An Analysis of Classical Multidimensional Scaling

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Abstract

Classical multidimensional scaling is an important tool for dimension reduction in many applications. Yet few theoretical results characterizing its statistical performance exist. In this paper, we provide a theoretical framework for analyzing the quality of embedded samples produced by classical multidimensional scaling. This lays down the foundation for various downstream statistical analysis. As an application, we study its performance in the setting of clustering noisy data. Our results provide scaling conditions on the sample size, ambient dimensionality, between-class distance and noise level under which classical multidimensional scaling followed by a clustering algorithm can recover the cluster labels of all samples with high probability. Numerical simulations confirm these scaling conditions are sharp in low, moderate, and high dimensional regimes. Applications to both human RNAseq data and natural language data lend strong support to the methodology and theory.

Keywords: Clustering; Dimension Reduction; Multidimensional Scaling.

1 Motivation and Background

Embedding high dimensional data into a low dimensional space is essential in many applications because the data structure is much easier to visualize and to study in low dimensions. Classical multidimensional scaling achieves this goal by searching for a few coordinates which preserve pairwise distances of data points in the original space (Torgerson, 1952; Borg & Groenen, 2005). What is intriguing is that multidimensional scaling does not require access to the original data coordinates. This property has been used for many applications in bioinformatics, psychology, and pattern recognition, etc., where only pairwise distances are available. For example, educational psychologists have collected comparisons between visual representations of chemical molecules to identify a small set of visual features that most significantly influence the judgments of beginning chemistry students (Mason et al., 2017). We refer readers to Borg & Groenen (2005) for a systematic overview of multidimensional scaling.

Despite the successes of multidimensional scaling in many applications, as pointed out by Fan et al. (2018a), few theoretical results characterizing its statistical performance under...
randomness exist. In this paper, we provide a theoretical framework for studying the quality of the low dimensional embedded samples provided by multidimensional scaling. Specifically, we establish an infinity norm bound for the embedding errors by focusing on classical multidimensional scaling, a version of multidimensional scaling where Euclidean norm is used to construct pairwise distances. This lays down the foundation for analyzing various downstream procedures. As an application, we apply a generic distance based clustering algorithm to the embedded samples, and analyze its clustering performance. The advantage of this two step procedure, referred to as the multidimensional scaling and clustering procedure, is that it can overcome the curse of dimensionality by reducing the dimensionality first. Theoretically, we provide scaling conditions for exact recovery with high probability using the multidimensional scaling and clustering procedure, where exact recovery means all cluster labels are inferred correctly, a term commonly used in community detection and stochastic block models (Abbe, 2018). According to the magnitude of the ambient dimension $d$, our main results imply three different regimes of scaling conditions. Both simulations and real data studies support our theoretical findings. To the best of our knowledge, we are the first to provide sharp scaling conditions for exact cluster detection using the multidimensional scaling and clustering procedure.

1.1 Review of Classical Multidimensional Scaling

We briefly review the procedure of classical multidimensional scaling. Given the distance matrix $D \in \mathbb{R}^{N \times N}$ of $N$ data points with the $(i, j)$th element being the Euclidean distance between the $i$th and $j$th samples, classical multidimensional scaling first obtains a matrix $B$ by applying double centering to the matrix of squared distances. Specifically, $B = -\frac{1}{2}JD^{(2)}J$ where $D_{i,j}^{(2)} = D_{i,j}^2$, $J = I_N - 11^T/N$ is the centering matrix, and $1 \in \mathbb{R}^N$ is the column vector of all 1’s. Let $X = (x_1, \ldots, x_N)^T \in \mathbb{R}^{N \times d}$ be the possibly unobserved data matrix. It can be shown

$$B = -\frac{1}{2}JD^{(2)}J = (X - 1\hat{\mu}^T)(X - 1\hat{\mu}^T)^T = (JX)(JX)^T,$$

where $\hat{\mu} = \sum_{i=1}^N x_i/N$ is the empirical mean of the data. See Borg & Groenen (2003) for details. The coordinates of an $r$-dimensional embedding are then given by the rows of $Y = V_r\Lambda_r^{1/2}$, where $\Lambda_r = \text{diag}(\lambda_1, \ldots, \lambda_r) \in \mathbb{R}^{r \times r}$ with $\lambda_i$ being the $i$th largest eigenvalue of $B$ and $V_r = (v_1, \ldots, v_r) \in \mathbb{R}^{N \times r}$ the matrix whose columns are the corresponding eigenvectors. Namely, each unobserved data point $x_i$ is mapped to the $i$th row of $V_r\Lambda_r^{1/2}$.

Mathematically, this embedding tries to preserve pairwise distances in $r$ dimensions by minimizing

$$\min_{Y \in \mathbb{R}^{N \times r}} \sum_{i,j=1}^N (D_{i,j}^X - D_{i,j}^Y)^2,$$

where $D^X, D^Y$ are the distance matrices corresponding to $X$ and $Y$ respectively.
We demonstrate how this procedure works on a toy example, by considering 5 Gaussian distributions with means $\mu_k \in \mathbb{R}^{1000}$ for $k = 1, \ldots, 5$, and a common covariance matrix $\Sigma = 0.25I_{1000}$. The first two coordinates of $\mu_k$’s are $(0, 0), (-1, 0), (1, 0), (0, 1),$ and $(0, -1)$ respectively, while the rest of the coordinates are 0. We sampled 200 data points from each Gaussian distribution. The central plot in Fig. 1 shows that the embedding obtained from multidimensional scaling with only two dimensions can cluster the data into five clusters with high accuracy while there is no visible separation using a randomly selected pair of original coordinates, as indicated by the left plot. The right plot in Fig. 1 shows the first two data coordinates colored by the labels returned by hierarchical clustering with Ward’s method (Ward Jr, 1963). It achieved reasonably high accuracy when clustering the embedded data points into five clusters.

Figure 1: Left: two randomly selected data coordinates. Middle: first two multidimensional scaling coordinates; color shows cluster identity. Right: the first two data coordinates; color shows the labels returned by hierarchical clustering.

1.2 Notation

We summarize the notation used throughout the paper. For any matrix $A = A_{i,j}$, the spectral norm is denoted by $\|A\|_2$ and the Frobenius norm by $\|A\|_F$. Furthermore, $\|A\|_{\text{max}} = \max_{i,j} |A_{i,j}|$, $\|A\|_{\infty} = \max_i \sum_j |A_{i,j}|$, $\|A\|_1 = \max_j \sum_i |A_{i,j}|$, and $A_i$ as the $i$th row of $A$. For any vector $v$, $\|v\|_2$ denotes the Euclidean norm and $\|v\|_{\infty} = \max_i |v(i)|$. Let $f(n)$ and $g(n)$ be functions that map integer $n$ to a positive real number, and let $c, b$ be positive constants and $n_0$ an integer. Then $f(n) = O(g(n))$ if $f(n) \leq cg(n)$ for all $n > n_0$; $f(n) = \Omega(g(n))$ if $f(n) \geq bg(n)$ for all $n > n_0$; and $f(n) = \Theta(g(n))$ if $f(n) = O(g(n))$ and $f(n) = \Omega(g(n))$. Sometimes $f(n) \lesssim g(n), f(n) \gtrsim g(n)$ are used to denote $f(n) = O(g(n)), f(n) = \Omega(g(n))$ respectively.

2 Model Formulation

Let $k$ be the number of clusters, $n_j$ be the number of samples in the $j$th cluster, $[k] := \{1, \ldots, k\}$ be the set of cluster labels, and $\ell$ be an $N$-dimensional cluster vector with each coordinate in $[k]$. Given pair-wise Euclidean distances of $N$ samples, we aim to recover the
unobserved cluster vector $\ell$ up to a permutation. To measure the clustering accuracy, we follow Abbe (2018) and define the permutation-invariant agreement function as
\[ A(u, v) = \max_{\pi \in O_k} \frac{1}{N} \sum_{i=1}^{N} I\{u_i = \pi(v_i)\}, \] (2.1)
where $u, v \in [k]^N$ are two vectors of cluster labels, and $O_k$ is the set of permutation operators on $[k]$. Consider $k$ Gaussian distributions with distinct mean vectors $\mu_j$ and a common covariance matrix $\Sigma$. Let $\sigma_1^2 \geq \ldots \geq \sigma_d^2$ be the $d$ eigenvalues of $\Sigma$. Suppose the $j$th cluster has $n_j$ identically and independently distributed samples. For simplicity, we assume $n_1 \mu_1 + \cdots + n_k \mu_k = 0$. For the $i$th sample $x_i \sim N(\mu_{\ell_i}, \Sigma)$ with $\ell_i \in [k]$ being its label, so we can formulate it as $x_i = \mu_{\ell_i} + \eta_i$ with $\eta_i \sim N(0, \Sigma)$.

**Remark 2.1.** We remark that the Gaussian assumption is only used to simplify the theoretical analysis. This assumption can be relaxed to sub-Gaussian assumptions.

Let $X$ be the unobserved $N \times d$ matrix whose rows consist of $x_i^T$’s. Through the double centering procedure as described in the introduction, we obtain the matrix $B$. For a prespecified $r$, the multidimensional scaling embedding of $X$ is then given by the matrix $Y = \tilde{V}_r \tilde{\Lambda}_r^{1/2}$, where the diagonal matrix $\tilde{\Lambda}_r$ contains the top $r$ eigenvalues of $B$ and the columns of $\tilde{V}_r$ are the corresponding $r$ eigenvectors. We define the maximal within cluster and minimal between cluster distances in the embedding as follows
\[ d_{\text{in}}(\tilde{V}_r \tilde{\Lambda}_r^{1/2}, \ell) = \max_{i,j,\ell_i=\ell_j} \left\| (\tilde{V}_r \tilde{\Lambda}_r^{1/2})_{ij} - (\tilde{V}_r \tilde{\Lambda}_r^{1/2})_{jj} \right\|_2, \]
\[ d_{\text{btw}}(\tilde{V}_r \tilde{\Lambda}_r^{1/2}, \ell) = \min_{i,j,\ell_i \neq \ell_j} \left\| (\tilde{V}_r \tilde{\Lambda}_r^{1/2})_{ij} - (\tilde{V}_r \tilde{\Lambda}_r^{1/2})_{jj} \right\|_2. \]
Using the same terminology as in Vu (2018), we say that the embedding $\tilde{V}_r \tilde{\Lambda}_r^{1/2}$ is a *perfect geometric representation* of the labels $\ell$ if $d_{\text{btw}}(\tilde{V}_r \tilde{\Lambda}_r^{1/2}, \ell) > 2d_{\text{in}}(\tilde{V}_r \tilde{\Lambda}_r^{1/2}, \ell)$. Here the choice of constant 2 is arbitrary. When the number of clusters, $k$, is given, the perfect geometric representation condition is sufficient to guarantee the exact recovery of cluster labels by several common clustering algorithms including single linkage and $k$-means clustering, that is, they produce an estimated cluster label vector $\hat{\ell} \in [k]^N$ with $A(\hat{\ell}, \ell) = 1$ as defined in (2.1). Specifically, when $d_{\text{btw}}(\tilde{V}_r \tilde{\Lambda}_r^{1/2}, \ell) > (3/2)^{1/2}d_{\text{in}}(\tilde{V}_r \tilde{\Lambda}_r^{1/2}, \ell)$, the true label $\ell$ corresponds to a local solution of the $k$-means objective which can be achieved by a modified Lloyd’s algorithm (Lloyd, 1982) as shown in the Supplemental Material. Since multiple algorithms can correctly recover the labels from a perfect geometric representation, in the remainder of the paper we say that the embedding obtained from multidimensional scaling *exactly recovers* the labels when it is a perfect geometric representation of the true labels.

We thus investigate the sampling regime when this embedding method produces a perfect geometric representation with high probability. By decomposing $X = M + H$, where $M_i^T = \mu_{\ell_i}$ and $H_i^T = \eta_i$, we can view $B = (JX)(JX)^T$ as a perturbation of $MM^T$. Intuitively, because the multidimensional scaling embedding of $M$ simply consists of $k$ distinct
points corresponding to the $k$ Gaussian communities, it trivially recovers the cluster labels. Let $MM^T = VΛV^T$ denote the spectral decomposition of $MM^T$, where $Λ = \text{diag}(λ_i)$ is a diagonal matrix containing the eigenvalues in descending order, and $V$ is the matrix whose columns are the associated eigenvectors. Then $VA^{1/2}$ represents the unperturbed, full rank multidimensional scaling embedding of $M$, which perfectly preserves all pairwise distances.

Let $n_{\min} = \min_{1 \leq j \leq k} n_j$, $σ_{\max} = \max_{1 \leq j \leq k} σ_j$, $μ_{\max} = \max_{1 \leq j \leq k} \|μ_j\|_2$, $μ_{\text{diff}} = \min_{j \neq m} \|μ_j - μ_m\|_2$ and $ζ = N/n_{\min}$, where $μ_{\text{diff}}$ measures the between-class separation and $ζ$ measures the unbalance of cluster sizes. Define the signal to noise ratio as

$$\text{SNR} = \frac{μ_{\text{diff}}^2}{σ_{\max}^2}.$$

We will derive conditions on the signal to noise ratio for exact recovery with high probability using the multidimensional scaling and clustering procedure. Let

$$ρ = \frac{λ_1}{λ_r}, \quad γ = \frac{d}{N}, \quad β = \left( (d \vee \log N) \wedge \left\{ (d \log N)^{1/2} \vee N^{1/2} \log N \right\} \right),$$

where $ρ$ measures the ratio between the largest and smallest eigenvalues in a rank $r$ multidimensional scaling embedding of $M$; $γ$ measures the ratio between the dimension and sample size, so that $γ \gg 1$ characterizes the high-dimension, low sample size regime; and $β$ is used to simplify notation.

To elucidate our results, we define the following regimes characterized by the relationship between $N$ and $d$:

1. the low dimensional regime assumes $d = O(N^{1/2} \log N)$;
2. the moderate dimensional regime assumes $Ω(N^{1/2} \log N) \leq d \leq O(N^2 \log N)$;
3. the high dimensional regime assumes $d = Ω(N^2 \log N)$.

## 3 Main Result

We need three regularity conditions before stating our results.

**Condition 1.** There exist constants $τ_1$ and $τ_2$ such that

$$0 < τ_1 < \min(κ, ζ, ρ) < \max(κ, ζ, ρ) < τ_2 < ∞.$$

**Condition 2.** For $s = \text{rank}(MM^T)$,

$$r ≤ s, \quad λ_{r+1} ≤ \left\{ \frac{λ_r}{2ζ(s-r)} \vee \frac{μ_{\text{diff}}^2 n_{\min}}{144(s-r)} \right\} (r < s).$$

**Condition 3.** $μ_{\max}/μ_{\text{diff}} ≤ \left\{ (β \vee γ)^{1/3} \vee N^{1/2} \right\}$.
For Condition 1, $\rho = O(1)$ requires the top $r$ eigenvalues of $MM^T$ to be of the same order, and $\zeta = O(1)$ requires approximately balanced clusters. Condition 2 ensures $\lambda_{r+1}$ is sufficiently small relative to $\lambda_r$ and $\mu_{\text{diff}}$, which guarantees $r$ dimensions are sufficient for dimension reduction. Condition 3 is generally nonrestrictive, since when $\rho = O(1)$, $\mu_{\text{diff}}$ and $\mu_{\text{max}}$ are of the same order unless the means are exactly colinear.

Our theoretical results are threefold and are derived by viewing the multidimensional scaling matrix $B = (JX)(JX)^T$ as a perturbation of $MM^T$. First the perturbation of the eigenspace is bounded (Theorem 3.1); secondly, the perturbation of the multidimensional scaling embedding matrix is bounded (Theorem 3.2); thirdly, a sufficient condition for exactly recovery is derived (Theorem 3.3). Finally, Theorems 3.4 and 3.8 extend Theorem 3.3 to provide a sharp characterization of the multidimensional scaling and clustering procedure in the high-dimensional regime under certain assumptions.

The first result, Theorem 3.1, bounds the perturbation of the eigenspace associated with the top $r$ eigenvalues of $B$ under max norm. The proof combines Theorem 2 in Fan et al. (2018b), which gives an entry-wise eigenvector perturbation bound well suited for low rank matrices with low coherence eigenvectors, with random matrix results, especially those in Vershynin (2012). It is given in Section S.2 of the Supplementary Material.

**Theorem 3.1.** Assume Condition 1 and the model in Section 2. Then with probability at least $1 - O(N^{-1})$ there exists a rotation matrix $R$ such that
\[
\|\hat{V}_r R - V_r\|_{\text{max}} \lesssim \frac{\sigma_{\text{max}}(\log N)^{1/2}}{\mu_{\text{max}}N^{1/2}} + \frac{\sigma_{\text{max}}^2(\gamma \lor \beta)}{\mu_{\text{max}}^2N^{1/2}}.
\]

As the rank $r$ multidimensional scaling embedding is obtained by rescaling the eigenvectors by the root of the associated eigenvalues, we desire a comparison not just of $V_r$ with $\hat{V}_r$ but of $V_r \Lambda_r^{-1/2}$ with $\hat{V}_r \tilde{\Lambda}_r^{-1/2}$. Since the output of a clustering algorithm remains the same under a fixed scaling and rotation of the data, it suffices to compare $V_s \Lambda_s^{-1/2}$ with $\alpha \hat{V}_r \tilde{\Lambda}_r^{-1/2}R$, where $\alpha$ is any constant and $R$ is any $r \times r$ rotation matrix. The following theorem bounds the perturbation of the multidimensional scaling embedding for a fixed choice of $\alpha$, and the proof is left in the Supplementary Material.

**Theorem 3.2.** Assume $\alpha = \left[\lambda_1 / \{\lambda_1 + \text{tr}(\Sigma)\}\right]^{1/2}$, $\text{SNR} \gtrsim (\log N)^{1/2}\{\gamma^{1/2} \lor (\log N)^{1/2}\}$, Conditions 1–2, and the model in Section 2. Then with probability at least $1 - O(N^{-1})$ there exists a rotation matrix $R$ such that
\[
\|V_r \Lambda_r^{-1/2} - \alpha \hat{V}_r \tilde{\Lambda}_r^{-1/2}R\|_{\text{max}} \lesssim (\sigma_{\text{max}}\mu_{\text{max}})^{1/2} + \sigma_{\text{max}}\{(\log N)^{1/2} \lor \gamma^{1/2}\} + \frac{\sigma_{\text{max}}^2}{\mu_{\text{max}}} (\gamma \lor \beta).
\]

A straightforward calculation given in the Supplementary Material shows that clustering the perturbed multidimensional scaling embedding $\alpha \hat{V}_r \tilde{\Lambda}_r^{-1/2}R$ perfectly recovers the community labels when $\mu_{\text{diff}} > 12\sqrt{\gamma}\|V_r \Lambda_r^{-1/2} - \alpha \hat{V}_r \tilde{\Lambda}_r^{-1/2}R\|_{\text{max}}$. The following theorem is obtained by combining this condition with the bound in Theorem 3.2, and gives a sufficient condition on the signal-to-noise ratio to ensure the multidimensional scaling and clustering
procedure exactly recovers the labels with high probability. The proof of Theorem 3.3 is in Appendix S.5 of the Supplementary Material.

**Theorem 3.3.** Assume Conditions 1–3 and the model in Section 2. Then with probability at least $1 - O(N^{-1})$ the multidimensional scaling and clustering procedure with rank $r$ embedding perfectly recovers the labels whenever:

$$\text{SNR} \gtrsim \beta \vee \gamma.$$  \hfill (3.1)

In this context, $\mu_{\text{diff}}^2, \sigma_{\text{max}}^2$ quantify the strength of the signal, noise respectively. Exact recovery is easier when $\text{SNR} = (\mu_{\text{diff}}/\sigma_{\text{max}})^2$ is large, namely when the classes are well separated relative to the noise, and Theorem 3.3 quantifies the scaling of the signal to noise ratio required for exact recovery. When (3.1) is satisfied, multidimensional scaling followed by a simple clustering algorithm such as $k$-means achieves exact recovery with high probability.

In the very high-dimensional setting, an alternate analysis using standard Davis Kahan perturbation gives sharper results as stated in Theorem 3.4. However the theorem assumes the top $r$ eigenvalues of $MM^T$ are approximately equal, i.e., $\lambda_1 \approx \lambda_r$, and is thus less general. The proof is in Section S.6 of the Supplementary Material.

**Theorem 3.4.** Let the assumptions of Theorem 3.3 hold, and in addition assume $\rho - 1 \leq C\mu_{\text{diff}}/\mu_{\text{max}}$ for some absolute constant $C < 1$. Then with probability at least $1 - O(N^{-1})$ the multidimensional scaling and clustering procedure with rank $r$ embedding perfectly recovers the labels whenever:

$$\text{SNR} \gtrsim N \vee (d \log N)^{1/2}.$$ \hfill (3.2)

**Remark 1.** The $d^{1/2}$ factor on the right hand side of (3.2) can be replaced by $\sqrt{\sum_{s=1}^d (\sigma_s/\sigma_{\text{max}})^4}$ to obtain a sharper scaling for highly nonisotropic distributions, see the application of the Matrix Bernstein Inequality in the proof of Lemma S.7.1 in the Supplementary Material. To write results as concisely as possible, the quantity is bounded by $d^{1/2}$.

By restricting to various regimes of interest, three corollaries are obtained from Theorems 3.3 and 3.4.

**Corollary 3.5 (Low Dimensional Regime).** Under the assumptions of Theorem 3.3, if $d = O(N^{1/2} \log N)$, then with probability at least $1 - O(N^{-1})$ the multidimensional scaling and clustering procedure with rank $r$ embedding perfectly recovers the labels whenever:

$$\text{SNR} \gtrsim \log N \vee d.$$  

The above condition is natural given that when $d = 1$, the maximum norm of a collection of $N$ independent $N(0, \sigma_{\text{max}}^2)$ random variables scales as $\sigma_{\text{max}}(\log N)^{1/2}$ (Vershynin, 2012). Thus clearly communities can be exactly recovered only for $\mu_{\text{diff}} \gtrsim \sigma_{\text{max}}(\log N)^{1/2}$, i.e., $\text{SNR} \gtrsim \log N$, and this scaling continues to hold for small $d$. 


Corollary 3.6 (Moderate Dimensional Regime). Under the assumptions of Theorem 3.3, if $\Omega(N^{1/2} \log N) \leq d \leq O(N^2 \log N)$, then with probability at least $1 - O(N^{-1})$ the multidimensional scaling and clustering procedure with rank $r$ embedding perfectly recovers the labels whenever:

$$\text{SNR} \gtrsim (\log N)^{1/2} \left\{ d^{1/2} \lor (N \log N)^{1/2} \right\}.$$  

This scaling is better with respect to the dimension than might naively be expected. Consider for example the isotropic case when $\sigma_j = \sigma_{\text{max}}$ for all $1 \leq j \leq d$. Since the data points essentially fall on spheres of radius $\sigma_{\text{max}}d^{1/2}$ about the means, one might expect for exact recovery to require $\mu_{\text{diff}}^2 \gtrsim \sigma_{\text{max}}^2 d$ (which gives SNR $\gtrsim d$). However, in high dimensions the measure of a sphere concentrates rapidly around the equator, which allows for perfect recovery of the communities even when the spheres of radius $\sigma_{\text{max}}d^{1/2}$ about the means intersect. Thus when $N$ is small, it is sufficient for SNR $\gtrsim d^{1/2}$.

Corollary 3.7 (High Dimensional Regime). Under the assumptions of Theorem 3.3, if $d = \Omega(N^2 \log N)$, then with probability at least $1 - O(N^{-1})$ the multidimensional scaling and clustering procedure with rank $r$ embedding perfectly recovers the labels whenever:

$$\text{SNR} \gtrsim \gamma.$$  

Furthermore, if $\rho - 1 \leq C \mu_{\text{diff}}/\mu_{\text{max}}$ for some absolute constant $C < 1$, then it is sufficient that:

$$\text{SNR} \gtrsim (d \log N)^{1/2}.$$  

Inequality (3.4) is a less restrictive condition than (3.3) in the high dimensional regime, but only valid when $\rho \approx 1$. To see this, observe that when $N = O(1)$, (3.3) reduces to SNR $\gtrsim d$ while (3.4) reduces to SNR $\gtrsim d^{1/2}$. This $\rho$-based discrepancy is due to the fact that in high dimensions estimating the eigenvalues of $MM^T$ from the eigenvalues of $(JX)(JX)^T$ is more problematic than the corresponding eigenspace estimation. Indeed, since $\lambda_i \left[ E \{(JX)(JX)^T\} \right] = \lambda_i(MM^T) + \text{tr}(\Sigma)$ ($i = 1, \ldots, N-1$), the multidimensional scaling eigenvalues are consistently over-estimated. However if tr$(\Sigma)$ is known or can be accurately approximated, a simple modification of the multidimensional scaling procedure makes (3.4) sufficient for general $\rho$, as stated in the following theorem. The proof is a simple modification of the proof of Theorem 3.4 and is omitted for brevity.

Theorem 3.8. Assume Conditions 1–3 and the model in Section 2. In addition, assume the multidimensional scaling embedding is computed by $\tilde{\Lambda}_r^{1/2} \tilde{V}_r$ instead of $\tilde{\Lambda}_r^{1/2} \tilde{V}_r$, where $\tilde{\Lambda}_r = \tilde{\Lambda}_r - \text{tr}(\Sigma) I_r$. Then with probability at least $1 - O(N^{-1})$ the multidimensional scaling and clustering procedure with rank $r$ embedding perfectly recovers the labels whenever:

$$\text{SNR} \gtrsim N \lor (d \log N)^{1/2}.$$
Table 1: Summary of the scaling conditions with isotropic noise

| Regime            | $\beta$ | $\beta \vee \gamma$ | Scaling Condition |
|-------------------|---------|-----------------------|-------------------|
| Low dimension     | $\log N \vee d$ | $\log N \vee d$ | $\text{SNR} \gtrsim \log N \vee d$ |
| Moderate dimension I | $N^{1/2}$ | $N^{1/2}$ | $\text{SNR} \gtrsim N^{1/2}$ |
| Moderate dimension II | $d^{1/2}$ | $d^{1/2}$ | $\text{SNR} \gtrsim d^{1/2}$ |
| High dimension    | $d^{1/2}$ | $\gamma$ | $\text{SNR} \gtrsim \gamma$ |

Remark 2. The rate given in Theorem 3.3 cannot be improved by incorporating the unbiasing procedure $\hat{\Lambda}_r = \tilde{\Lambda}_r - \text{tr}(\Sigma) I_r$, as the dominant terms arise from the eigenspace estimation.

Remark 3. When the covariance is isotropic, i.e., $\Sigma = \sigma_{\text{max}}^2 I_d$, some of the $\log N$ terms can be removed from our scaling conditions. Specifically, (3.1) in Theorem 3.3 will hold with $\beta = \{ (d \vee \log N) \wedge (d^{1/2} \vee N^{1/2}) \}$. See Table 1 for a summary of the resulting conditions; for brevity, we omit the proof.

4 Relationship with Existing Literature

Exact recovery using the multidimensional scaling and clustering procedure is related to the stochastic block model which is extensively studied in the literature. In a stochastic block model, there are $N$ points drawn from $k$ communities, and two points in communities $r$ and $m$ are connected with probability $P_{r,m}$ (Abbe, 2018). The resulting graph corresponds to an $N$ by $N$ adjacency matrix $A$, where $A_{ij} \in \{0, 1\}$. The matrix $A$ can be viewed as a similarity matrix analogous to the matrix $B$ in multidimensional scaling. However, in contrast to stochastic block models where the upper triangular entries of $A$ are independent, the corresponding entries of $B$ are dependent because, for example, both $B_{i,j}$ and $B_{i,k}$ depend on $x_i$. The $r$th row of $A$ can be treated as an $N$ dimensional random vector drawn from a probability distribution on $\{0, 1\}^N$ with mean $\mu_r = (P_{r,i})_{i \in [N]}$. With the $\{\mu_{r,1}^k\}$, $\mu_{\text{diff}}$ defined as before, and $\sigma_{\text{max}}^2 = \max_{r,m} P_{r,m}(1 - P_{r,m})$, McSherry (2001) showed that the communities can be exactly recovered with high probability when $\text{SNR} \gtrsim k(\zeta + \log N)$. See also Bickel & Chen (2009); Rohe et al. (2011). Recently, Abbe et al. (2016) showed that for two balanced communities, this characterization of exact recovery is sharp, i.e., exact recovery fails for $\text{SNR} \lesssim k^2$. In the low-dimensional regime and under some mild conditions, we obtain the same lower bound for the signal to noise ratio.

Our model is also closely related to the label recovery of a mixture of Gaussian distributions. Achlioptas & McSherry (2005) used spectral projection to show that when $N \gg \zeta k(d + \log k)$, the labels for general Gaussians are exactly recovered for $\text{SNR} \gtrsim \zeta + k \log(kN) + k^2$. Building upon the approach in Kumar & Kannan (2010), Awasthi &
A two-dimensional cube covariance matrix is defined as follows: \( \Sigma_{ij} = \sigma^2_{\max} |i-j| \). This construction.

The Toeplitz covariance matrix is defined by \( \mu_i(i) = 10^{-7}; \mu_i(j) = 0 \) for \( j \neq i \). Simulations 1b use balanced clusters (\( \zeta = k \)) and \( r = \text{rank}(MM^T) \). Thus for all simulations, Conditions 1–3 are satisfied, except \( \rho \gg 1 \) in Simulation 2d as described below.

Table 2 records the parameters, means, and covariance matrices used for all simulations. Covariance matrices considered include isotropic, Toeplitz, and \( K \) nearest neighbor (KNN). The Toeplitz covariance matrix is defined as \( \Sigma = \sigma^2_{\max}(0.7^{i-j}) \). The \( K \) nearest neighbor covariance matrix is defined as follows: \( d \) points \( z_1, \ldots, z_d \) are randomly sampling from a two-dimensional cube \( [0, c]^2 \), and \( \Sigma_{ij} = \sigma^2_{\max} \| z_i - z_j \|_2 \) if \( z_i \) is one of \( z_i's \) \( K \) nearest neighbors, with \( \Sigma_{ii} = \sigma^2_{\max} \). Simulations 1c, 2d use \( K = 4, 10 \) and \( c = 1, 0.5 \) in this construction.

Simulations 1a–1c target the small \( d \) regime. The probability of exact recovery using the multidimensional scaling and clustering procedure is estimated for fixed \( d, |\mu_{\text{diff}}| \) on a grid of

Table 2: Simulation settings

| Sim. | \( k \) | \( d/N \) | \( r \) | \( J \) | \( \Sigma \) | \( \{\mu_i\}^k_{i=1} \) | \( \rho \) | Plot |
|------|------|------|------|------|------|----------------|------|------|
| 1a   | 4    | 2    | 20   | \( \sigma^2_{\max} l_d \) | \( \pm(10^{-7}, 0), \pm(0, 10^{-7}) \) | 1    | Fig. 2a |
| 1b   | 4    | d = 10 | 3    | 50   | Toeplitz | \( \mu_i(i) = 10^{-7}; \mu_i(j) = 0 \) for \( j \neq i \) | 1    | Fig. 2b |
| 1c   | 4    | \( d = 20 \) | 3    | 50   | KNN\(^1\) | \( \mu_i(i) = 10^{-7}; \mu_i(j) = 0 \) for \( j \neq i \) | 1    | Fig. 2c |
| 2a   | 2    | \( N = 200 \) | 1    | 20   | \( \sigma^2_{\max} l_d \) | \( \mu_i(i) = 1; \mu_i(j) = 0 \) for \( j \neq i \) | 1    | Fig. 3a |
| 2b   | 5    | \( N = 100 \) | 4    | 20   | \( \sigma^2_{\max} I_d \) | \( \mu_i(i) = 0.5; \mu_i(j) = 0 \) for \( j \neq i \) | 1    | Fig. 3b |
| 2c   | 5    | \( N = 100 \) | 4    | 20   | Toeplitz | \( \mu_i(i) = 0.5; \mu_i(j) = 0 \) for \( j \neq i \) | 1    | Fig. 3c |
| 2d   | 5    | \( N = 100 \) | 4    | 20   | KNN\(^1\) | \( \mu_i(i) = 0.5; \mu_i(j) = 0 \) for \( j \neq i \) | 1    | Fig. 3d |
| 2e   | 3    | \( N = 60 \) | 2    | 20   | \( \sigma^2_{\max} I_d \) | \( (0, 0), (0.4, 0.6), (1, 1) \) | 75.19 | Fig. 3e |
| 2f   | 5    | \( N = 100 \) | 4    | 20   | \( \sigma^2_{\max} I_d \) | \( \pm(0, 0, 0, 0, 0), \pm(0.49, 0.51, 0, 0, 0), \sum_0 \in \mathbb{R}^{d-4} \) | 10,000 | Fig. 3f |

\(^{\dagger}\) \( K \) nearest neighbor.

Sheffet (2012) propose a spectral algorithm which improves the dependence on \( k \) and correctly classifies a fixed percentage of points when SNR \( \gtrsim 1 \). When the Gaussians are spherical and \( N \) is sufficiently large, the spectral algorithm proposed by Vempala & Wang (2004) exactly recovers the distribution labels when SNR \( \gtrsim \sqrt{\log N} \). This condition is less restrictive by a factor of \( \sqrt{\log N} \) than our result for the low \( d \) regime, but the method requires access to the data coordinates as well as isotropic covariance and is thus not directly comparable. All of the above methods for recovering a mixture of Gaussians require a singular value decomposition of the data matrix, which is generally not available in the multidimensional scaling context.

5 Numerical Studies

5.1 Simulations for Synthetic Data

This section reports simulation results for synthetic data which show the scaling conditions in Corollaries 3.5–3.7 are sharp in all three regimes. The simulations consider Gaussian distributions with both isotropic and more general covariance matrices, and for simplicity, use balanced clusters (\( \zeta = k \)) and \( r = \text{rank}(MM^T) \). Thus for all simulations, Conditions 1–3 are satisfied, except \( \rho \gg 1 \) in Simulation 2d as described below.

Table 2 records the parameters, means, and covariance matrices used for all simulations. Covariance matrices considered include isotropic, Toeplitz, and \( K \) nearest neighbor (KNN). The Toeplitz covariance matrix is defined by \( \Sigma_{ij} = \sigma^2_{\max}(0.7^{i-j}) \). The \( K \) nearest neighbor covariance matrix is defined as follows: \( d \) points \( z_1, \ldots, z_d \) are randomly sampling from a two-dimensional cube \( [0, c]^2 \), and \( \Sigma_{ij} = \Sigma_{ji} = \sigma^2_{\max} \| z_i - z_j \|_2 \) if \( z_i \) is one of \( z_i's \) \( K \) nearest neighbors, with \( \Sigma_{ii} = \sigma^2_{\max} \). Simulations 1c, 2d use \( K = 4, 10 \) and \( c = 1, 0.5 \) in this construction.

Simulations 1a–1c target the small \( d \) regime. The probability of exact recovery using the multidimensional scaling and clustering procedure is estimated for fixed \( d, \mu_{\text{diff}} \) on a grid of
σ_{\text{max}}, N values. For each grid point, J independent realizations are created, and we record the percentage of realizations for which single linkage clustering on the multidimensional scaling embedding perfectly recovers the labels.

The empirical probability estimates for this set of simulations are plotted in Fig. 2; the horizontal axis shows $\log \log N$ and the vertical axis $\log \text{SNR}$. Dark blue indicates exact recovery was achieved by 0% of the simulations; yellow indicates exact recovery was achieved by 100% of the simulations. Since the boundary between exact recovery and failure of exact recovery is linear with a slope of 1 (after an initial plateau in some of the simulations), the boundary is $\log \text{SNR} = \log \log N + C$ for some constant $C$, which is equivalent to $\text{SNR} = e^C \log N$. Since we fix a small $d$, the condition in Corollary 3.5 guaranteeing exact recovery reduces to $\text{SNR} \gtrapprox \log N$. The simulation results thus confirm that this lower bound for the signal to noise ratio is sharp.

Simulations 2a–2f target the moderate and large $d$ regimes. We estimate the probability of exact recovery for fixed $N$, $\mu_{\text{diff}}$ on a grid of $\sigma_{\text{max}}, d$ values in the same manner as for the first set of simulations. Except for Simulations 2c and 2d, $d$ ranges from 100 to 6,553, 600, so choice of $N$ ensures coverage of both the moderate and large $d$ regimes. For Simulations 2c and 2d, computational resources limited our investigation to the moderate $d$ regime.

The empirical probability estimates for the second set of simulations are plotted in Fig. 3; the horizontal axis shows $\log d$ and the vertical axis $\log \text{SNR}$. There is a qualitative similarity between Figures 3a–3d (where $\rho = 1$) and Figures 3e–3f (where $\rho > 1$). When $\rho = 1$ the boundary between exact recovery and failure of exact recovery is linear with a slope of 0.5. The boundary is thus characterized by $\log(\text{SNR}) = 0.5 \log d + C$ for some constant $C$, which is equivalent to $\text{SNR} = e^C d^{1/2}$. Since $N$ is small and fixed, the condition in Corollary 3.6 guaranteeing exact recovery in the moderate $d$ regime reduces to $\text{SNR} \gtrapprox d^{1/2}$, and since $\rho = 1$, the condition in Corollary 3.7 guaranteeing exact recovery in the large $d$ regime also reduces to $\text{SNR} \gtrapprox d^{1/2}$. Thus when $\rho = 1$, simulation results confirm that the lower bounds on the signal to noise ratio given by Corollaries 3.6 and 3.7 are sharp.

When $\rho \neq 1$ (Figures 3e and 3f), a phase transition occurs, as the boundary initially
Figure 3: Pink lines characterize the boundary and are defined by \( \log \text{SNR} = 0.5 \log d + C \) where \( C = 0, 1, -0.1, 1 \) for Figures 3a, 3b, 3c, 3d respectively. For Figures 3e, 3f, the left line is \( \log \text{SNR} = 0.5 \log d + C \) for \( C = 1.2, 1.7 \) and the right line is \( \log \text{SNR} = 0.78 \log d + C \) for \( C = -1.46, -0.82 \).

characterized by a line with slope 0.5 (moderate \( d \) regime) steepens to a line with slope 0.78 as the dimension is increased (high \( d \) regime). The authors hypothesize that the boundary converges to a line with slope 1 as \( d \to \infty \), but computational abilities limited \( d \leq 6,553,600 \). These results confirm that even when \( \rho \neq 1 \), the scaling condition \( \text{SNR} \gtrsim d^{1/2} \) given by Corollary 3.6 for the moderate \( d \) regime is sharp. In addition, the steepening of the boundary line suggests that when \( \rho \neq 1 \), the scaling condition \( \text{SNR} \gtrsim d \) given by Corollary 3.7 for the large \( d \) regime may also be sharp.

**Remark 4.** Additional simulation results confirm that if the eigenvalues are unbiased using the procedure described in Theorem 3.8, the steepening of the boundary line does not occur for general \( \rho \), and the boundary continues to be characterized by \( \text{SNR} = C d^{1/2} \) in the high dimensional regime.

### 5.2 Applications

This section illustrates the usefulness of multidimensional scaling for classification on cancer gene-expression and natural language datasets. We applied multidimensional scaling to the Pan-Cancer Atlas gene expression data downloaded from the University of California at Santa Cruz Xena Platform (Goldman et al., 2018). The Pan-Cancer Atlas, the output of The Cancer Genome Atlas project, consists of genomic, molecular, and clinical data of 11,060
Table 3: Classification accuracy for Pan-Cancer

| Cancer type                              | Sample size | Accuracy  |
|------------------------------------------|-------------|-----------|
| Breast invasive carcinoma                | 1,218       | 99.75%    |
| Kidney renal clear cell carcinoma        | 606         | 97.85%    |
| Lung adenocarcinoma                      | 576         | 98.78%    |
| Thyroid carcinoma                        | 572         | 99.83%    |
| Total                                    | 2,972       | 99.19%    |

tumors across 33 cancer types. We selected the four most prevalent cancer types from the Pan-Cancer Atlas: breast invasive carcinoma ($n_1 = 1,218$), kidney renal clear cell carcinoma ($n_2 = 606$), lung adenocarcinoma ($n_3 = 576$), and thyroid carcinoma ($n_4 = 572$). For each patient, $d = 20,531$ gene expressions with batch correction were recorded. After examining the eigenvalues of the multidimensional scaling matrix, we chose $r = 7$ to create the embedding as described in Section 2. Applying $k$-means clustering with $k = 4$ to the embedding, we obtained high accuracy in cancer type classification on the full data set; see Table 3 for the classification accuracies and Fig. 4a to visualize the multidimensional scaling embedding. We emphasize these results were obtained only through pair-wise distances between samples without the need to access full data.

We also applied multidimensional scaling to the natural language datasets available from http://www-alg.ist.hokudai.ac.jp/datasets.html. The data points considered are the names of famous individuals, taken from four possible classes: classical composers, artists, authors, and mathematicians; the data points thus do not have geometric coordinates. The pair-wise dissimilarity between data points is then defined using Google distance, a metric suggested by Cilibrasi & Vitanyi (2006) for sets of natural language terms. The Google distance between two terms is computed from the relative frequency count of the number of web pages containing both terms returned by an automated web search (Poland & Zeugmann, 2006). We analyzed three such datasets: people2 ($k = 2, N = 50$), a natural language data set containing the names of 25 classical composers and 25 artists; people3 ($k = 3, N = 75$), the people2 data set with the names of 25 authors added; and people4 ($k = 4, N = 100$), the people3 data set with the names of 25 mathematicians added.

We applied multidimensional scaling using $r = k - 1$, which corresponded to the maximal eigengap in the eigenvalues of the multidimensional scaling matrix for all three data sets, and ran $k$-means clustering on the resulting embedding. The resulting classification accuracies are in Table 4, and Fig. 4 shows the first two coordinates of the embedding. For people2, the second embedding coordinate was not used for clustering but is displayed in Fig. 4b; for people4, the third embedding coordinate is needed to separate the clusters but is not displayed in Fig. 4d.
Table 4: Classification accuracy for natural language data sets

| Data set | Sample size (N) | Number of classes (k) | Accuracy   |
|----------|----------------|-----------------------|------------|
| People2  | 50             | 2                     | 100.00%    |
| People3  | 75             | 3                     | 97.33%     |
| People4  | 100            | 4                     | 94.00%     |

Figure 4: First two coordinates of the embedding obtained by applying multidimensional scaling to Pan-Cancer and people data sets. Each color corresponds to a cancer type for Pan-Cancer and a people group for people data sets.

6 Discussion

This paper lays down a theoretical framework for analyzing the embedding quality of classical multidimensional scaling. Based on this framework, we further derive sharp scaling conditions on the signal-to-noise ratio required for a follow-up clustering procedure to exactly recover the labels of a collection of Gaussian (subGaussian) communities. These results generalize scaling conditions for exact recovery in stochastic block models to the more complex case of a network with dependent edges, giving the first strong theoretical guarantees for classical multidimensional scaling in the literature. We make no assumptions on the relationship between $N$ and $d$, and numerical simulations confirm the derived scaling conditions are sharp in the low, moderate, and high dimensional regimes. Many interesting open questions remain for future research, including extending the current framework to more general noise distributions and more general metrics and incorporating sparse measurement error in the pairwise distance matrix. Our results suggest that the performance of classical multidimensional scaling can be significantly improved by unbiasing the population eigenvalues in the high dimensional regime, and it remains to develop and analyze empirically robust unbiasing procedures.

7 Supplementary Material

Supplementary material available online includes (S.1) eigenspace perturbation results; (S.2) proof of Theorem 3.1; (S.3) proof of Theorem 3.2; (S.4) proof of Lemmas needed for Theorem 3.2; (S.5) proof of Theorem 3.3; (3.4) proof of Theorem 3.4; (S.7) proof of
random matrix lemmas; (S.8) clustering results.

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Supplementary Material to An Analysis of Classical Multidimensional Scaling

Abstract

This document contains Supplementary Material on (S.1) eigenspace perturbation results; (S.2) proof of Theorem 3.1; (S.3) proof of Theorem 3.2; (S.4) proof of Lemmas needed for Theorem 3.2; (S.5) proof of Theorem 3.3; (S.4) proof of Theorem 3.4; (S.7) proof of random matrix lemmas; (S.8) clustering results.

Appendices S.1–S.6 utilize $\lambda_1, \lambda_r = \Theta(N\mu_{\max}^2)$, which is guaranteed by Condition 1 since $n_1\nu_1^2 + \ldots + n_k\nu_k^2 = \lambda_1 + \ldots + \lambda_k$ implies $N\mu_{\max}^2 \leq \lambda_1 \leq N\mu_{\max}^2$ and $k = O(1)$ implies $s = O(1)$. The following matrix norm properties are also utilized. For any matrix product $AB$, $\|AB\|_{\max} \leq \|A\|_{\infty}\|B\|_{\max}$ and also $\|AB\|_{\max} \leq \|A\|_{\max}\|B\|_1$. For an $N$ by $r$ matrix $A$, $\|A\|_1 \leq N^{1/2}\|A\|_2$. $\|A\|_{\infty} \leq r^{1/2}\|A\|_2$, $\|A\|_2 \leq (Nr)^{1/2}\|A\|_{\max}$. The spectral norm is rotation invariant; namely, for any orthogonal matrix $R$, $\|A\|_2 = \|AR\|_2 = \|RA\|_2$.

S.1 Eigenspace Perturbation Results

This section reports two known theorems for bounding eigenvector perturbations of real, symmetric matrices. For both theorems, $A, \tilde{A} \in \mathbb{R}^{N \times N}$ are symmetric with eigenvalues $\lambda_1 \geq \ldots \geq \lambda_N, \tilde{\lambda}_1 \geq \ldots \geq \tilde{\lambda}_N$ and associated eigenvectors $v_1, \ldots, v_N$ and $\tilde{v}_1, \ldots, \tilde{v}_N$ respectively. The first is a recent result from Fan et al. (2018).

**Theorem S.1.1.** Let $A_r = \sum_{i=1}^r \lambda_i v_i v_i^T$ and $\kappa = (N/r) \max_i \sum_{j=1}^r v_j^2(i)$. Suppose $|\lambda_r| - \epsilon = \Omega((r^3\kappa^2\|A - \tilde{A}\|_{\infty})$, where $\epsilon = \|A - A_r\|_{\infty}$. Then, there exists an orthogonal matrix $R \in \mathbb{R}^{r \times r}$ such that

$$\|\tilde{V}_r R - V_r\|_{\max} = O\left\{ \frac{r^5/2\kappa^2\|A - \tilde{A}\|_{\infty}}{(|\lambda_r| - \epsilon)N^{1/2}} \right\},$$

where $V_r = (v_1, \ldots, v_r), \tilde{V}_r = (\tilde{v}_1, \ldots, \tilde{v}_r)$.

The second is a variation of the standard Davis Kahan Theorem given in Yu et al. (2014):

**Theorem S.1.2.** Fix $1 \leq m \leq s \leq N$ and assume that $\min(\lambda_{m-1} - \lambda_m, \lambda_s - \lambda_{s+1}) > 0$, where we define $\lambda_0 = \infty$ and $\lambda_{N+1} = -\infty$. Let $r = s - m + 1$, and $V_r = (v_m, v_{m+1}, \ldots, v_s) \in \mathbb{R}^{N \times r}, \tilde{V}_r = (\tilde{v}_m, \tilde{v}_{m+1}, \ldots, \tilde{v}_s) \in \mathbb{R}^{N \times r}$. We have

$$\|\sin \Theta(\tilde{V}_r, V_r)\|_F \leq \frac{2 \min(r^{1/2}\|\tilde{A} - A\|_2, \|\tilde{A} - A\|_F)}{\min(\lambda_{m-1} - \lambda_m, \lambda_s - \lambda_{s+1})},$$

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Lemma S.3.1. Let the assumptions of Theorem 3.2 hold. Then with probability at least 

$$\Pr(\|\tilde{V}_r - V_r\|_F \leq 2^{3/2} \min(r^{1/2}\|\tilde{A} - A\|_2, \|\tilde{A} - A\|_F) \min(\lambda_{m-1} - \lambda_m, \lambda_s - \lambda_{s+1})/\min(\lambda_{m-1} - \lambda_m, \lambda_s - \lambda_{s+1}))$$.

S.2 Proof of Theorem 3.1

We apply Theorem S.1.1 to obtain entry-wise control on the perturbation of the eigenspace from $MM^T \rightarrow (JX)(JX)^T$. We first bound $\kappa$ and $\epsilon$. Since $MM^T$ is block constant, so are its eigenvectors on the blocks defined by the community labels, so that $\|v_j\|_\infty \leq \frac{1}{n_{\min}}$ ($j = 1, \ldots, s$). Thus

$$\kappa \leq N \left(\|v_1\|_\infty^2 + \cdots + \|v_r\|_\infty^2\right) \leq \frac{N}{r} \left(\frac{r}{n_{\min}}\right) = \zeta,$$

i.e., we have low coherence since $\zeta = O(1)$ by Condition 1. Also since $\|v_i v_i^T\|_\infty \leq N\|v_i\|_\infty^2 \leq N\|v_i\|_\infty^2 \leq N\|v_i\|_\infty^2 \leq \zeta$, we have:

$$\epsilon = \left\|\sum_{i=r+1}^s \lambda_i v_i v_i^T\right\|_\infty \leq \lambda_{r+1}(s - r) \max_i \|v_i v_i^T\|_\infty \leq \lambda_{r+1}(s - r) \zeta \leq \frac{\lambda_r}{2},$$

since by assumption $\lambda_{r+1} \leq \lambda_r/\{2\zeta(s - r)\}$. Recalling $A$ is positive semi-definite, $|\lambda_r| - \epsilon \geq \lambda_r/2$. Thus defining $P = (JX)(JX)^T - MM^T$, by Theorem S.1.1 there exists a rotation matrix $R$ such that $\|\tilde{V}_r R - V_r\|_{\max} = O\{r^{5/2}\zeta^2\|P\|_{\infty}/(\lambda_r N^{1/2})\} = O\{\|P\|_{\infty}/(\mu_{\max}^2 N^{3/2})\}$ since $\lambda_r \geq N\mu_{\max}^2$. Now by Lemma S.7.2 with probability at least $1 - O(N^{-1})$,

$$\|\tilde{V}_r R - V_r\|_{\max} \lesssim \frac{\sigma_{\max}(\log N)^{1/2}}{\mu_{\max}^2 N^{3/2}} \lesssim \frac{\sigma_{\max}(\log N)^{1/2}}{\mu_{\max}^2 N^{3/2}} + \frac{\sigma_{\max}^2(\gamma \lor \beta)}{\mu_{\max}^2 N^{1/2}}$$

where $\gamma = d/N$, $\beta = \left[\left(d \lor \log N\right) \land \left\{(d \log N)^{1/2} \lor N^{1/2} \log N\right\}\right]$, which proves Theorem 3.1.

S.3 Proof of Theorem 3.2

The proof of Theorem 3.2 utilizes the following two lemmas, which are proved in Appendix S.4.

**Lemma S.3.1.** Let the assumptions of Theorem 3.2 hold. Then with probability at least $1 - O(N^{-1})$ there exists a rotation matrix $R$ such that

$$\alpha \lambda_1^{1/2}\|\tilde{V}_r R - V_r\|_{\max} \lesssim \sigma_{\max}(\log N)^{1/2} + \sigma_{\max}^2(\gamma \lor \beta).$$
Lemma S.3.2. Let the assumptions of Theorem 3.2 hold. Then with probability at least $1 - O(N^{-1})$ there exists a rotation matrix $R$ such that

$$\|V_r\|_{\max} \|\alpha \tilde{\Lambda}_{1/2}^r R - RA_{1/2}^r\|_{\max} \lesssim (\sigma_{\max} \mu_{\max})^{1/2} + \sigma_{\max}\{ (\log N)^{1/2} \vee \gamma^{1/2}\} + \frac{\sigma^2_{\max}}{\mu_{\max}}(\gamma \vee \beta).$$

In fact there exists a single rotation matrix $R$ such that the conclusions of Lemmas S.3.1 and S.3.2 hold simultaneously with high probability; see Appendix S.4. We have:

$$\|\alpha \tilde{V}_r \tilde{\Lambda}_{1/2}^r R - V_r A_{1/2}^r\|_{\max} \leq \|\tilde{V}_r R^{-1} \alpha \tilde{\Lambda}_{1/2}^r R - V_r R^{-1} \alpha \tilde{\Lambda}_{1/2}^r R\|_{\max}$$

$$+ \|V_r R^{-1} \alpha \tilde{\Lambda}_{1/2}^r R - V_r R^{-1} \alpha \tilde{\Lambda}_{1/2}^r R\|_{\max}$$

$$= \|\tilde{V}_r R - V_r\|_{\max} \|R^{-1} \alpha \tilde{\Lambda}_{1/2}^r R - \Lambda_{1/2}^r\|_{1}$$

$$+ \|V_r\|_{\max} \|R^{-1} \alpha \tilde{\Lambda}_{1/2}^r R - \Lambda_{1/2}^r\|_{1}$$

$$\leq r^{1/2} \|\tilde{V}_r R - V_r\|_{\max} \|R^{-1} \alpha \tilde{\Lambda}_{1/2}^r R\|_2$$

$$+ r^{1/2} \|V_r\|_{\max} \|R^{-1} \alpha \tilde{\Lambda}_{1/2}^r R - \Lambda_{1/2}^r\|_2$$

$$= \alpha(r\tilde{\lambda}_1)^{1/2} \|\tilde{V}_r R - V_r\|_{\max} + r^{1/2} \|V_r\|_{\max} \|\alpha \tilde{\Lambda}_{1/2}^r R - RA_{1/2}^r\|_2$$

$$\leq \alpha(r\tilde{\lambda}_1)^{1/2} \|\tilde{V}_r R - V_r\|_{\max}$$

$$+ r^{3/2} \|V_r\|_{\max} \|\alpha \tilde{\Lambda}_{1/2}^r R - RA_{1/2}^r\|_{\max}.$$ 

Applying Lemmas S.3.1 and S.3.2 to bound each of the above terms gives

$$\|\alpha \tilde{V}_r \tilde{\Lambda}_{1/2}^r R - V_r A_{1/2}^r\|_{\max} \lesssim (\sigma_{\max} \mu_{\max})^{1/2} + \sigma_{\max}\{ (\log N)^{1/2} \vee \gamma^{1/2}\} + \frac{\sigma^2_{\max}}{\mu_{\max}}(\gamma \vee \beta)$$

with probability at least $1 - O(N^{-1})$, which concludes the proof of Theorem 3.2.

S.4 Proof of Lemmas Needed for Theorem 3.2

The following framework for analyzing the perturbation $MM^T \rightarrow (JX)(JX)^T$ is used to prove both lemmas. We define the following relevant quantities:

$$A = MM^T;$$

$$\hat{A} = MM^T + \text{tr}(\Sigma)J;$$

$$\tilde{A} = (JX)(JX)^T;$$

$$P = \tilde{A} - A;$$

$$P - \text{tr}(\Sigma)J = \hat{A} - \tilde{A}.$$ 

The matrix $\tilde{A} = A + P$ is a perturbation of $A$; the quantity $\hat{A}$ will also be convenient in the proof, as we decompose the perturbation $A \rightarrow \hat{A}$ into two pieces: $A \rightarrow \tilde{A}$ and $\tilde{A} \rightarrow \hat{A}$. We let $\{\tilde{\lambda}_i\}_{i=1}^N$ denote the eigenvalues of $\tilde{A}$.

We first relate the eigendecompositions of $A$ and $\hat{A}$. The 1 vector is an eigenvector of $MM^T$ with corresponding eigenvalue $\lambda = 0$. Although $\lambda = 0$ has multiplicity greater
than 1, we choose a basis for its eigenspace so that \( v_N = 1 \) and the remaining eigenvectors \( v_1, \ldots, v_{N-1} \) are orthogonal to 1. The matrix \( J \) is a projection matrix which eliminates any component in the direction of 1 but has no affect on any other direction. Thus for \( i > N \)

\[
\hat{A}v_i = \{MM^T + \text{tr}(\Sigma)J\}v_i = \lambda_i v_i + \text{tr}(\Sigma)v_i = \{\lambda_i + \text{tr}(\Sigma)\}v_i,
\]

and also

\[
\hat{A}v_N = \{MM^T + \text{tr}(\Sigma)J\}1 = 0 = \lambda_N v_N.
\]

Thus all eigenvectors of \( A \) are still eigenvectors of \( \hat{A} \), that is, we may choose an eigenbasis \( \{\hat{v}_i\}_{i=1}^N \) for \( \hat{A} \) such that \( \hat{v}_i = v_i \) (\( i = 1, \ldots, N \)) with \( \hat{\lambda}_i = \lambda_i + \text{tr}(\Sigma) \) (\( i = 1, \ldots, N - 1 \)) and \( \hat{\lambda}_N = \lambda_N = 0 \). We let \( \hat{V}_r = (\hat{v}_1, \ldots, \hat{v}_r) \) so that \( V_r = \hat{V}_r \). Furthermore, by Weyl’s Inequality, \( |\hat{\lambda}_i - \lambda_i| \leq \|P\|_2 \) and \( |\lambda_i - \hat{\lambda}_i| \leq \|P - \text{tr}(\Sigma)J\|_2 \) for all \( i \).

### S.4.1 Proof of Lemma S.3.1

To obtain a bound for \( \alpha \hat{\lambda}_1^{1/2} \|\hat{V}_r R - V_r\|_{\text{max}} \), note

\[
\alpha \hat{\lambda}_1^{1/2} = \frac{\alpha^2 \hat{\lambda}_1 - \lambda_1}{\alpha \hat{\lambda}_1^{1/2} + \lambda_1^{1/2}} + \lambda_1^{1/2} \leq \frac{|\alpha^2 \hat{\lambda}_1 - \lambda_1|}{\lambda_1^{1/2}} + \lambda_1^{1/2}.
\]

Utilizing \( \alpha = [\lambda_1 / (\lambda_1 + \text{tr}(\Sigma))]^{1/2} \) and \( |\hat{\lambda}_i - \lambda_i| = |\lambda_i - \lambda_i - \text{tr}(\Sigma)| \leq \|P - \text{tr}(\Sigma)J\|_2 \), we have:

\[
\alpha \hat{\lambda}_1^{1/2} \leq \frac{|\lambda_1 \{\lambda_1 + \text{tr}(\Sigma)\}/\{\lambda_1 + \text{tr}(\Sigma)\} - \lambda_1|}{\lambda_1^{1/2}} + \lambda_1^{1/2}
\]

\[
= \frac{|\lambda_1 \|P - \text{tr}(\Sigma)J\|_2 / \{\lambda_1 + \text{tr}(\Sigma)\}|}{\lambda_1^{1/2}} + \lambda_1^{1/2}
\]

\[
= \frac{\|P - \text{tr}(\Sigma)J\|_2}{\lambda_1^{1/2}} \left( 1 + \frac{\text{tr}(\Sigma)}{\lambda_1} \right)^{-1} + \lambda_1^{1/2}.
\]

Since \( \text{SNR} \gtrsim (\log N)^{1/2} \{\gamma^{1/2} \lor (\log N)^{1/2}\} \), \( \|P - \text{tr}(\Sigma)J\|_2 / N = O(\mu_{\text{max}}^2) \) by Lemma S.7.1 with high probability. We obtain:

\[
\alpha \hat{\lambda}_1^{1/2} \|\hat{V}_r R - V_r\|_{\text{max}} \lesssim \left\{ \lambda_1^{1/2} + \frac{\|P - \text{tr}(\Sigma)J\|_2}{\lambda_1^{1/2}} \right\} \|\hat{V}_r R - V_r\|_{\text{max}}
\]

\[
\lesssim \left\{ \mu_{\text{max}} \lambda_1^{1/2} + \frac{\|P - \text{tr}(\Sigma)J\|_2}{\mu_{\text{max}} \lambda_1^{1/2}} \right\} \|\hat{V}_r R - V_r\|_{\text{max}}
\]

\[
\lesssim \mu_{\text{max}} \lambda_1^{1/2} \|\hat{V}_r R - V_r\|_{\text{max}}
\]

\[
\lesssim \sigma_{\text{max}} \lambda_1 \|\hat{V}_r R - V_r\|_{\text{max}}
\]

with probability at least \( 1 - O(N^{-1}) \), where the last line follows from Theorem 3.1.
S.4.2 Proof of Lemma S.3.2

As established in the proof of Theorem 3.1, there exists a rotation matrix $R$ satisfying $\|\tilde{V}_r R - V_r\|_{\text{max}} = O \left\{ \|P\|_{\infty} (\mu_{\text{max}} N^{3/2}) \right\}$. To control $\|\alpha \tilde{\lambda}_1^{1/2} R - R \Lambda_r^{1/2} \|_{\text{max}}$ for this rotation $R$, note $(\alpha \tilde{\lambda}_1^{1/2} R - R \Lambda_r^{1/2})_{ij} = (\alpha \tilde{\lambda}_1^{1/2} - \lambda_j^{1/2}) R_{ij}$. We partition the eigenvalues $\lambda_1, \ldots, \lambda_r$ into $\delta$-groups so that if $\lambda_{i+1} - \lambda_i < \delta$, they are in the same $\delta$-group, and if not, they are in different $\delta$-groups. We will show that when $\lambda_i, \lambda_j$ are in the same $\delta$ group, $\alpha \tilde{\lambda}_1^{1/2} - \lambda_j^{1/2}$ is small, and when they are in different $\delta$ groups, $|R_{ij}|$ is small, so that $(\alpha \Lambda_r^{1/2} R - R \Lambda_r^{1/2})_{ij}$ is always small. First we relate $\tilde{\lambda}_1^{1/2}$ to $\tilde{\lambda}_i$ by:

$$|\alpha \tilde{\lambda}_1^{1/2} - \lambda_j^{1/2}| = \left| \frac{\alpha^2 \tilde{\lambda}_i - \lambda_i}{\alpha^{1/2} \tilde{\lambda}_i + \lambda_1^{1/2}} + \frac{\lambda_i - \lambda_j}{\lambda_1^{1/2} + \lambda_j^{1/2}} \right| \leq |\frac{\alpha^2 \tilde{\lambda}_i - \lambda_i}{\lambda_1^{1/2}}| + |\frac{\lambda_i - \lambda_j}{\lambda_1^{1/2}}|.$$  

Utilizing $\alpha = \left[ \lambda_1 / \{ \lambda_1 + \text{tr}(\Sigma) \} \right]^{1/2}$, we bound $|\alpha^2 \tilde{\lambda}_i - \lambda_i|$ by

$$|\alpha^2 \tilde{\lambda}_i - \lambda_i| = \left| \left\{ \frac{\lambda_1}{\lambda_1 + \text{tr}(\Sigma)} \right\} \tilde{\lambda}_i - \lambda_i \right|$$

$$= \left| \left\{ \frac{\lambda_1}{\lambda_1 + \text{tr}(\Sigma)} \right\} \{ \lambda_i + \text{tr}(\Sigma) \} \pm \|P - \text{tr}(\Sigma) J\|_2 \right| - \lambda_i$$

$$= \left| \text{tr}(\Sigma)(\lambda_1 - \lambda_i) \pm \lambda_i \|P - \text{tr}(\Sigma) J\|_2 \right|$$

$$\leq \left| \frac{\lambda_1 - \lambda_i}{\lambda_1 / \text{tr}(\Sigma) + 1} \right| + \|P - \text{tr}(\Sigma) J\|_2.$$  

Thus letting $\tau_{\rho} = \frac{|\lambda_1 - \lambda_r|}{\lambda_1 / \text{tr}(\Sigma) + 1} = \frac{\lambda_r^{1/2}(\rho - 1)}{\{ \lambda_1 / \text{tr}(\Sigma) + 1 \}}$, we obtain

$$|\alpha \tilde{\lambda}_1^{1/2} - \lambda_j^{1/2}| \leq \left\{ \frac{\lambda_1}{\text{tr}(\Sigma)} + 1 \right\}^{1/2} + \frac{\|P - \text{tr}(\Sigma) J\|_2}{\lambda_1^{1/2}} + \frac{|\lambda_i - \lambda_j|}{\lambda_1^{1/2}}.$$  

Thus, when $\lambda_i, \lambda_j$ are in the same $\delta$ group, since $|R_{ij}| \leq 1$, we can bound:

$$|(\alpha \tilde{\lambda}_1^{1/2} R - R \Lambda_r^{1/2})_{ij}| = |\alpha \tilde{\lambda}_1^{1/2} - \lambda_j^{1/2}| |(|R_{ij}|)|$$

$$\leq \tau_{\rho} + \frac{\|P - \text{tr}(\Sigma) J\|_2}{\lambda_1^{1/2}} + \frac{\rho \delta}{\lambda_1^{1/2}}.$$  

To obtain a bound for $\lambda_i, \lambda_j$ in different $\delta$ groups, observe:

$$R = \tilde{V}_r^T V_r + \tilde{V}_r^T (\tilde{V}_r R - V_r)$$

$$|R_{ij}| \leq |\langle v_i, \tilde{v}_j \rangle| + \|V_r^T\|_{\infty} \|\tilde{V}_r R - V_r\|_{\text{max}}$$

$$\leq |\langle v_i, \tilde{v}_j \rangle| + N^{1/2} \|V_r^T\|_2 \|\tilde{V}_r R - V_r\|_{\text{max}}$$

$$= |\langle v_i, \tilde{v}_j \rangle| + N^{1/2} \|\tilde{V}_r R - V_r\|_{\text{max}}.$$  

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When \( i \) and \( j \) correspond to different \( \delta \)-groups, \(|\langle v_i, \tilde{v}_j \rangle| = |\langle \hat{v}_i, \tilde{v}_j \rangle| \leq 2 \|P - \text{tr}(\Sigma)J\|_2/(\delta - 2\|P - \text{tr}(\Sigma)J\|_2)\) by Davis-Kahan Theorem (see Theorem VII.3.2 in Bhatia (2013)).

Since \( \tau_\rho \leq |\lambda_1 - \lambda_r|/\lambda_r^{1/2} \), one has

\[
|\langle \alpha \Lambda_r^{1/2} R - R \Lambda_r^{1/2} \rangle_{ij}| \leq \begin{cases} 
\tau_\rho + (\|P - \text{tr}(\Sigma)J\|_2 + r\delta)/\lambda_r^{1/2} & (\lambda_i = \lambda_j) \\
\|I \times II\| & (\lambda_i \neq \lambda_j)
\end{cases},
\]

where \( \lambda_i \equiv \lambda_j \) if \( \lambda_i, \lambda_j \) are in the same \( \delta \) group and \( \lambda_i \neq \lambda_j \) if they are not, and

\[
I = \frac{\|P - \text{tr}(\Sigma)J\|_2^2 + 2|\lambda_1 - \lambda_r|}{\lambda_r^{1/2}}
\]

\[
II = \frac{2\|P - \text{tr}(\Sigma)J\|_2}{\delta - 2\|P - \text{tr}(\Sigma)J\|_2} + N^{-1/2}\|\tilde{\nu}_r R - V_r\|_{\text{max}}.
\]

We are free to choose \( \delta \) to optimize our bounds, and we choose \( \delta = \mu_{\text{max}} N^{1/2}\|P - \text{tr}(\Sigma)J\|_2^{1/2} \). Since SNR \( \gtrsim (\log N)^{1/2}\{\gamma^{1/2} \vee (\log N)^{1/2}\} \), \( \|P - \text{tr}(\Sigma)J\|_2 / N = O(\mu_{\text{max}}^2) \) by Lemma S.7.1 with probability \( 1 - O(N^{-1}) \), giving \( 2\|P - \text{tr}(\Sigma)J\|_2/(\delta - 2\|P - \text{tr}(\Sigma)J\|_2) \lesssim \|P - \text{tr}(\Sigma)J\|_2^{1/2}/(\mu_{\text{max}} N^{1/2}) \).

Since \( \|V_r\|_{\text{max}} \lesssim N^{-1/2} \), we have

\[
\|V_r\|_{\text{max}} \|\alpha \Lambda_r^{1/2} R - R \Lambda_r^{1/2}\|_{\text{max}} \lesssim \left\{ N^{-1/2} \left( \tau_\rho + \frac{\|P - \text{tr}(\Sigma)J\|_2}{\lambda_r^{1/2}} + \frac{r\delta}{\lambda_r^{1/2}} \right) \right\} \lor \{ N^{-1/2}(I)(II) \}.
\]

We now bound each term in the above maximum. The first term is bounded by

\[
N^{-1/2}(I)(II) \lesssim \left\{ \|P - \text{tr}(\Sigma)J\|_2^2 + \frac{|\lambda_1 - \lambda_r|}{N^{1/2} \lambda_r^{1/2}} \right\} \left\{ \|P - \text{tr}(\Sigma)J\|_2^{1/2} + \frac{\mu_{\text{max}} N^{1/2}}{\mu_{\text{max}} N} \right\} \lesssim \frac{\|P - \text{tr}(\Sigma)J\|_2^2}{N^{1/2}} + \frac{\|P - \text{tr}(\Sigma)J\|_2^{1/2}}{\mu_{\text{max}} N} + \frac{\mu_{\text{max}} N}{\mu_{\text{max}} N}.
\]

Since \( N^{1/2}\|\tilde{\nu}_r R - V_r\|_{\text{max}} \lesssim \mu_{\text{max}}^{-2} N^{-1}\|P\|_{\infty} \), the second term is bounded by

\[
\|V_r\|_{\text{max}} \|\alpha \Lambda_r^{1/2} R - R \Lambda_r^{1/2}\|_{\text{max}} \lesssim \left\{ \|P - \text{tr}(\Sigma)J\|_2^2 + \frac{|\lambda_1 - \lambda_r|}{N^{1/2} \lambda_r^{1/2}} \right\} \left\{ \frac{\|P - \text{tr}(\Sigma)J\|_2^{1/2}}{\mu_{\text{max}} N^{1/2}} + \frac{\|P\|_{\infty}}{\mu_{\text{max}} N} \right\} \lesssim \frac{\|P - \text{tr}(\Sigma)J\|_2^{1/2}}{N^{1/2}} + \frac{\|P\|_{\infty}}{\mu_{\text{max}} N},
\]

since \( \|P - \text{tr}(\Sigma)J\|_2/(\mu_{\text{max}} N) = O(\mu_{\text{max}}) \) with high probability. We have thus shown

\[
\|V_r\|_{\text{max}} \|\alpha \Lambda_r^{1/2} R - V_r \Lambda_r^{1/2}\|_{\text{max}} \lesssim \frac{\tau_\rho}{N^{1/2}} + \frac{\|P - \text{tr}(\Sigma)J\|_2}{N^{1/2}} + \frac{\|P - \text{tr}(\Sigma)J\|_2^{1/2}}{N^{1/2}} + \frac{\|P\|_{\infty}}{\mu_{\text{max}} N}.
\]

We use standard results from random matrix theory to control \( \|P - \text{tr}(\Sigma)J\|_2 \) and \( \|P\|_{\infty} \). By Lemma S.7.1,

\[
\frac{\|P - \text{tr}(\Sigma)J\|_2}{N} \lesssim \sigma_{\text{max}} \mu_{\text{max}} + \sigma_{\text{max}}^2 (\log N)^{1/2}\{\gamma^{1/2} \vee (\log N)^{1/2}\},
\]

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with probability at least $1 - O(N^{-1})$. By Lemma S.7.2,

$$\frac{\|P\|_\infty}{N} \leq \sigma_{\text{max}}\mu_{\text{max}}(\log N)^{1/2} + \sigma_{\text{max}}^2(\gamma \lor \beta),$$

with probability at least $1 - O(N^{-1})$. Applying these bounds and noting that $\tau_p/N^{1/2} \leq \sigma_{\text{max}}^2\gamma/\mu_{\text{max}}$, we obtain that with probability at least $1 - O(N^{-1})$

$$\|V_r\|_{\text{max}}\|\alpha \tilde{V}_r \tilde{\Lambda}_r^{1/2} R - V_r \Lambda_r^{1/2}\|_{\text{max}}$$

$$\leq (\sigma_{\text{max}}\mu_{\text{max}})^{1/2} + \sigma_{\text{max}}\{(\log N)^{1/2} \lor \gamma^{1/2}\} + \frac{\sigma_{\text{max}}^2(\gamma \lor \beta)}{\mu_{\text{max}}}.$$

### S.5 Proof of Theorem 3.3

Recall $s = \text{rank}(MM^T)$ and $r \leq s$ by Condition 2; because $M$ is centered, $1 \leq s \leq k - 1$. Let $V_r$ denote the $N \times r$ matrix whose columns are the top $r$ eigenvectors of $MM^T$, and $\Lambda_i$ ($i = 1, \ldots, s$) the $i \times i$ diagonal matrix of associated eigenvalues. Let $\tilde{V}_r, \tilde{\Lambda}_r$ denote the same quantities for the multidimensional scaling matrix $B$. Then the rows of $V_s \Lambda_s^{1/2}$ are the coordinates of the means $\{\mu_i^T\}_{i=1}^N$, obtained from a full rank multidimensional scaling embedding of $M$, and the rows of $\tilde{V}_r \tilde{\Lambda}_r^{1/2}$ are the coordinates of the points $\{x_i^T\}_{i=1}^N$ obtained from a rank $r$ multidimensional scaling embedding of $X$. We compare the classification obtained from $V_s \Lambda_s^{1/2}$, which is perfect, to that obtained from $\tilde{V}_r \tilde{\Lambda}_r^{1/2}$, which is noisy. Since the output of a clustering algorithm remains the same under a fixed scaling and rotation of the data, $V_s \Lambda_s^{1/2}$ can in fact be compared with $\alpha \tilde{V}_r \tilde{\Lambda}_r^{1/2} R$, where $\alpha$ is any constant and $R$ is any $r \times r$ rotation matrix. Note $(V_s \Lambda_s^{1/2})_i \in \mathbb{R}^s$ and $(\alpha V_r \Lambda_r^{1/2} R)_i \in \mathbb{R}^s$, but the coordinates $(\alpha V_r \Lambda_r^{1/2} R)_i$ are simply extended to coordinates in $\mathbb{R}^s$ by adding zeros in the remaining $s - r$ dimensions. Let $\{\phi_i^T\}_{i=1}^N$ denote the rows of $V_s \Lambda_s^{1/2}$ and $\{\tilde{\phi}_i^T\}_{i=1}^N$ denote the rows of $\alpha \tilde{V}_r \tilde{\Lambda}_r^{1/2} R$, augmented with zeros in $s - r$ dimensions.

Because $M$ has rank $s$ and zero mean, the pairwise distances are perfectly preserved by the multidimensional scaling embedding, and $\|\mu_i^T - \mu_j^T\|_2 = \|\phi_i^T - \phi_j^T\|_2$. Let

$$d_{\text{in}} = d_{\text{in}}(\alpha \tilde{V}_r \tilde{\Lambda}_r^{1/2} R, \ell) = \max_{i,j,\ell = i} \|\tilde{\phi}_i^T - \tilde{\phi}_j^T\|_2,$$

$$d_{\text{bow}} = d_{\text{bow}}(\alpha \tilde{V}_r \tilde{\Lambda}_r^{1/2} R, \ell) = \min_{i,j,\ell \neq j} \|\tilde{\phi}_i^T - \tilde{\phi}_j^T\|_2$$

be the maximal within and minimal between community distances respectively. Recall that to obtain a perfect geometric representation of the data, and thus exactly recover the true labels via a simple clustering algorithm, we must have $2d_{\text{in}} < d_{\text{bow}}$.

Since

$$\|\tilde{\phi}_i^T - \tilde{\phi}_j^T\|_2 \leq \|\phi_i^T - \phi_j^T\|_2 + \|\phi_i^T - \phi_j^T\|_2 + \|\phi_i^T - \phi_j^T\|_2,$$

$$= \|\phi_i^T - \phi_j^T\|_2 + \|\phi_i^T - \phi_j^T\|_2 + \|\mu_i^T - \mu_j^T\|_2,$$
we have
\[ d_{in} \leq 2 \max_i \|\tilde{\phi}_i^T - \phi_i^T\|_2. \]

By a similar argument, since
\begin{align*}
\|\phi_i^T - \phi_j^T\|_2 &\leq \|\tilde{\phi}_i^T - \phi_i^T\|_2 + \|\tilde{\phi}_j^T - \phi_j^T\|_2 + \|\tilde{\phi}_i^T - \tilde{\phi}_j^T\|_2, \\
\|\phi_i^T - \phi_j^T\|_2 &\geq \|\mu_i^T - \mu_j^T\|_2 - \|\hat{\phi}_i^T - \phi_i^T\|_2 - \|\hat{\phi}_j^T - \phi_j^T\|_2,
\end{align*}

we have
\[ d_{bow} \geq \mu_{diff} - 2 \max_i \|\tilde{\phi}_i^T - \phi_i^T\|_2. \]

Thus, \(2d_{in} < d_{bow}\) is guaranteed whenever
\[ \mu_{diff} > 6 \max_i \|\tilde{\phi}_i^T - \phi_i^T\|_2. \] (S.1)

With a slight abuse of notation we have:
\begin{align*}
\|\tilde{\phi}_i^T - \phi_i^T\|_2 &= \|(V_s \Lambda_s^{1/2})_i - \alpha (V_r \Lambda_r^{1/2})_i\|_2 \\
&\leq \|(V_s \Lambda_s^{1/2})_i - (V_r \Lambda_r^{1/2})_i\|_2 + \|(V_s \Lambda_s^{1/2})_i - \alpha (V_r \Lambda_r^{1/2})_i\|_2, \\
&\leq \|(V_s \Lambda_s^{1/2})_i - (V_r \Lambda_r^{1/2})_i\|_2 + \sqrt{r} \|V_s \Lambda_s^{1/2} - \alpha V_r \Lambda_r^{1/2} R\|_\text{max},
\end{align*}

where we assume \(r\)-dimensional rows have been augmented with zeros to become \(s\)-dimensional rows when needed. The first term represents the error incurred from discarding the small eigenvalues and eigenvectors of \(MM^T\), but this error is easily controlled when \(\lambda_{r+1}\) is small. Since \(MM^T\) is block constant, so are its eigenvectors on the blocks defined by the community labels, so that \(\|v_j\|_\infty \leq n^{-1/2}_\text{min} (j = 1, \ldots, s)\). Since the first \(r\) dimensions match exactly, we thus have for all \(i:\)
\[ \|(V_s \Lambda_s^{1/2})_i - (V_r \Lambda_r^{1/2})_i\|_2 \leq \|[0, \ldots, 0, \lambda_{r+1}^{1/2} v_{r+1}(i), \ldots, \lambda_s^{1/2} v_s(i)]\|_2 \leq \frac{\sqrt{r}}{n^{1/2}_\text{min}}. \]

Since \(\mu_{diff} > 12 (s - r)^{1/2} \lambda_{r+1}^{-1/2}\) by Condition 2, \(\mu_{diff} > 12 \max_i \|(V_s \Lambda_s^{1/2})_i - (V_r \Lambda_r^{1/2})_i\|_2\). Thus to guarantee (S.1), it is sufficient for:
\[ \mu_{diff} > 12 \sqrt{r} \|V_s \Lambda_s^{1/2} - \alpha V_r \Lambda_r^{1/2} R\|_\text{max}. \]

Applying Theorem 3.2 to bound \(\|V_s \Lambda_s^{1/2} - \alpha V_r \Lambda_r^{1/2} R\|_\text{max}\) with high probability, the multidimensional scaling and clustering procedure perfectly recovers the labels with probability \(1 - O(N^{-1})\) whenever
\[ \mu_{diff} \gtrsim (\sigma_{\text{max}} \mu_{\text{max}})^{1/2} + \sigma_{\text{max}} \{(\log N)^{1/2} \vee \gamma^{1/2}\} + \frac{\sigma_{\text{max}}^2}{\mu_{\text{max}}} (\gamma \vee \beta). \]

Writing this as three distinct inequalities (one for each term on the right hand side) and solving for \(\sigma_{\text{max}}^2\) yields
\[ \sigma_{\text{max}}^2 \lesssim \mu_{\text{diff}}^2 \left\{ \frac{\mu_{\text{diff}}^2}{\mu_{\text{max}}^2} \wedge \frac{1}{(\log N \vee \gamma)} \wedge \frac{\mu_{\text{max}}}{\mu_{\text{diff}}(\beta \vee \gamma)} \right\}. \]

Since \(\mu_{\text{max}}/\mu_{\text{diff}} \gtrsim O(1)\) and \(\mu_{\text{max}}/\mu_{\text{diff}} \leq (\beta \vee \gamma)^{1/3}\) by Condition 3, it is thus sufficient that \(\mu_{\text{diff}}^2 \gtrsim \sigma_{\text{max}}^2 (\beta \vee \gamma)\), which gives (3.1) in Theorem 3.3.
S.6 Proof of Theorem 3.4

We first establish Lemmas S.6.1 and S.6.2, alternate versions of Lemmas S.3.1 and S.3.2 which use Theorem S.1.2 instead of Theorem S.1.1 to bound \( \| \tilde{V}_r R - V_r \|_{\max} \).

**Lemma S.6.1.** Let the assumptions of Theorem 3.2 hold. Then with probability at least \( 1 - O(N^{-1}) \) there exists a rotation matrix \( R \) such that

\[
\alpha \tilde{\lambda}_1^{1/2} \| \tilde{V}_r R - V_r \|_{\max} \lesssim \sigma_{\max} N^{1/2} + \frac{\sigma_{\max}^2}{\mu_{\max}} (N \log N)^{1/2} \left\{ \gamma^{1/2} \lor (\log N)^{1/2} \right\}.
\]

**Proof.** Using the same notation and perturbation framework established in Appendix S.4, by Theorem S.1.2 there exists an orthogonal matrix \( R \) such that:

\[
\| \tilde{V}_r R - V_r \|_{\max} = \| \tilde{V}_r R - \tilde{V}_r \|_{\max}
\leq \| \tilde{V}_r R - \tilde{V}_r \|_F
\leq 2^{3/2} \tilde{\lambda}_{1/2} \| \tilde{A} - \tilde{A} \|_2
\leq \lambda_r - \lambda_{r+1}
\leq \lambda_r + \text{tr} (\Sigma) - \{ \lambda_{r+1} + \text{tr} (\Sigma) \}
\leq 2^{3/2} \tilde{\lambda}_{1/2} \| P - \text{tr} (\Sigma) J \|_2
\leq \frac{\lambda_r - \lambda_{r+1}}{\mu_{\max} N}
\leq \frac{\| P - \text{tr} (\Sigma) J \|_2}{\mu_{\max} N},
\]

where the next to last line follows since \( \lambda_r - \lambda_{r+1} \geq \lambda_r / 2 \). Thus by Lemma S.7.1, with probability at least \( 1 - O(N^{-1}) \),

\[
\| \tilde{V}_r R - V_r \|_{\max} \lesssim \frac{\sigma_{\max}}{\mu_{\max}} + \frac{\sigma_{\max}^2}{\mu_{\max}} (\log N)^{1/2} \left\{ \gamma^{1/2} \lor (\log N)^{1/2} \right\}.
\]

The remainder of the proof is identical to the proof of Lemma S.3.1, except we utilize the above bound for \( \| \tilde{V}_r R - V_r \|_{\max} \) to obtain that with probability \( 1 - O(N^{-1}) \):

\[
\alpha \tilde{\lambda}_1^{1/2} \| \tilde{V}_r R - V_r \|_{\max} \lesssim \mu_{\max} N^{1/2} \| \tilde{V}_r R - V_r \|_{\max}
\leq \sigma_{\max} N^{1/2} + \frac{\sigma_{\max}^2}{\mu_{\max}} (N \log N)^{1/2} \left\{ \gamma^{1/2} \lor (\log N)^{1/2} \right\}.
\]

\( \square \)

**Lemma S.6.2.** Let the assumptions of Theorem 3.2 hold. Then with probability at least \( 1 - O(N^{-1}) \) there exists a rotation matrix \( R \) such that

\[
\| V_r \|_{\max} \| \alpha \tilde{\lambda}_1^{1/2} R A_r^{1/2} \|_{\max} \lesssim \frac{\lambda_r^{1/2} (\rho - 1)}{\{ \lambda_l / \text{tr} (\Sigma) + 1 \} N^{1/2}} + (\sigma_{\max} \mu_{\max})^{1/2}
+ \sigma_{\max} \left\{ N^{1/2} \lor (\log N)^{1/4} \right\} + \frac{\sigma_{\max}^2}{\mu_{\max}} (N \log N)^{1/2} \left\{ \gamma^{1/2} \lor (\log N)^{1/2} \right\}.
\]
Proof. The proof is identical to that of Lemma S.3.2, except as in the proof of Lemma S.6.1 Theorem S.1.2 is applied to conclude there exists an orthogonal matrix $R$ such that $\|\hat{V}_r R - V_r\|_{\infty} \leq \mu_{\max}^{-2} N^{-1} \|P - \text{tr}(\Sigma)J\|_2$. One thus obtains the alternate bound:

$$N^{-1/2} (I)(II) \lesssim \mu_{\max} \left\{ \frac{\|P - \text{tr}(\Sigma)J\|_2^{1/2}}{\mu_{\max} N^{1/2}} + \frac{\|P - \text{tr}(\Sigma)J\|_2}{\mu_{\max} N^{1/2}} \right\},$$

so that

$$\|V_r\|_{\infty} \|\hat{V}_r \Lambda_r^{1/2} R - V_r \Lambda_r^{1/2}\|_{\infty} \lesssim \frac{\tau_{\rho}}{N^{1/2}} + \frac{\|P - \text{tr}(\Sigma)J\|_2^{1/2}}{N^{1/2}} + \frac{\|P - \text{tr}(\Sigma)J\|_2}{\mu_{\max} N^{1/2}},$$

where $\tau_{\rho} = \lambda_r^{1/2} (\rho - 1)/\{\lambda_1/\text{tr}(\Sigma) + 1\}$. Applying Lemma S.7.1 to bound $\|P - \text{tr}(\Sigma)J\|_2$ gives

$$\|V_r\|_{\infty} \|\hat{V}_r \Lambda_r^{1/2} R - V_r \Lambda_r^{1/2}\|_{\infty} \lesssim \frac{\tau_{\rho}}{N^{1/2}} + (\sigma_{\max} \mu_{\max})^{1/2} + \sigma_{\max}\{N^{1/2} \vee (\gamma \log N)^{1/4}\} + \frac{\sigma^2}{\mu_{\max}} (N \log N)^{1/2}\{\gamma^{1/2} \vee (\log N)^{1/2}\},$$

with probability $1 - O(N^{-1})$. □

We are ready to prove Theorem 3.4. An argument as in the proof of Theorem 3.2 gives:

$$\|\alpha \hat{V}_r \Lambda_r^{1/2} R - V_r \Lambda_r^{1/2}\|_{\infty} \lesssim \alpha \Lambda_r^{1/2} \|\hat{V}_r R - V_r\|_{\infty} + \|V_r\|_{\infty} \|\alpha \hat{V}_r \Lambda_r^{1/2} R - RA_r^{1/2}\|_{\infty}.$$ 

Choosing $\alpha = [\lambda_1/\{\lambda_1 + \text{tr}(\Sigma)\}]^{1/2}$, Lemmas S.6.1 and S.6.2 are applied to bound each of the above terms and conclude that there exists an orthogonal matrix $R$ such that

$$\|\alpha \hat{V}_r \Lambda_r^{1/2} R - V_r \Lambda_r^{1/2}\|_{\infty} \lesssim \frac{\lambda_r^{1/2} (\rho - 1)}{\{\lambda_1/\text{tr}(\Sigma) + 1\} N^{1/2}} + (\sigma_{\max} \mu_{\max})^{1/2}$$

$$\quad + \sigma_{\max}\{N^{1/2} \vee (\gamma \log N)^{1/4}\} + \frac{\sigma^2}{\mu_{\max}} (N \log N)^{1/2}\{\gamma^{1/2} \vee (\log N)^{1/2}\},$$

with probability at least $1 - O(N^{-1})$. An argument as in the proof of Theorem 3.3 guarantees the multidimensional scaling and clustering procedure perfectly recovers the labels whenever $\mu_{\text{diff}} \gtrsim \|\alpha \hat{V}_r \Lambda_r^{1/2} R - V_r \Lambda_r^{1/2}\|_{\infty}$. Thus with probability at least $1 - O(N^{-1})$, it is sufficient for

$$\mu_{\text{diff}} \gtrsim \frac{\lambda_r^{1/2} (\rho - 1)}{\{\lambda_1/\text{tr}(\Sigma) + 1\} N^{1/2}} + (\sigma_{\max} \mu_{\max})^{1/2} + \sigma_{\max}\{N^{1/2} \vee (\gamma \log N)^{1/4}\}$$

$$\quad + \frac{\sigma^2}{\mu_{\max}} (N \log N)^{1/2}\{\gamma^{1/2} \vee (\log N)^{1/2}\}. $$

Since $\rho - 1 \leq C \mu_{\text{diff}}/\mu_{\max}$ guarantees $\mu_{\text{diff}} \gtrsim \lambda_r^{1/2} (\rho - 1)/\{\lambda_1/\text{tr}(\Sigma) + 1\} N^{1/2}$ for appropriate choice of $C$, it is in fact sufficient for

$$\mu_{\text{diff}} \gtrsim (\sigma_{\max} \mu_{\max})^{1/2} + \sigma_{\max}\{N^{1/2} \vee (\gamma \log N)^{1/4}\} + \frac{\sigma^2}{\mu_{\max}} (N \log N)^{1/2}\{\gamma^{1/2} \vee (\log N)^{1/2}\}. $$
Since $\mu_{\text{max}}/\mu_{\text{diff}} \leq N^{1/2}$ by Condition 3, a straightforward calculation shows the above condition is implied by:

$$
\sigma_{\text{max}}^2 \lesssim \mu_{\text{diff}}^2 \left\{ \frac{1}{N} \land \frac{\mu_{\text{max}}}{\mu_{\text{diff}}(d \log N)^{1/2}} \right\}.
$$

Since $\mu_{\text{max}}/\mu_{\text{diff}} \gtrsim O(1)$, it is thus sufficient that $\mu_{\text{diff}}^2 \gtrsim \sigma_{\text{max}}^2 \left\{ N \lor (d \log N)^{1/2} \right\}$, and we obtain (3.2) in Theorem 3.4.

### S.7 Proof of Random Matrix Lemmas

This section states and proves Lemmas S.7.1 and S.7.2, two random matrix lemmas which are needed in the proofs of Theorem 3.1 and Lemmas S.3.1-S.3.2 and S.6.1–S.6.2.

**Lemma S.7.1.** Let $M$ be a deterministic $N$ by $d$ matrix with zero row mean, and $\mu_{\text{max}} = \max_{1 \leq i \leq N} \|M_i\|_2$ its maximal row norm. Let $H$ be a random $N$ by $d$ matrix, with independent rows each having distribution $N(0, \Sigma)$, and let $\sigma_{\text{max}}^2$ denote the largest eigenvalue of $\Sigma$. Then

$$
P = \{ J(M + H) \} \{ J(M + H) \}^T - MM^T,
$$

where $J = I_N - (1/N)11^T$, satisfies

$$
\frac{1}{N} \| P - \text{tr}(\Sigma)J \|_2 \lesssim \sigma_{\text{max}}\mu_{\text{max}} + \sigma_{\text{max}}^2 \left( \log N \right)^{1/2} \left\{ \gamma^{1/2} \lor \left( \log N \right)^{1/2} \right\},
$$

with probability at least $1 - O(N^{-1})$, where $\gamma = d/N$.

**Lemma S.7.2.** Let $M$ be a deterministic $N$ by $d$ matrix with $O(1)$ distinct rows and zero row mean, and $\mu_{\text{max}} = \max_{1 \leq i \leq N} \|M_i\|_2$ its maximal row norm. Let $H$ be a random $N$ by $d$ matrix, with independent rows each having distribution $N(0, \Sigma)$, and let $\sigma_{\text{max}}^2$ denote the largest eigenvalue of $\Sigma$. Then

$$
P = \{ J(M + H) \} \{ J(M + H) \}^T - MM^T,
$$

where $J = I_N - (1/N)11^T$, satisfies

$$
\frac{1}{N} \| P \|_\infty \lesssim \sigma_{\text{max}}\mu_{\text{max}} \left( \log N \right)^{1/2} + \gamma \sigma_{\text{max}}^2 + \sigma_{\text{max}}^2 \left[ (d \lor \log N) \land \left\{ \left( d \log N \right)^{1/2} \lor N^{1/2} \log N \right\} \right],
$$

with probability at least $1 - O(N^{-1})$, where $\gamma = d/N$.

Throughout this section we utilize $JM = M$ and $M^TJ = M^T$ (since the rows of $M$ are centered), so that the matrix $P$ defined in Lemmas S.7.1 and S.7.2 has form:

$$
P = JMH^T J + JHM^T J + JHH^T J = M^T J + JHM^T + JHH^T J.
$$
Since Lemmas S.7.1 and S.7.2 assume the rows of $H$ are $N(0, \Sigma)$, we further decompose $H = G\Sigma^{1/2}$ throughout this section for an $N$ by $d$ matrix $G$ with independent $N(0, 1)$ entries, and let $\nu_1^T, \ldots, \nu_N^T$ denote the rows of $G$.

We also let $u_1, \ldots, u_d \in \mathbb{R}^d$ denote the eigenvectors of the covariance matrix $\Sigma$ and decompose $\Sigma$ as:

$$\Sigma = \sum_{s=1}^d \sigma_s^2 u_s u_s^T.$$

### S.7.1 Proof of Lemma S.7.1

Since $J^2 = J$ and $\|J\|_2 = 1$, we have

$$P - \text{tr}(\Sigma)J = MH^T J + JHM^T + J(HH^T - \text{tr}(\Sigma)I_N)J$$

$$\|P - \text{tr}(\Sigma)J\|_2 \leq \|MH^T\|_2 \|J\|_2 + \|J\|_2 \|HM^T\|_2 + \|J\|_2 \|HH^T - \text{tr}(\Sigma)I_N\|_2 \|J\|_2$$

$$= (I) + (II).$$

We now bound each term.

**Bounding (I)**

We decompose

$$MH^T = M\Sigma^{1/2}G^T = \|M\Sigma^{1/2}\|_2 \frac{M\Sigma^{1/2}G^T}{\|M\Sigma^{1/2}\|_2} \leq \mu_{\max} N^{1/2} \sigma_{\max} \frac{M\Sigma^{1/2}G^T}{\|M\Sigma^{1/2}\|_2}.$$

Observing that $\left(M\Sigma^{1/2}/\|M\Sigma^{1/2}\|_2\right)G^T$ is the product of a deterministic unit norm matrix and a random matrix, we use Lemma 4.5 from Vershynin (2011) to conclude that with probability $1 - O(N^{-1})$

$$\frac{M\Sigma^{1/2}G^T}{\|M\Sigma^{1/2}\|_2} \leq \{N + \log(2N)\}^{1/2} + C(\log N)^{1/2},$$

and thus

$$\|MH^T\|_2 \leq \sigma_{\max} \mu_{\max} N^{1/2} \left[\{N + \log(2N)\}^{1/2} + C(\log N)^{1/2}\right]$$

$$\lesssim \sigma_{\max} \mu_{\max} N$$

with probability $1 - O(N^{-1})$.

**Bounding (II)**

We have

$$HH^T = G\Sigma G^T = \sum_{s=1}^d \sigma_s^2 G u_s u_s^T G^T = \sum_{s=1}^d \sigma_s^2 g_s g_s^T,$$
where we let $g_s = Gu_s$. The $g_s$ are random vectors in $\mathbb{R}^N$. We will show that $g_s$ and $g_\ell$ are independent for $s \neq \ell$ so that $HH^T$ can be written as a sum of $d$ independent rank 1 matrices, which will allow for the application of a matrix Bernstein inequality. We also verify that for each $s$, the vector $g_s$ has independent $N(0, 1)$ entries.

To show $g_s$ and $g_\ell$ are independent, it is sufficient to verify that for $s \neq \ell$, $\langle g, u_s \rangle$ and $\langle g, u_\ell \rangle$ are independent for a random vector $g \in \mathbb{R}^d$ with independent $N(0, 1)$ entries. We have

$$\text{cov}(\langle g, u_s \rangle, \langle g, u_\ell \rangle) = \sum_{i=1}^{d} E\{ (g(i))^2 \} u_s(i)u_\ell(i) = \langle u_s, u_\ell \rangle = 0,$$

since $u_s, u_\ell$ are orthogonal eigenvectors of $\Sigma$. Since $\langle g, u_s \rangle$ and $\langle g, u_\ell \rangle$ are Gaussian random variables with zero covariance, we can conclude they are independent.

We observe that clearly $g_s$ has independent entries, since $g_s = Gu_s$ and the rows of $G$ are independent. Also each entry is $N(0, 1)$ since for any random vector $g \in \mathbb{R}^d$ with independent $N(0, 1)$ entries, $\langle g, u_s \rangle$ is also Gaussian with mean zero and unit variance since $\|u_s\|_2 = 1$.

Thus, clearly we have:

$$E(g_sg_s^T) = I_N, \quad E(HH^T) = I_N \sum_{s=1}^{d} \sigma_s^2.$$

We can thus decompose

$$HH^T - \text{tr}(\Sigma)I_N = HH^T - E(HH^T) = \sum_{s=1}^{d} \sigma_s^2(g_sg_s^T - I_N),$$

and apply the following matrix Bernstein inequality (Theorem 5.29 from Vershynin (2012)):

**Theorem S.7.3.** Consider a finite sequence $X_s$ of independent centered self-adjoint random $N \times N$ matrices. Assume we have for some numbers $K$ and $B$ that $\|X_s\|_2 \leq K$ almost surely, and that $\|\sum_s E(X_s^2)\|_2 \leq B^2$. Then, for every $t \geq 0$ we have

$$\text{pr}\left(\|\sum_s X_s\|_2 > t\right) \leq 2N \exp\left(-c \min\left(\frac{t^2}{B^2}, \frac{t}{K}\right)\right).$$

To apply the theorem we must compute $B$ and $K$ for $X_s = \sigma_s^2(g_sg_s^T - I_N)$. Since $g_s^T$ is a 1 by $N$ isotropic Gaussian random vector in $\mathbb{R}^N$, we have by Theorem 5.39 in Vershynin (2012) that with probability at least $1 - 2e^{-t^2/2}$:

$$1 - CN^{1/2} - t \leq s_{\min}(g_s^T) \leq s_{\max}(g_s^T) \leq 1 + CN^{1/2} + t$$

for an absolute constant $C$. Letting $\delta = CN^{1/2} + t$, by Lemma 5.36 from Vershynin (2012), the above implies that

$$\|g_sg_s^T - I_N\|_2 \leq (\delta \vee \delta^2)$$

$$\|\sigma_s^2(g_sg_s^T - I_N)\|_2 \leq \sigma_s^2(\delta \vee \delta^2),$$

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and by taking a union bound over $1 \leq s \leq d$, we have that $\max_s \|\sigma^2_s(g_s g_s^T - I_N)\|_2 \leq \sigma^2_{\text{max}}(\delta \lor \delta^2)$ with probability at least $1 - 2de^{-t^2/2}$. Choosing $t \sim (\log N + \log d)^{1/2}$, we have $\delta^2 > \delta$ and we obtain that with probability at least $1 - O(N^{-1})$:

$$\max_s \|\sigma^2_s(g_s g_s^T - I_N)\|_2 \leq C\sigma^2_{\text{max}}(N + \log d),$$

and we can thus choose $K = C\sigma^2_{\text{max}}(N + \log d)$ in the Bernstein inequality. To compute $B$, we have

$$(g_s g_s^T - I_N)^2 = \|g_s\|^2 g_s g_s^T - 2g_s g_s^T + I_N.$$  

Because $g_s$ has independent and identically distributed $N(0, 1)$ entries, the off diagonal entries of $g_s g_s^T$ are mean zero. To compute the expectation on the diagonal, note that

$$\left(\|g_s\|^2 g_s g_s^T\right)_{jj} = g_s(j)^2 \sum_{i=1}^N g_s(i)^2 = g_s(j)^4 + \sum_{i \neq j} g_s(i)^2 g_s(j)^2$$

$$E\left(\|g_s\|^2 g_s g_s^T\right)_{jj} = 3 + (N - 1) = N + 2.$$  

Thus, we have

$$E\{\sigma^4_s(g_s g_s^T - I_N)^2\} = \sigma^4_s \{(N + 2)I_N - 2I_N + I_N\} = \sigma^4_s(N + 1)I_N,$$

so that

$$\left\|\sum_s E(X_s^2)\right\|_2 = \left\|\sum_{s=1}^d \sigma^4_s(N + 1)I_N\right\|_2 = (N + 1)\sum_{s=1}^d \sigma^4_s \leq (N + 1)d\sigma^4_{\text{max}},$$

and we can thus choose $B^2 = CNd\sigma^4_{\text{max}}$. Thus by the matrix Bernstein inequality,

$$\text{pr}\left(\left\|\sum_{s=1}^d \sigma^2_s(g_s g_s^T - I_N)\right\|_2 > t\right) \leq 2N\exp\left\{-c\min\left(\frac{t^2}{B^2}, \frac{t}{K}\right)\right\}. $$

Choosing $t = C\{B(\log N)^{1/2} \lor K \log N\}$, we obtain that with probability at least $1 - O(N^{-1})$

$$\left\|\sum_{s=1}^d \sigma^2_s(g_s g_s^T - I_N)\right\|_2 \leq C\{B(\log N)^{1/2} \lor K \log N\}$$

$$\|HH^T - E(HH^T)\|_2 \leq C\sigma^2_{\text{max}}\{(dN \log N)^{1/2} \lor (N + \log d) \log N\}$$

$$\leq C\sigma^2_{\text{max}}(N \log N)^{1/2}\{d^{1/2} \lor (N \log N)^{1/2}\}.$$  

In sum, we have

$$\textbf{I} \lesssim \sigma_{\text{max}}\mu_{\text{max}} N$$

$$\textbf{II} \lesssim \sigma^2_{\text{max}}(N \log N)^{1/2}\{d^{1/2} \lor (N \log N)^{1/2}\}. $$

We can thus bound the spectral norm of $\{P - \text{tr}(\Sigma) J\}/N$ by

$$\frac{\|P - \text{tr}(\Sigma) J\|_2}{N} \lesssim \sigma_{\text{max}}\mu_{\text{max}} + \sigma^2_{\text{max}}(\log N)^{1/2}\{\gamma^{1/2} \lor (\log N)^{1/2}\}.$$  

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S.7.2 Proof of Lemma S.7.2

Since \( J^2 = J \), we decompose \( P \) as follows:

\[
P = J(MH^T + HM^T)J + J(HH^T - \text{tr}(\Sigma)I_N)J + \text{tr}(\Sigma)J
\]

\[
\|P\|_\infty \leq \|J(MH^T + HM^T)J\|_\infty + \|J(HH^T - \text{tr}(\Sigma)I_N)J\|_\infty + \|\text{tr}(\Sigma)J\|_\infty
\]

:= (I) + (II) + (III),

and proceed to bound each term. Recall that for any matrix product \( AB \), \( \|AB\|_{\text{max}} \leq \|A\|_\infty \|B\|_{\text{max}} \) and also \( \|AB\|_{\text{max}} \leq \|A\|_{\text{max}} \|B\|_1 \). Since \( \|J\|_\infty = \|J\|_1 = 2(N - 1)/N \leq 2 \), we can conclude that for any matrix \( A \), \( \|JAJ\|_{\text{max}} \leq 4\|A\|_{\text{max}} \), a property we will apply throughout the proof. For a random variable \( X \), \( \|X\|_{\psi_2}, \|X\|_{\psi_1} \) denote the subgaussian, subexponential norm of \( X \).

**Bounding (I)**

We have

\[
\|J(MH^T + HM^T)J\|_\infty \leq N\|J(MH^T + HM^T)J\|_{\text{max}}
\]

\[
\leq 4N\|HM^T + MH^T\|_{\text{max}}.
\]

As in the proof of Lemma S.7.1, we may write \( H = G\Sigma^{1/2} \) for \( G \) having independent standard Gaussian entries. Assuming \( M \) has \( k \) distinct rows, and letting \( \nu_i^T = G_i \) and \( \mu_i^T = M_i \) for \( \ell_i \in [k] \), we have

\[
(HM^T + MH^T)_{i,j} = (G\Sigma^{1/2}M^T + M\Sigma^{1/2}G^T)_{i,j}
\]

\[
= \langle \nu_i^T, \Sigma^{1/2}\mu_{\ell_j} \rangle + \langle \Sigma^{1/2}\mu_{\ell_i}, \nu_j^T \rangle,
\]

so that

\[
\|HM^T + MH^T\|_{\text{max}} \leq 2 \max_{i,j} |\langle \Sigma^{1/2}\mu_{\ell_j}, \nu_i^T \rangle|
\]

For a fixed \( \ell_j \), consider the random variable \( w_i = |\langle \Sigma^{1/2}\mu_{\ell_j}, \Sigma^{1/2}\mu_{\ell_i} \rangle| \). By definition of subgaussian norm of random vector (see 5.22 in Vershynin (2012)) and by Lemma 5.24 of Vershynin (2012):

\[
\|w_i\|_{\psi_2} = \| \left\langle \frac{\Sigma^{1/2}\mu_{\ell_j}}{\|\Sigma^{1/2}\mu_{\ell_j}\|_2}, \nu_i^T \right\rangle \|_{\psi_2}
\]

\[
\leq \sup_{x \in S^{d-1}} \|\langle x, \nu_i^T \rangle\|_{\psi_2}
\]

\[
= \|\nu_i^T\|_{\psi_2}
\]

\[
\leq C \left( \max_s \|\nu_i(s)\|_{\psi_2} \right)
\]

\[
= C,
\]
since \( \nu_i \) is standard Gaussian. Because every subgaussian random variable satisfies \( \Pr(|X| \geq t) \leq e^{1-ct^2/\|X\|_\psi^2} \), we obtain

\[
\Pr(w_i \geq t) \leq e^{1-ct^2} \\
\Pr \left( \max_i w_i < t \right) \geq 1 - Ne^{1-ct^2} \geq 1 - e^{1-ct^2},
\]

for any \( ct^2 \geq 2 \log N \). Choosing \( t^2 = (2/c) \log N \) we obtain

\[
\Pr \left\{ \| \Sigma^{1/2} \mu_{\ell_j} \|_2 (\max_i w_i) < C \| \Sigma^{1/2} \mu_{\ell_j} \|_2 (\log N)^{1/2} \right\} \geq 1 - O(N^{-1}).
\]

Observing that \( \| \Sigma^{1/2} \mu_{\ell_j} \|_2 \leq \mu_{\max} \sigma_{\max} \) and taking a union bound over \( j = 1, \ldots, k \), we can conclude that

\[
\| HM^T + MH^T \|_{\max} \leq C \mu_{\max} \sigma_{\max} (\log N)^{1/2}
\]

with probability \( 1 - O(N^{-1}) \).

**Bounding (II)**

Since

\[
(II) = \| J \{ HH^T - \text{tr}(\Sigma) I_N \} J \|_{\infty} = \| J \{ HH^T - E(HH^T) \} J \|_{\infty}
\]

we have

\[
(II) \leq \min \{ 4N \| HH^T - E(HH^T) \|_{\max}, N^{1/2} \| HH^T - E(HH^T) \|_2 \}.
\]

Recall from the bound for \( \| HH^T - E(HH^T) \|_2 \) in the proof of Lemma S.7.1 that we can decompose

\[
HH^T - E(HH^T) = \sum_{s=1}^d \sigma_s^2 (g_s g_s^T - I_N),
\]

where the \( g_s \) are independent, standard, Gaussian random vectors, i.e., \( g_s \sim N(0, I_N) \).

Consider the entries of \( HH^T - E(HH^T) \).

\[
\{ HH^T - E(HH^T) \}_{i,j} = \begin{cases} 
\sum_{s=1}^d \sigma_s^2 g_s(i) g_s(j) & i \neq j \\
\sum_{s=1}^d \sigma_s^2 \{ g_s(i)^2 - 1 \} & i = j
\end{cases}.
\]

Since \( g_s(i), g_s(j) \) are subgaussian, the product is subexponential. When \( i = j \), by Lemma 5.14 in Vershynin (2012),

\[
\| \sigma_s^2 g_s(i)^2 \|_{\psi_1} \leq 2 \| \sigma_s g_s(i) \|_{\psi_2}^2 = C \sigma_s^2,
\]

and since \( \| X - E(X) \|_{\psi_1} \leq 2 \| X \|_{\psi_1} \) (see Vershynin (2012)), we also have \( \| \sigma_s^2 \{ g_s(i)^2 - 1 \} \|_{\psi_1} \leq C \sigma_s^2 \).

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When \( i \neq j \), observe that by independence and the subgaussian condition:

\[
\Pr \left\{ |\sigma_s^2 g_s(i) g_s(j)| < t \right\} \geq \Pr \left[ \left\{ |\sigma_s g_s(i)| < t^{1/2} \right\} \cap \left\{ |\sigma_s g_s(j)| < t^{1/2} \right\} \right] \\
\geq (1 - e^{-ct/\sigma_s^2})^2 \\
\geq 1 - e^{-ct/\sigma_s^2}.
\]

Thus, \( \|\sigma_s^2 g_s(i) g_s(j)\|_{\psi_1} = C\sigma_s^2 \) by the subexponential condition, and we have in fact \( \|\sigma_s^2 g_s(i) g_s(j) - (1 - \epsilon)\sigma_s^2\|_{\psi_1} \leq C\sigma_s^2 \) for all \( i, j \). Next we apply the following Corollary 5.17 from Vershynin (2012):

**Corollary S.7.4.** Let \( X_1, \ldots, X_N \) be independent centered subexponential random variables, and let \( K = \max_i \|X_i\|_{\psi_1} \). Then, for every \( \epsilon \geq 0 \), we have

\[
\Pr \left( \left| \sum_{i=1}^N X_i \right| \geq \epsilon N \right) \leq \exp \left\{ -c \left( \frac{\epsilon^2}{K^2} \wedge \frac{\epsilon}{K} \right) N \right\}
\]

where \( c > 0 \) is an absolute constant.

When \( i \neq j \) this becomes:

\[
\Pr \left\{ |\langle \sigma_s^2 g_s(i) g_s(j) \rangle| \geq \epsilon d \right\} \leq 2\exp \left\{ -c \left( \frac{\epsilon^2}{\sigma_{\max}^2} \wedge \frac{\epsilon}{\sigma_{\max}} \right) d \right\} = 2\exp \left( -\frac{c\epsilon d}{\sigma_{\max}^2} \right)
\]

and for \( i = j \) this becomes

\[
\Pr \left\{ |\sigma_s^2 \{g_s(i)^2 - 1\}| \geq \epsilon d \right\} \leq 2\exp \left( -\frac{c\epsilon d}{\sigma_{\max}^2} \right)
\]

for any \( \epsilon \geq \sigma_{\max}^2 \). Taking a union bound over all \( i, j \) thus gives

\[
\Pr \left\{ \max_{i,j} |HH^T - E(HH^T)| < \epsilon d \right\} \geq 1 - 2N^2\exp \left( -\frac{c\epsilon d}{\sigma_{\max}^2} \right) \geq 1 - 2\exp(-\log N)
\]

as long as \( \epsilon \geq \max \{ (\log N/\epsilon d) \vee 1 \} \). We thus obtain:

\[
\Pr \left\{ \max_{i,j} |HH^T - E(HH^T)| < C\sigma_{\max}^2 (\log N \vee d) \right\} \geq 1 - O(N^{-1})
\]

giving:

\[
N \|HH^T - E(HH^T)\|_{\max} \leq C\sigma_{\max}^2 N (d \vee \log N).
\]

Note however when \( d \) is large a better bound is obtained by spectral norm concentration. As shown in the proof of Lemma S.7.1, we have:

\[
N^{1/2} \|HH^T - E(HH^T)\|_2 \lesssim \sigma_{\max}^2 N (\log N)^{1/2} \{ d^{1/2} \vee (N \log N)^{1/2} \}
\]

with probability \( 1 - O(N^{-1}) \).

Combining the two bounds:

\[
\|J\{HH^T - E(HH^T)\}J\|_{\infty} \lesssim \sigma_{\max}^2 N \left[ (d \vee \log N) \wedge \{(d \log N)^{1/2} \vee N^{1/2} \log N \} \right]
\]

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with probability at least $1 - O(N^{-1})$.

To summarize, we have with probability at least $1 - O(N^{-1})$:

\[
(\text{I}) \leq C\sigma_{\max} \mu_{\max} N (\log N)^{1/2}
\]

\[
(\text{II}) \leq C\sigma_{\max}^2 N \left( (d \lor \log N) \land \{ (d \log N)^{1/2} \lor N^{1/2} \log N \} \right)
\]

\[
(\text{III}) = \| \text{tr}(\Sigma) J \|_{\infty} = \text{tr}(\Sigma) \| J \|_{\infty} \leq 2 \text{tr}(\Sigma) = 2 \sum_{s=1}^{d} \sigma_s^2 \leq 2\sigma_{\max}^2.
\]

Dividing the above bounds by $N$, we thus obtain

\[
\frac{\| P \|_{\infty}}{N} \lesssim \sigma_{\max} \mu_{\max} (\log N)^{1/2}
\]

\[
+ \sigma_{\max}^2 \left( (d \lor \log N) \land \{ (d \log N)^{1/2} \lor N^{1/2} \log N \} \right) + \gamma \sigma_{\max}^2,
\]

and the Lemma is proved.

### S.8 Clustering Results

#### S.8.1 $k$-means

Given $k$ initial centroids $c_1, \ldots, c_k$, the standard $k$-means algorithm known as Loyd’s algorithm partitions a data set by iteratively assigning each data point to its closest centroid and then recomputing the centroids until convergence. The goal is to recover a partition $S = \{S_1, \ldots, S_k\}$ which minimizes the $k$-means objective

\[
G(S) = \sum_{m=1}^{k} \frac{1}{2|S_m|} \sum_{x_i, x_j \in S_m} \| x_i - x_j \|_2^2.
\] (S.1)

The following lemma guarantees that any perfect geometric representation $S$ as defined in Section 2 is a local minimum of the $k$-means objective, so that Loyd’s algorithm will converge to $S$ when appropriately initialized. Indeed, if Loyd’s algorithm is run with furthest point initialization, the initial centroids will consist of one point from each set $S_i$, and Loyd’s algorithm will perfectly recover the partition $S$. The furthest point initialization procedure randomly selects a data point as the first centroid $c_1$ and then for $i = 2, \ldots, k$ iteratively defines centroid $c_{i+1}$ by selecting the data point $x \in X \setminus \{c_1, \ldots, c_i\}$ which maximizes $\min_{1 \leq j \leq i} \| x - c_j \|_2$.

**Lemma S.8.1.** Let $S = \{S_1, \ldots, S_k\}$ be a partition of the data into clusters with $S_m = \{x_i : \ell_i = m\}$, and let

\[
d_{\text{in}}(X, \ell) = \max_{m \in [k]} \max_{x_i, x_j \in S_m} \| x_i - x_j \|_2, \quad d_{\text{btw}}(X, \ell) = \min_{m \neq l} \min_{x_i \in S_m, x_j \in S_l} \| x_i - x_j \|_2
\]

be the maximal within cluster and minimal between cluster distances respectively. Then if $d_{\text{btw}} > (3/2)^{1/2} d_{\text{in}}$, the partition $S$ is a local minimum of the $k$-means objective.
Proof. We use contradiction to prove this lemma. Suppose not. Then there is a point reassignment that increases the $k$-means objective $G(S)$ defined in (S.1). Specifically, there exists a point $x \in S_m$ such that moving it to another cluster $S_l$ decreases $G(S)$. Let $\hat{S} = \{\hat{S}_1, \ldots, \hat{S}_k\}$ denote the same clustering as $S$ except point $x$ is moved from $S_m$ to $S_l$, i.e., $\hat{S}_m = S_m \setminus x$ and $\hat{S}_l = S_l \cup x$. We have $G(\hat{S}) < G(S)$ and

$$G(S) - G(\hat{S}) = \sum_{g=1}^{k} \frac{1}{2|S_g|} \sum_{x_i, x_j \in S_g} \|x_i - x_j\|_2^2 - \sum_{g=1}^{k} \frac{1}{2|\hat{S}_g|} \sum_{x_i', x_j' \in \hat{S}_g} \|x_i' - x_j'\|_2^2$$

$$= \left( \frac{1}{2|S_m|} \sum_{x_i, x_j \in S_m} \|x_i - x_j\|_2^2 - \frac{1}{2|S_m|} \sum_{x_i, x_j \in S_m} \|x_i' - x_j'\|_2^2 \right) + \left( \frac{1}{2|S_l|} \sum_{x_i, x_j \in S_l} \|x_i - x_j\|_2^2 - \frac{1}{2|S_l|} \sum_{x_i, x_j \in S_l} \|x_i' - x_j'\|_2^2 \right)$$

$$:= (A) + (B),$$

where

$$(A) = \frac{1}{2|S_m|} \sum_{x_i, x_j \in S_m} \|x_i - x_j\|_2^2 - \frac{1}{2|S_m|} \sum_{x_i, x_j \in S_l} \|x_i - x_j\|_2^2 \left( \frac{|S_m|}{|S_m| - 1} \right) - \frac{1}{2|S_m|} \sum_{x_i, x_j \in S_m \setminus x} \|x_i - x_j\|_2^2$$

$$(B) = \frac{1}{2|S_l|} \sum_{x_i, x_j \in S_l} \|x_i - x_j\|_2^2 - \frac{1}{2|S_l|} \sum_{x_i, x_j \in S_l} \|x_i - x_j\|_2^2 \left( \frac{|S_l|}{|S_l| + 1} \right) - \frac{1}{2|S_l|} \sum_{x_i, x_j \in S_l} \|x_i - x_j\|_2^2.$$
Thus, we have

\[ G(S) - G(\hat{S}) = \frac{1}{2|S_m|} \sum_{x_i, x_j \in \{S_m \setminus x\}} ||x_i - x_j||^2_2 \left( 1 - \frac{|S_m|}{|S_m| + 1} \right) + \frac{1}{|S_m|} \sum_{x_i \in S_m \setminus x} ||x_i - x||^2_2 \]

\[ + \frac{1}{2|S_i|} \sum_{x_i, x_j \in S_i} ||x_i - x_j||^2_2 \left( 1 - \frac{|S_i|}{|S_i| + 1} \right) - \frac{1}{|S_i|} \sum_{x_i \in S_i} ||x_i - x||^2_2 \]

\[ \leq \frac{1}{|S_m|} \sum_{x_i \in \{S_m \setminus x\}} d^2_{in} + \frac{1}{2|S_i|} \sum_{x_i, x_j \in S_i} d^2_{in} \left( \frac{1}{|S_i| + 1} \right) - \frac{1}{|S_i|} \sum_{x_i \in S_i} d^2_{bw} \]

\[ = \frac{|S_m| - 1}{|S_m|} d^2_{in} + \frac{|S_i|(|S_i| - 1)}{2|S_i|(|S_i| + 1)} d^2_{in} - \frac{|S_i| d^2_{bw}}{|S_i|} \]

\[ = \frac{|S_m| - 1}{|S_m|} d^2_{in} + \frac{|S_i| - 1}{2(|S_i| + 1)} d^2_{in} - d^2_{bw} \]

\[ \leq d^2_{in} + \frac{1}{2} d^2_{in} - d^2_{bw} \]

\[ = \frac{3}{2} d^2_{in} - d^2_{bw}. \]

Since moving the point \( x \) decreases the \( k \)-means objective, we have:

\[ 0 < G(S) - G(\hat{S}) \leq \frac{3}{2} d^2_{in} - d^2_{bw}, \]

which gives \( d_{bw} \leq (3/2)^{1/2} d_{in} \), which contradicts the assumptions of Lemma S.8.1. Thus the partition \( S \) corresponds to a local minimum of the \( k \)-means objective. \( \square \)

### S.8.2 Single Linkage

Single linkage clustering is an agglomerative procedure in which each data point is initially a singleton cluster and clusters are iteratively merged by choosing clusters \( C_m, C_l \) which minimize the linkage function

\[ d(C_m, C_l) = \min_{x_i \in C_m, x_j \in C_l} ||x_i - x_j||_2. \]

Iterating this procedure until all points are joined in a single cluster creates the hierarchical structure known as the single linkage dendrogram. If a level \( \epsilon \) is specified, and clusters are merged only as long as \( d(C_m, C_l) \leq \epsilon \), a fixed partition of the data \( X \) is obtained, which we denote by \( SL(X, \epsilon) \). In fact \( SL(X, \epsilon) \) consists of the connected components of a graph defined on the data by creating an edge between \( x_i \) and \( x_j \) if \( ||x_i - x_j|| \leq \epsilon \) (see Section 3 of Gower & Ross (1969)). The following lemma is a direct consequence of the single linkage clustering procedure and the definition of a perfect geometric representation \( S \); it ensures that \( S \) can be recovered from single linkage clustering by selecting the hierarchical clustering which corresponds to \( k \) clusters.

**Lemma S.8.2.** Let \( S = \{S_1, \ldots, S_k\} \) be a partition of the data into clusters with \( S_m = \{x_i : \ell_i = m\} \), and let

\[ d_{in}(X, \ell) = \max_{m \in \ell} \max_{x_i, x_j \in S_m} ||x_i - x_j||_2, \quad d_{bw}(X, \ell) = \min_{m \neq l} \min_{x_i \in S_m, x_j \in S_l} ||x_i - x_j||_2 \]

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be the maximal within cluster and minimal between cluster distances respectively. Then $S = \text{SL}(X, \epsilon)$ for all $d_{in} \leq \epsilon < d_{bew}$.

**Proof.** Let $\epsilon$ satisfy $d_{in} \leq \epsilon < d_{bew}$ and construct a graph on $X$ by creating an edge between $x_i$ and $x_j$ if $\|x_i - x_j\|_2 \leq \epsilon$. Then for $m = 1, \ldots, k$, every pair of points $x_i, x_j \in S_m$ is connected, and every pair of points $x_i \in S_m, x_j \in S_l$ where $l \neq m$ is not connected. Thus $S = \text{SL}(X, \epsilon)$.

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