A Central Limit Theorem for Classical Multidimensional Scaling

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Abstract

Classical multidimensional scaling (CMDS) is a widely used method in manifold learning. It takes in a dissimilarity matrix and outputs a coordinate matrix based on a spectral decomposition. However, there are not yet any statistical results characterizing the performance of CMDS under randomness, such as perturbation analysis when the objects are sampled from a probabilistic model. In this paper, we present such an analysis given that the objects are sampled from a suitable distribution. In particular, we show that the resulting embedding gives rise to a central limit theorem for noisy dissimilarity measurements, and provide compelling simulation and real data illustration of this CLT for CMDS.

Keywords: classical multidimensional scaling, central limit theorem, error model, dissimilarity matrix.

1 Background and Overview

Inference based on dissimilarities is of fundamental importance in statistics, data mining and machine learning [1], with applications ranging from neuroscience to psychology to economics [2]. In each of these fields, rather than directly observing the feature values of the objects, often we observe only the dissimilarities or “distances” between pairs of objects (inter-point distances). A common approach to manifold learning and subsequent inference problems involving dissimilarities is to embed the observed distances into some (usually Euclidean) space to recover a configuration

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that faithfully preserves observed distances, and then proceed to perform inference based on the resulting configuration. The popular Classical Multidimensional Scaling (CMDS) manifold learning method provides an example of such an embedding scheme into Euclidean space, in which we have readily available tools to perform statistical inference \cite{3}. However, several recent papers have pointed out that there is still little known about the behavior of CMDS under noise: Fan et al. \cite{4} write “[W]e are not aware of any statistical results measuring the performance of MDS under randomness, such as perturbation analysis when the objects are sampled from a probabilistic model.”; Peterfreund and Gavish \cite{5} write “To the best of our knowledge, the literature does not offer a systematic treatment on the influence of ambient noise on MDS embedding quality.” This paper presents such an analysis.

1.1 Review of Classical Multidimensional Scaling

First we give a brief review of CMDS:

Given an $n \times n$ hollow symmetric dissimilarity matrix $D = [d_{ij}]$, the fundamental goal of multidimensional scaling is to find a suitable embedding dimension $d$ and $x_1, \ldots, x_n \in \mathbb{R}^d$ such that the inter-point distance between $x_i$ and $x_j$ is “as close as possible” to the distance given in the dissimilarity matrix $D$. One of the most widely used multidimensional scaling techniques is the classical multidimensional scaling (CMDS) and involves the following steps:

1. Compute the matrix $B = -\frac{1}{2}PD^2P$, where $D^2$ is $D$ matrix entry-wise squared, and $P = I - \frac{1}{n}11^\top$ is the double centering matrix. Here $I$ denotes the $n \times n$ identity matrix and $1 = (1, \ldots, 1)^\top \in \mathbb{R}^n$.

2. Extract the $d$ largest positive eigenvalues $s_1, \ldots, s_d$ of $B$ and the corresponding eigenvectors $u_1, \ldots, u_d$.

3. Let $X = U_BS_B^{\frac{1}{2}} \in \mathbb{R}^{n \times d}$, where $U_B = (u_1, \ldots, u_d)$ and $S_B = \text{diag}(s_1, \ldots, s_d)$, where each row of $X$ represents the coordinate of a point in $\mathbb{R}^d$.

The resulting configuration $X$ centers all points around the origin, resulting in an inherent issue of
identifiability: $X$ is unique only up to an orthogonal transformation. In the following presentation, we will write $X = U_B S_B^{\frac{1}{2}} W$ for some orthogonal matrix $W$ for a suitably transformed $X$.

## 2 Noise Model and Embedding

Suppose we have the inter-point distances of $n$ points in $\mathbb{R}^d$, and that the resulting distance matrix is $D \in \mathbb{R}^{n \times n}$, i.e. $D_{ij} = \|x_i - x_j\|_2$. As before, let $D^2$ denote the entry-wise square of $D$. Let $\Delta$ be the distance matrix we observed (measured via a scientific experiment, say). A realistic error model could be $\Delta = D + E$, where we can think $D$ as “signal” and $E$ as “noise”. Furthermore, the random matrix $E$ should ideally satisfy the following conditions:

1. $\mathbb{E}[E] = 0$.
2. $E$ is hollow; that is, $\Delta$ still has 0’s on its diagonal.
3. Entries $E_{ij}$ are independent and $\text{Var}(E_{ij}) = \sigma^2$.
4. Each $E_{ij}$ follows a sub-Gaussian distribution.
5. As a technical condition, we also require that $\max_{1 \leq i \leq n} \sum_{j=1}^{n} D_{ij}^2 \gg \log^4 n$. This is a relatively mild condition to ensure the distance matrix is not too sparsely populated.

We then apply CMDS to $\Delta$ to get the resulting configuration matrix $\hat{X}$, and we use the following notations for this procedure:

1. Let $\hat{B} = -\frac{1}{2} P \Delta^2 P$.
2. Let $S_B \in \mathbb{R}^{d \times d}$ be the diagonal matrix of $d$ largest eigenvalues of $\hat{B}$ and $U_B \in \mathbb{R}^{n \times d}$ be the matrix whose orthogonal columns are the corresponding eigenvectors.
3. The matrix $\hat{X} = U_B S_B^{\frac{1}{2}} \in \mathbb{R}^{n \times d}$ is the “embedding of $\Delta$” into $\mathbb{R}^d$.

A natural question arises regarding how the added noise affects the embedding configuration. That is, what is the relationship between the embedding $X$ from $D$ as in Section 1.1 and this embedding $\hat{X}$ from $\Delta$?
3 Main Results

3.1 Sub-Gaussian Random Vectors

Recall that a random variable $X$ is sub-Gaussian if $\mathbb{P}[|X| > t] \leq 2e^{-\frac{t^2}{2K^2}}$ for some constant $K$ and for all $t \geq 0$. Associated with a sub-Gaussian random variable is a Orlicz norm defined as $||X||_{\psi_2} = \inf\{t > 0 : \mathbb{E}\exp(\frac{X^2}{t^2}) \leq 2\}$. A random vector $X$ in $\mathbb{R}^n$ is called sub-Gaussian if the one-dimensional marginals $\langle X, x \rangle$ are sub-Gaussian random variables for all $x \in \mathbb{R}^n$, and the corresponding sub-Gaussian norm of $X$ is defined as $||X||_{\psi_2} = \sup_{x \in S^{n-1}} ||\langle X, x \rangle||_{\psi_2}$.

3.2 Main Theorem

We have the following consistency results relating $X$ and $\hat{X}$:

**Theorem 3.1.** (Central Limit Theorem for the rows of CMDS) Let $Z_1, Z_2, \ldots, Z_n \overset{i.i.d.}{\sim} F$ for some sub-Gaussian distribution $F$ on $\mathbb{R}^d$. Let $D$ be the Euclidean distance matrix generated by the $Z_i$’s, $D_{ij} = ||Z_i - Z_j||$. Let the noise matrix $E$ satisfy the conditions in Section 2 and let $\Delta = D + E$. Suppose that $X$ and $\hat{X}$ are the CMDS embedding configurations in $\mathbb{R}^d$ of $D$ and $\Delta$. Then there exists a sequence of orthogonal matrices $\{W_n\}_{n=1}^\infty \in \mathbb{R}^{d \times d}$, such that for any $\alpha \in \mathbb{R}^d$ and any fixed row index $i$,

$$\lim_{n \to \infty} \mathbb{P}\{\sqrt{n}[(\hat{X}_nW_n)_i - (Z_i - \bar{Z})] \leq \alpha\} = \int_{\text{supp} F} \Phi(\alpha, \Sigma(z))dF(z)$$

where $\bar{Z}$ is the mean of $Z_i$’s and $\Phi(\alpha, \Sigma)$ denotes the CDF of a multivariate Gaussian with mean 0 and covariance matrix $\Sigma$, evaluated at $\alpha$.

Here

$$\Sigma(z) = \Xi^{-1}\tilde{\Sigma}(z)\Xi^{-1}$$

in which

$$\Xi := \text{Var}(Z_i) \in \mathbb{R}^{d \times d}, \text{ and}$$

$$\tilde{\Sigma}(z) := \mathbb{E}_{Z_k}[\sigma^2||z - Z_k||^2 + \frac{1}{4}\mathbb{E}[E_{ij}^4] - \frac{\sigma^4}{4})(Z_k - \mu_z)(Z_k - \mu_z)^\top] \in \mathbb{R}^{d \times d}$$

is a covariance matrix depending on $z$, and $\mu_z = \mathbb{E}[Z_i] \in \mathbb{R}^{d \times 1}$.
Intuitively, this theorem claims that the rows of $\hat{X}$, after some orthogonal transformation, will be (approximately) centered around the rows of $X$ when $n$ is large. Furthermore, the more inter-point distances we have, the more tightly the rows of $\hat{X}$ will center around the corresponding rows of $X$. The covariance of the centering will depend on the noise and the true distribution of the points in the underlying space. We refer the reader to the Appendix for a detailed proof of this theorem.

**Remark 1.** Note that the entries of $\Delta$ should be nonnegative. Consider a modification of our conditions to have noise added only to large entries of $D$, provided that $D$ has sufficiently many large entries. That is, if $||E_{ij}||_\psi^2 = \gamma$, we will add noise only to entries of $D$ for which $D_{ij} > \gamma C$ for some constant $C$. In this case, a variant of our Theorem 3.1 can be established.

### 4 Empirical Results

#### 4.1 Three Point-mass Simulated Data

As a simple illustration of our CMDS CLT, we embed noisy Euclidean distances obtained from $n$ points into $\mathbb{R}^2$. We consider three points $x_1, x_2, x_3 \in \mathbb{R}^2$ for which the inter-point distances are 3, 4 and 5 (these three points form a right triangle) and generate $n_k = \pi_k n$ points equal to $x_k$, $k = 1, 2, 3$, where $\pi = [0.2, 0.3, 0.5]^\top$. The resulting Euclidean inter-point distance matrix $D$ is then subjected to uniform noise, yielding $\Delta = D + E$ where $E_{ij} \overset{i.i.d.}{\sim} \text{Uniform}(-4, +4)$ for $i < j$ and $E_{ij} = E_{ji}$. For this case, our CLT for CMDS embedding into two dimensions gives class-conditional Gaussians. For each $n \in \{50, 100, 500, 1000\}$, Figure 1 compares, for one realization, the theoretical vs. estimated means and covariances matrices (95% level curves). Table 4.1 shows the empirical covariance matrix for one of the point masses, $\hat{\Sigma}^{(1)}$, behaving in accordance with Theorem 3.1.
Figure 1: Simulation results for $n=50$, 100, 500 and 1000 points, as described in Section 4.1. The blue ellipses are the 95% level curves of the empirical covariance matrix, and the blue dots are the empirical centers for three classes. The black dots are the true positions of $x_1$, $x_2$ and $x_3$, and the black ellipses are the 95% level curve for the theoretical covariance matrices as in Theorem 3.1. Note that the blue and black centers and ellipses coincide for large $n$. 
Table 4.1 investigates the empirical covariance matrix for one of the point masses, and its entry-wise variance, as a function of \( n \). The theoretical covariance matrix is \( \Sigma^{(1)} = \begin{bmatrix} 13.56 & -3.06 \\ -3.06 & 22.65 \end{bmatrix} \).

\[
\begin{array}{cccc}
  n=50 & n=100 & n=500 & n=1000 \\
  \hat{\Sigma}^{(1)} : & \begin{bmatrix} 14.15 & 0.25 \\ 0.25 & 79.07 \end{bmatrix} & \begin{bmatrix} 13.67 & -0.79 \\ -0.79 & 98.96 \end{bmatrix} & \begin{bmatrix} 13.65 & -2.34 \\ -2.34 & 41.02 \end{bmatrix} & \begin{bmatrix} 13.63 & -2.70 \\ -2.70 & 31.76 \end{bmatrix} \\
  \text{Var} & \begin{bmatrix} \hat{\Sigma}_{11}^{(1)} \end{bmatrix} : & \begin{bmatrix} 41.25 \end{bmatrix} & \begin{bmatrix} 19.29 \end{bmatrix} & \begin{bmatrix} 3.67 \end{bmatrix} & \begin{bmatrix} 1.71 \end{bmatrix} \\
  & \begin{bmatrix} \hat{\Sigma}_{12}^{(1)} \end{bmatrix} : & \begin{bmatrix} 113.31 \end{bmatrix} & \begin{bmatrix} 68.06 \end{bmatrix} & \begin{bmatrix} 7.87 \end{bmatrix} & \begin{bmatrix} 3.25 \end{bmatrix} \\
  & \begin{bmatrix} \hat{\Sigma}_{22}^{(1)} \end{bmatrix} : & \begin{bmatrix} 829.52 \end{bmatrix} & \begin{bmatrix} 984.45 \end{bmatrix} & \begin{bmatrix} 31.71 \end{bmatrix} & \begin{bmatrix} 11.08 \end{bmatrix} \\
\end{array}
\]

Table 1: Empirical average of covariance matrix \( \hat{\Sigma}^{(1)} \), and entry-wise variance, via 500 simulations.

Remark 2. In this simulation we relax the requirement that the entries of \( \Delta \) should be nonnegative in order to illustrate the phenomenon of decreasing covariance with increasing \( n \).

4.2 Shape clustering

As a second illustration of the effect of noise on CMDS, we examine a more involved clustering experiment in the (non-Euclidean) shape space of closed curves. In this experiment, we consider boundary curves obtained from silhouettes of the Kimia shape database. Specifically, we restrict attention to three predefined classes of objects (bottle, bone, and wrench) and take from each class three different examples of shapes all given by planar closed polygonal curves representing the objects’ outline. Figure 2 shows one instance for each of the bottle, bone, and wrench class. A database of noisy curves is then created as follows: for each of the nine template shapes, we generate 100 noisy realizations in which vertices of the curve are moved along the curve’s normal vectors with random distances drawn from independent Gaussian distributions at each vertex. This results in a total of 900 noisy versions of the initial curves such as the ones displayed in Figure 3.
We then compute the pairwise distance matrix between all the curves (including the noiseless templates) based on a shape distance which was introduced in [6] and later extended in the work of [7]. This type of metric is based on the representation of shapes in a particular distribution space called currents, see [7] for details. In our context, this metric offers several advantages: (i) the distance is completely geometrical in the sense that it is independent of the sampling of the curves and does not rely on predefined pointwise correspondences between vertices; (ii) it has an intrinsic smoothing effect that provides robustness to noise to a certain degree; (iii) it can be computed in closed form with minimal computational time which is critical given the large number of pairwise distances to evaluate. In this setting, we can view the resulting distance matrix as a
noisy perturbation of the ideal distances between the 9 template curves, which fits into the generic framework of our model. (Note that we leave aside the issue of checking the technical assumptions on the matrix $E$, which may be quite involved for this noise model and distance.)

We proceed to perform CMDS on this distance matrix. A scree plot investigation shows that an appropriate embedding dimension here is $\hat{d} = 3$ (the top three eigenvalues are 2.20, 0.68, 0.06 with the fourth $\ll 0.01$). The resulting embedding configuration is shown in Figure 4. This configuration exhibits nine fairly well-separated clusters roughly centered around the position of each of the noiseless template curves. Those, in turn, form 3 ‘super-clusters’ consistent with the classes. Furthermore, the ellipsoidal shape of each cluster suggests that the configuration approximately follows a Gaussian distribution.
One immediate consequence of our Main Theorem is that when the variance of the noise $E$ increases, the covariance matrix $\Sigma$ gets larger. To further illustrate this point, we repeated the same experiment but with larger variance Gaussian noise on the curves before applying CMDS, and we observe that larger noise indeed leads to larger covariances of the clusters in the configuration space.

While these preliminary shape clustering results are obtained with a specific and simple distance on the space of curves, future work will investigate whether similar properties hold with different, more elaborate metrics and/or geometric noise models. The central limit theorem derived here could then constitute a useful theoretical tool to evaluate the discriminating power of
shape clustering methods based on CMDS.

5 Discussion

In [8], [9] and [10], the authors prove that adjacency spectral embedding of the random dot product graph gives rise to a central limit theorem for the rows of the latent positions. In this work we extend these results to distance matrix embedding.

We have avoided any discussion of the model selection problem of choosing a suitable embedding dimension $\hat{d}$. Instead, we assume $d$ is known – except in Section 4.2. There are many methods for choosing (spectral) embedding dimensions, see [11, 12, 13].

A practically relevant and conceptually illustrative example comes from relaxing the assumption of common variance for the entries of the noise matrix $E$ model in Section 2: the consistency result from Theorem 3.1 no longer holds. To illustrate this point, we return to our three-point-mass simulation presented in Section 4.1 and modify our noise model as follows: Let $\tilde{E}_{ij} \overset{i.i.d.}{\sim} \text{Uniform}(-D_{ij}, +D_{ij})$ for $i < j$ and $\tilde{E}_{ij} = \tilde{E}_{ji}$. (The noise now depends on the entries of $D$, and $\Delta = D + \tilde{E}$ no longer has negative entries.) The embedding of $\Delta$ into two dimensions gives class-conditional Gaussians; however, we have introduced bias into the embedding configuration. Figure 5 shows, for one realization, the embedding result. Note that the empirical mean and the theoretical positions do not coincide in simulation with large $n$, and theoretically even in the limit.
Figure 5: Simulation of CMDS with heteroscedastic noise $\tilde{E}$. The black dots are the true positions for the three points. The blue dots are the empirical means and the blue ellipses are the 95% level curve of the empirical covariance matrix. Note that $\tilde{E}$ used in this simulation is of the same order for the off-diagonal blocks as that used in Figure 1. NB: there is asymptotic bias.
CMDS is just one of a wide variety of multidimensional scaling techniques. Minimizing the raw stress criterion is another commonly used MDS technique [14]. This method seeks to minimize the raw stress, defined as \( \sigma_r = \sigma_r(X) = \sum_{(i,j)} [d_{ij} - \delta_{ij}(X)] \) where \( d_{ij} \) is the \((i,j)\)th entry in the given distance matrix \( D \) and \( \delta \) is a distance metric. We minimize \( \sigma_r \) by an iterative algorithm which updates the configuration matrix \( X \) until the stopping criteria is met [15]. Keeping the simulation settings as in Section 4.1, the resulting configuration is shown in Figure 6. This suggests that the CLT may hold for raw stress just as well as for CMDS. However, this claim is at best a conjecture at present as the analysis seems significantly more involved.

Another possible, albeit naive model of \( \Delta \) is \( \Delta^2 = D^2 + E \) (as opposed to \( \Delta^2 = (D + E)^2 \)) where \( E \) still satisfies the conditions in Section 2. This is the error model on the squared distance matrix \( D^2 \) rather than the distance matrix \( D \). Our central limit theorem still holds for this situation, with a greatly-simplified covariance matrix. For the sake of completeness, we present this version below. The proof is essentially a simplified version of the Appendix.

**Theorem 5.1.** Keep the setting as in 3.1 and replace \( \Delta = D + E \) with \( \Delta^2 = D^2 + E \). Then there exists a sequence \( \{W_n\}_{n=1}^\infty \in \mathbb{R}^{d \times d} \) such that for any \( \alpha \in \mathbb{R}^d \) and any fixed row index \( i \), we have

\[
\lim_{n \to \infty} \mathbb{P}\{\sqrt{n}[(\hat{X}_nW_n)_i - (Z_i - \bar{Z})] \leq \alpha\} = \int_{\text{supp}\Phi} \Phi(\alpha, \Sigma(z))dF(z)
\]

where \( \bar{Z} \) is the mean of \( Z_i \)'s and \( \Phi(\alpha, \Sigma) \) denotes the CDF of a multivariate Gaussian with mean \( 0 \) and covariance matrix \( \Sigma \), evaluated at \( \alpha \). Here

\[
\Sigma(z) = \frac{1}{4} \Xi^{-1} \tilde{\Sigma}(z) \Xi^{-1},
\]

in which \( \tilde{\Sigma}(z) := \mathbb{E}_Z[\text{Var}(E_{ij})(z - \mu_z)(z - \mu_z)^\top] \) is a covariance matrix depending on \( z \) where \( \mu_z = \mathbb{E}[Z] \), and \( \Xi = \text{Var}(Z_i) \in \mathbb{R}^{d \times d} \) where \( W \) is some orthogonal matrix.
Figure 6: Simulation of MDS using raw stress criterion for \( n = 50, 100, 500 \) and 1000 points. The black dots are the true positions of \( x_1, x_2 \) and \( x_3 \), the blue dots are the empirical mean of the simulation and the blue ellipses are the 95% level curve of the empirical covariance matrix.
## Appendix: Proof of Lemmas and Theorems

Throughout this Appendix, $||A||$ denotes the spectral norm of matrix $A$, and $||A||_F$ denotes the Frobenius norm of matrix $A$. There are two simple observations we will utilize repeatedly in the following presentation.

**Observation A.1.** Let matrices $A$ and $B$ be of appropriate dimensions, then $||AB||_F \leq ||A|| ||B||_F$.

**Observation A.2.** Let matrices $A$ and $S$ be of appropriate dimensions, and let $S$ be a diagonal matrix, then $||AS||_F \leq ||S|| ||A||_F$.

**Proposition A.3.** $||B - \hat{B}|| = O(\sqrt{n})$ with high probability.

**Proof.** We have:

\[
||B - \hat{B}|| = || - \frac{1}{2} PD^2 P + \frac{1}{2} P(D + E)^2 P || \\
= ||PD \circ EP + \frac{1}{2} P E^2 P || \text{ (where } \circ \text{ is the Hadamard product)} \\
\leq ||D \circ E|| + \frac{1}{2} ||P E^2 P||, \text{ (since } ||P|| = 1.)
\]

Note that $E[D \circ E] = 0$ and $E[\frac{1}{2} P E^2 P] = 0$. A direct application of Theorem 6 in [16] gives the desired result.

**Lemma A.4.** Let $X_1, \ldots, X_n, Y \overset{i.i.d.}{\sim} F$ for some sub-Gaussian distribution $F$, where $X_i$ is the $i$th row of the configuration matrix $X$ of $B$ viewed as a column vector. Let $\Xi = E[X_1 X_1^\top]$ be of rank $d$, then $\lambda_i(B) = \Omega(n)$ almost surely.

**Proof.** For any matrix $H$, the nonzero eigenvalues of $H^\top H$ are the same as those $HH^\top$, so $\lambda_i(X X^\top) = \lambda_i(X^\top X)$. In what follows, we remind the reader that $X$ is a matrix whose rows are the transposes of the column vectors $X_i$, and $Y$ is a $d$-dimensional vector that is independent from and has the same distribution as that of the $X_i$. We observe that $(X^\top X - nE[YY^\top])_{ij} = \sum_{k=1}^{n} (X_{ki} X_{kj} - E[Y_i Y_j])$ is a sum of $n$ independent mean-zero sub-Gaussian random variables. By general Hoeffding’s inequality [17], for all $i, j \in [d]$,

\[
P[|(X^\top X - nE[YY^\top])_{ij}| \geq t] \leq 2 \exp\left\{ -\frac{ct^2}{nM} \right\},
\]

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where $M = \max_k ||(X_{ki}X_{kj} - E[Y_iY_j])||^2_{F^2}$, which gives

$$\mathbb{P}[||(X^TX) - nE[YY^T]|_{ij} \geq C\sqrt{n\log n}] \leq 2n^{-2c^2}.$$  

A union bound over all $i, j \in [d]$ implies that $||X^TX - nE[YY^T]||_F^2 \leq C^2d^2n\log n$ with probability at least $1 - \frac{2}{nM^2}$, i.e. $||X^TX - nE[YY^T]||_F \leq Cd\sqrt{n\log n}$ with high probability for any $C > \frac{M}{\sqrt{2}}$. By Hoffman-Wielandt inequality, $|\lambda_i(XX^T) - n\lambda_i(E[YY^T])| \leq Cd\sqrt{n\log n}$, and by reverse triangle inequality, we obtain

$$\lambda_i(XX^T) \geq \lambda_d(XX^T) \geq |n\lambda_d(\Xi)| - Cd\sqrt{n\log n} = \Omega(n)$$  

holds almost surely. \hfill\qed

**Proposition A.5.** Let $W_1 \Sigma W_2^T$ be the singular value decomposition of $U_B^T U_B$, then with high probability, $||U_B^T U_B - W_1 W_2^T|| = \mathcal{O}(n^{-1})$.

**Proof.** Let $\sigma_1, \sigma_2, \ldots, \sigma_d$ be the singular values of $U_B^T U_B$ (the diagonal entries of $\Sigma$). Then $\sigma_i = \cos(\theta_i)$ where $\theta_i$’s are the principal angles between the subspace spanned by $U_B$ and $U_B^\ast$. Then Davis-Kahan sin($\Theta$) theorem \cite{18} gives

$$||U_B U_B^\ast - U_B^\ast U_B|| = \max_i |\sin(\theta_i)| \leq \frac{C||B - \hat{B}||}{\lambda_d(B)} = \mathcal{O}(n^{-\frac{1}{2}})$$  

for sufficiently large $n$. Note in the last equality we used the previous two lemmas. Thus,

$$||U_B^T U_B - W_1 W_2^T||_F = ||\Sigma - I||_F = \sqrt{\sum_{i=1}^d (1 - \sigma_i)^2} \leq \sum_{i=1}^d (1 - \sigma_i) \leq \sum_{i=1}^d (1 - \sigma_i^2)$$  

$$= \sum_{i=1}^d \sin(\theta_i)^2 \leq d||U_B^T U_B^\ast - U_B^\ast U_B||^2 = \mathcal{O}(n^{-1})$$  

\hfill\qed

Recall that a random vector $X$ is sub-exponential if $\mathbb{P}[|X| > t] \leq 2e^{-\frac{t^2}{K}}$ for some constant $K$ and for all $t \geq 0$. Associated with a sub-exponential random variable there is a Orlicz norm defined as $||X||_{\psi_1} = \inf\{t > 0 : \mathbb{E}\exp(\frac{|X|}{t}) \leq 2\}$. Furthermore, a random variable $X$ is sub-Gaussian if and only if $X^2$ is sub-exponential, and $||X^2||_{\psi_1} = ||X||_{\psi_2}^2$.  

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Lemma A.6. Let $W^* = W_1W_2^\top$, then asymptotically almost surely, $||W^*S_B - S_BW^*||_F = \mathcal{O}(\log n)$ and $||W^*S_B^{\frac{1}{2}} - S_B^{\frac{1}{2}}W^*||_F = \mathcal{O}(n^{-\frac{1}{2}} \log n)$.

Proof. Let $R = U_B - U_BU_B^\top U_B$. Note $R$ is the residual after projecting $U_B$ orthogonally onto the column space of $U_B$, and thus

$$||U_B - U_BU_B^\top U_B||_F \leq \min_W ||U_B - U_BW||_F$$

where the minimization is over all orthogonal matrices $W$. By a variant of the Davis-Kahan sin $\Theta$ theorem [19], we have

$$\min_W ||U_BW - U_B||_F \leq \frac{C\sqrt{d}||B - \hat{B}||}{\lambda_d(B)},$$

then we have

$$||R||_F \leq \mathcal{O}(n^{-\frac{1}{2}}).$$

Now consider

$$W^*S_B = (W^* - U_B^\top U_B)S_B + U_B^\top U_B S_B$$

$$= (W^* - U_B^\top U_B)S_B + U_B^\top U_B S_B$$

$$= (W^* - U_B^\top U_B)S_B + U_B^\top (\hat{B} - B)U_B + U_B^\top opBU_B$$

$$= (W^* - U_B^\top U_B)S_B + U_B^\top (\hat{B} - B)R + U_B^\top (\hat{B} - B)U_BU_B^\top U_B + S_BU_B^\top U_B.$$

Note here we use the fact $U_B S_B = \hat{B}U_B$. Now write

$$S_BU_B^\top U_B = S_B(U_B^\top U_B - W^*) + S_BW^*,$$

then we have

$$W^*S_B - S_BW^* = (W^* - U_B^\top U_B)S_B + U_B^\top (\hat{B} - B)R + U_B^\top (\hat{B} - B)U_BU_B^\top U_B + S_B(U_B^\top U_B - W^*).$$
This gives

\[
||W^* S_B - S_B W^*||_F
\]
\[
\leq ||(U_B^T U_B - W^*)(S_B + S_B)||_F + ||U_B^T (\hat{B} - B) R||_F + ||U_B^T (\hat{B} - B) U_B U_B^T U_B||_F
\]
\[
\leq ||(U_B^T U_B - W^*)||_F(||S_B|| + ||S_B||) + ||U_B^T (\hat{B} - B) R||_F + ||U_B^T (\hat{B} - B) U_B U_B^T U_B||_F
\]
\[
\leq ||W_1 W_2^T - U_B^T U_B||_F(O(n) + O(n)) + ||U_B^T (\hat{B} - B) R||_F + ||U_B^T (\hat{B} - B) U_B||_F||U_B^T U_B||_F
\]
\[
\leq O(n^{-1})(O(n^4) + O(n)) + O(1) + ||U_B^T (\hat{B} - B) U_B||_F||U_B^T U_B||_F
\]
\[
= O(1) + ||U_B^T (\hat{B} - B) U_B||_F.
\]

Consider the term \(U_B^T (\hat{B} - B) U_B \in \mathbb{R}^{d \times d}\). If we denote \(U_i\) be the \(i\)th column of \(U_B\), then for each \(i, j\)th entry, we have

\[
(U_B^T (\hat{B} - B) U_B)_{ij} = U_i^T (\hat{B} - B) U_j = \frac{1}{2} V_i^T (\Delta^2 - D^2) V_j
\]

where \(V = PU_B\). Furthermore, we have

\[
V_i^T (\Delta^2 - D^2) V_j = \sum_{k, l} V_{ik} (\Delta_{kl}^2 - D_{kl}^2) V_{jl}. \tag{1}
\]

Recall, since \(X_k\)'s are sub-Gaussian, thus equation (1) is a sum of mean zero sub-exponential random variables. By Bernstein’s inequality [17], we have

\[
\mathbb{P}[|\sum_{k, l} (\Delta_{kl}^2 - D_{kl}^2) V_{ik} V_{jl}| > t] \leq 2 \exp\{-C \min\left(\frac{t^2}{M^2 \sum_{k, l} V_{ik}^2 V_{jl}^2}, \frac{t}{M \max_{k, l} (V_{ik} V_{jl})}\right)\}
\]

where \(M := \max_{k, l} ||\Delta_{kl}^2 - D_{kl}^2||_{\psi_1}\). Note since \(\sum_{k} V_{ik}^2 \leq 1 \forall i\), we have that each entry of \(U_B^T (\hat{B} - B) U_B \in \mathbb{R}^{d \times d}\) is \(O(\log n)\), and \(||U_B^T (\hat{B} - B) U_B||_F = O(\log n)\). This then gives \(||W^* S_B - S_B W^*||_F = O(\log n)\), with high probability.

Now, consider \(||W^* S_B^{\frac{1}{2}} - S_B^{\frac{1}{2}} W^*||_F\). The \(i, j\)th entry of \(W^* S_B^{\frac{1}{2}} - S_B^{\frac{1}{2}} W^*\) is

\[
W_{ij}^*(\lambda_i^{\frac{1}{2}}(\hat{B}) - \lambda_j^{\frac{1}{2}}(B)) = W_{ij}^* \frac{\lambda_i(\hat{B}) - \lambda_j(B)}{\lambda_i^{\frac{1}{2}}(\hat{B}) + \lambda_j^{\frac{1}{2}}(B)}
\]
\[
\leq W_{ij}^* \frac{\lambda_i(\hat{B}) - \lambda_j(B)}{\Omega(\sqrt{n})}
\]
\[
= O(n^{-\frac{1}{2}} \log n).
\]
Lemma A.7. There exists an orthogonal matrix $W$, such that 

$$
\hat{X} - XW = (\hat{B} - B)U_BW^*S_B^{-\frac{1}{2}} - U_BU_B^\top(\hat{B} - B)U_BW^*S_B^{-\frac{1}{2}} + (I - U_BU_B^\top)(\hat{B} - B)R_3S_B^{\frac{1}{2}} + R_1S_B^{\frac{1}{2}} + U_BR_2,
$$

where $R_1 = U_BU_B^\top U_B$, $R_2 = W^*S_B^{\frac{1}{2}} - S_B^{\frac{1}{2}}W^*$, and $R_3 = \hat{B} - U_BW^*$.

Proof. We have 

$$
\hat{X} - U_BS_B^{\frac{1}{2}}W^* = U_BS_B^{\frac{1}{2}} - U_BW^*S_B^{\frac{1}{2}} + U_B(W^*S_B^{\frac{1}{2}} - S_B^{\frac{1}{2}}W^*)
$$

$$
= U_BS_B^{\frac{1}{2}} - U_BU_B^\top U_BS_B^{\frac{1}{2}} + U_BU_B^\top U_BS_B^{\frac{1}{2}} - U_BW^*S_B^{\frac{1}{2}} + U_B(W^*S_B^{\frac{1}{2}} - S_B^{\frac{1}{2}}W^*)
$$

$$
= U_BS_B^{\frac{1}{2}} - U_BU_B^\top U_BS_B^{\frac{1}{2}} + R_1S_B^{\frac{1}{2}} + U_BR_2
$$

$$
= BU_BS_B^{-\frac{1}{2}} - BU_BS_B^{-\frac{1}{2}} + U_BU_B^\top BU_BS_B^{\frac{1}{2}} - U_BU_B^\top BU_BS_B^{\frac{1}{2}} + R_1S_B^{\frac{1}{2}} + U_BR_2
$$

$$
= (\hat{B} - B)U_BS_B^{-\frac{1}{2}} - U_BU_B^\top (\hat{B} - B)U_BS_B^{-\frac{1}{2}} + R_1S_B^{\frac{1}{2}} + U_BR_2
$$

Note we used the facts that $U_BU_B^\top B = B$ and $U_BS_B^{\frac{1}{2}} = \hat{B}U_BS_B^{-\frac{1}{2}}$ in the above equalities.

Writing

$$
R_3 = U_B - U_BW^*
$$

$$
= U_B - U_BU_B^\top U_B + U_BU_B^\top U_B - U_BW^*
$$

$$
= U_B - U_BU_B^\top U_B + R_1,
$$

we have that 

$$
\hat{X} - U_BS_B^{\frac{1}{2}}W^*
$$

$$
= (\hat{B} - B)(U_BW^* + R_3)S_B^{-\frac{1}{2}} - U_BU_B^\top (\hat{B} - B)(R_3 + U_BU_B^\top W^*)S_B^{-\frac{1}{2}} + R_1S_B^{\frac{1}{2}} + U_BR_2
$$

$$
= (\hat{B} - B)U_BU_B^\top \hat{B}U_BS_B^{\frac{1}{2}} + (I - U_BU_B^\top) (\hat{B} - B)R_3S_B^{-\frac{1}{2}} + R_1S_B^{\frac{1}{2}} + U_BR_2
$$

Lemma A.8. There exists an orthogonal matrix $W$ such that with high probability, $||\hat{X} - XW||_F = ||(\hat{B} - B)U_BS_B^{-\frac{1}{2}}||_F + O(n^{-\frac{1}{2}} \log n)$.

Proof. By Lemma A.7, we have 

$$
\hat{X} - U_BS_B^{\frac{1}{2}}W^*
$$

$$
= (\hat{B} - B)U_BU_B^\top \hat{B}U_BS_B^{\frac{1}{2}} + (I - U_BU_B^\top) (\hat{B} - B)R_3S_B^{-\frac{1}{2}} + R_1S_B^{\frac{1}{2}} + U_BR_2.
$$
Recall that
\[ \|U_B - U_B U_B^\top U_B\|_F = O(n^{-\frac{1}{2}}), \]
\[ \|R_1\|_F \leq \|U_B\| \|U_B^\top U_B - W^*\|_F = O(1)O(n^{-1}) = O(n^{-1}) \]
\[ \|R_2\|_F = O(n^{-\frac{1}{2}} \log n) \]
\[ \|R_3\|_F = \|U_B - U_B W^*\|_F = \|U_B - U_B U_B^\top U_B + R_1\|_F \leq \|U_B - U_B U_B^\top U_B\|_F + \|R_1\|_F = O(n^{-\frac{1}{2}}) \]
A similar application of Hoeffding’s inequality as in previous lemma gives
\[ \|U_B U_B^\top (\hat{B} - B) U_B W^* S_B^{-\frac{1}{2}}\|_F \leq \|U_B U_B^\top (\hat{B} - B) U_B\|_F \|S_B^{-\frac{1}{2}}\|_F = O(n^{-\frac{1}{2}} \log n). \]
Furthermore, we have
\[ \| (I - U_B U_B^\top) (\hat{B} - B) R_3 S_B^{-\frac{1}{2}} \|_F \leq \| (I - U_B U_B^\top) \| \| (\hat{B} - B) \| \| R_3 \|_F \| S_B^{-\frac{1}{2}} \| \]
\[ = (\| I \| + \| U_B U_B^\top \|) \| (\hat{B} - B) \| \| R_3 \|_F \| S_B^{-\frac{1}{2}} \|
\[ = O(1)O(\sqrt{n})O(n^{-\frac{1}{2}})O(n^{-\frac{1}{2}})
\[ = O(n^{-\frac{1}{2}}) \]
and
\[ \| R_1 S_B^{-\frac{1}{2}} \|_F \leq \| R_1 \|_F \| S_B^{-\frac{1}{2}} \| = O(n^{-1})O(n^{\frac{1}{2}}) = O(n^{-\frac{1}{2}}) \]
with
\[ \| U_B R_2 \|_F \leq \| U_B \| \| R_2 \|_F = O(n^{-\frac{1}{2}} \log n). \]
Together, we get
\[ \| \hat{X} - U_B S_B^{\frac{1}{2}} W^* \|_F = \| (\hat{B} - B) U_B W^* S_B^{-\frac{1}{2}} \|_F + O(n^{-\frac{1}{2}} \log n) \]
\[ = \| (\hat{B} - B) U_B S_B^{-\frac{1}{2}} W^* - (\hat{B} - B) U_B (S_B^{-\frac{1}{2}} W^* - W^* S_B^{-\frac{1}{2}}) \|_F + O(n^{-\frac{1}{2}} \log n) \]
\[ \leq \| (\hat{B} - B) U_B S_B^{-\frac{1}{2}} W^* \|_F + \| (\hat{B} - B) U_B \| \| S_B^{-\frac{1}{2}} W^* - W^* S_B^{-\frac{1}{2}} \|_F + O(n^{-\frac{1}{2}} \log n) \]
\[ \leq \| (\hat{B} - B) U_B S_B^{-\frac{1}{2}} \|_F + O(n^{-\frac{1}{2}} \log n) O(n^{\frac{1}{2}}) + O(n^{-\frac{1}{2}} \log n) \]
\[ = \| (\hat{B} - B) U_B S_B^{-\frac{1}{2}} \|_F + O(n^{-\frac{1}{2}} \log n) \]
Note we implicitly used the fact that \( \| S_B^{-\frac{1}{2}} W^* - W S_B^{-\frac{1}{2}} \|_F = O(n^{-\frac{3}{2}} \log n) \), which can be proved completely analogous to Lemma A.6.

**Theorem A.9.** There exist orthogonal matrices \( W_n \in \mathbb{R}^{d \times d} \), such that
\[
\max_i \| (\hat{X}_n)_i - W_n(X_n)_i \| \leq \frac{C \sqrt{d \log^2 n}}{\sqrt{n}} \] asymptotically almost surely.

**Proof.** By previous theorem
\[
\| \hat{X} - XW \|_F = \| (\hat{B} - B)U_BS_B^{-\frac{1}{2}} \|_F + O(n^{-\frac{3}{2}} \log n),
\]
hence,
\[
\max_i \| \hat{X}_i - WX_i \| \leq \frac{1}{\lambda_d(B)^2} \max_i \| (\hat{B} - B)U_B \| + O(n^{-\frac{3}{2}} \log n)
\]
\[
\leq \frac{\sqrt{d}}{\lambda_d(B)^2} \max_i \| (\hat{B} - B)U_{B,j} \|_\infty + O(n^{-\frac{3}{2}} \log n)
\]

where \( U_{B,j} \) is the \( j \)th column of \( U_B \). Now for a given \( j \) and a given index \( i \), the \( i \)th element of the vector \( (\hat{B} - B)U_{B,j} \) is of the form \( \sum_k (\hat{B}_{ik} - B_{ik})U_{Bkj} \), and again by Hoeffding’s inequality, is \( O(\log n) \) a.a.s.. Taking the union bound over all \( i \) and all \( j \), we get
\[
\max_i \| \hat{X}_i - WX_i \| \leq \frac{C \sqrt{d} \log^2 n}{\lambda_d(B)^2} + O(n^{-\frac{3}{2}} \log n)
\]
\[
\leq \frac{C \sqrt{d} \log^2 n}{\sqrt{n}}
\]

**Lemma A.10.** We have
\[
\sqrt{n}[(\hat{B} - B)U_B(U^*_BS_B^{-\frac{1}{2}} - S_B^{-\frac{1}{2}}W^*)]_h \overset{P}{\to} 0 \tag{2}
\]
\[
\sqrt{n}[U_BU_B^\top(\hat{B} - B)U_BW^*S_B^{-\frac{1}{2}}]_h \overset{P}{\to} 0 \tag{3}
\]
\[
\sqrt{n}[(I - U_BU_B^\top)(\hat{B} - B)R_3S_B^{-\frac{1}{2}}]_h \overset{P}{\to} 0 \tag{4}
\]
and with high probability

\[ \| R_1 S_{B}^{\frac{1}{2}} + U_B R_2 \|_F \leq \frac{C \log n}{\sqrt{n}}. \]  

(5)

**Proof.** For (5), note

\[
\| R_1 S_{B}^{\frac{1}{2}} + U_B R_2 \|_F \leq \| R_1 S_{B}^{\frac{1}{2}} \|_F + \| U_B R_2 \|_F \\
\leq \| R_1 \|_F \| S_{B}^{\frac{1}{2}} \| + \| U_B \| \| R_2 \|_F \\
\leq \mathcal{O}(n^{-1})\mathcal{O}(n^{\frac{1}{2}}) + \mathcal{O}(n^{-\frac{1}{2}} \log n) \\
= \mathcal{O}(n^{-\frac{1}{2}} \log n).
\]

For (2), we have

\[
\sqrt{n}\| (\hat{B} - B) U_B (W^* S_{B}^{\frac{1}{2}} - S_{B}^{\frac{1}{2}} W^*) \|_F \leq \sqrt{n}\| (\hat{B} - B) U_B \| \| W^* S_{B}^{\frac{1}{2}} - S_{B}^{\frac{1}{2}} W^* \|_F \\
\leq \sqrt{n}\| (\hat{B} - B) \| \| W^* S_{B}^{\frac{1}{2}} - S_{B}^{\frac{1}{2}} W^* \|_F \\
= \sqrt{n}\mathcal{O}(\sqrt{n})\mathcal{O}(n^{-\frac{1}{2}} \log n) \\
= C \log n \rightarrow 0 \text{ as } n \rightarrow \infty.
\]

Consider (3), recall that \( X = U_B S_{B}^{\frac{1}{2}} W \) for some orthogonal matrix \( W \), and since \( X_i \)'s are sub-Gaussian, \( \| X_i \| \) is bounded by some constant \( C \) w.h.p., i.e., \( \| X_i \| = \sqrt{\sum_{j=1}^{d} \sigma_{j} U_{B_{ij}}^2} \leq C \) w.h.p. where \( \sigma_i \)'s are the diagonal entries of \( S_{B}^{\frac{1}{2}} \). Note \( \sigma_i = \Omega(n) \geq C' n \) for all \( i \) and some constant \( C' \), thus we get \( \sqrt{\sum_{j=1}^{d} U_{B_{ij}}^2} \leq \frac{C}{\sqrt{n}} \), i.e., \( \| U_B \|_2 \rightarrow \infty \leq \frac{C}{\sqrt{n}} \).

Hence,

\[
\| [U_B U_B] (\hat{B} - B) U_B W^* S_{B}^{\frac{1}{2}} \|_h \leq \| U_B \|_2 \| U_B (\hat{B} - B) U_B \| \| S_{B}^{\frac{1}{2}} \| \\
\leq \frac{C}{\sqrt{n}} \mathcal{O}(\log n) \mathcal{O}(n^{-\frac{1}{2}}) \\
\leq \frac{C \log n}{n} \rightarrow 0 \text{ as } n \rightarrow \infty.
\]

To show (4), we must bound the Euclidean norm of the vector

\[
\| (I - U_B U_B^\top)(\hat{B} - B) R_3 S_{B}^{\frac{1}{2}} \|_h.
\]
Define
\[ G_1 = (I - U_B U_B^\top)(\hat{B} - B)(I - U_B U_B^\top)U_B S_B^{-\frac{1}{2}}, \]
\[ G_2 = (I - U_B U_B^\top)(\hat{B} - B)U_B(U_B^\top U_B - W)S_B^{-\frac{1}{2}}. \]

Note that \((I - U_B U_B^\top)(\hat{B} - B)R_3 S_B^{-\frac{1}{2}} = G_1 + G_2\). We now only need to bound the \(h\)th row of \(G_1\) and \(G_2\).

\[
\|G_2\|_F \leq \|(I - U_B U_B^\top)(\hat{B} - B)U_B\|\|U_B^\top U_B - W^*\|_F\|S_B^{-\frac{1}{2}}\| \\
\leq \|(I - U_B U_B^\top)\|\|\hat{B} - B\|\|U_B\|\|U_B^\top U_B - W^*\|_F\|S_B^{-\frac{1}{2}}\| \\
= \mathcal{O}(1)\mathcal{O}(n^{\frac{1}{2}})\mathcal{O}(n^{-1})\mathcal{O}(n^{-\frac{1}{2}}) \\
= \mathcal{O}(n^{-1})
\]

Thus
\[
\|\sqrt{n}G_2\|_F = \mathcal{O}(n^{-\frac{1}{2}}) \to 0 \text{ as } n \to \infty.
\]

Let us consider the \(G_1\) term. Note, \(U_B^\top U_B = I\), we then have
\[
\|(G_1)_h\| = \||(I - U_B U_B^\top)(\hat{B} - B)(I - U_B U_B^\top)U_B S_B^{-\frac{1}{2}}\|_h \\
= \||(I - U_B U_B^\top)(\hat{B} - B)(I - U_B U_B^\top)U_B U_B^\top U_B S_B^{-\frac{1}{2}}\|_h \\
= \|U_B S_B^{-\frac{1}{2}}\|\||(I - U_B U_B^\top)(\hat{B} - B)(I - U_B U_B^\top)U_B U_B^\top\|_h \\
\leq \frac{C}{\sqrt{n}}\||(I - U_B U_B^\top)(\hat{B} - B)(I - U_B U_B^\top)U_B U_B^\top\|_h.
\]

Define
\[ H_1 = (I - U_B U_B^\top)(\hat{B} - B)(I - U_B U_B^\top)U_B U_B^\top, \]
and assume row-exchangability on \(H_1\), i.e., we assume \(n\mathbb{E}\|(H_1)_h\|^2 = \|H_1\|_F^2\), then Markov’s inequality gives
\[
P[\|\sqrt{n}(H_1)_h\| > t] \leq \frac{n\mathbb{E}\||(I - U_B U_B^\top)(\hat{B} - B)(I - U_B U_B^\top)U_B U_B^\top\|_h^2}{t^2} \\
= \frac{\|(I - U_B U_B^\top)(\hat{B} - B)(I - U_B U_B^\top)U_B U_B^\top\|_F^2}{t^2}.
\]

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Furthermore,
\[
\|(I - U_BU_B^\top)(\hat{B} - B)(I - U_BU_B^\top)U_BU_B^\top\|_F \leq O(1)\|\hat{B} - B\|_F \|U_B - U_BU_B^\top U_B\|_F \|U_B\|
\]

We now recall the following two observations

- The optimization problem \( \min_{T \in \mathbb{R}^{d \times d}} \|U_B - U_BT\|_F^2 \) is solved by \( T = U_B^\top U_B \).
- By theorem 2 of [19], there exists \( W \in \mathbb{R}^{d \times d} \) orthogonal, such that \( \|U_B - U_BW\|_F \leq C\|U_BU_B^\top - U_BU_B^\top\|_F \).

Combining the two facts above, we conclude that \( \|U_B - U_BU_B^\top U_B\|_F^2 \leq \frac{C}{n} \) with high probability, as in Lemma A.6, hence
\[
\|(I - U_BU_B^\top)(\hat{B} - B)(I - U_BU_B^\top)U_BU_B^\top\|_F \leq O(\sqrt{n})\frac{C}{\sqrt{n}} = O(1),
\]
which gives
\[
\mathbb{P}(\|\sqrt{n}(H_1)h\| > t) \leq \frac{C}{t^2}.
\]

Thus
\[
\lim_{n \to \infty} \frac{C}{\sqrt{n}} \|\sqrt{n}(H_1)h\| = 0,
\]
which completes the proof.

**Lemma A.11.** Let rows of \( X: X_k \overset{i.i.d.}{\sim} F \) for some sub-Gaussian distribution \( F \). Fix some \( i \in [n] \), there exists a sequence of \( d \times d \) orthogonal matrices \( W_n \), such that
\[
\sqrt{n}W_n^\top \left[(\hat{B} - B)U_BS_B^{-\frac{1}{2}}\right]_i \overset{p}{\to} N(0, \Sigma(x_i))
\]
where
\[
\Sigma(x_i) = \Xi^{-1}\hat{\Sigma}(x_i)\Xi^{-1},
\]
in which
\[
\Xi = \mathbb{E}[X_kX_k^\top] \in \mathbb{R}^{d \times d}.
\]
and
\[
\hat{\Sigma}(x_i) = \mathbb{E}_X[(\sigma^2\|x_i - X_k\|^2 + \frac{1}{4}\mathbb{E}[E_{ij}^4] - \frac{\sigma^4}{4})(X_k - \bar{\mu})(X_k - \bar{\mu})^\top] \in \mathbb{R}^{d \times d}
\]
is a covariance matrix depending on \( x_i \), and \( \bar{\mu} = \mathbb{E}[X_k] \in \mathbb{R}^d \)
Proof. Recall, since $X = U_B S_B^\frac{1}{2} W_n$, we can write
\[
\sqrt{n} W_n^\top [(\hat{B} - B)U_B S_B^{-\frac{1}{2}}]_i = \sqrt{n} W_n^\top [(\hat{B} - B)XW_n^\top S_B^{-1}]_i,
\]
\[
= \sqrt{n} W_n^\top S_B^{-1} W_n[(\hat{B} - B)X]_i
\]
\[
= \sqrt{n} W_n^\top S_B^{-1} W_n[P(D \circ E + \frac{E^2}{2})P X]_i,
\]
\[
= \sqrt{n} W_n^\top S_B^{-1} W_n[(I - \frac{11^\top}{n})(D \circ E + \frac{E^2}{2})P X]_i
\]
\[
= \sqrt{n} W_n^\top S_B^{-1} W_n[(I - \frac{11^\top}{n})(D \circ E + \frac{E^2}{2})(X - \mu)]_i
\]
\[
= \sqrt{n} W_n^\top S_B^{-1} W_n[(I - \frac{11^\top}{n})(D \circ E + \frac{E^2}{2} - \frac{\sigma^2 11^\top}{2} + \frac{\sigma^2 11^\top}{2}))(X - \mu)]_i
\]
\[
= \sqrt{n} W_n^\top S_B^{-1} W_n[(I - \frac{11^\top}{n})(D \circ E + \frac{E^2}{2} - \frac{\sigma^2 11^\top}{2}))(X - \mu)]_i
\]
\[
(\text{since } (I - \frac{11^\top}{n})\frac{\sigma^2 11^\top}{2}(X - \mu) = 0)
\]
\[
= \sqrt{n} W_n^\top S_B^{-1} W_n[(D \circ E + \frac{E^2}{2} - \frac{\sigma^2 11^\top}{2}))(X - \mu)]_i
\]
\[
(\text{since } (X - \mu) \text{ has mean } 0 \text{ and } \frac{11^\top}{n}(D \circ E + \frac{E^2}{2} - \frac{\sigma^2 11^\top}{2}))(X - \mu) \xrightarrow{n \to \infty} 0)
\]
\[
= n W_n^\top S_B^{-1} W_n[\frac{1}{\sqrt{n}}(\sum_{j \neq i}^n((D \circ E + \frac{E^2}{2} - \frac{\sigma^2 11^\top}{2}))_{ij}(X - \mu)_j)]
\]
\[
- \frac{1}{\sqrt{n}}(D \circ E + \frac{E^2}{2} - \frac{\sigma^2 11^\top}{2}))_{ii}(X - \mu)_i.
\]

Note $\frac{1}{\sqrt{n}}(D \circ E + \frac{E^2}{2} - \frac{\sigma^2 11^\top}{2}))_{ii}(X - \mu)_i \xrightarrow{n \to \infty} 0$, hence when $n \to \infty$, the above expression yields:
\[
n W_n^\top S_B^{-1} W_n[\frac{1}{\sqrt{n}}(\sum_{j \neq i}^n((D_{ij} \circ E_{ij} + \frac{E_{ij}^2}{2} - \frac{\sigma^2 11^\top}{2}))_{ij}(X_j - \bar{\mu})_j)]
\]
\[
\text{(6)}
\]
Condition on $X_i = x_i$, [6] is then the sum of $n - 1$ independent mean 0 random variables, each with covariance matrix given by:
\[
\text{cov}[(E_{ij}||x_i - X_j|| + \frac{E_{ij}^2}{2} - \sigma^2)(X_j - \bar{\mu})_j)] = \sum_{j \neq i}^n \text{var}(E_{ij}||x_i - X_j|| + \frac{E_{ij}^2}{2} - \sigma^2)(X_j - \bar{\mu})(X_j - \bar{\mu})^\top
\]

Consider
\[
\text{var}(E_{ij}||x_i - X_j|| + \frac{E_{ij}^2}{2} - \sigma^2),
\]

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which can be written as:

\[
\mathbb{E}[E^2_{ij}||x_i - X_j||^2 + E^2_{ij}||x_i - X_j|| (E^2_{ij} - \sigma^2) + \frac{(E^2_{ij} - \sigma^2)^2}{4}] - (\mathbb{E}[E_{ij}||x_i - X_j|| + \frac{E^2_{ij} - \sigma^2}{2})^2.
\]

Hence

\[
\tilde{\Sigma}(x_i) = \mathbb{E}_{X_k}[(\sigma^2||x_i - X||^2 + \frac{1}{4}\mathbb{E}[E^4_{ij}] - \frac{\sigma^4}{4})(X_k - \bar{\mu}^\top)(X_k - \bar{\mu}^\top)^\top].
\]

Finally, by the strong law of large numbers, we have

\[
\frac{W_n^\top S_B W_n}{n} = \frac{1}{n} X^\top X \rightarrow \Xi \in \mathbb{R}^{d \times d}
\]

almost surely, hence, \((nW_n^\top S_B^{-1}W_n) \rightarrow \Xi^{-1}\) almost surely. Multivariate Slutsky’s theorem then yields

\[
\sqrt{n}W_n^\top[(\hat{B} - B)U_BS_B^{-\frac{1}{2}}] \xrightarrow{\mathcal{D}} \mathcal{N}(0, \Xi^{-1}\tilde{\Sigma}(x_i)\Xi^{-1})
\]

\[
\square
\]

We can now prove Theorem [3.1].

\textbf{Proof.} Note that \(X_i = (Z_i - \bar{Z})W\), where \(W\) is an orthogonal matrix, that is \(X_i\)’s are just centered \(Z_i\)’s after some orthogonal transformation. Substituting \(X_i\)’s with \(Z_i\)’s on the right hand side of the equality in Lemma [A.11], we get the desired result.

\[
\square
\]

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