf{x} = 1$ ;
- 74 (d)  $\|K\|_2^2 := \int_{\mathbb{R}^2} K^2(\mathbf{x}) d\mathbf{x} < \infty$ .
- 75 (e) *There exists a positive integer  $s$ , such that for all non-negative integers  $s_1, s_2$  satisfying*  
76  $1 \leq s_1 + s_2 < s$ ,

$$\int_{\mathbf{x} \in \mathbb{R}^2} x_1^{s_1} x_2^{s_2} K(\mathbf{x}) d\mathbf{x} = 0.$$

- 77 (f)  $K$  is  $L_K$ -Lipchitz with respect to the  $\ell_2$  norm on  $\mathbb{R}^2$ .

### 78 B.3 Minimax lower bound for estimating the persistence intensity function

79 Below we provide a minimax lower bound on the  $L_\infty$  estimation error of the persistence intensity  
80 function by leveraging well-known minimax arguments for estimating a smooth probability density  
81 function based on an i.i.d. sample; see [GN21] for details, as well for the definition of Besov norms.

82 **Theorem B.4** *Let  $\mathcal{F}$  denote the set of functions on  $\Omega$  with Besov norm bounded by  $B > 0$ :*

$$\mathcal{F} = \{f : \Omega \rightarrow \mathbb{R}, \|f\|_{B_{\infty, \infty}^s} \leq B\}.$$

83 *Then,*

$$\inf_{\hat{p}_n} \sup_P \mathbb{E}_{\mu_1, \dots, \mu_n \stackrel{i.i.d.}{\sim} P} \sup_{\omega \in \Omega} \|\omega - \partial\Omega\|_2^q |\hat{p}_n(\omega) - p(\omega)| \geq O(n^{-\frac{s}{2(s+1)}}),$$

84 *where the infimum is taken over estimator  $\hat{p}_n$  mapping  $\mu_1, \dots, \mu_n$  to an intensity function in  $\mathcal{F}$ , the*  
85 *supremum is over the set of all probability distribution on  $\mathcal{Z}_{L, M}^q$  and  $p$  is the intensity function of*  
86  $\mathbb{E}_P[\mu]$ .

### 87 B.4 Estimating the persistence surface

88 For estimating the persistence surface in (6), we directly generate the persistence surface from the  
89 empirical averaged persistence measure  $\bar{\mu}_n$  given by

$$A \in \mathcal{B} \mapsto \bar{\mu}_n(A) = \frac{1}{n} \sum_{i=1}^n \mu_i(A).$$

90 Since  $\bar{\mu}_n$  is unbiased for  $\mathbb{E}[\mu]$  and  $\rho$  is a linear transformation,  $\rho_h(\bar{\mu}_n)$  is also unbiased for  $\rho_h(\mathbb{E}[\mu])$ .  
91 The following theorem bounds its variation.

92 **Theorem B.5** *With the choice of the weight function*

$$f(\boldsymbol{\omega}) = \|\boldsymbol{\omega} - \partial\Omega\|_2^q,$$

93 *when Assumptions 3.3(a) and 3.4 hold true, there exists a constant  $C$  depending on  $L, M, L_K, \|K\|_\infty$*   
 94 *and  $\|\bar{p}\|_\infty$ , such that for any  $\delta \in (0, 1)$ , it can be guaranteed with probability at least  $1 - \delta$  that*

$$\|\rho_h(\bar{\mu}_n) - \rho_h(\mathbb{E}[\mu])\|_\infty \leq C \max \left\{ \frac{1}{nh^2} \log \frac{1}{\delta h^2}, \sqrt{\frac{1}{nh^2}} \sqrt{\log \frac{1}{\delta h^2}} \right\}.$$

95 **B.5 Estimating the persistent betti number by the empirical averaged persistence measure**

96 As an alternative to the kernel-based estimator for the persistent betti number in (10), we can directly  
 97 use the empirical persistent betti number as the estimator:

$$\bar{\beta}_{\mathbf{x}} = \bar{\mu}_n(B_{\mathbf{x}}).$$

98 Since  $\bar{\mu}_n$  is an unbiased estimator for  $\mathbb{E}[\mu]$ ,  $\bar{\beta}_{\mathbf{x}}$  is an unbiased estimator for  $\beta_{\mathbf{x}}$ . As for the variation  
 99 of the estimator, we provide the following theorem.

100 **Theorem B.6** *Under Assumptions 3.2, 3.3(a) and 3.4, for any  $\delta \in (0, 1)$ , there exists a universal*  
 101 *constant  $C$  such that with probability at least  $1 - \delta$ , it can be guaranteed that*

$$\begin{aligned} \sup_{\mathbf{x} \in \Omega_\ell} |\bar{\beta}_{\mathbf{x}} - \beta_{\mathbf{x}}| &\leq C \left( \frac{M\ell^{-q}}{n} \left( 2 \log(M\ell^{-q}n + 1) + \log \frac{1}{\delta} \right) \right. \\ &\quad \left. + \sqrt{\min \left\{ \frac{M^2\ell^{-2q}}{n}, \frac{\sqrt{2}ML\ell^{1-2q} \|\bar{p}\|_\infty}{(q-1)_+ n} \right\}} \left( \sqrt{2 \log(M\ell^{-q}n + 1)} + \sqrt{\log \frac{1}{\delta}} \right) \right), \end{aligned}$$

102 *where  $(q-1)_+ = \max\{q-1, 0\}$ .*

## 103 C Preliminary facts

104 In this section we present and prove various auxiliary results that are needed in the proofs of the main  
 105 theorems.

### 106 C.1 Preliminary facts for the proof of Theorem B.1

107 Bounding the weighted intensity function as in Theorem B.1 requires a detailed exploration of the  
 108 persistent diagram for the Vietoris-Rips filtration. Throughout this section, we will consider the  
 109 filtering function corresponding to the Vietoris-Rips filtration

$$\varphi[J](\mathbf{X}) = \min_{i,j \in J, i \neq j} \|\mathbf{X}_i - \mathbf{X}_j\|_2.$$

110 Firstly, we state a form of the **area formula** given by [Mor16], which would be useful for a change  
 111 of variable in deriving the intensity function for the expected persistence measure.

112 **Theorem C.1** *Denote  $\mathcal{L}^M$  as the  $M$ -dimensional Lebesgue measure and  $\mathcal{H}^M$  as the  $M$ -*  
 113 *dimensional Hausdorff measure. Consider a Lipschitz function  $f : \mathbb{R}^M \rightarrow \mathbb{R}^N$  for  $M \leq N$ . If*  
 114  *$h : \mathbb{R}^M \rightarrow \mathbb{R}$  is an  $\mathcal{L}^M$ -integrable function, then*

$$\int_{\mathbb{R}^M} h(\mathbf{X}) J_{\mathbf{X}} f(\mathbf{X}) d\mathcal{L}^M(\mathbf{X}) = \int_{\mathbb{R}^N} \sum_{\mathbf{X} \in f^{-1}\{\mathbf{Y}\}} h(\mathbf{X}) d\mathcal{H}^M \mathbf{Y},$$

115 *where  $J_{\mathbf{X}} f(\mathbf{X})$  is the Jacobian determinant of the function  $f$ :*

$$J_{\mathbf{X}} f(\mathbf{X}) = \sqrt{\det \left( \left( \frac{df}{d\mathbf{X}} \right)^\top \left( \frac{df}{d\mathbf{X}} \right) \right)}.$$

116 Theorem C.1 directly implies the following corollary, the proof of which would be omitted.

117 **Corollary C.2** Let  $\psi : \mathbb{R}^M \rightarrow \mathbb{R}^N$  be a Lipchitz bijection with  $M \leq N$ , and  $\kappa : \mathbb{R}^N \rightarrow \mathbb{R}$  be a  
 118 function which satisfies that  $h := \kappa \circ \psi$  is  $\mathcal{L}^M$ -integrable. Then

$$\int_{\mathbb{R}^M} \kappa \circ \psi(\mathbf{X}) J_{\mathbf{X}} \psi(\mathbf{X}) d\mathcal{L}^M(\mathbf{X}) = \int_{\mathbb{R}^N} \kappa(\mathbf{Y}) d\mathcal{H}^M(\mathbf{Y}).$$

119 The following proposition considers two kinds of partitions of the unit cube  $[0, 1]^{d \times n}$ , with each part  
 120 satisfying some desired properties.

121 **Proposition C.3** There exists a set  $S$  with cardinality  $\text{card}(S) = 4d^2$ , such that for any  $J_1, J_2 \subset [N]$   
 122 that satisfies  $J_1 \neq J_2, |J_1| = |J_2| = 2$ , bearing a zero-measured set,  $[0, 1]^{d \times n}$  can be partitioned as

$$[0, 1]^{d \times n} = \bigcup_{s \in S} W_{J_1, J_2}^s,$$

123 such that within each part  $W_{J_1, J_2}^s$ , there exists a diffeomorphism  $\Psi_{J_1, J_2}^s : W_{J_1, J_2}^s \rightarrow \mathbb{R}^2 \times [0, 1]^{nd-2}$ ,  
 124 such that:

- 125 1. For every  $\mathbf{X} \in W_{J_1, J_2}^s$ ,  $\Psi_{J_1, J_2}^s(\mathbf{X})_1 = \varphi[J_1](\mathbf{X})$  and  $\Psi_{J_1, J_2}^s(\mathbf{X})_2 = \varphi[J_2](\mathbf{X})$ ;
- 126 2. The Jacobian determinant  $J_{\mathbf{X}} \Psi_{J_1, J_2}^s(\mathbf{X}) \geq \frac{1}{d}$ .

127 *Proof:* Let  $S = [d]^2 \times \{-1, +1\}^2$ , then it is easy to see that  $|S| = 4d^2$ . For any  $J_1, J_2 \subset [n]$  with  
 128  $J_1 \neq J_2$  and  $|J_1| = |J_2| = 2$ , let denote  $J_1 = \{i_1, j_1\}$ ,  $J_2 = \{i_2, j_2\}$  with  $j_2 = \max\{j \in J_2 : j \notin$   
 129  $J_1\}$ . For any  $s = (k_1, k_2, s_1, s_2) \in S$ , let

$$\begin{aligned} W_{J_1, J_2}^s &= \{ \mathbf{X} : \{k_1\} = \operatorname{argmax}_k |X_{i_1}^k - X_{j_1}^k|, s_1(X_{j_1}^k - X_{i_1}^k) > 0, \\ &\quad \{k_2\} = \operatorname{argmax}_k |X_{i_2}^k - X_{j_2}^k|, s_2(X_{j_2}^k - X_{i_2}^k) > 0. \} \end{aligned}$$

130 Notice here that  $\{k_1\} = \operatorname{argmax}_k |X_{i_1}^k - X_{j_1}^k|$  means  $k_1$  is the *only* index for  $|X_{i_1}^k - X_{j_1}^k|$  to reach its  
 131 maximum.

132 We begin by proving that  $\{W_{J_1, J_2}^s\}_{s \in S}$  forms a partition of  $[0, 1]^{d \times n}$  bearing a zero-measured set.  
 133 Firstly, for  $s, s' \in S$  with  $s \neq s'$ , it is easy to see that  $W_{J_1, J_2}^s$  and  $W_{J_1, J_2}^{s'}$  are disjoint. Secondly, if

$$\mathbf{X} \in [0, 1]^{d \times n} - \bigcup_{s \in S} W_{J_1, J_2}^s,$$

134 then by definition, there exists  $k, k' \in [d]$ , such that  $k \neq k'$  and that either

$$|X_{j_1}^k - X_{i_1}^k| = |X_{j_1}^{k'} - X_{i_1}^{k'}|$$

135 or

$$|X_{j_2}^k - X_{i_2}^k| = |X_{j_2}^{k'} - X_{i_2}^{k'}|.$$

136 Notice that for any  $k, k' \in [d]$  with  $k \neq k'$ , the set

$$\begin{aligned} &\left\{ \mathbf{X} : |X_{j_1}^k - X_{i_1}^k| = |X_{j_1}^{k'} - X_{i_1}^{k'}| \right\} \\ &= \left\{ \mathbf{X} : X_{j_1}^k - X_{i_1}^k = |X_{j_1}^{k'} - X_{i_1}^{k'}| \right\} \cup \left\{ \mathbf{X} : X_{j_1}^k - X_{i_1}^k = -|X_{j_1}^{k'} - X_{i_1}^{k'}| \right\}, \end{aligned}$$

137 where the sets

$$\begin{aligned} &\left\{ \mathbf{X} \in [0, 1]^{d \times n} : X_{j_1}^k - X_{i_1}^k = |X_{j_1}^{k'} - X_{i_1}^{k'}| \right\} \quad \text{and} \\ &\left\{ \mathbf{X} \in [0, 1]^{d \times n} : X_{j_1}^k - X_{i_1}^k = -|X_{j_1}^{k'} - X_{i_1}^{k'}| \right\} \end{aligned}$$

138 are a subsets of  $(nd - 1)$  dimensional linear manifolds in  $[0, 1]^{d \times n}$ , and are therefore zero-measured  
 139 in  $\mathcal{L}^{nd}$ . Similarly, we can prove that the set  $[0, 1]^{d \times n} - \bigcup_{s \in S} W_{J_1, J_2}^s$  is the union of a finite number  
 140 of subsets of  $(nd - 1)$  dimensional linear manifolds in  $[0, 1]^{d \times n}$ . Consequently,

$$\bigcup_{s \in S} W_{J_1, J_2}^s$$

141 is a partition of  $[0, 1]^{d \times n}$  bearing a zero-measured set.

142 Furthermore, define  $\Psi_{J_1, J_2}^s$  as

$$\Psi_{J_1, J_2}^s(\mathbf{X}) = \left( \varphi[J_1](\mathbf{X}), \varphi[J_2](\mathbf{X}), \{X_j^k\}_{\substack{1 \leq j \leq n \\ 1 \leq k \leq d \\ (j,k) \neq (j_1, k_1) \\ (j,k) \neq (j_2, k_2)}} \right), \quad \forall \mathbf{X} \in W_{J_1, J_2}^s.$$

143 Then we can firstly notice that

$$X_{j_1}^{k_1} = s_1 \sqrt{u_1^2 - \sum_{k \neq k_1} (X_{j_1}^k)^2} + X_{i_1}^{k_1} \quad \text{and}$$

$$X_{j_2}^{k_2} = s_2 \sqrt{u_2^2 - \sum_{k \neq k_2} (X_{j_2}^k)^2} + X_{i_2}^{k_2},$$

144 for  $u_1 = \varphi[J_1](X)$  and  $u_2 = \varphi[J_2](X)$ . This validates  $\Psi_{J_1, J_2}^s$  as a diffeomorphism. The proof now  
 145 boils down to bounding the Jacobian of  $\Psi_{J_1, J_2}^s$ . Towards this end, notice that the partial derivative of  
 146  $\varphi$  is bounded by

$$\begin{aligned} \left| \frac{\partial \varphi[J_1](\mathbf{X})}{\partial X_{j_1}^{k_1}} \right| &= \left| \frac{\partial}{\partial X_{j_1}^{k_1}} \sqrt{\sum_{k=1}^d (X_{i_1}^k - X_{j_1}^k)^2} \right| \\ &= \left| \frac{X_{j_1}^{k_1} - X_{i_1}^{k_1}}{\sqrt{\sum_{k=1}^d (X_{i_1}^k - X_{j_1}^k)^2}} \right| \\ &\geq \frac{1}{\sqrt{d}}, \end{aligned}$$

147 where in the last line we applied the fact that

$$\left| X_{j_1}^{k_1} - X_{i_1}^{k_1} \right| = \max_{1 \leq k \leq d} |X_{j_1}^k - X_{i_1}^k| \geq \sqrt{\frac{1}{d} \sum_{k=1}^d (X_{i_1}^k - X_{j_1}^k)^2}.$$

148 Similarly,

$$\left| \frac{\partial \varphi[J_2](\mathbf{X})}{\partial X_{j_2}^{k_2}} \right| = \left| \frac{\partial}{\partial X_{j_2}^{k_2}} \sqrt{\sum_{k=1}^d (X_{i_2}^k - X_{j_2}^k)^2} \right| \geq \frac{1}{\sqrt{d}}.$$

149 Furthermore, since  $j_2 \notin J_1$ , it is easy to see that

$$\frac{\partial \varphi[J_1](\mathbf{X})}{\partial X_{j_2}^{k_2}} = 0.$$

150 Therefore, the Jacobian determinant of  $\Psi_{J_1, J_2}^s$  is bounded by

$$\begin{aligned} J_{\mathbf{X}} \Psi_{J_1, J_2}^s(\mathbf{X}) &= \left| \det \left( \frac{d\Psi_{J_1, J_2}^s(\mathbf{X})}{d\mathbf{X}} \right) \right| \\ &= \left| \det \left( \begin{pmatrix} \mathbf{I}_{nd-2} & \mathbf{0}_{(nd-2) \times 1} & \mathbf{0}_{(nd-2) \times 1} \\ \mathbf{0}_{1 \times (nd-2)} & \frac{\partial \varphi[J_1](\mathbf{X})}{\partial X_{j_1}^{k_1}} & \frac{\partial \varphi[J_1](\mathbf{X})}{\partial X_{j_2}^{k_2}} \\ \mathbf{0}_{1 \times (nd-2)} & \frac{\partial \varphi[J_2](\mathbf{X})}{\partial X_{j_1}^{k_1}} & \frac{\partial \varphi[J_2](\mathbf{X})}{\partial X_{j_2}^{k_2}} \end{pmatrix} \right) \right| \\ &= \left| \frac{\partial \varphi[J_1](\mathbf{X})}{\partial X_{j_1}^{k_1}} \cdot \frac{\partial \varphi[J_2](\mathbf{X})}{\partial X_{j_2}^{k_2}} \right| \geq \frac{1}{d}. \end{aligned}$$

151 This completes the proof. ■

152 The following is important for representing of the persistence intensity function  $p$  and the persistence  
 153 density function  $\tilde{p}$ .

154 **Proposition C.4** Bearing a zero-measured set,  $[0, 1]^{d \times n}$  can be partitioned as

$$[0, 1]^{d \times n} = \bigcup_{r=1}^R V_r,$$

155 such that

- 156 1. For every  $\mathbf{X}, \mathbf{X}' \in V_r$ ,  $J_1, J_2 \subset [n]$  with  $|J_1| = |J_2| = 2$ , it is guaranteed that  $\varphi[J_1](\mathbf{X}) \neq$   
 157  $\varphi[J_2](\mathbf{X})$ ; furthermore, if  $\varphi[J_1](\mathbf{X}) < \varphi[J_2](\mathbf{X})$ , then  $\varphi[J_1](\mathbf{X}') < \varphi[J_2](\mathbf{X}')$ ;
- 158 2. For every  $\mathbf{X}, \mathbf{X}' \in V_r$ ,  $J_1, J_2, J_3, J_4 \subset [n]$  with  $|J_1| = |J_2| = |J_3| = |J_4| = 2$ ,  
 159 it is guaranteed that  $\varphi[J_1](\mathbf{X}) - \varphi[J_2](\mathbf{X}) \neq \varphi[J_3](\mathbf{X}) - \varphi[J_4](\mathbf{X})$ ; furthermore, if  
 160  $\varphi[J_1](\mathbf{X}) - \varphi[J_2](\mathbf{X}) > \varphi[J_3](\mathbf{X}) - \varphi[J_4](\mathbf{X}) > 0$ , then  $\varphi[J_1](\mathbf{X}') - \varphi[J_2](\mathbf{X}') >$   
 161  $\varphi[J_3](\mathbf{X}') - \varphi[J_4](\mathbf{X}') > 0$ .
- 162 3. For every  $r \in [R]$  and  $\mathbf{X} \in V_r$ , there are  $N_r$  points in  $\text{Dgm}(\mathbf{X}, \varphi)$ ; furthermore, all these  
 163 points can be ordered by their orthogonal distance to the diagonal, and the order is fixed for  
 164 all  $\mathbf{X} \in V_r$ .

165 Furthermore, the expected persistence measure  $\mathbb{E}[\mu]$  and its normalized counterpart  $\mathbb{E}[\tilde{\mu}]$  can be  
 166 characterized such that for any Borel set  $B \subset \Omega$ ,

$$\mathbb{E}[\mu](B) = \sum_{r=1}^R \sum_{i=1}^{N_r} \int_{x \in \Phi^{-1}[J_{i_r}^1, J_{i_r}^2](B) \cap V_r} \kappa(\mathbf{X}) d\mathbf{X} \quad \text{and}$$

$$\mathbb{E}[\tilde{\mu}](B) = \sum_{r=1}^R \frac{1}{N_r} \sum_{i=1}^{N_r} \int_{x \in \Phi^{-1}[J_{i_r}^1, J_{i_r}^2](B) \cap V_r} \kappa(\mathbf{X}) d\mathbf{X}$$

167 , in which

$$\Phi[J_1, J_2](\mathbf{X}) = (\varphi[J_1](\mathbf{X}), \varphi[J_2](\mathbf{X})),$$

168 and  $J_{i_r}^1, J_{i_r}^2$  are the simplicial complexes corresponding to the birth and death of the  $i$ -th persistence  
 169 homology for all  $\mathbf{X} \in V_r$ .

170 *Proof:* For simplicity, we only give a sketch of the proof for this proposition. A weaker version  
 171 of this proposition is proved in [CD19], where the second property of the partition is not required.  
 172 Therefore, the partition we aim to construct here is a refinement of the partition given in [CD19]. In  
 173 order to see that the second condition can be reached, we firstly prove that the set

$$A = \{ \mathbf{X} \in [0, 1]^{d \times n} : \exists J_1, J_2, J_3, J_4 \subset [n], \text{ s.t.} \\
|J_1| = |J_2| = |J_3| = |J_4| = 2, \\
J_1 \neq J_2, J_3 \neq J_4, (J_1, J_2) \neq (J_3, J_4), \\
\varphi[J_1](\mathbf{X}) - \varphi[J_2](\mathbf{X}) = \varphi[J_3](\mathbf{X}) - \varphi[J_4](\mathbf{X}) \}$$

174 is zero-measured. For this step, the technique in proving Lemma 4.1 in [CD19] can be applied to  
 175 prove that  $A$  does not contain any open set, and all its points are singular.

176 We can further define

$$\mathcal{F}_n^2 = \{(J_1, J_2) : J_1, J_2 \subset [n], |J_1| = |J_2| = 2, J_1 \neq J_2\}.$$

177 Since  $A$  is zero-measured, we can only consider the set  $[0, 1]^{d \times n} - A$ , on which

$$\{\Delta\varphi[J_1, J_2](\mathbf{X}) := \varphi[J_1](\mathbf{X}) - \varphi[J_2](\mathbf{X})\}_{(J_1, J_2) \in \mathcal{F}_n^2}$$

178 must take different values for different  $(J_1, J_2) \in \mathcal{F}_n^2$ . Denote these values as  $r_1 < r_2 < \dots <$   
 179  $r_L$ , and let  $E_\ell(\mathbf{X})$  denote the element  $(J_1, J_2) \in \mathcal{F}_n^2$  such that  $\Delta\varphi[J_1, J_2](\mathbf{X}) = r_\ell$ . The sets  
 180  $E_1(\mathbf{X}), E_2(\mathbf{X}), \dots, E_L(\mathbf{X})$  then form a partition of  $\mathcal{F}_n^2$ . With similar techniques as Lemma 4.2 in  
 181 [CD19], we can prove that the map  $\mathbf{X} \mapsto \mathcal{A}^2(\mathbf{X})$  is locally constant almost surely everywhere. This  
 182 essentially completes the proof.

183

184 The following lemma is a direct application of Proposition 4.6 in [DP19], and guarantees that the  
 185 number of points in the persistence diagram  $\text{Dgm}(\mathbf{X}, \varphi)$  that are far enough from the diagonal is  
 186 upper bounded in terms of the expectation. ■

187 **Lemma C.5** *Let  $\kappa$  be a probability density function on  $[0, 1]^d$  that satisfies  $0 < \inf \kappa < \sup \kappa < \infty$ .  
 188 Denote  $\mathbb{X}_n$  as a binomial process with parameters  $n$  and  $\kappa$  or a Poisson process with parameter  $n\kappa$   
 189 on  $[0, 1]^d$ . In the  $k$ th dimensional persistence diagram of the Vietoris-Rips filtration of  $\mathbb{X}_n$ , let  $N_\ell$  be  
 190 the number of points with persistence of at least  $\ell$ . Then there are some universal constant  $C$  that the  
 191 expectation of  $N_\ell$  is upper bounded as*

$$\mathbb{E}[N_\ell] \leq Cn \exp(-Cn\ell^d),$$

192 where  $C$  is a constant depends only on  $k$ .

193 *Proof:* Let  $\mu$  be the persistence measure corresponding to the  $k$ -th dimensional persistence diagram  
 194 of the Vietoris-Rips filtration of  $\mathbb{X}_n$ . From Proposition 4.6 in [DP19],

$$P(\mu(\mathbb{R} \times [\ell, \infty)) > t) \leq c_1 \exp\left(-c_2 \left(n\ell^d + \left(\frac{t}{n}\right)^{1/(k+1)}\right)\right).$$

195 And hence the expectation of  $\mu(\mathbb{R} \times [\ell, \infty))$  is bounded as

$$\begin{aligned} \mathbb{E}[\mu(\mathbb{R} \times [\ell, \infty))] &\leq \int_0^\infty c_1 \exp\left(-c_2 \left(n\ell^d + \left(\frac{t}{n}\right)^{1/(k+1)}\right)\right) dt \\ &= c_1 \exp(-c_2(n\ell^d)) \int_0^\infty \exp\left(-c_2 \left(\frac{t}{n}\right)^{1/(k+1)}\right) dt \\ &= c_1 \exp(-c_2(n\ell^d)) \int_0^\infty (k+1)nu^k \exp(-c_2u) du \\ &= Cn \exp(-Cn\ell^d), \end{aligned}$$

196 for some constant  $C$  that depends on  $k$ . Now,  $\mathbb{R} \times [\ell, \infty)$  contains all the homological features whose  
 197 persistence is at least  $\ell$ , so

$$N_\ell \leq \mu(\mathbb{R} \times [\ell, \infty)).$$

198 And hence

$$\mathbb{E}[N_\ell] \leq Cn \exp(-Cn\ell^d).$$

199 ■

## 200 C.2 Uniform tail bounds

201 In this section, we provide some uniform tail bound theorems that are important for bounding the  
 202 variation of estimators. We will omit the proofs of these theorems in the paper.

203 **The Talagrand's inequality.** The following form of the Talagrand's inequality was shown in  
 204 [SC08].

205 **Theorem C.6** *Let  $(\mathcal{Z}, \mathcal{F}, P)$  be a probability space and  $(T, d)$  be a separable metric space. Con-  
 206 sider a function class  $\mathcal{G} = \{g_t : t \in T\} \in L_0(\mathcal{Z})$ , such that the function  $t \mapsto g_t(z)$  is continuous in  
 207  $t$  for all  $z \in \mathcal{Z}$ . Furthermore, suppose that there exists a constant  $B > 0, \sigma^2 > 0$  such that for all  
 208  $g \in \mathcal{G}$ ,  $\mathbb{E}[g] = 0, \mathbb{E}[g^2] \leq \sigma^2, \|g\|_\infty \leq B$ . Let  $Z_1, Z_2, \dots, Z_n \sim$  i.i.d.  $P$ , and define*

$$G = \sup_{g \in \mathcal{G}} \left| \frac{1}{n} \sum_{i=1}^n g(Z_i) \right|.$$

209 Then for any  $\delta \in (0, 1)$ , with probability of at least  $1 - \delta$ ,

$$G \leq 4\mathbb{E}[G] + \sqrt{\frac{2\sigma^2}{n} \log \frac{1}{\delta}} + \frac{B}{n} \log \frac{1}{\delta}. \quad (2)$$



210 Theorem C.6 implies that the expectation of  $G$  is an important factor in bounding  $G$ . The following  
 211 theorem gives an upper bound of  $\mathbb{E}[G]$  by the covering number of  $\mathcal{G}$ .

212 **Theorem C.7** Under the same conditions as in Theorem C.6, if for any  $\eta \in (0, B)$ , there exists  
 213  $A > 0, \nu > 0$  such that for any probability measure  $Q$  on  $\mathcal{Z}$ , the covering number

$$\mathcal{N}(\mathcal{G}, L_2(Q), \eta) \leq \left( \frac{AB}{\eta} \right)^\nu,$$

214 then there exists a constant  $C$  such that

$$\mathbb{E}[G] \leq C \left( \frac{\nu B}{n} \log \left( \frac{AB}{\sigma} \right) + \sqrt{\frac{\nu \sigma^2}{n} \log \left( \frac{AB}{\sigma} \right)} \right).$$

215 **Tail bound by polynomial discrimination.** As an alternative to the Talagrand's inequality, the  
 216 following theorem bounds  $G$  with high probability when the function class  $\mathcal{G}$  has *polynomial*  
 217 *discrimination*. The proof applies the Bernstein's inequality and a straightforward union bound  
 218 argument.

219 **Theorem C.8** Under the same conditions as in Theorem C.6, define

$$\mathcal{G}(\mathbf{Z}_1^n) = \{(g(Z_1), g(Z_2), \dots, g(Z_n)) : g \in \mathcal{G}\}. \quad (3)$$

220 If the cardinality of the set  $\mathcal{G}(\mathbf{Z}_1^n)$  is bounded by

$$\text{Card}(\mathcal{G}(\mathbf{Z}_1^n)) \leq (An + 1)^\nu \quad (4)$$

221 for some  $\nu > 0$ , then there exists a universal constant  $C$  such that with probability at least  $1 - \delta$ ,

$$G \leq C \left( \sqrt{\frac{\sigma^2}{n}} \left( \sqrt{\nu \log(An + 1)} + \sqrt{\log \frac{1}{\delta}} \right) + \frac{B}{n} \left( \nu \log(An + 1) + \log \frac{1}{\delta} \right) \right) \quad (5)$$

222 The following lemma shows that for persistent measures with bounded total persistence, the total  
 223 mass of the set away from the diagonal  $\partial\Omega$  is upper bounded.

224 **Lemma C.9** Let  $\Omega_\ell$  denote the set of points in  $\Omega$  that are at least  $\ell$  away from the diagonal:

$$\Omega_\ell = \{\boldsymbol{\omega} \in \Omega : \|\boldsymbol{\omega} - \partial\Omega\|_2 \geq \ell\}.$$

225 Then for a persistent measure  $\mu$ , if  $\text{Pers}_q(\mu) \leq M$ , then  $\mu(\Omega_\ell) \leq M\ell^{-q}$ .

226 The following theorem shown in [DL21] provides a standard lower bound for the minimax rate of  
 227 estimating a probability density function using independent samples. This is useful for deducing the  
 228 minimax rate for estimating the (weighted) intensity functions.

229 **Theorem C.10** Let  $\mathcal{F}$  denote the set of probability density functions on  $[0, 1]^2$  with Bounded Besov  
 230 norm:

$$\mathcal{F} = \{f : [0, 1]^2 \rightarrow \mathbb{R}, \int_{[0, 1]^2} f(x) dx = 1, \|f\|_{\infty, \infty}^r \leq B\}.$$

231 Then for any estimator (measurable function)

$$\hat{f}_n : ([0, 1]^2)^n \rightarrow \mathcal{F},$$

232 there exists  $f \in \mathcal{F}$ , such that if  $X_1, X_2, \dots, X_n \sim \text{i.i.d. } f$ , then

$$\mathbb{E} \|\hat{f}_n(X_1, X_2, \dots, X_n) - f\|_\infty \geq O(n^{-\frac{r}{2r+2}}).$$

## 233 D Proof of theorems and supportive propositions

### 234 D.1 Proof of Theorem 3.1

235 In order to prove Theorem 3.1, we firstly show the following supportive lemma.

236 **Lemma D.1** Let  $\Omega$  and  $\partial\Omega$  be defined as in (1) and (2). Then for any  $q > 0$ ,

$$\int_{\Omega} \|\mathbf{x} - \partial\Omega\|_2^q d\mathbf{x} = \frac{2}{(q+1)(q+2)} \left(\frac{L}{\sqrt{2}}\right)^{q+2}.$$

237 *Proof of Lemma D.1:* Take the coordinate transformation

$$\begin{cases} y_1 = \frac{x_2 - x_1}{\sqrt{2}} = \|\mathbf{x} - \partial\Omega\|_2; \\ y_2 = \frac{x_2 + x_1}{\sqrt{2}}. \end{cases}$$

238 Then it can be easily verified that the determinant of the Jacobian matrix between  $\mathbf{x}$  and  $\mathbf{y}$  coordinates  
239 is 1, and that the  $\ell_1$  ball  $\Omega$  can be represented using  $\mathbf{y}$  coordinates by

$$\Omega = \{(y_1, y_2) : 0 < y_1 \leq \frac{L}{\sqrt{2}}, y_1 \leq y_2 \leq \sqrt{2}L - y_1\}.$$

240 Therefore,

$$\begin{aligned} \int_{\Omega} \|\mathbf{x} - \partial\Omega\|_2^q d\mathbf{x} &= \int_0^{\frac{L}{\sqrt{2}}} \left( \int_{y_1}^{\sqrt{2}L - y_1} dy_2 \right) y_1^q dy_1 \\ &= \int_0^{\frac{L}{\sqrt{2}}} (\sqrt{2}L - 2y_1) y_1^q dy_1 \\ &= \frac{2}{(q+1)(q+2)} \left(\frac{L}{\sqrt{2}}\right)^{q+2}. \end{aligned}$$

241 With this lemma, we can now prove Theorem 3.1.

242 *Proof of Theorem 3.1:* The main idea of bounding the OT distance is to construct an admissible  
243 transport between  $\mu$  and  $\nu$ , and then control the cost of this transport. We will separate the proof into  
244 three steps accordingly.

245 **Step 1: Construct an admissible transport from  $\mu$  to  $\nu$ .** Define  $\hat{\pi}$  as a measure on  $\bar{\Omega} \times \bar{\Omega}$  such  
246 that for any Borel sets  $A, B \subset \bar{\Omega}$ ,

$$\begin{aligned} \hat{\pi}(A \times B) &= \int_{A \cap B \cap \Omega} \min\{p_{\mu}(\mathbf{x}), p_{\nu}(\mathbf{x})\} d\mathbf{x} + \\ &\quad \int_{A \cap \text{Proj}_{\partial\Omega}^{-1}(B) \cap \Omega} [p_{\mu}(\mathbf{x}) - p_{\nu}(\mathbf{x})]^+ d\mathbf{x} + \int_{B \cap \text{Proj}_{\partial\Omega}^{-1}(A) \cap \Omega} [p_{\nu}(\mathbf{x}) - p_{\mu}(\mathbf{x})]^+ d\mathbf{x}. \end{aligned} \quad (6)$$

247 Here, for any set  $A \subset \bar{\Omega}$ ,

$$\text{Proj}_{\partial\Omega}^{-1}(A) = \{\omega \in \Omega : \text{Proj}_{\partial\Omega}(\omega) \in A\}.$$

248 Intuitively,  $\hat{\pi}$  represents such a transport: at each point  $\mathbf{x} \in \Omega$ , if  $p_{\mu}(\mathbf{x}) > p_{\nu}(\mathbf{x})$ , then we transport the  
249 mass of  $p_{\nu}$  from  $\mathbf{x}$  to  $\mathbf{x}$ , and the remaining mass from  $\mathbf{x}$  to its projection onto  $\partial\Omega$ ; if  $p_{\nu}(\mathbf{x}) > p_{\mu}(\mathbf{x})$ ,  
250 then the opposite is done.

251 Firstly, we prove that this is an admissible transport between  $\mu$  and  $\nu$ . Notice that for any Borel set  
252  $A \subset \Omega$ ,  $A \cap \bar{\Omega} \cap \Omega = A$ ,  $A \cap \text{Proj}_{\partial\Omega}^{-1}(\bar{\Omega}) \cap \Omega = A$  and  $\text{Proj}_{\partial\Omega}^{-1}(A) = \emptyset$ . Therefore, by taking  $B = \bar{\Omega}$   
253 in (6), we get

$$\begin{aligned} \hat{\pi}(A \times \bar{\Omega}) &= \int_A \min\{p_{\mu}(\mathbf{x}), p_{\nu}(\mathbf{x})\} d\mathbf{x} + \int_A [p_{\mu}(\mathbf{x}) - p_{\nu}(\mathbf{x})]^+ d\mathbf{x} + 0 \\ &= \int_A \{\min\{p_{\mu}(\mathbf{x}), p_{\nu}(\mathbf{x})\} + [p_{\mu}(\mathbf{x}) - p_{\nu}(\mathbf{x})]^+\} d\mathbf{x} \\ &= \int_A p_{\mu}(\mathbf{x}) d\mathbf{x} = \mu(A). \end{aligned}$$

254 Similarly, we can prove that  $\hat{\pi}(\bar{\Omega} \times B) = \nu(B)$  for any Borel set  $B \subset \Omega$ . Therefore,  $\hat{\pi}$  is an  
255 admissible transport between  $\mu$  and  $\nu$ .

256 **Step 2: Present  $d\hat{\pi}$ .** In order to calculate the transport cost of  $\hat{\pi}$ , we firstly need to present  $d\hat{\pi}$ . For  
 257 this, we would make use of *pushforward measures*. Define  $\iota : \bar{\Omega} \rightarrow \bar{\Omega} \times \bar{\Omega}$  by  $\iota(\mathbf{x}) = (\mathbf{x}, \mathbf{x})$ , and  
 258 let  $j : \bar{\Omega} \times \bar{\Omega} \rightarrow \bar{\Omega}$  be satisfying  $j \circ \iota = id$ . Furthermore, let  $\iota_*(\lambda_\Omega)$  be the pushforward measure on  
 259  $\bar{\Omega} \times \bar{\Omega}$  generated by  $\iota$ . Then for any Borel sets  $A, B \subset \bar{\Omega}$ , one has  $\iota^{-1}(A \times B) = A \cap B$ , and the  
 260 first term in (6) can be presented as

$$\begin{aligned} & \int_{A \cap B \cap \Omega} \min \{p_\mu(\mathbf{x}), p_\nu(\mathbf{x})\} d\mathbf{x} \\ &= \int_{\iota^{-1}(A \times B)} \min \{(p_\mu \circ j)(\iota(\mathbf{x})), (p_\nu \circ j)(\iota(\mathbf{x}))\} d\lambda_\Omega(\mathbf{x}) \\ &= \int_{A \times B} \min \{(p_\mu \circ j)(\mathbf{x}, \mathbf{y}), (p_\nu \circ j)(\mathbf{x}, \mathbf{y})\} d\iota_*(\lambda_\Omega)(\mathbf{x}, \mathbf{y}). \end{aligned}$$

261 For the second term in (6), we can similarly, define  $\iota^{(1)} : \bar{\Omega} \rightarrow \bar{\Omega} \times \bar{\Omega}$  by  $\iota^{(1)}(\mathbf{x}) = (\mathbf{x}, \text{Proj}_{\partial\Omega}(\mathbf{x}))$ ,  
 262 let  $j^{(1)} : \bar{\Omega} \times \bar{\Omega} \rightarrow \bar{\Omega}$  be satisfying  $j^{(1)} \circ \iota^{(1)} = id$ , and consider the pushforward measure  $\iota_*^{(1)}(\lambda_\Omega)$ .  
 263 Then  $(\iota^{(1)})^{-1}(A \times B) = A \cap \text{Proj}_{\partial\Omega}^{-1}(B)$ , and

$$\begin{aligned} & \int_{A \cap \text{Proj}_{\partial\Omega}^{-1}(B) \cap \Omega} [p_\mu(\mathbf{x}) - p_\nu(\mathbf{x})]^+ d\mathbf{x} \\ &= \int_{(\iota^{(1)})^{-1}(A \times B)} \left[ (p_\mu \circ j^{(1)})(\iota^{(1)}(\mathbf{x})) - (p_\nu \circ j^{(1)})(\iota^{(1)}(\mathbf{x})) \right]^+ d\lambda_\Omega(\mathbf{x}) \\ &= \int_{A \times B} \left[ (p_\mu \circ j^{(1)})(\mathbf{x}, \mathbf{y}) - (p_\nu \circ j^{(1)})(\mathbf{x}, \mathbf{y}) \right]^+ d\iota_*^{(1)}(\lambda_\Omega)(\mathbf{x}, \mathbf{y}). \end{aligned}$$

264 For the third term in (6), we can similarly define  $\iota^{(2)} : \bar{\Omega} \rightarrow \bar{\Omega} \times \bar{\Omega}$  by  $\iota^{(2)}(\mathbf{x}) = (\text{Proj}_{\partial\Omega}(\mathbf{x}), \mathbf{x})$ , let  
 265  $j^{(2)} : \bar{\Omega} \times \bar{\Omega} \rightarrow \bar{\Omega}$  be satisfying  $j^{(2)} \circ \iota^{(2)} = id$ , and consider a pushforward measure  $\iota_*^{(2)}(\lambda_\Omega)$ . Then  
 266  $(\iota^{(2)})^{-1}(A \times B) = \text{Proj}_{\partial\Omega}^{-1}(A) \cap B$ , and

$$\begin{aligned} & \int_{\text{Proj}_{\partial\Omega}^{-1}(A) \cap B \cap \Omega} [p_\mu(\mathbf{x}) - p_\nu(\mathbf{x})]^+ d\mathbf{x} \\ &= \int_{(\iota^{(2)})^{-1}(A \times B)} \left[ (p_\mu \circ j^{(2)})(\iota^{(2)}(\mathbf{x})) - (p_\nu \circ j^{(2)})(\iota^{(2)}(\mathbf{x})) \right]^+ d\lambda_\Omega(\mathbf{x}) \\ &= \int_{A \times B} \left[ (p_\mu \circ j^{(2)})(\mathbf{x}, \mathbf{y}) - (p_\nu \circ j^{(2)})(\mathbf{x}, \mathbf{y}) \right]^+ d\iota_*^{(2)}(\lambda_\Omega)(\mathbf{x}, \mathbf{y}). \end{aligned}$$

267 Combining these results, we can obtain the following presentation of  $d\hat{\pi}$ :

$$\begin{aligned} d\hat{\pi} &= \min \{(p_\mu \circ j)(\mathbf{x}, \mathbf{y}), (p_\nu \circ j)(\mathbf{x}, \mathbf{y})\} d\iota_*(\lambda_\Omega) \\ &\quad + \left[ (p_\mu \circ j^{(1)})(\mathbf{x}, \mathbf{y}) - (p_\nu \circ j^{(1)})(\mathbf{x}, \mathbf{y}) \right]^+ d\iota_*^{(1)}(\lambda_\Omega) \\ &\quad + \left[ (p_\mu \circ j^{(2)})(\mathbf{x}, \mathbf{y}) - (p_\nu \circ j^{(2)})(\mathbf{x}, \mathbf{y}) \right]^+ d\iota_*^{(2)}(\lambda_\Omega). \end{aligned}$$

268 **Step 3: Calculate the transportation cost of  $\hat{\pi}$ .** Based on our presentation of  $d\hat{\pi}$ , the  $q$ -th order  
 269 transportation cost of  $\hat{\pi}$  is, by definition:

$$\begin{aligned} C_q^q(\hat{\pi}) &= \int_{\bar{\Omega} \times \bar{\Omega}} \|\mathbf{x} - \mathbf{y}\|_2^q d\hat{\pi}(\mathbf{x}, \mathbf{y}) \\ &= \int_{\bar{\Omega} \times \bar{\Omega}} \|\mathbf{x} - \mathbf{y}\|_2^q \min \{(p_\nu \circ j)(\mathbf{x}, \mathbf{y}), (p_\mu \circ j)(\mathbf{x}, \mathbf{y})\} d\iota_*(\lambda_\Omega) \\ &\quad + \int_{\bar{\Omega} \times \bar{\Omega}} \|\mathbf{x} - \mathbf{y}\|_2^q \left[ (p_\mu \circ j^{(1)})(\mathbf{x}, \mathbf{y}) - (p_\nu \circ j^{(1)})(\mathbf{x}, \mathbf{y}) \right]^+ d\iota_*^{(1)}(\lambda_\Omega) \\ &\quad + \int_{\bar{\Omega} \times \bar{\Omega}} \|\mathbf{x} - \mathbf{y}\|_2^q \left[ (p_\mu \circ j^{(2)})(\mathbf{x}, \mathbf{y}) - (p_\nu \circ j^{(2)})(\mathbf{x}, \mathbf{y}) \right]^+ d\iota_*^{(2)}(\lambda_\Omega). \end{aligned} \quad (7)$$

270 We now explore the three terms in (7). First of all, since  $\iota_*(\lambda_\Omega)$  is a pushforward measure generated  
 271 by the function  $\iota(\mathbf{x}) = (\mathbf{x}, \mathbf{x})$ , it is easy to see that

$$\iota_*(\lambda_\Omega)(\{(\mathbf{x}, \mathbf{y}) \in \Omega \times \Omega : \mathbf{x} \neq \mathbf{y}\}) = 0.$$

272 Therefore, the first term in (7) is simply

$$\begin{aligned} & \int_{\overline{\Omega} \times \overline{\Omega}} \|\mathbf{x} - \mathbf{y}\|_2^q \min \{(p_\nu \circ j)(\mathbf{x}, \mathbf{y}), (p_\mu \circ j)(\mathbf{x}, \mathbf{y})\} d\iota_*(\lambda_\Omega) \\ &= \int_{(\mathbf{x}, \mathbf{y}) \in \overline{\Omega} \times \overline{\Omega}, \mathbf{x} = \mathbf{y}} \|\mathbf{x} - \mathbf{y}\|_2^q \min \{(p_\nu \circ j)(\mathbf{x}, \mathbf{y}), (p_\mu \circ j)(\mathbf{x}, \mathbf{y})\} d\iota_*(\lambda_\Omega) \\ &= \int_{\mathbf{x} \in \overline{\Omega}} \|\mathbf{x} - \mathbf{x}\|_2^q \min \{p_\mu(\mathbf{x}), p_\nu(\mathbf{x})\} d\mathbf{x} = 0. \end{aligned}$$

273 As for the second term, notice that  $\iota_*^{(1)}(\lambda_\Omega)$  is a pushforward measure generated by the function  
 274  $\iota^{(1)}(\mathbf{x}) = (\mathbf{x}, \text{Proj}_{\partial\Omega}(\mathbf{x}))$ . Therefore by definition,

$$\iota_*^{(1)}(\lambda_\Omega)(\{(\mathbf{x}, \mathbf{y}) \in \Omega \times \Omega : \mathbf{y} \neq \text{Proj}_{\partial\Omega}(\mathbf{x})\}) = 0.$$

275 Hence, the second term in (7) is equal to

$$\begin{aligned} & \int_{\overline{\Omega} \times \overline{\Omega}} \|\mathbf{x} - \mathbf{y}\|_2^q \left[ (p_\mu \circ j^{(1)})(\mathbf{x}, \mathbf{y}) - (p_\nu \circ j^{(1)})(\mathbf{x}, \mathbf{y}) \right]^+ d\iota_*^{(1)}(\lambda_\Omega) \\ &= \int_{(\mathbf{x}, \mathbf{y}) \in \overline{\Omega} \times \overline{\Omega}, \mathbf{y} = \text{Proj}_{\partial\Omega}(\mathbf{x})} \|\mathbf{x} - \mathbf{y}\|_2^q \\ & \quad \times \left[ (p_\mu \circ j^{(1)})(\mathbf{x}, \text{Proj}_{\partial\Omega}(\mathbf{x})) - (p_\nu \circ j^{(1)})(\mathbf{x}, \text{Proj}_{\partial\Omega}(\mathbf{x})) \right]^+ d\iota_*^{(1)}(\lambda_\Omega) \\ &= \int_{\mathbf{x} \in \overline{\Omega}} \|\mathbf{x} - \text{Proj}_{\partial\Omega}(\mathbf{x})\|_2^q \left[ (p_\mu \circ j^{(1)} \circ \iota^{(1)})(\mathbf{x}) - (p_\nu \circ j^{(1)} \circ \iota^{(1)})(\mathbf{x}) \right] d\mathbf{x} \\ &= \int_{\Omega} \|\mathbf{x} - \partial\Omega\|_2^q [p_\mu(\mathbf{x}) - p_\nu(\mathbf{x})]^+ d\mathbf{x}. \end{aligned}$$

276 Similarly, we can obtain that the third term of (7) is equal to

$$\begin{aligned} & \int_{\overline{\Omega} \times \overline{\Omega}} \|\mathbf{x} - \mathbf{y}\|_2^q \left[ (p_\mu \circ j^{(2)})(\mathbf{x}, \mathbf{y}) - (p_\nu \circ j^{(2)})(\mathbf{x}, \mathbf{y}) \right]^+ d\iota_*^{(2)}(\lambda_\Omega) \\ &= \int_{\Omega} [p_\nu(\mathbf{x}) - p_\mu(\mathbf{x})]^+ \|\mathbf{x} - \partial\Omega\|_2^q d\mathbf{x}. \end{aligned}$$

277 Combining these results, we obtain

$$\begin{aligned} C_q^q(\hat{\pi}) &= \int_{\Omega} [p_\mu(\mathbf{x}) - p_\nu(\mathbf{x})]^+ \|\mathbf{x} - \partial\Omega\|_2^q d\mathbf{x} + \int_{\Omega} [p_\nu(\mathbf{x}) - p_\mu(\mathbf{x})]^+ \|\mathbf{x} - \partial\Omega\|_2^q d\mathbf{x} \\ &= \int_{\Omega} |p_\mu(\mathbf{x}) - p_\nu(\mathbf{x})| \|\mathbf{x} - \partial\Omega\|_2^q d\mathbf{x} \\ &\leq \|p_\mu - p_\nu\|_\infty \int_{\Omega} \|\mathbf{x} - \partial\Omega\|_2^q d\mathbf{x} = \frac{2}{(q+1)(q+2)} \left( \frac{L}{\sqrt{2}} \right)^{q+2} \|p_\mu - p_\nu\|_\infty. \end{aligned}$$

278 Notice that the last equality uses Lemma D.1.

279 Finally, since  $\hat{\pi}$  is an admissible transport from  $\mu$  to  $\nu$ , the optimal transport distance between  $\mu$  and  
 280  $\nu$ ,  $\text{OT}_q(\mu, \nu)$ , should be at most  $C_q(\hat{\pi})$ . The bound (7) follows naturally.

281 **Example of converging OT distance while intensity functions diverge.** Consider the following  
 282 sequences of intensity functions

$$\begin{aligned} p_{\mu_n} &= \frac{4^n}{L^2} \mathbb{1} \left\{ \|\mathbf{x} - \mathbf{u}_n\|_1 < \frac{\sqrt{2}L}{2^{n+1}} \right\} \\ p_{\nu_n} &= \frac{4^n}{L^2} \mathbb{1} \left\{ \|\mathbf{x} - \mathbf{d}_n\|_1 < \frac{\sqrt{2}L}{2^{n+1}} \right\}, \end{aligned}$$

283 in which

$$\mathbf{u}_n = \left( \frac{\sqrt{2}L}{4}, \frac{\sqrt{2}L}{4} + \frac{\sqrt{2}L}{2^{n+1}} \right)$$

$$\mathbf{d}_n = \left( \frac{\sqrt{2}L}{4} - \frac{\sqrt{2}L}{2^{n+1}}, \frac{\sqrt{2}L}{4} \right).$$

284 Essentially,  $\mu_n$  and  $\nu_n$  are uniform distributions on two adjacent  $\ell_1$  balls. It is easy to verify that the  
 285 total mass of both  $\mu_n$  and  $\nu_n$  is 1, and the optimal transport distance between  $\mu_n$  and  $\nu_n$  is upper  
 286 bounded by

$$\text{OT}_q(\mu_n, \nu_n) \leq \frac{L}{2^n} \rightarrow 0;$$

287 on the other hand, the  $\ell_\infty$  distance between the intensity functions clearly diverges as  $n \rightarrow \infty$ :

$$\|p_{\mu_n} - p_{\nu_n}\|_\infty \geq |p_{\mu_n}(\mathbf{u}_n) - p_{\nu_n}(\mathbf{u}_n)| = \frac{4^n}{L^2} \rightarrow \infty.$$

288 ■

289 *A remark on the bottleneck distance.* We argue that there can be no meaningful upper bound for the  
 290 bottleneck distance  $\text{OT}_\infty$  by the  $\ell_\infty$  distance between the intensity or density functions. Consider  
 291 the following example: define  $T_h$  as an upper-left triangle in  $\Omega$ :

$$T_h := \{\boldsymbol{\omega} \in \Omega \mid \|\boldsymbol{\omega} - \partial\Omega\|_2 \geq \frac{L-h}{\sqrt{2}}\},$$

292 and  $T'_h$  as a triangle tangent to the diagonal:

$$T'_h := \left\{ \boldsymbol{\omega} \in \Omega \mid \left\| \boldsymbol{\omega} - \left( \frac{L}{2}, \frac{L}{2} \right) \right\|_\infty \leq \frac{h}{2} \right\}.$$

293 We define  $\mu_h$  as the uniform distribution on  $T_h$ , so that

$$p_{\mu_h}(\boldsymbol{\omega}) = \frac{2}{h^2} \mathbb{1}\{\boldsymbol{\omega} \in T_h\};$$

294 on the other hand  $\nu$  is very similar to  $\mu$  but has a small part of its mass on  $T'_h$ :

$$p_{\nu_h}(\boldsymbol{\omega}) = \left( \frac{2}{h^2} - h \right) \mathbb{1}\{\boldsymbol{\omega} \in T_h\} + h \mathbb{1}\{\boldsymbol{\omega} \in T'_h\}.$$

295 As  $h \rightarrow 0$ , it is easy to verify that  $\|p_{\mu_h} - p_{\nu_h}\|_\infty = h \rightarrow 0$ , while  $\text{OT}(\mu_h, \nu_h) \rightarrow L/\sqrt{2}$ . This is  
 296 because although the densities for  $\mu$  and  $\nu$  becomes very close, there is always a small part of the  
 297 mass of  $\mu$  in  $T_h$  that has to be transported to  $T'_h$ ; since the bottleneck distance only considers the  
 298 *maximum* transport cost, it would converge to the limiting distance between  $T_h$  and  $T'_h$ , which is  
 299  $L/\sqrt{2}$ . It is easy to generalize this example to the case where  $p_{\mu_h}$  and  $p_{\nu_h}$  are smooth.

## 300 **D.2 Proof of Theorem 3.5**

301 Both theorems are classic results on the bias of kernel estimators and are proved by the smoothness  
 302 of the target functions as supposed by Assumption 3.2. We here provides the proof of Theorem 3.5  
 303 (a), and part (b) can be proved in a completely similar fashion.

304 We firstly clarify the specific smoothness condition proposed by Assumption 3.2. It guarantees Hence,  
 305 we can represent the bias of  $\mathbb{E}[\hat{p}_h(\boldsymbol{\omega})]$  as an integral. Since  $\bar{\mu}_n$  is an unbiased estimator for  $\mathbb{E}[\mu]$ ,

$$\begin{aligned} \mathbb{E}[\hat{p}_h(\boldsymbol{\omega})] - p(\boldsymbol{\omega}) &= \mathbb{E} \left[ \int_{\mathbf{x}} \frac{1}{h^2} K \left( \frac{\mathbf{x} - \boldsymbol{\omega}}{h} \right) d\bar{\mu}_n \right] - p(\boldsymbol{\omega}) \\ &= \int_{\mathbf{x}} \frac{1}{h^2} K \left( \frac{\mathbf{x} - \boldsymbol{\omega}}{h} \right) d\mathbb{E}[\bar{\mu}_n] - p(\boldsymbol{\omega}) \\ &= \int_{\mathbf{x}} \frac{1}{h^2} K \left( \frac{\mathbf{x} - \boldsymbol{\omega}}{h} \right) p(\mathbf{x}) d\mathbf{x} - p(\boldsymbol{\omega}) \\ &= \int_{\mathbf{x}} \frac{1}{h^2} K \left( \frac{\mathbf{x} - \boldsymbol{\omega}}{h} \right) [p(\mathbf{x}) - p(\boldsymbol{\omega})] d\mathbf{x}, \end{aligned}$$

306 where in the last line we applied the property that the kernel function  $K(\cdot)$  integrals to 1. We can  
 307 then apply the smoothness of  $p(\cdot)$  as in (1) and obtain that

$$\begin{aligned} & |\mathbb{E}[\hat{p}_h(\boldsymbol{\omega})] - p(\boldsymbol{\omega})| \\ & \leq \left| \int_{\mathbf{x}} \frac{1}{h^2} K\left(\frac{\mathbf{x} - \boldsymbol{\omega}}{h}\right) \sum_{t=1}^{s-1} \frac{1}{t!} \sum_{t_1+t_2=t} \frac{d^t p(\boldsymbol{\omega})}{d\omega_1^{t_1} d\omega_2^{t_2}} (x_1 - \omega_1)^{t_1} (x_2 - \omega_2)^{t_2} d\mathbf{x} \right| \\ & \quad + \int_{\mathbf{x}} \frac{1}{h^2} \left| K\left(\frac{\mathbf{x} - \boldsymbol{\omega}}{h}\right) \right| L_p \|\mathbf{x} - \boldsymbol{\omega}\|_2^s d\mathbf{x} \end{aligned}$$

308 By taking a change of variable  $\mathbf{v} = \frac{\mathbf{x} - \boldsymbol{\omega}}{h}$ , the first term can be represented as

$$\sum_{t=1}^{s-1} \frac{1}{t!} \sum_{t_1+t_2=t} \frac{d^t p(\boldsymbol{\omega})}{d\omega_1^{t_1} d\omega_2^{t_2}} \int_{\|\mathbf{v}\|_2 \leq 1} K(\mathbf{v}) h^t v_1^{t_1} v_2^{t_2} d\mathbf{v}.$$

309 The zero-moment condition of the kernel function in Assumption B.3 guarantees that this term equals  
 310 to 0. Hence,

$$\begin{aligned} |\mathbb{E}[\hat{p}_h(\boldsymbol{\omega})] - p(\boldsymbol{\omega})| & \leq \int_{\mathbf{x}} \frac{1}{h^2} \left| K\left(\frac{\mathbf{x} - \boldsymbol{\omega}}{h}\right) \right| L_p \|\mathbf{x} - \boldsymbol{\omega}\|_2^s d\mathbf{x} \\ & \quad \stackrel{\mathbf{v}=(\mathbf{x}-\boldsymbol{\omega})/h}{=} L_p h^s \int_{\|\mathbf{v}\|_2 \leq 1} |K(\mathbf{v})| \|\mathbf{v}\|_2^s d\mathbf{v}. \end{aligned}$$

### 311 D.3 Proof of Theorem 3.6 (a)

312 **A useful claim.** The following claim can be applied for easing calculation in Theorem 3.6.

313 **Claim D.2** For  $q \in \mathbb{R}$  and  $x \in [0, 1]$ ,

$$1 - x^q \leq (q \vee 1)(1 - x),$$

314 where  $q \vee 1 = \max\{q, 1\}$ .

315 **Proof of Claim D.2.** If  $q \geq 1$  or  $q \leq 0$ , let  $f(x) = 1 - x^q$ . Then  $f'(x) = -qx^{q-1}$  and  
 316  $f''(x) = -q(q-1)x^{q-2}$ , so  $f''(x) \leq 0$  for  $x \in [0, 1]$  and  $f$  is concave on  $[0, 1]$ . Then by Jensen's  
 317 inequality,

$$1 - x^q = f(x) \leq f(1) + f'(1)(x - 1) = q(1 - x).$$

318 If  $q \in [0, 1]$ , then  $x^q \geq x$  implies

$$1 - x^q \leq 1 - x.$$

319 Hence combining these gives

$$1 - x^q \leq (q \vee 1)(1 - x).$$

320 ■

321 This proof applies the Talagrand's inequality. For this purpose, we firstly define an auxiliary family  
 322 of functions, and then verify the conditions in Theorems C.6 and C.7 .

323 **Defining an auxiliary function class.** Let  $\mu_1, \mu_2, \dots, \mu_n$  be i.i.d. random measures in  $\mathcal{Z}_{L,M}^q$ ,  
 324  $\ell_{\boldsymbol{\omega}} = \|\boldsymbol{\omega} - \partial\Omega\|_2 - h$  and  $g_{\boldsymbol{\omega}}$  be defined as

$$g_{\boldsymbol{\omega}}(\mu) = \ell_{\boldsymbol{\omega}}^q \left( \int_{\Omega} \frac{1}{h^2} K\left(\frac{\mathbf{x} - \boldsymbol{\omega}}{h}\right) d\mu - \int_{\Omega} \frac{1}{h^2} K\left(\frac{\mathbf{x} - \boldsymbol{\omega}}{h}\right) d\mathbb{E}[\mu] \right), \quad (8)$$

325 and  $K$  satisfy Assumption B.3. Take  $\mathcal{Z} = \mathcal{Z}_{L,M}^q$ ,  $(T, d) = (\Omega_{2h}, \|\cdot\|_2)$ , and for all  $\mu \in \mathcal{Z}_{L,M}^q$ ,  
 326 define  $\mathcal{G} = \{g_{\boldsymbol{\omega}} : \boldsymbol{\omega} \in \Omega_{2h}\}$ . By definition,  $g_{\boldsymbol{\omega}}(\mu)$  has zero mean and the variation of the kernel  
 327 estimator  $\hat{p}_h(\cdot)$  can be represented by

$$\sup_{\boldsymbol{\omega} \in \Omega_{2h}} \ell_{\boldsymbol{\omega}}^q |\hat{p}_h(\boldsymbol{\omega}) - \mathbb{E}[\hat{p}_h(\boldsymbol{\omega})]| = \sup_{\boldsymbol{\omega} \in \Omega_{2h}} \left| \frac{1}{n} \sum_{i=1}^n g_{\boldsymbol{\omega}}(\mu_i) \right|.$$

328 Hence, in order to apply the Talagrand's inequality, we need to bound  $\|g_{\boldsymbol{\omega}}(\mu)\|_{\infty}$ ,  $\mathbb{E}[g_{\boldsymbol{\omega}}(\mu)^2]$  and the  
 329 covering number of  $\mathcal{G}$ . We provide these upper bound accordingly in the following paragraphs.

330 **Bounding**  $\|g_\omega(\mu)\|_\infty$  **and**  $\mathbb{E}[g_\omega(\mu)^2]$ . Notice that since  $K$  vanishes outside the unit circle of  $\mathbb{R}^2$ ,  
 331 for any  $\mathbf{x} \notin \Omega_{\ell_\omega}$ , we have  $\|\frac{\mathbf{x}-\omega}{h}\|_2 > 1$  and therefore  $K\left(\frac{\mathbf{x}-\omega}{h}\right) = 0$ . Hence, for all  $\omega \in \Omega_{2h}$ ,

$$\begin{aligned}
 |g_\omega(\mu)| &= \ell_\omega^q \left| \int_\Omega \frac{1}{h^2} K\left(\frac{\mathbf{x}-\omega}{h}\right) d\mu - \int_\Omega \frac{1}{h^2} K\left(\frac{\mathbf{x}-\omega}{h}\right) d\mathbb{E}[\mu] \right| \\
 &\leq \ell_\omega^q \max \left\{ \left| \int_\Omega \frac{1}{h^2} K\left(\frac{\mathbf{x}-\omega}{h}\right) d\mu \right|, \left| \int_\Omega \frac{1}{h^2} K\left(\frac{\mathbf{x}-\omega}{h}\right) d\mathbb{E}[\mu] \right| \right\} \\
 &= \ell_\omega^q \max \left\{ \left| \int_{\Omega_{\ell_\omega}} \frac{1}{h^2} K\left(\frac{\mathbf{x}-\omega}{h}\right) d\mu \right|, \left| \int_{\Omega_{\ell_\omega}} \frac{1}{h^2} K\left(\frac{\mathbf{x}-\omega}{h}\right) d\mathbb{E}[\mu] \right| \right\} \\
 &\leq \ell_\omega^q \frac{\|K\|_\infty}{h^2} \max \{(\mu(\Omega_{\ell_\omega}), \mathbb{E}[\mu](\Omega_{\ell_\omega}))\} \\
 &\leq \ell_\omega^q \frac{\|K\|_\infty M}{h^2 \ell_\omega^q} = \frac{\|K\|_\infty M}{h^2}
 \end{aligned} \tag{9}$$

332 where in the last inequality we used Lemma C.9. On the other hand, the variance of  $g_\omega$  is bounded by

$$\begin{aligned}
 \mathbb{E}[g_\omega(\mu)^2] &= \ell_\omega^{2q} \mathbb{E} \left| \int \frac{1}{h^2} K\left(\frac{\mathbf{x}-\omega}{h}\right) d\mu - \int \frac{1}{h^2} K\left(\frac{\mathbf{x}-\omega}{h}\right) d\mathbb{E}[\mu] \right|^2 \\
 &\leq \ell_\omega^{2q} \mathbb{E} \left| \int_{\Omega_{\ell_\omega}} \frac{1}{h^2} K\left(\frac{\mathbf{x}-\omega}{h}\right) d\mu \right|^2 \\
 &\leq \ell_\omega^{2q} \mathbb{E} \left\{ \mu(\Omega_{\ell_\omega}) \cdot \int_{\Omega_{\ell_\omega}} \frac{1}{h^4} K^2\left(\frac{\mathbf{x}-\omega}{h}\right) d\mu \right\} \\
 &= \ell_\omega^{2q} \mu(\Omega_{\ell_\omega}) \int_{\Omega_{\ell_\omega}} \frac{1}{h^4} K^2\left(\frac{\mathbf{x}-\omega}{h}\right) d\mathbb{E}[\mu]
 \end{aligned} \tag{10}$$

$$\begin{aligned}
 &\leq \ell_\omega^{2q} \cdot \frac{M}{\ell_\omega^q} \int_{\|\mathbf{x}-\omega\|_2 \leq h} \frac{1}{h^4} K^2\left(\frac{\mathbf{x}-\omega}{h}\right) p(\mathbf{x}) d\mathbf{x} \\
 &\stackrel{\mathbf{v}=(\mathbf{x}-\omega)/h}{=} \ell_\omega^q M \int_{\|\mathbf{v}\|_2 \leq 1} \frac{1}{h^2} K^2(\mathbf{v}) p(\omega + \mathbf{v}h) d\mathbf{v} \\
 &\leq \ell_\omega^q M \frac{1}{h^2} \frac{\|\bar{p}\|_\infty}{\ell_\omega^q} \int_{\|\mathbf{v}\|_2 \leq 1} K^2(\mathbf{v}) d\mathbf{v} = \frac{M \|\bar{p}\|_\infty \|K\|_2^2}{h^2}.
 \end{aligned} \tag{11}$$

333 **Bounding the covering number of  $\mathcal{G}$ .** For any probability measure  $Q$  on  $\mathcal{Z}_{L,M}^q$  and any  $\eta \in$   
 334  $(0, \frac{\|K\|_\infty M}{h^2})$ , we aim to bound the covering number of  $\mathcal{G}$  with respect to  $L_2(Q)$  distance. This  
 335 requires relating the  $L_2(Q)$  distance in  $\mathcal{G}$  and the  $\ell_2$  distance in  $\mathbb{R}^2$ . Specifically, for any  $\omega, \omega' \in \Omega_{2h}$   
 336 and  $\mu \in \mathcal{Z}_{L,M}^q$ , we can assume without loss of generality that  $\ell_\omega \leq \ell_{\omega'}$ . In this case, we firstly  
 337 observe that

$$\begin{aligned}
 &\left| \ell_\omega^q \int K\left(\frac{\mathbf{x}-\omega}{h}\right) d\mu - \ell_{\omega'}^q \int K\left(\frac{\mathbf{x}-\omega'}{h}\right) d\mu \right| \\
 &\leq \left| \int \ell_\omega^q \left[ K\left(\frac{\mathbf{x}-\omega}{h}\right) - K\left(\frac{\mathbf{x}-\omega'}{h}\right) \right] d\mu \right| + \left| \int (\ell_\omega^q - \ell_{\omega'}^q) K\left(\frac{\mathbf{x}-\omega'}{h}\right) d\mu \right| \\
 &\leq \ell_\omega^q \int_{\Omega_{\ell_\omega}} \frac{L_k}{h} \|\omega - \omega'\|_2 d\mu + \int_{\Omega_{\ell_{\omega'}}} (\ell_{\omega'}^q - \ell_\omega^q) \|K\|_\infty d\mu \\
 &\leq \ell_\omega^q \frac{L_k}{h} \|\omega - \omega'\|_2 \mu(\Omega_{\ell_\omega}) + \|K\|_\infty (\ell_{\omega'}^q - \ell_\omega^q) \mu(\Omega_{\ell_{\omega'}}) \\
 &\leq \frac{M L_k}{h} \|\omega - \omega'\|_2 + M \|K\|_\infty \left[ 1 - \left( \frac{\ell_\omega}{\ell_{\omega'}} \right)^q \right].
 \end{aligned} \tag{12}$$

338 Since  $\ell_\omega \geq \ell_{\omega'} - \|\omega - \omega'\|_2$ , the last term of (12) can be bounded by using Claim D.2 and  
 339  $\ell_\omega \geq \ell_{\omega'} - \|\omega - \omega'\|_2$  as

$$\begin{aligned} 1 - \left(\frac{\ell_\omega}{\ell_{\omega'}}\right)^q &\leq (q \vee 1) \left(1 - \frac{\ell_\omega}{\ell_{\omega'}}\right) \\ &\leq \frac{q \vee 1}{\ell_{\omega'}} \|\omega - \omega'\|_2 \\ &\leq \frac{q \vee 1}{h} \|\omega - \omega'\|_2. \end{aligned} \quad (13)$$

340 Notice that in the last line, we applied the fact that since  $\omega' \in \Omega_{2h}$ ,  $\ell_{\omega'} = \|\omega - \partial\Omega\|_2 - h \geq h$ .

341 From now on, we use  $q'$  to denote  $q \vee 1$  for simplicity. Equations (12) and (13) imply that

$$\left| \ell_\omega^q \int K\left(\frac{\mathbf{x} - \omega}{h}\right) d\mu - \ell_{\omega'}^q \int K\left(\frac{\mathbf{x} - \omega'}{h}\right) d\mu \right| \leq \frac{M(L_K + q' \|K\|_\infty)}{h} \|\omega - \omega'\|_2.$$

342 Therefore, the difference between  $g_\omega(\mu)$  and  $g_{\omega'}(\mu)$  can be bounded by

$$\begin{aligned} |g_\omega(\mu) - g_{\omega'}(\mu)| &\leq \left| \ell_\omega^q \int \frac{1}{h^2} K\left(\frac{\mathbf{x} - \omega}{h}\right) d\mu - \ell_{\omega'}^q \int \frac{1}{h^2} K\left(\frac{\mathbf{x} - \omega'}{h}\right) d\mu \right| \\ &\quad + \left| \ell_\omega^q \int \frac{1}{h^2} K\left(\frac{\mathbf{x} - \omega}{h}\right) d\mathbb{E}[\mu] - \ell_{\omega'}^q \int \frac{1}{h^2} K\left(\frac{\mathbf{x} - \omega'}{h}\right) d\mathbb{E}[\mu] \right| \\ &\leq \frac{2M(L_K + q' \|K\|_\infty)}{h^3} \|\omega - \omega'\|_2. \end{aligned}$$

343 In this way, we have related the distance between  $g_\omega$  and  $g_{\omega'}$  to the distance between  $\omega$  and  $\omega'$ . Now,  
 344 for any  $\eta \in (0, \frac{\|K\|_\infty M}{h^2})$ , we can set  $\epsilon = \frac{\eta h^3}{2M(L_K + q' \|K\|_\infty)}$ . It is easy to verify that

$$\epsilon < \frac{h^3}{2M(L_K + q' \|K\|_\infty)} \frac{\|K\|_\infty M}{h^2} = \frac{\|K\|_\infty}{2(L_K + q' \|K\|_\infty)} h < h.$$

345 Hence, we can construct a  $\epsilon$ -covering of  $\Omega_{2h}$  in the  $\ell_2$  distance, denoted as  $S$ . It is easy to show that  
 346 the covering number

$$\mathcal{N}(\Omega_{2h}, \|\cdot\|_2, \epsilon) \leq \frac{2L^2}{\epsilon^2}.$$

347 By definition, for any  $\omega \in \Omega_{2h}$ , there exists  $\omega' \in S$ , such that  $\|\omega - \omega'\|_2 \leq \epsilon < h < \ell_{\omega'}$ . Therefore,  
 348 for any measure  $Q$  on  $\mathcal{Z}_{L,M}^q$ ,

$$\begin{aligned} \|g_\omega(\mu) - g_{\omega'}(\mu)\|_{L_2(Q)} &\leq \sup_{\mu \in \mathcal{Z}_{L,M}^q} |g_\omega(\mu) - g_{\omega'}(\mu)| \\ &\leq \frac{2M(L_K + q' \|K\|_\infty)}{h^3} \|\omega - \omega'\|_2 \leq \frac{2M(L_K + q' \|K\|_\infty)}{h^3} \epsilon = \eta. \end{aligned}$$

349 In conclusion,

$$\begin{aligned} \mathcal{N}(\mathcal{G}, L_2(Q), \eta) &\leq \mathcal{N}\left(\Omega_{2h}, \|\cdot\|_2, \frac{\eta h^3}{2M(L_K + q' \|K\|_\infty)}\right) \\ &< \left(\frac{4LM(L_K + q' \|K\|_\infty)}{\eta h^3}\right)^2. \end{aligned} \quad (14)$$

350 **Completing the proof.** With  $\|g_\omega(\mu)\|_\infty$ ,  $\mathbb{E}[g_\omega(\mu)^2]$  and the covering number of  $\mathcal{G}$  bounded as in  
 351 (9), (10) and (14), we can apply Theorems C.6 and C.7 with

$$\begin{cases} AB = \frac{4LM(L_K + q' \|K\|_\infty)}{h^3}; \\ B = \frac{\|K\|_\infty M}{h^2}; \\ \sigma^2 = \frac{M \|\bar{p}\|_\infty}{h^2} \|K\|_2^2; \\ \nu = 2. \end{cases}$$



352 This gives us the conclusion that with probability at least  $1 - \delta$ ,

$$\sup_{\omega \in \Omega_{2h}} \left| \frac{1}{n} \sum_{i=1}^n g_{\omega}(\mu_i) \right| \lesssim \frac{2\|K\|_{\infty} M}{nh^2} \log \left( \frac{4L(L_K + q'\|K\|_{\infty})}{\delta h^2 \|K\|_2} \sqrt{\frac{M}{\|\bar{p}\|_{\infty}}} \right) +$$

$$\sqrt{\frac{2M\|\bar{p}\|_{\infty}}{n}} \frac{\|K\|_2}{h} \sqrt{\log \left( \frac{4L(L_K + q'\|K\|_{\infty})}{\delta h^2 \|K\|_2} \sqrt{\frac{M}{\|\bar{p}\|_{\infty}}} \right)}.$$

353 ■

#### 354 **D.4 Proof of Theorem 3.6(b)**

355 Part (b) of Theorem 3.6 can be proved in a similar, though slightly easier, fashion to part (a). We  
356 therefore provide a sketch of the proof and omit the details.

357 **Defining an auxiliary function class.** For every  $\tilde{\mu}$  and  $\omega \in \Omega$ , define

$$g_{\omega}(\tilde{\mu}) = \int_{\Omega} \frac{1}{h^2} K \left( \frac{\mathbf{x} - \omega}{h} \right) d\tilde{\mu} - \int_{\Omega} \frac{1}{h^2} K \left( \frac{\mathbf{x} - \omega}{h} \right) d\mathbb{E}[\tilde{\mu}],$$

358 and let  $\mathcal{G} = \{g_{\omega} : \omega \in \Omega\}$ . It is easy to verify that  $\mathbb{E}[g] \equiv 0$  for all  $\omega \in \Omega$ , and that

$$\|\tilde{p}_h(\omega) - \tilde{p}(\omega)\| = \sup_{g \in \mathcal{G}} \left| \frac{1}{n} \sum_{i=1}^n g(\mu_i) \right|.$$

359 **Bounding  $\|g\|_{\infty}$  and  $\mathbb{E}[g^2]$ .** Since  $\tilde{\mu}$  and  $\mathbb{E}[\tilde{\mu}]$  are normalized measures with a total mass of 1,  
360  $\|g\|_{\infty}$  can be bounded by

$$\|g\|_{\infty} \leq \frac{\|K\|_{\infty}}{h^2};$$

361 in the mean time, Assumption 3.3 (b) guarantees that  $\mathbb{E}[g_{\omega}(\tilde{\mu})^2]$  can be bounded by

$$\mathbb{E}[g_{\omega}(\tilde{\mu})^2] \leq \frac{\|\tilde{p}\|_{\infty} \|K\|_2^2}{h^2}.$$

362 **Bounding the covering number of  $\mathcal{G}$ .** We again apply the Lipchitz property of the kernel function  
363  $K(\cdot)$  to conclude that for any  $\omega, \omega' \in \Omega$ ,

$$|g_{\omega}(\tilde{\mu}) - g_{\omega'}(\tilde{\mu})| \leq \frac{2L_K}{h^3} \|\omega - \omega'\|_2.$$

364 Hence, using a similar reasoning to the proof of part (a), we can bound the covering number of  $\mathcal{G}$  by

$$\mathcal{N}(\mathcal{G}, L^2(Q), \eta) < \left( \frac{4LL_K}{\eta h^3} \right)^2.$$

365 **Completing the proof.** Theorem 3.6 (b) is a direct corollary of Theorems C.6 and C.7 with the  
366 following choice of parameters:

$$\begin{cases} AB = \frac{4LL_K}{h^3}; \\ B = \frac{\|K\|_{\infty}}{h^2}; \\ \sigma^2 = \frac{\|\tilde{p}\|_{\infty}}{h^2} \|K\|_2^2; \\ \nu = 2. \end{cases}$$

#### 367 **D.5 Proof of Theorems 3.7 and B.4**

368 In this section, we provide the proof of Theorem B.4, which gives a minimax lower bound for  
369 estimating the weighted persistence intensity function. Theorem 3.7, which gives the minimax lower

370 bound for estimating the persistence density function, can be proved in a similar while simpler  
 371 fashion, so we omit its proof for brevity.

372 The main idea of this proof is to build a connection of weighted intensity function  $\bar{p}(\cdot)$  and a  
 373 probability density function. First of all, we can observe the conclusion of Theorem C.10 holds true  
 374 also when the support for the density function is  $\Omega$  instead of  $[0, 1]^2$ . Now, notice that for any  $\mathbf{x} \in \Omega$ ,  
 375 we can define the following measure:

$$\mu_{\mathbf{x}} = M\delta_{\mathbf{x}}\|\mathbf{x} - \partial\Omega\|_2^{-q}. \quad (15)$$

376 It is easy to verify that  $\text{Pers}_q(\mu_{\mathbf{x}}) = M$ , so  $\mu_{\mathbf{x}} \in \mathcal{Z}_{L,M}^q$ . Therefore, for any estimator  $\hat{p}_n :$   
 377  $(\mathcal{Z}_{L,M}^q)^n \rightarrow \mathcal{F}$ , we can construct the following estimator  $\hat{f}_n$ :

$$\hat{f}_n(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n) = \hat{p}_n(\mu_{\mathbf{x}_1}, \mu_{\mathbf{x}_2}, \dots, \mu_{\mathbf{x}_n}).$$

378 Theorem C.10 states that there exists a probability density function  $f : \Omega \rightarrow \mathbb{R}$  with  $\|f\|_{\infty, \infty}^r \leq B$   
 379 such that when  $X_1, X_2, \dots, X_n \sim \text{i.i.d. } f$ ,

$$\mathbb{E}\|\hat{f}_n(X_1, X_2, \dots, X_n) - f\|_{\infty} \geq O(n^{-\frac{r}{2r+2}}).$$

380 We can apply the probability density function  $f$  to construct a probability measure on  $\mathcal{Z}_{L,M}^q$ . First,  
 381 define a map  $\Phi : \Omega \rightarrow \mathcal{Z}_{L,M}^q$  by  $\Phi(\mathbf{x}) = \mu_{\mathbf{x}}$  in (15). Impose a measure structure on  $\mathcal{Z}_{L,M}^q$  by  
 382 pushforwarding the measure structure on  $\Omega$ , i.e.  $\mathcal{Y} \subset \mathcal{Z}_{L,M}^q$  is measurable if and only if  $\Phi^{-1}(\mathcal{Y})$  is  
 383 measurable in  $\Omega$ . Define a probability measure  $P$  on  $\mathcal{Z}_{L,M}^q$  as a pushforward measure, i.e., for any  
 384 measurable set  $\mathcal{Y} \subset \mathcal{Z}_{L,M}^q$ ,

$$P(\mathcal{Y}) = \int_{\Phi^{-1}(\mathcal{Y})} f(\mathbf{x})d\mathbf{x}.$$

385 Then from the change of variables,

$$\int_{\mathcal{Y}} g(\mu)dP(\mu) = \int_{\Phi^{-1}(\mathcal{Y})} g(\Phi(\mathbf{x}))f(\mathbf{x})d\mathbf{x}.$$

386 Now, the intensity for  $P$  can be represented as follows: let  $p(\cdot)$  be the intensity function for  $\mathbb{E}[\mu]$   
 387 when  $\mu \sim P$ , then for all  $\mathbf{u} \in \Omega$ ,

$$\bar{p}(\mathbf{u}) := \|\mathbf{u} - \partial\Omega\|_2^q p(\mathbf{u}) = Mf(\mathbf{u}). \quad (16)$$

388 To see this fact, consider any Borel set  $\mathcal{A} \subset \Omega$ . By definition, the expected measure  $\mathbb{E}[\mu]$  satisfies

$$\begin{aligned} \mathbb{E}[\mu](\mathcal{A}) &= \mathbb{E}[\mu(\mathcal{A})] = \int_{\mathcal{Z}_{L,M}^q} \mu(\mathcal{A})dP(\mu) \\ &= \int_{\Phi^{-1}(\mathcal{Z}_{L,M}^q)} \Phi(\mathbf{x})(\mathcal{A})f(\mathbf{x})d\mathbf{x} \\ &= \int_{\Omega} \mu_{\mathbf{x}}(\mathcal{A})f(\mathbf{x})d\mathbf{x} \\ &= \int_{\Omega} M\|\mathbf{x} - \partial\Omega\|_2^{-q} \mathbf{1}\{\mathbf{x} \in \mathcal{A}\}f(\mathbf{x})d\mathbf{x} \\ &= \int_{\mathcal{A}} M\|\mathbf{x} - \partial\Omega\|_2^{-q} f(\mathbf{x})d\mathbf{x}. \end{aligned}$$

389 Since  $\mathcal{A}$  can be any Borel set, we get  $p(\mathbf{u}) = M\|\mathbf{u} - \partial\Omega\|_2^{-q}$  by definition, and Equation (16)  
 390 follows naturally. Since the  $\ell_{\infty}$  difference between  $\hat{f}_n$  and  $f$  is lower bounded, we can obtain

$$\mathbb{E}_P \sup_{\omega \in \Omega} \|\omega - \partial\Omega\|_2^q |\hat{p}_n(\omega) - p(\omega)| = M\mathbb{E}_f \|\hat{f}_n - f\|_{\infty} \geq O(n^{-\frac{r}{2r+2}}).$$

391

■

392 **D.6 Proof of Theorems and Corollaries regarding linear representations of the persistence**  
 393 **measure**

394 The theoretical results regarding linear representations of the persistence measure in Section 3.3 are  
 395 rather direct applications of the theoretical results on estimating the persistence intensity and density  
 396 functions. We therefore combine their proofs in this section.

397 **Proof of Theorem 3.8.** Theorem 3.5 directly implies that under Assumption 3.2, for any  $\Psi \in$   
 398  $\mathcal{F}_{2h,R}$ , the bias of  $\hat{\Psi}$  is bounded by

$$\begin{aligned} \left| \mathbb{E}[\hat{\Psi}] - \Psi \right| &= \left| \int_{\omega \in \Omega} f(\omega) (\mathbb{E}[\hat{p}_h(\omega)] - p(\omega)) d\omega \right| \\ &\leq \int_{\omega \in \Omega} f(\omega) |\mathbb{E}[\hat{p}_h(\omega)] - p(\omega)| d\omega \\ &\leq \sup_{\omega \in \Omega} |\mathbb{E}[\hat{p}_h(\omega)] - p(\omega)| \int_{\omega \in \Omega} f(\omega) d\omega \\ &\leq L_p h^s R \int_{\|v\|_2 \leq 1} |K(v)| \|v\|_2^2 dv, \end{aligned}$$

399 where in the last line we applied Theorem 3.5 and the definition of  $\mathcal{F}_{2h,R}$ . The upper bound for the  
 400 bias of  $\check{\Psi}$  follows similarly.

401 **Proof of Theorem 3.9.** The upper bound for the variation of  $\hat{\Psi}$  is a direct corollary of Theorem 3.6  
 402 (a) and the fact that

$$\begin{aligned} \sup_{\Psi \in \mathcal{F}_{2h,R}} \left| \hat{\Psi} - \mathbb{E}[\hat{\Psi}] \right| &= \sup_{\Psi \in \mathcal{F}_{2h,R}} \left| \int_{\omega \in \Omega} f(\omega) [\hat{p}_h(\omega) - \mathbb{E}[\hat{p}_h](\omega)] d\omega \right| \\ &\leq \int_{\omega \in \Omega} \ell_{\omega}^{-q} f(\omega) d\omega \cdot \sup_{\omega \in \Omega} \ell_{\omega}^q |\hat{p}_h(\omega) - \mathbb{E}[\hat{p}_h](\omega)| \\ &\leq R \cdot \sup_{\omega \in \Omega} \ell_{\omega}^q |\hat{p}_h(\omega) - \mathbb{E}[\hat{p}_h](\omega)|; \end{aligned}$$

403 The upper bound for the variation of  $\check{\Psi}$  follows from Theorem 3.6 (b) and a similar relation:

$$\sup_{\check{\Psi} \in \mathcal{F}_R} |\check{\Psi} - \mathbb{E}[\check{\Psi}]| \leq R \cdot \sup_{\omega \in \Omega} |\check{p}_h(\omega) - \mathbb{E}[\check{p}_h](\omega)|.$$

404 **Proof of Corollaries 3.10 and 3.11.** For every  $x \in \Omega_{2h}$ , define

$$f_x(\omega) = \mathbb{1} \{ \omega \in B_x \},$$

405 and let

$$\mathcal{F}_{2h,R} = \left\{ \Psi = \int_{\Omega_{2h}} f_x(\omega) d\mathbb{E}[\mu] \mid x \in \Omega_{2h} \right\}.$$

406 Corollary 3.10 follows from Theorem 3.8 and the fact that

$$\int_{\omega \in \Omega_{2h}} f_x(\omega) d\omega \leq \frac{L^2}{4}$$

407 for every  $x \in \Omega_{2h}$ . Similarly, Corollary 3.11 follows from Theorem 3.9 and the fact that

$$\int_{\omega \in \Omega_{2h}} \ell_{\omega}^{-q} f_x(\omega) d\omega \leq C \ell_x^{2-q},$$

408 for a constant  $C$ .

409 **Proof of Corollary 3.12.** For every  $\mathbf{x} \in \Omega$ , we define

$$f_{\mathbf{x}}(\boldsymbol{\omega}) = \mathbb{1}\{\boldsymbol{\omega} \in B_{\mathbf{x}}\},$$

410 and let

$$\widetilde{\mathcal{F}}_R = \left\{ \widetilde{\Psi} = \int_{\Omega} f_{\mathbf{x}} \boldsymbol{\omega} d\mathbb{E}[\tilde{\mu}] \mid \mathbf{x} \in \Omega \right\}.$$

411 Corollary 3.12 follows directly from Theorem 3.9 and the fact that for every  $\mathbf{x} \in \Omega$ ,

$$\int_{\boldsymbol{\omega} \in \Omega} f_{\mathbf{x}}(\boldsymbol{\omega}) d\boldsymbol{\omega} \leq \frac{L^2}{4}.$$

#### 412 **D.7 Proof of Theorem B.5**

413 This proof again involves the Talagrand's inequality, and therefore takes a similar shape to the proof  
414 of Theorem 3.6. We begin by defining an auxiliary function class.

415 **Defining the auxiliary function class  $\mathcal{G}$ .** Recall that we choose the weight function as  $f(\boldsymbol{\omega}) =$   
416  $\|\boldsymbol{\omega} - \partial\Omega\|_2^q$ . Therefore, for any persistence measure  $\mu \in \mathcal{Z}_{L,M}^q$ , its corresponding persistence surface  
417 is characterized by

$$\rho_h(\mu)(\mathbf{u}) = \int_{\Omega} \|\boldsymbol{\omega} - \partial\Omega\|_2^q \frac{1}{h^2} K\left(\frac{\mathbf{u} - \boldsymbol{\omega}}{h}\right) d\mu(\boldsymbol{\omega});$$

418 hence, by defining

$$g_{\mathbf{u}}(\mu) = \int_{\Omega} \|\boldsymbol{\omega} - \partial\Omega\|_2^q \frac{1}{h^2} K\left(\frac{\mathbf{u} - \boldsymbol{\omega}}{h}\right) d(\mu - \mathbb{E}[\mu])(\boldsymbol{\omega})$$

419 and letting  $\mathcal{G} = \{g_{\mathbf{u}}(\mu) : \mathbf{u} \in \Omega\}$ , we observe that  $\mathbb{E}[g] = 0$  for all  $g \in \mathcal{G}$  and

$$\|\rho_h(\boldsymbol{\mu}_n) - \mathbb{E}[\rho_h(\boldsymbol{\mu})]\|_{\infty} = \sup_{g \in \mathcal{G}} \left\| \frac{1}{n} \sum_{i=1}^n g(\mu_i) \right\|.$$

420 **Bounding  $\|g\|_{\infty}$  and  $\mathbb{E}[g^2]$ .** Assumptions 3.4 and B.3 directly implies that for any  $g \in \mathcal{G}$  and any  
421  $\mathbf{u} \in \Omega$ ,

$$\begin{aligned} |g_{\mathbf{u}}(\mu)| &\leq \frac{\|K\|_{\infty}}{h^2} \max \left\{ \int_{\Omega} \|\boldsymbol{\omega} - \partial\Omega\|_2^q d\mu, \int_{\Omega} \|\boldsymbol{\omega} - \partial\Omega\|_2^q d\mathbb{E}[\mu] \right\} \\ &= \frac{\|K\|_{\infty}}{h^2} \max \{ \text{Pers}_q(\mu), \text{Pers}_q(\mathbb{E}[\mu]) \} \leq \frac{M\|K\|_{\infty}}{h^2}. \end{aligned}$$

422 Regarding the variance of  $g$ , Assumption 3.3 implies that

$$\begin{aligned} \mathbb{E}[g_{\mathbf{u}}(\mu)^2] &\leq \|g\|_{\infty} \cdot \int_{\Omega} \|\boldsymbol{\omega} - \partial\Omega\|_2^q \frac{1}{h^2} \left| K\left(\frac{\mathbf{u} - \boldsymbol{\omega}}{h}\right) \right| d\mathbb{E}[\mu] \\ &\leq \frac{M\|K\|_{\infty}}{h^2} \int_{\Omega} \frac{1}{h^2} \left| K\left(\frac{\mathbf{u} - \boldsymbol{\omega}}{h}\right) \right| \|\boldsymbol{\omega} - \partial\Omega\|_2^q p(\boldsymbol{\omega}) d\boldsymbol{\omega} \\ &\leq \frac{M\|K\|_{\infty}}{h^2} \int_{\|\mathbf{v}\|_2 \leq 1} |K(\mathbf{v})| d\mathbf{v} \cdot \sup_{\boldsymbol{\omega} \in \Omega} \|\boldsymbol{\omega} - \partial\Omega\|_2^q p(\boldsymbol{\omega}) \\ &\leq \frac{M\|K\|_1 \|K\|_{\infty} \|\bar{p}\|_{\infty}}{h^2}, \end{aligned}$$

423 where in the third line we applied the change of variable  $\mathbf{v} = (\mathbf{u} - \boldsymbol{\omega})/h$ , and let

$$\|K\|_1 := \int_{\|\mathbf{v}\|_2 \leq 1} |K(\mathbf{v})| d\mathbf{v}.$$

424 **Covering number of  $\mathcal{G}$ .** Similar to the proof of Theorem 3.6, we bound the covering number of  $\mathcal{G}$   
 425 by the Lipchitz property of the kernel function  $K$ . For any two points  $\mathbf{u}, \mathbf{u}' \in \Omega$ , Assumption B.3  
 426 guarantees that

$$\left| K\left(\frac{\mathbf{u} - \boldsymbol{\omega}}{h}\right) - K\left(\frac{\mathbf{u}' - \boldsymbol{\omega}}{h}\right) \right| \leq \frac{L_K \|\mathbf{u} - \mathbf{u}'\|_2}{h}.$$

427 Therefore, it is easy to verify that

$$|g_{\mathbf{u}}(\mu) - g_{\mathbf{u}'}(\mu)| \leq \frac{ML_K \|\mathbf{u} - \mathbf{u}'\|_2}{h^3}.$$

428 A similar reasoning to the proof of Theorem 3.6 yields that the covering number of  $\mathcal{G}$  is upper  
 429 bounded by

$$\mathcal{N}(\mathcal{G}, L^2(Q), \eta) \leq \mathcal{N}\left(\Omega, \|\cdot\|_2, \frac{\eta h^3}{ML_K}\right) \leq 2 \left(\frac{LML_K}{\eta h^3}\right)^2.$$

430 **Completing the proof.** Theorem B.5 is a direct application of Theorems C.6 and C.7 with the  
 431 following choice of parameters:

$$\begin{cases} AB = \frac{2LML_K}{h^3}; \\ B = \frac{M\|K\|_\infty}{h^2}; \\ \sigma^2 = \frac{M\|K\|_1\|K\|_\infty\|\bar{\rho}\|_\infty}{h^2}; \\ \nu = 2. \end{cases}$$

## 432 D.8 Proof of Theorems B.1 and B.2

433 Observe that the persistence diagram of the Vietoris-Rips filtration of  $\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_N)$  is  
 434 decided purely by  $\{\varphi[J](\mathbf{X})\}_{J \subset [N], |J|=2}$ , in which

$$\varphi[J](\mathbf{X}) = \|\mathbf{X}_i - \mathbf{X}_j\|_2,$$

435 for  $J = \{i, j\}$ . In what follows, we firstly focus on the proof of Theorem B.1, and apply the  
 436 techniques to that of Theorem B.2 in a similar manner.

437 **Proof of Theorem B.1.** Propositions C.4 and C.3 imply that for any Borel set  $B \subseteq \Omega$ ,

$$\begin{aligned} \mathbb{E}[\mu](B) &= \sum_{r=1}^R \sum_{i=1}^{N_r} \sum_{s \in S} \int_{V_r \cap W_{J_{i_r}^1, J_{i_r}^2}^s \cap \Phi[J_{i_r}^1, J_{i_r}^2]^{-1}(B)} \kappa(\mathbf{X}) d\mathbf{X} \\ &= \sum_{r=1}^R \sum_{i=1}^{N_r} \sum_{s \in S} \int_{\Psi_{J_{i_r}^1, J_{i_r}^2}^s (V_r \cap W_{J_{i_r}^1, J_{i_r}^2}^s \cap \Phi[J_{i_r}^1, J_{i_r}^2]^{-1}(B))} \kappa((\Psi_{J_{i_r}^1, J_{i_r}^2}^s)^{-1}(u, y)) J[\Psi_{J_{i_r}^1, J_{i_r}^2}^s]^{-1}(\mathbf{u}, \mathbf{Y}) d\mathbf{Y} du, \end{aligned}$$

438 where in the second line we change the variable from  $\mathbf{X} \in [0, 1]^{d \times n}$  to  $(\mathbf{Y}, \mathbf{u})$  with  $\mathbf{Y} \in [0, 1]^{nd-2}$   
 439 and  $\mathbf{u} \in \Omega$ . Now, a change of order of summation gives

$$\begin{aligned}
 \mathbb{E}[\mu](B) &= \sum_{s \in S} \sum_{\substack{J_1, J_2 \subset [N] \\ |J_1|=|J_2|=2 \\ J_1 \neq J_2}} \sum_{r=1}^R \sum_{i=1}^{N_r} I(J_{ir}^1 = J_1, J_{ir}^2 = J_2) \\
 &\quad \times \int_{\Psi_{J_1, J_2}^s (V_r \cap W_{J_1, J_2}^s \cap \Phi[J_1, J_2]^{-1}(B))} \kappa((\Psi_{J_1, J_2}^s)^{-1}(\mathbf{u}, \mathbf{Y})) J[\Psi_{J_{ir}^1, J_{ir}^2}^s]^{-1}(u, y) d\mathbf{Y} d\mathbf{u} \\
 &\leq \sum_{s \in S} \sum_{\substack{J_1, J_2 \subset [N] \\ |J_1|=|J_2|=2 \\ J_1 \neq J_2}} \sum_{r=1}^R \sum_{i=1}^{N_r} I(J_{ir}^1 = J_1, J_{ir}^2 = J_2) \\
 &\quad \times \int_{\Psi_{J_1, J_2}^s (V_r \cap W_{J_1, J_2}^s \cap \Phi[J_1, J_2]^{-1}(B))} d \sup \kappa d\mathbf{Y} d\mathbf{u} \\
 &\leq \sum_{s \in S} \sum_{\substack{J_1, J_2 \subset [N] \\ |J_1|=|J_2|=2 \\ J_1 \neq J_2}} N(B) \int_{\Psi_{J_1, J_2}^s (W_{J_1, J_2}^s \cap \Phi[J_1, J_2]^{-1}(B))} d \sup \kappa d\mathbf{Y} d\mathbf{u}, \tag{17}
 \end{aligned}$$

440 where  $N(B)$  is the number of persistent homology points in  $B$ , and in the second line we use the  
 441 facts that  $\{V_r\}_{r=1}^R$  are disjoint,  $\kappa \leq \sup \kappa$  and  $J[\Psi_{J_{ir}^1, J_{ir}^2}^s]^{-1} \leq d$ . Hence, bounding  $\mathbb{E}[\mu](B)$  boils  
 442 down to characterizing the domain of integration on the right hand side of (17). For this, notice that  
 443 by definition,

$$\begin{aligned}
 &(\mathbf{Y}, \mathbf{u}) \in \Psi_{J_1, J_2}^s (W_{J_1, J_2}^s \cap \Phi[J_1, J_2]^{-1}(B)) \\
 &\Leftrightarrow \exists \mathbf{X} \in W_{J_1, J_2}^s, \text{ such that } \Phi[J_1, J_2](\mathbf{X}) \in B, \Psi_{J_1, J_2}^s(\mathbf{X}) = (\mathbf{Y}, \mathbf{u}) \\
 &\rightarrow \exists \mathbf{X} \in W_{J_1, J_2}^s, \text{ such that } \Phi[J_1, J_2](\mathbf{X}) \in B, \Phi[J_1, J_2](\mathbf{X}) = \mathbf{u}, \text{ and } \mathbf{Y} \in [0, 1]^{Nd-2} \\
 &\rightarrow \mathbf{u} \in B, \text{ and } \mathbf{Y} \in [0, 1]^{Nd-2}.
 \end{aligned}$$

444 Hence,  $\mathbb{E}[\mu](B)$  is upper bounded by

$$\begin{aligned}
 \mathbb{E}[\mu](B) &\leq N(B) \sum_{s \in S} \sum_{\substack{J_1, J_2 \subset [N] \\ |J_1|=|J_2|=2 \\ J_1 \neq J_2}} \int_{\mathbf{u} \in B, \mathbf{Y} \in [0, 1]^{Nd-2}} d \sup \kappa d\mathbf{Y} d\mathbf{u} \\
 &= d \sup \kappa N(B) \sum_{s \in S} \sum_{\substack{J_1, J_2 \subset [N] \\ |J_1|=|J_2|=2 \\ J_1 \neq J_2}} \int_{[0, 1]^{Nd-2}} d\mathbf{Y} \int_B d\mathbf{u} \\
 &= d \sup \kappa N(B) \sum_{s \in S} \sum_{\substack{J_1, J_2 \subset [N] \\ |J_1|=|J_2|=2 \\ J_1 \neq J_2}} \int_B d\mathbf{u}.
 \end{aligned}$$

445 This effectively means that the intensity function  $p(\mathbf{u})$  is upper bounded by

$$p(\mathbf{u}) \leq \mathbb{E}[N(\{\mathbf{u}\})] d \sup \kappa \sum_{s \in S} \sum_{\substack{J_1, J_2 \subset [N] \\ |J_1|=|J_2|=2 \\ J_1 \neq J_2}} 1$$

$$< \mathbb{E}[N(\{\mathbf{u}\})] \text{card}(S) |\{(J_1, J_2) : |J_1| = |J_2| = 2, J_1 \neq J_2, J_1 \subset [N], J_2 \subset [N]\}| d \sup \kappa.$$

446 Now,  $N(\{\mathbf{u}\}) \leq N_\ell$ , so Lemma C.5 implies  $\mathbb{E}[N(\{\mathbf{u}\})] \leq CN$ . And  $\text{card}(S) \leq 4d^2$  and  
 447  $|\{(J_1, J_2) : |J_1| = |J_2| = 2, J_1 \neq J_2, J_1 \subset [N], J_2 \subset [N]\}| \leq \frac{N^4}{4}$ , so

$$\begin{aligned}
 p(\mathbf{u}) &\leq (CN) \cdot (4d^2) \cdot \left(\frac{N^4}{4}\right) \cdot d \sup \kappa \\
 &= C' N^5 d^3 \sup \kappa.
 \end{aligned}$$

448 Theorem B.1 follows with the choice of

$$\text{poly}(N, d) = N^5 d^3.$$

449 **Proof of Theorem B.2.** Propositions C.4 and C.3 imply that for any Borel set  $B \subseteq \Omega$ , the  
450 normalized persistence measure of  $B$  is expressed by

$$\begin{aligned} \mathbb{E}[\tilde{\mu}](B) &= \sum_{r=1}^R \frac{1}{N_r} \sum_{i=1}^{N_r} \sum_{s \in S} \int_{V_r \cap W_{J_{ir}^1, J_{ir}^2}^s \cap \Phi[J_{ir}^1, J_{ir}^2]^{-1}(B)} \kappa(\mathbf{X}) d\mathbf{X} \\ &\leq \sum_{r=1}^R \max_{1 \leq i \leq N_r} \sum_{s \in S} \int_{V_r \cap W_{J_{ir}^1, J_{ir}^2}^s \cap \Phi[J_{ir}^1, J_{ir}^2]^{-1}(B)} \kappa(\mathbf{X}) d\mathbf{X}. \end{aligned}$$

451 Hence, same techniques can be applied to show that the persistence density function is upper bounded  
452 by

$$\begin{aligned} \tilde{p}(\mathbf{u}) &\leq d \sup \kappa \mathbb{E} \left[ \frac{N(\{\mathbf{u}\})}{N(\{\mathbf{u}\})} \right] \sum_{s \in S} \sum_{\substack{J_1, J_2 \subset [N] \\ |J_1| = |J_2| = 2 \\ J_1 \neq J_2}} 1 \\ &\leq d \sup \kappa \max_{1 \leq i \leq N(\mathbf{u})} \sum_{s \in S} \sum_{\substack{J_1, J_2 \subset [N] \\ |J_1| = |J_2| = 2 \\ J_1 \neq J_2}} 1 \\ &\leq \text{card}(S) |\{(J_1, J_2) : |J_1| = |J_2| = 2, J_1 \neq J_2, J_1 \subset [N], J_2 \subset [N]\}| d \sup \kappa \\ &\leq (4d^2) \cdot \left( \frac{N^4}{4} \right) \cdot d \sup \kappa. \end{aligned}$$

453 Theorem B.2 follows from choosing

$$\text{poly}(N, d) = N^4 d^3.$$

## 454 D.9 Proof of Theorem B.6

455 In this proof, we firstly define an auxiliary family of functions, and then verify the conditions in  
456 Theorem C.8.

457 **Defining the auxiliary function class.** For every  $\mathbf{x} \in \Omega_\ell$  and  $\mu \in \mathcal{Z}_{L,M}^q$ , define

$$g_{\mathbf{x}}(\mu) = \mu(B_{\mathbf{x}}) - \mathbb{E}[\mu](B_{\mathbf{x}}), \quad (18)$$

458 and let  $\mathcal{G} = \{g_{\mathbf{x}} : \mathbf{x} \in \Omega_\ell\}$ . It is easy to verify that  $\mathbb{E}[g_{\mathbf{x}}(\mu)] = 0$  for all  $\mathbf{x} \in \Omega_\ell$ , and that

$$\sup_{\mathbf{x} \in \Omega_\ell} \left| \hat{\beta}_{\mathbf{x}} - \mathbb{E}[\hat{\beta}_{\mathbf{x}}] \right| = \left| \sup_{g \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^n g(\mu_i) \right|.$$

459 **Bounding  $\|g_{\mathbf{x}}\|_\infty$  and  $\mathbb{E}[g_{\mathbf{x}}(\mu)^2]$ .** For any  $\mathbf{x} \in \Omega_\ell$ , the set  $B_{\mathbf{x}}$  is contained in  $\Omega_\ell$ . Hence for any  
460  $\mu \in \mathcal{Z}_{L,M}^q$ ,  $\mu(B_{\mathbf{x}})$  and  $\mathbb{E}[\mu](B_{\mathbf{x}})$  can be bounded as

$$\begin{aligned} \mu(B_{\mathbf{x}}) &\leq \mu(\Omega_\ell) \leq \ell^{-q} \text{Pers}_q(\mu) \leq M \ell^{-q}, \\ \mathbb{E}[\mu](B_{\mathbf{x}}) &\leq \mathbb{E}[\mu](\Omega_\ell) \leq \ell^{-q} \text{Pers}_q(\mathbb{E}[\mu]) \leq M \ell^{-q}. \end{aligned} \quad (19)$$

461 Hence  $\|g_{\mathbf{x}}\|_\infty$  can be bounded as

$$\|g_{\mathbf{x}}\|_\infty \leq \sup_{\mu \in \mathcal{Z}_{L,M}^q} \max \{\mu(B_{\mathbf{x}}), \mathbb{E}[\mu](B_{\mathbf{x}})\} \leq M \ell^{-q}. \quad (20)$$

462 As for the variance of  $g_{\mathbf{x}}(\mu)$ , we firstly observe that

$$\mathbb{E}[g_{\mathbf{x}}(\mu)^2] \leq \|g_{\mathbf{x}}\|_\infty \mathbb{E}[\mu](B_{\mathbf{x}}) \quad (21)$$

463 Now, apart from using the bound  $\mathbb{E}[\mu](B_{\mathbf{x}}) \leq M\ell^{-q}$  from (19), we can also have tighter bound with  
 464 respect to  $\ell$  when  $q > 1$ . To do this, we again take the coordinate transformation

$$\begin{cases} y_1 = \frac{x_2 - x_1}{\sqrt{2}} = \|\mathbf{x} - \partial\Omega\|_2, \\ y_2 = \frac{x_2 + x_1}{\sqrt{2}}. \end{cases}$$

465 It can be easily verified that the determinant of the Jacobian matrix between  $\mathbf{x}$  and  $\mathbf{y}$  coordinates is 1,  
 466 and that the  $\Omega_\ell$  can be represented using  $\mathbf{y}$  coordinates by

$$\Omega_\ell = \left\{ (y_1, y_2) : \ell < y_1 \leq \frac{L}{\sqrt{2}}, y_1 \leq y_2 \leq \sqrt{2}L - y_1 \right\}.$$

467 Then, we have a tighter bound with respect to  $\ell$  of  $\mathbb{E}[\mu](B_{\mathbf{x}})$  when  $q > 1$  as

$$\begin{aligned} \mathbb{E}[\mu](B_{\mathbf{x}}) &\leq \mathbb{E}[\mu](\Omega_\ell) = \int_{\Omega_\ell} p(\mathbf{u}) d\mathbf{u} \\ &= \int_{\Omega_\ell} \|\mathbf{u} - \partial\Omega\|_2^{-q} \bar{p}(\mathbf{u}) d\mathbf{u} \\ &\leq \|\bar{p}\|_\infty \int_\ell^{\frac{L}{\sqrt{2}}} \left( \int_{y_1}^{\sqrt{2}L - y_1} dy_2 \right) y_1^{-q} dy_1 \\ &\leq \|\bar{p}\|_\infty \int_\ell^{\frac{L}{\sqrt{2}}} \sqrt{2}L y_1^{-q} dy_1 \\ &\leq \frac{\sqrt{2}L\ell^{1-q} \|\bar{p}\|_\infty}{q-1}. \end{aligned}$$

468 Hence when we let  $(q-1)_+ = \max\{q-1, 0\}$ ,

$$\mathbb{E}[\mu](B_{\mathbf{x}}) \leq \min \left\{ M\ell^{-q}, \frac{\sqrt{2}L\ell^{1-q} \|\bar{p}\|_\infty}{(q-1)_+} \right\}. \quad (22)$$

469 And hence by applying (22) to (21), the variance of  $g_{\mathbf{x}}(\mu)$  can be upper bounded as

$$\begin{aligned} \mathbb{E}[g_{\mathbf{x}}(\mu)^2] &\leq \|g_{\mathbf{x}}\|_\infty \mathbb{E}[\mu](B_{\mathbf{x}}) \\ &\leq \min \left\{ M^2\ell^{-2q}, \frac{\sqrt{2}ML\ell^{1-2q} \|\bar{p}\|_\infty}{(q-1)_+} \right\} \end{aligned} \quad (23)$$

470 **Polynomial discrimination of  $\mathcal{G}$ .** By definition, the empirical persistent measure  $\mu_i$  can be repre-  
 471 sented as

$$\mu_i = \sum_j \delta_{\mathbf{r}_{ij}},$$

472 in which  $\mathbf{r}_{ij} = (b_{ij}, d_{ij})$  represents the  $j$ -th point in the corresponding persistent diagram, with  $b_{ij}$   
 473 and  $d_{ij}$  being its birth and death weight respectively. Without loss of generality, we can sort the  
 474 points in descending order of their distance to the diagonal  $\partial\Omega$ . Let  $N_i = \mu_i(\Omega_\ell)$ , then we have  
 475  $N_i \leq M\ell^{-q}$ . Hence, for every  $\mathbf{x}$  with  $\|\mathbf{x} - \partial\Omega\|_2 = \ell$ ,  $\mu_i(B_{\mathbf{x}})$  can be represented as

$$\mu_i(B_{\mathbf{x}}) = \sum_{j=1}^{N_i} \mathbb{1}(b_{ij} < x_1) \mathbb{1}(d_{ij} > x_2). \quad (24)$$

476 With this expression, we are ready to bound the cardinality of  $\mathcal{G}(\mu_1^n)$ . Notice that for any fixed  $\mathbf{x}$ , the  
 477 value of the tuple  $(g_{\mathbf{x}}(\mu_1), \dots, g_{\mathbf{x}}(\mu_n))$  is completely decided by the Cartesian product of indicator  
 478 functions

$$\{\mathbb{1}(b_{ij} < x_1)\}_{i \in [n], j \in [N_i]} \times \{\mathbb{1}(d_{ij} > x_2)\}_{i \in [n], j \in [N_i]} := S_b \times S_d.$$

479 It is easy to see that with the variation of  $\mathbf{x} = (x_1, x_2)$ , the number of different values taken by  $S_b$   
 480 and  $S_d$  can be bounded by

$$1 + \sum_{i=1}^n N_i \leq 1 + n \cdot M\ell^{-q}.$$

481 Hence, the cardinality of  $\mathcal{G}(\mu_1^n)$  is bounded by

$$\text{Card}(\mathcal{G}(\mu)) \leq (M\ell^{-q}n + 1)^2. \quad (25)$$



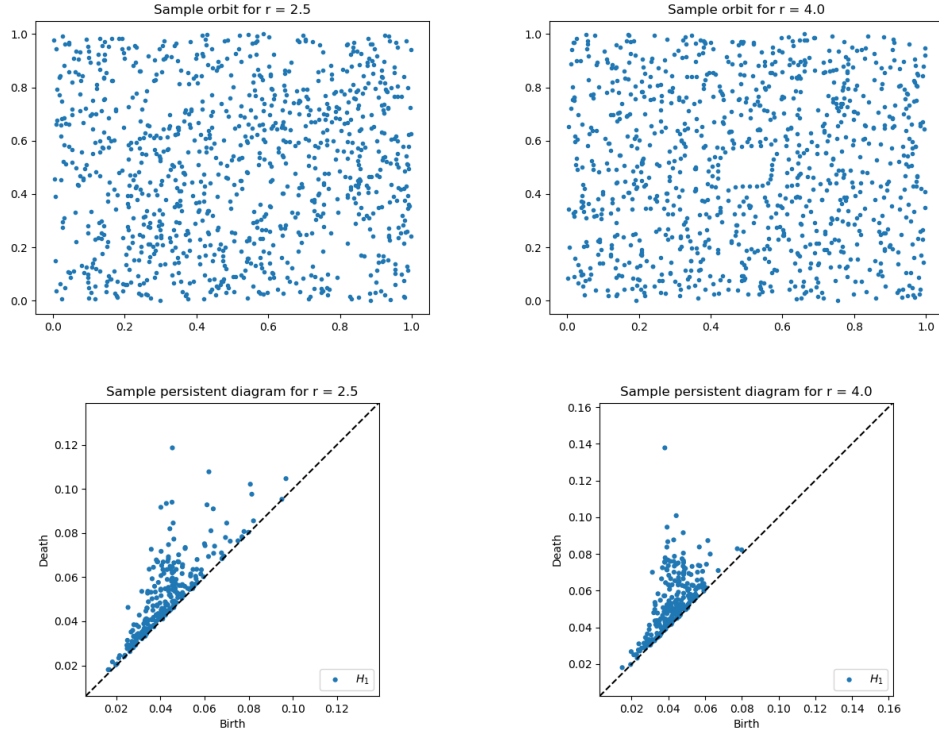


Figure 1: Top row: sample orbits from the ORBIT5K data set with  $r = 2.5$  (left) and  $r = 4.0$  (right). Bottom row: sample persistent diagrams.

482 **Completing the proof.** The theorem is a direct result for applying Theorem C.8 with the following  
 483 parameters:

$$\begin{cases} A = M\ell^{-q}; \\ B = M; \\ \sigma^2 = \min \left\{ M^2\ell^{-2q}, \frac{\sqrt{2}ML\ell^{1-2q}\|\bar{p}\|_\infty}{(q-1)_+} \right\}; \\ \nu = 2. \end{cases}$$

## 484 E Experimental details

485 Figure 1 shows two ORBIT5K simulations with different values of  $r$  (2.5 and 4) and the corresponding  
 486 persistent diagrams. Figure 2 displays the kernel intensity functions for the ORBIT5K simulations set  
 487 with  $r = 2.5$  and  $r = 4$  for varying sample sizes, while Figure 3 shows persistence density functions.  
 488 Figures 4 and 5 show the Betti curves and estimated Betti curves using the kernel density function for  
 489 the ORBIT5K simulations for  $r = 2.5$  and  $r = 4$ .

490 Finally, Figure 6 displays the estimated persistence density functions computed over random draws  
 491 of varying size of the digits “4” and “8” from the MNIST dataset.

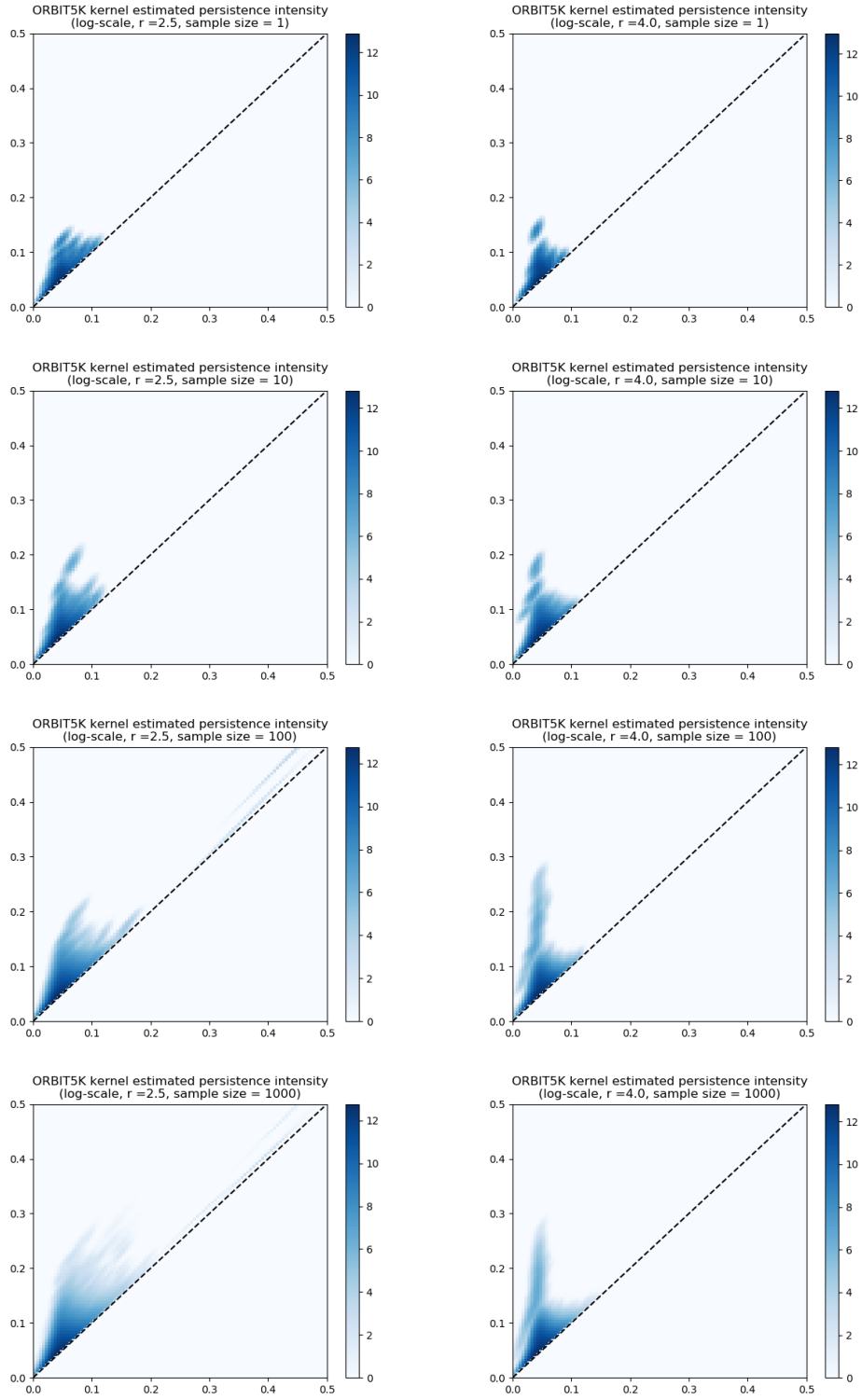


Figure 2: Kernel estimators for the persistence intensity function from the ORBIT5K data set with  $r = 2.5$  (left) and  $r = 4.0$  (right) and sample sizes 1, 10, 100 and 1000 (top to bottom).

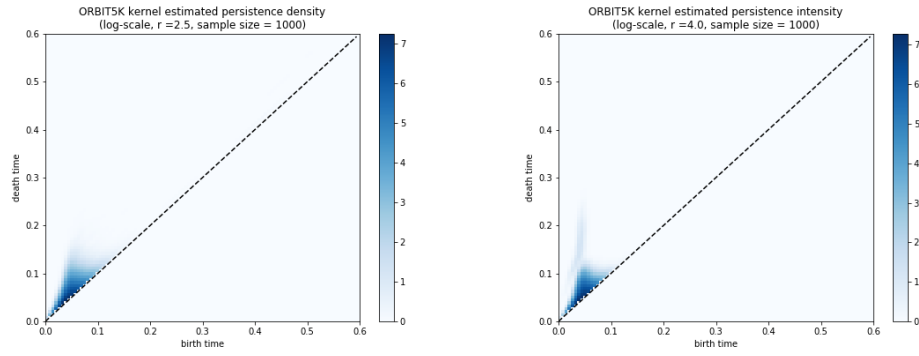


Figure 3: Kernel estimators for the persistence density function from the ORBIT5K data set with  $r = 2.5$  (left) and  $r = 4.0$  (right) and sample size  $n = 1000$ .

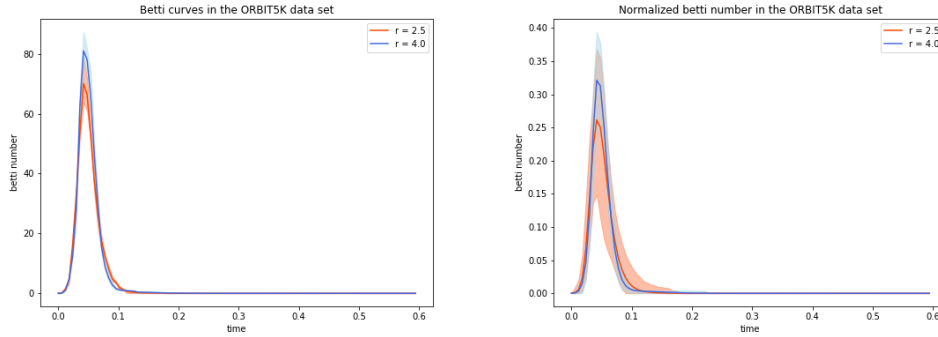


Figure 4: Empirical betti curves (left) and normalized betti curves (right) from the ORBIT5K data set with  $r = 2.5$  and  $r = 4.0$ . Solid lines show sample average and the shades depict the lower and upper 2.5 percentiles.

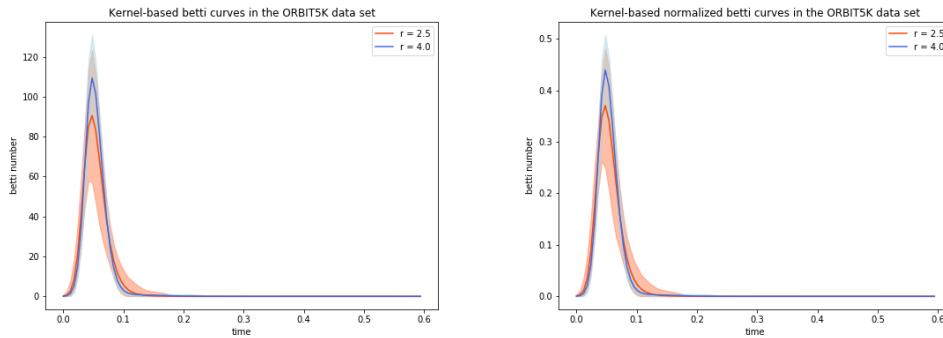


Figure 5: Kernel-based betti curves (left) and normalized betti curves (right) from the ORBIT5K data set with  $r = 2.5$  and  $r = 4.0$ . Solid lines show sample average and the shades depict the lower and upper 2.5 percentiles.

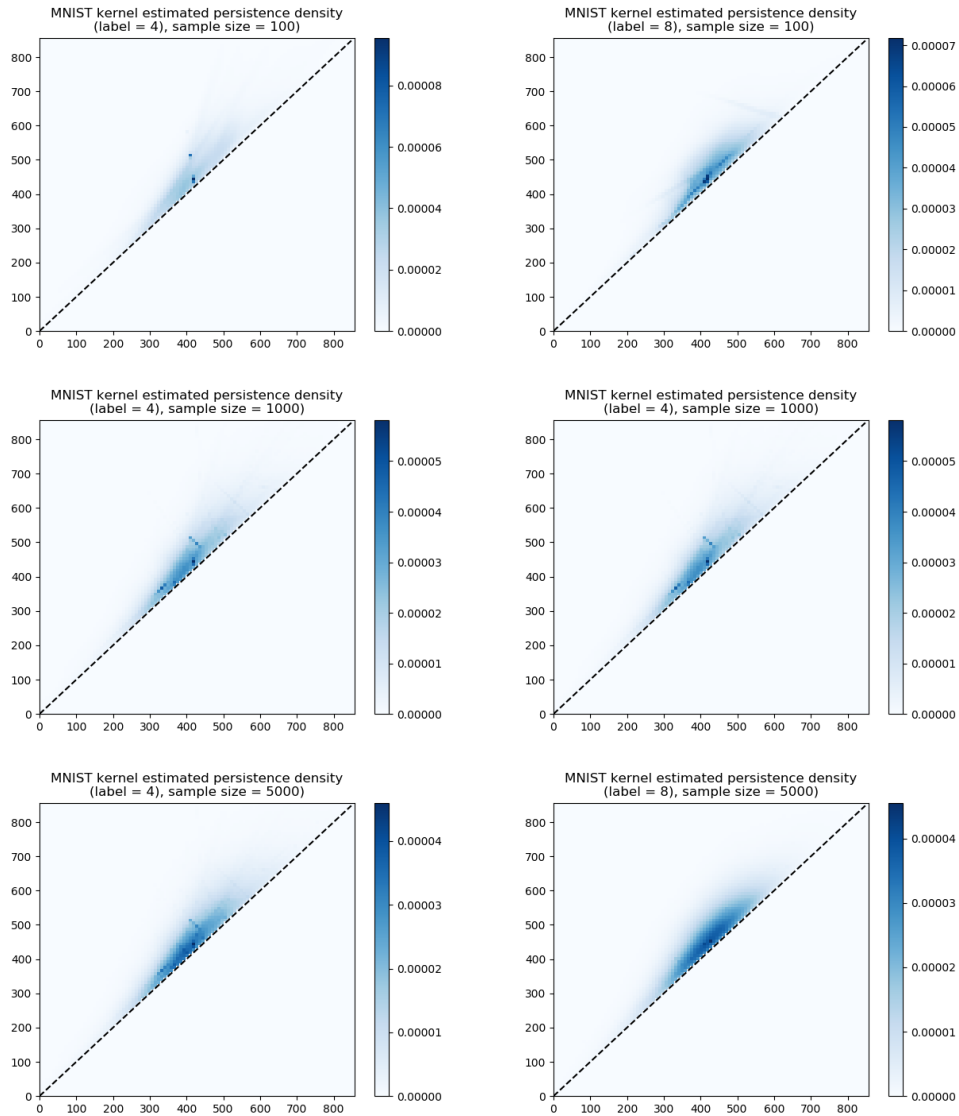


Figure 6: Kernel estimators for the persistence density function from the MNIST data set for the digits 4 (left column) and 8 (right column) based on random draws of sample sizes 100, 1000 and 5000 (top to bottom).

492 **References**

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