Laplacian Eigenmaps from Sparse, Noisy Similarity Measurements

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Abstract—Manifold learning and dimensionality reduction techniques are ubiquitous in science and engineering, but can be computationally expensive procedures when applied to large data sets or when similarities are expensive to compute. To date, little work has been done to investigate the tradeoff between computational resources and the quality of learned representations. We present both theoretical and experimental results in this direction. Experimentally, we explore the effects of noise and occlusion on Laplacian eigenmaps embeddings of two real-world data sets, one from speech processing and one from neuroscience, as well as a synthetic data set.

I. INTRODUCTION AND MOTIVATION

MANIFOLD-BASED dimensionality reduction techniques operate under the assumption that data observed in a high-dimensional space lie on a low-dimensional manifold [4], [5], [25], [56]. Owing to the ubiquity of large high-dimensional data sets, these techniques have been well studied, with applications across many disparate fields [59]. In addition to the classical linear techniques (e.g., PCA [37], MDS [23] and CCA [29], [33]), numerous manifold embedding procedures have been proposed to discover intrinsic low-dimensional structure in nonlinear data (e.g., ISOMAP [50] and Laplacian eigenmaps [4], among others). These nonlinear techniques typically attempt to preserve some notion of local geometry in the embedding. As such, they tend to be empirically robust to modest noise and outliers [4], though general theoretical results in this direction are comparatively few.

Herein, we theoretically and practically explore the robustness of Laplacian eigenmaps to very general noise conditions. The present work differs from most manifold embedding robustness results in two key ways: first, we assume that the uncertainty lies not in the observations themselves, but rather in our measurement of the pairwise similarities used to construct the kernel matrix. Second, the noise model is entirely nonparametric: we make no distributional assumptions on the noise other than unbiasedness (see Equation (2) below).

A. Problem Description

Suppose that $\mathcal{X}$ is a set of objects, endowed with a notion of similarity captured by a kernel function $\kappa: \mathcal{X} \times \mathcal{X} \rightarrow [0, 1]$; i.e., $x, y \in \mathcal{X}$ are similar if $\kappa(x, y) \approx 1$, and $x, y \in \mathcal{X}$ are not similar if $\kappa(x, y) \approx 0$. Given $n$ observations $x_1, x_2, \ldots, x_n \in \mathcal{X}$, we can represent their similarities via a hollow (i.e., no self-loops), undirected weighted graph with adjacency matrix $\mathcal{K}$ given by

$$
\mathcal{K}_{ij} = \begin{cases} 
\kappa(x_i, x_j) & \text{if } i \neq j \\
0 & \text{otherwise.}
\end{cases}
$$

Manifold-based dimensionality reduction techniques seek to recover the low-dimensional structure intrinsic in the similarities captured by $\mathcal{K}$. We note that some manifold embedding algorithms rely on distance or dissimilarity measures rather than similarities, but the distinction is immaterial here.

The quality of the embedding of $\mathcal{K}$ depends upon the quality of the similarity measure $\kappa$ and upon our ability to compute the similarity accurately. If $\kappa$ only approximately captures the “correct” notion of similarity between observations, it is natural to ask how this influences the quality of the embedding. Similarly, when $\kappa(x, y)$ is expensive to compute, we might ask whether an embedding of similar quality is possible based on an inexpensive approximation or by computing $\kappa(x, y)$ for only a fraction of all pairs of observations, and inferring the rest of $\mathcal{K}$, for example, by applying Chatterjee’s universal singular value thresholding (USVT) [13].

The Laplacian eigenmaps embeddings constructed in [43] and serve as an illustrative example. The authors’ data consists of a set of 10,383 word examples, each represented by a time series of acoustic feature vectors. For word examples $x_i$ and $x_j$, the corresponding entry in the kernel matrix is

$$
\mathcal{K}_{ij} = \exp\{-d^2(x_i, x_j)/\sigma^2\},
$$

where $d(x_i, x_j)$ is a function of the dynamic time warping (DTW) alignment cost [53] between $x_i$ and $x_j$. We refer the reader to [43] and references therein for technical details. The inadequacies of DTW as a word similarity measure are well documented in the speech processing literature [43], [44]. Additionally, DTW cost is computationally expensive, requiring time that scales as the product of the lengths of the two aligned sequences. As such, a fast estimate of $d(x_i, x_j)$ or $\kappa(x_i, x_j)$ is acceptable, and it is preferable to avoid computing all $O(n^2)$ alignments required to populate the kernel matrix.

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B. Our Model

In light of the above, we consider the following model. We assume a fixed set of observations \(x_1, x_2, \ldots, x_n \in \mathcal{X}\), and a similarity function \(\kappa\) defined on \(\mathcal{X} \times \mathcal{X}\), giving rise to a true but unknown symmetric kernel matrix \(\mathcal{K} = [\mathcal{K}_{ij}] \in [0,1]^{n \times n}\). The embedding learned from \(\mathcal{K}\) is the best embedding we could hope to learn, in that it accurately and completely captures all the information available to us about \(x_1, x_2, \ldots, x_n\). The data processing inequality [22] implies that given the data, kernel function and embedding procedure, adding noise and occlusion to \(\mathcal{K}\) cannot improve the embeddings from the standpoint of subsequent inference or classification. Suppose, however, that rather than observing \(\mathcal{K}\), we observe a random symmetric matrix \(\mathcal{Y} \in \mathbb{R}^{n \times n}\), whose entries are generated independently as

\[
Y_{ij} = Y_{ji} = \begin{cases} K_{ij} & \text{with probability } p \\ 0 & \text{with probability } (1-p), \end{cases}
\]

where the \(K_{ij} \in [0,1]\) are independent random variables with \(\mathbb{E}K_{ij} = \mathcal{K}_{ij}\) and \(p \in [0,1]\) is the (expected) fraction of entries of \(\mathcal{Y}\) that are observed. We note that our results hold for similarity functions bounded by any constant, and our use of the range \([0,1]\) is without loss of generality. We can think of \(K\) as a corrupted version of \(\mathcal{K}\), with errors reflecting, for example, our failure to fully capture the correct notion of similarity on \(\mathcal{X}\), or approximation error arising from estimating a computationally expensive \(\kappa(x,y)\). Similarly, we can view the sparsity of \(\mathcal{Y}\) as reflecting the fact that when \(n\) is large or \(\kappa\) is expensive to compute, we would like to avoid computing all \(O(n^2)\) pairwise similarities in \(\mathcal{K}\). Our model is meant to account for general uncertainty in the kernel matrix, which may come from many sources (e.g., computational restrictions, estimation, etc.). Ultimately, we require only that errors be entry-wise independent and unbiased.

When \(\mathcal{K}_{ij} \approx 0\) or \(\mathcal{K}_{ij} \approx 1\), our model allows \(K_{ij}\) very little variance. In many applications, the cases when \(\kappa(x,y) \approx 0\) or \(\kappa(x,y) \approx 1\) are less prone to error, which is reflected in our model. Indeed, it is often easy to detect when two observations are very similar or very dissimilar, whereas one expects higher variance in estimation of similarity when, say, \(\kappa(x,y) = 1/2\).

Remark 1 (Error Generalization): Our model is a good approximation to more complicated error models. As an example, consider the Gaussian kernel \(\kappa(x,y) = \exp(-d^2(x,y)/\sigma^2)\), where \(\sigma > 0\) is the kernel bandwidth. A more natural but less tractable error model is one in which \(D_{ij}\) is an estimate (possibly biased) of \(d(x_i, x_j)\) and our kernel matrix is \(K_{ij} = \exp(-D_{ij}/\sigma^2)\), say, \(D_{ij} = d_0 + E_{ij}\) where \(E_{ij}\) is a random error term. A Taylor expansion of \(\exp(-d^2/\sigma^2)\) about \(d_0 = d(x_i, x_j)\) shows that (taking \(\sigma = 1\) without loss of generality and using the fact that \(\mathcal{K}_{ij} = e^{d^2}K_{ij} = e^{d_0^2}E_{ij} - 2d_0e^{-d_0^2}E_{ij} + (4d_0^2 - 2)e^{-d_0^2}E_{ij}^2 + O(E_{ij}^3)\).

We see that so long as \(E_{ij}\) is reasonably well-behaved, we still have \(\mathbb{E}K_{ij} \approx \mathcal{K}_{ij}\), and an approximate version of the results presented in this paper will hold. More broadly, we note that so long as \(\mathbb{E}K_{ij} - \mathcal{K}_{ij}\) is suitably small for most entries, our results can be extended to the case of biased errors. These observations are borne out by experiment (See Figures 5 and 9).

In this paper, we theoretically and practically explore under what conditions it is suitable to use the embedding learned using \(\mathcal{Y}\) in place of \(\mathcal{K}\). Under such conditions, we can obtain embeddings with quality comparable to those produced from \(\mathcal{K}\), at a greatly reduced computational cost. In the present work, we consider the performance of Laplacian eigenmaps [4], [5] under this model, though we believe that the results extend to other embedding techniques, as well.

C. Laplacian Eigenmaps

As originally described in [4], [5], Laplacian eigenmaps embeds the observed data \(\mathcal{X}\) into \(\mathbb{R}^d\) by first constructing the \(k\)-nearest-neighbor (\(k\)-NN) or \(\epsilon\)-graph \(G = (V,E)\) from \(\mathcal{X}\). In the \(k\)-NN graph, an edge is present between \(i\) and \(j\) if \(x_i\) is among the \(k\) nearest neighbors (according to some distance defined on \(\mathcal{X}\)) of \(x_j\) or vice versa. In the \(\epsilon\)-graph, \(i\) and \(j\) are adjacent if \(\|x_i - x_j\|^2 < \epsilon\) for a given threshold parameter \(\epsilon\).

We define \(W\), the weighted adjacency matrix of \(G\), by

\[
W_{ij} = \begin{cases} \mathcal{K}_{ij} & \text{if } (i,j) \in E \\ 0 & \text{else}, \end{cases}
\]

and let \(D \in \mathbb{R}^{n \times n}\) be the diagonal matrix defined by \(D_{ii} = \sum_j W_{ij}\) for \(i \in [n]\). Then the normalized weighted graph Laplacian of \(G\) [13] is given by \(\mathcal{L}(W) = D^{-1/2}W D^{-1/2}\). If the eigendecomposition of \(\mathcal{L}(W)\) is given by \(\mathcal{L}(W) = U \Lambda U^\top\) with the diagonal entries of \(\Lambda\) nonincreasing, then Laplacian eigenmaps embeds \(\mathcal{X}\) via \(U[;1 : d+1] - \text{the first } d\) nontrivial eigenvectors of \(\mathcal{L}(W)\). (note that \(U[;1] = 1\), the trivial all-ones vector). This embedding optimally preserves the local geometry of \(\mathcal{X}\) in a least squares sense.

In the event that \(\mathcal{X}\) is noisily and incompletely observed as \(Y\), how does the \(d\)-dimensional Laplacian eigenmaps embedding of \(Y\) compare with that of \(\mathcal{X}\)? Our main result, Theorem 1 deals with the regularized matrix \(Y_{ij} + r\) rather than \(Y\) itself, owing to the fact that when \(p\) is small, the matrix \(p\mathcal{K} = \mathcal{Y}\) may be quite sparse, in the sense that some or all of the row sums \(\sum_{j=1}^n \mathcal{K}_{ij}\) are too small to guarantee necessary concentration inequalities [40], [46], [57]. Regularization prevents this pitfall, at the cost of changing the matrix to which we converge. We discuss regularization at more length in Subsection 1.C. Intuitively, our main theorem states that the embedding produced from a regularized version of \(Y\) is similar to that produced by \(\mathcal{K}\). This implies that we can avoid the \(O(n^2)\) exact computations for \(\mathcal{K}\), using instead the potentially less computationally expensive \(Y\), with little loss in downstream performance.

Remark 2: We depart from Laplacian eigenmaps as originally described [4] in that we do not build a \(k\)-NN graph or \(\epsilon\)-graph from \(\mathcal{X}\). However, a suitably-chosen kernel function (e.g., the Gaussian kernel) ensures that \(\mathcal{K}\) approximates a \(k\)-NN or \(\epsilon\)-graph, with \(Y\) a noisily-observed subgraph of \(\mathcal{X}\).

D. Notation

For a set \(S\), we denote the complement of \(S\) by \(S^c\). For a matrix \(B \in \mathbb{R}^{n \times n}\), we let \(\lambda(B)\) denote the multi-set of
eigenvalues of $B$, and for $S \subset \mathbb{R}$, we define $\lambda_S(B) = \lambda(B) \cap S$. We let $J$ denote the matrix of all ones.

We make use of standard big-$O$ notation, writing $f(n) = O(g(n))$ to mean that there exists a constant $C > 0$ such that $f(n) \leq C g(n)$ for suitably large $n$. Similarly, we write $f(n) = o(g(n))$ to mean that $f(n)/g(n) \to 0$ as $n \to \infty$. We use $f(n) = \Omega(g(n))$ to denote that $f$ grows at least as quickly as $g$ does, i.e., to denote that $g(n) = O(f(n))$, and we write $f(n) = \omega(g(n))$ when $g(n) = o(f(n))$.

Throughout this paper, all quantities are assumed to depend on $n$, a fact that we highlight by subscripting or superscripting with $n$ (e.g., $\mathcal{X} = \mathcal{X}^{(n)}$), but which we will suppress in much of the text for ease of notation. Our main theorem, Theorem 1, is a finite-sample result, with $\mathcal{X}^{(n)}$ viewed as fixed for each $n$, and $K^{(n)}$ and $Y^{(n)}$ randomly generated from $\mathcal{X}^{(n)}$. We note that all of our results can be restated as holding almost surely as $n \to \infty$ by assuming suitable lower bounds on the constants in the supporting Lemmas so as to ensure that the probabilities of the various “bad events” are summably small. An application of the Borel-Cantelli lemma then implies that our desired events hold almost surely. This modification can be made to work either in the case (a) where we view our desired events hold almost surely. This modification can be made to work either in the case (a) where we view $Y, K$ and $\mathcal{X}$ as (growing, “nested”) principle submatrices of infinite matrices, or (b) in the case where we consider a sequence of fixed matrices $\mathcal{X}^{(n)} \to \infty$.

In this work, we assume $\mathcal{X}$ to be fixed (i.e., not random—the randomness lies entirely in $Y$ and $K$). This assumption is made primarily for the sake of brevity and simplicity, since randomness in $\mathcal{X}$ would have to come from random selection of the sample $x_1, x_2, \ldots, x_n \in \mathcal{X}$ according to some distribution $F$ on $\mathcal{X}$. Clearly, the properties of $\mathcal{X}$ depend on the properties of $F$ and $\mathcal{X}$, but a thorough exploration of precisely how $F$ and $\mathcal{X}$ influence $\mathcal{X}$ is beyond the scope of this paper, and we leave it for future work.

E. Roadmap

Section II surveys robust manifold-based dimensionality reduction and related problems. We present our theoretical results in Section III and explore these results experimentally in Section IV. We close with a brief discussion in Section V.

II. RELATED WORK

A. Manifold Learning

Manifold learning is a general class of techniques for nonlinear dimensionality reduction that seek to embed a collection of observations into Euclidean space in a way that preserves some aspect of the structure of those observations. For example, given a collection of objects and some notion of distance on those objects, we may wish to embed the objects into Euclidean space in such a way that all pairwise distances are (approximately) preserved [35, 45]. A host of different embedding techniques have been proposed in the literature (see, for example, [21, 23, 45, 51, 52, 56]) to preserve the numerous different notions of structure in the data. As outlined in [62], it is possible to view many of these approaches as special cases of a more general framework.

There is a large amount of literature dedicated to improving the performance of manifold learning and dimensionality reduction algorithms in the presence of noise and missing data; see, for example, [8, 12, 30, 54]. The present work differs from most such results in the following key ways: We assume that the uncertainty lies not in the observations themselves, but rather in the computation of the pairwise similarities or distances used to construct the kernel matrix, and our model of this uncertainty is nonparametric. Additionally, we make no assumption that the observations lie in Euclidean space. Rather, the objects under study are arbitrary (e.g., they may be time series, graphs, etc.), and information about the geometry of $\mathcal{X}$ comes through the kernel function $\kappa$.

With the rise of big data and the continued popularity of kernel methods, much research has gone toward faster construction and embedding of the kernel matrix by speeding up the evaluation of the kernel function itself [42, 61], the embedding procedure [3, 7], and construction of the kernel matrix as a whole [27]. Construction of the kernel matrix is often the major bottleneck in machine learning systems [32, 43, 44]. In our model, embedding the partially observed noisy kernel matrix $Y$ allows for potentially dramatic speedups compared to the computation of the full, clean kernel $\mathcal{X}$. A similarly-motivated idea was explored in [15], where the authors presented a pair of divide-and-conquer algorithms for approximately constructing $k$-NN graphs on observations in Euclidean space. However, unlike our approach, they do not consider noise in the observations themselves or in the assessment of distances between observations.

Another close analogue to our present work is [51], in which the authors theoretically and empirically explored the robustness properties of spectral clustering: i.e., Laplacian eigenmaps applied to a binary adjacency matrix followed by $k$-means clustering. In the language of the present paper, they considered the inner product kernel matrix $\mathcal{X} \in \mathbb{R}^{n \times n}$ on a fixed (but unknown) subset $\mathcal{X} \subset \mathbb{R}^d$. From this kernel, they observed the matrix $Y \in \{0, 1\}^{n \times n}$ with independent entries

$$Y_{ij} = Y_{ji} = \begin{cases} 1 & \text{with probability } \mathcal{X}_{ij} \\ 0 & \text{with probability } (1 - \mathcal{X}_{ij}) \end{cases}$$

They compared the Laplacian spectral embedding based on $\mathcal{X}$ with that based on $Y$. Their key result showed that, under some mild assumptions on the spectrum of $\mathcal{X}(\mathcal{X})$ (the normalized Laplacian of $\mathcal{X}$), the eigenspace of $\mathcal{X}(Y)$ does not significantly differ from the corresponding eigenspace of $\mathcal{X}(\mathcal{X})$ (after suitable rotation). As a result, they prove that spectral clustering of $\mathcal{X}(Y)$ consistently estimates the clusters obtained by spectrally clustering $\mathcal{X}(\mathcal{X})$. While our main theorem uses results [51, Prop. 2.1 and Thm. 2.2]) developed in that paper, the generality of our occlusion model compared to [5] requires new proof techniques. Additionally, our manifolds do not necessarily have a well-defined cluster structure (as the stochastic blockmodel graphs of [51] do), and so we do not consider consistency of clustering of our embedding. Rather, in Theorem 1 we prove that the relevant eigenvectors of $\mathcal{X}(Y)$ do not significantly differ from the corresponding eigenvectors of $\mathcal{X}(\mathcal{X})$. As in [51], we expect the consistency of subsequent inference to similarly follow.
B. Matrix Completion and Data Imputation

A natural approach to applying Laplacian eigenmaps to $Y$ is to first impute the missing entries of $Y$ using matrix completion techniques. For example, with the additional assumption that $\mathcal{X}$ is approximately low-rank, it would be possible to impute the missing data via the techniques developed in compressed sensing [10]. While some compressed sensing papers have considered matrix completion in the presence of both noise and occlusion [9], [17], most also require bounds on the incoherence of matrix $\mathcal{X}$, a requirement that need not hold in general for the kernel matrices we consider here.

Some matrix completion work has considered imputing missing entries in a distance matrix [11, 46, 58]. Among these works, [56] is closest in spirit to the problem considered in the present work. In [56], the authors considered the problem of placing $n$ objects into $d$-dimensional Euclidean space based on noisy, occluded measurements of the $O(n^3)$ pairwise distances. Their semidefinite programming-based approach solves this problem under a very general error model, where nothing is known about the errors other than a bound on their magnitude. However, their model differs from ours in two key ways. First, the observations in question are assumed to lie in $d$-dimensional Euclidean space, while ours need only be endowed with a kernel function. Second, they assume that distance measurements are taken on all pairs of points within a fixed radius of one another. However, under our model, all entries of $\mathcal{X}$ are equally likely to be (noisily) observed.

Chatterjee [13] considered the problem of completing an arbitrary matrix based on partial, noisy observations, with no specific assumptions on the matrix structure. His universal singular value thresholding (USVT) procedure constructs a minimax optimal estimate for $\mathcal{X}$ based on its occluded, noisy measurement $Y$ (as defined in (2)). Though we believe that the results obtained in this paper would hold in a qualitatively similar way if we used USVT applied to matrix $Y$ prior to embedding, analyzing the behavior of the USVT estimate of $\mathcal{X}$ under the graph Laplacian is theoretically challenging, and we do not pursue it further here. In empirical comparisons, we found our method and Chatterjee’s USVT performed nearly identically across our data sets. We do note that USVT requires an expensive SVD computation, and yields a dense matrix as an estimate of $\mathcal{X}$, instead of the sparse $Y$, which may be computationally intractable for large $n$.

C. Matrix Concentration

Recent years have seen a flurry of results proving concentration results for sums of random matrices [2], [14], [38], [40], [41], [46], [49], [57], in the spirit of the well-established scalar analogues [19]. Many existing concentration results require assumptions about the density of the underlying graphs [46], [51]. For example, many such results hold only in the dense regime and require a lower bound on the average degree (i.e., a lower bound on the row sums of the expected value of the random matrix). It is well known that the high variance associated with small average degree precludes concentration of the Laplacian for general weighted graphs [20], [25], [39], [40]. This is an issue for the problem considered in the present work, especially when we observe only a small fraction of the matrix entries.

Existing empirical and theoretical results show that regularization yields the desired concentration of the graph Laplacian for sparse graphs (see [2], [14], [38], [40], [41], [49] and references therein). This regularization typically takes the form of either adding a small number to each entry of the adjacency matrix, as in [40], or by adding to the degree matrix directly, as in [49]. Our result draws on this line of work by investigating the behavior of the Laplacian eigenmaps embeddings when regularization is applied. In this sense, the current work is a natural outgrowth of [51] and [49] in that the former considers concentration of the Laplacian eigenmaps embeddings under the Frobenius norm, and the latter considers concentration of the regularized graph Laplacian under the spectral norm. We follow the former of these two works and consider concentration under the Frobenius norm, rather than spectral norm. This differs from the bounds established in [40], [41], [46], [57], which show concentration of the adjacency matrix and graph Laplacian under the spectral norm. We prefer the Frobenius norm formulation of Theorem 1 as the Frobenius norm between the (suitably rotated) eigenspaces has a natural interpretation as the Procrustes alignment error of the orthogonal bases of the two different embeddings.

III. Main Results

Our goal is to theoretically and empirically understand the impact of observation error on the embedding obtained via Laplacian eigenmaps. That is, how much does the embedding obtained using matrix $Y$ degrade with respect to that obtained using matrix $\mathcal{X}$? We prove that Laplacian eigenmaps is indeed robust to certain amounts of both occlusion and noise by first proving that (a suitably regularized version of) $\mathcal{L}^2(Y)$ concentrates about (a regularized version of) $\mathcal{L}^2(p,\mathcal{X})$, where $Y$ and $p$ are defined as in Equation (2). Combining this result with the Davis-Kahan theorem [24], we obtain in Theorem 1 a guarantee that the embedding learned from the occluded noisy kernel matrix is similar (up to rotation) to that learned from the regularized clean kernel matrix. We provide relevant details below and in the appendix.

Let $G = (V, E)$ be an undirected, loop-free, weighted graph on $n$ vertices with edge weights $w_{ij} \geq 0$. We represent $G$ by its adjacency matrix $A \in \mathbb{R}^{n \times n}$, with entries

$$A_{ij} = A_{ji} = \begin{cases} w_{ij} & \text{if } \{i, j\} \in E \\ 0 & \text{if } \{i, j\} \notin E. \end{cases}$$

Given $A$, we define its normalized graph Laplacian by

$$\mathcal{L}(A) = (\mathcal{D}(A))^{-1/2} A \mathcal{D}(A)^{-1/2},$$

where $\mathcal{D}(A) \in \mathbb{R}^{n \times n}$, the degree matrix, is diagonal with $\mathcal{D}(A)_{ii} = \sum_{j=1}^{n} A_{ij}$ and inverse square root defined as

$$(\mathcal{D}(A)^{-1/2})_{ii} = \begin{cases} 1/\sqrt{\mathcal{D}(A)_{ii}} & \text{if } \mathcal{D}(A)_{ii} \neq 0 \\ 0 & \text{otherwise}. \end{cases}$$

We note that the graph Laplacian as we have defined it differs from the more commonly used $I - \mathcal{D}(A)^{-1/2} A \mathcal{D}(A)^{-1/2}$
(e.g., in [18]). We will be interested in the eigenspace of \( \mathcal{L}(A) \), and one can easily check that both our \( \mathcal{L}(A) \) and the more commonly used definition have the same eigenspaces.

In general, neither the adjacency matrix nor the graph Laplacian of sparse random graphs concentrate about their means owing to high variance in degree distributions [26], [40], [41]. This suggests that we should not expect that \( \mathcal{L}(Y) \) will concentrate for arbitrary kernel matrices, and hence we turn to regularization. Let \( J \in \mathbb{R}^{n \times n} \) denote the matrix of all ones. Our main result will require us to bound \( \|\mathcal{L}^2(Y + rJ) - \mathcal{L}^2(p\mathcal{X} + rJ)\|_F \), where \( Y \) is the sparse, noisy version of \( \mathcal{X} \) as specified in (2), and \( r \geq 0 \) is a regularization parameter. We deal with the squared Laplacians for reasons discussed in [51] Section 2]. Namely, we require that \( \mathcal{L}(Y + rJ) \) converge to \( \mathcal{L}(p\mathcal{X} + rJ) \) in Frobenius norm. To ensure convergence for a suitably broad class of matrices, we must instead consider the squared Laplacians in combination with the following Lemma, proved in [51], which ensures that if certain eigenvectors of \( \mathcal{L}(Y + rJ) \) converge, then so do the relevant eigenvectors of \( \mathcal{L}(Y + rJ) \).

**Lemma 1 ([57] Lemma 2.1):** Let \( B \in \mathbb{R}^{n \times n} \) be symmetric.

1) \( \lambda^2 \) is an eigenvalue of \( B^2 \) if and only if either \( \lambda \) or \( -\lambda \) is an eigenvalue of \( B \).

2) If \( Bx = \lambda x \), then \( B^2x = \lambda^2 x \).

3) If \( B^2x = \lambda^2 x \), then \( x \) can be written as a linear combination of eigenvectors of \( B \) with corresponding eigenvalues \( \lambda \) or \( -\lambda \).

Our main theorem, Theorem 1, shows that the span of the eigenvectors corresponding to the largest eigenvalues of the Laplacian of \( \mathcal{X} \) and the Laplacian of the sparse noisy kernel matrix \( Y \) are close. As a consequence, subsequent inference performed on the Laplacian eigenmaps embeddings will be robust to the errors introduced in \( Y \), since the embeddings will be (nearly) isometric to one another. In the statement of the theorem, we include subscript or superscript \( n \) on all quantities that depend on \( n \), though we will drop these subscripts in the sequel for notational convenience. Recall that for \( B \in \mathbb{R}^{n \times n} \), \( \lambda(B) \) denotes the multi-set of eigenvalues of \( B \) and for \( S \subset \mathbb{R} \), we define \( \lambda_S(B) = \lambda(B) \cap S \).

**Theorem 1:** Under the model described in (2), for an open interval \( S_n \subset \mathbb{R} \), let \( k_n = |\lambda_{S_n}(\mathcal{L}(Y^{(n)} + r_n J))| \) be the cardinality of \( \lambda_{S_n}(\mathcal{L}(Y^{(n)} + r_n J)) \) (counting multiplicities), and let \( X_n \in \mathbb{R}^{n \times k_n} \) be the matrix whose columns form an orthonormal basis for the subspace spanned by the eigenvectors of \( \mathcal{L}(Y^{(n)} + r_n J) \) with corresponding eigenvalues in \( \lambda_{S_n}(\mathcal{L}(Y^{(n)} + r_n J)) \). Let \( \hat{k}_n = |\lambda_{S_n}(\mathcal{L}(p\mathcal{X}^{(n)} + r_n J))| \) and let \( X_n \) be the analogue of \( X_n \) for \( \mathcal{L}(p\mathcal{X}^{(n)} + r_n J) \). Define

\[
\delta_n = \inf\{|\ell - s| : \ell \in \lambda_{S_n}(\mathcal{L}(p\mathcal{X}^{(n)} + r_n J)), s \in S_n\}.
\]

Let \( r_n \) depend on \( n \) in such a way that \( r_n \geq n^{-1} \log n \) for suitably large \( n \). There exist constants \( C, c > 0 \) and a positive integer \( N \) such that \( n \geq N \) implies that \( k_n = \hat{k}_n \), and there exists orthonormal rotation matrix \( O_n \) such that with probability at least \( 1 - n^{-c} \),

\[
\|X_n - X_n O_n\|_F \leq C \left( \frac{\log^{1/2} n}{\delta_n r_n n^{1/2}} \right).
\]

**Proof:** Combining Theorems 2 and 3 yields the result. ■

**Remark 3:** A key difference between the main theorem in [51] and our result is that we do not require a restriction on the degrees of \( p\mathcal{X} \) directly. Rather, we use regularization to ensure that no row sum is too small. We note that letting \( p = 1 \) and making minor adjustments to the arguments in our concentration inequalities (namely, lower bounds on the entries of the degree matrix \( D \)), we recover the main result of [51], with a slightly better convergence rate. Namely, if we define \( \tau = n^{-1} \min_{i \in [n]} D_{ii} \), our result has \( \tau^{-1} \) controlling to rate of convergence of the eigenspaces rather than \( \tau^{-2} \) as in [51] (with dependence on \( n \) and \( \delta \) unchanged).

**Remark 4:** We note the somewhat surprising fact that the bound in (4) does not depend explicitly on \( p \). This is a result of the presence of regularization parameter \( r \), which prevents \( p\mathcal{X} + r \) from becoming too sparse. We note that if one imposes stronger assumptions on the growth of \( p \) (namely, restricting the speed with which \( p \) can approach 0), our proofs can be adapted to dispense with \( r \) altogether, in which case \( p \) appears in the bounds instead.

Our main tool for proving Theorem 1 is the Davis-Kahan theorem [24], which we use in the form presented in [51]. We here index all quantities by \( n \) to reiterate that all quantities are allowed to depend on \( n \), but remind the reader that we will drop this indexing in much of the sequel for ease of notation.

**Theorem 2:** Let \( S_n \subset \mathbb{R} \) be an interval and let \( \mathcal{X}_n \) be a matrix with orthonormal columns that span the same subspace as that spanned by the eigenvectors of \( \mathcal{L}^2(p\mathcal{X}^{(n)}(n)) \) with corresponding eigenvalues in \( \lambda_{S_n}(\mathcal{L}^2(p\mathcal{X}^{(n)} + r_n J)) = \lambda_{S_n}(\mathcal{L}^2(p\mathcal{X}^{(n)} + r_n J)) \). Define \( X_n \) analogously for \( \mathcal{L}^2(Y^{(n)} + r_n J) \). Let \( \delta_n \) be defined for \( \mathcal{L}^2(p\mathcal{X}^{(n)} + r_n J) \) as in (4).

If \( \mathcal{X}_n \) and \( X_n \) are of the same dimension, then there exists orthonormal matrix \( O_n \), which depends on \( \mathcal{X}_n \) and \( X_n \), such that

\[
\frac{1}{2} \|X_n - X_n O_n\|_F^2 \leq \frac{\|\mathcal{L}^2(Y^{(n)} + r_n J) - \mathcal{L}^2(p\mathcal{X}^{(n)} + r_n J)\|_F^2}{\delta_n^2}.
\]

To apply Theorem 2 toward Theorem 1 we need a concentration bound for \( \mathcal{L}^2(Y + rJ) \) about \( \mathcal{L}^2(p\mathcal{X} + rJ) \). We note that, \( Y, \mathcal{X}, J \) and \( r \) all implicitly depend on \( n \), a fact

![Fig. 1. Points sampled from a 3-dimensional Swiss roll.](image-url)
that we do not generally make explicit in the sequel for ease of notation, but which we highlight here for clarity. For each \( n = 1, 2, \ldots, \) let \( \mathcal{X}^{(n)} \) be a weighted adjacency matrix for a graph on \( n \) points in \( \mathcal{X} \) as defined in (1). Similarly, let \( Y^{(n)} \) be the corresponding sparse noisy kernel matrix as defined in (2).

The corresponding sparse noisy kernel matrix as defined in (2). graph on \( n \) with \( \alpha = 1 \). Of notation, but which we highlight here for clarity. For each

\[ n = 1, 2, \ldots, \] let \( \mathcal{X}^{(n)} \) be a weighted adjacency matrix for a graph on \( n \) points in \( \mathcal{X} \) as defined in (1). Similarly, let \( Y^{(n)} \) be the corresponding sparse noisy kernel matrix as defined in (2).

Theorem 3: Assume that regularization parameter \( r \) grows with \( n \) in such a way that \( r = \omega(n^{-1} \log n) \). There exist constants \( C, c > 0 \) such that for suitably large \( n \),

\[ \| \mathcal{L}^2(Y + rJ) - \mathcal{L}^2(p\mathcal{X} + rJ) \|_F \leq C \frac{\log^{1/2} n}{r n^{1/2}} \]

with probability at least \( 1 - n^{-c} \).

Proof: This theorem is proven in the Appendix.

Remark 5: A number of results exist concerning concentration of the adjacency matrix and the graph Laplacian of random graphs (see, for example, [26], [40], [41], [46], [51], [57]). In general, these results show that the graph Laplacian concentrates in spectral norm about its mean when the quantity \( d = n \max_{1 \leq i < j \leq n} p_{ij} \) is of size \( \Omega(\log n) \) (here \( p_{ij} \) is the probability of an edge appearing between nodes \( i \) and \( j \) in the random graph). Our result differs from most of these, in that we are concerned with concentration under the Frobenius norm, rather than the spectral norm. We obtain results in a similar regime, as captured by our lower bound requirements on the regularization term \( r \).

A key quantity in Theorem 2 is the spectral gap \( \delta_n \) as defined in (4). \( \delta_n \) measures how well the eigenvalues in \( \lambda_S(\mathcal{L}^2(p\mathcal{X}^{(n)})) \) are isolated from the rest of the spectrum. \( \delta_n \) must grow in such a way that for suitably large \( n \), the eigenvalues falling in \( S_n \) correspond to the eigenvectors of interest, and the rate of this growth is one of the factors controlling the convergence in Theorem 1. The existence of this eigengap is crucial for the application of the Davis-Kahan Theorem [23], [51]. The eigengap depends on the matrix \( p\mathcal{X}^{(n)} \) (i.e., on the topology of the graph this matrix encodes). As discussed in [60], the existence of such a gap is a reasonable assumption when, for example, the data set (viewed through similarity function \( \kappa \)) has a cluster structure.

Typically, computing the Laplacian eigenmaps embedding of a data set is not an end in itself, but rather a processing step performed prior to subsequent inference, classification, or data exploration. Such tasks depend entirely upon the geometry of the embedded data points produced by Laplacian eigenmaps. If the geometry of the points produced from the inexpensive embedding based on \( Y \) is approximately equal (up to rotation) to that of the embedding based on \( \mathcal{X} \), then we can expect comparable performance on downstream tasks that are invariant under rotations of the data (e.g., clustering). Thus, our results show that we can obtain performance comparable to that obtained when using the dense, computationally intensive \( \mathcal{X} \) while avoiding the expense of working with \( \mathcal{X} \) directly.

IV. EXPERIMENTS

In this section, we present simulation and real-world data to complement our theoretical results in Section III.

A. Data Sets

We consider three data sets, one synthetic, one from connectomics, and one from the speech processing literature.

1) Synthetic Data (Fig. 2, 3): We consider a high-dimensional analogue of the 3-dimensional swiss roll manifold (see Fig. 1). We sample \( n \) points uniformly at random from the \( d^* \)-dimensional unit cube and embed those points into \( (d^*+1) \)-dimensional space by applying the swiss roll transform

\[ (x, y) \mapsto (cx \cos(cx), y, cx \sin(cx)), \quad x \in \mathbb{R}, y \in \mathbb{R}^{d^*} \]

where \( c \) controls the curvature of the manifold. In all experiments we use \( n = 5000, d^* = 6 \) and \( c = 5 \). We chose this higher-dimensional version of the well-understood, simple swiss roll manifold to examine the effect of both under- and over-estimating the dimension \( d^* \). We obtain a kernel matrix \( \mathcal{X} \) from these points by applying a Gaussian kernel with bandwidth \( \sigma \). Results are fairly stable for a wide range of values of \( \sigma \). We use \( \sigma = 0.2 \) in all experiments, while stressing that the task of selecting parameters in dimensionality reduction techniques warrants much additional study.
the expected value of beta-distributed spoken word examples, representing $K$ with word examples to obtain a DTW alignment cost, we define a radial basis kernel on the types. We refer the reader to [43] for technical details. Using distinction distinguishes word types as measured by average precision serves as our starting point for constructing embeddings. The (AP), which runs between $\alpha$, which depends on many factors, e.g., choice of acoustic features, performance. Performance on this task for this data set varies a small amount of positive bias in the errors causes a marked decrease in performance at all noise and occlusion levels.

$$b = -0.1$$  $$b = -0.01$$  $$b = -0.001$$  $$b = 0.001$$

Fig. 4. Relative error (RelErr) in recovering the clean embedding of the high-dimensional swiss roll as a function of occlusion and noise level for different levels of bias $b$. Each tile is the mean of 50 independent trials. We see that Laplacian eigenmaps embedding is quite robust to negative bias, but that even a small amount of positive bias in the errors causes a marked decrease in performance at all noise and occlusion levels.

$$b = -0.1$$  $$b = -0.01$$  $$b = -0.001$$  $$b = 0.001$$

Fig. 5. Performance on the speech task, measured by average precision, as a function of embedding dimension. We see that performance peaks at an embedding dimension of $d = 500$, with a severe degradation in the case where embedding dimension is chosen too small.

$C. elegans$ Connectome (Fig. 8): We consider the task of clustering the 253 non-isolated neurons in the C. elegans, a nematode commonly used as a simple biological model (see [16] and citations therein). These neurons are categorized according to their function: sensory neurons, interneurons and motor neurons, which make up 27.96%, 29.75% and 42.29% of the connectome, respectively. Our data consists of the symmetric binary adjacency matrix corresponding to the C. elegans brain graph, in which each node corresponds to an individual neuron, with an edge between two neurons if they share a synapse. As discussed in [16], this brain graph can be constructed in multiple ways. Here we consider the subgraph of the chemical connectome induced by the non-isolated vertices of the electrical gap junction connectome. Our goal is to embed the nodes of this graph via Laplacian eigenmaps so that clustering (e.g., by k-means) recovers the three neuron categories enumerated above. We assess the quality of these embeddings using adjusted Rand index (ARI), which measures how well two partitions agree, adjusted for chance.

c) Speech Data (Fig. 5, 7 and 9): We consider a speech processing data set used in [43, 44], consisting of 10,383 spoken word examples, representing 5,539 distinct word types. We refer the reader to [43] for technical details. Using DTW alignment cost, we define a radial basis kernel on the word examples to obtain a $10,383 \times 10,383$ kernel matrix that serves as our starting point for constructing embeddings. The evaluation, developed in [11], assesses how well a representation distinguishes word types as measured by average precision (AP), which runs between 0 and 1, with 1 representing perfect performance. Performance on this task for this data set varies depends on many factors, e.g., choice of acoustic features, and better performance than reported here has been obtained. However, the aim of this paper is not to best that performance, but rather to examine how noise and occlusion influence performance for a given set of observations.

B. Noise Conditions

We consider the effects of additive noise and occlusion both in isolation and in tandem on the quality of Laplacian eigenmaps embeddings.

a) Additive Noise: Given a kernel matrix $\mathcal{K} \in \{0, 1\}^{n \times n}$, we produce a random symmetric matrix $K \in \{0, 1\}^{n \times n}$ where $K_{ii} = 0$ for all $i \in [n]$, and $\{K_{ij}\}_{1 \leq i < j \leq n}$ are independent with $K_{ij}$ beta-distributed with $\mathbb{E}[K_{ij}] = \alpha \mathcal{X}_{ij}$. We constrain the expected value of beta-distributed $K_{ij}$ in this way by fixing one of the two shape parameters of the beta distribution, and varying the other to change the variance of the $K_{ij}$. In particular, $K_{ij} \sim \text{Beta}(\alpha_{ij}, \eta_{ij})$ with $\alpha_{ij} > 0$ and $\eta_{ij} > 0$. fixing $\eta_{ij} = \alpha_{ij}(1 - \mathcal{X}_{ij})/\mathcal{X}_{ij}$ ensures that $\mathbb{E}[K_{ij}] = \mathcal{X}_{ij}$ with

$$\text{Var}[K_{ij}] = \frac{\mathcal{X}_{ij}^2(1 - \mathcal{X}_{ij})}{\alpha_{ij} + \mathcal{X}_{ij}},$$

so that we can vary our level of uncertainty on the $K_{ij}$ variables by varying $\alpha_{ij}$. We select a single global value $\alpha > 0$, and take $K_{ij} \sim \text{Beta}(\alpha, \alpha(1 - \mathcal{X}_{ij})/\mathcal{X}_{ij})$. In the limit $\alpha \to 0$, the $K_{ij}$ are simply Bernoulli random variables with probability of success $p_{ij} = 1/\mathcal{X}_{ij}$. In the limit $\alpha \to \infty$, we have $K_{ij} = \mathcal{X}_{ij}$ almost surely. Thus, we can think of our parameter $\alpha$ as a measure of the accuracy of our measurements of $\mathcal{X}$. We note also that our parameterization implies that the $K_{ij}$ variables do not all have the same variance. Rather, variances are smaller for $\mathcal{X}_{ij}$ nearer to 0 and 1. As discussed in Section I this is a good model for applications in which the cases $\mathcal{X}_{ij} \approx 0$ and $\mathcal{X}_{ij} \approx 1$ are comparatively easy to handle from an estimation or computation standpoint, and the trouble arises from the cases where $\mathcal{X}_{ij} \approx 1/2$.

b) Occlusion: We observe an occluded version of $\mathcal{X}$, where entries above the diagonal are observed independently with probability $p$. We proceed with our embedding using this sparse kernel matrix, with zeros in the unobserved entries.

c) Additive Noise with Occlusion: We consider the effects of additive noise and occlusion both in isolation and in tandem on the quality of Laplacian eigenmaps embeddings.

1. Additive Noise: Given a kernel matrix $\mathcal{K} \in \{0, 1\}^{n \times n}$, we produce a random symmetric matrix $K \in \{0, 1\}^{n \times n}$ where $K_{ii} = 0$ for all $i \in [n]$, and $\{K_{ij}\}_{1 \leq i < j \leq n}$ are independent with $K_{ij}$ beta-distributed with $\mathbb{E}[K_{ij}] = \alpha \mathcal{X}_{ij}$. We constrain the expected value of beta-distributed $K_{ij}$ in this way by fixing one of the two shape parameters of the beta distribution, and varying the other to change the variance of the $K_{ij}$. In particular, $K_{ij} \sim \text{Beta}(\alpha_{ij}, \eta_{ij})$ with $\alpha_{ij} > 0$ and $\eta_{ij} > 0$. fixing $\eta_{ij} = \alpha_{ij}(1 - \mathcal{X}_{ij})/\mathcal{X}_{ij}$ ensures that $\mathbb{E}[K_{ij}] = \mathcal{X}_{ij}$ with

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b) Occlusion: We observe an occluded version of $\mathcal{X}$, where entries above the diagonal are observed independently with probability $p$. We proceed with our embedding using this sparse kernel matrix, with zeros in the unobserved entries.

c) Additive Noise with Occlusion: This condition combines the preceding two. We observe an occluded, noisy version of matrix $\mathcal{X}$. That is, we generate noisy matrix $K$ from $\mathcal{X}$ with entries drawn independently from suitably chosen beta-distributions, then occlude $K$ by independently observing entries with probability $p$. 
the expressiveness of the model (i.e., higher embedding dimension) comes at the cost of increased variance (i.e., higher relative error in recovering the clean data point is the mean of 50 independent trials, with error bars indicating one standard error. We see a pattern typical of model selection problems, in which the target dimension is fixed at recovering the clean Laplacian eigenmaps embedding. Here, Fig. 2 shows how noise and occlusion influence the error in maps embeddings should be robust to noise and occlusion. As discussed in Section I, provided these errors are errors influence the quality of Laplacian eigenmaps embedding. Rather than the unbiased additive noise considered above, we consider how more complicated multiplicative and biased errors model.

\[ d \] Multiplicative and Biased Errors with Occlusion:

Rather than the unbiased additive noise considered above, we consider how more complicated multiplicative and biased errors influence the quality of Laplacian eigenmaps embeddings. As discussed in Section I, provided these errors are sufficiently well-behaved, we can adapt the results presented in this paper to make similar statements about this more general error model.

C. Effect of Noise and Occlusion on Embeddings

Our main theoretical result suggests that Laplacian eigenmaps embeddings should be robust to noise and occlusion. Fig. 2 shows how noise and occlusion influence the error in recovering the clean Laplacian eigenmaps embedding. Here, the target dimension is fixed at \( d = d^* = 6 \), while the noise and occlusion vary on the two axes. Each tile is the relative error averaged over 50 independent trials. We see that the clean Laplacian eigenmaps embedding is recovered with low error over a wide range of noise levels and occlusion rates, with performance degrading only when the fraction of observed entries goes below 0.25 in high-noise conditions.

Fig. 7 further illuminates the results seen in the synthetic data. Rather than looking at the relative error in recovering the clean embedding, we examine how noise and occlusion in the kernel matrix influence the down-stream speech task of distinguishing word types. The plot shows average precision as a function of both noise level and occlusion for three different embedding dimensions. We see that performance decays similarly in all three embedding dimensions, but that choice of embedding dimension has a large effect on overall performance. For example, comparing the \( d = 100 \) case with the \( d = 500 \) case, we see that both exhibit similar deterioration patterns with respect to noise level and expected fraction of observed entries, but the 500-dimensional embeddings outperform the 100-dimensional ones when noise and occlusion are not so severe as to drown out the signal in the kernel matrix.

D. Effect of Multiplicative Error and Bias

Our theoretical results are for the case of unbiased noise, \( \mathbb{E}K_{ij} = \mathcal{K}_{ij} \), and it is natural to ask whether similar results hold for a broader class of error models. As mentioned in Section I, our results can be extended to biased errors (\( \mathbb{E}K_{ij} \neq \mathcal{K}_{ij} \)), provided those errors are suitably well-behaved. Fig. 3 and 4 lend experimental support to this point.

Using the same synthetic high-dimensional swiss roll setup as in Fig. 2, we consider biased noise, with \( K_{ij} \) beta-distributed, but with \( \mathbb{E}K_{ij} = \mathcal{K}_{ij} + b \), where \( b \in \mathbb{R} \) is a bias, clipping \( \mathcal{K}_{ij} + b \) to lie in \([0, 1] \) in the event that the bias \( b \) pushes \( \mathcal{K}_{ij} \) out of its allowed range. Note that this corresponds to making \( K_{ij} \) either identically 0 or identically 1, according to whether \( \mathcal{K}_{ij} + b \) is less than 0 or greater than 1, respectively. We again vary the parameter \( \alpha \) as described above, but now the errors are biased away from \( \mathcal{K}_{ij} \). Fig. 4 shows relative error in recovering the clean embeddings, again as a function of the parameters \( p \) and \( \alpha \), for four different levels of bias \( b = -0.1, -0.01, -0.001, 0.001 \). The first thing we notice is that performance is far more sensitive to positive bias than it is to negative bias, with negative bias as large as \(-0.1 \) (a full one tenth of the dynamic range of the similarity measure) having comparatively little effect while a positive bias of just \( 0.001 \) results in notably worse relative error at all levels of noise and occlusion when compared to the unbiased errors in Fig. 2. This performance makes sense. Positive bias in our estimation of \( \mathcal{K} \) results in us embedding a graph that looks highly connected, and the signal present in the comparatively sparse \( \mathcal{K} \) is swamped. On the other hand, negative bias in our estimates only serves to further accentuate the few high-weighted observed entries, since only those entries for which \( \mathcal{K}_{ij} \) is suitably far from 0 survive the bias. We have observed empirically that a similarly-motivated technique, in which small entries of the kernel matrix are clamped to 0, yields slight performance improvements in speech applications.

We further explore how general errors influence the quality of Laplacian eigenmaps embeddings by considering an error
model in which
\[ K_{ij} = \exp\{-D_{ij}^2/\sigma^2\}, \tag{5} \]
where \( D_{ij} = d(x_i, x_j) + Z_{ij}, \) and \( Z_{ij} \) is a one-dimensional normal random variable with mean 0 and variance \( \nu^2. \) Thus, we have a distance measure corrupted by unbiased noise, corresponding to the common scenario in which the kernel function \( \kappa(x, y) \) is a function of the distance between objects \( x \) and \( y \) and uncertainty lies in the measurement of that distance. The result, in the case of a nonlinear kernel function, is (typically) non-additive, biased, error, so that \( \mathbb{E}K_{ij} \neq \mathbb{E} \kappa(x_i, x_j). \) We again use the same high-dimensional swiss roll as described above. We generate noisy versions of the kernel matrix \( \mathcal{K}, \) using the same Gaussian kernel with bandwidth \( \sigma = 0.2, \) but now noise takes the form described in Equation (5). Fig. 7 shows relative error in our recovery of the clean embeddings, as a function of the fraction of observed entries \( p \) and the variance \( \nu^2 \) of the noise term \( Z_{ij}. \) We see that Laplacian eigenmaps embeddings are robust to fairly large amounts of uncertainty in the distance measurement. Indeed, we see that relative error is near zero for variance \( \nu^2 \leq 1, \) with the exception of particularly small values of \( p, \) when nearly all of the kernel matrix is occluded. This performance is impressive in light of the fact that \( \nu^2 = 1 \) corresponds to a standard deviation a full five times larger than the kernel bandwidth in these experiments.

\section*{E. Model Misspecification}

Selecting the target dimension is of the utmost importance for good embeddings. Fig. 6 shows how embedding dimension interacts with noise and occlusion on the synthetic data. The two plots show that relative error in recovering the clean embedding is smaller at lower target dimensionalities, and this pattern holds over a wide range of noise levels and occlusion rates. In particular, we note that relative error in the presence of high noise and high occlusion remains comparable to the relative error in low noise and low occlusion conditions. Of course, this only tells part of the story. Fig. 5 shows average precision on the speech data set under clean conditions, as a function of embedding dimension. While a low-dimensional embedding performs under noise or occlusion might very closely resemble the corresponding clean embedding as in Fig. 6, Fig. 5 suggests that such an embedding would not yield satisfactory performance on downstream tasks such as classification. Indeed, we see here a pattern typical of model selection tasks: one must balance estimation error of model parameters against error in fitting the observed data [28, 50, 55]. The noisy embedding can only be as good as the clean embedding we are attempting to recover.

\section*{F. Effect of regularization}

In the setting of the current work, when \( p \) is too small, we are in the sparse graph setting [2, 14, 38, 40, 41, 49], and it is natural to consider whether applying regularization might ease the deterioration of embedding quality in this regime. We follow the regularization procedure described in [40], in which a regularization parameter \( r \) is added to each entry of the observed matrix. That is, letting \( Y \) denote the occluded version of the noisy matrix \( K, \) we apply Laplacian eigenmaps to the matrix \( [Y_{ij} + r] \) rather than \( Y \) itself. Our main theoretical results suggest that under suitable conditions, such an approach will be beneficial. The \textit{C. elegans} brain graph is extremely sparse, and occlusion makes this sparsity still more dramatic. Fig. 8 shows how regularization influences downstream performance on the \textit{C. elegans} data under different levels of occlusion. We see that when \( r \) is chosen too small, regularization is not enough to significantly change the learned embedding. Similarly, when \( r \) is chosen too large, regularization overpowers the signal present in the occluded matrix. However, with the \textit{C. elegans} data, we see that there exists a level \( (r \approx 0.01) \) at which regularization greatly improves ARI, even when only half of the edges of the graph are known. We note that embeddings produced by the regularization procedure described in [49] resulted in nearly identical performance.

The performance seen here is especially exciting from the neuroscience standpoint– these results suggest that we can recover structural and functional information in connectome data even when accurate assessment of all possible neural connections is impossible. We note the similarity of this phenomenon to that explored in [48], where the authors considered graph inference in the setting where one can trade the accuracy of edge assessment against the number of edges assessed. Of course, the usefulness of this result requires that can determine an appropriate value for \( r \) for a given data set, a problem that we leave for future work.

We close by illustrating conditions under which regularization does not appear to be a benefit. One would think, initially, and especially given the improvement seen in the \textit{C. elegans} data, that regularization would yield similar gains in our speech task. Fig. 9 shows how regularization influences downstream performance on the speech task. We see that
neurons even when much of the structure of the brain graph is occluded, with performance consistently superior to that obtained without regularization.

The regularization does not appear to confer the benefit seen in this phenomenon to future work.

In a similar vein, it stands to reason that a design technique might enable convergence of the regularized estimate to the true expected graph, rather than to its regularized counterpart as in the current work. For example, if only a small fraction of the nodes in a given graph require regularization, then the Frobenius error between the regularized and non-regularized Laplacians can still go to zero even if \( r \) goes to zero slowly.

In a similar vein, it stands to reason that a technique that evaluates entries of the kernel matrix adaptively rather than the edge-independent occlusion model considered here might achieve more accurate recovery of the clean embeddings.

B. Other Error Models

The noise model we have considered is additive, unbiased and entry-wise independent. As discussed in Section II our results can be (approximately) extended to multiplicative, biased noise models, at least for certain kernels. However, the concentration bounds we have used require a certain independence structure. As such, it seems likely that novel techniques will be required to handle entry-wise dependent noise and occlusion in the kernel matrix. For example, the techniques in [47] might be brought to bear, except that they require structural assumptions on \( \mathcal{X} \) that seem unlikely to hold for a non-linear kernel function.

C. Graph Construction

We have largely ignored the problem of constructing the \( k \)-NN or \( \epsilon \)-graph, the first step in Laplacian eigenmaps and spectral clustering. Rather than using either of these constructions, we have relied on the fact that the kernel matrix can be made to resemble these graphs by using, for example, a Gaussian kernel. We believe that the our analysis can be extended to many of these constructions simply by taking advantage of this resemblance. We leave this extension for future work.

D. Other Dimensionality Reduction Techniques

To what extent are different embedding techniques robust to uncertainty in similarity measures (as opposed to errors on the observations themselves)? To the best of our knowledge, MDS and Laplacian eigenmaps remain the only techniques for which such questions have been explored. We believe that analyses similar to that pursued in the current work should apply to other dimensionality reduction techniques. Indeed, given the results in [62], it would be a surprise to learn that no such general result is possible.

Fig. 8. Adjusted Rand index (ARI) on the C. elegans data set for different levels of regularization as a function of dimension at different values of \( p \), the expected fraction of observed entries. Each data point is the mean of 50 independent trials. We see that regularization enables us to accurately cluster the neurons even when much of the structure of the brain graph is occluded, with performance consistently superior to that obtained without regularization.
those reported using $Y$ alone at all noise and occlusion rates. Indeed, USVT performed remarkably similarly to our method on all three data sets, a fact that warrants further exploration.

Some well-known dimensionality reduction techniques can be adapted fairly easily to the model in Equation (2) by using Chatterjee’s USVT to impute the missing entries of $X$. While direct comparison of the relative merits might be adapted to lessen the impact of uncertainty (as in Section III), the results seen for Laplacian eigenmaps are more severe in the presence of noise and occlusion when compared with USVT. While a direct comparison (experimental or otherwise) of Laplacian eigenmaps with other dimensionality reduction techniques is not the focus of this paper, a more thorough exploration of how different methods fare in the presence of noise and occlusion (and how those methods might be adapted to lessen the impact of uncertainty) warrants additional work in the future.

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APPENDIX

CONCENTRATION OF $\mathcal{L}^2(Y + rJ)$

In what follows, we suppress dependence on $n$ for ease of notation. We remind the reader that all quantities involved, including the parameters $r$ and $p$ all implicitly depend on $n$. We let $\hat{Y} = Y + rJ$ denote the regularized version of matrix $Y$, and define $\hat{D}$ to be the corresponding degree matrix, so that $\hat{D}_{ii} = nr + \sum_{j=1}^{n} Y_{ij}$. Denote the regularized version of $p\mathcal{X}$ by $\mathcal{X} = p\mathcal{X} + rJ$, with $\hat{\mathcal{X}}$ the corresponding degree matrix, $\hat{\mathcal{X}}_{ii} = nr + \sum_{j=1}^{n} p\mathcal{X}_{ij}$.

Throughout, $C > 0$ denotes a constant (independent of $n$), which may change from line to line or from one lemma to another; $\beta$ and $\gamma$ denote quantities (both depending on $n$) that will control convergence of the node degrees and the Frobenius norm in Theorem 3 respectively. We will see that the constraints on $\beta$ and $\gamma$ required for our concentration bounds are such that when we plug in $\gamma = C' n^{-1/2} r^{-1} \log^{1/2} n$ and $\beta = C'' n^{-1/2} r^{-1/2} \log^{1/2} n$ for suitably chosen constants $C', C'' > 0$, we obtain the bound claimed in Theorem 3.

We first establish that with high probability, the row sums of $\hat{Y}$ concentrate about their expected value.

Lemma 2: Suppose that there exists constant $c_1 > 0$ such that for all suitably large $n$ we have

$$\frac{\beta^2 r}{1 + \beta} \geq c_1 \frac{\log n}{n}.$$  

(6)

Then for all suitably large $n$, with probability at least $n^{1-c_1}$, it holds for all $i \in [n]$ that $|\hat{D}_{ii} - \hat{\mathcal{X}}_{ii}| \leq \beta \hat{\mathcal{X}}_{ii}$.

Proof: Fix $i \in [n]$. By definition,

$$\hat{D}_{ii} - \hat{\mathcal{X}}_{ii} = \sum_{j=1}^{n} (Y_{ij} + r) - (p\mathcal{X}_{ij} + r) = \sum_{j=1}^{n} Y_{ij} - p\mathcal{X}_{ij},$$

and $\mathbb{E} Y_{ij} = p\mathcal{X}_{ij}$. By a standard Chernoff-style bound [19],

$$\Pr \left[ |\hat{D}_{ii} - \hat{\mathcal{X}}_{ii}| \geq \beta \hat{\mathcal{X}}_{ii} \right] \leq 2 \exp \left\{ \frac{-3\beta^2 \hat{\mathcal{X}}_{ii}^2}{6V + 2\beta \hat{\mathcal{X}}_{ii}} \right\},$$

where $V = \sum_{j=1}^{n} \mathbb{E} Y_{ij}^2$. Since

$$V = \sum_{j=1}^{n} p\mathcal{X}_{ij}^2 \leq p \sum_{j=1}^{n} \mathcal{X}_{ij} \leq \hat{\mathcal{X}}_{ii},$$

we have

$$\Pr \left[ |\hat{D}_{ii} - \hat{\mathcal{X}}_{ii}| \geq \beta \hat{\mathcal{X}}_{ii} \right] \leq 2 \exp \left\{ \frac{-c_1}{1 + \beta} \hat{\mathcal{X}}_{ii} \right\},$$

where $C > 0$ is a constant. Since $\hat{\mathcal{X}}_{ii} \geq nr$ by virtue of regularization, our assumption in (6) ensures that

$$\Pr \left[ |\hat{D}_{ii} - \hat{\mathcal{X}}_{ii}| \geq \beta \hat{\mathcal{X}}_{ii} \right] \leq n^{-c_1}.$$ Applying the union bound over all $i \in [n]$ yields the result.

Lemma 3: Suppose that $\gamma$ depends on $n$ in such a way that there exist constants $C', C'' > 0$ so that for suitably large $n$,

$$C' \gamma^2 \geq \frac{16}{n^2 r^2} + \frac{16}{n^2}$$

and

$$\gamma \geq C'' \frac{\log^{1/2} n}{n^{3/2} r^2}.$$  

(7)

(8)
Then there exists a constant $c_2 > 0$ such that with probability at least $1 - n^{-c_2}$, we have
\[
\sum_{i=1}^{n} \sum_{k=1}^{n} \frac{(\hat{Y}_{ik}^2 - \hat{X}_{ik}^2)^2}{\hat{P}_{ii}^2 \hat{P}_{kk}^2} \leq C \gamma^2,
\]
where $C > 0$ is a constant.

**Proof:** For ease of notation, define
\[
X_{ik} = \frac{(\hat{Y}_{ik}^2 - \hat{X}_{ik}^2)^2}{\hat{P}_{ii}^2 \hat{P}_{kk}^2}.
\]
We will bound $\Pr \left[ \sum_{i,k} X_{ik} \geq \gamma^2 \right]$ and show
\[
\mathbb{E} \sum_{i,k} X_{ik} \leq C' \gamma^2,
\]
which implies that $\Pr \left[ \sum_{i,k} X_{ik} \geq C \gamma^2 \right]$. A standard Chernoff-style bound lets us write
\[
\Pr \left[ \sum_{i,k} X_{ik} \geq \gamma^2 + \mathbb{E} \sum_{i,k} X_{ik} \right] \leq \exp \left\{ \frac{-3 \gamma^4}{6V + 2\gamma^2 M} \right\},
\]
where
\[
V = \sum_{i,k} \mathbb{E} X_{ik}^2 = \sum_{i,k} \frac{\mathbb{E} (\hat{Y}_{ik}^2 - \hat{X}_{ik}^2)^4}{\hat{P}_{ii}^4 \hat{P}_{kk}^4},
\]
and $M = \max \left\{ 1/(\hat{P}_{ii}^2 \hat{P}_{kk}^2) : i, k \in [n] \right\}$. Bounding $V \leq n^{-6r-8}$ and $M \leq (nr)^{-4}$,
\[
\Pr \left[ \sum_{i,k} X_{ik} \geq \gamma^2 + \mathbb{E} \sum_{i,k} X_{ik} \right] \leq \exp \left\{ \frac{-3(\gamma n r)^4}{6n^{-2r} + 2\gamma^2} \right\},
\]
and using our assumption in (8) to lower bound the denominator inside the exponent by $\Omega(n \gamma^4)$, we can guarantee the existence of a constant $c_2 > 0$ such that
\[
\Pr \left[ \sum_{i,k} X_{ik} \geq \gamma^2 + \mathbb{E} \sum_{i,k} X_{ik} \right] \leq n^{-c_2}.
\]

It remains for us to show that $\mathbb{E} \sum_{i,k} X_{ik} \leq C' \gamma^2$. We have
\[
\mathbb{E} \sum_{i,k} X_{ik} \leq \sum_{i,k} \frac{\mathbb{E} (\hat{Y}_{ik}^2 + \hat{X}_{ik}^2)}{\hat{P}_{ii}^2 \hat{P}_{kk}^2} \leq 8 \left( \mathbb{E} K_{ik}^4 + r^4 \right) + \hat{X}_{ik}^4,
\]
where we have used the fact that $(a + b)^2 \leq 2a^2 + 2b^2$ for all $a, b \in \mathbb{R}$. Since $\hat{P}_{ii} \geq nr$ for all $i \in [n]$, we have
\[
\sum_{i=1}^{n} \frac{1}{r} \leq \frac{1}{r} \text{ and } \sum_{i=1}^{n} \frac{r^4}{\hat{P}_{ii}^2 \hat{P}_{kk}^2} \leq \frac{1}{n^2 r^2}.
\]
Noting that $\mathbb{E} K_{ik}^4 \leq \mathbb{E} K_{ik} = X_{ik}$ and applying (10), we have
\[
\sum_{i=1}^{n} \sum_{k=1}^{n} \frac{p\mathbb{E} K_{ik}^4}{\hat{P}_{ii}^2 \hat{P}_{kk}^2} \leq \sum_{i=1}^{n} \frac{1}{\hat{P}_{ii} n^2 r^2} \leq \frac{1}{n^2 r^3}.
\]
Recalling that $\hat{X}_{ik} = p \mathcal{X}_{ik} + r$ by definition and applying the definition of $\hat{D}_{ii}$, (11) implies
\[
\sum_{i=1}^{n} \sum_{k=1}^{n} \frac{\hat{X}_{ik}^4}{\hat{P}_{ii}^2 \hat{P}_{kk}^2} \leq 8 \sum_{i=1}^{n} \sum_{k=1}^{n} \frac{p^4 \mathcal{X}_{ik}^4 + r^4}{\hat{P}_{ii}^2 \hat{P}_{kk}^2} \leq \frac{8p^3}{n^4 r} + \frac{8}{n^2 r^2}.
\]
Combining this with (9) and (11) and applying (7) completes the proof.

**Lemma 4:** Under the same conditions as Lemma 2, and assuming there exists a constant $C > 0$ such that
\[
C \gamma^2 \geq \frac{\beta^2}{mr^2},
\]
with probability at least $n^{-1-c_1}$, we have
\[
\sum_{i=1}^{n} \sum_{k=1}^{n} \frac{(\hat{Y}_{ik}^2 - \hat{X}_{ik}^2)(\hat{Y}_{ik}^2 - \hat{X}_{ik}^2)}{\hat{P}_{ii}^2 \hat{P}_{kk}^2} \leq C \gamma^2.
\]

**Proof:** Observing that $\hat{Y}_{ik} + \hat{X}_{ik} \leq 1 + p + 2r$,
\[
\sum_{i=1}^{n} \sum_{k=1}^{n} \sum_{\ell=1}^{n} \frac{(\hat{Y}_{ik} - \hat{X}_{ik})(\hat{Y}_{i\ell} - \hat{X}_{i\ell})}{\hat{P}_{ii}^2 \hat{P}_{kk}^2} \leq \frac{(1 + p + 2r)^2}{n^2 r^2} \sum_{i=1}^{n} \sum_{k=1}^{n} \sum_{\ell=1}^{n} \frac{(\hat{Y}_{ik} - \hat{X}_{ik})(\hat{Y}_{i\ell} - \hat{X}_{i\ell})}{\hat{P}_{ii}^2 \hat{P}_{kk}^2}.
\]
By Lemma 2 with probability at least $1 - n^{-1-c_1}$, it holds for all $i \in [n]$ that
\[
\left| \sum_{k=1}^{n} \hat{Y}_{ik} - \hat{X}_{ik} \right| \leq \beta \hat{D}_{ii},
\]
and hence, since $p, r \in [0, 1]$ and $\hat{D}_{ii} \geq nr$,
\[
\sum_{i=1}^{n} \sum_{k=1}^{n} \sum_{\ell=1}^{n} \frac{(\hat{Y}_{ik} - \hat{X}_{ik})(\hat{Y}_{i\ell} - \hat{X}_{i\ell})}{\hat{P}_{ii}^2 \hat{P}_{kk}^2} \leq 16 \beta^2.
\]
Our assumption in (12) yields the desired result.

**Lemma 5:**
\[
\sum_{i,j,k,\ell} \frac{p^4 \mathcal{X}_{ik} \mathcal{X}_{jk} \mathcal{X}_{i\ell} \mathcal{X}_{j\ell}}{\hat{D}_{ii} \hat{D}_{jj} \hat{D}_{kk} \hat{D}_{\ell \ell}} \leq \frac{p}{r}.
\]

**Proof:** Using the following facts:
(i) $\hat{D}_{ii} \geq nr$ for all $i \in [n]$,
(ii) $\mathcal{X}_{ik} \in [0, 1]$ for all $i, j \in [n]$,
(iii) $\sum_{k=1}^{n} p \mathcal{X}_{ik} \leq \hat{D}_{ii}$ for all $i \in [n]$,
we have
\[
\sum_{i,j,k,\ell} \frac{p^4 \mathcal{X}_{ik} \mathcal{X}_{jk} \mathcal{X}_{i\ell} \mathcal{X}_{j\ell}}{\hat{D}_{ii} \hat{D}_{jj} \hat{D}_{kk} \hat{D}_{\ell \ell}} \leq \frac{p}{nr} \sum_{i,j,k,\ell} \frac{p^2 \mathcal{X}_{ik} \mathcal{X}_{jk} \mathcal{X}_{i\ell} \mathcal{X}_{j\ell}}{\hat{D}_{ii} \hat{D}_{jj} \hat{D}_{kk} \hat{D}_{\ell \ell}} \leq \frac{p}{nr} \sum_{i,j,k} \frac{p^2 \mathcal{X}_{ik} \mathcal{X}_{jk}}{\hat{D}_{ii} \hat{D}_{kk}} \leq \frac{p}{r}.
\]
Lemma 6: For ease of notation, let
\[ X_{ijkt} = \frac{\hat{Y}_{ik}Y_{jk} - \hat{X}_{ik}\hat{X}_{jk}(\hat{Y}_{it}Y_{jt} - \hat{X}_{it}\hat{X}_{jt})}{\hat{D}_{ii}\hat{D}_{jj}\hat{D}_{kk}\hat{D}_{tt}} \tag{13} \]
and define \( T = \{(i, j, k, \ell) : i, j, k, \ell \in [n] \text{ distinct}\} \). There exists a constant \( C > 0 \) such that
\[
\sum_{(i, j, k, \ell) \in T} \text{Var} X_{ijkt} \leq \frac{C}{n^4 r^5}.
\]

Proof: Since \( i, j, k, \ell \) are distinct for each \((i, j, k, \ell) \in T\),
\[
\text{Var} X_{ijkt} = \mathbb{E} X_{ijkt}^2
\]
\[
= d_{ijkt}^2 \mathbb{E} \left[ \hat{Y}_{ik}\hat{Y}_{jk} - \hat{X}_{ik}\hat{X}_{jk} \right]^2 \mathbb{E} \left[ \hat{Y}_{it}\hat{Y}_{jt} - \hat{X}_{it}\hat{X}_{jt} \right]^2,
\]
where \( d_{ijkt} = \hat{D}_{ii}\hat{D}_{jj}\hat{D}_{kk}\hat{D}_{tt} \). Expanding \( \hat{Y}_{ik} = Y_{ik} + r + \hat{X}_{ik} \) and \( \hat{X}_{ik} = p\hat{X}_{ik} + r \) and using linearity of expectation, we have
\[
\mathbb{E} \left[ \hat{Y}_{ik}\hat{Y}_{jk} - \hat{X}_{ik}\hat{X}_{jk} \right]^2
\]
\[
= \mathbb{E} \left[ Y_{ik}Y_{jk} - p^2\hat{X}_{ik}\hat{X}_{jk} \right] + r \left[ Y_{ik} - p\hat{X}_{ik} \right] + r \left[ Y_{jk} - p\hat{X}_{jk} \right]
\]
\[
= \mathbb{Var} Y_{ik} + r^2 + 2pr \mathbb{Var} \hat{X}_{ik} + 2pr \mathbb{Var} \hat{X}_{jk}.
\]
For ease of notation, define
\[
Q_{ijkt} = p^2\hat{X}_{ik}\hat{X}_{jk} + r^2 + 2pr \mathbb{Var} \hat{X}_{ik} + 2pr \mathbb{Var} \hat{X}_{jk}.
\]
The Bhatia-Davis inequality [6] states that if a random variable \( Z \) satisfies \( \mathbb{P}[m \leq Z \leq M] = 1 \), then \( \mathbb{Var} Z \leq (EZ - m)(M - EZ) \). Since \( \hat{X}_{ik} \in [0, 1] \) for all \( i, k \in [n] \), we have \( \mathbb{Var} Y_{ik} \leq p^2\hat{X}_{ik}\hat{X}_{jk} \) and \( \mathbb{Var} Y_{jk} \leq p^2\hat{X}_{ik}\hat{X}_{jk} \), and hence
\[
\mathbb{E} \left[ \hat{Y}_{ik}\hat{Y}_{jk} - \hat{X}_{ik}\hat{X}_{jk} \right]^2 \leq Q_{ijkt}.
\]
Combining this with (13), we have
\[
\text{Var} X_{ijkt} \leq d_{ijkt}^2 \mathbb{E} X_{ijkt}^2 \leq \sum_{(i, j, k, \ell) \in T} d_{ijkt}^2 \mathbb{E} X_{ijkt}^2 \leq \frac{C}{n^4 r^5}.
\]
Summing, we have
\[
\sum_{(i, j, k, \ell) \in T} \text{Var} X_{ijkt} \leq \sum_{(i, j, k, \ell) \in T} d_{ijkt}^2 Q_{ijkt} Q_{ijkt}.
\]
\[
= \sum_{(i, j, k, \ell) \in T} d_{ijkt}^2 \left[ p^4\hat{X}_{ik}\hat{X}_{jk}\hat{X}_{il}\hat{X}_{lj} + 4 \left( \sum_{(i, j, k, \ell) \in T} d_{ijkt}^2 r^2 \right) + 2 \left( \sum_{(i, j, k, \ell) \in T} d_{ijkt}^2 r^2 \right)^2 \right]
\]
\[
\leq \frac{p}{n^4 r^5} + \frac{4 (r + 2p)}{n^4 r^5} + \frac{4 (r + 2p)^2}{n^4 r^5},
\]
where we have used \( \hat{D}_{ii} \geq nr \) along with Lemma 5 to bound the first sum after the equality, and the other sums are bounded using reasoning nearly identical to that in the proof of Lemma 5. The result then follows from \( r, p \in [0, 1] \).
Now, consider the situation where \((i, j, k, \ell)\) is not a permutation of \((a, b, c, d)\). Clearly, if \(\{i, j, k, \ell\} \cap \{a, b, c, d\} = \emptyset\), then \(\text{Cov}(X_{ijkl}, X_{abcd}) = 0\). Indeed, \(\text{Cov}(X_{ijkl}, X_{abcd}) \neq 0\) requires that each term of the form \((\hat{Y}_{ik} \hat{Y}_{jk} - \hat{X}_{ik} \hat{X}_{jk})\) be dependent on one of the other three such terms in \(X_{ijkl} X_{abcd}\), since otherwise a term of the form \(\mathbb{E}(\hat{Y}_{ik} \hat{Y}_{jk} - \hat{X}_{ik} \hat{X}_{jk})\) factors out and the covariance is zero. Indeed, only one other choice (up to permutations of the indices) of \((i, j, k, \ell)\) and \((a, b, c, d)\) gives rise to a non-zero covariance, namely \(\mathbb{E}X_{ijkl} X_{abcd}\). By symmetry, to handle the terms of this form, it will suffice for us to bound

\[
\sum_{\{i, j, k, \ell\} \in T \setminus \{i, j, k, \ell\}} \sum_{\{i, j, k, \ell\}} \text{Cov}(X_{ijkl}, X_{abcd})
\]

Using the fact that \(\text{Var} \hat{Y}_{ik} \leq \hat{X}_{ik}\) by the Bhatia-Davis inequality, and applying reasoning similar to that in Lemma 5,

\[
\sum_{\{i, j, k, \ell\} \in T \setminus \{i, j, k, \ell\}} \sum_{\{i, j, k, \ell\}} \text{Cov}(X_{ijkl}, X_{abcd})
= \sum_{\{i, j, k, \ell\} \in T \setminus \{i, j, k, \ell\}} \sum_{\{i, j, k, \ell\}} \frac{\hat{X}_{ik} \hat{X}_{jk} \hat{X}_{ij} \hat{X}_{kl} \text{Var} \hat{Y}_{ik} \text{Var} \hat{Y}_{ij}}{D_{ii} D_{jj} D_{kk} D_{ll}}
\leq \sum_{\{i, j, k, \ell\} \in T \setminus \{i, j, k, \ell\}} \sum_{\{i, j, k, \ell\}} \frac{\hat{X}_{ik} \hat{X}_{jk} \hat{X}_{ij} \hat{X}_{kl} \text{Var} \hat{Y}_{ik} \text{Var} \hat{Y}_{ij}}{D_{ii} D_{jj} D_{kk} D_{ll}}
\leq \frac{(1 + r)^2}{(nr)^4} \sum_{i, j, k, \ell \in [n]} \text{distinct}
\leq \frac{(1 + r)^2}{n^2 r^n}.
\]

Combining this with (14) and noting that \(r > n^{-1}\) implies \((n^2 r^n)^{-1} \geq (n^4 r^4)^{-1}\), we have our result.

**Lemma 8:** Let \(T = \{(i, j, k, \ell) : i, j, k, \ell \in [n]\} \) distinct. For each \((i, j, k, \ell) \in T\), define variable

\[
X_{ijkl} = \frac{(\hat{Y}_{ik} \hat{Y}_{jk} - \hat{X}_{ik} \hat{X}_{jk})(\hat{Y}_{ij} \hat{Y}_{kl} - \hat{X}_{ij} \hat{X}_{kl})}{D_{ii} D_{jj} D_{kk} D_{ll}}.
\]

There exist constants \(C, C_T > 0\) such that with probability at least \(1 - C_T (\gamma^4 n^3 r^4)^{-1}\),

\[
\sum_{\{i, j, k, \ell\} \in T} \frac{X_{ijkl} \hat{X}_{ij} \hat{X}_{kl} \hat{X}_{ij}}{D_{ii} D_{kk} D_{ll}} \leq C_T C^2.
\]

**Proof:** By Chebyshev’s inequality,

\[
\text{Pr} \left[ \sum_{\{i, j, k, \ell\} \in T} X_{ijkl} \geq C_T C^2 \right] \leq \frac{\text{Var} \sum_{\{i, j, k, \ell\} \in T} X_{ijkl}}{C_T C^2}.
\]

We have

\[
\text{Var} \sum_{\{i, j, k, \ell\} \in T} X_{ijkl}
= \sum_{\{i, j, k, \ell\} \in T} \text{Var} X_{ijkl}
+ \sum_{\{i, j, k, \ell, (i', j', k', \ell')\} \in \{\mathcal{Z}\}} \text{Cov}(X_{ijkl}, X_{i'j'k'\ell'}).\]

Lemma 6 bounds the first of these two sums by

\[
\sum_{\{i, j, k, \ell\} \in T} \text{Var} X_{ijkl} \leq \frac{C'}{n^4 r^4},
\]

where \(C' > 0\) is a constant, and Lemma 7 ensures that

\[
\sum_{\{(i, j, k, \ell, (i', j', k', \ell')) \in \{\mathcal{Z}\}} \text{Cov}(X_{ijkl}, X_{i'j'k'\ell'}) \leq \frac{C''}{n^3 r^4}
\]

for some constant \(C'' > 0\). Since \((n^4 r^5)^{-1} \leq (n^3 r^4)^{-1}\) for \(r > 1/n\), we have

\[
\text{Pr} \left[ \sum_{\{i, j, k, \ell\} \in T} X_{ijkl} \geq C_T C^2 \right] \leq \frac{C_T C^2}{C'' r^4}.
\]

Choosing \(C_T = (C'' + C) / C_T\) yields the result.

**Lemma 9:** Under the conditions of the above lemmata, there exist constants \(C, C_T > 0\) such that for all suitably large \(n\), with probability at least \(1 - 3 n^{-c}\), we have

\[
||\hat{\mathcal{L}} - (\hat{\mathcal{G}}^{-1/2} \hat{\mathcal{G}}^{-1/2}) ||_{p} \leq C \gamma.
\]

**Proof:** Expanding the sum and recalling our earlier definition of \(T = \{(i, j, k, \ell) : i, j, k, \ell \in [n]\} \) distinct, we have

\[
||\hat{\mathcal{L}} - (\hat{\mathcal{G}}^{-1/2} \hat{\mathcal{G}}^{-1/2}) ||_{p}^2
= \sum_{i, j, k, \ell} \hat{Y}_{ij} \hat{Y}_{jk} - \hat{X}_{ij} \hat{X}_{jk} \hat{Y}_{ij} \hat{Y}_{kl} - \hat{X}_{ij} \hat{X}_{kl}
\]

\[
\leq \sum_{i, j, k, \ell} \frac{\hat{Y}_{ij} \hat{Y}_{jk} - \hat{X}_{ij} \hat{X}_{jk}}{D_{ii} D_{jj} D_{kk} D_{ll}}
+ \sum_{i, j, k, \ell} \frac{\hat{Y}_{ij} \hat{Y}_{jk} - \hat{X}_{ij} \hat{X}_{jk}}{D_{ii} D_{kk} D_{ll}}
\]

Each of these three summations is bounded (with high probability) by \(C_T \gamma^2\) by Lemma 5 and 8 respectively. Let constants \(c_1, c_2 > 0\) be as defined in Lemma 2 and Lemma 3 respectively, and choose \(c_3 > 0\) so that \(C_T (\gamma^4 n^3 r^4)^{-1} \leq n^{-c_3}\) for suitably large \(n\), where \(C_T\) is as defined in Lemma 8.

By the union bound, with probability at least \(1 - (1 - n^{-c_1} + n^{-c_2} + n^{-c_3})\), all three sums are bounded at once, and the result follows by taking

\[
c = \min\{c_1, c_2, c_3\}.
\]

**Lemma 10:** Suppose that \(\beta \rightarrow 0\) as \(n \rightarrow \infty\). Under the conditions of Lemma 2 there exists a constant \(C > 0\) such that with probability at least \(1 - n^{-c_1}\),

\[
||\hat{\mathcal{L}} - (\hat{\mathcal{G}}^{-1/2} \hat{\mathcal{G}}^{-1/2}) ||_{p} \leq C \gamma^2 r^{1/2}.
\]

**Proof:** Under the conditions of Lemma 2 with probability at least \(1 - n^{-c_1}\), it holds for all \(i \in [n]\) that \(\|\mathcal{L}_i - \sum_{k=1}^n \hat{Y}_{ik}\| \leq \beta \mathcal{L}_i\). It follows that for a suitably chosen constant \(C' > 0\), for all \(i, j, k \in [n]\) we have

\[
\frac{1}{D_{ii} D_{jj} D_{kk}} - \frac{1}{D_{ii} D_{jj} D_{kk}} \leq \frac{C' \beta}{D_{ii} D_{jj} D_{kk}}.
\]

To see why this is the case (here we are following the argument motivating Equation A.6 in [5]), note that when \(\|\mathcal{L}_i - \sum_{k=1}^n \hat{Y}_{ik}\| \leq \beta \mathcal{L}_i\) for all \(i \in [n]\), we have

\[
\frac{1}{D_{ii} D_{jj} D_{kk}} \leq \frac{1}{D_{ii} D_{jj} D_{kk}} \leq \frac{1}{D_{ii} D_{jj} D_{kk}}.
\]
and Equation [16] follows, since \( \beta \to 0 \) as \( n \to \infty \), and thus

\[
(1 + \beta)^{-2} \geq \frac{\beta^2 - 1}{(\beta - 1 + 1)^2} = \frac{\beta^2 - 1}{\beta^2 - 1} \geq 1 - C'\beta,
\]

\[
(1 - \beta)^{-2} = 1 + \frac{2}{\beta^2 - 1} + \frac{1}{(\beta - 1 - 1)^2} \leq 1 + C''\beta.
\]

Using (16), we have

\[
\| \hat{L}L - (\hat{G}^{-1/2}\hat{Y}^{-1/2}) \|_F^2 \leq C'\beta^2 \sum_{i,j,k,t} \hat{Y}_{ik}\hat{Y}_{jk}\hat{Y}_{it}\hat{Y}_{jt} D_{ii}D_{jj}D_{kk}D_{tt}.
\]

Under the same event, we have \( \sum_{k=1}^n \hat{Y}_{jk} \leq (1 + \beta) D_{tt} \) for all \( i \in [n] \), and making repeated use of this and the facts that \( \hat{Y}_{jk} \leq (1 + r) D_{ii} \), and \( D_{ii} \geq n r \), it follows that

\[
\| \hat{L}L - (\hat{G}^{-1/2}\hat{Y}^{-1/2}) \|_F^2 \leq C'\beta^2 \sum_{i,j,k,t} \hat{Y}_{ik}\hat{Y}_{jk}\hat{Y}_{it}\hat{Y}_{jt} D_{ii}D_{jj}D_{kk}D_{tt} \leq \frac{\beta^2(1 + r)(1 + \beta)^3}{r}.
\]

The result follows since \( r \) and \( \beta \) are bounded above by 1.

To obtain our result in Theorem 3 let \( \gamma = C''n^{-1/2} - 1 \log^2 n \) and \( \beta = C''n^{-1/2} - 1 \log^2 n \) for suitably large constants \( C', C'' > 0 \). Note first that these choices of \( \gamma \) and \( \beta \) satisfy all of the constraints of the lemmata required for Lemma 9 so long as \( r = \omega(n^{-1} \log n) \). Further, note that \( \beta r^{-1/2} = C' \gamma \) for some constant \( C > 0 \), and hence Lemma 10 implies that \( \| \hat{L}L - (\hat{G}^{-1/2}\hat{Y}^{-1/2}) \|_F \leq C'\gamma \) with high probability. Combining Lemma 9 and Lemma 10 and applying the triangle inequality then yields Theorem 3.

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