Multi-sample estimation of centered log-ratio matrix in microbiome studies

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Abstract

In microbiome studies, one of the ways of studying bacterial abundances is to estimate bacterial composition based on the sequencing read counts. Various transformations are then applied to such compositional data for downstream statistical analysis, among which the centered log-ratio (clr) transformation is most commonly used. Due to limited sequencing depth and DNA dropouts, many rare bacterial taxa might not be captured in the final sequencing reads, which results in many zero counts. Naive composition estimation using count normalization leads to many zero proportions, which makes clr transformation infeasible. This paper proposes a multi-sample approach to estimation of the clr matrix directly in order to borrow information across samples and across species. Empirical results from real datasets suggest that the clr matrix over multiple samples is approximately low rank, which motivates a regularized maximum likelihood estimation with a nuclear norm penalty. An efficient optimization algorithm using the generalized accelerated proximal gradient is developed. Theoretical upper bounds of the estimation errors and of its corresponding singular subspace errors are established. Simulation studies demonstrate that the proposed estimator outperforms the naive estimators. The method is analyzed on Gut Microbiome dataset and the American Gut project.

Keywords: Approximate low rank, Generalized accelerated proximal gradient, Metagenomics

1. Introduction

Recent studies have demonstrated that the microbiome composition varies across individuals due to different health and environmental conditions [8, 10]. Microbiome is associated with many complex diseases such as obesity, atherosclerosis, and Crohn’s disease [20, 24, 35]. With the development of next-generation sequencing technologies, the human microbiome can be quantified by using direct DNA sequencing of either marker genes or the whole metagenomes. After aligning the sequence reads to the reference microbial genomes, one obtains counts of sequencing reads that can be assigned to a set of bacterial taxa observed in the samples. Such count data provide information about the relative abundance of different bacteria in different samples.

Due to limited sequencing depths and DNA dropouts during sequencing, count results many zeros and therefore the relative proportional of bacterial taxa often include many zeros. Excessive zeros in the proportions complicate many downstream data analyses. Since the pioneering work of [1, 2, 14], several techniques have been proposed to deal with zeros in compositional or count data (see [27] for an overview). When the data are compositional, they need to be scaled so that subsequent analysis are scale-invariant, and geometrically this means to force them into the open simplex. A common practice to analyze compositional data is to map bijectively the compositions into the ordinary Euclidean space through a suitable transformation, so that standard multivariate analysis techniques can be used [2, 14]. Among many such transformations [2, 3, 14], the center log-ratio (clr) tranformation, defined as the logarithms of the bacterial composition subtracted by logarithm of the geometric mean, is most widely used in practical analysis of microbiome data. After such transformation, one can then apply the standard statistical analysis methods such as the principal component analysis based on the clr transformed data [2, 16].

Since the original data observed are counts instead of compositions in microbiome studies, one has to first estimate the compositions before applying the clr transformation. The most commonly applied methods in composition data

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analysis involve a two-step procedure. One first estimates the composition using the observed count data and then performs the clr transformation [8, 26]. Since the counts often includes many zeros, such zeros can just be replaced by an arbitrarily small numbers so that one can furtherly apply the clr transformation. One drawback of estimating the clr matrix from the estimated compositions is that the uncertainty in the estimated compositions is not accounted when they are transformed using the clrs.

In this paper, we propose a method to estimate the clr matrix directly based on the observed count data. One key idea of the proposed method is to estimate the clr matrix of compositions of multiple samples together, i.e., the clr matrix estimated from the count data from multiple samples. This effectively borrows information across multiple samples in order to obtain better estimate of the clr matrix for each of the samples. More specifically, our proposed approach is based on a penalized likelihood estimation parameterized directly based on the clr matrix, where a nuclear norm penalty on the clr matrix is imposed to capture the expected approximate low-rank structure of the clr matrix. The low rank assumption is based on the empirical observations that the bacteria taxa abundances tend to be highly correlated and individual gut microbiome samples tend to cluster together to form discrete microbial communities. This is different from the approach of [8], where the low-rank assumption is directly imposed on the compositional matrix. Since there is no constraints on the clr matrix (except trivial constraints that sum of each rows to be zero), we develop a generalized accelerated proximal gradient algorithm to efficiently perform the optimization. The computation is faster than that of [8] where a simplex projection step is needed to account for the bounded simplex constraints.

We obtain the estimation bounds of the proposed estimator and its corresponding singular vector under both the exact low-rank and approximate low-rank settings. We present simulation results to compare our estimate and commonly used zero-replacement estimate. Finally, we demonstrate the methods using the data set from [38] and data set from the American Gut Project [29].

2. A Poisson-Multinomial Model for Microbiome Count Data

We refer to any \( u \in \mathbb{R}^p \) as a composition vector if \( u_i > 0 \) for \( i = 1, 2, \ldots, p \) and \( \sum_{i=1}^{p} u_i = 1 \). The data observed in typical marker gene-based microbiome studies (i.e., 16S rRNA marker gene) can be summarized as follows. Let \( N_i \) be the total number of sequencing reads for the \( i \)th sample that can be assigned to one of the \( p \) bacterial taxa, and \( W_{ij} \) be the read count that can be assigned to the \( j \)th taxon for \( j = 1, \cdots, p \), where \( N_i = \sum_{j=1}^{p} W_{ij} \). It is natural to model the count data \( W_i = (W_{ij}, j = 1, \cdots, p) \) using a multinomial distribution with composition parameter \( X_i^* = (X_{ij}^*, j = 1, \cdots, p) \) with \( \sum_{j=1}^{p} X_{ij}^* = 1 \). Let \( X^* = (X_{ij}^*) \in \mathbb{R}^{n \times p} \) denote the \( n \times p \) compositional matrix.

Since each row of the compositional matrix \( X \) (\( X \) can be true parameter \( X^* \) or estimated one \( \hat{X} \)) is within the \( p - 1 \) dimensional simplex with a unit sum constraint, certain transformation is often needed for downstream statistical analysis, including principal component analysis, estimation of covariance and regression analysis. One of the transformations that has been widely used in compositional data analysis is the clr transformation [1, 2], which is defined as \( Z_{ij} = \log(X_{ij}/g(X_{ij})) \) where \( g(a) = \left( \prod_{i=1}^{p} a_i \right)^{1/p} \) is the geometric mean of the \( p \) proportions. This can be written as a vector form as

\[
Z_i = \text{clr}(X_i) = \log X_i \cdot \left( 1_p - \frac{1}{p} 1_p 1_p^T \right).
\]

The inverse of the clr transformation, which returns the original compositional vector \( X_i^* \), is actually the softmax function defined as

\[
X_i = \text{clr}^{-1}(Z_i) = \text{softmax}(Z_i) = \left( \frac{\exp(Z_{ij})}{\sum_{k=1}^{p} \exp(Z_{ik})} \right)_{i \times p},
\]

and the gradient of the softmax function is

\[
\nabla \text{softmax}(Z_i) = \text{diag}[\text{softmax}(Z_i)] - [\text{softmax}(Z_i)]^T \text{softmax}(Z_i) \in \mathbb{R}^{p \times p}.
\]
We let $Z^* = (Z_i^*) \in \mathbb{R}^{n \times p}$ denote the matrix of the underlying true centered log-ratio transformation of $n$ samples over $p$ taxa. Different from the work focusing on estimating $X^* \in \mathbb{R}^{n \times p}$ [8, 26], our goal is to estimate this clr matrix $Z^*$ based on the observed counts $W \in \mathbb{R}^{n \times p}$.

Using the clr matrix $Z^*$ as the parameter, the proposed Poisson-multinomial model for count-compositional data can be written as

$$N_i \sim \text{Pois}(v_i), i = 1, 2, \ldots, n;$$

$$P_{Z^*}(W_{i1}, \ldots, W_{ip}|N_i) = \frac{N_i!}{\prod_{j=1}^{p} W_{ij}!} \prod_{j=1}^{p} (Z_{ij}^*)^{W_{ij}}, i = 1, 2, \ldots, n. \quad (1)$$

where $X_{ij}^* = \text{softmax}(Z_{ij}^*) = \text{clr}^{-1}(Z_{ij}^*)$.

The maximum likelihood estimation (of each composition vector in each row) provides one naive estimation $\hat{Z}_{\text{MLE}}$ of the clr matrix $Z^*$, which is equivalent to estimating each row $Z_i^* \in \mathbb{R}^{1 \times p}$ separately using only the data observed for the $i$th sample. However, $\hat{Z}_{\text{MLE}}$ cannot resolve zero-count issue: $\hat{Z}_{ij}^\text{MLE} = -\infty$ and then softmax $\left(\hat{Z}_{ij}^\text{MLE}\right) = 0$ when $W_{ij} = 0$. One standard and commonly used method of avoiding assigning zeros to $\hat{X}_{ij}$ is the zero-replacement estimation $\hat{X}_{ij}^{\text{ZF}}$:

$$\hat{X}_{ij}^{\text{ZF}} = \frac{W_{ij} \wedge a}{\sum_{j=1}^{p} (W_{ij} \wedge a)},$$

where $a$ is an arbitrarily small number, but commonly set $a = 0.5$ [2, 7, 8, 27, 28].

On the other hand, empirical observations in real microbiome data suggest that the clr matrix $Z^*$ or composition matrix $X^*$ is usually approximate low-rank due to dependency among the bacterial taxa. In this paper, we explore this low-rank structure of $Z^*$ to provide an improved estimate of $Z^*$. This is different from [8], where composition matrix $X^*$ is assumed to be approximate low-rank.

### 3. Regularized Estimation of the Centered-Log-Ratio Matrix and the Computational Algorithm

#### 3.1. Regularized estimation of the centered-log-ratio matrix

In order to improve the estimate of the clr matrix $Z^*$, the approximate low-rank structure of the $Z^*$ is explored. The co-occurrence patterns [15], various symbiotic relationships in microbial communities [9, 18, 37] and samples in similar microbial communities are expected to lead to an approximately low-rank structure of the clr matrix in the sense that the singular values of $Z^*$ decay to zero in a fast rate. Such a low-rank structure of $Z^*$ is further investigated in our real data analysis in \S 6, showing the empirical evidence of approximate low-rank clr matrix. We propose the following nuclear-norm penalized estimation of the clr matrix $Z^*$ by exploring the low-rank structure of such a matrix,

$$\hat{Z}(\lambda) \in \arg \min_{Z_i, \neq 0} \mathcal{L}_N(Z; W) + \lambda \|Z\|_1, \quad (2)$$

where

$$\mathcal{L}_N(Z; W) \triangleq -\frac{1}{N} \sum_{i=1}^{n} N_i \mathcal{L}_N(Z_i; W) \triangleq -\frac{1}{N} \sum_{i=1}^{n} \sum_{j=1}^{p} W_{ij} \log \left(\text{softmax}(Z_{ij})\right)$$

$$= -\frac{1}{N} \sum_{i=1}^{n} \sum_{j=1}^{p} W_{ij} \log \left(\frac{e^{Z_{ij}}}{\sum_{j=1}^{p} e^{Z_{ij}}}\right) = \frac{1}{N} \sum_{i=1}^{n} \left( N_i \log \left(\sum_{j=1}^{p} e^{Z_{ij}}\right) - \sum_{j=1}^{p} W_{ij} Z_{ij} \right).$$

The proposed estimator (2) is a regularized nuclear norm minimization which can be solved by either semidefinite programming via interior-point semidefinite programming (SDP) solver, or first-order method via Templates for First-Order Conic Solvers (TFOCs). However the interior-point SDP solver computes the nuclear norm via a less efficient eigenvalue decomposition, which does not scale well with large $n$ and $p$. TFOCs on the other hand often results in the oscillations or overshoots along the trajectory of the iterations.
To achieve a stable and efficient optimization for (2) with large $n$ and $p$, we propose an algorithm based on the generalized accelerated proximal gradient method and Nesterov’s scheme. Compared to [8] which focus on estimating $X^*$ and introducing nuclear norm regularization of $X^*$, we do not need further projections and the zero-sum constraints of each row is automatically satisfied in our optimization algorithm. Algorithm with fixed tuning parameter $\lambda$ is in §3.2 and auto-tuning procedure is in §3.3. More details of §3.2 and §3.3 are provided in appendix Appendix A.

3.2. A generalized accelerated proximal gradient algorithm

We present an optimization algorithm for (2) based on the generalized accelerated Nesterov’s scheme, which follows the formulation of [5, 8] and the spirit of [34].

The algorithm involves the following steps: First, based on the count matrix, we initialize $Z^{(0)}, Y^{(0)} \in \mathbb{R}^{n \times p}$ as

\[
\begin{align*}
Z_{ij}^{(0)} &\leftarrow \hat{Z}_{ij} + \epsilon_{ij} = \text{CLR} \left( \frac{W_{ij} \wedge 0.5}{\sum_{j=1}^{p} (W_{ij} \wedge 0.5)} \right) + \epsilon_{ij}, \\
Y_{ij}^{(0)} &\leftarrow \hat{Z}_{ij}^{(0)}.
\end{align*}
\]

where $\epsilon \in \mathbb{R}^{n \times p}$ is the perturbation and $\epsilon = \hat{e} \cdot (I_p - \frac{1}{p}1_p 1_p^T)$ with $\hat{e} \in \mathbb{R}^{n \times p}$ and summation of each row of $\epsilon$ is guaranteed to be zeros while $\hat{e}$ have $n \times p$ independent and randomly-generated entries. It is worth noticing the perturbation $\epsilon$ does not appear in [8] and theoretically is not needed in convex optimization, but more likely to appear in non-convex optimization scenarios (for example, neural network scenarios). However due to numerical instability of centroid-log-ratio and softmax function [17], perturbation $\epsilon$ is important to ensure the stability of the proposed algorithm in our simulations in §5.

Next we update $Z^{(k)}$ and $Y^{(k)}$ as

\[
\begin{align*}
Z^{(k)} &\in \arg \min_{Z \in \mathbb{R}^{n \times p}} \frac{L_{k-1}}{2} \left\| Z - Z^{(k-1)} \right\|_2^2 + L_{k-1}^{-1} \nabla L_N \left( Y^{(k-1)}; W \right) + \lambda ||Z||_1, \\
Y^{(k)} &\leftarrow Z^{(k)} + \frac{k-1}{k+\rho} - 1 \left( Z^{(k)} - Z^{(k-1)} \right).
\end{align*}
\]

until convergence or a maximum number of iterations is reached. Here $\nabla L_N(Z; W)$ is the gradient function of $L_N(Z; W)$:

\[
\nabla L_N(Z; W) \triangleq \left( \frac{\partial L_N}{\partial z_{ij}} \right)_{n \times p} = \left( \frac{N_j}{N} e_{ij} - \frac{W_{ij}}{N} \sum_{k=1}^{p} e_{ak} \right)_{n \times p} = \left[ \frac{N_j}{N} \nabla L_N(z_{ij}; W_{1}) \right]_{n \times p} \in \mathbb{R}^{n \times p}
\]

and $L_k$ is the reciprocal of step size in the $k$th iteration, which can be chosen by the following line search strategy: denote

\[
f_L(Z, Y; W) = L_N(Z; W) - L_N(Y; W) - (Z - Y, \nabla L_N(Y)) - \frac{1}{2} \langle L||X - Y\rangle^2
\]

as the error of approximating $L_N(Z; W)$ by the second order Taylor expansion with the second order coefficient as $L$. In the $k$th iteration, we start with integer $n_k = 1$ and let $L_k = \gamma^n L_{k-1}$ for certain scaling parameter $\gamma > 1$, then repeatedly increasing $n_k = 1, 2, \ldots$ until $f_L(\hat{X}^{(k)}, \hat{Y}^{(k-1)}) \leq 0$. In the optimization literature, $\frac{k}{k+\rho - 1}$ and $\rho$ are, respectively, referred to as the momentum term and friction parameter. We follow the suggestions by [8, 34] and set a high friction rate that $\rho \geq \frac{\gamma}{2}$.

More details of this algorithm with fixed tuning parameter $\lambda$ are summarized in Algorithm 1 in appendix Appendix A.1, denoted as NuclearCLR $(W, \lambda)$. 

4
3.3. An auto-tuning procedure

Different from [8], we only have one tuning parameter $\lambda$ in (2) and we search within a larger search region of $\lambda$ [4, 42], that is, $\lambda$ is selected from $[2^{-3}, 2^{-2}, \ldots, 2^3, 2^4]$. Similar to [4], our tuning parameter selection procedure is based on the criteria

$$R(Z) \equiv \frac{\mathcal{L}_N(Z)}{||Z||_F} + \frac{||Z||_A}{\mathcal{L}_N(Z)},$$

(6)
motivated by the intuition that $\mathcal{L}_N(Z)$ and $\lambda \cdot ||Z||_F$ has to be of same magnitude [4]; otherwise, one of $\mathcal{L}_N(Z)$ or nuclear-regularization $\lambda ||Z||_A$ dominates the other in the optimization procedure: for example, if $\mathcal{L}_N(Z)$ is much larger than $\lambda ||Z||_A$, then the estimator might not be likely to have low-rank property since $\lambda ||Z||_A$ affects the optimization procedure in a limited way.

In first step, we initialize $\lambda^{(0)} = \mathcal{L}_N(\hat{Z}^{(0)})$ with $\hat{Z}^{(0)}$ in (3), and for $l = 0, 1, 2, \ldots$, is to empirically set $\lambda \geq \mathcal{L}_N(\hat{Z})$; similar way of setting initial value for the tuning parameter appears in [4] as well. Theoretically speaking, this is consistent with the idea of $\lambda$ having a lower bound [32]; however, we are unable to establish the lower bounds since we are unable to analytically derive duality of our objective function like [32].

In following iterative steps, we estimate $R(\hat{Z}(\lambda^{(l)}))$ and expects it decreases in first several iterations and stop when $R(\hat{Z}(\lambda^{(l)}))$ starts increasing, that is, when $R(\hat{Z}(\lambda^{(l)}))$ is close to its local minimum. Similar to [4], our search region is $[\gamma_{\lambda}^{(l)}, 0, l = 0, 1, \ldots]$ we set the empirical scaling factor $\gamma_{\lambda}$ set to 1.5.

More details are summarized in Algorithm 2 in Section Appendix .1.

4. Theoretical Properties of the Proposed Estimator

In this section, we investigate the theoretical properties of $\hat{Z}$ proposed in (2) in §3; in particular, the upper bounds of the estimation accuracy for clr matrix $Z^*$ are provided in Theorem 1 for the exact low-rank settings and Theorem 3 for the approximate low-rank settings. The following assumption appears in both settings to ensure that total number of the read counts are comparable across all the samples, which implies that the samples have similar read depths.

**Assumption 1.** Denote $R_i$, for $i \in [n]$ which quantifies the proportion of the total count for the $i$th subject. Assume there exist constants $\alpha, \beta$ such that, for any $i \in [n]$, $\frac{\alpha R_i}{n} \leq R_i \leq \frac{\beta R_i}{n}$.

This assumption also appears in [8].

4.1. Estimation bounds under the exact low-rank matrix assumption

The following theorem shows the estimation upper bound results over a class of bounded low-rank clr matrices:

$$\mathcal{B}_0(r) \triangleq \{ Z \in \mathbb{R}^{n \times p} : \text{rank}(Z) \leq r \}.$$

(7)

**Theorem 1.** Under Assumption 1 and $Z^* \in \mathcal{B}_0(r)$, with tuning parameter selected as

$$\lambda = \beta R \vee \left( \frac{p \max_{i,j} X_{ij}^*}{\min_{i,j} X_{ij}^*} \right)^2 \log(n + p) \frac{n}{N},$$

(8)

Suppose that $N \geq (n + p) \log(n + p)$, then there exists constant $C$ independent of $n, p, r$ such that

$$\frac{1}{n} \mathbb{E} \left[ \|\hat{Z}(\lambda) - Z^*\|_F^2 \right] \leq C_1(p) \cdot \frac{r(n + p) \log(n + p)}{pN},$$

with probability at least $1 - \frac{1}{n + p}$ where

$$C_1(p) = \frac{C}{\min_{i,j} X_{ij}^*} \left( \max_{i,j} X_{ij}^* \right)^2 \cdot \left( \beta R \vee \left( \frac{p \max_{i,j} X_{ij}^*}{\min_{i,j} X_{ij}^*} \right)^2 \right) \alpha R \left( \min_{i,j} X_{ij}^* \right)^2.$$
From Theorem 1, by using the softmax transformation, we can obtain an estimate of the compositional matrix $X^*$, denoted as $\hat{X}$. The following Corollary 2 gives an estimation error bound on KL divergence of estimation matrix

**Corollary 2.** Under Assumption 1 and $Z^* \in B_0(r)$, with tuning parameter selected in (8). Given a fixed constant $C_0 \geq \frac{6}{\rho_{\min_i, X^*_i, \alpha_R}}$, if $(n+p) \log(n+p) \leq N < C_0(n+p)^2 \log(n+p)$, we have

$$
\frac{1}{n} \sum_{i=1}^{n} D_{KL}\left(\text{softmax}(Z^*), \text{softmax}(Z(\lambda))\right) \leq C_3(p) \cdot \frac{r(n+p) \log(n+p)}{pN}.
$$

where

$$
C_3(p) = C \left[ \frac{\max_{i,j} X^*_i j^2}{\beta_R \vee \left( \rho \max_{i,j} X^*_i j \right)} \right], C \text{ is independent of } n, p, N, \alpha_R, \beta_R.
$$

The techniques are related to recent work on matrix completion [8, 31], although our problem setup, method and sampling procedure are all distinct from matrix completion. We apply a peeling scheme by partitioning the set of all possible values of $\hat{Z}$, and then derive estimation upper bounds for each of these subsets based on concentration inequalities.

### 4.2. Estimator bounds under approximate low-rank matrix assumption

We now consider the setting of approximately low-rank $\text{clr}$ matrix with singular values of $\text{clr}$ matrix $Z^*$ belonging to an $\ell_q$ ball,

$$
\mathcal{B}_q(\rho_q) \triangleq \left\{ Z \in \mathbb{R}^{n \times p} : \text{Z1}_p = \hat{0}_n, \sum_{i=1}^{n+p} \|Z_i\|_q^q \leq \rho_q \right\},
$$

where $0 \leq q \leq 1$. In particular, if $q = 0$ the $\ell_0$ ball $\mathcal{B}_0(\rho_0)$ corresponds to the set of bounded matrices with rank at most $\rho_0$. In general, we have the following upper bound result:

**Theorem 3.** Under Assumption 1 and $Z^* \in \mathcal{B}_q(\rho_q)$, with tuning parameter selected by (8), if $N \geq (n+p) \log(n+p)$, $N = O\left(\rho_0 p \frac{(n+p)^{\frac{1}{2}}}{n^{\frac{1}{2}}} \log(n+p)\right)$, the estimator $\hat{Z}(\lambda)$ in (2) satisfies:

$$
\frac{1}{n} \mathbb{E} \left\| \hat{Z}(\lambda) - Z^* \right\|_F^2 \leq C(n, p, q, \rho_q) \left( \frac{(n+p) \log(n+p)}{N} \right)^{1 - \frac{1}{q}}
$$

$n+p$ with probability at least $1 - \frac{1}{n^p}$ where

$$
C(n, p, q, \rho_q) = \left\{ \frac{\max_{i,j} X^*_i j^2}{\beta_R \vee \left( \rho \max_{i,j} X^*_i j \right)} \right\}^{1 - \frac{1}{q}}.
$$

and $C_1$ is independent of $n, p, N, \alpha_R, \beta_R$.

The rates of convergence of Theorem 3 with $q = 0$ and $\rho_0 = r$ reduces to the exact low-rank setting in Theorem 1.

### 4.3. Estimation of singular subspace in the low-rank setting

We assume that the true $\text{clr}$ matrix $Z^*$ with rank $r$ has the singular value decomposition

$$
Z^* = UDV^T = \sum_{i=1}^{r} d_i U_i V_i^T,
$$

where $D = \text{diag}(d_1, \ldots, d_r)$ consists of the singular values of $Z^*$ with $d_1 > d_2 > \cdots > d_r$; $U = (U_1, \cdots, U_r)$ and $V = (V_1, \cdots, V_r)$ are $\ell^2$ normalized left and right singular vectors. Given an estimate of the sample $\text{clr}$ matrix $\hat{Z}$, it is often of interest to estimate its corresponding singular vectors by the corresponding singular value decomposition [2], denote them as $\hat{U}$ and $\hat{V}$. Similar to [40, 41], we can provide an upper bound for singular subspace distance based on Theorem 1 as well as Weyl’s lemma 14 [36] and Davis-Kahan’s $\sin \Theta$ theorem [11–13].
Theorem 4. Under all the assumptions in Theorem 3 and with tuning parameter selected as in (8) and by further imposing a lower bound on the $r$th largest singular value:

$$
\sigma_{r+1}(Z^*) \leq \frac{1}{2} \sigma_r(Z^*),
$$

then for right singular vectors $V_{Z^*}$, $V_{Z(\hat{\lambda})}$ and left singular vectors $U_{Z^*}$, $U_{Z(\hat{\lambda})}$ we have

$$
\frac{4 \left\| \sin \Theta (V_{Z(\hat{\lambda})}, V_{Z^*}) \right\|_F^2}{\sigma_r^2(Z^*)} \leq C(n, p, q, \rho_q) \left( \frac{(n + p) \log(n + p)}{N} \right)^{1 - \frac{1}{2}}.
$$

with probability at least $1 - \frac{3}{n^p}$ where

$$
C(n, p, q, \rho_q) = \frac{2C_1 n}{\sigma_r^2(Z^*) \min_{i,j} X_{ij}^*} \cdot \rho_q p^2 \frac{\left\{ \max_{i,j} X_{ij}^* \right\}^4}{\alpha R \left[ \min_{i,j} X_{ij}^* \right]^4} \left( \beta R \vee \left( p \max_{i,j} X_{ij}^* \right) \right)^{1 - \frac{1}{2}}.
$$

5. Simulation Studies

We now evaluate the numerical performances of the proposed estimator $\hat{Z}_{\text{nuc}}$ under exact low-rank settings and approximate low-rank settings by simulations in §5.1, §5.2. To avoid confusion, estimator $\hat{Z}_{\text{nuc}}$ is different from estimator $\hat{Z}(\hat{\lambda})$ mentioned in §4: the estimator $\hat{Z}_{\text{nuc}}$ utilizes auto-tuning procedure in §3.3 but $\hat{Z}(\hat{\lambda})$ in §4 are for fixed tuning parameter $\lambda$.

Data generating procedures are divided into two steps:

(1) generate clr matrix $Z^*$;

(2) generate count matrix $W$ according to Poisson-Multinomial model (1): generate $R_i = \frac{P_i}{\sum_{k=1}^n P_k}$ with $P_i \sim \text{Uniform}[1, 10]$ for each individual $i \in [n]$. Based on $R_i$ and $X^* = \text{softmax}(Z^*)$, the read counts are generated from the multinomial model, i.e. $W_i \sim \text{Mult}(N_i; X^*)$, where $N_i = \gamma n p R_i$, $\gamma = 1, 2, 3, 4, 5$. The sample size is $n = 100$ and the number of taxa is $p \in \{50, 100, 150\}$.

The second step is the same for low-rank settings in §5.1 and approximate low-rank settings in §5.2. As a result, it suffices to focus on generating procedures of clr matrix $Z^*$.

5.1. Low-rank simulation settings

As we explained in the beginning of §5, it suffices to focus on generating procedure of clr matrices $Z^*$. Let $U \in \mathbb{R}^{n \times r}$ with $U_{ij} \sim N(0, 0.5)$ and $r = 20$. In order to simulate correlated compositional data arising from metagenomics, let $V = 0.2V^{(1)} + V^{(2)} \in \mathbb{R}^{n \times r}$, where

$$
V_{ij}^{(1)} = \begin{cases} 
1, & i = j; \\
0, & i \neq j \text{ with probability } q; \\
1, & i \neq j \text{ with probability } 1 - q.
\end{cases}
$$

V_{ij}^{(2)} \sim N(0, 10^{-2}),

(11)

where the choice of $(v, q)$ is specified in Table 2 and such choice is the same for low-rank settings in Table 1. Further steps of generating count matrices $W^*$ are specified in the beginning of §5.

The results are summarized in Table 1 and Table 2. The proposed estimator $\hat{Z}_{\text{nuc}}$ outperforms the zero-replacement estimator $\hat{Z}_{\text{zr}}$ and singular value thresholding estimator $\hat{Z}_{\text{svt}}$ in almost all settings. In particular, the difference between th loss of $\hat{Z}_{\text{nuc}}$ and the other two becomes more significant for smaller $\gamma$, i.e., when the number of total read counts is small; and the settings with $p = 50, 100$ has more significant loss than the settings with $p = 150$. Improvement of
Table 1: Comparison of estimation errors measured by means of squared Frobenius norm error \((\times 10^{-2})\) of for \(\hat{Z}_nuc\), \(\hat{Z}_{zr}\), \(\hat{Z}_{svt}\) for both exact and approximate low rank settings for various dimension \(p\) and parameter \(\gamma\).

| \(\gamma\) | \(\hat{Z}_nuc\) \(p = 50\) | \(\hat{Z}_{zr}\) \(p = 100\) | \(\hat{Z}_{svt}\) \(p = 150\) |
|---|---|---|---|
| Low rank settings | | | |
| 1 | 16.64 | 42.31 | 38.06 |
| 2 | 9.74 | 43.63 | 41.77 |
| 3 | 6.32 | 42.31 | 41.28 |
| 4 | 5.77 | 40.38 | 39.67 |
| 5 | 4.36 | 38.55 | 38.07 |
| Approximate low-rank settings | | | |
| 1 | 31.77 | 43.43 | 42.33 |
| 2 | 28.49 | 41.53 | 40.96 |
| 3 | 28.18 | 39.99 | 36.45 |
| 4 | 23.87 | 39.53 | 39.29 |
| 5 | 19.48 | 36.77 | 36.65 |

estimation errors measured by \(\sin \Theta\) distance for right singular subspaces in Table 2 is generally more modest than improvement of \(clr\) matrices \(\hat{Z}\): for settings with \(p = 150\), we can hardly see improvement in Table 2 although such an improvement is still significant for \(\hat{Z}\) in low-rank settings (Table 1).

To further compare the resulting estimates, Fig. 1 shows two scatter plots comparing the true \(clr\) matrix \(Z^*\) and the estimated \(\hat{Z}\) for two low-rank settings in Table 1. Although slightly biased due to the nuclear norm penalty in the estimation, it still greatly outperforms the commonly used zero-replacement estimator \(\hat{Z}_{zr}\).

5.2. Approximate low-rank simulation settings

For the approximation low-rank settings, we try to identify a data generating procedure different from the exact low-rank settings in §5.1. As we explained in the beginning of §5, it suffices to focus on generating procedure of \(clr\) matrices \(Z^*\). Different from Section §5.1, we put \(r = \min\{n, p\}\) but have \(Z^* = \tilde{U}\tilde{D}\tilde{V}^T\) (instead of \(Z^* = UV^T\)) where

(a) \(\tilde{U} \in \mathbb{R}^{n \times r}\), \(\tilde{V} \in \mathbb{R}^{p \times r}\) are (column-wise \(\ell_2\) normalized) right eigenvectors of \(U \in \mathbb{R}^{n \times r}\), \(V \in \mathbb{R}^{p \times \min\{n, p\}}\) to ensure diagonals of \(D\) can represent singular values of \(Z^*\).

(b) \(\tilde{D} = \text{diag}\left\{i^{-2}, i = 1, 2, \ldots, \min\{n, p\}\right\}\) satisfy approximate low-rank assumption (9) with \(q = 1\) (since \(\sum_{i=1}^{\infty} i^{-2} = \frac{6}{\pi^2} < \infty\))

(c) generate \(U \in \mathbb{R}^{n \times r}\) and \(V = 0, 2V^{(1)} + V^{(2)} \in \mathbb{R}^{p \times r}\) in the following way:

\[
V^{(1)}_{ij} = \begin{cases} 
1, & i = j; \\
v, & i \neq j \text{ with probability } q; \\
1, & i \neq j \text{ with probability } 1 - q.
\end{cases}
\]

\(V^{(2)}_{ij} \sim \mathcal{N}(0, 5 \cdot 10^{-2})\),

where the choice of \((v, q)\) is specified in Table 3 and this choice is the same for approximate low-rank settings in Table 1.

Further steps of generating count matrices \(W^*\) are specified in the beginning of §5.

We can see improvement in terms of estimation of \(\hat{Z}_{nuc}\) in Table 1 but not much improvement \(\hat{V}_{nuc}\) in Table 3. While in exact low-rank settings, we have already seen that estimation of singular spaces are more difficult than estimating \(clr\) matrix \(Z^*\), here such phenomena appear again in the approximate low-rank settings.
Table 2: Exact low-rank simulation settings: comparison of estimation errors measured by $\sin \Theta$ distance for right singular subspaces for $\hat{Z}_{\text{nuc}}$, $\hat{Z}_{\text{zr}}$ and $\hat{Z}_{\text{svt}}$. Data generating procedure follows §5 with $(v, q) = (-2, 0.5)$ in (11) in Section 5.1. This data generating procedure is the same for low-rank settings in Table 1.

| $p$ | $\hat{V}_{\text{nuc}}$ | $\hat{V}_{\text{zr}}$ | $\hat{V}_{\text{svt}}$ | $\|\sin \Theta\|_F^{(\times 10^{-2})}$ $\hat{V}_{\text{nuc}}, \hat{V}_{\text{zr}}, \hat{V}_{\text{svt}} \in \mathbb{R}^{p \times 1}$ | $\|\sin \Theta\|_F^{(\times 10^{-1})}$ $\hat{V}_{\text{nuc}}, \hat{V}_{\text{zr}}, \hat{V}_{\text{svt}} \in \mathbb{R}^{p \times 1}$ | $\|\sin \Theta\|_F^{(\times 10^{-1})}$ $\hat{V}_{\text{nuc}}, \hat{V}_{\text{zr}}, \hat{V}_{\text{svt}} \in \mathbb{R}^{p \times 2}$ | $\|\sin \Theta\|_F^{(\times 10^{-1})}$ $\hat{V}_{\text{nuc}}, \hat{V}_{\text{zr}}, \hat{V}_{\text{svt}} \in \mathbb{R}^{p \times 20}$ |
|-----|----------------|----------------|----------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| 50  |                |                |                | $1$ 66.25 173.47 166.67 109.80 183.52 183.81 187.68 188.40 187.12 | $2$ 62.88 172.27 173.38 79.59 185.81 186.86 186.74 | $3$ 47.02 178.15 184.54 55.36 191.11 186.30 189.71 | $4$ 45.37 170.72 182.15 50.32 181.99 184.17 197.25 | $5$ 44.81 174.84 177.70 49.34 180.63 187.62 190.09 |
| 100 |                |                |                | $1$ 239.72 330.85 328.30 283.10 351.66 352.75 364.49 363.49 363.48 | $2$ 234.11 330.45 332.03 257.10 351.48 357.89 360.79 360.95 | $3$ 230.72 331.90 334.49 280.47 356.61 359.76 360.94 358.99 | $4$ 231.13 325.36 332.15 235.63 362.28 361.96 361.58 | $5$ 238.78 333.65 335.11 220.25 361.18 359.02 359.80 |
| 150 |                |                |                | $1$ 394.14 472.05 472.84 450.04 514.22 512.28 531.68 528.68 530.43 | $2$ 388.94 475.94 476.22 423.53 511.51 512.25 526.91 528.88 529.81 | $3$ 384.03 480.26 472.65 447.31 515.79 512.42 527.39 528.44 527.09 | $4$ 383.81 473.70 479.97 402.53 516.39 515.56 527.69 531.43 528.90 | $5$ 387.86 478.80 480.26 389.71 518.93 512.66 529.37 529.42 531.04 |

9
Figure 1: Scatter plots showing comparison of shrinkage of entries between $\hat{Z}^\gamma$ and $\hat{Z}^{\text{nmuc}}$. Two settings are from the low-rank settings in Table 1, Table 2. Two figures in (1a) correspond to the setting with $\gamma = 3$, $p = 50$ and other two figures in (1b) correspond to the setting with $\gamma = 5$, $p = 50$. 
Table 3: Approximate low-rank simulation settings: comparison of estimation errors measured by $\sin \Theta$ distance for right singular subspaces for $\hat{Z}_{\text{nuc}}$, $\hat{Z}_{\text{zr}}$ and $\hat{Z}_{\text{svt}}$ in the low rank model over 50 replications (we run 50 replications since this is much slower than “low-rank” settings). Data generating procedure follows §5 with $(v, q) = (-1, 0.5)$ in Section 5.2. This data generating procedure is the same as for approximate low-rank settings in Table 1.

| $p$ | $\gamma$ | $\hat{V}_{\text{nuc}}$ | $\hat{V}_{\text{zr}}$ | $\hat{V}_{\text{svt}}$ | $\|\sin \Theta\|_F^2 \left(10^{-2}\right)$ | $\hat{V}_{\text{nuc}}, \hat{V}_{\text{zr}}, \hat{V}_{\text{svt}} \in \mathbb{R}^{p \times 1}$ | $\|\sin \Theta\|_F^2 \left(10^{-1}\right)$ | $\hat{V}_{\text{nuc}}, \hat{V}_{\text{zr}}, \hat{V}_{\text{svt}} \in \mathbb{R}^{p \times 2}$ | $\|\sin \Theta\|_F^2 \left(10^{-2}\right)$ | $\hat{V}_{\text{nuc}}, \hat{V}_{\text{zr}}, \hat{V}_{\text{svt}} \in \mathbb{R}^{p \times 3}$ | $\|\sin \Theta\|_F^2 \left(10^{-1}\right)$ | $\hat{V}_{\text{nuc}}, \hat{V}_{\text{zr}}, \hat{V}_{\text{svt}} \in \mathbb{R}^{p \times 20}$ |
|-----|-----|-----|-----|-----|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|
| $p = 50$ | 1 | 170.96 | 172.75 | 173.88 | 177.80 | 186.74 | 170.86 | 187.33 | 184.54 | 188.53 |
| | 2 | 180.30 | 175.97 | 182.29 | 179.70 | 182.22 | 180.70 | 188.56 | 186.28 | 187.65 |
| | 3 | 175.88 | 178.53 | 169.75 | 180.56 | 177.31 | 180.01 | 188.24 | 186.55 | 187.24 |
| | 4 | 180.29 | 180.16 | 175.62 | 183.38 | 184.16 | 185.00 | 186.80 | 187.23 | 188.73 |
| | 5 | 176.49 | 180.79 | 175.45 | 187.91 | 182.89 | 182.60 | 184.18 | 188.16 | 189.31 |
| $p = 100$ | 1 | 333.34 | 331.12 | 339.27 | 351.64 | 347.54 | 345.49 | 361.45 | 358.81 |
| | 2 | 329.49 | 333.59 | 337.45 | 350.35 | 352.69 | 352.94 | 363.64 | 359.81 | 360.31 |
| | 3 | 338.77 | 343.03 | 333.04 | 353.88 | 349.34 | 350.01 | 364.20 | 357.38 | 365.85 |
| | 4 | 343.73 | 343.84 | 334.12 | 353.46 | 356.75 | 355.17 | 363.32 | 367.29 | 365.61 |
| | 5 | 331.76 | 334.34 | 342.92 | 357.04 | 353.80 | 357.61 | 358.72 | 361.38 | 368.84 |
| $p = 150$ | 1 | 464.15 | 488.80 | 472.40 | 512.67 | 507.97 | 507.28 | 527.99 | 522.48 | 525.37 |
| | 2 | 478.23 | 480.28 | 477.62 | 510.23 | 506.52 | 512.77 | 526.78 | 531.88 | 528.96 |
| | 3 | 468.29 | 491.70 | 472.51 | 513.62 | 508.42 | 517.00 | 527.73 | 530.37 | 530.40 |
| | 4 | 488.29 | 486.52 | 480.52 | 505.49 | 517.41 | 515.26 | 536.24 | 536.76 | 531.08 |
| | 5 | 477.98 | 472.42 | 484.11 | 522.21 | 518.09 | 512.62 | 524.05 | 531.84 | 536.62 |

11
6. Analysis of Real Datasets

We apply our clr matrix estimation algorithm in §3 to two real datasets, the gut microbiome data set in a cohort of 98 individuals [38] and the data set from the American Gut Project [29].

6.1. Gut Microbiome Dataset

The gut microbiome plays an important role in regulating metabolic functions and influences human health and disease [30, 39]. [38] reported a cohort gut microbiome data set that includes the counts of 87 bacteria for 98 healthy volunteers.

Fig. 2 shows the decay singular values \( \hat{Z}_{nuc} \) indicating an approximate low-rank clr matrix. Fig. 3 shows boxplots for clr matrices \( \hat{Z}_{zr}, \hat{Z}_{nuc} \). To compare the results, define

\[
\Omega = \{(i, j) : i = 1, \ldots, n; j = 1, \ldots, p | W_{ij} > 0\}
\]

(12)

and \( \Omega^c \) as the support of the nonzero and zero entries in \( \mathbf{W} \), respectively. Similar to [8], Fig. (3b) shows that the observed nonzero counts have an effect on estimating the clr matrix of the genera that were observed as zeros. The estimated centered-log-ratio \( \hat{Z}_{nuc} \) in \( \Omega^c \) tends to shrink towards those in \( \Omega \). In contrast, the zero-replacement estimator \( \hat{Z}_{zr} \) in Fig. (3a) provides almost the same estimates for all the samples/taxa in \( \Omega^c \) and \( \{W_{ij} | (i, j) \in \Omega\} \), i.e. the observed nonzero counts have little effect on

\[
\{\hat{Z}_{zr} \}_{(i, j) \in \Omega^c}.
\]

6.2. American Gut Project

The microbiome data of the American Gut Project [29] includes the counts of 70 bacteria for 3,566 individuals collected through an open platform for citizen science. Fig. 4 shows the decay of singular values \( \hat{Z}_{zr} \) indicating an approximate low-rank composition matrix.

Fig. 5 shows the boxplots of the estimated clr matrices \( \hat{Z}_{zr}, \hat{Z}_{nuc} \) ordered by their columns. To compare the results, Fig. (5b) shows that the observed nonzero counts have much more effect on estimating the centered-log-ratio \( Z_{ij}^* \) of the genera that were observed as zeros than \( \hat{Z}_{zr} \) in Fig. (5a).
Figure 3: Analysis of the gut microbiome dataset of [38]. Boxplots of the estimated center log-ratio transformation for the genera corresponding to non-zero observations (Ω) and zero observations (Ωc). Fig. 3a: the zero replacement estimator $\hat{Z}^{\text{zr}}$. Fig. 3b: the proposed estimator $\hat{Z}^{\text{auto}}$ with tuning parameter set following §3.3 where the tuning parameter is auto-tuned as $\lambda = 2.15$. 
Figure 4: Analysis of the American Gut Project dataset: Fig. (4) shows decay of singular values \( \hat{d}_i \) (versus \( i \)) based on the singular value decomposition of \( \hat{Z}_{\text{nuc}} = \hat{U}_{\text{nuc}} \text{diag} \{ \hat{d}_1, \ldots, \hat{d}_{\min(n,p)} \} [\hat{V}_{\text{nuc}}]^T \), indicating the low-rank structure of the compositional matrix.

7. Discussion

Centroid-log-ratio transformation is one of the most commonly used transformations in compositional data analysis. Traditionally the centroid-log-ratios are estimated from the compositional vectors. However, in many studies such as microbiome studies that motivated our method in this paper, the raw data are counts instead of the compositions, let alone centroid-log-ratios. Treating the centroid-log-ratios as a parameter in Poisson-multinomial model for high dimensional count data, we have developed a nuclear-norm penalized maximum likelihood method for estimating the clr matrix of all the samples. The method effectively borrows information across the samples and taxa in order to achieve better estimation. We have demonstrated this using simulations and analysis of the large real datasets of Gut Microbiome Dataset and the American Gut Project. The method can be efficiently implemented using the generalized accelerated proximal gradient method.

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Supplementary Material

Supplementary material related to this article can be found online.

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| Genera                      |
|-----------------------------|
| Acinetobacter               |
| Actinomyces                 |
| Adlercreutzia               |
| Akkermansia                 |
| Alistipes                   |
| Anaerococcus                |
| Anaerostipes                |
| Anaerotruncus               |
| Bacillus                    |
| Bacteroides                 |
| Bifidobacterium             |
| Bilophila                   |
| Blautia                     |
| Butyricimonas               |
| Campylobacter               |
| Clostridium                 |
| Collinsella                 |
| Coprobacillus               |
| Coprococcus                 |
| Corynebacterium             |
| Dehalobacterium             |
| Desulfovibrio               |
| Dialister                   |
| Dorea                       |
| Eggerthella                 |
| Enterobacter                |
| Enterococcus                |
| Erwinia                     |
| Faecalibacterium            |
| Finegoldia                  |
| Fusobacterium               |
| Granulicatella              |
| Haemophilus                 |
| Holdemania                  |
| Klebsiella                  |
| Lachnobacterium             |
| Lachnospira                 |
| Lactobacillus               |
| Lactococcus                 |
| Listeria                    |
| Methanobrevibacter          |
| Odoribacter                 |
| Oscillospira                |
| Oxalobacter                 |
| Paludibacter                |
| Pantoea                     |
| Parabacteroides             |
| Paraprevotella              |
| Peptoniphilus               |
| Phascolarctobacterium       |
| Plesiomonas                 |
| Porphyromonas               |
| Prevotella                  |
| Proteus                     |
| Pseudomonas                 |
| Roseburia                   |
| Rothia                      |
| Ruminococcus                |
| Serratia                    |
| Staphylococcus              |
| Stenotrophomonas            |
| Streptococcus               |
| Sutterella                  |
| Thiothrix                   |
| Turicibacter                |
| Varibaculum                 |
| Veillonella                 |
| X. Eubacterium              |
| X. Prevotella               |
| X. Ruminococcus             |

Figure 5: Analysis of the American Gut Project dataset, showing the boxplots of the estimated center log-ratio transformation of the compositions for the genera corresponding to non-zero observations ($\Omega$) and zero observations ($\Omega^c$) in combo data set. Top panel: the zero replacement estimator $\hat{Z}^{zr}$. Bottom panel: the proposed estimator $\hat{Z}^{auto}$ with the tuning parameter set following §3.3, where the tuning parameter is auto-tuned as $\lambda = 5.99$. 
Appendix A. Details of the algorithms

This section provides more details of the algorithms described in §3.2 and §3.3.

Algorithm 1 (denoted by NuclearCLR (W, \lambda)) provides more details than those appeared in §3.2, the generalized accelerated proximal gradient algorithm solving (2) with fixed tuning parameter \lambda. 

**Algorithm 1: NuclearCLR (W, \lambda), the algorithm described in Section 3.1 for (2).**

Let \(
\begin{align*}
    &\textbf{Require:} \quad \text{Count matrix } W \in \mathbb{N}^{n \times p}, \text{tuning parameter } \lambda. \\
    &\text{Auxiliary parameters: scaling parameter } \gamma_L = 1.5, \text{initial step size } L_0, \text{friction rate } \rho = 5, \text{zero-criterion parameter } \epsilon_{\gamma_{L,0}} = 10^{-7}; \text{maximum number of iterations } K_{L,\text{max}} = 10^4. \\
    &\textbf{Ensure:} \quad \text{Estimator of centroid log ratio matrix } \hat{Z}^{(k)} \in \mathbb{R}^{n \times p}. \\
    &\text{Initialize } k = 0; \\
    &\text{(3): } 2^{(0)} = \hat{Y}^{(0)} = \text{softmax} \left( \frac{W_{i,j} - 0.5}{\sum_j (W_{i,j} - 0.5)} \right) + \epsilon, \text{ where } \epsilon \text{ is the random perturbation with } \epsilon = \tilde{\epsilon} \cdot \left( I_p - \frac{1}{p} I_p I_p \right) \text{ (and run } 4, 8, 16,... \text{ initializers due to this perturbation)}; \\
    &\text{while } k \leq K_{L,\text{max}} \text{ do} \\
    &\quad k \leftarrow k + 1; \\
    &\quad \text{Determine } \hat{Z}^{(k)}, \hat{Y}^{(k)} \text{ by (4), (4) in the following way:} \\
    &\quad \text{Set } L_0 \leftarrow L_0; \\
    &\quad \text{while True do} \\
    &\quad \quad (4) \hat{Z}^{(k)} \in \arg \min_{Z \in \mathbb{R}^{n \times p}} \frac{L_{k-1}}{2} \left\| Z - \hat{Z}^{(k-1)} + L_{k-1} \nabla L_N(\hat{Y}^{(k-1)}; W) \right\|^2_2 + \lambda \| Z \|, \text{ by SVD and singular value thresholding;} \\
    &\quad \quad (4) \hat{Y}^{(k)} \leftarrow \hat{Z}^{(k)} + \frac{1}{\sqrt{p-1}} \left( \hat{Z}^{(k)} - \hat{Z}^{(k-1)} \right); \\
    &\quad \quad \text{if } \mathcal{F}_k \left( \hat{Z}^{(k)}, \hat{Y}^{(k)}; W \right) < 0 \text{ then} \\
    &\quad \quad \quad \text{break;} \\
    &\quad \quad \text{end if} \\
    &\quad \quad L_0 \leftarrow \gamma_L L_0. \\
    &\quad \text{end while} \\
    &\quad \text{if } \mathcal{F}_k \left( \hat{Z}^{(k)}, \hat{Y}^{(k)}; W \right) \leq \epsilon_{\gamma_{L,0}} \text{ then} \\
    &\quad \quad \text{return } \hat{Z}^{(k)} \text{ (exit)}; \\
    &\quad \text{end if} \\
    &\quad \text{end while} \\
    &\quad \text{return } \hat{Z}^{(k)} \text{ (exit)}.
\end{align*}
\)
Appendix 2. Proof of Theorems

For any integer \( n > 0 \), we write \([n] = \{1, \ldots, n\}\) and denote \( e_i(n)\) as the canonical basis in \( \mathbb{R}^n \) with \( i\)th entry being one and others being zero.

Before our derivation, we present Lemma 5, which is a consequence of Davis-Kahan sin \( \Theta \) theorem. While some classical forms are in [13, 33], we present Davis-Kahan sin \( \Theta \) theorem in the context of our setting, which is analogous to [19]:

**Lemma 5** (Davis-Kahan sin \( \Theta \)). Denote singular value decomposition of symmetric matrix \( \hat{A}_m \in \mathbb{R}^{m \times n} \) as \( \hat{A}_m = V_{\hat{A}} \Sigma_{\hat{A}} V_{\hat{A}}^T + V_{\hat{A}} \Sigma_{\hat{A}} V_{\hat{A}}^T \), and similarly for \( Z_m \). Suppose \( \| \Sigma_{\hat{A}} \|_2 < \| \Sigma_{\hat{A}}^{-1} \|_2 \), where \( \| \Sigma_{\hat{A}}^{-1} \|_2 \) is the \( r \)th (absolutely) largest eigenvalue of \( \hat{A}_m \), \( \| \Sigma_{\hat{A}} \|_2 \) is the \( (r+1) \)th (absolutely) largest eigenvalue of \( \hat{A}_m \). Then for any unitarily-invariant norm \( \| \cdot \|_U \) and (we focus on ||\cdot||_F),

\[
\| (V_{\hat{A}}^T V_{\hat{A}}) \|_U \leq \frac{\| (\hat{A}_m - A_m) V_{\hat{A}} \|_U}{\| \Sigma_{\hat{A}}^{-1} \|_2 - \| \Sigma_{\hat{A}} \|_2} = O_P \left( \frac{\| \hat{A}_m - A_m \|_U}{\sigma_r (A_m)} \right).
\]

**Appendix 2.1. Proof of Theorem 1 and Theorem 3**

Theorem 1 and Theorem 3 can be considered as two special cases of following theorem:
Theorem 6 (Upper bounds). With tuning parameter selected as (8)

$$\lambda = \delta \frac{\beta^R \vee \left( p \max_{i,j} X^*_i \right)}{\left(p \min_{i,j} X^*_i \right)^2} \cdot \frac{\log(n + p)}{N},$$

$$\frac{1}{n} \|Z^* - \tilde{Z}\|_F^2 \leq \frac{C}{\min_{i,j} \text{softmax}(Z^*_i)_j}
\frac{\left[ \beta^R \vee \left( \max_{i,j} \text{softmax}(Z^*_i)_j p \right) \right]^2}{\left( \min_{i,j} \text{softmax}(Z^*_i)_j p \right)^2} \cdot \frac{\log(n + p)}{N} \sum_{i=1}^{n+p} \sigma_i(Z^*)$$

$$+ \frac{\left[ \max_{i,j} \text{softmax}(Z^*) \right]^4 \cdot \left[ \beta^R \vee \left( \max_{i,j} \text{softmax}(Z^*_i)_j p \right) \right]}{\min_{i,j} \text{softmax}(Z^*_i)_j p} \cdot \frac{\log(n + p)}{N} \sum_{i=1}^{n+p} \sigma_i(Z^*)$$

$$+ \frac{\alpha_R \left[ \min_{i,j} \text{softmax}(Z^*_i)_j \right]^3}{\left[ \beta^R \vee \left( \max_{i,j} \text{softmax}(Z^*_i)_j p \right) \right]} \cdot \frac{\log(n + p)}{N} \sum_{i=1}^{n+p} \sigma_i(Z^*)$$

$$\leq \frac{C}{\min_{i,j} \text{softmax}(Z^*_i)_j}
\frac{\left[ \max_{i,j} \text{softmax}(Z^*) \right]^4 \cdot \left[ \beta^R \vee \left( \max_{i,j} \text{softmax}(Z^*_i)_j p \right) \right]}{\min_{i,j} \text{softmax}(Z^*_i)_j p} \cdot \frac{\log(n + p)}{N} \sum_{i=1}^{n+p} \sigma_i(Z^*)$$

$$+ \frac{\alpha_R \left[ \min_{i,j} \text{softmax}(Z^*_i)_j \right]^3}{\left[ \beta^R \vee \left( \max_{i,j} \text{softmax}(Z^*_i)_j p \right) \right]} \cdot \frac{\log(n + p)}{N} \sum_{i=1}^{n+p} \sigma_i(Z^*)$$

In addition, given a fixed constant $C_0 \geq \frac{6}{p \min_{i,j} \text{softmax}(Z^*_i)_j \sigma_R}$, if $N < C_0(n + p)^2 \log(n + p)$, we have

$$\frac{1}{n} \sum_{i=1}^{n} D_{KL}(Z^*; \hat{Z})$$

$$\leq \frac{C}{\min_{i,j} \text{softmax}(Z^*_i)_j}
\frac{\left[ \max_{i,j} \text{softmax}(Z^*) \right]^4 \cdot \left[ \beta^R \vee \left( \max_{i,j} \text{softmax}(Z^*_i)_j p \right) \right]}{\min_{i,j} \text{softmax}(Z^*_i)_j p} \cdot \frac{\log(n + p)}{N} \sum_{i=1}^{n+p} \sigma_i(Z^*)$$

$$+ \frac{\alpha_R \left[ \min_{i,j} \text{softmax}(Z^*_i)_j \right]^3}{\left[ \beta^R \vee \left( \max_{i,j} \text{softmax}(Z^*_i)_j p \right) \right]} \cdot \frac{\log(n + p)}{N} \sum_{i=1}^{n+p} \sigma_i(Z^*)$$

with probability at least $1 - \frac{1}{n^p}$.

Proof. Similar to [8], the count matrix $W$ follows a multinomial distribution: $W = \sum_{k=1}^{N} E_k$ where $E_k$ are independent and identically distributed copies of a Bernoulli random matrix $E$ that satisfies

$$\mathbb{P} \left( E = e_i(n) e_j(p)^T \right) = \left[ R \cdot 1_p^T; \text{softmax}(Z^*) \right]_{ij},$$

where $R$ is specified in §4.
Consequently,

\[
\mathcal{L}_N(Z) = \frac{1}{N} \sum_{k=1}^{N} \log(\text{softmax}(Z), E_k) = \frac{1}{N} \sum_{k=1}^{N} \log(\text{softmax}(Z), E_k)
\]

\[
= \frac{1}{N} \sum_{k=1}^{N} \sum_{i=1}^{n} \log(e_i(n)e_i(n)^T \text{softmax}(Z), E_k)
\]

\[
= \frac{1}{N} \sum_{k=1}^{N} \sum_{i=1}^{n} \log(\text{softmax}(Z)^T, E_k e_i(n)).
\]  

(1)

Any solution \( \hat{Z} \) to (2) satisfies

\[
\mathcal{L}_N(\hat{Z}) - \mathcal{L}_N(Z^*)
\]

\[
\leq \frac{1}{N} \sum_{i=1}^{n} \sum_{j=1}^{p} \left[ W_{ij} \log \left( \text{softmax} \left( Z_i^* \right) \right) - W_{ij} \log \left( \text{softmax} \left( \hat{Z}_{ij} \right) \right) \right]
\]

\[
\leq \lambda \left( \|Z\|_\infty - \|\hat{Z}\|_\infty \right). 
\]

(2)

Next we present following Lemmas to derive a lower bound for (.1):

**Lemma 7.** Given the selected tuning parameter from Theorem 6, with probability at least \( 1 - \frac{1}{n^p} \), we have the following upper bound for \( \|Z^* - \hat{Z}\|_\infty \):

\[
\|Z^* - \hat{Z}\|_\infty \leq 4 \sqrt{r} \|Z^* - \hat{Z}\|_F + 4 \sum_{i=r+1}^{n+p} \sigma_i(Z^*). 
\]

(3)

**Lemma 8.** If \( Z^* \) satisfies (3) as well as \( Z1_p = \hat{0}_m \), we have

\[
\frac{1}{N} \sum_{i=1}^{n} \mathbb{R}_D KL \left( \text{softmax} \left( Z_i^* \right), \text{softmax} \left( \hat{Z} \right) \right)
\]

\[
\leq \mathcal{L}_N(\hat{Z}) - \mathcal{L}_N(Z^*) + C_2 \beta_1 \left( \frac{\max_{i,j} \text{softmax}(Z_i^*)}{p} \right)^2 \cdot \frac{\log(n + p)}{N} \sum_{i=r+1}^{n+p} \sigma_i(Z^*)
\]

\[
+ C_2 \left( \frac{\max_{i,j} \text{softmax}(Z_i^*)}{p} \right)^2 \cdot \left[ \beta_2 \vee \left( \frac{\max_{i,j} \text{softmax}(Z_i^*)}{p} \right) \right] \cdot \frac{r(n + p) \log(n + p)}{N},
\]

with probability proceeding \( 1 - \frac{2}{n^p} \).

**Lemma 9.** For any \( Z, \hat{Z} \in \mathbb{R}^{n \times p} \) such that \( Z1_p = \hat{Z}1_p = \hat{0}_m \), we have

\[
\min_{i,j} X_{ij} \leq \frac{\sum_{i=1}^{n} D_{KL} \left( \text{softmax} \left( Z_i^* \right), \text{softmax} \left( \hat{Z} \right) \right)}{\|Z^* - \hat{Z}\|_F} \leq \max_{i,j} X_{ij}.
\]

1. First regime: \( N < (n + p) \log(n + p) \). By applying Lemma 7, 9, we obtain the upper bound of \( \|Z\|_\infty - \|\hat{Z}\|_\infty \) as

\[
\|Z^* - \hat{Z}\|_\infty \leq 4 \sqrt{r} \|Z^* - \hat{Z}\|_F + 4 \sum_{i=r+1}^{n+p} \sigma_i(Z^*)
\]

\[
\leq \sqrt{\sum_{i=1}^{n} D_{KL} \left( \text{softmax} \left( Z_i^* \right), \text{softmax} \left( \hat{Z}_i^* \right) \right)} + 4 \sum_{i=r+1}^{n+p} \sigma_i(Z^*). 
\]
Therefore, combining (.2), Lemma 7 and Lemma 8 imply
\[
\frac{\beta_R}{n} \sum_{i=1}^{n} D_{KL} \left( \text{softmax}(Z_i^\ast), \text{softmax}(\hat{Z}_i) \right)
\]
\[
\leq \frac{1}{N} \sum_{i=1}^{n} R D_{KL} \left( \text{softmax}(Z_i^\ast), \text{softmax}(\hat{Z}_i) \right)
\]
\[
\leq \lambda \left[ \frac{\sum_{i=1}^{n} D_{KL} \left( \text{softmax}(Z_i^\ast), \text{softmax}(\hat{Z}_i) \right)}{n \min_{i,j} \text{softmax}(Z_i^\ast)_{j}} + 4 \sum_{i=r+1}^{n \cap p} \sigma_j(Z^\ast) \right]
\]
\[
+ \frac{\beta_R}{N} \left( \max_{i,j} \text{softmax}(Z_i^\ast)p \right) \cdot \frac{\log(n + p)}{n} \sum_{i=r+1}^{n \cap p} \sigma_j(Z^\ast) + C_2 \left( \text{softmax}(Z^\ast)p^2 \cdot [\beta_R \vee (\text{softmax}(Z^\ast)p)] \cdot \frac{r(n + p) \log(n + p)}{N} \right)
\]
with probability at least \(1 - \frac{3}{np}\). The above formula can be treated as a quadratic inequality for \(\sum_{i=1}^{n} D_{KL} \left( \text{softmax}(Z_i^\ast), \text{softmax}(\hat{Z}_i) \right)\).

We plug \(\lambda\) in Theorem 6, and obtain
\[
\frac{1}{n} \sum_{i=1}^{n} D_{KL} \left( \text{softmax}(Z_i^\ast), \text{softmax}(\hat{Z}_i) \right)
\]
\[
\leq C_3 \left\{ \frac{\beta_R}{N} \left( \max_{i,j} \text{softmax}(Z_i^\ast)p \right) \cdot \frac{\log(n + p)}{n} \sum_{i=r+1}^{n \cap p} \sigma_j(Z^\ast) + \frac{(\text{softmax}(Z^\ast)p^2 \cdot [\beta_R \vee (\text{softmax}(Z^\ast)p)] \cdot \frac{r(n + p) \log(n + p)}{N} \right) \}
\]

2. Second regime: \(N > C_0(n + p) \log(n + p)\). We denote \(\Delta = \hat{Z} - Z^\ast\). According to (.1) and Taylor expansion, that is, there exists \(t \in (0, 1)\) such that
\[
L_N(\hat{Z}) - L_N(Z^\ast) = \langle \nabla L_N(\hat{Z}), \Delta \rangle
\]
\[
= \frac{1}{N} \text{vec}(\Delta)^T \text{vec} \left( \nabla \text{vec} \left( \nabla L_N(\hat{Z} + tZ^\ast) \right) \right) \text{vec}(\Delta)
\]
\[
= \frac{1}{N} \text{vec}(\Delta)^T \sum_{i=1}^{n} \text{vec} \left( \nabla \text{vec} \left( \nabla L_N(\hat{Z} + tZ^\ast) \right) \right) \text{vec}(\Delta),
\]

\(\square\)

**Appendix .3. Proof of Lemmas**

**Appendix .3.1. Proof of Lemma 7**

For notational simplicity, we denote \(\Delta = \hat{Z} - Z^\ast \in \mathbb{R}^{exp}\), and
\[
\nabla L_N(Z) = \frac{\partial L_N}{\partial Z_{ij}} \in \mathbb{R}^{exp}
\]
\[
\nabla L_N(Z) \triangleq \left( \frac{\partial L_N}{\partial Z_{ij}} \right)_{n \times p} = \left\{ \frac{N_i}{N} e^{z_{i,j}} - \frac{W_{ij}}{N} \right\}_{n \times p} \in \mathbb{R}^{exp}
\]
and furtherly we obtain

\[ \sum_{i=1}^{n} \left( \sqrt{\sum_{j=1}^{p} \left( \frac{\partial L}{\partial Z^{i}} \right)^{2}} \right) \leq \frac{M}{3} + \sqrt{\frac{M^{2}}{9} + \frac{\sigma^{2}}{\log(n + p)}} \cdot \frac{2 \log(n + p)}{N} \leq \epsilon \cdot \frac{\log(n + p)}{N}, \]

Denote \( \text{vec}(\Delta), \text{vec}(\nabla L_{N}) \in \mathbb{R}^{np} \) vectorized forms of corresponding matrices. According to Taylor expansion,

\[ \mathcal{L}_{N}(\bar{Z}) - \mathcal{L}_{N}(Z^{*}) - \left( \nabla \mathcal{L}_{N}(Z) \cdot \Delta \right) \]

\[ = \frac{1}{N} \text{vec}(\Delta)^{T} \text{vec} \left( \nabla \text{vec} \left( \nabla \mathcal{L}_{N}(Z + i\Delta Z) \right) \right) \text{vec}(\Delta) \]

and furtherly we obtain

\[ 0 \leq \frac{1}{N} \text{vec}(\Delta)^{T} \sum_{i=1}^{n} \text{vec} \left( \nabla \text{vec} \left( \nabla \mathcal{L}_{N}(Z + i\Delta Z) \right) \right) \text{vec}(\Delta) \]

\[ = \mathcal{L}_{N}(\bar{Z}) - \mathcal{L}_{N}(Z^{*}) - \left( \nabla \mathcal{L}_{N}(Z) \cdot \Delta \right) \]

\[ \leq -\left( \nabla \mathcal{L}_{N}(\bar{Z}) \cdot \Delta \right) + \lambda \left( \|\Delta\|_{*} - \|\bar{Z}\|_{*} \right) \]

To further upper bound the nuclear norm \( \|\bar{Z} - Z^{*}\|_{*} \), we state two technical results:

**Lemma 10.** With probability at least \( 1 - \frac{1}{p^{2}} \), we have

\[ \|\nabla \mathcal{L}_{N}(Z^{*})\|_{2} \leq \frac{M}{3} + \sqrt{\frac{M^{2}}{9} + \frac{\sigma^{2}}{\log(n + p)}} \cdot \frac{2 \log(n + p)}{N} \leq \epsilon \cdot \frac{\log(n + p)}{N}, \]

\[ \sigma^{2} = 1 - \sum_{i=1}^{n} \nu_{i} \|\text{softmax}(Z_{i})\|_{2}^{2}, \]

\[ M = \sqrt{1 + \max_{i \in [n]} \left( \|c^{l-1}(Z_{i})\|_{2}^{2} - 2 \min_{j \in [p]} \|c^{l-1}(Z_{j})\|_{2}^{2} \right)} \cdot \left( \frac{512 \log(n + p)}{\log 4 \sigma_{R}^{2} N} \right), \]

Based on Lemma 10, with probability proceeding \( 1 - \frac{1}{p^{2}} \), the selected tuning parameter \( \lambda \geq 2 \|\nabla \mathcal{L}_{N}(Z^{*})\|_{2} \).

According to Lemma 1 (B.2) in [31] as well as Lemma 5 in [8], we obtain Lemma 7.

**Proof of Lemma 8**

For notational simplicity, we denote

\[ \eta \triangleq n \log \frac{\max_{i,j} X_{ij}}{\min_{i,j} X_{ij}} \left[ \frac{512 \log(n + p)}{\log 4 \sigma_{R}^{2} N} \right]^{1/2}, \]

\[ D_{R} (\text{softmax}(Z^{*}), \text{softmax}(Z)) \triangleq \sum_{i=1}^{n} R_{KL} (\text{softmax}(Z^{*}), \text{softmax}(Z_{i})). \]
The main lines of this proof are in the same spirit as Lemma 2 in [8] as well as Lemma 3 in [31]. We use a peeling argument to prove the probability of the following "bad" event is small:

\[
\mathcal{B} \triangleq \left\{ Z \in \mathbb{R}^{n \times p} : \left| \frac{1}{N} \sum_{k=1}^{N} \log(\text{softmax}(Z) - \text{softmax}(Z^*)) - D_{\mathbb{R}}(\text{softmax}(Z^*), \text{softmax}(Z)) \right| \geq D_{\mathbb{R}}(\text{softmax}(Z^*), \text{softmax}(Z)) + E(n, p, r) \right\},
\]

where \( E(n, p, r) \) is defined by

\[
E(n, p, r) \triangleq \left[ \frac{(\beta_{\mathbb{R}}/n) \vee \max_{i,j} X_{ij}}{N} \left\{ \log(n + p) \right\} + \log(n + p) \right] \]
\[
\cdot \left[ 2048 \left( \max_{i,j} \text{softmax}(Z^*) \right)^2 nr \left( \max_{i,j} X_{ij} \right)^2 \right] \left[ \min_{i,j} \text{softmax}(Z^*) \right] \frac{\alpha_{\mathbb{R}}}{\min_{i,j} X_{ij}} \]
\[
\cdot \left[ \frac{(\beta_{\mathbb{R}}/n) \vee \max_{i,j} X_{ij}}{N} \left\{ \log(n + p) \right\} \right] \]
\[
\cdot \left[ \frac{16 \max_{i,j} \text{softmax}(Z^*) \sum_{j=1}^{n \times p} \sigma_j(Z^*)}{(\log(n + p))} \right],
\]

We separate the constraint set \( \{ Z : Z1_p = \vec{0}_n \} \) into pieces and focus on a sequence of small sets:

\[
C_l \triangleq \left\{ Z : Z1_p = \vec{0}_n, 2^{l-1} \eta \leq \sum_{j=1}^{n} D_{KL}(\text{softmax}(Z^*_j), \text{softmax}(Z_j)) \leq 2\eta, l = 1, 2, 3, \ldots \right\}
\]

Notice

\[
D_{\mathbb{R}}(\text{softmax}(Z^*), \text{softmax}(Z)) \geq \frac{\alpha_{\mathbb{R}}}{n} \sum_{j=1}^{n} D_{KL}(\text{softmax}(Z^*_j), \text{softmax}(Z_j)),
\]

it suffices to estimate the probability of the following events and then apply the union bound,

\[
\mathcal{B}_l \triangleq \left\{ \exists Z : \left| \frac{1}{N} \sum_{k=1}^{N} \log(\text{softmax}(Z) - \text{softmax}(Z^*)) - D_{\mathbb{R}}(\text{softmax}(Z^*), \text{softmax}(Z)) \right| \geq \frac{2\eta \alpha_{\mathbb{R}}}{4n} + E(n, p, r), Z1_p = \vec{0}_n \right\},
\]

Since \( C_l \subset \mathcal{D}(2\eta) \triangleq \left\{ Z : Z1_p = \vec{0}_n, D_{\mathbb{R}}(\text{softmax}(Z^*), \text{softmax}(Z)) \leq 2\eta \right\} \) we can establish the upper bound of the
probability of event $\mathcal{B}$ by using the union bound, the fact that $x \geq \log x$ and Lemma 13:

$$
P(\mathcal{B}) \leq \sum_{i=1}^{\infty} P(\mathcal{D}(2^i\eta) \cap \mathcal{B})
$$

$$
\leq \sum_{i=1}^{\infty} \exp \left[ -\frac{\alpha^2 N \eta^2 4^i}{512 \left( n \log \frac{\max_i \text{softmax}(Z_i^*)}{\min_i \text{softmax}(Z_i^*)} \right)^2} \right]
$$

$$
\leq \sum_{i=1}^{\infty} \exp \left[ -\frac{\alpha^2 N \eta^2 \log 4}{512 \left( n \log \frac{\max_i \text{softmax}(Z_i^*)}{\min_i \text{softmax}(Z_i^*)} \right)^2} \right]
$$

$$
\leq \sum_{i=1}^{\infty} (n + p)^{-i} \leq \frac{2}{n + p}
$$

Note that by the conditions that $N > (n + p) \log(n + p)$, these exists some constant $C_2 > 0$ such that

$$
E(n, p, r) \leq C_2 \beta R \vee \left( \max_{i,j} \text{softmax}(Z_i^*), p \right) \log(n + p) \sum_{i=r+1}^{n+p} \sigma_i (Z^*) + C_2 \left( \max_{i,j} \text{softmax}(Z_i^*), p \right) \beta R \vee \left( \max_{i,j} \text{softmax}(Z_i^*), p \right) \alpha R \left( \min_{i,j} \text{softmax}(Z_i^*), p \right)^3 \cdot r(n + p) \log(n + p),
$$

which completes the proof.

**Proof of Lemma 9** By using Taylor expansion, we can rewrite KL divergence as

$$
\sum_{i=1}^{n} D_{KL} \left( \text{softmax}(Z_i^*), \text{softmax}(\hat{Z}_i) \right)
$$

$$
= \sum_{i=1}^{n} \left[ \log \sum_{k=1}^{p} e^{\lambda_k} - \log \sum_{k=1}^{p} e^{\lambda_k} - \sum_{k=1}^{p} \text{softmax}(Z_i^*) \cdot (\hat{Z}_{ij} - Z_{ij}^*) \right]
$$

$$
= -\sum_{i=1}^{n} \left( \hat{Z}_i - Z_i^* \right)^T \nabla^2 \text{softmax} \left( (1+t)Z_i^* + t\hat{Z}_i \right) (Z_i - Z_i^*),
$$

where $\nabla^2 \text{softmax}(\xi) = -\text{diag} \left[ \text{softmax}(\xi) \right] + \text{softmax}(\xi)^T \text{softmax}(\xi)$. Let us denote $u \triangleq \text{softmax}(\xi)$ and then for any $x \in \mathbb{R}^p \setminus \{0_p\}$ such that $x^T \mathbf{I}_p = 0$,

$$
-x^T \nabla^2 \text{softmax}(\xi) x = \frac{x^T \left( \text{diag}(u) - uu^T \right) x}{x^T x}
$$

$$
= \frac{\left( \text{diag}(u)^{\frac{1}{2}} x \right)^T \left( I_p - \text{diag}(u)^{-\frac{1}{2}} u \left[ \text{diag}(u)^{-\frac{1}{2}} u \right]^T \text{diag}(u)^{\frac{1}{2}} x \right)}{x^T x}
$$

$$
= \frac{\left( \text{diag}(u)^{\frac{1}{2}} x \right)^T \left[ I_p - \text{diag}(u)^{-\frac{1}{2}} u \left[ \text{diag}(u)^{-\frac{1}{2}} u \right]^T \text{diag}(u)^{\frac{1}{2}} x \right] \text{diag}(u)^{\frac{1}{2}} x}{x^T x}
$$

$$
= \frac{\left( \text{diag}(u)^{\frac{1}{2}} x \right)^T \text{diag}(u)^{\frac{1}{2}} x}{x^T x}
$$

24
and thus
\[
\min_j U_f (\xi_j) = \min_j u_j \cdot \inf_{y^T 1_p = 0} \frac{y^T \left( I_p - \text{diag}(u)^{-\frac{1}{2}} u \left[ \text{diag}(u)^{-\frac{1}{2}} u \right]^T \right) y}{y^T y} \leq \frac{-x^T \nabla^2 \text{softmax} (\xi) x}{x^T x} \leq \max_j u_j \cdot \sup_{y^T 1_p = 0} \frac{y^T \left( I_p - \text{diag}(u)^{-\frac{1}{2}} u \left[ \text{diag}(u)^{-\frac{1}{2}} u \right]^T \right) y}{y^T y} = \max_j \text{softmax} (\xi_j).
\]

As a result, we have (.4).

**Proof of Lemma 11**

According to (.4), we rewrite \( \nabla \mathcal{L}_N (Z^*) = -\frac{1}{N} \sum_{k=1}^N Y^{(k)} \) with \( Y^{(k)} \triangleq \begin{bmatrix} \text{softmax}(Z^-) \end{bmatrix} \) for which we have to provide upper bounds for \( \text{softmax}(Z^-)^T E_k \mathbb{I}_u \).

Notice

**Lemma 11.** \( E Y^{(k)} = 0_{n \times p} \).

**Proof.**
\[
E \left[ Y^{(k)} \right] = E \left[ \begin{bmatrix} e_i(n)^T E_k \cdot \nabla \text{clr}^{-1} (Z^*_i) \\ \langle \text{softmax}(Z^-)^T, E_k^T e_i(n) \rangle \end{bmatrix} \right] = E \left[ \begin{bmatrix} e_i(n)^T E_k \cdot \nabla \text{clr}^{-1} (Z^*_i) \\ \langle \text{softmax}(Z^-)^T, E_k^T e_i(n) \rangle \end{bmatrix} \right] \left. E_k = 1 \right| \mathbb{P}(e_i(n)^T E_k 1_p = 1),
\]
where \( \mathbb{E} \left[ \begin{bmatrix} e_i(n)^T E_k \cdot \nabla \text{clr}^{-1} (Z^*_i) \\ \langle \text{softmax}(Z^-)^T, E_k^T e_i(n) \rangle \end{bmatrix} \right] E_k = 1 \) is just having \( \xi \triangleq e_i(n)^T E_k \) as multinomial distribution with \( \text{softmax} (Z^-) \) as true composition and 1 as total count; that is,
\[
\begin{align*}
\mathbb{E} \left[ \begin{bmatrix} e_i(n)^T E_k \cdot \nabla \text{clr}^{-1} (Z^*_i) \\ \langle \text{softmax}(Z^-)^T, E_k^T e_i(n) \rangle \end{bmatrix} \right] E_k = 1 = \mathbb{E} \left[ \begin{bmatrix} e_i(n)^T E_k \cdot \nabla \text{clr}^{-1} (Z^*_i) \\ \langle \text{softmax}(Z^-)^T, E_k^T e_i(n) \rangle \end{bmatrix} \right] \left. E_k = 1 \right| \mathbb{P}(e_i(n)^T E_k 1_p = 1),
\end{align*}
\]
\[
\sum_{j=1}^p \text{softmax}(Z^-)_j \cdot \frac{\xi \cdot \nabla \text{clr}^{-1} (Z^*_j)}{\langle \text{softmax}(Z^-)_j, \xi \rangle} = \sum_{j=1}^p e_i(p)^T \nabla \text{clr}^{-1} (Z^*_j) = 0^T.
\]

As a result, \( E Y^{(k)} = 0_{n \times p} \).

Next we are to use Lemma 6 in [8], for which we have to provide upper bounds for \( \| Y^{(k)} \|_2, \| E \left[ Y^{(k)} \right]^T Y^{(k)} \|_2, \| E Y^{(k)} Y^{(k)} \|_2 \):
1. As for $\|Y^{(k)}\|_2$,

\[
\|Y^{(k)}\|_2^2 \leq \max_{ij} \left\| \frac{e_j(p)^T \cdot \nabla \text{clr}^{-1}(Z_i^*)}{(\text{softmax}(Z_i^*)^T \cdot e_j(p))^2} \right\|_2 = \max_{ij} \left\| e_j(p) - \text{clr}^{-1}(Z_i^*)^T \right\|_2^2 \\
= 1 + \max_{i \in [n]} \left[ \|\text{clr}^{-1}(Z_i^*)\|_2^2 - 2 \min_{j \in [p]} \text{clr}^{-1}(Z_i^*) \right].
\]

(8)

2. Speaking of $\|E[Y^{(k)}]^T Y^{(k)}\|_2$,

\[
E[Y^{(k)}]^T Y^{(k)} = \left[ \begin{array}{c} e_i(n)^T E_k \cdot \nabla \text{clr}^{-1}(Z_i^*) \\ \vdots \\ e_i(n)^T E_k \cdot \nabla \text{clr}^{-1}(Z_i^*) \end{array} \right]^T \left[ \begin{array}{c} E_k \cdot e_i(n) \\ \vdots \\ E_k \cdot e_i(n) \end{array} \right] \\
= \sum_{i=1}^n E \sum_{j=1}^n \frac{e_i(n)^T E_k \cdot \nabla \text{clr}^{-1}(Z_i^*)}{(\text{softmax}(Z_i^*)^T \cdot E_k e_i(n))^2} \left( e_j(n)^T E_k \cdot \nabla \text{clr}^{-1}(Z_i^*) \right) \\
= \sum_{i=1}^n E \left\{ \left( e_i(n)^T E_k \cdot \nabla \text{clr}^{-1}(Z_i^*) \right) \cdot (\text{softmax}(Z_i^*)^T, E_k^T e_i(n)) \right\} \\
= \sum_{i=1}^n P(\epsilon_i(n)^T E_k 1_p = 1) \\
E_{\epsilon_i \in \{0,1\}^{1 \times \rho} - \text{Mult}(1, \text{softmax}(Z_i^*))} \left\{ \nabla \text{clr}^{-1}(Z_i^*)^T \xi \cdot \nabla \text{clr}^{-1}(Z_i^*) \right\} \\
= \sum_{i=1}^n v_i \sum_{j=1}^p \text{softmax}(Z_i^*)_j \left( [\epsilon_j(p) - \text{softmax}(Z_i^*^T)](e_j(p)^T - \text{softmax}(Z_i^*)) \right) \\
= \sum_{i=1}^n v_i \left( (X_i^*)^T X_i^* + \text{diag}(X_i^*) \right) \left( X_i^* + \sum_{j=1}^p [\epsilon_j(p)X_i^* + (e_j(p)X_i^*)^T] \right),
\]

hence

\[
\|E[Y^{(k)}]^T Y^{(k)}\|_2 \leq 1 - \sum_{i=1}^n v_i \|\text{softmax}(Z_i^*)\|_2^2.
\]

(9)

3. Lastly, for $\|EY^{(k)}[Y^{(k)}]^T\|_2$,

\[
EY^{(k)}[Y^{(k)}]^T = \text{diag} \left\{ \frac{e_i(n)^T E_k \cdot \nabla \text{clr}^{-1}(Z_i^*)}{(\text{softmax}(Z_i^*)^T, E_k^T e_i(n))^2} \right\} \\
= \text{diag} \left\{ P(\epsilon_i(n)^T E_k 1_p = 1) \right\} \\
E \frac{e_i(n)^T E_k \cdot \nabla \text{clr}^{-1}(Z_i^*)}{(\text{softmax}(Z_i^*)^T, E_k^T e_i(n))^2} e_i(n)^T E_k 1_p \\
= \text{diag} \left\{ v_i E_{\epsilon_i \in \{0,1\}^{1 \times \rho} - \text{Mult}(1, \text{softmax}(Z_i^*))} \left[ \xi \cdot \nabla \text{clr}^{-1}(Z_i^*) \right] \cdot (\text{softmax}(Z_i^*)^T, E_k)^T \right\}
\]

26
By applying Lemma 6 in [8], (.8), (.9), (.10) imply
\[
\text{where } E
\]
\[
\text{And denote by } Z
\]
\[
\text{We define a constraint set } \mathcal{D}(T) \text{ with some constant } T > 0,
\]
\[
\mathcal{D}(T) \triangleq \left\{ \mathbf{Z} \left| \sum_{i=1}^{n} D_{KL} \left( \text{softmax}(\mathbf{Z}_i), \text{softmax}(\mathbf{Z}_i) \right) \leq T \right. \right\}.
\]

Consequently,
\[
\|\mathbf{E} \mathbf{y}^{(k)} (\mathbf{y}^{(k)})^T\|_2 = \max_{i \in [p]} v_i \left( 1 - \|\text{softmax}(\mathbf{Z}_i)\|_2 \right).
\]

By applying Lemma 6 in [8], (.8), (.9), (.10) imply
\[
P \left( \left\| \frac{1}{N} \sum_{k=1}^{N} \mathbf{y}_k \right\|_2 \geq t \right) \leq (n + p) \exp \left( -\frac{N^2 t^2 / 2}{\sigma^2 + MNt/3} \right),
\]
where \( M, \sigma^2 \) are in Lemma 10. Since Lemma 6 in [8] implies
\[
\| \frac{1}{N} \sum_{k=1}^{N} \mathbf{y}_k \|_2 \leq M \left( \frac{M^2}{9} + \frac{\sigma^2}{\log(n + p)} \right) 2 \log(n + p) / N,
\]
with probability at least 1 - \( 1 / n^{2p} \).

**Appendix 4. Concentration inequalities**

**Lemma 12.** Let \( n \times p \) random matrices \( \{ \mathbf{E}_k \}_{k=1}^{N} \) be independent and identically distributed with distribution \( \Pi = R^{i} \circ \text{softmax}(\mathbf{Z}^*) \) on \( [e_i(p)]^T, (i, j) \in [n] \times [p] \) and \( \{ \mathbf{E}_k \}_{k=1}^{N} \) is an i.i.d. Rademacher sequence. Assume \( \alpha_n / n \leq R \leq \beta_n / n \) for any \( \mathbf{Z}^* \in \mathcal{S} \) we have the upper bound
\[
\mathbf{E} \left\| \sum_{k=1}^{N} \mathbf{E}_k \right\|_2 \leq \left\{ 28 \log(n + p) \left( \frac{\beta_n}{n} \vee \max_{i,j} \text{softmax}(\mathbf{Z}^*_i) \right) \right\} \frac{1}{N} + 28 \log(n + p) / N.
\]

**Lemma 13.** We define a constraint set \( \mathcal{D}(T) \) with some constant \( T > 0 \),
\[
\mathcal{D}(T) \triangleq \left\{ \mathbf{Z} \left| \sum_{i=1}^{n} D_{KL} \left( \text{softmax}(\mathbf{Z}_i), \text{softmax}(\mathbf{Z}_i) \right) \leq T \right. \right\}.
\]

And denote by \( \mathbf{Z}_T \) the function on the constraint set \( \mathcal{D}(T) \)
\[
\mathbf{U}_T \triangleq \sup_{\mathbf{Z} \in \mathcal{D}(T)} \left| L_N (\mathbf{Z}) - L_N (\mathbf{Z}^*) - \sum_{i=1}^{n} R_i D_{KL} \left( \text{softmax}(\mathbf{Z}_i), \text{softmax}(\mathbf{Z}_i) \right) \right|.
\]

Under the assumption that \( \alpha_n / n \leq R \leq \beta_n / n \), if \( \hat{\mathbf{Z}} \) satisfies \( \| \hat{\mathbf{Z}} - \mathbf{Z}^* \| \leq 4 \sqrt{T} \), then
\[
P \left( \mathbf{U}_T \geq \frac{\alpha_n T}{n} + E(n, p, r) \right) \leq \exp \left[ -\frac{\alpha_n^2 N T^2}{512 \left( n \log \min_{i} \text{softmax}(\mathbf{Z}_i) \right)^2} \right],
\]
where \( E(n, p, r) \) is defined in (.6).
Proof. Since
\[
\sup_{\mathbf{Z} \in \mathcal{S}} \max_{i,j} |\log \text{softmax} (\mathbf{Z})_{ij} - \log \text{softmax} (\hat{\mathbf{Z}})_{ij}| \leq \log \frac{\max_{i,j} \text{softmax} (\mathbf{Z})_{ij}}{\min_{i,j} \text{softmax} (\mathbf{Z})_{ij}},
\]
we obtain the following concentration inequality by a version of Hoeffding’s inequality due to Theorem 14.2 of [6],
\[
P \left( U_T - \mathbf{E} U_T \geq \frac{\alpha_T}{8n} \right) \leq \exp \left[ -\frac{\alpha^2 T^2}{512 \left( n \log \frac{\max_{i,j} \text{softmax} (\mathbf{Z})_{ij}}{\min_{i,j} \text{softmax} (\mathbf{Z})_{ij}} \right)^2} \right]. \tag{15}
\]
It remains to upper bound the quantity \( \mathbf{E} U_T \). By using a standard symmetrization argument, we obtain
\[
\mathbf{E} U_T = \mathbf{E} \sup_{\mathbf{Z} \in \mathcal{D}(T)} \left| \mathcal{L}_N (\hat{\mathbf{Z}}) - \mathcal{L}_N (\mathbf{Z}^*) - \sum_{j=1}^n R_f D_{KL} (\text{softmax} (\mathbf{Z}^*), \text{softmax} (\hat{\mathbf{Z}})) \right|
\leq 2 \mathbf{E} \left( \sup_{\mathbf{Z} \in \mathcal{D}(T)} \left| \mathcal{L}_N (\hat{\mathbf{Z}}) - \mathcal{L}_N (\mathbf{Z}^*) \right| \right)
= 2 \mathbf{E} \left( \sup_{\mathbf{Z} \in \mathcal{D}(T)} \left| \frac{N}{\sqrt{t}} \sum_{j=1}^n e_j (\log \text{softmax} (\mathbf{Z}^*) - \log \text{softmax} (\hat{\mathbf{Z}}), E_k) \right| \right)
= 2 \mathbf{E} \left( \sup_{\mathbf{Z} \in \mathcal{D}(T)} \left| \frac{N}{\sqrt{t}} \sum_{j=1}^n e_j \sum_{i,j} \mathbf{1}_{(E_k = e_i (E_j))} \log \frac{\text{softmax} (\mathbf{Z}^*)_{ij}}{\text{softmax} (\hat{\mathbf{Z}})_{ij}} \right| \right),
\]
where \( \{e_k\}_{k=1}^n \) is an independent and identically distributed Rademacher sequence. Then the contraction principle from Theorem 4.12 in [23], together with Holder’s inequality between nuclear and operator norm, yields
\[
\mathbf{E} U_T \leq \frac{4}{\min_{i,j} \text{softmax} (\mathbf{Z}^*)_{ij}} \cdot \mathbf{E} \left( \sup_{\mathbf{Z} \in \mathcal{D}(T)} \left| \frac{N}{\sqrt{t}} \sum_{j=1}^n e_j (\log \text{softmax} (\mathbf{Z}^*) - \log \text{softmax} (\hat{\mathbf{Z}}), E_k) \right| \right)
\leq \frac{4}{\min_{i,j} \text{softmax} (\mathbf{Z}^*)_{ij}} \cdot \sup_{\mathbf{Z} \in \mathcal{D}(T)} \left\| \mathbf{Z}^* - \hat{\mathbf{Z}} \right\| \cdot \mathbf{E} \left\| \frac{N}{\sqrt{t}} \sum_{j=1}^n e_j E_k \right\|_2.
\]
We bound \( \mathbf{E} \left\| \frac{N}{\sqrt{t}} \sum_{j=1}^n e_j E_k \right\|_2 \) by applying Lemma 12. Under the assumption that \( \left\| \hat{\mathbf{Z}} - \mathbf{Z}^* \right\|_F \leq 4 \sqrt{T} \left\| \mathbf{Z} - \mathbf{Z}^* \right\|_F + 4 \sum_{i=1}^n \sigma_i (\mathbf{Z}^*) \), applying Lemma 9, we can bound \( \left\| \hat{\mathbf{Z}} - \mathbf{Z}^* \right\|_F \) by
\[
\sup_{\mathbf{Z} \in \mathcal{D}(T)} \left\| \hat{\mathbf{Z}} - \mathbf{Z}^* \right\|_F
\leq 4 \sum_{i=1}^n \sigma_i (\mathbf{Z}^*) + 4 \sqrt{T} \sup_{\mathbf{Z} \in \mathcal{D}(T)} \left\| \mathbf{Z} - \mathbf{Z}^* \right\|_F
\leq 4 \sum_{i=1}^n \sigma_i (\mathbf{Z}^*) + \frac{8 \max_{i,j} \text{softmax} (\mathbf{Z}^*)_{ij} \sqrt{T} \sum_{i=1}^n D_{KL} (\text{softmax} (\hat{\mathbf{Z}}), \text{softmax} (\mathbf{Z}^*)_{ij})}{\sqrt{n}}
\leq 4 \sum_{i=1}^n \sigma_i (\mathbf{Z}^*) + \frac{8 \max_{i,j} \text{softmax} (\mathbf{Z}^*)_{ij} \sqrt{T}}{\sqrt{n}}.
\]
As a result,

\[
\mathbf{E}U_T \leq \frac{16}{\min_{i,j} \text{softmax}(Z_i^j)} \left[ \frac{2^8 \log(n+p) \left( \beta'R/n \right)}{N} \max_{i,j} \text{softmax}(Z_i^j) \right] + \frac{2^8 \log(n+p)}{N} \\
\leq \frac{\sigma_r(Z^*) \left( \hat{Z} - Z^* \right) V_Z \text{diag} \{ \sigma_1(Z^*), \ldots, \sigma_r(Z^*) \}^{-1}}{\sigma_r(Z^*)} \leq E(n, p, r) + \frac{\alpha R T}{8n}.
\]

Finally, plugging the upper bound of \( \mathbf{E}U_t \) into concentration inequality (.15), we obtain (.14). \( \Box \)

\textbf{Proof of main results}

\textbf{Appendix .5. Proof of upper bound on singular subspace distance}

\textbf{A simple proof of the upper bound}

\textbf{Lemma 14 (Weyl’s lemma).} \( \left| \sigma_r(\hat{Z}) - \sigma_r(Z^*) \right| \leq \| \hat{Z} - Z^* \|. \)

Weyl’s lemma 14 and Davis-Kahan \text{sin} \Theta theorem (see a version from [19, 25]), for right singular vectors \( V_{Z^*}, V_{\hat{Z}} \) and an unitarily invariant norm \( \| \cdot \|_U \) we obtain

\[
\| \text{sin} \Theta(V_{\hat{Z}}, V_{Z^*}) \|_U \leq \frac{\left\| (\hat{Z} - Z^*) V_Z \right\|_U}{\sigma_r(Z^*)} \leq (10) \frac{2\left\| (\hat{Z} - Z^*) V_Z \right\|_U}{\sigma_r(Z^*)},
\]

and if we pick \( \| \cdot \|_U = \| \cdot \|_F \), Theorem 1 implies Theorem 4. Same for left singular vectors of course.

\textbf{Proofs of the asymptotic expansion of the singular subspace distance}

As an extension, we can also derive Theorem 4 from following result similar to asymptotic expansion results under Frobenius norm in [21, 22, 25, 40]:

\textbf{Theorem 15.} Under assumptions and selection of tuning parameter in Theorem 1 and by furtherly imposing a lower bound on rth largest singular value (10), then we have

\[
\frac{\sigma_r(Z)}{\| Z - Z^* \|_U} \| \text{sin} \Theta(V_{Z^*}, V_{Z^*}) \|_F = \left( \frac{\sigma_r(Z)}{\| Z - Z^* \|_U} \| (\hat{Z} - Z^*) V_{Z^*} \text{diag} \{ \sigma_1(Z^*), \ldots, \sigma_r(Z^*) \}^{-1} \|_F \right) + O_p \left( r^{-1} \frac{\| \hat{Z} - Z^* \|_U}{\sigma_r(Z^*)} \log(n) \right).
\]