

# Out-of-sample Extension for Latent Position Graphs

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**Editor:**

## Abstract

We consider the problem of vertex classification for graphs constructed from the latent position model. It was shown previously that the approach of embedding the graphs into some Euclidean space followed by classification in that space can yield a universally consistent vertex classifier. However, a major technical difficulty of the approach arises when classifying unlabeled out-of-sample vertices without including them in the embedding stage. In this paper, we studied the out-of-sample extension for the graph embedding step and its impact on the subsequent inference tasks. We show that, under the latent position graph model and for sufficiently large  $n$ , the mapping of the out-of-sample vertices is close to its true latent position. We then demonstrate that successful inference for the out-of-sample vertices is possible.

**Keywords:** out-of-sample extension, inhomogeneous random graphs, latent position model, convergence of eigenvectors

## 1. Introduction

The classical statistical pattern recognition setting involves

$$(X, Y), (X_1, Y_1), (X_2, Y_2), \dots, (X_n, Y_n) \stackrel{\text{i.i.d.}}{\sim} F_{X,Y}$$

where the  $X_i \in \mathcal{X} \subset \mathbb{R}^d$  are observed feature vectors and the  $Y_i \in \mathcal{Y} = \{-1, 1\}$  are observed class labels, for some probability distribution  $F_{X,Y}$  on  $\mathcal{X} \times \mathcal{Y}$ . This setting has been extensively investigated and many important and interesting theoretical concepts and results, e.g., universal consistency, structural complexities, and arbitrary slow convergence are available. See, e.g., [Devroye et al. \(1996\)](#) for a comprehensive overview.

Now, suppose that the feature vectors are unobserved, and we observe instead a graph  $G$  on  $n + 1$  vertices. Suppose also that  $G$  is constructed in a manner such that there is a one-to-one relationship between the vertices of  $G$  and the feature vectors  $X, X_1, \dots, X_n$ . The question of classifying the vertices based on  $G$  and the observed labels  $Y_i$  then arises naturally.

A general approach to this classification problem is illustrated by Algorithm 1 wherein inference, e.g., classification or clustering, proceeds by first embedding the graph  $G$  into some

**Algorithm 1** Vertex classifier on graphs

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**Input:**  $\mathbf{A} \in \{0, 1\}^{n \times n}$ , training set  $\mathcal{T} \subset [n] = \{1, 2, \dots, n\}$  and labels  $\mathbf{Y}_{\mathcal{T}} = \{Y_i : i \in \mathcal{T}\}$ .

**Output:** Class labels  $\{\hat{Y}_j : j \in [n] \setminus \mathcal{T}\}$ .

*Step 1:* Compute the eigen-decomposition of  $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{U}^T$ .

*Step 2:* Let  $d$  be the “elbow” in the scree plot of  $\mathbf{A}$ ,  $\mathbf{S}_{\mathbf{A}}$  the diagonal matrix of the top  $d$  eigenvalues of  $\mathbf{A}$  and  $\mathbf{U}_{\mathbf{A}}$  the corresponding columns of  $\mathbf{U}$ .

*Step 3:* Define  $\mathbf{Z}$  to be  $\mathbf{U}_{\mathbf{A}}\mathbf{S}_{\mathbf{A}}^{1/2}$ . Denote by  $Z_i$  the  $i$ -th row of  $\mathbf{Z}$ . Define  $\mathbf{Z}_{\mathcal{T}}$  to be the rows of  $\mathbf{Z}$  corresponding to the index set  $\mathcal{T}$ .  $\mathbf{Z}$  is called the adjacency spectral embedding of  $\mathbf{A}$ .

*Step 4:* Find a *linear* classifier  $\tilde{g}_n$  that minimizes the empirical  $\varphi$ -loss when trained on  $(\mathbf{Z}_{\mathcal{T}}, \mathbf{Y}_{\mathcal{T}})$  where  $\varphi$  is a *convex* loss function that is a surrogate for 0 – 1 loss.

*Step 5:* Apply  $\tilde{g}_n$  on the  $\{Z_j : j \in [n] \setminus \mathcal{T}\}$  to obtain the  $\{\hat{Y}_j : j \in [n] \setminus \mathcal{T}\}$ .

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Euclidean space  $\mathbb{R}^d$  followed by inference in that space. This approach is well-represented in the literature of multidimensional scaling, spectral clustering, and manifold learning. The approach’s popularity is due partly to its simplicity, as after the embedding step, the vertices of  $G$  are now points in  $\mathbb{R}^d$  and classification or clustering can proceed in an almost identical manner to that of the classical setting, with a plethora of well-established and robust inference procedures available. In addition, theoretical justifications for the embedding step are also available. For example in the spectral clustering and manifold learning literature, the embedding step is often based on the spectral decomposition of the (combinatorial or normalized) Laplacians matrices of the graph. It can then be shown that, under mild conditions on the construction of  $G$ , the Laplacian matrices converge in some sense to the corresponding Laplace-Beltrami operators on the domain. Thus, the eigenvalues and eigenvectors of the graph Laplacians converge to the eigenvalues and eigenfunctions of the corresponding operator. See for example von Luxburg et al. (2008); Hein et al. (2007); von Luxburg (2007); Coifman and Lafon (2006); Belkin and Niyogi (2005); Hein et al. (2005); Singer (2006); Rosasco et al. (2010) and the references therein for a survey of the results.

The above cited results suggest that the embedding is conducive to the subsequent inference task, but as they are general convergence results and do not explicitly consider the subsequent inference problem, they do not directly demonstrate that inference using the embeddings are meaningful. Recently, there has been investigations that coupled the embedding step with the subsequent inference step for several widely-used random models for constructing  $G$ . For example, Rohe et al. (2011); Sussman et al. (2012a); Fishkind et al. (2013); Chaudhuri et al. (2012) showed that clustering using the embeddings can be consistent for graphs constructed based on the stochastic block model (Holland et al., 1983), the random dot product model (Young and Scheinerman, 2007), and the extended partition model (Karrer and Newman, 2011). In related works, Sussman et al. (2012b); Tang et al. (2013) showed that one can obtain universally consistent vertex classification for graphs constructed based on the random dot product model or its generalization, the latent position model (Hoff et al., 2002). However, a major technical difficulty of the approach arises when one tries to use it to classify unlabeled *out-of-sample* vertices without including

them in the embedding stage. A possible solution is to recompute the embedding for each new vertex. However, as many of the popular embedding methods are spectral in nature, e.g., classical multidimensional scaling (Torgerson, 1952), Isomap (Tenenbaum et al., 2000), Laplacian eigenmaps (Belkin and Niyogi, 2003) and diffusion maps (Coifman and Lafon, 2006), the computational costs for each new embedding is of order  $O(n^3)$ , making this solution computationally expensive. To circumvent this technical difficulty, out-of-sample extensions for many of the popular embedding methods such as those listed above have been devised, see e.g. Faloutsos and Lin (1995); Platt (2005); Bengio et al. (2004); Williams and Seeger (2001); de Silva and Tenenbaum (2003); Wang et al. (1999); Trosset and Priebe (2008). In these out-of-sample extensions, the embedding for the in-sample points is kept fixed and the out-of-sample vertices are inserted into the configuration of the in-sample points. The computational costs are thus much less, e.g., linear in the number of in-sample vertices for each insertion of an out-of-sample vertex into the existing configuration.

In this paper, we study the out-of-sample extension for the embedding step in Algorithm 1 and its impact on the subsequent inference tasks. In particular we show that, under the latent position graph model and for sufficiently large  $n$ , the mapping of the out-of-sample vertices is close to its true latent position. This suggests that inference for the out-of-sample vertices is possible.

The structure of our paper is as follows. We introduce the framework of latent position graphs in § 2. We describe the out-of-sample extension for the adjacency spectral embedding and analyze its properties in § 3. In § 4, we investigate via simulation the implications of performing inference using these out-of-sample embeddings. We conclude the paper with discussion of related work, how the results presented herein can be extended, and other implications.

## 2. Framework

Let  $\mathcal{X}$  be a compact metric space and let  $\kappa: \mathcal{X} \times \mathcal{X} \mapsto [0, 1]$  be a continuous positive definite kernel on  $\mathcal{X}$ . Let  $F$  be a probability measure on the Borel  $\sigma$ -field of  $\mathcal{X}$ . Now, for a given  $n$ , let  $X_1, X_2, \dots, X_n \stackrel{\text{i.i.d.}}{\sim} F$ . Let  $\rho_n \in (0, 1)$  be arbitrary ( $\rho_n$  can depend on  $n$ ). Define  $\mathbf{K} = (\rho_n \kappa(X_i, X_j))_{i,j=1}^n$ . Let  $\mathbf{A}$  be a symmetric, hollow, random binary matrix where the entries  $\{\mathbf{A}_{ij}\}_{i < j}$  of  $\mathbf{A}$  are *conditionally independent* Bernoulli random variables given the  $\{X_i\}_{i=1}^n$ , with  $\mathbb{P}[\mathbf{A}_{ij} = 1] = \mathbf{K}_{ij} = \rho_n \kappa(X_i, X_j)$  for all  $i, j \in \{1, 2, \dots, n\}$ ,  $i < j$ . A graph  $G$  whose adjacency matrix  $\mathbf{A}$  is constructed as above is an instance of a latent position graph. The factor  $\rho_n$  controls the sparsity of the resulting graph. For example, if  $\kappa > 0$  on  $\mathcal{X} \times \mathcal{X}$ , then  $\rho_n = (\log n)/n$  leads to sparse, connected graphs almost surely,  $\rho_n = 1/n$  leads to graphs with a single giant connected component, and  $\rho_n = C > 0$  for some fixed  $C$  leads to dense graphs. We will denote by  $G \sim \text{LPM}(\mathcal{X}, F, \kappa, \rho_n)$  an instance of a latent position graph on  $\mathcal{X}$  with distribution  $F$ , link function  $\kappa$ , and sparsity factor  $\rho_n$ . We shall assume throughout this paper that  $n\rho_n = \omega(\log n)$  for some  $k \geq 1$ . That is, the expected average degree of  $\mathbf{A}$  grows at least as fast as  $\omega(\log n)$ .

An example of a latent position graph model is the random dot product graph (RDPG) model of Young and Scheinerman (2007). In the RDPG model,  $\mathcal{X}$  is taken to be the unit simplex in  $\mathbb{R}^d$  and the link function  $\kappa$  is the Euclidean inner product. One can then take  $F$  to be a Dirichlet distribution on the unit simplex. Another example of a latent position

graph model takes  $\mathcal{X}$  as a compact subset of  $\mathbb{R}^d$  and the link function  $\kappa$  is a radial basis function, e.g., a Gaussian kernel  $\exp(-\|X_i - X_j\|^2)$ . This model is similar to the method of constructing graphs based on point clouds in  $\mathbb{R}^d$  in the manifold learning literature. The small difference is that in the case presented here, the Gaussian kernel is used for generating the edges probabilities in the Bernoulli trials, i.e., the edges are unweighted but random, whereas in the manifold learning literature, the Gaussian kernel is used to assign weights to the edges i.e., the edges are weighted but deterministic.

The latent position graph model and the related latent space approach (Hoff et al., 2002) is widely used in network analysis. It is a generalization of the stochastic block model (SBM) (Holland et al., 1983) and variants such as the degree-corrected SBM (Karrer and Newman, 2011), the mixed-membership SBM (Airoldi et al., 2008) and the random dot product graph model (Young and Scheinerman, 2007). It is also closely related to the inhomogeneous random graph model (Bollobás et al., 2007) and the exchangeable graph model (Diaconis and Janson, 2008).

We now define a feature map  $\Phi: \mathcal{X} \mapsto l_2$  for  $\kappa$ .  $\Phi$  will serve as our *canonical* feature map, i.e., our subsequent results for the out-of-sample extension are based on bounds for the deviation of the out-of-sample embedding from the canonical feature map representation, e.g., Theorem 2. The kernel  $\kappa$  defines an integral operator  $\mathcal{K}$  on  $L^2(\mathcal{X}, F)$ , the space of  $F$ -square-integrable functions on  $\mathcal{X}$ , via

$$(\mathcal{K}g)(x) = \int_{\mathcal{X}} \kappa(x, x')g(x')F(dx'). \quad (1)$$

$\mathcal{K}$  is then a compact operator and is of trace class (see e.g., Theorem 4.1 in Blanchard et al. (2007)). Let  $\{\lambda_j(\mathcal{K})\}$  be the set of eigenvalues of  $\mathcal{K}$  in non-increasing order. The  $\{\lambda_j\}$  are non-negative and discrete, and their only accumulation point is at 0. Let  $\{\psi_j\}$  be a set of orthonormal eigenfunctions of  $\mathcal{K}$  corresponding to the  $\{\lambda_j(\mathcal{K})\}$ . Then by Mercer's representation theorem (Cucker and Smale, 2002), one can write

$$\kappa(x, x') = \sum_{j=1}^{\infty} \lambda_j \psi_j(x) \psi_j(x')$$

with the above sum converging absolutely and uniformly for each  $x$  and  $x'$  in  $\text{supp}(F) \times \text{supp}(F)$ . We define the feature map  $\Phi: \mathcal{X} \mapsto l_2$  via

$$\Phi(x) = (\sqrt{\lambda_j} \psi_j(x) : j = 1, 2, \dots). \quad (2)$$

We define a related feature map  $\Phi_d: \mathcal{X} \mapsto \mathbb{R}^d$  for  $d \geq 1$  by

$$\Phi_d(x) = (\sqrt{\lambda_j} \psi_j(x) : j = 1, 2, \dots, d). \quad (3)$$

We will refer to  $\Phi_d$  as the *truncated* feature map or as the truncation of  $\Phi$ . We note that the feature map  $\Phi$  and  $\Phi_d$  are defined in terms of the spectrum and eigenfunctions of  $\mathcal{K}$  and thus do not depend on the scaling parameter  $\rho_n$ .

We conclude this section with some notations that will be used in the remainder of the paper. Let us denote by  $\mathcal{M}_d$  and  $\mathcal{M}_{d,n}$  the set of  $d \times d$  matrices and  $d \times n$  matrices on  $\mathbb{R}$ , respectively. For a given adjacency matrix  $\mathbf{A} \in \mathcal{M}_n$ , let  $\mathbf{U}\mathbf{S}\mathbf{U}^T$  be the eigen-decomposition

of  $\mathbf{A}$ . For a given  $d \geq 1$ , let  $\mathbf{S}_{\mathbf{A}} \in \mathcal{M}_d$  be the diagonal matrix comprising of the  $d$  largest eigenvalues of  $\mathbf{A}$  and let  $\mathbf{U}_{\mathbf{A}} \in \mathcal{M}_{n,d}$  be the matrix comprising of the corresponding eigenvectors. The matrices  $\mathbf{S}_{\mathbf{K}}$  and  $\mathbf{U}_{\mathbf{K}}$  are defined similarly. For a matrix  $\mathbf{M}$ ,  $\|\mathbf{M}\|$  denotes the spectral norm of  $\mathbf{M}$  and  $\|\mathbf{M}\|_F$  denotes the Frobenius norm of  $\mathbf{M}$ . For a vector  $\mathbf{v} \in \mathbb{R}^n$ ,  $v_i$  denote the  $i$ -th component of  $\mathbf{v}$  and  $\|\mathbf{v}\|$  denotes the Euclidean norm of  $\mathbf{v}$ .

### 3. Out-of-sample extension

We now introduce the out-of-sample extension for the adjacency spectral embedding of Algorithm 1.

**Definition 1** Suppose  $\mathbf{A}$  is an instance of  $\text{LPM}(\mathcal{X}, F, \kappa, \rho_n)$  on  $n$  vertices. Let  $\mathbf{Z} = \mathbf{U}_{\mathbf{A}} \mathbf{S}_{\mathbf{A}}^{1/2} \in \mathcal{M}_{n,d}$  and denote by  $\mathbf{Z}^\dagger \in \mathcal{M}_{d,n}$  the matrix  $(\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T$ ;  $\mathbf{Z}^\dagger$  is the Moore-Penrose pseudo-inverse of  $\mathbf{Z}$ . Let  $Z_i^\dagger$  be the  $i$ -th column of  $\mathbf{Z}^\dagger$ . For a given  $X \in \mathcal{X}$ , let  $T_n(X; \{X_i\}_{i=1}^n)$  be the (random) mapping defined by

$$T_n(X) := T_n(X; \{X_i\}_{i=1}^n) := \sum_{i=1}^n \xi_i Z_i^\dagger = \mathbf{Z}^\dagger \boldsymbol{\xi} \quad (4)$$

where  $\boldsymbol{\xi}$  is a vector of independent Bernoulli random variables with  $\mathbb{P}[\xi_i = 1] = \rho_n \kappa(X, X_i)$ . The map  $T_n$  is the out-of-sample extension of  $X$ ; that is,  $T_n(X)$  extends the embedding  $X_i$  for the sampled  $\{X_i\}_{i=1}^n$  to any  $X \in \mathcal{X}$ .

We make some quick remarks regarding Definition 1. First, we note that the out-of-sample extension give rise to i.i.d. random variables, i.e., if  $X'_1, X'_2, \dots, X'_m$  are i.i.d from  $F$ , then the  $T_n(X'_1; \{X_i\}_{i=1}^n), T_n(X'_2; \{X_i\}_{i=1}^n), \dots, T_n(X'_m; \{X_i\}_{i=1}^n)$  are i.i.d. random variables in  $\mathbb{R}^d$ . Secondly,  $T_n(X; \{X_i\}_{i=1}^n)$  is a random mapping for any given  $X$ , even when conditioned on the  $\{X_i\}$ . The randomness of  $T_n$  arises from the randomness in the adjacency matrix  $\mathbf{A}$  induced by the in-sample points  $\{X_i\}_{i=1}^n$  as well as the randomness in the Bernoulli random variables  $\boldsymbol{\xi}$  used in Eq. (4). Thirdly, Eq. (4) states that the out-of-sample extension  $T_n(X)$  of  $X$  is the least square solution to  $\|\mathbf{Z} \zeta - \boldsymbol{\xi}\|$ , i.e.,  $\mathbf{Z} T_n(X)$  is the least square projection of the (random) vector  $\boldsymbol{\xi}$  onto the subspace spanned by the columns of  $\mathbf{Z}$ . The use of the least square solution to  $\boldsymbol{\xi}$ , or equivalently the projection of  $\boldsymbol{\xi}$  onto the subspace spanned by the configuration of the in-sample points, is standard in many of the out-of-sample extensions to the popular embedding methods, see e.g. Bengio et al. (2004); Anderson and Robinson (2003); Faloutsos and Lin (1995); de Silva and Tenenbaum (2003); Wang et al. (1999). In general,  $\boldsymbol{\xi}$  is a vector containing the proximity (similarity or dissimilarity) between the out-of-sample point and the in-sample points and the least square solution can be related to the Nyström method for approximating the eigenvalues and eigenvectors of a large matrix, see e.g. Bengio et al. (2004); Platt (2005); Williams and Seeger (2001).

Finally, the motivation for Definition 1 can be gleaned by considering the setting of random dot product graphs. In this setting,  $\mathbf{K} = \rho_n \mathbf{X} \mathbf{X}^T$  where  $\mathbf{X}$  is the matrix whose rows correspond to the sampled latent positions as points in  $\mathbb{R}^d$ . Then  $\tilde{\mathbf{Z}} = \mathbf{U}_{\mathbf{K}} \mathbf{S}_{\mathbf{K}}^{1/2}$  is equivalent (up to rotation) to  $\rho_n^{1/2} \mathbf{X}$ . Now let  $\boldsymbol{\xi}$  be a vector of Bernoulli random variables with  $\mathbb{E}[\boldsymbol{\xi}] = \mathbf{X} \mathbf{X}$ . Then  $\tilde{\mathbf{Z}}^\dagger \mathbb{E}[\boldsymbol{\xi}] = \rho_n^{-1/2} \mathbf{X}^\dagger \rho_n \mathbf{X} \mathbf{X} = \rho_n^{1/2} \mathbf{X}$ . Thus, if we can show that  $T_n(X; \{X_i\}_{i=1}^n) = \mathbf{Z}^\dagger \boldsymbol{\xi} \approx \tilde{\mathbf{Z}}^\dagger \mathbb{E}[\boldsymbol{\xi}]$ , then we have  $\rho_n^{-1/2} T_n(X; \{X_i\}_{i=1}^n) \approx X$ . As  $\mathbf{Z}$  is “close”

to  $\tilde{\mathbf{Z}}$  (Tang et al., 2013; Sussman et al., 2012b) and  $(\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)(\boldsymbol{\xi} - \mathbb{E}[\boldsymbol{\xi}])$  is “small” with high probability, see e.g. Tropp (2012); Yurinsky (1995), the relationship  $\rho_n^{-1/2} T_n(X; \{X_i\}_{i=1}^n) \approx X$  holds for random dot product graphs. As the latent position graphs with positive definite kernels  $\kappa$  can be thought of as being random dot product graphs with latent positions being “points” in  $l_2$ , one expects a relationship of the form  $\rho_n^{-1/2} T_n(X; \{X_i\}_{i=1}^n) \approx \Phi_d(X)$  for the (truncated) feature map  $\Phi$  of  $\kappa$ . Precise statements of the relationships are given in Theorem 2 and Corollary 3 below.

### 3.1 Out-of-sample extension and Nyström approximation

In the following discussion, we give a brief description of the relationship between Definition 1 and the Nyström approximation of Drineas and Mahoney (2005); Gittens and Mahoney (2013) which they called “sketching”. Let  $\mathbf{A} \in \mathcal{M}_n$  be symmetric and let  $\mathbf{S} \in \mathcal{M}_{n,l}$  with  $l \ll n$ . Following Gittens and Mahoney (2013), let  $\mathbf{C} = \mathbf{A}\mathbf{S}$  and  $\mathbf{A}_\mathbf{S} = \mathbf{S}^T \mathbf{A} \mathbf{S}$ . Then  $\mathbf{C} \mathbf{A}_\mathbf{S}^\dagger \mathbf{C}^T$  serves as a low-rank approximation to  $\mathbf{A}$  with rank at most  $l$  and Gittens and Mahoney (2013) refers to  $\mathbf{S}$  as the sketching matrix. The different choices for  $\mathbf{S}$  leads to different low-rank approximations. For example, a subsampling scheme correspond to the entries of  $\mathbf{S}$  being binaries  $\{0, 1\}$  variable with a single non-zero entry in each row or column. More general entries for  $\mathbf{S}$  correspond to a linear projection of the columns of  $\mathbf{A}$ . There are times when  $\mathbf{A}_\mathbf{S}$  is ill-conditioned and one is instead interested in the best rank  $d$  approximation to  $\mathbf{A}_\mathbf{S}$ , i.e., the sketched version of  $\mathbf{A}$  is  $\mathbf{C} \tilde{\mathbf{A}}_\mathbf{S}^\dagger \mathbf{C}^T$  where  $\tilde{\mathbf{A}}_\mathbf{S}$  is a rank  $d$  approximation to  $\mathbf{A}_\mathbf{S}$ .

Suppose now that  $\mathbf{S}$  correspond to a subsampling scheme. Then  $\mathbf{A}_\mathbf{S} = \mathbf{S}^T \mathbf{A} \mathbf{S}$  correspond to a sub-matrix of  $\mathbf{A}$ , i.e.,  $\mathbf{A}_\mathbf{S}$  correspond to the rows and columns indexed by  $\mathbf{S}$ . Without loss of generality, we assume that  $\mathbf{A}_\mathbf{S}$  is the first  $l$  rows and columns of  $\mathbf{A}$ . That is, we have the following decomposition

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{S,S} & \mathbf{A}_{S,S^c} \\ \mathbf{A}_{S^c,S} & \mathbf{A}_{S^c,S^c} \end{bmatrix} \quad (5)$$

where  $S = \{1, 2, \dots, l\}$  and  $S^c = \{1, 2, \dots, n\} \setminus S$ . We have abused notations slightly by writing  $\mathbf{A}_\mathbf{S} = \mathbf{A}_{S,S}$ . Then  $\mathbf{C} \mathbf{A}_\mathbf{S}^\dagger \mathbf{C}^T$  can be written as

$$\begin{aligned} \mathbf{C} \mathbf{A}_\mathbf{S}^\dagger \mathbf{C}^T &= \begin{bmatrix} \mathbf{A}_{S,S} & \mathbf{A}_{S,S^c} \\ \mathbf{A}_{S^c,S} & \mathbf{A}_{S^c,S^c} \end{bmatrix} \begin{bmatrix} \mathbf{I}_l \\ \mathbf{0} \end{bmatrix} \mathbf{A}_{S,S}^\dagger [\mathbf{I}_l | \mathbf{0}] \begin{bmatrix} \mathbf{A}_{S,S} & \mathbf{A}_{S,S^c} \\ \mathbf{A}_{S^c,S} & \mathbf{A}_{S^c,S^c} \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{A}_{S,S} \\ \mathbf{A}_{S^c,S} \end{bmatrix} \mathbf{A}_{S,S}^\dagger [\mathbf{A}_{S,S} | \mathbf{A}_{S,S^c}] \\ &= \begin{bmatrix} \mathbf{A}_{S,S} \mathbf{A}_{S,S}^\dagger \mathbf{A}_{S,S} & \mathbf{A}_{S,S} \mathbf{A}_{S,S}^\dagger \mathbf{A}_{S,S^c} \\ \mathbf{A}_{S^c,S} \mathbf{A}_{S,S}^\dagger \mathbf{A}_{S,S} & \mathbf{A}_{S^c,S} \mathbf{A}_{S,S}^\dagger \mathbf{A}_{S^c,S^c} \end{bmatrix}. \end{aligned} \quad (6)$$

Let us now take  $\tilde{\mathbf{A}}_\mathbf{S}$  to be the best rank  $d$  approximation to  $\mathbf{A}_\mathbf{S}$  in the positive semidefinite cone. Then  $\mathbf{C} \tilde{\mathbf{A}}_\mathbf{S}^\dagger \mathbf{C}^T$  can be written as

$$\mathbf{C} \tilde{\mathbf{A}}_\mathbf{S}^\dagger \mathbf{C}^T = \begin{bmatrix} \mathbf{A}_{S,S} \tilde{\mathbf{A}}_{S,S}^\dagger \mathbf{A}_{S,S} & \mathbf{A}_{S,S} \tilde{\mathbf{A}}_{S,S}^\dagger \mathbf{A}_{S,S^c} \\ \mathbf{A}_{S^c,S} \tilde{\mathbf{A}}_{S,S}^\dagger \mathbf{A}_{S,S} & \mathbf{A}_{S^c,S} \tilde{\mathbf{A}}_{S,S}^\dagger \mathbf{A}_{S^c,S^c} \end{bmatrix}. \quad (7)$$

Now let  $\mathbf{X} \in \mathcal{M}_{l,d}$  be such that  $\mathbf{X}\mathbf{X}^T = \mathbf{A}_{S,S}\tilde{\mathbf{A}}_{S,S}^\dagger\mathbf{A}_{S,S} = \tilde{\mathbf{A}}_{S,S}$  and let  $\mathbf{Y} = (\mathbf{X}^\dagger\mathbf{A}_{S,S^c})^T \in \mathcal{M}_{n-l,d}$ . Then Eq. (7), can be written as

$$\begin{aligned} \mathbf{C}\tilde{\mathbf{A}}_S^\dagger\mathbf{C}^T &= \begin{bmatrix} \mathbf{A}_{S,S}\tilde{\mathbf{A}}_{S,S}^\dagger\mathbf{A}_{S,S} & \mathbf{A}_{S,S}\tilde{\mathbf{A}}_{S,S}^\dagger\mathbf{A}_{S,S^c} \\ \mathbf{A}_{S^c,S}\tilde{\mathbf{A}}_{S,S}^\dagger\mathbf{A}_{S,S} & \mathbf{A}_{S^c,S}\tilde{\mathbf{A}}_{S,S}^\dagger\mathbf{A}_{S^c,S^c} \end{bmatrix} \\ &= \begin{bmatrix} \tilde{\mathbf{A}}_{S,S} & \mathbf{A}_{S,S}\tilde{\mathbf{A}}_{S,S}^\dagger\mathbf{A}_{S,S^c} \\ \mathbf{A}_{S^c,S}\tilde{\mathbf{A}}_{S,S}^\dagger\mathbf{A}_{S,S} & \mathbf{A}_{S^c,S}\tilde{\mathbf{A}}_{S,S}^\dagger\mathbf{A}_{S^c,S^c} \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{X}\mathbf{X}^T & \mathbf{X}\mathbf{Y}^T \\ \mathbf{Y}\mathbf{X}^T & \mathbf{Y}\mathbf{Y}^T \end{bmatrix}. \end{aligned} \quad (8)$$

We thus note that if  $\mathbf{A}$  is an adjacency matrix on a graph  $G$  with  $n$  vertices then  $\mathbf{A}_S$  is the adjacency matrix of the induced subgraph of  $G$  on  $l$  vertices. Then  $\tilde{\mathbf{A}}_S = \mathbf{U}_\mathbf{A}\mathbf{S}_\mathbf{A}\mathbf{U}_\mathbf{A}$  is the rank  $d$  approximation to  $\mathbf{A}$  that arises from the adjacency spectral embedding of  $\mathbf{A}$ . Thus  $\mathbf{X} = \mathbf{U}_\mathbf{A}\mathbf{S}_\mathbf{A}^{1/2}$  and therefore  $\mathbf{Y} = (\mathbf{X}^\dagger\mathbf{A}_{S,S^c})^T$  is the matrix each of whose rows correspond to an out-of-sample embedding of the rows of  $\mathbf{A}_{S,S^c}$  into  $\mathbb{R}^d$  as defined in Definition 1.

In summary, in the context of adjacency spectral embedding, the embeddings of the in-sample and out-of-sample vertices generate a Nyström approximation to  $\mathbf{A}$  and a Nyström approximation to  $\mathbf{A}$  can be used to derive the embeddings (through an eigen-decomposition) for the in-sample and out-of-sample vertices.

### 3.2 Estimation of feature map

The main result of this paper is the following result on the out-of-sample mapping error  $T_n(X) - \Phi_d(X)$ . Its proof is given in the appendix. We note that the dependency on  $\kappa$  and  $F$  is hidden in the spectral gap  $\delta_d$  of  $\mathcal{K}$ , the integral operator induced by  $\kappa$  and  $F$ .

**Theorem 2** *Let  $d \geq 1$  be given. Denote by  $\delta_d$  the quantity  $\lambda_d(\mathcal{K}) - \lambda_{d+1}(\mathcal{K})$  and suppose that  $\delta_d > 0$ . Let  $\eta \in (0, 1/2)$  be arbitrary. Then there exists an orthogonal  $\mathbf{W}$  such that*

$$\mathbb{P}\left[\|\rho_n^{-1/2}\mathbf{W}T_n(X) - \Phi_d(X)\| \leq C\delta_d^{-3}\sqrt{d\frac{\log(n/\eta)}{n\rho_n}}\right] \geq 1 - 2\eta \quad (9)$$

for some constant  $C$  independent of  $n, \eta, \kappa, d$ , and  $F$ .

We note the following corollary of the above result for the case where the latent position model is the random dot product graph model. For this case, the operator  $\mathcal{K}$  is of rank  $d$  and the truncated feature map  $\Phi_d(X)$  is equal (up to rotation) to the latent position  $X$ .

**Corollary 3** *Let  $\mathbf{A} \in \mathcal{M}_n$  be an instance of RDPG( $\mathbb{R}^d, F$ ). Denote by  $\delta_d$  the smallest eigenvalue of  $\mathbb{E}[XX^T]$ . Let  $\eta \in (0, 1/2)$  be arbitrary. Then there exists an orthogonal  $\mathbf{W}$  such that*

$$\mathbb{P}\left[\|\rho_n^{-1/2}\mathbf{W}T_n(X) - X\| \leq C\delta_d^{-3}\sqrt{d\frac{\log(n/\eta)}{n\rho_n}}\right] \geq 1 - 2\eta \quad (10)$$

for some constant  $C$  independent of  $n, \eta, d$ , and  $F$ .



We note the following result from [Tang et al. \(2013\)](#) that serves as an analogue of Theorem 2 for the in-sample points. We note that, other than the possibly different hidden constants, the bound for the out-of-sample points in Eq. (9) is almost identical to that of the in-sample points in Eq. (11). The main difference is in the power of the spectral gap in the bounds, i.e.,  $\delta_d^{-3}$  against  $\delta_d^{-2}$ . This difference might be due to the proof technique and not inherent in the distinction of out-of-sample versus in-sample points. We also note that one can take the orthogonal matrix  $\mathbf{W}$  for the out-of-sample points to be the same as the in-sample points, i.e., the rotation that makes the in-sample points “close” to the truncated feature map  $\Phi_d$  also makes the out-of-sample points “close” to  $\Phi_d$ .

**Theorem 4** *Let  $d \geq 1$  be given. Denote by  $\delta_d$  the quantity  $\lambda_d(\mathcal{X}) - \lambda_{d+1}(\mathcal{X})$  and suppose that  $\delta_d > 0$ . Let  $\eta \in (0, 1/2)$  be arbitrary. Let  $\hat{\Phi}_d(X_i)$  denote the  $i$ -th row of  $\mathbf{U}_\mathbf{A} \mathbf{S}_\mathbf{A}^{1/2}$ . Then there exists a unitary matrix  $\mathbf{W} \in \mathcal{M}_d(\mathbb{R})$  such that for all  $i \in [n]$*

$$\mathbb{P}\left[\|\rho_n^{-1/2} \mathbf{W} \hat{\Phi}_d(X_i) - \Phi_d(X_i)\| \leq C \delta_d^{-2} \sqrt{\frac{d \log(n/\eta)}{n \rho_n}}\right] \geq 1 - 2\eta \quad (11)$$

for some constant  $C$  independent of  $n, \eta, \kappa, d$ , and  $F$ .

Theorem 2 and its corollary states that in the latent position model, the out-of-sample embedded points can be rotated to be very close to the true feature map with high probability. This suggests that successful statistical inference on the out-of-sample points is possible. As an example, we investigate the problem of vertex classification for latent position graphs whose link functions  $\kappa$  belong to the class of universal kernels. Specifically, we consider an approach that proceeds by embedding the vertices into some  $\mathbb{R}^d$  followed by finding a linear discriminant in that space. It was shown in [Tang et al. \(2013\)](#) that such an approach can be made to yield a universally consistent vertex classifier if the vertex to be classified is embedded in-sample as the number of in-sample vertices increases to  $\infty$ . In the following discussion we present a variation of this result in the case where the vertex to be classified is embedded out-of-sample and the number of in-sample vertices is fixed and finite. We show that under this out-of-sample setting, the misclassification rate can be made arbitrarily small provided that the number of in-sample vertices is sufficiently large (see Theorem 7).

**Definition 5** *A continuous kernel on a metric space  $\mathcal{X}$  is said to be a universal kernel, if for some choice of feature map  $\Phi: \mathcal{X} \mapsto H$  of  $\kappa$  to some Hilbert space  $H$ , the class of functions of the form*

$$\mathcal{F}_\Phi = \{\langle w, \Phi \rangle_H : w \in H\} \quad (12)$$

*is dense in  $\mathcal{C}(\mathcal{X})$ , i.e., for any continuous  $g: \mathcal{X} \mapsto \mathbb{R}$  and any  $\epsilon > 0$ , there exists  $f \in \mathcal{F}_\Phi$  such that  $\|f - g\|_\infty < \epsilon$ .*

We note that if  $\kappa$  is such that  $\mathcal{F}_\Phi$  is dense in  $\mathcal{C}(\mathcal{X})$  for some feature map  $\Phi$  of  $\kappa$ , then  $\mathcal{F}_{\Phi'}$  is dense in  $\mathcal{C}(\mathcal{X})$  for any feature map  $\Phi'$  of  $\kappa$ , i.e., the universality of  $\kappa$  is independent of its choice of feature map. In addition, any feature map  $\Phi$  of a universal kernel  $\kappa$  is injective. The following result lists several well-known universal kernels. For more on universal kernels, the reader is referred to [Steinwart \(2001\)](#); [Micchelli et al. \(2006\)](#).



**Proposition 6** *Let  $S$  be a compact subset of  $\mathbb{R}^d$ . Then the following kernels are universal on  $S$ .*

- *exponential kernel  $\kappa(x, y) = \exp(\langle x, y \rangle)$ .*
- *Gaussian kernel  $\kappa(x, y) = \exp(-\|x - y\|^2/\sigma^2)$  for  $\sigma > 0$ .*
- *The binomial kernel  $\kappa(x, y) = (1 - \langle x, y \rangle)^{-\alpha}$  for  $\alpha > 0$ .*
- *inverse multiquadratics  $\kappa(x, y) = (c^2 + \|x - y\|^2)^{-\beta}$  for  $\beta > 0$ .*

Let  $\mathcal{C}_\Phi^{(d)}$  be the class of linear functions on  $\mathbb{R}^d$  induced by the feature map  $\Phi_d$  whose linear coefficients are normalized to have norm at most  $d$ , i.e.,  $g \in \mathcal{C}_\Phi^{(d)}$  if and only if  $g$  is of the form

$$g(X) = \langle w, \Phi_d(X) \rangle_{\mathbb{R}^d}$$

for some  $w \in \mathbb{R}^d, \|w\| \leq d$ . We note that the  $\{\mathcal{C}_\Phi^{(d)}\}$  is a nested increasing sequence and furthermore that

$$\bigcup_{d \geq 1} \mathcal{C}_\Phi^{(d)} = \mathcal{F}_\Phi = \{\langle w, \Phi \rangle_{\mathcal{H}} : w \in \mathcal{H}\}.$$

Now, given  $\{X_i\}_{i=1}^n$ , let  $\mathcal{C}_{T_n}^{(d)}$  be the class of linear functions on  $\mathbb{R}^d$  induced by the out-of-sample extension  $T_n(X; \{X_i\}_{i=1}^n)$ , i.e.,  $g \in \mathcal{C}_{T_n}^{(d)}$  if and only if  $g$  is of the form

$$g(X) = \langle w, T_n(X; \{X_i\}_{i=1}^n) \rangle_{\mathbb{R}^d}. \quad (13)$$

**Theorem 7** *Let  $\kappa$  be a universal kernel on  $\mathcal{X}$ . Let  $\eta > 0$  be arbitrary. Then for any  $F_{X,Y}$  and any  $\epsilon > 0$ , there exists  $d$  and  $n_0$  such that if  $n \geq n_0$  then*

$$L_{T_n}^* \leq L^* + \epsilon, \quad (14)$$

where  $T_n: \mathcal{X} \mapsto \mathbb{R}^d$  is the out-of-sample mapping as defined in Definition 1 and  $L^*$  is the Bayes risk for the classification problem with distribution  $F_{X,Y}$ .

We make a brief remark regarding Theorem 7. The term  $L_{T_n}^*$  in Eq. (14) refers to the Bayes risk for the classification problem given by the out-of-sample mapping  $T_n$ . As noted earlier,  $T_n(X; \{X_i\}_{i=1}^n)$  is a random mapping for any given  $X$ , even when conditioned on the  $\{X_i\}$  as  $T_n(X)$  also depends on the latent position graph  $\mathbf{A}$  generated by the  $\{X_i\}$ . As such, with slight abuse of notations,  $L_{T_n}^*$  refers to the Bayes-risk of the mapping  $T_n$  when not conditioned on any set of  $\{X_i\}$ . That is,  $L_{T_n}^*$  is the Bayes-risk for out-of-sample embedding in the presence of  $n$  in-sample latent positions, i.e., the latent positions of the in-sample points are integrated out. As the information processing lemma implies  $L_{T_n}^* \geq L^*$ , one can view Eq. (14) as a sort of converse to the information processing lemma in that the degradation due to the out-of-sample embedding transformation  $T_n$  can be made negligible if the number of in-sample points is sufficiently large.

**Proof** Let  $\varphi$  be any classification-calibrated (see Bartlett et al. (2006)) convex surrogate of the 0–1 loss. For any measurable function  $f: \mathcal{X} \mapsto \mathbb{R}$ , let  $R_{\varphi,f}$  be defined by  $\mathbb{E}[\varphi(Yf(X))]$ .

Let  $f^*$  be a measurable function such that  $R_{\varphi, f^*} = R_{\varphi}^* = \inf R_{\varphi, f}$  where the infimum is taken over the set of all measurable functions on  $\mathcal{X}$ . As  $\mathcal{F}_{\Phi}$  is dense in the set of measurable functions on  $\mathcal{X}$ , without loss of generality we can take  $f^* \in \mathcal{F}_{\Phi}$ . Now let  $\epsilon > 0$  be arbitrary. As  $\mathcal{F}_{\Phi} = \bigcup_{d \geq 1} \mathcal{C}_{\Phi}^{(d)}$ , and the  $\{\mathcal{C}_{\Phi}^{(d)}\}$  is a nested increasing sequence, there exists a  $d \geq 1$  such that for some  $\tilde{f} \in \mathcal{C}_{\Phi}^{(d)}$ , we have  $\|\tilde{f} - f^*\|_{\infty} < \epsilon$ . Thus, for any  $\epsilon > 0$ , there exists a  $d \geq 1$  such that for some  $\tilde{f} \in \mathcal{C}_{\Phi}^{(d)}$ ,  $R_{\varphi, \tilde{f}} - R_{\varphi}^* < \epsilon$ . Now let  $f \in \mathcal{C}_{\Phi}^{(d)}$  be arbitrary. Then  $f = \langle w, \Phi_d \rangle_{\mathbb{R}^d}$  for some  $w \in \mathbb{R}^d, \|w\| \leq d$ . Let  $g = \langle w, T_n \rangle_{\mathbb{R}^d}$  and consider the difference  $R_{\varphi, f} - R_{\varphi, g}$ . As  $\varphi$  is convex, it is locally-Lipschitz and

$$\begin{aligned} |R_{\varphi, f} - R_{\varphi, g}| &= |\mathbb{E}[\varphi(Yf(X)) - \varphi(Yg(X))]| \leq \mathbb{E}[|M(Yf(X) - Yg(X))|] \\ &\leq \mathbb{E}[M|\langle w, \Phi_d(X) - T_n(X) \rangle_{\mathbb{R}^d}|] \leq \mathbb{E}[M\sqrt{d}\|\Phi_d(X) - T_n(X)\|] \\ &\leq (1 - n^{-2}) * C\delta_d^{-3} \sqrt{\frac{d \log n}{n\rho_n}} + n^{-2}, \end{aligned} \quad (15)$$

for some constant  $M > 0$ . Furthermore, we can take  $M$  to be independent of  $f$ . Thus, there exists some  $n_0$  such that for all  $n \geq n_0$ ,  $\sup |R_{\varphi, f} - R_{\varphi, g}| \leq \epsilon$  where the supremum is taken over all  $w \in \mathbb{R}^d, \|w\| \leq d$ . Now let  $w^*$  be such that  $\langle w^*, \Phi_d \rangle = \operatorname{arginf}_{f \in \mathcal{C}_{\Phi}^{(d)}} R_{\varphi, f}$ . We then have

$$\inf_{g \in \mathcal{C}_{T_n}^{(d)}} R_{\varphi, g} \leq R_{\varphi, \langle w^*, T_n \rangle} \leq R_{\varphi, \langle w^*, \Phi_d \rangle} + \epsilon \leq \inf_{f \in \mathcal{C}_{\Phi}^{(d)}} R_{\varphi, f} + \epsilon \leq R_{\varphi}^* + 2\epsilon. \quad (16)$$

If  $\varphi$  is a classification-calibrated convex surrogate of the 0 – 1 loss, then there exists a non-decreasing function  $\psi: [0, 1] \mapsto [0, \infty)$  such that  $L(f) - L^* \leq \psi^{-1}(R_{\varphi, f} - R_{\varphi}^*)$  (Bartlett et al., 2006). Thus by Eq. (16) we have

$$L_{T_n}^* - L^* \leq L(\operatorname{sign}(\operatorname{arginf}_{g \in \mathcal{C}_{T_n}^{(d)}} R_{\varphi, g})) - L^* \leq \psi^{-1}(2\epsilon). \quad (17)$$

As  $\epsilon$  is arbitrary, the proof is completed. ■

## 4. Experimental Results

In this section, we illustrate the out-of-sample extension described in § 4 by studying its impact on classification performance through two simulation examples and a real data example. In our first example, data is simulated using a mixture of two multivariate normals in  $\mathbb{R}^2$ . The components of the mixture have equal prior and the first component of the mixture has mean parameter  $(1, 1)$  and identity covariance matrix while the second component has mean  $(-1, -1)$  and identity covariance matrix. We sample 10000 data points from this mixture and assign class labels in  $\{-1, 1\}$  to them according to the quadrant in which they fall, i.e., if  $X_i = (a, b) \in \mathbb{R}^2$  then  $Y_i = \operatorname{sign}(ab)$ . Fig 1a depicts the scatter plot of the sampled data colored according to their class labels. The Bayes risk is 0 for classifying the  $X_i$ . A latent position graph  $G$  is then generated based on the sampled data points with  $\kappa$  being the Gaussian kernel.

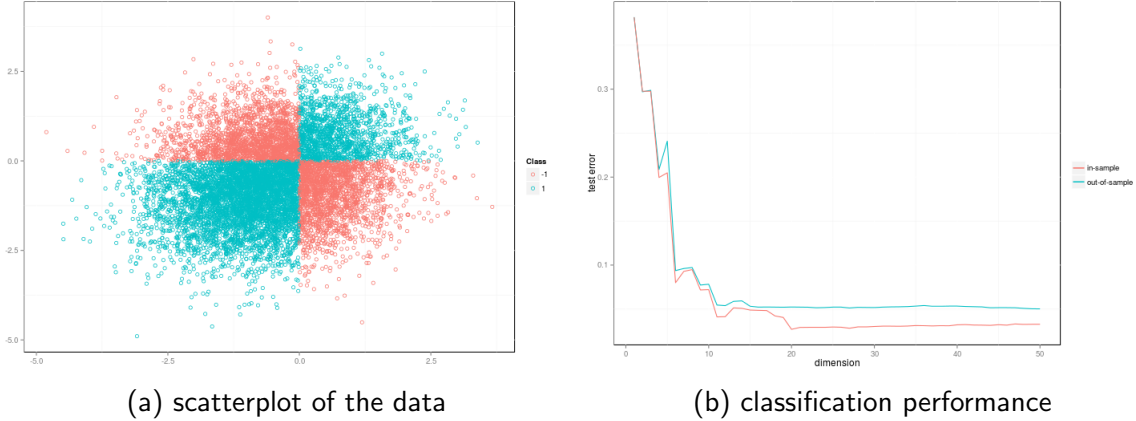


Figure 1: Comparison of the in-sample against out-of-sample classification performance for a simulated data example. The performance degradation due to out-of-sample embedding is less than 2%.

To measure the in-sample classification performance, we embed  $G$  into  $\mathbb{R}^d$  for  $d$  ranging from 1 through 50. A subset of 2000 vertices is then selected uniformly at random and designated as the training data set. The remaining 8000 vertices constitute the testing data set. For each choice of dimension  $d$ , we select a linear classifier  $g_d$  by performing a least square regression on the 2000 training data points and measure the classification error of  $g_d$  on the 8000 testing data points. The results are plotted in Fig 1b.

For the out-of-sample classification performance, we embed the induced graph  $G'$  formed by the 2000 training vertices in the above description. For each choice of dimension  $d$ , we out-of-sample embed the 8000 testing vertices into  $\mathbb{R}^d$ . For each choice of dimension  $d$ , a linear classifier  $g_d$  is once again selected by linear regression using the in-sample training data points and tested on the out-of-sample embedded testing data points. The classification errors are also plotted in Fig 1b. A quick glance at the plots in Fig 1b suggests that the classification performance degradation due to the out-of-sample embedding is negligible.

Our next example uses the abalone dataset from the UCI machine learning repository (Bache and Lichman, 2013). The data set consists of 4177 observations of nine different abalones attributes. The attributes are sex, number of rings, and seven other physical measurements of the abalones, e.g., length, diameter, and shell weight. The number of rings in an abalone is an estimate of its age in years. We consider the problem of classifying an abalone based on its physical measurements. Following the description of the data set, the class labels are as follows. An abalone is classified as class 1 if its number of rings is eight or less. It is classified as class 2 if its number of rings is nine or ten, and it is classified as class 3 otherwise. The dataset is partitioned into a training set of 3133 observations and a test set of 1044 observations. The lowest misclassification rate is reported to be 35.39% (Vaugh, 1995).

We form a graph  $G$  on 4177 vertices following a latent position model with a Gaussian kernel  $\exp(-2\|X_i - X_j\|^2)$  where  $X_i \in \mathbb{R}^7$  represents the physical measurements of the

$i$ -th abalone observation. To measure the in-sample classification performance, we embed the vertices of  $G$  into  $\mathbb{R}^{50}$  and train a multi-class linear SVM on the embedding of the 3133 training vertices. We then measure the mis-classification rate of this classifier on the embedding of the 1044 testing vertices. For the out-of-sample setting, we randomly chose a subset of  $m$  vertices from the training set and embed the resulting induced subgraph  $G_m$  into  $\mathbb{R}^{50}$  then out-of-sample embed the remaining  $4177 - m$  vertices. We then train a multi-class linear SVM on the  $3133 - m$  out-of-sample embedded vertices in the training set and measure the mis-classification error on the vertices in the testing set. The results for various choices of  $m \in \{200, 600, 1000, \dots, 2600\}$  are given in Table 1.

$m = 200$	$m = 600$	$m = 1000$	$m = 1400$	$m = 1800$	$m = 2200$	$m = 2600$
0.444	0.386	0.391	0.375	0.382	0.374	0.401

Table 1: Out-of-sample classification performance for the abalone dataset. The in-sample classification performance is 0.358. The lowest reported mis-classification rate is 0.354. The performance degradation due to the out-of-sample embedding is as low as 2%.

Our final example is on the CharityNet dataset. The data set consists of 2 years of anonymized donations transactions between anonymized donors and charities. There are in total 3.3 million transactions representing donations from 1.8 million donors to 5700 charities. Note that the data set does not contains any explicit information on the charities to charities relationship, i.e., the charities relate to one another through the donations transactions between donors and charities. We investigate the problem of clustering the charities under the assumption that there are additional information on the donors, but virtually no information on the charities.

We can view the problem as embedding an adjacency matrix  $\mathbf{A} = \begin{bmatrix} \mathbf{A}_{dd} & \mathbf{A}_{dc} \\ \mathbf{A}_{dc}^T & \mathbf{A}_{cc} \end{bmatrix}$  follows by clustering the vertices of  $\mathbf{A}$ . Here  $\mathbf{A}_{dd}$  represent the (unobserved) donors to donors graph,  $\mathbf{A}_{dc}$  represents the donors to charities graph and  $\mathbf{A}_{cc}$  represents the (unobserved) charities to charities graph. Because we only have transactions between donors and charities, we do not observe any part of  $\mathbf{A}$  except  $\mathbf{A}_{dc}$ . Using the additional information on the donors, e.g., geographical information of city and state, we can simulate  $\mathbf{A}_{dd}$  by modeling each of  $\mathbf{A}_{dd}(i, j) \sim \text{Bern}(\exp(-d_{ij}^2))$ , where  $d_{ij}$  is a pairwise distance between donors  $i$  and  $j$ . We then use  $\mathbf{A}_{dd}$  to obtain an embedding of the donors. Given this embedding, we out-of-sample embed the charities and cluster them using the Mclust implementation of (Fraley and Raftery, 1999) for Gaussian mixture models. We note that for this example, a biclustering of  $\mathbf{A}_{dc}$  is also applicable.

For this experiment, we randomly sub-sample 10,000 donors and use the associated charities and transactions, which yields 1,722 unique charities, 9,877 unique donors, and 17,764 transactions. There are 52 unique states for the charities, and the model-based clustering yields  $\hat{K} = 17$  clusters. We validate our clustering via calculating the adjusted Rand Index (ARI) between the clustering labels and the true labels of the charities. We use the state information of the charities as the true labels, and we obtain an ARI of 0.01. This number appears small at first sight so we generate a null distribution of the adjusted Rand Index by shuffling the true labels. Figure 2 depicts the null distribution of the ARI

with 10,000 trials. It shows that  $\mu = 3.5e - 05$  and  $\sigma = 0.003$ . The shaded area indicates the number of times the null ARIs are larger than the alternative ARI, which is the  $p$ -value. With the  $p$ -value of  $6e - 04$ , we claim that the ARI obtained by clustering the out-of-sample embedded charities is significantly better than chance. In addition, this example also illustrates the applicability of out-of-sample embedding to scenarios where the lack of information regarding the relationships between a subset of the rows might prevents the use of spectral decomposition algorithms for embedding the whole matrix.

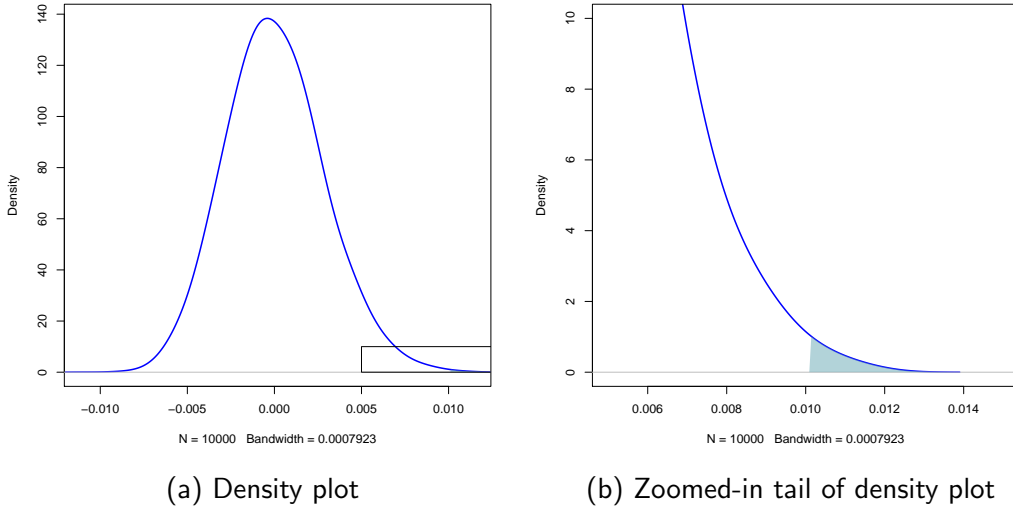


Figure 2: Density plots for the null distribution, under a permutation test, of the ARI values between the clustering labels and the permuted true labels (state information of the charities). The shaded area above the ARI value between the clustering labels and the true labels represent the estimated  $p$ -value. The plot indicates that the ARI value of the clustering of the out-of-sample charities is (statistically significant) better than chance.

## 5. Conclusions

In this paper we investigated the out-of-sample extension for embedding out-of-sample vertices in graphs arising from a latent position model with positive definite kernel  $\kappa$ . We showed, in Theorem 2, that if the number of in-sample vertices is sufficiently large, then with high-probability, the embedding into  $\mathbb{R}^d$  given by the out-of-sample extension is close to the true (truncated) feature map  $\Phi_d$ . This implies that inference for the out-of-sample vertices using their embeddings is appropriate, e.g., Theorem 7. Experimental results on simulated data suggest that under suitable conditions, the degradation due to the out-of-sample extension is negligible.

The out-of-sample extension described in this paper is related to the notion of “sketching” and Nyström approximation for matrices (Bengio et al., 2004; Williams and Seeger,

2001; Gittens and Mahoney, 2013; Drineas and Mahoney, 2005; Platt, 2005). This connection suggests inquiry on how to select the in-sample vertices via consideration of the Nyström approximation so as to yield the best inferential performance on the out-of-sample vertices, i.e., whether one can use results on error bounds in the Nyström approximation to augment the selection of the in-sample vertices. A possible approach might be to select the sketching matrix  $\mathbf{S}$ , and hence the in-sample vertices, via a non-uniform importance sampling based on the leverage scores of the rows of  $\mathbf{A}$ . The leverage score of row  $i$  of  $\mathbf{A}$  is the  $l_2$  norm of the  $i$ -th row of  $\mathbf{U}$  in the eigen-decomposition  $\mathbf{U}\Sigma\mathbf{U}^T$  of  $\mathbf{A}$ , and fast approximation methods to compute the leverage scores are available, see e.g. Clarkson and Woodruff (2013); Drineas et al. (2012). We believe the investigation of this and other approaches to selecting the in-sample vertices will yield results that are useful and relevant for application domains.

Finally, as mentioned in Section 3, the out-of-sample extension as defined in this paper depends only on the in-sample vertices. Hence, the embedding of a batch of out-of-sample vertices does not use the information contained in the relationship between the out-of-sample vertices. A modification of the out-of-sample extension presented herein that uses this information in the batch setting is possible, see e.g. Trosset and Priebe (2008) for such a modification in the case of classical multidimensional scaling. However, the construction similar to that in Trosset and Priebe (2008) will yield a convex but non-linear optimization problem with no closed-form solution and is much more complicated to analyze. We thus note that it is of potential interest to introduce an out-of-sample extension in the batch setting that is simple and amenable to analysis.

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## Appendix A: Proof of Theorem 2

We now proceed to prove Theorem 2. First recall the definition of  $T_n(X)$  in terms of the Moore-Penrose pseudo-inverse  $\mathbf{Z}^\dagger$  of  $\mathbf{Z} = \mathbf{U}_A \mathbf{S}_A^{1/2}$  and  $\boldsymbol{\xi}$  from Definition 1. We consider the expression

$$T_n(X) = \mathbf{Z}^\dagger \boldsymbol{\xi} = (\mathbf{Z} - \mathbf{W}\tilde{\mathbf{Z}}^\dagger)\boldsymbol{\xi} + \mathbf{W}\tilde{\mathbf{Z}}^\dagger(\boldsymbol{\xi} - \mathbb{E}[\boldsymbol{\xi}]) + \mathbf{W}\tilde{\mathbf{Z}}^\dagger \mathbb{E}[\boldsymbol{\xi}] \quad (18)$$

where  $\tilde{\mathbf{Z}}^\dagger$  is the Moore-Penrose pseudo-inverse of  $\tilde{\mathbf{Z}} = \mathbf{U}_K \mathbf{S}_K^{1/2}$  and  $\mathbf{W}$  is some orthogonal matrix in  $\mathcal{M}_d$ . A rough sketch of the argument then goes as follows. We first show that  $\mathbf{Z}^\dagger$  is “close” (up to rotation) in operator norm to  $\tilde{\mathbf{Z}}^\dagger$ . This allows us to conclude that  $(\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)\boldsymbol{\xi}$  is “small”. We then show that  $\tilde{\mathbf{Z}}^\dagger(\boldsymbol{\xi} - \mathbb{E}[\boldsymbol{\xi}])$  is “small” as it is a sum of zero-mean random vectors in  $\mathbb{R}^d$ . We then relate  $\rho_n^{-1/2}\tilde{\mathbf{Z}}^\dagger \mathbb{E}[\boldsymbol{\xi}]$  to the projection  $\hat{\mathcal{P}}_d$  of the feature map  $\Phi$  into  $\mathbb{R}^d$  where  $\hat{\mathcal{P}}_d$  is induced by the eigenvectors of  $\mathbf{K}$ . Finally, we use results on the convergence

of spectra of  $\mathbf{K}$  to the spectra of  $\mathcal{K}$  to show that the projection  $\hat{\mathcal{P}}_d$  of  $\Phi$  is “close” (up to rotation) to the projection that maps  $\Phi$  into  $\Phi_d$ . We thus arrive at an expression of the form  $\rho_n^{-1/2} \mathbf{W} T_n(X) \approx \Phi_d(X)$  as in the statement of Theorem 2.

We first collect some assorted bounds for the eigenvalues of  $\mathbf{A}$  and  $\mathbf{K}$  and bounds for the projection onto the subspaces of  $\mathbf{A}$  or  $\mathbf{K}$  in the following proposition.

**Proposition 8** *Let  $\mathcal{P}_{\mathbf{A}}$  and  $\mathcal{P}_{\mathbf{K}}$  be the projection operators onto the subspace spanned by the eigenvectors corresponding to the  $d$  largest eigenvalues of  $\mathbf{A}$  and  $\mathbf{K}$ , respectively. Denote by  $\delta_d$  the quantity  $\lambda_d(\mathcal{K}) - \lambda_{d+1}(\mathcal{K})$  and suppose that  $\delta_d > 0$ . Assume also that  $n$  satisfies  $\delta_d(\mathcal{K}) > 4\sqrt{2}\sqrt{(n\rho_n)^{-1} \log(n/\eta)}$ . Then with probability at least  $1 - 2\eta$ , the following inequalities hold simultaneously.*

$$\|\mathbf{A} - \mathbf{K}\| \leq 2\sqrt{n\rho_n \log(n/\eta)} \quad (19)$$

$$\lambda_1(\mathbf{A}) \leq n\rho_n; \quad \lambda_1(\mathbf{K}) \leq n\rho_n \quad (20)$$

$$\lambda_d(\mathbf{A}) \geq n\rho_n \lambda_d(\mathcal{K})/2; \quad \lambda_d(\mathbf{K}) \geq n\rho_n \lambda_d(\mathcal{K})/2 \quad (21)$$

$$\|\mathcal{P}_{\mathbf{A}} - \mathcal{P}_{\mathbf{K}}\| \leq 4\delta_d^{-1} \sqrt{n\rho_n \log(n/\eta)} \quad (22)$$

$$\|(\mathcal{P}_{\mathbf{A}}\mathbf{A}) - (\mathcal{P}_{\mathbf{K}}\mathbf{K})\| \leq 6\delta_d^{-1} \sqrt{n\rho_n \log(n/\eta)} \quad (23)$$

**Proof** [Sketch] Eq. (19) is from Oliveira (2010). The bound for  $\lambda_1(\mathbf{K})$  follows from the assumption that the range of  $\kappa$  is in  $[0, 1]$ . The bound for  $\lambda_d(\mathbf{K})$  follows from Theorem 14 below. The bounds for the eigenvalues of  $\mathbf{A}$  follow from the bounds for the corresponding eigenvalues of  $\mathbf{K}$ , Eq. (19), and perturbation results, e.g. Corollary III.2.6 in Bhatia (1997). Eq. (22) follows from Eq. (19) and the sin  $\Theta$  theorem (Davis and Kahan, 1970). Eq. (23) follows from Eq. (22), Eq. (19), and an application of the triangle inequality.  $\blacksquare$

We also note the following result on perturbation for pseudo-inverses from Wedin (1973).

**Lemma 9** *Let  $\mathbf{A}$  and  $\mathbf{B}$  be matrices with  $\text{rk}(\mathbf{A}) = \text{rk}(\mathbf{B})$ . Let  $\mathbf{A}^\dagger$  and  $\mathbf{B}^\dagger$  be the Moore-Penrose pseudo-inverses of  $\mathbf{A}$  and  $\mathbf{B}$ , respectively. Then*

$$\|\mathbf{A}^\dagger - \mathbf{B}^\dagger\| \leq \frac{(1 + \sqrt{5})}{2} (\|\mathbf{A}^\dagger\|)(\|\mathbf{B}^\dagger\|) \|\mathbf{A} - \mathbf{B}\| \quad (24)$$

We now provide a bound for the spectral norm of the difference  $\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger$ .

**Lemma 10** *Let  $\mathbf{Z} = \mathbf{U}_{\mathbf{A}} \mathbf{S}_{\mathbf{A}}^{1/2}$  and  $\tilde{\mathbf{Z}} = \mathbf{U}_{\mathbf{K}} \mathbf{S}_{\mathbf{K}}^{1/2}$ . Then, with probability at least,  $1 - 2\eta$ , there exists an orthogonal  $\mathbf{W} \in \mathcal{M}_d$  such that*

$$\|\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger\| \leq 24(1 + \sqrt{5}) \frac{\sqrt{\log(n/\eta)}}{n\rho_n \delta_d^3} \quad (25)$$

**Proof** We have  $\mathbf{Z}^\dagger(\mathbf{Z}^\dagger)^T = \mathbf{S}_{\mathbf{A}}^{-1}$  and  $\tilde{\mathbf{Z}}^\dagger(\tilde{\mathbf{Z}}^\dagger)^T = \mathbf{S}_{\mathbf{K}}^{-1}$ . Thus,  $\|\mathbf{Z}^\dagger\| = \|\mathbf{S}_{\mathbf{A}}^{-1}\|^{1/2} = (\lambda_d(\mathbf{A}))^{-1/2}$  and  $\|\tilde{\mathbf{Z}}^\dagger\| = \|\mathbf{S}_{\mathbf{K}}^{-1}\|^{1/2} = (\lambda_d(\mathbf{K}))^{-1/2}$ . Then by Lemma 9, we have

$$\|\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger\| \leq \frac{1 + \sqrt{5}}{2} (\|\mathbf{S}_{\mathbf{A}}^{-1}\|^{1/2})(\|\mathbf{S}_{\mathbf{K}}^{-1}\|^{1/2}) \|\mathbf{Z}\mathbf{W}^T - \tilde{\mathbf{Z}}\|$$



for any orthogonal  $\mathbf{W} \in \mathcal{M}_d$ . By Proposition 8, with probability at least  $1 - 2\eta$ ,

$$(\|\mathbf{S}_{\mathbf{A}}^{-1}\|^{1/2})(\|\mathbf{S}_{\mathbf{K}}^{-1}\|^{1/2}) = 1/\sqrt{\lambda_d(\mathbf{A})\lambda_d(\mathbf{K})} \leq 2/(n\rho_n\lambda_d(\mathcal{K})).$$

To complete the proof, we show that with probability at least  $1 - 2\eta$ , there exists some orthogonal  $\mathbf{W} \in \mathcal{M}_d$  such that

$$\|\mathbf{Z}\mathbf{W}^T - \tilde{\mathbf{Z}}\| \leq 24\delta_d^{-2}\sqrt{\log(n/\eta)}.$$

We proceed as follows. We note that  $\mathbf{Z}$  and  $\tilde{\mathbf{Z}}$  are matrices in  $\mathcal{M}_{n,d}$  and are of full column rank. Then by Lemma A.1 in Tang et al. (2013), there exists an orthogonal matrix  $\mathbf{W} \in \mathcal{M}_d$  such that

$$\|\mathbf{Z}\mathbf{W}^T - \tilde{\mathbf{Z}}\| \leq \|\mathbf{Z}\mathbf{Z}^T - \tilde{\mathbf{Z}}\tilde{\mathbf{Z}}^T\| \frac{\sqrt{\|\mathbf{Z}\mathbf{Z}^T\|} + \sqrt{\|\tilde{\mathbf{Z}}\tilde{\mathbf{Z}}^T\|}}{\lambda_d(\tilde{\mathbf{Z}}\tilde{\mathbf{Z}}^T)}$$

As  $\mathbf{Z}\mathbf{Z}^T = \mathbf{U}_{\mathbf{A}}\mathbf{S}_{\mathbf{A}}\mathbf{U}_{\mathbf{A}} = (\mathcal{P}_{\mathbf{A}}\mathbf{A})$  and  $\tilde{\mathbf{Z}}\tilde{\mathbf{Z}}^T = (\mathcal{P}_{\mathbf{K}}\mathbf{K})$ , we thus have

$$\begin{aligned} \|\mathbf{Z}\mathbf{W}^T - \tilde{\mathbf{Z}}\| &\leq \|(\mathcal{P}_{\mathbf{A}}\mathbf{A}) - (\mathcal{P}_{\mathbf{K}}\mathbf{K})\| \frac{\sqrt{\lambda_1(\mathbf{A})} + \sqrt{\lambda_1(\mathbf{K})}}{\lambda_d(\mathbf{K})} \\ &\leq 6\delta_d^{-1}\sqrt{n\rho_n \log(n/\eta)} \frac{2\sqrt{n\rho_n}}{n\rho_n\delta_d/2} \\ &\leq 24\delta_d^{-2}\sqrt{\log(n/\eta)} \end{aligned} \tag{26}$$

where the inequalities in Eq. (26) follows from Proposition 8 and hold with probability  $1 - 2\eta$ . Eq. (25) is thus established.  $\blacksquare$

We now provide a bound for  $\|(\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)\boldsymbol{\xi}\|$  which, as sketched earlier, is one of the key step in the proof of Theorem 2. We note that application of the multiplicative bound for the norm of a matrix vector product, i.e.,  $\|(\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)\boldsymbol{\xi}\| \leq (\|(\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)\|)(\|\boldsymbol{\xi}\|)$  leads to a bound that is worse by a factor of  $\rho_n^{-1/2}$ . This is due to the fact that  $\boldsymbol{\xi}$  is a vector whose components are independent Bernoulli random variables and thus the scaling of the probabilities  $\mathbb{E}[\boldsymbol{\xi}]$  by a constant  $c$  changes  $\|\boldsymbol{\xi}\|$  by a factor that is roughly  $c^{1/2}$ .

**Lemma 11** *With probability at least  $1 - 2\eta$ , there exists an orthogonal  $\mathbf{W} \in \mathcal{M}_d$  such that*

$$\|(\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)\boldsymbol{\xi}\| \leq C\delta_d^{-3}\sqrt{\frac{\log(n/\eta)}{n}} \tag{27}$$

The proof of Lemma 11 uses the following concentration inequality for sums of independent matrices from Tropp (2012).

**Theorem 12** *Consider a finite sequence  $\mathbf{B}_k$  of independent random matrices with dimensions  $d_1 \times d_2$ . Assume that each  $\mathbf{B}_k$  satisfies  $\mathbb{E}[\mathbf{B}_k] = \mathbf{0}$  and that, for some  $R \geq 0$  independent of the  $\mathbf{B}_k$ ,  $\|\mathbf{B}_k\| \leq R$  almost surely. Define*

$$\sigma^2 := \max\left\{\left\|\sum_k \mathbb{E}[\mathbf{B}_k\mathbf{B}_k^*]\right\|, \left\|\sum_k \mathbb{E}[\mathbf{B}_k^*\mathbf{B}_k]\right\|\right\}$$

*Then, for all  $t \geq 0$ , one has*

$$\mathbb{P}\left[\left\|\sum_k \mathbf{B}_k\right\| \geq t\right] \leq (d_1 + d_2) \exp\left(\frac{-t^2/2}{\sigma^2 + Rt/3}\right). \tag{28}$$

**Proof** [Lemma 11] Let  $\mathbf{W}$  be the matrix that minimizes  $\|\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger\|$  over the set of orthogonal matrices. Let  $\mathbf{b}_i$  be the  $i$ -th column of  $\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger$ . We have

$$\begin{aligned} \|(\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)\boldsymbol{\xi}\| &= \|(\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)\mathbb{E}[\boldsymbol{\xi}]\| + \|(\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)(\boldsymbol{\xi} - \mathbb{E}[\boldsymbol{\xi}])\| \\ &= \|(\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)\mathbb{E}[\boldsymbol{\xi}]\| + \left\| \sum_{i=1}^n \mathbf{b}_i(\xi_i - \mathbb{E}[\xi_i]) \right\| \end{aligned}$$

By Lemma 10, we have

$$\|(\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)\mathbb{E}[\boldsymbol{\xi}]\| \leq (\|\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger\|)\|\mathbb{E}[\boldsymbol{\xi}]\| \leq 24(1 + \sqrt{5})\delta_d^{-3} \sqrt{\frac{\log(n/\eta)}{n}}$$

with probability at least  $1 - 2\eta$ . We now apply Theorem 12 to the term  $\sum_{i=1}^n \mathbf{b}_i(\xi_i - \mathbb{E}[\xi_i])$ . We note that

$$\begin{aligned} \sum_{i=1}^n \mathbb{E}[\mathbf{b}_i \mathbf{b}_i^T (\xi_i - \mathbb{E}[\xi_i])^2] &= \sum_{i=1}^n \mathbf{b}_i \mathbf{b}_i^T \rho_n \kappa(X, X_i) (1 - \rho_n \kappa(X, X_i)) \\ &\prec \sum_{i=1}^n \rho_n \mathbf{b}_i \mathbf{b}_i^T \\ &\prec \rho_n (\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger) (\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)^T \end{aligned}$$

where  $\prec$  refers to the positive semidefinite ordering for matrices. Similarly, we have

$$\sum_{i=1}^n \mathbb{E}[\mathbf{b}_i^T \mathbf{b}_i (\xi_i - \mathbb{E}[\xi_i])^2] \leq \rho_n \sum_{i=1}^n \mathbf{b}_i^T \mathbf{b}_i = \rho_n \text{Tr}[(\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)^T (\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)]$$

We thus have

$$\sigma^2 \leq \rho_n \|(\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)\|_F^2$$

Theorem 12 now applies to give

$$\|(\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)(\boldsymbol{\xi} - \mathbb{E}[\boldsymbol{\xi}])\| \leq \sqrt{2d\rho_n \log(n/\eta)} \|\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger\|_F$$

with probability at least  $1 - 2\eta$ . We therefore have

$$\|(\mathbf{W}\mathbf{Z}^\dagger - \tilde{\mathbf{Z}}^\dagger)\boldsymbol{\xi}\| \leq C_1 \delta_d^{-3} \sqrt{\frac{\log(n/\eta)}{n}} + C_2 \delta_d^{-3} \frac{d \log(n/\eta)}{n \sqrt{\rho_n}}$$

Under our assumption of  $n\rho_n = o(1)$ , the above bound simplifies to Eq. (27) as desired.  $\blacksquare$

Theorem 12 also allows us to bound the term  $\mathbf{W}_2 \tilde{\mathbf{Z}}^\dagger (\boldsymbol{\xi} - \mathbf{p})$  with a bound of the form  $C \delta_d^{-3} n^{-1/2} \sqrt{\log(n/\eta)}$ . Thus, the last key step of the proof is to relate  $\tilde{\mathbf{Z}}^\dagger \mathbb{E}[\boldsymbol{\xi}] \in \mathbb{R}^d$  to the truncated feature map  $\Phi_d$ . This will be done by relating the eigenvalues and eigenvectors of  $\mathbf{K}$  to the eigenvalues and eigenfunctions of  $\mathcal{K}$ . But as  $\mathbf{K}$  is an operator on  $\mathbb{R}^n$  and  $\mathcal{K}$  is an operator on  $L^2(\mathcal{X}, F)$ , we will relate these eigenvalues, eigenvectors and eigenfunctions through some auxiliary operators on the reproducing kernel Hilbert space  $\mathcal{H}$  of  $\kappa$ . Following

Rosasco et al. (2010), we introduce the operators  $\mathcal{K}_{\mathcal{H}}: \mathcal{H} \mapsto \mathcal{H}$  and  $\mathcal{K}_{\mathcal{H},n}: \mathcal{H} \mapsto \mathcal{H}$  defined by

$$\begin{aligned}\mathcal{K}_{\mathcal{H}}\eta &= \int_{\mathcal{X}} \langle \eta, \kappa(\cdot, x) \rangle_{\mathcal{H}} \kappa(\cdot, x) dF(x) \\ \mathcal{K}_{\mathcal{H},n}\eta &= \frac{1}{n} \sum_{i=1}^n \langle \eta, \kappa(\cdot, X_i) \rangle_{\mathcal{H}} \kappa(\cdot, X_i).\end{aligned}$$

The operator  $\mathcal{K}_{\mathcal{H}}$  and  $\mathcal{K}_{\mathcal{H},n}$  are defined on the same Hilbert space  $\mathcal{H}$ , in contrast to  $\mathcal{K}$  and  $\mathbf{K}$  which are defined on the different spaces  $L^2(\mathcal{X}, F)$  and  $\mathbb{R}^n$ , and we can relate  $\mathcal{K}_{\mathcal{H},n}$  to  $\mathcal{K}_{\mathcal{H}}$  (Theorem 14). In addition, we can relate the eigenvalues and eigenfunctions of  $\mathcal{K}$  to that of  $\mathcal{K}_{\mathcal{H}}$  as well as the eigenvalues and eigenvectors of  $\mathbf{K}$  to the eigenvalues and eigenfunctions of  $\mathcal{K}_{\mathcal{H},n}$ , therefore giving us a relationship between the eigenvalues/eigenfunctions of  $\mathcal{K}$  and the eigenvalues/eigenvectors of  $\mathbf{K}$ . A precise statement of the relationships is contained in Proposition 13 and Theorem 14.

**Proposition 13** (Rosasco et al. (2010), von Luxburg et al. (2008)) *The operators  $\mathcal{K}_{\mathcal{H}}$  and  $\mathcal{K}_{\mathcal{H},n}$  are positive, self-adjoint operators and are of trace class with  $\mathcal{K}_{\mathcal{H},n}$  being of finite rank. The spectra of  $\mathcal{K}$  and  $\mathcal{K}_{\mathcal{H}}$  are contained in  $[0, 1]$  and are the same, possibly up to the zero eigenvalues. If  $\lambda$  is a non-zero eigenvalue of  $\mathcal{K}$  and  $u$  and  $v$  are associated eigenfunction of  $\mathcal{K}$  and  $\mathcal{K}_{\mathcal{H}}$ , normalized to norm 1 in  $L^2(\mathcal{X}, F)$  and  $\mathcal{H}$ , respectively, then*

$$u(x) = \frac{v(x)}{\sqrt{\lambda}}; \quad v(x) = \frac{1}{\sqrt{\lambda}} \int_{\mathcal{X}} \kappa(x, x') u(x') dF(x') \quad (29)$$

*Similarly, the spectra of  $\mathbf{K}/(n\rho_n)$  and  $\mathcal{K}_{\mathcal{H},n}$  are contained in  $[0, 1]$  and are the same, possibly up to the zero eigenvalues. If  $\hat{\lambda}$  is a non-zero eigenvalue of  $\mathbf{K}/(n\rho_n)$  and  $\hat{u}$  and  $\hat{v}$  are the corresponding eigenvector and eigenfunction of  $\mathbf{K}/(n\rho_n)$  and  $\mathcal{K}_{\mathcal{H},n}$ , normalized to norm 1 in  $\mathbb{R}^n$  and  $\mathcal{H}$ , respectively, then*

$$\hat{u}_i = \frac{\hat{v}(x_i)}{\sqrt{\hat{\lambda}}}; \quad \hat{v}(\cdot) = \frac{1}{\sqrt{\hat{\lambda}n}} \sum_{i=1}^n \kappa(\cdot, x_i) \hat{u}_i \quad (30)$$

Eq. (30) in Proposition 13 states that an eigenvector  $\hat{u}$  of  $\mathbf{K}/(n\rho_n)$ , which is only defined for  $X_1, X_2, \dots, X_n$ , can be extended to an eigenfunction  $\hat{v} \in \mathcal{H}$  of  $\mathcal{K}_{\mathcal{H},n}$  defined for all  $x \in \mathcal{X}$ , and furthermore, that  $\hat{u}_i = \hat{v}(X_i)$  for all  $i = 1, 2, \dots, n$ .

**Theorem 14** (Rosasco et al. (2010); Zwald and Blanchard (2006)) *Let  $\eta > 0$  be arbitrary. Then with probability at least  $1 - 2e^{-\eta}$ ,*

$$\|\mathcal{K}_{\mathcal{H}} - \mathcal{K}_{\mathcal{H},n}\|_{HS} \leq 2\sqrt{2}\sqrt{\frac{\eta}{n}} \quad (31)$$

*where  $\|\cdot\|_{HS}$  is the Hilbert-Schmidt norm. Let  $\delta_d = \lambda_d(\mathcal{K}) - \lambda_{d+1}(\mathcal{K})$ . For a given  $d \geq 1$  and an arbitrary  $\eta > 0$ , if the number  $n$  of samples  $X_i \sim F$  satisfies*

$$4\sqrt{2}\sqrt{\frac{\eta}{n}} < \delta_d$$

then with probability greater than  $1 - 2e^{-\eta}$

$$\|\mathcal{P}_d - \hat{\mathcal{P}}_d\|_{HS} \leq \frac{2\sqrt{2}\sqrt{\eta}}{\delta_d\sqrt{n}} \quad (32)$$

where  $\mathcal{P}_d$  is the projection onto the subspace spanned by the eigenfunctions corresponding to the  $d$  largest eigenvalues of  $\mathcal{K}$  and  $\hat{\mathcal{P}}_d$  is the projection onto the subspace spanned by the eigenfunctions corresponding to the  $d$  largest eigenvalues of  $\mathcal{K}_{\mathcal{H},n}$ .

With the above technical details in place, the following result states that  $\rho_n^{-1/2}\tilde{\mathbf{Z}}^\dagger\mathbb{E}[\boldsymbol{\xi}]$  is equivalent to the isometric embedding of  $\hat{\mathcal{P}}_d\kappa(\cdot, X)$  into  $\mathbb{R}^d$ .

**Lemma 15** *Let  $\hat{\mathcal{P}}_d$  be the projection onto the subspace spanned by the eigenfunctions corresponding to the  $d$  largest eigenvalues of  $\mathcal{K}_{\mathcal{H},n}$ . Then*

$$\rho_n^{-1/2}\tilde{\mathbf{Z}}^\dagger\mathbb{E}[\boldsymbol{\xi}] = \iota(\hat{\mathcal{P}}_d\kappa(\cdot, X)) \quad (33)$$

where  $\iota$  is the isometric isomorphism of the finite-dimensional subspace corresponding to the projection  $\hat{\mathcal{P}}_d$  into  $\mathbb{R}^d$ .

**Proof** Let  $\{\lambda_r\}$  and  $\{\psi_r\}$  be the eigenvalues and eigenfunctions of  $\mathcal{K}$ . Let  $\hat{\lambda}_1, \hat{\lambda}_2, \dots, \hat{\lambda}_d$  be the eigenvalues of  $\mathbf{K}/(n\rho_n)$  and let  $\hat{u}^{(1)}, \hat{u}^{(2)}, \dots, \hat{u}^{(d)}$  be the associated eigenvectors, normalized to have norm 1 in  $\mathbb{R}^n$ . Also let  $\hat{v}^{(1)}, \hat{v}^{(2)}, \dots, \hat{v}^{(d)}$  be the corresponding eigenfunctions of  $\mathcal{K}_{\mathcal{H},n}$ , normalized to have norm 1 in  $\mathcal{H}$ . Let  $\Psi_{r,n} = (\sqrt{\lambda_r}\psi_r(X_i))_{i=1}^n \in \mathbb{R}^n$ . Then the  $s$ -th component of  $\mathbf{U}_{\mathbf{K}}^T\mathbb{E}[\boldsymbol{\xi}] \in \mathbb{R}^d$  for  $s = 1, 2, \dots, d$  is of the form

$$\begin{aligned} \sum_{i=1}^n \hat{u}_j^{(s)} \rho_n \kappa(X, X_i) &= \rho_n \sum_{i=1}^n \hat{u}_i^{(s)} \sum_{r=1}^{\infty} \lambda_r \psi_r(X) \psi_r(X_i) \\ &= \rho_n \sum_{r=1}^{\infty} \sqrt{\lambda_r} \psi_r(X) \sum_{i=1}^n \hat{u}_i^{(s)} \sqrt{\lambda_r} \psi_r(X_i) \\ &= \rho_n \sum_{r=1}^{\infty} \sqrt{\lambda_r} \psi_r(X) * \langle \hat{u}^{(s)}, \Psi_{r,n} \rangle_{\mathbb{R}^n} \end{aligned} \quad (34)$$

where  $\hat{u}_j^{(s)}$  is the  $j$ -th component of  $\hat{u}^{(s)}$ . Now we note that

$$\begin{aligned} \langle \hat{v}^{(s)}, \sqrt{\lambda_r} \psi_r \rangle_{\mathcal{H}} &= \left\langle \frac{1}{\sqrt{\hat{\lambda}_s n}} \sum_{i=1}^n \kappa(\cdot, X_i) \hat{u}_i^{(s)}, \sqrt{\lambda_r} \psi_r \right\rangle_{\mathcal{H}} \\ &= \frac{1}{\sqrt{\hat{\lambda}_s n}} \sum_{i=1}^n \hat{u}_i^{(s)} \left\langle \kappa(\cdot, X_i), \sqrt{\lambda_r} \psi_r \right\rangle_{\mathcal{H}} \\ &= \frac{1}{\sqrt{\hat{\lambda}_s n}} \sum_{i=1}^n \psi_r(X_i) \sqrt{\lambda_r} \hat{u}_i^{(s)} \\ &= \frac{1}{\sqrt{\hat{\lambda}_s n}} \langle \hat{u}^{(s)}, \Psi_{r,n} \rangle_{\mathbb{R}^n} \end{aligned}$$

where we have used the reproducing kernel property of  $\kappa$ , i.e.,  $\langle \kappa(\cdot, X), g \rangle_{\mathcal{H}} = g(X)$  for any  $g \in \mathcal{H}$ . Thus, the  $s$ -th component of  $\mathbf{U}_{\mathbf{K}}^T \mathbb{E}[\boldsymbol{\xi}]$  can be written as

$$\rho_n \sqrt{\hat{\lambda}_s n} \sum_{r=1}^{\infty} \sqrt{\lambda_r} \psi_r(X) * \langle \hat{v}^{(s)}, \sqrt{\lambda_r} \psi_r \rangle_{\mathcal{H}} \quad (35)$$

Therefore, as  $\tilde{\mathbf{Z}}^\dagger = \mathbf{S}_{\mathbf{K}}^{-1/2} \mathbf{U}_{\mathbf{K}}^T$ , the  $s$ -th component of  $\rho_n^{-1/2} \tilde{\mathbf{Z}}^\dagger \mathbb{E}[\boldsymbol{\xi}]$  is just

$$\rho_n^{-1/2} (\hat{\lambda}_s n \rho_n)^{-1/2} \mathbf{U}_{\mathbf{K}}^T \mathbb{E}[\boldsymbol{\xi}] = \sum_{r=1}^{\infty} \sqrt{\lambda_r} \psi_r(X) * \langle \hat{v}^{(s)}, \sqrt{\lambda_r} \psi_r \rangle_{\mathcal{H}} = \hat{v}^{(s)}(X) \quad (36)$$

We now consider the projection  $\hat{\mathcal{P}}_d \kappa(\cdot, X)$ . We have

$$\hat{\mathcal{P}}_d \kappa(\cdot, X) = \sum_{s=1}^d \langle \hat{v}^{(s)}, \kappa(\cdot, X) \rangle_{\mathcal{H}} \hat{v}^{(s)} = \sum_{s=1}^d \hat{v}^{(s)}(X) \hat{v}^{(s)} \quad (37)$$

Let us now define  $\tilde{T}_n: \mathcal{X} \mapsto \mathbb{R}^d$  to be the mapping  $\tilde{T}_n(X) = \rho_n^{-1/2} \tilde{\mathbf{Z}}^\dagger \mathbf{p}_X$  where  $\mathbf{p}_X = (\rho_n \kappa(X_i, X))_{i=1}^n \in \mathbb{R}^n$ .  $\tilde{T}_n$  is a deterministic mapping given the  $\{X_i\}_{i=1}^n$  and furthermore, that

$$\langle \tilde{T}_n(X), \tilde{T}_n(X') \rangle_{\mathbb{R}^d} = \langle \hat{\mathcal{P}}_d \kappa(\cdot, X), \hat{\mathcal{P}}_d \kappa(\cdot, X') \rangle_{\mathcal{H}} \quad (38)$$

as the  $\{\hat{v}^{(s)}\}$  are orthogonal with respect to  $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ . As  $\hat{\mathcal{P}}_d$  is a projection onto a finite-dimensional subspace of  $\mathcal{H}$ , we thus have that there exists an isometric isomorphism  $\iota$  of the finite-dimensional subspace of  $\mathcal{H}$  spanned by the  $\{\hat{v}^{(s)}\}$  into  $\mathbb{R}^d$  such that  $\tilde{T}_n(X) = \rho_n^{-1/2} \tilde{\mathbf{Z}}^\dagger \mathbf{p}(X) = \iota(\hat{\mathcal{P}}_d \kappa(\cdot, X))$  for all  $X \in \mathcal{X}$  as desired.  $\blacksquare$

Lemma 15 states that there is an isometric isomorphism  $\hat{\iota}$  of  $\mathbb{R}^d$  into  $\hat{\mathcal{P}}_d \mathcal{H}$  such that  $\rho_n^{-1/2} \tilde{\mathbf{Z}}^\dagger \mathbb{E}[\boldsymbol{\xi}] \in \mathbb{R}^d$  is mapped into  $\hat{\mathcal{P}}_d \kappa(\cdot, X) \in \hat{\mathcal{P}}_d \mathcal{H}$ . By the definition of the truncated feature map  $\Phi_d$ , we also have that there is an isometric isomorphism  $\iota$  of  $\mathbb{R}^d$  into  $\mathcal{P}_d \mathcal{H}$  such that  $\Phi_d$  is mapped into  $\mathcal{P}_d \kappa(\cdot, X)$ . We can thus compare  $\rho_n^{-1/2} \tilde{\mathbf{Z}}^\dagger \mathbb{E}[\boldsymbol{\xi}]$  and  $\Phi_d$  via their difference in  $\mathcal{H}$ , i.e., via  $\|\hat{\iota}(\rho_n^{-1/2} \tilde{\mathbf{Z}}^\dagger \mathbb{E}[\boldsymbol{\xi}]) - \iota(\Phi_d(X))\|_{\mathcal{H}}$ . However, a comparison between  $\rho_n^{-1/2} \tilde{\mathbf{Z}}^\dagger \mathbb{E}[\boldsymbol{\xi}]$  and  $\Phi_d(X)$  as points in  $\mathbb{R}^d$  via the Euclidean distance on  $\mathbb{R}^d$  might be more useful. The following result facilitates such a comparison.

**Lemma 16** *With probability  $1 - 2\eta$  there exists an orthogonal  $\mathbf{W} \in \mathcal{M}_d$  such that*

$$\|\rho_n^{-1/2} \mathbf{W} \tilde{\mathbf{Z}}^\dagger \mathbf{p}_X - \Phi_d(X)\|_{\mathbb{R}^d} \leq C \sqrt{\frac{\log(n/\eta)}{n}} \quad (39)$$

for all  $X \in \mathcal{X}$ , where  $\mathbf{p}_X = (\rho_n \kappa(X_i, X))_{i=1}^n = \mathbb{E}[\boldsymbol{\xi}] \in \mathbb{R}^n$ .

**Proof** Let  $\nu, \nu' \in \hat{\mathcal{P}}_d \mathcal{H}$  be arbitrary. Thus,  $\nu = \hat{\mathcal{P}}_d \zeta$  and  $\nu' = \hat{\mathcal{P}}_d \zeta'$  for some  $\zeta, \zeta' \in \mathcal{H}$ . The polarization identity gives

$$\langle \mathcal{P}_d \nu, \mathcal{P}_d \nu' \rangle_{\mathcal{H}} = \frac{1}{4} \left( \|\mathcal{P}_d(\nu + \nu')\|_{\mathcal{H}}^2 - \|\mathcal{P}_d(\nu - \nu')\|_{\mathcal{H}}^2 \right) \quad (40)$$

$$\langle \nu, \nu' \rangle_{\mathcal{H}} = \frac{1}{4} \left( \|\nu + \nu'\|_{\mathcal{H}}^2 - \|\nu - \nu'\|_{\mathcal{H}}^2 \right) \quad (41)$$

By the Pythagorean theorem, we have

$$\|\zeta - \mathcal{P}_d \zeta\|_{\mathcal{H}}^2 = \|\zeta\|_{\mathcal{H}}^2 - \|\mathcal{P}_d \zeta\|_{\mathcal{H}}^2 \quad (42)$$

for any  $\zeta \in \mathcal{H}$ . Therefore,

$$\begin{aligned} \langle \nu, \nu' \rangle_{\mathcal{H}} - \langle \mathcal{P}_d \nu, \mathcal{P}_d \nu' \rangle_{\mathcal{H}} &= \frac{1}{4} \|(\nu + \nu') - \mathcal{P}_d(\nu + \nu')\|_{\mathcal{H}}^2 \\ &\quad - \frac{1}{4} \|(\nu - \nu') - \mathcal{P}_d(\nu - \nu')\|_{\mathcal{H}}^2 \end{aligned} \quad (43)$$

Eq. (43) then implies

$$\begin{aligned} |\langle \nu, \nu' \rangle_{\mathcal{H}} - \langle \mathcal{P}_d \nu, \mathcal{P}_d \nu' \rangle_{\mathcal{H}}| &\leq \frac{1}{4} \sup_{\hat{\mathcal{P}}_d \mathcal{H}} \{\|\tilde{\nu} - \mathcal{P}_d \tilde{\nu}\|_{\mathcal{H}}^2\} \\ &\leq \frac{1}{4} \sup_{\mathcal{H}} \|\hat{\mathcal{P}}_d \tilde{\zeta} - \mathcal{P}_d \hat{\mathcal{P}}_d \tilde{\zeta}\|_{\mathcal{H}}^2 \\ &\leq \frac{1}{4} \sup_{\mathcal{H}} \|(\hat{\mathcal{P}}_d - \mathcal{P}_d) \hat{\mathcal{P}}_d \tilde{\zeta}\|_{\mathcal{H}}^2 \\ &\leq \frac{1}{4} \|\hat{\mathcal{P}}_d - \mathcal{P}_d\|_{HS(\mathcal{H})}^2 \|\hat{\mathcal{P}}_d \tilde{\zeta}\|_{\mathcal{H}}^2 \end{aligned}$$

Therefore, by Eq. (32) in Proposition 13, we have for  $n$  satisfying  $4\sqrt{2}n^{-1}\sqrt{\log(1/\eta)} < \delta_d$ , that with probability at least  $1 - 2\eta$ .

$$|\langle \nu, \nu' \rangle_{\mathcal{H}} - \langle \mathcal{P}_d \nu, \mathcal{P}_d \nu' \rangle_{\mathcal{H}}| \leq \frac{2\log(1/\eta)}{\delta_d^2 n} \quad (44)$$

holds for all  $\nu, \nu' \in \hat{\mathcal{P}}_d \mathcal{H}$ . Suppose that Eq. (44) holds. Thus, the projection  $\mathcal{P}_d$  when restricted to  $\hat{\mathcal{P}}_d \mathcal{H}$  is almost an isometry from  $\hat{\mathcal{P}}_d \mathcal{H}$  to  $\mathcal{P}_d \mathcal{H}$ . There thus exists a unique isometry  $\tilde{i}$  from  $\hat{\mathcal{P}}_d \mathcal{H}$  to  $\mathcal{P}_d \mathcal{H}$  such that

$$\|\tilde{i}(\nu) - \mathcal{P}_d \nu\|_{\mathcal{H}} \leq 3 \frac{\sqrt{2\log(1/\eta)}}{\delta_d \sqrt{n}} \quad (45)$$

holds for all  $\nu \in \hat{\mathcal{P}}_d \mathcal{H}$  (Theorem 1 in Chmielinski (2000)). Now let  $\xi \in \mathcal{P}_d \mathcal{H}$  be arbitrary. Then  $\xi = \mathcal{P}_d \zeta$  for some  $\zeta \in \mathcal{H}$ . Let  $\nu = \hat{\mathcal{P}}_d \zeta$ . We then have

$$\begin{aligned} \|\tilde{i}(\nu) - \xi\|_{\mathcal{H}} &\leq \|\tilde{i}(\nu) - \mathcal{P}_d \nu\|_{\mathcal{H}} + \|\mathcal{P}_d \nu - \xi\|_{\mathcal{H}} \\ &\leq \|\tilde{i}(\nu) - \mathcal{P}_d \nu\|_{\mathcal{H}} + \|\mathcal{P}_d \hat{\mathcal{P}}_d \zeta - \mathcal{P}_d \zeta\|_{\mathcal{H}} \\ &\leq 3 \frac{\sqrt{2\log(1/\eta)}}{\delta_d \sqrt{n}} + \|\hat{\mathcal{P}}_d - \mathcal{P}_d\|_{HS(\mathcal{H})} \|\zeta\|_{\mathcal{H}} \end{aligned} \quad (46)$$

By Proposition 13, the right hand side of Eq. (46) can be bounded to give

$$\|\tilde{i}(\nu) - \xi\| \leq C \frac{\sqrt{\log(1/\eta)}}{\delta_d \sqrt{n}} \quad (47)$$

for some constant  $C$ . Thus, for any  $\xi \in \mathcal{P}_d\mathcal{H}$ , there exists a  $\nu \in \hat{\mathcal{P}}_d\mathcal{H}$  with  $\|\tilde{i}(\nu) - \xi\|_{\mathcal{H}} < C\delta_d^{-1}n^{-1/2}\sqrt{\log(1/\eta)}$ , i.e.,  $\tilde{i}$  is  $C\delta_d^{-1}n^{-1/2}\sqrt{\log(1/\eta)}$ -surjective. Thus  $\tilde{i}$  is an isometric isomorphism from  $\hat{\mathcal{P}}_d\mathcal{H}$  into  $\mathcal{P}_d\mathcal{H}$  (Proposition 1 in Chmielński (1997)).

To complete the proof, we note that  $(\tilde{i} \circ \hat{i}^{-1})(\tilde{\mathbf{Z}}^\dagger \mathbf{p}_X)$  is the image of the isometric isomorphism taking  $\tilde{\mathbf{Z}}^\dagger \mathbf{p}_X$  in  $\mathbb{R}^d$  to some  $\nu \in \mathcal{P}_d\mathcal{H}$ . By our previous reasoning, we have that  $(\tilde{i} \circ \hat{i}^{-1})(\tilde{\mathbf{Z}}^\dagger \mathbf{p}_X)$  is “close” to  $\mathcal{P}_d\hat{\mathcal{P}}_d\kappa(\cdot, X)$  which is “close” to  $\mathcal{P}_d\mathcal{P}_d\kappa(\cdot, X) = \mathcal{P}_d\kappa(\cdot, X)$ . Formally, let  $\varphi = \iota \circ \tilde{i} \circ \hat{i}^{-1}$ . We then have

$$\begin{aligned} \|\varphi(\tilde{\mathbf{Z}}^\dagger \mathbf{p}_X) - \Phi_d(X)\|_{\mathbb{R}^d} &= \|\tilde{i} \circ \hat{i}^{-1}(\tilde{\mathbf{Z}}^\dagger \mathbf{p}_X) - \iota^{-1}(\Phi_d(X))\|_{\mathcal{H}} \\ &= \|\tilde{i}(\hat{\mathcal{P}}_d\kappa(\cdot, X)) - \mathcal{P}_d\kappa(\cdot, X)\|_{\mathcal{H}} \\ &\leq \|\tilde{i}(\hat{\mathcal{P}}_d\kappa(\cdot, X)) - \mathcal{P}_d\hat{\mathcal{P}}_d\kappa(\cdot, X)\|_{\mathcal{H}} + \|\mathcal{P}_d\hat{\mathcal{P}}_d\kappa(\cdot, X) - \mathcal{P}_d\kappa(\cdot, X)\|_{\mathcal{H}} \\ &\leq C \frac{\sqrt{\log(1/\eta)}}{\delta_d\sqrt{n}}. \end{aligned} \tag{48}$$

As  $\varphi$  is a composition of isometric isomorphisms between finite-dimensional Hilbert spaces, it is an isometric isomorphism from  $\mathbb{R}^d$  to  $\mathbb{R}^d$ , i.e.,  $\varphi$  correspond to an orthogonal matrix  $\mathbf{W}$ , as desired.  $\blacksquare$

We now proceed to complete the proof of Theorem 2.

**Proof** [Theorem 2] Let  $\mathbf{W}, \mathbf{W}_1, \mathbf{W}_2 \in \mathcal{M}_d$  be orthogonal matrices with  $\mathbf{W}_2\mathbf{W}_1 = \mathbf{W}$ . Recall that  $\mathbb{E}[\boldsymbol{\xi}] = (\rho_n\kappa(X, X_i))_{i=1}^n$ . We then have

$$\begin{aligned} \|\rho_n^{-1/2}\mathbf{W}T_n(X) - \Phi_d(X)\| &\leq \|\rho_n^{-1/2}(\mathbf{W}_2\mathbf{W}_1\mathbf{Z}^\dagger - \mathbf{W}_2\tilde{\mathbf{Z}}^\dagger)\boldsymbol{\xi}\| + \|\rho_n^{-1/2}\mathbf{W}_2\tilde{\mathbf{Z}}^\dagger(\boldsymbol{\xi} - \mathbb{E}[\boldsymbol{\xi}])\| \\ &\quad + \|\rho_n^{-1/2}\mathbf{W}_2\tilde{\mathbf{Z}}^\dagger\mathbb{E}[\boldsymbol{\xi}] - \Phi_d(X)\| \end{aligned}$$

The first term in the right hand side of the above can be bounded by Lemma 10, i.e., there exists an orthogonal  $\mathbf{W}_1$  such that

$$\|\rho_n^{-1/2}(\mathbf{W}_2\mathbf{W}_1\mathbf{Z}^\dagger - \mathbf{W}_2\tilde{\mathbf{Z}}^\dagger)\boldsymbol{\xi}\| \leq C\delta_d^{-3}\sqrt{\frac{\log(n/\eta)}{n\rho_n}} \tag{49}$$

with probability at least  $1 - 2\eta$ . The second term  $\|\rho_n^{-1/2}\mathbf{W}_2\tilde{\mathbf{Z}}^\dagger(\boldsymbol{\xi} - \mathbb{E}[\boldsymbol{\xi}])\|$  can be bounded by Theorem 12, i.e.,

$$\|\rho_n^{-1/2}\mathbf{W}_2\tilde{\mathbf{Z}}^\dagger(\boldsymbol{\xi} - \mathbb{E}[\boldsymbol{\xi}])\| < C\delta_d^{-3}\sqrt{\frac{\log(n/\eta)}{n\rho_n}} \tag{50}$$

Finally, the third term is bounded by Lemma 16. Thus, with probability at least  $1 - \eta$ , there exists some unitary  $\mathbf{W}$  such that

$$\|\rho_n^{-1/2}\mathbf{W}T_n(X) - \Phi_d(X)\| \leq C\delta_d^{-3}\sqrt{\frac{\log(n/\eta)}{n\rho_n}} \tag{51}$$

as desired.  $\blacksquare$



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