Consistent Estimation of Low-Dimensional Latent Structure in High-Dimensional Data

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Abstract

We consider the problem of extracting a low-dimensional, linear latent variable structure from high-dimensional random variables. Specifically, we show that under mild conditions and when this structure manifests itself as a linear space that spans the conditional means, it is possible to consistently recover the structure using only information up to the second moments of these random variables. This finding, specialized to one-parameter exponential families whose variance function is quadratic in their means, allows for the derivation of an explicit estimator of such latent structure. This approach serves as a latent variable model estimator and as a tool for dimension reduction for a high-dimensional matrix of data composed of many related variables. Our theoretical results are verified by simulation studies and an application to genomic data.

Keywords: exponential family distribution, factor analysis, high-dimensional data, latent variable model, spectral decomposition

1. Introduction

Low-dimensional latent variable models are often used to capture systematic structure in the conditional mean space of high-dimensional random variables (rv's). This has been a popular strategy in high-dimensional probabilistic modeling and data analysis, and it serves as an attractive strategy for dimension reduction and recovering latent structure. Examples include factor analysis (Bartholomew et al., 2011), probabilistic principal components analysis (PCA) (Tipping and Bishop, 1999), non-negative matrix factorization (Lee

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and Seung, 1999), asymptotic PCA (Leek, 2011), latent Dirichlet allocation (LDA) (Blei et al., 2003), and exponential family distribution extensions of PCA (Collins et al., 2001).

Let $\mathbf{Y}_{k \times n} = (y_{ij})$ be an observed data matrix of k variables (one variable per row), each with n observations, whose entries are rv's such that

$$\theta_{ij} = \mathbb{E}\left[y_{ij}|\mathbf{M}\right] = (\mathbf{\Phi}\mathbf{M})\left(i,j\right) \text{ or } \mathbf{\Theta} = \mathbb{E}\left[\mathbf{Y}|\mathbf{M}\right] = \mathbf{\Phi}\mathbf{M},\tag{1}$$

where \mathbb{E} is the expectation operator, $\mathbf{M}_{r \times n}$ is a matrix of r latent variables, and $\mathbf{\Phi}_{k \times r}$ is a matrix of coefficients relating the latent variables to the observed variables. Furthermore, the dimensions are such as $k \gg n \ge r$. In model (1), the conditional mean θ_{ij} of y_{ij} for a fixed i only depends on the jth column \mathbf{m}^j of \mathbf{M} , and each row of the conditional mean matrix $\mathbf{\Theta}$ lies in the row space $\Pi_{\mathbf{M}}$ of \mathbf{M} . The latent structure in $\mathbf{\Theta}$ is therefore induced by $\Pi_{\mathbf{M}}$.

The above model is a general form of several highly used models. This includes instances of factor analysis (Bartholomew et al., 2011), probabilistic PCA (Tipping and Bishop, 1999), mixed membership clustering in population genetics (Pritchard et al., 2000; Alexander et al., 2009) which is closely related to LDA, and non-negative matrix factorization (Lee and Seung, 1999). Whereas the specialized models are often focused on the probabilistic interpretation of the columns of \mathbf{M} , we are instead here interested in its row space, $\Pi_{\mathbf{M}}$. This row space is sufficient for: (i) characterizing systematic patterns of variation in the data **Y**, which can be used for exploratory data analysis or dimension reduction; (ii) accounting for the latent variables in downstream modeling of **Y** (Leek and Storey, 2007, 2008) that requires adjustment for these variables; (iii) potentially identifying suitable initial values or geometric constraints for algorithms that estimate probabilistically constrained versions of \mathbf{M} ; (iv) or recovering \mathbf{M} itself if additional geometric properties are known (e.g., as in Arora et al. (2013)). Furthermore, many of the above models make assumptions about the probability distribution of \mathbf{M} that may be untrue on a given data set. One can compare our estimate of $\Pi_{\mathbf{M}}$ (which makes minimal assumptions) to the space induced by the model-based estimates of \mathbf{M} to gauge the accuracy of the model assumptions and fit. Therefore, we focus on estimation of the latent variable space $\Pi_{\mathbf{M}}$. Estimation of Φ may be tractable, but we do not focus on that here.

Leek (2011) and Anandkumar et al. (2012, 2015) have carried out work that is complementary to that presented here. They both study moment estimators of linear latent variable models applied to high-dimensional data. We explain how our work is related to Leek (2011) in Section 4.3 and how it is related to Anandkumar et al. (2012, 2015) in Appendix A. The strategies employed in these papers have ties to what we do here; however, they each consider different probabilistic models with theory that does not directly apply to the models we study.

We show that both the row space $\Pi_{\mathbf{M}}$ of \mathbf{M} (in Section 2) and the row rank of \mathbf{M} (in Section 3) can be consistently estimated using information from a suitably adjusted $n \times n$ matrix $k^{-1}\mathbf{Y}^T\mathbf{Y}$. In Section 4, we specialize these general results to y_{ij} 's that, conditional on \mathbf{M} , come from exponential family distributions. In particular, we explicitly construct a nonparametric, consistent estimator of the row space $\Pi_{\mathbf{M}}$ of \mathbf{M} for y_{ij} rv's that follow the natural exponential family (NEF) with quadratic variance function (QVF) using information only up to their second moments, and the estimator is computationally straightforward to implement. In Section 5, we extend the results of previous sections to the case where $\mathbf{\Phi}$ is random. A simulation study is conducted in Section 6 to check and confirm our theoretical findings, and we apply the estimators to a genomics data set in Section 7. Finally, we end the article with a discussion in Section 8, collect in Appendix B all technical proofs, and present the full set of results from simulation studies in Appendix C and Appendix D.

2. Almost Surely Estimating the Latent Linear Space

The big picture strategy we take is summarized as follows. Carrying out a decomposition related to Leek (2011), we first expand $k^{-1}\mathbf{Y}^T\mathbf{Y}$ into four components:

$$k^{-1}\mathbf{Y}^{T}\mathbf{Y} = k^{-1}(\mathbf{Y} - \mathbf{\Phi}\mathbf{M} + \mathbf{\Phi}\mathbf{M})^{T}(\mathbf{Y} - \mathbf{\Phi}\mathbf{M} + \mathbf{\Phi}\mathbf{M})$$
$$= \underbrace{k^{-1}(\mathbf{Y} - \mathbf{\Phi}\mathbf{M})^{T}(\mathbf{Y} - \mathbf{\Phi}\mathbf{M})}_{(i)} + \underbrace{k^{-1}(\mathbf{Y} - \mathbf{\Phi}\mathbf{M})^{T}(\mathbf{\Phi}\mathbf{M})}_{(ii)}$$
(2)

$$+\underbrace{k^{-1}(\mathbf{\Phi}\mathbf{M})^{T}(\mathbf{Y}-\mathbf{\Phi}\mathbf{M})}_{(iii)}+\underbrace{k^{-1}(\mathbf{\Phi}\mathbf{M})^{T}(\mathbf{\Phi}\mathbf{M})}_{(iv)}$$
(3)

We then show the following about each of the components as $k \to \infty$, under the assumptions given in detail below:

- (i): this term may be estimated arbitrarily well as $k \to \infty$ by a diagonal matrix defined and studied below;
- (*ii*) and (*iii*): these terms converge to the zero matrix;

• (*iv*): this term converges to a symmetric matrix with r positive eigenvalues whose leading r eigenvectors span the row space of **M**.

Once the convergence of these terms is rigorously established, the strategy we take is to form an estimate of term (i), denoted by $\hat{\mathbf{D}}_k$, and show that the space spanned by the leading r eigenvectors of $k^{-1}\mathbf{Y}^T\mathbf{Y} - \hat{\mathbf{D}}_k$ converges to the row space of \mathbf{M} as $k \to \infty$. We then also provide a framework to estimate the dimension r of the row space of \mathbf{M} and incorporate it into this estimation framework.

2.1 Model Assumptions

We first define the matrix norm $\|\mathbf{X}\| = \sqrt{\sum_{i,j} x_{ij}^2}$ for any real matrix $\mathbf{X} = (x_{ij})$ and let C > 0 denote a generic, finite constant whose value may vary at different occurrences. We first assume that $\boldsymbol{\Phi}$ is deterministic; the results in this section are extended to the case where $\boldsymbol{\Phi}$ is random in Section 5. The assumptions on model (1) are as follows:

- **A1)** $1 \leq \operatorname{rank}(\mathbf{M}) = r < n \text{ and } n \text{ is finite; } \{y_{ij} | \mathbf{M} \}_{i,j} \text{ are jointly independent with variance}$ $\mathbb{V}[y_{ij} | \mathbf{M}] = \delta_{ij} \text{ such that } \sup_{k} \max_{i,j} \mathbb{E}\left[y_{ij}^{8} | \mathbf{M}\right] \leq C \text{ (which implies } \sup_{k} \max_{i,j} \mathbb{E}\left[y_{ij}^{4} | \mathbf{M}\right] \leq C$), where \mathbb{V} is the variance operator.
- A2) $\sup_{k\geq 1} \max_{1\leq i\leq k} \|\phi_i\| \leq C$, where ϕ_i is the *i*th row of Φ . Further, for some $\mathbf{W}_{r\times r} > 0$ and some non-negative sequence $c_k \to 0$,

$$\left\|k^{-1}\boldsymbol{\Phi}^{T}\boldsymbol{\Phi} - \mathbf{W}\right\| = c_k. \tag{4}$$

Since we are considering model (1) for which \mathbf{Y} is conditioned on \mathbf{M} , all random vectors in this model are by default conditioned on \mathbf{M} unless otherwise noted (e.g., Section 5). For conciseness we will omit stating "conditional on \mathbf{M} " in this default setting.

We state a consequence of the assumption A2) as Lemma 1, whose proof is straightforward and omitted.

Lemma 1 If the assumption A2 holds, then

$$\lim_{k \to \infty} k^{-1} \sum_{i=1}^{k} \theta_{ij}^{2} = \left(\mathbf{M}^{T} \mathbf{W} \mathbf{M} \right)_{jj}$$

for each $1 \leq j \leq n$ and $\sup_{k} \max_{i,j} |\theta_{ij}| \leq C$.

The uniform boundedness results provided by Lemma 1 will be used to prove the convergence results later.

2.2 $k^{-1}\mathbf{Y}^T\mathbf{Y}$ Asymptotically Preserves the Latent Linear Space

We first derive the asymptotic form of $k^{-1}\mathbf{Y}^T\mathbf{Y}$ with the aid of the strong law of large numbers (SLLN) in Walk (2005). Let $\bar{\delta}_{kj} = k^{-1}\sum_{l=1}^k \delta_{lj}$ be the column-wise average variance of $\mathbf{Y}|\mathbf{M}$ (where $\mathbb{V}[y_{ij}|\mathbf{M}] = \delta_{ij}$ as defined above) and

$$\mathbf{D}_{k} = \operatorname{diag}\left\{\bar{\delta}_{k1}, \dots, \bar{\delta}_{kn}\right\}$$
(5)

the $n \times n$ diagonal matrix composed of these average variances.

Theorem 2 Under the assumptions for model (1),

$$\lim_{k \to \infty} \left\| k^{-1} \mathbf{Y}^T \mathbf{Y} - \mathbf{D}_k - \mathbf{H} \right\| = 0 \text{ almost surely (a.s.)},\tag{6}$$

where $\mathbf{H} = \mathbf{M}^T \mathbf{W} \mathbf{M}$.

Theorem 2 shows that $\mathbf{R}_k = k^{-1}\mathbf{Y}^T\mathbf{Y} - \mathbf{D}_k$ becomes arbitrarily close to \mathbf{H} as the number of variables $k \to \infty$. In fact, it gives much more information on the eigensystem of \mathbf{R}_k (as we take the convention that an eigenvector always has norm 1). Let $\{\beta_{k,i}\}_{i=1}^n$ be the eigenvalues of \mathbf{R}_k ordered into $\beta_{k,i} \ge \beta_{k,i+1}$ for $1 \le i \le n-1$ (where here we take the convention that the ordering of the designated multiple copies of a multiple eigenvalue is arbitrary),

 $S = \bigcup_{i=1}^{r} \left\{ \mathbf{u} : \mathbf{u} \text{ is an eigenvector of } \mathbf{R}_{k} \text{ corresponding to } \beta_{k,i} \right\},\$

and $\{\alpha_i\}_{i=1}^n$ be the eigenvalues of **H** ordered into $\alpha_i \ge \alpha_{i+1}$ for $1 \le i \le n-1$.

Corollary 3 Under the assumptions for model (1),

$$\lim_{k \to \infty} \max_{1 \le i \le n} |\beta_{k,i} - \alpha_i| = 0 \ a.s.$$
(7)

Further, $\lim_{k\to\infty} |S| = r$ a.s. and

$$\lim_{k \to \infty} \left\langle \{ \mathbf{u} \in S \} \right\rangle \triangle \Pi_{\mathbf{M}} = \emptyset \ a.s., \tag{8}$$

where $\langle \cdot \rangle$ denotes the linear space spanned by its arguments, and \triangle the symmetric set difference.

Corollary 3 reveals that asymptotically as $k \to \infty$ the eigenvalues of \mathbf{R}_k converge to those of \mathbf{H} when both sets of eigenvalues are ordered the same way, that the dimension of the space spanned by all the eigenvectors corresponding to the r largest eigenvalues of \mathbf{R}_k converges to r as $k \to \infty$, and that $\Pi_{\mathbf{M}}$ is asymptotically spanned by the leading rdimensional joint eigenspace induced by \mathbf{R}_k as $k \to \infty$. When the nonzero eigenvalues of \mathbf{H} are distinct, we easily have

$$\lim_{k \to \infty} \langle \mathbf{u}_{k,i} \rangle \bigtriangleup \langle \mathbf{v}_i \rangle = \emptyset \text{ a.s. for each } i = 1, \dots, r,$$
(9)

where, modulo a sign, $\mathbf{u}_{k,i}$ is the eigenvector corresponding to $\beta_{k,i}$ and \mathbf{v}_i that to α_i .

When the dimension r of the latent space $\Pi_{\mathbf{M}}$ and the diagonal matrix \mathbf{D}_k of the column-wise average variances are known, it follows by Corollary 3 that $\tilde{\Pi}_{\mathbf{M}} = \langle \{\mathbf{u} \in S\} \rangle$ asymptotically spans the latent space $\Pi_{\mathbf{M}}$, and $\tilde{\Pi}_{\mathbf{M}}$ converges to the row space $\Pi_{\mathbf{M}}$ with probability 1. However, in practice both r and \mathbf{D}_k need to be estimated, which is the topic of the next three sections. Estimating the number of latent variables r is in general a difficult problem. In our setting we also must accurately estimate \mathbf{D}_k , which can be a difficult task when the variances δ_{ij} may all be different (i.e., heteroskedastic).

3. Consistently Estimating the Latent Linear Space Dimension

The strategy we take to consistently estimate the dimension of the latent variable space r is to carefully scale the ordered eigenvalues of $\mathbf{R}_k = k^{-1}\mathbf{Y}^T\mathbf{Y} - \mathbf{D}_k$ and identify the index of the eigenvalue whose magnitude separates the magnitudes of these eigenvalues into two particular groups when k is large. Recall that, by Theorem 2 and Corollary 3, the difference between the vector of descendingly ordered eigenvalues of \mathbf{R}_k and that of those of $\mathbf{H} = \mathbf{M}^T \mathbf{W} \mathbf{M}$ converges to zero as $k \to \infty$. However, since rank (\mathbf{H}) = r and $\mathbf{W} > 0$, we know that the r largest eigenvalues of \mathbf{H} are positive but the rest are zero. This means that the r largest eigenvalues of \mathbf{R}_k are all strictly positive as $k \to \infty$, while the smallest

n-r eigenvalues of \mathbf{R}_k converge to 0 as $k \to \infty$. Depending on the speed of convergence of the n-r smallest eigenvalues of \mathbf{R}_k to 0, if we suitably scale the eigenvalues of \mathbf{R}_k , then the scaled, ordered eigenvalues will eventually separate into two groups, those with very large magnitudes and the rest very small. The index of the scaled, ordered eigenvalues for which such a separation happens is then a consistent estimator of r. If we replace \mathbf{R}_k with an estimator $\hat{\mathbf{R}}_k = k^{-1}\mathbf{Y}^T\mathbf{Y} - \hat{\mathbf{D}}_k$ that satisfies a certain level of accuracy detailed below, then the previous reasoning applied to the eigenvalues of $\hat{\mathbf{R}}_k$ will also give a consistent estimator of r.

To find the scaling sequence for the magnitudes of the eigenvalues of \mathbf{R}_k or equivalently the speed of convergence of the n-r smallest eigenvalues of \mathbf{R}_k to 0, we define the $k \times n$ matrix \mathbf{E} with entry $\mathbf{E}(i, j) = e_{ij} = y_{ij} - \theta_{ij}$, and study as a whole the random part of $k^{-1}\mathbf{Y}^T\mathbf{Y}$ defined by

$$\mathbf{F} = \underbrace{k^{-1}\mathbf{E}^T\mathbf{E}}_{(i)} + \underbrace{k^{-1}\mathbf{E}^T\mathbf{\Theta}}_{(ii)} + \underbrace{k^{-1}\mathbf{\Theta}^T\mathbf{E}}_{(iii)}.$$
(10)

Note that the terms (i), (ii) and (iii) in **F** correspond to those from equation (3). We will show that **F** configured as a $2n^2$ vector possesses asymptotic Normality after centering and scaling as $k \to \infty$. This then reveals that the scaling sequence for the eigenvalues of \mathbf{R}_k should be no smaller than being proportional to $k^{-1/2}$.

Let $\boldsymbol{\Delta} = (\delta_{ij}), \, \boldsymbol{\Delta}_i = \text{diag} \{\delta_{i1}, ..., \delta_{in}\}$ and define

$$\mathbf{z}_{i} = k^{-1} \left(e_{i1} \mathbf{e}_{i}, ..., e_{in} \mathbf{e}_{i}, \boldsymbol{\phi}_{i} \mathbf{m}^{1} \mathbf{e}_{i}, ..., \boldsymbol{\phi}_{i} \mathbf{m}^{n} \mathbf{e}_{i} \right)$$
(11)

for $1 \leq i \leq k$, where \mathbf{e}_i and \mathbf{m}^j are respectively the *i*th row of \mathbf{E} and the *j*th column of \mathbf{M} . We have:

Proposition 4 Under model (1), **F** is a linear function of $\sum_{i=1}^{k} \mathbf{z}_{i}$ with global Lipschitz constant 1. If we assume A1) and A2) from Section 2 and also

A3) The sequences $k^{-1} \sum_{i=1}^{k} \mathbb{E}\left[e_{ij}^{4}|\mathbf{M}\right], k^{-1} \sum_{i=1}^{k} \phi_{i} \mathbb{E}\left[e_{ij}^{3}|\mathbf{M}\right] and k^{-1} \sum_{i=1}^{k} \phi_{i} \mathbf{m}^{j} \phi_{i} \mathbf{m}^{l} \boldsymbol{\Delta}_{i} for$ any $1 \leq j \leq l \leq n$ are all convergent as $k \to \infty$,

then $\sum_{i=1}^{\kappa} \sqrt{k} (\mathbf{z}_i - \mathbb{E}[\mathbf{z}_i | \mathbf{M}])$ converges in distribution to a multivariate Normal random vector with mean zero.

With the concentration property of \mathbf{F} established by Proposition 4, we will be able to explore the possibility of consistently estimating r by studying the magnitudes of eigenvalues $\{\hat{\alpha}_{k,i}\}_{i=1}^n$ of

$$\hat{\mathbf{R}}_{k} = k^{-1} \mathbf{Y}^{T} \mathbf{Y} - \hat{\mathbf{D}}_{k} \text{ with } \hat{\mathbf{D}}_{k} = \operatorname{diag} \left\{ \hat{\delta}_{k1}, \dots, \hat{\delta}_{kn} \right\},$$
(12)

where each $\hat{\delta}_{kj}$ is an estimate of $\bar{\delta}_{kj}$ for $1 \leq j \leq n$, and the $\hat{\alpha}_{k,i}$'s are ordered into $\hat{\alpha}_{k,i} \geq \hat{\alpha}_{k,i+1}$ for $1 \leq i < n-1$.

Theorem 5 Under the assumptions A1), A2) and A3), if

A4) for some non-negative ε_k such that $\varepsilon_k \to 0$,

$$\left\|\hat{\mathbf{D}}_{k} - \mathbf{D}_{k}\right\| = \varepsilon_{k},\tag{13}$$

then

$$\left\| \hat{\mathbf{R}}_{k} - \mathbf{H} \right\| = O_{\Pr}\left(\tau_{k}\right) \text{ and } \left\| \hat{\alpha}_{k,i} - \alpha_{i} \right\| = O_{\Pr}\left(\tau_{k}\right), \tag{14}$$

where Pr is the probability measure and

$$\tau_k = \max\left\{k^{-1/2}, \varepsilon_k, c_k\right\}.$$
(15)

Further, for any $\tilde{\tau}_k > 0$ such that $\tilde{\tau}_k = o(1)$ and $\tau_k = o(\tilde{\tau}_k)$, as $k \to \infty$,

$$\begin{cases} \Pr\left(\tilde{\tau}_{k}^{-1}\hat{\alpha}_{k,i} > \tilde{c}\right) \to 0 & \text{if } r+1 \le i \le n, \\ \Pr\left(\tilde{\tau}_{k}^{-1}\hat{\alpha}_{k,i} \to \infty\right) \to 1 & \text{if } 1 \le i \le r, \end{cases}$$
(16)

for any fixed $\tilde{c} > 0$. Therefore, letting

$$\hat{r} = \sum_{i=1}^{n} \mathbb{1}_{\left\{\tilde{\tau}_{k}^{-1}\hat{\alpha}_{k,i} > \tilde{c}\right\}}$$
(17)

gives

$$\Pr\left(\hat{r}=r\right) \to 1 \ as \ k \to \infty,\tag{18}$$

where 1_A is the indicator of a set A.

Theorem 5 shows that the speed of convergence, $\{\tau_k\}_{k\geq 1}$, of the eigenvalues of $\hat{\mathbf{R}}_k$ (and those of \mathbf{R}_k) is essentially is determined by those related to $k^{-1} \boldsymbol{\Phi}^T \boldsymbol{\Phi}$ and \mathbf{D}_k ; see equations (13)–(15). Further, it reveals that, when $\{\tau_k\}_{k\geq 1}$ is known, with probability approaching

to 1 as $k \to \infty$, the scaled, ordered eigenvalues $\{\tilde{\tau}_k^{-1}\hat{\alpha}_{k,i}\}_{i=1}^n$ eventually separates into two groups: $\tilde{\tau}_k^{-1}\hat{\alpha}_{k,i}$ for $1 \leq i \leq r$ all lie above \tilde{c} but the rest all lie below \tilde{c} for any chosen $\tilde{c} > 0$. In other words, for a chosen $\tilde{c} > 0$, the number of $\tilde{\tau}_k^{-1}\hat{\alpha}_{k,i} > \tilde{c}$ when k is large is very likely equal to r. However, in practice $\{\varepsilon_k\}_{k\geq 1}$ and $\{c_k\}_{k\geq 1}$ are unknown, and even if they are known or can be estimated, unfortunately the hidden constants in (14) are unknown (even when $k = \infty$). Further, when k is finite, the n - r smallest eigenvalues of $\hat{\mathbf{R}}_k$ may not yet be identically zero, the hidden constants may have a large impact on estimating the scaling sequence $\tilde{\tau}_k$, and rates slightly different than $\tilde{\tau}_k$ may have to be chosen to balance the effects of the hidden constants; see in Section 6 a brief discussion on the estimation of $\tilde{\tau}_k$ and the effects of choosing $\tilde{\tau}_k$ on estimating r for finite k.

Before we apply our theory to y_{ij} 's that follow specific parametric distributions, we pause to comment on the key results obtained so far. Theorem 2 and Corollary 3 together ensure that asymptotically as $k \to \infty$ we can span the row space $\Pi_{\mathbf{M}}$ of \mathbf{M} by the rleading eigenvectors of $\mathbf{R}_k = k^{-1}\mathbf{Y}^T\mathbf{Y} - \mathbf{D}_k$ (see the definition of \mathbf{D}_k in (5)). However, the conclusions in these results are based on a known r and \mathbf{D}_k . In contrast, Proposition 4 and Theorem 5 retain similar assertions to those of Theorem 2 and Corollary 3 by replacing the unknown \mathbf{D}_k by its consistent estimate $\hat{\mathbf{D}}_k$, and they enable us to construct a consistent estimate \hat{r} of r such that the linear space spanned by the leading \hat{r} eigenvectors of $\hat{\mathbf{R}}_k = k^{-1}\mathbf{Y}^T\mathbf{Y} - \hat{\mathbf{D}}_k$ consistently estimates $\Pi_{\mathbf{M}}$ as $k \to \infty$. This reveals that to consistently estimate $\Pi_{\mathbf{M}}$ in a fully data driven approach using our theory, it is crucial to develop a consistent estimate $\hat{\mathbf{D}}_k$ of \mathbf{D}_k .

4. Specializing to Exponential Family Distributions

We specialize the general results obtained in Section 2 and Section 3 for model (1) to the case when y_{ij} follow the single parameter exponential family probability density function (pdf) given by

$$f(y;\theta) = h(y) \exp\left\{\eta(\theta)y - g(\eta(\theta))\right\},\tag{19}$$

where η is the canonical link function, and g and h are known functions such that $f(y;\theta)$ is a proper pdf. The values that θ can take are $\Omega = \{\theta \in \mathbb{R} : \int f(y;\theta) = 1\}$. The following corollary says that our general results on consistent estimation of the latent space $\Pi_{\mathbf{M}}$ and its dimension r hold when the link function η is bounded on the closure of the parameter space $\Omega_0 \subseteq \Omega$. **Corollary 6** Suppose Ω_0 is an open subset of Ω such that its closure lies in the interior of Ω . If conditional on \mathbf{M} each y_{ij} has pdf of the form (19) with $\theta_{ij} \in \Omega_0$ and η is bounded as a function of θ in the closure of Ω_0 , then $\sup_k \max_{i,j} \mathbb{E}\left[y_{ij}^8 | \mathbf{M}\right] \leq C$, which implies that Theorem 2, Corollary 3, Proposition 4 and Theorem 5 hold.

We remark that the boundedness of η on the closure of Ω_0 is not restrictive, in that in practice either Ω_0 is bounded in Euclidean norm or η is bounded in supremum norm. The proof of Corollary 6 is a simple observation that g is analytic in η when $\theta \in \Omega_0$ (see, e.g. Letac and Mora, 1990) and that the derivative of g in η of any order is bounded when η is bounded; the proof is thus omitted.

4.1 Estimating D_k

With Corollary 6 (see also the discussion at the end of Section 3), we only need to estimate $\bar{\delta}_{kj}$ (which in turn yields \mathbf{D}_k) in order to consistently estimate r and $\Pi_{\mathbf{M}}$. To obtain an estimate $\hat{\delta}_{kj}$ of $\bar{\delta}_{kj}$ when potentially all δ_{ij} are different from each other (i.e., complete heteroskedasticity), we exploit the intrinsic relationship between θ_{ij} and δ_{ij} when y_{ij} come from a certain class of natural exponential family (NEF) distributions.

Lemma 7 Let y have marginal pdf (19). Then there exists a quadratic function $v(\cdot)$ such that $\mathbb{E}[v(y)] = \mathbb{V}[y]$ if and only if f parametrized by η forms an NEF with quadratic variance function (QVF) defined by Morris (1982) such that

$$\mathbb{V}[y] = b_0 + b_1 \mathbb{E}[y] + b_2 (\mathbb{E}[y])^2 \quad with \ b_2 \neq -1$$
(20)

for some $b_0, b_1, b_2 \in \mathbb{R}$. Specifically, (20) implies

$$v(t) = (1+b_2)^{-1} (b_0 + b_1 t + b_2 t^2).$$
(21)

The proof of Lemma 7 is straightforward and omitted. Table 1 lists $v(\cdot)$ for the six NEFs with QVF.

Inspired by the availability of the function $v(\cdot)$ obtained in Lemma 7, we now state a general result on how to explicitly construct a $\hat{\mathbf{D}}_k$ that properly estimates \mathbf{D}_k .

Lemma 8 Let y_{ij} have pdf(19) such that $\mathbb{V}[y_{ij}|\mathbf{M}] = \mathbb{E}[v(y_{ij})|\mathbf{M}]$ for some function $v(\cdot)$ satisfying

$$\sup_{k} \max_{i,j} \mathbb{E}\left[v^{4}\left(y_{ij}\right) | \mathbf{M}\right] \le C < \infty.$$
(22)

Table 1: The function $v(\cdot)$ such that $\mathbb{E}[v(y)] = \mathbb{V}[y]$ when y has pdf (19) and comes from a NEF with QVF in Morris (1982). Note that $\text{logit}(x) = \log \frac{x}{1-x}$ for $x \in (0,1)$ and "GHS" stands for "generalized hyperbolic secant distribution".

	θ	$\mathbb{V}[y]$	v(y)	$\eta(heta)$
$Normal(\mu, 1)$	μ	1	1	θ
$Poisson(\lambda)$	λ	θ	y	$\log(heta)$
$\operatorname{Binomial}(s, p)$	sp	$\theta - \theta^2/s$	$(sy - y^2)/(s - 1)$	$\operatorname{logit}(\theta/s)$
$\operatorname{NegBin}(s, p)$	sp/(1-p)	$\theta + \theta^2/s$	$(sy + y^2)/(s + 1)$	$\log(\theta/(s+\theta))$
$\operatorname{Gamma}(s,\lambda)$	s/λ	$ heta^2/s$	$y^2/(1+s)$	-1/ heta
$\operatorname{GHS}(s,\lambda)$	$s\lambda$	$s + \theta^2/s$	$(s^2 + y^2)/(1+s)$	$\arctan(\theta/s)$

Then

$$\hat{\delta}_{kj} = k^{-1} \sum_{l=1}^{k} v(y_{lj})$$
(23)

satisfies $\lim_{k\to\infty} \left| \hat{\delta}_{kj} - \bar{\delta}_{kj} \right| = 0$ a.s. for each $1 \leq j \leq n$. If additionally, for each $1 \leq j \leq n$ and some $\sigma_j > 0$,

$$\lim_{k \to \infty} k^{-1} \sum_{l=1}^{k} \mathbb{V} \left[v \left(y_{lj} \right) | \mathbf{M} \right] = \sigma_j,$$
(24)

then $\sqrt{k}\left(\hat{\delta}_{kj}-\bar{\delta}_{kj}\right)$ converges in distribution to a Normal random variable as $k\to\infty$.

Lemma 8 shows that $\hat{\mathbf{D}}_k$ in (12) with $\hat{\delta}_{kj}$ defined by (23) satisfies $\lim_{k\to\infty} \left\| \hat{\mathbf{D}}_k - \mathbf{D}_k \right\| \stackrel{\text{a.s.}}{=} 0$. Note that the first assertion in Lemma 8, i.e., $\lim_{k\to\infty} \left| \hat{\delta}_{kj} - \bar{\delta}_{kj} \right| = 0$ a.s., clearly applies to y_{ij} that follow NEFs with QVF when their corresponding θ_{ij} are in a set Ω_0 described in Corollary 6. We remark that requiring the closure of Ω_0 to be in the interior of Ω is not restrictive, since in practice the θ_{ij} 's are not the boundary points of Ω .

4.2 Simultaneously Consistently Estimating the Latent Linear Space and Its Dimension

We are ready to present a consistent estimator of the latent linear space $\Pi_{\mathbf{M}}$:

- 1. Set $\hat{\mathbf{R}}_k = k^{-1} \mathbf{Y}^T \mathbf{Y} \hat{\mathbf{D}}_k$ as (12) with $\hat{\delta}_{kj}$ as in (23).
- 2. Estimate r as \hat{r} using (18) as given in Theorem 5.

- 3. From the spectral decomposition $\hat{\mathbf{R}}_k = \mathbf{V}\mathbf{K}\mathbf{V}^T$ where $\mathbf{V}^T\mathbf{V} = \mathbf{I}$ and $\mathbf{K} = \text{diag}\left\{\hat{\alpha}_{k,i}\right\}_{i=1}^n$, pick \hat{r} columns $\left\{\hat{\mathbf{u}}_{k,i}\right\}_{i=1}^{\hat{r}}$ of \mathbf{V} corresponding to the \hat{r} largest $\left\{\hat{\alpha}_{k,i}\right\}_{i=1}^{\hat{r}}$.
- 4. Set

$$\hat{\Pi}_{\mathbf{M}} = \left\langle \{ \hat{\mathbf{u}}_{k,i} \}_{i=1}^{\hat{r}} \right\rangle \tag{25}$$

to be the estimate of $\Pi_{\mathbf{M}}$. Note that $\hat{\mathbf{M}} = (\hat{\mathbf{u}}_{k,1}, ..., \hat{\mathbf{u}}_{k,\hat{r}})^T$ can be regarded as an estimator of \mathbf{M} even though it is not our focus.

The above procedure is supported by the following theorem, whose proof is straightforward and omitted. More specifically, $\hat{\Pi}_{\mathbf{M}}$ in (25) consistently estimates $\Pi_{\mathbf{M}}$.

Theorem 9 Under the assumptions of Theorem 2 and Lemma 8, $\lim_{k\to\infty} \left\| \hat{\mathbf{R}}_k - \mathbf{H} \right\| = 0$ a.s. and $\lim_{k\to\infty} \left\langle \{ \hat{\mathbf{u}}_{k,i} \}_{i=1}^r \right\rangle \Delta \Pi_{\mathbf{M}} = \emptyset$ a.s.. If additionally the conditions of Theorem 5 are satisfied, then equation (18) holds and $\lim_{k\to\infty} \Pr\left(\left\{ \hat{\Pi}_{\mathbf{M}} \Delta \Pi_{\mathbf{M}} = \emptyset \right\} \right) = 1.$

4.3 Normal Distribution with Unknown Variances

One of the exponential family distributions we considered above is $y_{ij}|\theta_{ij} \sim \text{Normal}(\theta_{ij}, 1)$. Suppose instead we assume that $y_{ij}|\theta_{ij} \sim \text{Normal}(\theta_{ij}, \sigma_i^2)$, where $\sigma_1^2, \ldots, \sigma_k^2$ are unknown. Leek (2011) studies this important case, and obtains several results related to ours. Let $a_1 \geq a_2 \geq \ldots \geq a_n$ be the *n* ordered singular values resulting from the singular value decomposition (SVD) of **Y**. If we regress the top t-1 right singular vectors in this SVD from each row of **Y**, this yields total residual variation that is of proportion $(\sum_{j=t}^n a_j^2)/(\sum_{j'=1}^n a_{j'}^2)$ to the total variation in **Y**. In order to estimate $\sigma_{\text{average}}^2 = k^{-1} \sum_{j=1}^k \sigma_j^2$, Leek (2011) employs the estimate

$$\hat{\sigma}_{\text{average}}^2 = \frac{1}{k(n-t)} \frac{\sum_{j=t}^n a_j^2}{\sum_{j'=1}^n a_{j'}^2} \|\mathbf{Y}\|^2.$$

Using our notation, Leek (2011) then sets $\hat{\mathbf{D}}_k = \hat{\sigma}_{average}^2 \mathbf{I}$, where \mathbf{I} is the $n \times n$ identity matrix, and proceeds to estimate $\Pi_{\mathbf{M}}$ based on $k^{-1}\mathbf{Y}^T\mathbf{Y} - \hat{\mathbf{D}}_k$ as we have done. However, it must be the case that t > r in order for $\hat{\sigma}_{average}^2$ to be well-behaved, so the assumptions and theory in Leek (2011) have several important differences from ours. We refer the reader to Leek (2011) for specific details on this important case. We note that taking our results together with those of Leek (2011), this covers a large proportion of the models utilized in practice.

5. Letting the Latent Variable Coefficients Φ Be Random

We now discuss the case where Φ is random but then conditioned. Assume that Φ is a random matrix with entries ϕ_{ij} defined on the probability space $(\Omega_1, \mathcal{F}_1, \mathbb{P}_1)$, and that the entries y_{ij} of \mathbf{Y} , conditional on Φ and \mathbf{M} , are defined on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Rather than model (1), consider the following model:

$$\theta_{ij} = \mathbb{E}\left[y_{ij}|\mathbf{\Phi}, \mathbf{M}\right] = \left(\mathbf{\Phi}\mathbf{M}\right)(i, j) \text{ or } \mathbf{\Theta} = \mathbb{E}\left[\mathbf{Y}|\mathbf{\Phi}, \mathbf{M}\right] = \mathbf{\Phi}\mathbf{M}.$$
(26)

Suppose assumption A4) holds (see (13)) and:

- **A1'**) $1 \leq \operatorname{rank}(\mathbf{M}) = r < n \text{ and } n \text{ is finite; conditional on } \mathbf{M} \text{ and } \mathbf{\Phi}, \{y_{ij}\}_{i,j} \text{ are jointly}$ independent with variance $\mathbb{V}[y_{ij}|\mathbf{M}, \mathbf{\Phi}] = \delta_{ij}$ such that $\sup_{k} \max_{i,j} \mathbb{E}\left[y_{ij}^{8}|\mathbf{M}, \mathbf{\Phi}\right] \leq C$ (which implies $\sup_{k} \max_{i,j} \mathbb{E}\left[y_{ij}^{4}|\mathbf{M}, \mathbf{\Phi}\right] \leq C$), where \mathbb{E} and \mathbb{V} are the expectation and variance wrt \mathbb{P} .
- **A2'**) Either A2) holds \mathbb{P}_1 -a.s., i.e., $\mathbb{P}_1\left(\sup_{k\geq 1} \max_{1\leq i\leq k} \|\boldsymbol{\phi}_i\|\leq C\right)=1$ and

$$\mathbb{P}_1\left(\left\|k^{-1}\boldsymbol{\Phi}^T\boldsymbol{\Phi} - \mathbf{W}\right\| = c_k, \exists c_k \to 0, \exists \mathbf{W}_{r \times r} > 0\right) = 1,$$
(27)

or A2) holds in probability \mathbb{P}_1 , i.e., as $k \to \infty$, $\mathbb{P}_1\left(\sup_{k\geq 1} \max_{1\leq i\leq k} \|\phi_i\|\leq C\right) \to 1$ and

$$\mathbb{P}_1\left(\left\|k^{-1}\boldsymbol{\Phi}^T\boldsymbol{\Phi} - \mathbf{W}\right\| = c_k, \exists c_k \to 0, \exists \mathbf{W}_{r \times r} > 0\right) \to 1.$$
(28)

A3') Conditional on \mathbf{M} , $k^{-1} \sum_{i=1}^{k} \mathbb{E}\left[e_{ij}^{4} | \mathbf{M}\right]$, $k^{-1} \sum_{i=1}^{k} \phi_{i} \mathbb{E}\left[e_{ij}^{3} | \mathbf{M}\right]$ and $k^{-1} \sum_{i=1}^{k} \phi_{i} \mathbf{m}^{j} \phi_{i} \mathbf{m}^{l} \Delta_{i}$ for any $1 \leq j \leq l \leq n$ are all convergent \mathbb{P}_{1} -a.s. as $k \to \infty$.

Note that assumptions A1'), A2') and A3') are the probabilistic versions of assumptions A1), A2 and A3) that also account for the randomness of $\mathbf{\Phi}$. Recall assumption A2) when $\mathbf{\Phi}$ is deterministic, i.e., for some $\mathbf{W}_{r\times r} > 0$ and some non-negative sequence $c_k \to 0$, $||k^{-1}\mathbf{\Phi}^T\mathbf{\Phi} - \mathbf{W}|| = c_k$. Assumption A2) implies that (see also Lemma 1):

$$\sup_{k \ge 1} \max_{1 \le i \le k} \|\phi_i\| \le C \quad \text{and} \quad \sup_{k \ge 1} \max_{1 \le i \le k, 1 \le j \le n} |\theta_{ij}| \le C.$$

$$\tag{29}$$

These two uniform boundedness results in equation (29) are then used to show the a.s. convergence in Theorem 2 which induces the a.s. convergence in Corollary 3, the validity

of Lindeberg's condition as (34) that induces Proposition 4, convergence in probability in equations (14) and (16) that induces Theorem 5, Corollary 6, and Theorem 9.

Let $\tilde{N}_1 \in \mathcal{F}_1$ be such that (27) does not hold, then $\mathbb{P}_1\left(\tilde{N}_1\right) = 0$. On the other hand, if (28) holds, then for any positive constants C and $\tilde{\varepsilon}$ there exists a $k_0 = k_0(C, \tilde{\varepsilon})$ such that the set

$$N_1^*(C,\tilde{\varepsilon}) = \left\{ \omega \in \Omega_1 : \sup_{k \ge 1} \max_{1 \le i \le k} \|\boldsymbol{\phi}_i\| > C \right\}$$

satisfies

$$\mathbb{P}_1\left(N_1^*\left(C,\tilde{\varepsilon}\right)\right) < \tilde{\varepsilon}$$

whenever $k > k_0$. Now if (27) holds, then the results on the a.s. convergence and on convergence in probability for $y_{ij}|\mathbf{M}$ remain true with respect to \mathbb{P} when $y_{ij}|\mathbf{M}$ is replaced by $y_{ij}|(\mathbf{\Phi}, \mathbf{M})$, as long as each $\phi_{ij}(\omega)$ is such that $\omega \in \Omega_1 \setminus \tilde{N}_1$. In contrast, if (28) holds, then the results on the a.s. convergence for $y_{ij}|\mathbf{M}$ reduce to convergence in probability in \mathbb{P} . But those on convergence in probability for $y_{ij}|\mathbf{M}$ remain true with respect to \mathbb{P} when $y_{ij}|\mathbf{M}$ is replaced by $y_{ij}|(\mathbf{\Phi}, \mathbf{M})$, as long as each $\phi_{ij}(\omega)$ is with $\omega \in \Omega_1 \setminus N_1^*(C, \tilde{\varepsilon})$ (where $\tilde{\varepsilon}$ can be chosen to be small). Therefore, the results (except Lemmas 7 and 8) obtained in the previous sections hold with their corresponding probability statements, whenever, for some $\mathbf{W}_{r \times r} > 0$,

$$\left\|k^{-1}\boldsymbol{\Phi}^{T}\boldsymbol{\Phi} - \mathbf{W}\right\| = c_{k} \to 0 \tag{30}$$

holds a.s. or in probability in \mathbb{P}_1 , and they allow Φ to be random (and conditioned) or deterministic. Statistically speaking, an event with very small or zero \mathbb{P}_1 probability is very unlikely to occur. This means that the practical utility of these results is not affected when (30) holds in the sense of (27) or (28) when k is large.

Finally, we remark that Lemmas 7 and 8 are independent of the assumptions A1), A2) and A3), and of A1'), A2') and A3'). In other words, for model (26), Lemma 7 remains valid, and so does Lemma 8 when the assumptions involved there are replaced by those on $y_{ij} | (\mathbf{\Phi}, \mathbf{M})$.

6. A Simulation Study

We conducted a simulation study to demonstrate the validity of our theoretical results. The quality of $\hat{\Pi}_{\mathbf{M}}$ is measured by

$$d\left(\mathbf{M}, \hat{\mathbf{M}}\right) = \left(\sqrt{n\hat{r}}\right)^{-1} \sqrt{\left\|\mathbf{M}^{T} - \hat{\mathbf{M}}^{T}\mathbf{M}_{\mathbf{V}}\right\|^{2} + \left\|\hat{\mathbf{M}}^{T} - \mathbf{M}^{T}\mathbf{V}_{\mathbf{M}}\right\|^{2}},$$

where \hat{r} is an estimate of r, $\mathbf{M}_{\mathbf{V}} = \hat{\mathbf{M}}\mathbf{M}^{T}$ and $\mathbf{V}_{\mathbf{M}} = (\mathbf{M}\mathbf{M}^{T})^{-1}\mathbf{M}\hat{\mathbf{M}}^{T}$. In fact, $d(\mathbf{M}, \hat{\mathbf{M}})$ measures the difference between the orthogonal projections (as linear operators) induced by the rows of $\hat{\mathbf{M}}$ and those of \mathbf{M} respectively, and $d(\mathbf{M}, \hat{\mathbf{M}}) = 0$ if and only if $\hat{\mathbf{\Pi}}_{\mathbf{M}} = \mathbf{\Pi}_{\mathbf{M}}$. We propose a rank estimator \hat{r} , directly applied to $\hat{\mathbf{R}}_k$, based on Theorem 5. Specifically, $\tilde{\tau}_k = \tilde{c}_k k^{-\eta}$ for some positive \tilde{c}_k and η is used to scale the eigenvalues of $\hat{\mathbf{R}}_k$, for which \tilde{c}_k (dependent on k) is determined by a strategy of Hallin and Liska (2007) (that was also used by Leek, 2011); for more details, we refer the reader to these two references. We do so since the assertions in Theorem 5 are valid only for $k = \infty$, assumption A3) may not be satisfied in our simulation study, and the unknown constants in equation (14) for the speed of convergence need to be estimated. However, we caution that, if the scaling sequence $\tilde{\tau}_k$ in Theorem 5 defined via (15) is not well estimated to capture the speed of convergence of the eigenvalues of $\hat{\mathbf{R}}_k$, \hat{r} defined by (17) as an estimate of r can be inaccurate; see our simulation study results.

6.1 Simulation Study Design

The settings for our simulation study are described below:

- 1. We consider $n = 15, 100, 200, k = 10^3, 5 \times 10^3, 10^4, 10^5$ and r = 1, 2, 3, 4, 5, 6, 8, 10, 12.
- 2. The mean matrix $\Theta = \Phi \mathbf{M}$ and the observed data $y_{ij}|\theta_{ij}$ are generated within the following scenarios:
 - (a) $y_{ij}|\theta_{ij} \sim \text{Normal}(\theta_{ij}, 1), \ \mathbf{\Phi}(i, j) = \phi_{ij} \stackrel{i.i.d.}{\sim} \text{Normal}(0, 1), \text{ and } \mathbf{M}(i, j) = m_{ij} \stackrel{i.i.d.}{\sim} \text{Uniform } (1, 10).$
 - (b) $y_{ij}|\theta_{ij} \sim \text{Poisson}(\theta_{ij}), \phi_{ij} \overset{i.i.d.}{\sim} \text{Chi-square}(9,1)$ with degrees of freedom 9 and non-centrality 1, and $m_{ij} \overset{i.i.d.}{\sim} \text{Uniform}(1,5).$

Table 2: Assessment of the estimator \hat{r} . Data were simulated under model (1) with n = 15and r = 5 under the five distributions listed. Shown is the number of times that $\hat{r} = r$ among 100 simulated data sets for each scenario. Also shown in parentheses is the number of times that $\hat{r} < r$, if any instances occurred. Results from several additional scenarios are considered in Appendix C.

k	Binomial	Gamma	NegBin	Normal	Poisson
1000	3(97)	24(4)	3	100	84(6)
5000	95~(5)	30(9)	4	96	94
10,000	100	33(22)	27(9)	96	89
100,000	100	90	43	99	94

- (c) $y_{ij}|\theta_{ij} \sim \text{Binomial}(s,\theta_{ij})$ with s = 20 and $\phi_{ij} \stackrel{i.i.d.}{\sim}$ Uniform (0.05, 0.95). **M** is such that $m_{ij} = 1$ for $1 \le i = j \le r$, $m_{ij} = r^{-1}$ for $1 \le i \le r$ and $r+1 \le j \le n$, and $m_{ij} = 0$ otherwise.
- (d) $y_{ij}|\theta_{ij} \sim \text{NegBin}(s,\theta_{ij})$ with $s = 10, \phi_{ij} \stackrel{i.i.d.}{\sim} \text{Uniform}(0.5,2)$, and $m_{ij} \stackrel{i.i.d.}{\sim} \text{Uniform}(0.3, 1.5)$.
- (e) $y_{ij}|\theta_{ij} \sim \text{Gamma}(s,\theta_{ij})$ with shape s = 10 and mean $\theta_{ij}, \phi_{ij} \stackrel{i.i.d.}{\sim}$ Uniform (0.5, 2), and $m_{ij} \stackrel{i.i.d.}{\sim}$ Uniform (0.3, 1.5).
- 3. For each combination of values in Step 1 and distributions in Step 2 above, the data matrix **Y** is generated independently 100 times and then the relevant statistics are calculated.

For each simulated data set, we measure the quality of $\hat{\mathbf{D}}_k$ by $\rho_k = \max_{1 \leq j \leq n} \left| \hat{\delta}_{kj} - \bar{\delta}_{kj} \right|$, that of $\hat{\Pi}_{\mathbf{M}}$ by $d\left(\mathbf{M}, \hat{\mathbf{M}}\right)$, and we record \hat{r} .

6.2 Simulation Study Results

Figure 1 and Table 2 display the performance of the nonparametric estimator $\hat{\Pi}_{\mathbf{M}}$ of $\Pi_{\mathbf{M}}$, that of $\hat{\mathbf{D}}_k$, and that of \hat{r} when n = 15 and r = 5; for other values of n and r, the performance of \hat{r} is provided in Appendix C and that of $\hat{\Pi}_{\mathbf{M}}$ in Appendix D. The following conclusions can be drawn from the simulation study:



Figure 1: Performance of the nonparametric estimator $\hat{\Pi}_{\mathbf{M}}$ of $\Pi_{\mathbf{M}}$ when n = 15 and r = 5. Column 1: Boxplots of the difference between the row spaces spanned by \mathbf{M} and $\hat{\mathbf{M}}$ as measured by $d(\mathbf{M}, \hat{\mathbf{M}})$ when the true dimension of \mathbf{M} is utilized to form $\hat{\mathbf{M}}$ (i.e., setting $\hat{r} = r$). Column 2: Boxplots of $d(\mathbf{M}, \hat{\mathbf{M}})$ when using the proposed estimator \hat{r} of the row space dimension in forming $\hat{\mathbf{M}}$. Column 3: An assessment of the estimate $\hat{\mathbf{D}}_k$ of \mathbf{D}_k , where the latter term is the average of the column-wise variances of \mathbf{Y} . The difference is measured by $\|\hat{\mathbf{D}}_k - \mathbf{D}_k\| = \max_{1 \le j \le n} |\hat{\delta}_{kj} - \bar{\delta}_{kj}|$. Results from several additional scenarios are shown in Appendix \mathbf{D} .

- 1. $\hat{\Pi}_{\mathbf{M}}$ with \hat{r} set as the true r approximates $\Pi_{\mathbf{M}}$ with increasing accuracy as measured by the difference between their induced orthogonal projections $d\left(\mathbf{M}, \hat{\mathbf{M}}\right)$ when k gets larger. In all settings, strong trends of convergence of $\hat{\Pi}_{\mathbf{M}}$ to $\Pi_{\mathbf{M}}$ can be observed, even when \hat{r} is used. However, the speed of convergence can be slightly different for different settings due to the hidden constants in (4) and (14).
- 2. As k gets larger $\hat{\mathbf{D}}_k$ becomes more accurate, and strong trends of convergence of $\hat{\mathbf{D}}_k$ to \mathbf{D}_k can be observed in all settings. This is similar to the behavior of $\hat{\mathbf{\Pi}}_{\mathbf{M}}$. However, the accuracy of $\hat{\mathbf{D}}_k$ in estimating \mathbf{D}_k does not seem to have a drastic impact on $\hat{\mathbf{\Pi}}_{\mathbf{M}}$, since $\hat{\mathbf{D}}_k$ induces a shift by a diagonal matrix to the matrix $k^{-1}\mathbf{Y}^T\mathbf{Y}$ and such a shift does not necessarily have a huge impact on the leading eigenvectors of $\hat{\mathbf{R}}_k$ and hence on $\hat{\mathbf{\Pi}}_{\mathbf{M}}$. We do not report the performance of $\hat{\mathbf{D}}_k$ in the scenarios where $y_{ij}|\theta_{ij} \sim \mathsf{Normal}(\theta_{ij}, 1)$ since in this case $\delta_{ij} = 1$ and $\mathbf{D}_k = \mathbf{I}$, and $\hat{\mathbf{D}}_k = \mathbf{I}$ has been set.
- 3. In all settings, \hat{r} can under- or over-estimate r, and as k increases \hat{r} becomes more accurate. However, when $\hat{r} > r$ it does not reduce the accuracy of the estimate $\hat{\Pi}_{\mathbf{M}}$ when \hat{r} is used to pick the number of leading eigenvectors of $\hat{\mathbf{R}}_k$ to estimate $\Pi_{\mathbf{M}}$. In fact, when $\hat{r} > r$, additional linearly independent eigenvectors $\hat{\mathbf{u}}_{k,i}$ for $i = 1, \ldots, r$ may be used to span $\Pi_{\mathbf{M}}$, giving better estimate than using the true r. When $\hat{r} < r$, the accuracy of $\hat{\Pi}_{\mathbf{M}}$ is reduced, since in this case the original row space $\Pi_{\mathbf{M}}$ can not be sufficiently spanned by $\hat{\Pi}_{\mathbf{M}}$. This is clearly seen from the plots on performance of $\hat{\Pi}_{\mathbf{M}}$.
- 4. The scaling sequence $\{\tilde{\tau}_k\}_{k\geq 1}$ plays a critical role on the accuracy of \hat{r} as an estimator of r, since it decides where to "cut" the spectrum of $\hat{\mathbf{R}}_k$ for finite k to give \hat{r} , where numerically all eigenvalues of $\hat{\mathbf{R}}_k$ are non-zero. In all settings, the non-adaptive choice of the sequence $\{\tilde{\tau}_k\}_{k\geq 1}$ with $\tilde{\tau}_k = \tilde{c}_k k^{-1/3}$ has been used, and it can cause inaccurate scaling of the spectrum of $\hat{\mathbf{R}}_k$ and hence inaccurate estimate of r. This explains why r has been under-estimated when y_{ij} 's follow Binomial distributions, $n \in \{100, 200\}$ and $r \geq 2$, since in these cases the magnitudes of the eigenvalues of $\hat{\mathbf{R}}_k$ have more complicated behavior, and $\tilde{\tau}_k$ are too large compared the magnitudes of these eigenvalues; see Tables S1–S3 in Appendix C for results when n = 100 and those when n = 200. We found that when y_{ij} follow Binomial distributions in the simulation study, in order to accurately estimate r, $\tilde{\tau}_k = O(k^{-1/1.1})$ should be set

for n = 100 and that $\tilde{\tau}_k = O(k^{-1/1.5})$ should be set for n = 200. The non-adaptive choice of $\tilde{\tau}_k$ also explains why \hat{r} over-estimates r when y_{ij} 's follow the Negative Binomial distributions or gamma distributions in the simulation study, since these two types of distributions are more likely to generate outliers that counterbalance the speed of concentration as k gets larger, and affect the separation of the spectrum of the limiting matrix $\hat{\mathbf{R}}_k$. In other words, for these two cases, $\tilde{\tau}_k$ are too small in magnitudes in order to scale up the spectrum of $\hat{\mathbf{R}}_k$ to the point of separation in order to estimate r. In general, the magnitude of n plays a role in the asymptotic property of $\hat{\mathbf{R}}_k$ as $k \to \infty$, and it affects the speed of convergence of $\hat{\mathbf{R}}_k$ through the hidden constants in (14) even when all needed assumptions are satisfied for Theorem 5. This explains why larger n does not necessarily induce more accurate \hat{r} when r increases but k does not increase at a compatible speed when k is finite; see Tables S1–S3 in Appendix C. However, deciding the hidden constants in (14) is usually very hard, and accurately estimating $r = \operatorname{rank}(\mathbf{M})$, being also the number of factors in factor models, is in general a very challenging problem.

7. Application to an RNA-Seq Study

In Robinson et al. (2015), we measured genome-wide gene expression in the budding yeast *Saccharomyces cerevisiae* in a nested factorial experimental design that allowed us to carefully partition gene expression variation due to both biology and technology. The technology utilized to measure gene expression is called "RNA-seq", short for RNA sequencing. This technology provides a digital measure of gene expression in that mRNA molecules are discretely sequenced and therefore counted (Wang et al., 2009). The resulting 6575×16 matrix of RNA-seq counts represents gene expression measurements on 6575 genes across 16 samples. We also have a design matrix of dimension 9×16 that captures the experimental design and apportionment of variation throughout the data. The data here are counts, and RNA-seq count data are typically modeled as overdispersed Poisson data (McCarthy et al., 2012). It can be verified on these data that, because of the experimental design, there is very little over-dispersion once the experimental design is taken into account; we therefore utilize the Poisson distribution in this analysis.

We set **Y** to be the 6575×16 matrix of RNA-seq counts and **M** the 9×16 design matrix, where each row of **M** is normalized to have unit Euclidean norm. Ignoring our knowledge of **M**, we applied the proposed estimator using the Poisson distribution formula



Figure 2: A measure of how well $\hat{\mathbf{M}}$ captures the row space of \mathbf{M} as the dimension \hat{r} of $\hat{\mathbf{M}}$ increases in the RNA-seq data set. This measure $d(\mathbf{M}, \hat{\mathbf{M}})$ is plotted versus \hat{r} over $\hat{r} \in \{1, 2, ..., 16\}$. The true dimension of the row space of \mathbf{M} is r = 9, shown by vertical dotted line.



Figure 3: A measure of how well $\hat{\mathbf{M}}$ captures the row space of \mathbf{M} as the number of variables k increases in the RNA-seq data set. For each value of k, we randomly sampled k rows from the RNA-seq data matrix and computed $d(\mathbf{M}, \hat{\mathbf{M}})$ as defined in the text; this was repeated 50 times and the median was plotted.

to yield an estimate $\hat{\mathbf{M}}$ over a range of values of $\hat{r} \in \{1, 2, \dots, 16\}$. In evaluating $\hat{\mathbf{M}}$, we utilized the measure $d(\mathbf{M}, \hat{\mathbf{M}})$ defined in Section 6.

Figure 2 shows how $d(\mathbf{M}, \hat{\mathbf{M}})$ changes with the dimension \hat{r} of $\hat{\mathbf{M}}$. It can be seen that the minimum value is at $\hat{r} = 9$ (where r = 9 is the true dimension of \mathbf{M}). We then randomly sampled rows of \mathbf{Y} to quantify how $d(\mathbf{M}, \hat{\mathbf{M}})$ changes as the number of variables k grows. Figure 3 shows the median $d(\mathbf{M}, \hat{\mathbf{M}})$ values over 50 random samplings for each k value, where a convergence with respect to k can be observed. In summary, this analysis shows that the proposed methodology is capable of accurately capturing the linear latent variable space on real data that is extremely heteroskedastic and does not follow the Normal distribution.

8. Discussion

We have proposed a general method to consistently estimate the low-dimensional, linear latent variable structure in a set of high-dimensional rv's. Further, by exploiting the intrinsic relationship between the moments of natural exponential family (NEF) distributions that have quadratic variance functions (QVFs), we are able to explicitly recover this latent structure by using just the second moments of the rv's even when these rv's have heteroskedastic variances. Empirical evidence confirms our theoretical findings and the utility of our methodology. Once the latent structure has been well estimated, the variable-specific coefficients of the latent variables can be estimated via appropriate estimation methods.

We point out that, under the same assumptions A1), A2), A3) and A4), the theoretical results in Sections 2, 3 and 4 hold for the unconditional model

$$\boldsymbol{\Theta} = \mathbb{E}\left[\mathbf{Y}\right] = \boldsymbol{\Phi}\mathbf{M} \tag{31}$$

when both Φ and \mathbf{M} are deterministic with rank $(\mathbf{M}) = r$. In this case the conditional distribution of each y_{ij} given \mathbf{M} in model (1), i.e., $\Theta = \mathbb{E}[\mathbf{Y}|\mathbf{M}] = \Phi \mathbf{M}$ when \mathbf{M} is a realization of a random matrix $\tilde{\mathbf{M}}$, becomes the marginal distribution of y_{ij} in model (31) and the proofs proceed almost verbatim as those for model (1). Further, for the model

$$\boldsymbol{\Theta} = \mathbb{E}\left[\mathbf{Y}|\boldsymbol{\Phi}\right] = \boldsymbol{\Phi}\mathbf{M} \tag{32}$$

when Φ is random but **M** is deterministic with rank (**M**) = r, under the assumptions A1'), A2'), A3') and A4), similar arguments as those given in Section 5 imply that the theoretical results obtained in Sections 2, 3 and 4 hold when the probabilistic statements in the conclusions there are adjusted in the way detailed in Section 5.

We have observed that for certain NEF distribution configurations, estimating the rank of the linear space generated by the latent structure can can be challenging, even with the theory we provided, if the scaling sequence to separate the limiting spectrum of the adjusted gram matrix of the data is not adaptively specified. The need for choosing an adaptive scaling sequence comes from the hidden constants that describe the asymptotic speed of convergence, and it can be a delicate task to do so in non-asymptotic settings. This is reflective of the more general challenge of estimating the dimension of a latent variable model.

Finally, we briefly point out that, when the y_{ij} have pdf $f(y_{ij}; \theta_{ij}, \psi)$ such that

$$f(y;\theta,\psi) = h(y,\psi) \exp\left\{\psi^{-1}\left[\eta(\theta)y - g(\eta(\theta))\right]\right\}$$

form an exponential dispersion family (see, e.g., Jørgensen, 1987), an explicit estimator of \mathbf{D}_k (and hence that of $\Pi_{\mathbf{M}}$) will require results beyond those provided in this work, even if the unknown dispersion parameter ψ is constant. We leave this case to future research.

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References

- D. H Alexander, J Novembre, and K Lange. Fast model-based estimation of ancestry in unrelated individuals. *Genome Research*, 19(9):1655–1664, 2009.
- Anima Anandkumar, Dean P. Foster, Daniel Hsu, Sham M. Kakade, and Yi-Kai Liu. A spectral algorithm for latent Dirichlet allocation. Advances in Neural Information Processing Systems, 25, 2012.
- Anima Anandkumar, Dean P. Foster, Daniel Hsu, Sham M. Kakade, and Yi-Kai Liu. A spectral algorithm for latent Dirichlet allocation. *Algorithmica*, 72:193C–214, 2015.

- Sanjeev Arora, Rong Ge, Yonatan Halpern, David Mimno, Ankur Moitra, David Sontag, Yichen Wu, and Michael Zhu. A practical algorithm for topic modeling with provable guarantees. In *Proceedings of The 30th International Conference on Machine Learning*, pages 280–288, 2013.
- D. J. Bartholomew, M. Knott, and I. Moustaki. Latent Variable Models and Factor Analysis: A Unified Approach. Wiley Series in Probability and Statistics, 3rd edition, 2011.
- David M. Blei, Andrew Ng, and Michael Jordan. Latent dirichlet allocation. *JMLR*, 3: 993–1022, 2003.
- Michael Collins, Sanjoy Dasgupta, and Robert E Schapire. A generalization of principal components analysis to the exponential family. In *Advances in neural information* processing systems, pages 617–624, 2001.
- Marc Hallin and Roman Liska. Determining the number of factors in the general dynamic factor model. J. Amer. Statist. Assoc., 102(478):603C617, 2007.
- A.J. Hoffman and H.W. Wielandt. The variation of the spectrum of a normal matrix. Duke Math. J., 20(1):37–39, 1953.
- Bent Jørgensen. Exponential dispersion models. J. R. Statist. Soc. B, 49(2):127–162, 1987.
- D. D. Lee and S. Seung. Learning the parts of objects by non-negative matrix factorization. *Nature*, 401:788–791, 1999.
- Jeffrey T. Leek. Asymptotic conditional singular value decomposition for high-dimensional genomic data. *Biometric*, 67(2):344–352, 2011.
- Jeffrey T Leek and John D Storey. Capturing heterogeneity in gene expression studies by surrogate variable analysis. *PLoS Genet*, 3(9):e161, 2007.
- Jeffrey T. Leek and John D. Storey. A general framework for multiple testing dependence. Proc. Natl. Acad. Sci. U.S.A., 105(48):18718–18723, 2008.
- Gerard Letac and Marianne Mora. Natural real exponential families with cubic variance functions. Ann. Statist., 18(1):1–37, 1990.

- Davis J McCarthy, Yunshun Chen, and Gordon K Smyth. Differential expression analysis of multifactor RNA-Seq experiments with respect to biological variation. *Nucleic Acids Research*, 40(10):4288–4297, 2012.
- Carl N. Morris. Natural exponential families with quadratic variance functions. Ann. Statist., 10(1):65–80, 1982.
- J. K. Pritchard, M. Stephens, and P. Donnelly. Inference of population structure using multilocus genotype data. *Genetics*, 155(2):945–959, 2000.
- David G. Robinson, Jean Y. Wang, and John D. Storey. A nested parallel experiment demonstrates differences in intensity-dependence between rna-seq and microarrays. Nucleic acids research, 2015. doi: 10.1093/nar/gkv636.
- Michael E. Tipping and Christopher M. Bishop. Probabilistic principal component analysis. Journal of the Royal Statistical Society: Series B, 61(3):611–622, 1999. doi: 10.1111/ 1467-9868.00196.
- A. W. Van der Vaart. Asymptotic Statistics. Cambridge Univ. Press, 1998.
- Harro Walk. Strong laws of large numbers by elementary Tauberian arguments. Monatsh. Math., 144(4):329–346, 2005.
- H. S. Wang, B. Li, and C. L. Leng. Shrinkage tuning parameter selection with a diverging number of parameters. *Journal of the Royal Statistical Society Series B-Statistical Methodology*, 71:671–683, 2009.

Appendix A. Relationship to Anandkumar et al.

Anandkumar et al. (2012, 2015) consider a different class of probabilistic models than we consider. We establish this by rewriting their model in our notation. We consider the model

$$\mathbb{E}\left[\mathbf{Y}|\mathbf{M}\right] = \mathbf{\Phi}_{k \times r} \mathbf{M}_{r \times n},$$

where $\mathbf{Y}_{k \times n}$ is a matrix of *n* observations on *k* variables. The data points y_{ij} can take on a wide range of classes of variables, from Binomial outcomes, to count data, to continuous data (see Table 1, for example). Variable *i* can be written as $\mathbf{y}_i = (y_{i1}, \ldots, y_{in})$, which is a $1 \times n$ vector. In terms of this variable, our model assumes that

$$\mathbb{E}\left[\mathbf{y}_{i}|\mathbf{M}\right] = \boldsymbol{\phi}_{i}\mathbf{M},$$

where $\phi_i \in \mathbb{R}^{1 \times r}$ is row *i* of Φ .

Anandkumar et al. (2012, 2015), on the other hand, assume that $y_{ij} \in \{0, 1\}^n$ with the restriction that $\sum_{j=1}^n y_{ij} = 1$. This construction is meant to represent an observed document of text where there are n words in the dictionary. They consider a single document with an infinite number of words. The vector $\mathbf{y}_i = (y_{i1}, \ldots, y_{in})$ tells us which of the n words is present at location i in the document. When they let $k \to \infty$, this means the number of words in the document grows to infinity.

The model studied in Anandkumar et al. (2012, 2015) is

$$\mathbb{E}\left[\mathbf{y}_{i}^{T}|\mathbf{m}\right] = \mathbf{O}_{n \times r}\mathbf{m}_{r \times 1},$$

where there are r topics under consideration and the r-vector \mathbf{m} gives the mixture of topics in this particular document. Each column of \mathbf{O} gives the multinomial probabilities of the nwords for the corresponding topic. Note that the linear latent variable model \mathbf{Om} does not vary with i, whereas in our model it does. Also, the dimensionality of the latent variable model is different than ours. Therefore, this is a different model than we consider.

Anandkumar et al. (2012, 2015) take the approach of calculating, projecting and decomposing the expectations of tensor products involving $(\mathbf{y}_1, \mathbf{y}_2)$ and $(\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3)$, and then suggesting that these expectations can be almost surely estimated as $k \to \infty$ by utilizing the analogous sample moments. In order to exactly recover **O** modulo a permutation of its columns, additional assumptions are made by Anandkumar et al. (2012, 2015), such as knowledge of the sum of the unknown exponents in the Dirichlet distribution in the LDA model of Blei et al. (2003). It is also assumed that the number of topics r is known.

Appendix B. Proofs

Since we are considering the conditional model (1), i.e., $\Theta = \mathbb{E}[\mathbf{Y}|\mathbf{M}] = \Phi \mathbf{M}$, to maintain concise notations we introduce the conditional expectation and variance operators respectively as $\tilde{\mathbb{E}}[\cdot] = \mathbb{E}[\cdot|\mathbf{M}]$ and $\tilde{\mathbb{V}}[\cdot] = \mathbb{V}[\cdot|\mathbf{M}]$. In the proofs, unless otherwise noted, the random vectors are conditioned on \mathbf{M} and the arguments for these random vectors are conditional on \mathbf{M} .

B.1 Proof of Theorem 2

Denote the terms in the order in which they appear in the expansion

$$k^{-1}\mathbf{Y}^{T}\mathbf{Y} = k^{-1}\mathbf{\Theta}^{T}\mathbf{\Theta} + k^{-1} \left(\mathbf{Y} - \mathbf{\Theta}\right)^{T}\mathbf{\Theta} + k^{-1}\mathbf{\Theta}^{T} \left(\mathbf{Y} - \mathbf{\Theta}\right)$$
$$+ k^{-1} \left(\mathbf{Y} - \mathbf{\Theta}\right)^{T} \left(\mathbf{Y} - \mathbf{\Theta}\right)$$

as \mathbf{A}_1 , \mathbf{A}_2 and \mathbf{A}_2^T and \mathbf{A}_3 , we see that $\lim_{k \to \infty} \mathbf{A}_1 = \mathbf{H}$ by assumption (4). We claim that $\lim_{k \to \infty} \|\mathbf{A}_2\| = 0 = \lim_{k \to \infty} \|\mathbf{A}_2^T\|$ a.s. The (i, j) entry $a_{2,ij}$ of \mathbf{A}_2 is $a_{2,ij} = k^{-1} \sum_{l=1}^k \tilde{a}_{2,ij,l}$, where $\tilde{a}_{2,ij,l} = (y_{li} - \theta_{li}) \theta_{lj}$ for $1 \le l \le k$. Clearly, $\tilde{\mathbb{E}}[\tilde{a}_{2,ij,l}] = 0$. Set $\tilde{y}_{li} = y_{li} - \theta_{li}$. By Lemma 1, uniformly bounded 4th conditional moments of y_{ij} and Hölder's inequality,

$$\sup_{k\geq 1} \max_{1\leq l\leq k} \tilde{\mathbb{V}}\left[\tilde{a}_{2,ij,l}\right] \leq C \sup_{k\geq 1} \max_{1\leq l\leq k} \left(\tilde{\mathbb{E}}\left[\tilde{y}_{li}^{4}\right]\right)^{1/2} \leq C.$$

By independence conditional \mathbf{M} ,

$$\sum_{k \ge 1} \frac{1}{k} \tilde{\mathbb{V}}\left[a_{2,ij}\right] \le C \sum_{k \ge 1} \frac{1}{k^3} \sum_{l=1}^k \left(\tilde{\mathbb{E}}\left[\tilde{y}_{li}^4\right]\right)^{1/2} \le C \sum_{k \ge 1} \frac{1}{k^2} = \frac{C\pi^2}{6}.$$

Therefore, Theorem 1 of Walk (2005) implies that $\lim_{k\to\infty} a_{2,ij} = 0$ a.s., which validates the claim.

Consider the last term \mathbf{A}_3 , whose (i, j)th off-diagonal entry $a_{3,ij}$ can be written as $a_{3,ij} = k^{-1} \sum_{l=1}^{k} \tilde{a}_{3,ij,l}$, where $\tilde{a}_{3,ij,l} = (y_{li} - \theta_{li}) (y_{lj} - \theta_{lj})$. Clearly, $\tilde{\mathbb{E}} [\tilde{a}_{3,ij,l}] = 0$. The same

reasoning as above implies

$$\sum_{k \ge 1} \frac{1}{k} \tilde{\mathbb{V}}\left[a_{3,ij}\right] \le C \sum_{k \ge 1} \frac{1}{k^3} \sum_{l=1}^k \left(\tilde{\mathbb{E}}\left[\tilde{y}_{li}^4\right]\right)^{1/2} \left(\tilde{\mathbb{E}}\left[\tilde{y}_{lj}^4\right]\right)^{1/2} \le C \sum_{k \ge 1} \frac{1}{k^2} = \frac{C\pi^2}{6}$$

when $i \neq j$. So, Theorem 1 of Walk (2005) implies that $\lim_{k\to\infty} a_{3,ij} = 0$ a.s. The diagonal entries of \mathbf{A}_3 can be written as $a_{3,ii} = k^{-1} \sum_{l=1}^k \tilde{a}_{3,ii,l}$, where $\tilde{a}_{3,ii,l} = (y_{li} - \theta_{li})^2$. Since $\tilde{\mathbb{E}}[\tilde{a}_{3,ii,l}] = \delta_{li}$ and

$$\tilde{\mathbb{V}}\left[\tilde{a}_{3,ii,l}\right] \le \delta_i^2 + \tilde{\mathbb{E}}\left[\tilde{y}_{li}^4\right] \le 2\tilde{\mathbb{E}}\left[\tilde{y}_{li}^4\right] \le C,$$

it follows that

$$\sum_{k\geq 1} \frac{1}{k} \tilde{\mathbb{V}}\left[a_{3,ii}\right] \leq \sum_{k\geq 1} \frac{C}{k^2} = \frac{C\pi^2}{6}.$$

Hence, Theorem 1 of Walk (2005) implies $\lim_{k\to\infty} |a_{3,ii} - \bar{\delta}_{ki}| = 0$ a.s. and $\lim_{k\to\infty} ||\mathbf{A}_3 - \mathbf{D}_k|| = 0$. Combining the limiting terms obtained above completes the proof.

B.2 Proof of Corollary 3

We show (7) first. By (6) and Wielandt-Hoffman (WH) inequality of Hoffman and Wielandt (1953), we immediately have (7), i.e.,

$$\lim_{k \to \infty} \max_{1 \le i \le n} |\beta_{k,i} - \alpha_i| = 0 \text{ a.s.}.$$
(33)

Now we show the rest of the assertions. Let $\{\lambda_l\}_{l=1}^s$ with $1 \leq s \leq n$ be the distinct eigenvalues of **H** ordered into $\lambda_l > \lambda_{l+1}$ for $1 \leq l \leq s-1$. Note that $s_l = 0$ since the rank of **H** is r and **H** is positive semi-definite. Let $\varepsilon_0 = \min_{1 \leq l \leq s_0} \{\lambda_l - \lambda_{l+1}\}$ and pick $\varepsilon > 0$ such that $\varepsilon < 4^{-1}\varepsilon_0$, where $s_0 = \max\{l : \lambda_l > 0\} \leq r < n$. From (33), we see that there exists some $k_0 \in \mathbb{N}$ and a partition of $\{1, ..., n\}$ into its subsets $\{A_l\}_{l=1}^s$ for which, whenever $k \geq k_0$, $\max_{1 \leq l \leq s} \max_{i \in A_l} |\beta_{k,i} - \lambda_l| < 4^{-1}\varepsilon$ but

$$\min_{1 \le l < l' \le s} \min\left\{ |\beta_{k,i} - \beta_{k,j}| : i \in A_l, j \in A_{l'}, l \ne l' \right\} > 4^{-1} \varepsilon_0.$$

Namely, $\{\beta_{k,i}\}_{i=1}^{n}$ separate into s groups $\{\beta_{k,i} : i \in A_l\}$ for $1 \leq l \leq s$ each with center λ_l but diameter at most $2^{-1}\varepsilon$. Therefore, $\lim_{k\to\infty} \{\beta_{k,i} : i = 1, \ldots, n\} = \{\lambda_l : l = 1, \ldots, s\}$ a.s..

Since $\mathbf{W} > 0$, rank $(\mathbf{M}) = r$ and \mathbf{H} is symmetric, \mathbf{H} is diagonalizable with rank $(\mathbf{H}) = r$ and the geometric multiplicity (gm) of each λ_l equals its algebraic multiplicity (am). Therefore, the linear space spanned by the union of the eigenvectors corresponding to all non-zero eigenvalues of \mathbf{H} must be $\langle \{\mathbf{v}_i\}_{i=1}^r \rangle$ and rank $(\langle \{\mathbf{v}_i\}_{i=1}^r \rangle) = r$ must hold, where \mathbf{v}_i is an eigenvector corresponding to some α_j for $1 \leq j \leq r$. Moreover, $\langle \{\mathbf{v}_i\}_{i=1}^r \rangle = \Pi_{\mathbf{M}}$. Fix an l and any $\boldsymbol{\gamma} \in \mathbb{R}^n$ with $\|\boldsymbol{\gamma}\| < \infty$. Let $\mathbf{u}_{k,i}$ be any eigenvector that is part of the basis for the eigenspace $U_{k,i}$ of $\beta_{k,i}$. Then, from (6) and (7), we see that

$$b_{k}(\boldsymbol{\gamma}) = (\mathbf{R}_{k} - \beta_{k,i}\mathbf{I})\boldsymbol{\gamma} - (\mathbf{R}_{k} - \beta_{k,j}\mathbf{I})\boldsymbol{\gamma}$$

satisfies $\lim_{k\to\infty} \|b_k(\boldsymbol{\gamma})\| = 0$ a.s. for all $i, j \in A_l$. Therefore, $\lim_{k\to\infty} U_{k,i} \Delta U_{k,j} = \emptyset$ a.s. for all $i, j \in A_l$ and asymptotically there are only s linearly independent eigenspaces $\{U_{k,i_l}\}_{l=1}^s$ with $1 \leq i_l \leq n$ corresponding to $\left\{\lim_{k\to\infty} \beta_{k,i} : i \in A_l, 1 \leq l \leq s\right\}$. On the other hand, for any $i \in A_l$,

$$a_{k}\left(\boldsymbol{\gamma}\right) = \left(\mathbf{R}_{k} - \beta_{k,i}\mathbf{I}\right)\boldsymbol{\gamma} - \left(\mathbf{H} - \lambda_{l}\mathbf{I}\right)\boldsymbol{\gamma}$$

satisfies $\lim_{k\to\infty} ||a_k(\gamma)|| = 0$ a.s.. Let **v** be any eigenvector that is part of the basis for the eigenspace V_l of λ_l . Then, for any $i \in A_l$,

$$\|(\mathbf{R}_{k} - \beta_{k,i}\mathbf{I})\mathbf{v}\| \leq \|(\mathbf{H} - \lambda_{l}\mathbf{I})\mathbf{v}\| + \|a_{k}(\boldsymbol{\gamma})\| \to 0 \text{ a.s.}$$

and

$$\| (\mathbf{H} - \lambda_l \mathbf{I}) \mathbf{u}_{k,i} \| \le \| (\mathbf{R}_k - \beta_{k,i} \mathbf{I}) \mathbf{u}_{k,i} \| + \| a_k (\boldsymbol{\gamma}) \| \to 0 \text{ a.s.}$$

since $\|\mathbf{v}\| = 1$ and $\Pr(\|\mathbf{u}_{k,i}\| < \infty) = 1$. Consequently, $V_l \subseteq \lim_{k \to \infty} U_{k,i}$ and $\lim_{m \to \infty} U_{k,i} \subseteq V_l$ a.s. for any $i \in A_l$. Since we have already shown that $\{U_{k,i}\}_{i=1}^n$ asymptotically reduces to $\{U_{k,i_l}\}_{l=1}^s$ corresponding to $\{\beta_{k,i_l}\}_{l=1}^s \subseteq \{\beta_{k,i}\}_{i=1}^n$ for which $\lim_{k \to \infty} \max_{1 \le l \le s} |\beta_{k,i_l} - \lambda_l| = 0$ a.s., we see that all eigenvectors corresponding to the *r* largest eigenvalues of \mathbf{R}_k together asymptotically spans $\langle \{\mathbf{v}_i\}_{i=1}^r \rangle$ a.s.. This yields $\lim_{k \to \infty} |S| = r$ a.s. and (8). The proof is completed.

B.3 Proof of Proposition 4

We remark that our proof of Proposition 4 follows a similar strategy given in Leek (2011) but uses slightly different techniques.

We show the first claim. Recall $\boldsymbol{\Theta} = \boldsymbol{\Phi} \mathbf{M}$. It suffices to show that each of $k^{-1} \boldsymbol{\Theta}^T \mathbf{E}$ and $k^{-1} \mathbf{E}^T \mathbf{E}$ is a linear mapping of $\sum_{i=1}^k \mathbf{z}_i$ with Lipschitz constant 1 as follows. The (i, j)th entry of $k^{-1} \mathbf{E}^T \mathbf{E}$ is

$$k^{-1}\sum_{l=1}^{k}e_{li}e_{lj} = k^{-1}\sum_{l=1}^{k} \langle \mathbf{q}_j, e_{li}\mathbf{e}_l \rangle = \left\langle \mathbf{q}_j, k^{-1}\sum_{l=1}^{k}e_{li}\mathbf{e}_l \right\rangle,$$

where $\mathbf{q}_i = (0, ..., 0, 1, 0, ..., 0)$ (i.e., only the *i*th entry is 1; others are 0) and $\langle \cdot, \cdot \rangle$ is the inner product in Euclidean space. In other words, the (i, j)th entry of $k^{-1}\mathbf{E}^T\mathbf{E}$ is exactly the (in + j)th entry of $\sum_{i=1}^k \mathbf{z}_i$. Further, the (i, j)th entry of $k^{-1}\mathbf{\Theta}^T\mathbf{E}$ is

$$k^{-1}\sum_{l=1}^{k}\phi_{l}\mathbf{m}^{i}e_{lj} = k^{-1}\sum_{l=1}^{k}\left\langle \mathbf{q}_{j},\phi_{l}\mathbf{m}^{i}\mathbf{e}_{l}\right\rangle = \left\langle \mathbf{q}_{j},k^{-1}\sum_{l=1}^{k}\phi_{l}\mathbf{m}^{i}\mathbf{e}_{l}\right\rangle,$$

i.e., the $(n^2 + ni + j)$ th entry of $\sum_{i=1}^{k} \mathbf{z}_i$.

Notice that linearity of picking an entry as a mapping described above is invariant under matrix transpose, we see that $k^{-1}\mathbf{E}^T\boldsymbol{\Theta}$ is also a linear mapping of $\sum_{i=1}^k \mathbf{z}_i$ with Lipschitz constant 1. Consequently, \mathbf{F} is a linear mapping of $\{\mathbf{z}_i\}_{i=1}^k$ with Lipschitz constant 1.

Now we show the second claim. Set $\sum_{i=1}^{k} \tilde{\mathbf{z}}_{i}$ with $\tilde{\mathbf{z}}_{i} = \sqrt{k} \left(\mathbf{z}_{i} - \tilde{\mathbb{E}} \left[\mathbf{z}_{i} \right] \right)$. We will verify

that $\sum_{i=1}^{k} \tilde{\mathbf{z}}_{i}$ is asymptotically Normally distributed. Clearly, among the long vector $\tilde{\mathbb{E}}[\mathbf{z}_{i}]$, only the *j*th entry of $\tilde{\mathbb{E}}[e_{ij}\mathbf{e}_{i}]$ is nonzero and it is $k^{-1}\delta_{ij}$, which means that $\tilde{\mathbb{E}}[\mathbf{z}_{i}]$ has an easy form. By the multivariate central limit theorem (MCLT), e.g., see page 20 of Van der Vaart (1998), to show the asymptotic normality of $\sum_{i=1}^{k} \tilde{\mathbf{z}}_{i}$ as $k \to \infty$, it suffices to show

$$v_{k}^{\varepsilon} = \sum_{i=1}^{k} \tilde{\mathbb{E}} \left[\|\tilde{\mathbf{z}}_{i}\|^{2} \mathbf{1}_{\{\|\tilde{\mathbf{z}}_{i}\| > \varepsilon\}} \right] \to 0 \text{ as } k \to \infty$$
(34)

for any $\varepsilon > 0$ and

$$\sum_{i=1}^{k} \widetilde{Cov} \left[\tilde{\mathbf{z}}_{i} \right] \to \mathbf{\Sigma}_{\infty} \text{ as } k \to \infty$$
(35)

for some matrix Σ_{∞} in order that $\sum_{i=1}^{k} \tilde{\mathbf{z}}_{i} \rightsquigarrow N(\mathbf{0}, \Sigma_{\infty})$, where \widetilde{Cov} is the conditional covariance operator given \mathbf{M} and \rightsquigarrow denotes weak convergence.

We verify (34) first. Since $\sup_{k} \max_{i,j} \tilde{\mathbb{E}}\left[y_{ij}^{8}\right] \leq C$, $\sup_{k} \max_{i} \|\phi_{i}\| < \infty$ and *n* is finite, the identity

$$k \|\tilde{\mathbf{z}}_{i}\|^{2} = \sum_{j \neq l; 1 \le j, l \le n} e_{il}^{2} e_{ij}^{2} + \sum_{j=1}^{n} \left(e_{ij}^{2} - \delta_{ij}\right)^{2} + \sum_{j=1}^{n} \sum_{l=1}^{n} \left(\phi_{i} \mathbf{m}^{j} e_{il}\right)^{2}$$
(36)

for each $1 \le i \le k$ implies, via Hölder's inequality,

$$\tilde{\mathbb{E}}\left[\|\tilde{\mathbf{z}}_{i}\|^{2} \mathbf{1}_{\{\|\tilde{\mathbf{z}}_{i}\| > \varepsilon\}}\right] \leq k^{-1} \left(\tilde{\mathbb{E}}\left[\vartheta_{i}^{2}\right] \Pr\left(\vartheta_{i} > k\varepsilon^{2}\right)\right)^{1/2} \leq \frac{C}{k^{3/2}\varepsilon}$$

and $v_k^{\varepsilon} \leq Ck^{-1/2}\varepsilon^{-1} \to 0$ as $k \to \infty$, where ϑ_i denotes the right hand side (RHS) of (36). Hence, (34) is valid.

It is left to verify (35). Let $\Sigma_i^* = \widetilde{Cov}(\tilde{\mathbf{z}}_i)$. Then $k\Sigma_i^*$ has entries zero except at the blocks $\mathbf{S}_{i1,jl} = \widetilde{Cov}(e_{ij}\mathbf{e}_i, e_{il}\mathbf{e}_i)$, $\mathbf{S}_{i2,jl} = \widetilde{Cov}(\phi_i \mathbf{m}^j \mathbf{e}_i, \phi_i \mathbf{m}^l \mathbf{e}_i)$ and $\mathbf{S}_{i4,jl} = \widetilde{Cov}(e_{ij}\mathbf{e}_i, \phi_i \mathbf{m}^l \mathbf{e}_i)$. Specifically, $\mathbf{S}_{i1,jl}(r,r') = \tilde{\mathbb{E}}(e_{ir}^4)$ if r = r' = j = l and is 0 otherwise; $\mathbf{S}_{i2,jl} = \phi_i \mathbf{m}^j \phi_i \mathbf{m}^l \Delta_i$ with $\Delta_i = \text{diag}\{\delta_{i1}, ..., \delta_{in}\}$; $\mathbf{S}_{i4,jl}(r,r') = \phi_i \mathbf{m}^l \tilde{\mathbb{E}}[e_{ir}^3]$ if r = r' = j and is 0 otherwise. By the joint independence among $\{\tilde{\mathbf{z}}_i\}_{i=1}^k$, we have $\widetilde{Cov}\left[\sum_{i=1}^k \tilde{\mathbf{z}}_i\right] = \Sigma_k^* = \sum_{i=1}^k \Sigma_i^*$. Further, $\Sigma_k^* \to \Sigma_\infty$ as $k \to \infty$ when, for each $1 \le j, l \le n$,

By assumption A3), the above needed convergence is ensured, meaning that $\Sigma_k^* \to \Sigma_\infty$ for some $\Sigma_\infty \ge 0$, i.e., (35) holds. Therefore, $\sum_{i=1}^k \tilde{\mathbf{z}}_i$ is asymptotically Normally distributed as $N(\mathbf{0}, \Sigma_\infty)$. The proof is completed.

B.4 Proof of Theorem 5

We will use the notations in the proof of Proposition 4 and aim to show $\left\| \hat{\mathbf{R}}_k - \mathbf{H} \right\| = O_{\Pr}(\tau_k)$, which then by Wielandt-Hoffman (WH) inequality of Hoffman and Wielandt (1953) implies $\left\| \hat{\boldsymbol{\alpha}}_k - \boldsymbol{\alpha} \right\| = O_{\Pr}(\tau_k)$, where $\hat{\boldsymbol{\alpha}}_k = (\hat{\alpha}_{k,1}, ..., \hat{\alpha}_{k,n})$ and $\boldsymbol{\alpha} = (\alpha_1, ..., \alpha_n)$. Recall $k^{-1}\mathbf{Y}^T\mathbf{Y} = \mathbf{F} + k^{-1}\Theta^T\Theta$ and $\mathbf{F} = f_0\left(\sum_{i=1}^k \mathbf{z}_i\right)$ by Proposition 4, where f_0 is linear with Lipschitz constant 1. We see that the linearity of f_0 and that the only nonzero entries of $\tilde{\mathbb{E}}[\mathbf{z}_i]$ are $k^{-1}\delta_{ij}$ at indices (j-1)n+j for $1 \leq j \leq n$ together imply

$$\sqrt{k}\mathbf{F} = f_0\left(\sum_{i=1}^k \sqrt{k}\left(\mathbf{z}_i - \tilde{\mathbb{E}}\left[\mathbf{z}_i\right]\right)\right) + \sqrt{k}\mathbf{D}_k = f_0\left(\sum_{i=1}^k \tilde{\mathbf{z}}_i\right) + \sqrt{k}\mathbf{D}_k.$$

Therefore, the Lipschitz property of f_0 and the asymptotic normality of $\sum_{i=1}^{k} \tilde{\mathbf{z}}_i$ force

$$\sqrt{k} \left(\hat{\mathbf{R}}_{k} - \mathbf{H} \right) = f_{0} \left(\sum_{i=1}^{k} \tilde{\mathbf{z}}_{i} \right) + \sqrt{k} \left(\hat{\mathbf{D}}_{k} - \mathbf{D}_{k} \right) + \sqrt{k} \left(\mathbf{M}^{T} \left(k^{-1} \boldsymbol{\Phi}^{T} \boldsymbol{\Phi} - \mathbf{W} \right) \mathbf{M} \right)$$
$$= O_{\mathrm{Pr}} \left(1 \right) + \sqrt{k} \varepsilon_{k} + \sqrt{k} O \left(c_{k} \right),$$

where we have used assumptions (13) and (4). Hence, (14) holds with τ_k set by (15). Finally, we show (16) and (18). From (14), we see that $\max \{\alpha_i - \tilde{c}_i \tau_k, 0\} \leq \hat{\alpha}_{k,i} \leq \alpha_i + \tilde{c}_i \tau_k$ for some finite constant $\tilde{c}_i \geq 0$ for each $1 \leq i \leq n$. Since $\alpha_r > 0$ but $\alpha_{r+1} = 0$, we see that $\tilde{\tau}_k^{-1} \hat{\alpha}_{k,i} \geq \tilde{\tau}_k^{-1} \alpha_r - \tilde{c}_i \tilde{\tau}_k^{-1} \tau_k \to \infty$ for $1 \leq i \leq r$ but $\tilde{\tau}_k^{-1} \hat{\alpha}_{k,i} \leq \tilde{c}_i \tilde{\tau}_k^{-1} \tau_k \to 0$ for $r+1 \leq i \leq n$. So, (16) and (18) hold. The proof is completed.

B.5 Proof of Lemma 8

Let $w_{ij} = v(y_{ij})$. Then w_{ij} are mutually independent and

$$\sum_{k\geq 1} k^{-1} \tilde{\mathbb{V}}\left[\hat{\delta}_{kj}\right] = \sum_{k\geq 1} k^{-2} \max_{1\leq i\leq k} \tilde{\mathbb{V}}\left[w_{ij}\right] \leq C \sum_{k\geq 1} k^{-2} < \infty.$$

Therefore, Theorem 1 of Walk (2005) implies that $\tilde{d}_{kj} = \hat{\delta}_{kj} - \bar{\delta}_{kj} = \hat{\delta}_{kj} - \tilde{\mathbb{E}}\left[\hat{\delta}_{kj}\right] \to 0$ a.s. as $k \to \infty$. Now we show the second claim. Let $\tilde{y}_{ij} = v(y_{ij}) - \delta_{ij}$ and $b_{ij} = k^{-1/2}\tilde{y}_{ij}$. Then

 $\sum_{l=1}^{k} b_{lj} = \sqrt{k} \tilde{d}_{kj}.$ For any $\varepsilon > 0$, assumption (22) implies

$$\tilde{a}_{i} = \tilde{\mathbb{E}}\left[b_{lj}^{2} \mathbb{1}_{\left\{|b_{lj}| > \varepsilon\right\}}\right] \leq k^{-1} \left(\tilde{\mathbb{E}}\left[\tilde{y}_{ij}^{4}\right] \Pr\left(|\tilde{y}_{ij}| > k^{1/2}\varepsilon\right)\right)^{1/2} \leq \frac{C}{k^{5/4}\varepsilon}$$

and

$$\lim_{k \to \infty} \sum_{i=1}^{k} \tilde{a}_i \le \lim_{k \to \infty} \frac{kC}{k^{5/4}\varepsilon} = 0.$$

By assumption (24), $\lim_{k\to\infty}\sum_{i=1}^{k} \tilde{\mathbb{V}}[b_{ij}] = \sigma_j$ for each $1 \leq j \leq n$. Thus, the conditions of MCLT (e.g., see Van der Vaart, 1998) are satisfied and $\sum_{l=1}^{k} b_{lj}$ converges in distribution to a Normal random variable with mean 0 and variance σ_j . The proof is completed.

Appendix C. Performance of \hat{r} in estimating r

In the following tables, we provide an assessment of the estimator \hat{r} in several scenarios that extend beyond that shown in Table 2. Data were simulated under model (1) over a range of n and r values under the five distributions listed. Shown is the number of times that $\hat{r} = r$ among 100 simulated data sets for each scenario. Also shown in parentheses is the number of times that $\hat{r} < r$, if any instances occurred.

k	Binomial	Gamma	NegBin	Normal	Poisson		
n = 15 and $r = 1$							
1000	96	82	82	100	91		
5000	99	89	86	100	92		
10,000	96	76	91	99	93		
100,000	100	90	86	99	94		
n = 15 and $r = 2$							
1000	96	92	5(85)	100	94		
5000	96	90	93	98	97		
10,000	97	93	90	96	95		
100,000	99	96	93	99	97		
n = 15 and $r = 3$							
1000	95	27(68)	36(51)	96	94		
5000	97	44 (46)	45 (46)	99	93		
10,000	100	89	76 (20)	96	95		
100,000	97	95	90	98	96		
n = 15 and $r = 4$							
1000	51 (48)	25(29)	9 (2)	100	94		
5000	99	20(72)	49 (5)	97	94		
10,000	100	60 (27)	28 (35)	97	93		
100,000	98	91	90	97	93		

Table S1: Performance of \hat{r} as an estimator of r when n = 15 and $r \in \{1, 2, 3, 4\}$.

k	Binomial	Gamma	NegBin	Normal	Poisson		
n = 100 and r = 1							
1000	100	99 (1)	99	100	100		
5000	100	100	100	100	100		
10,000	100	100	100	100	100		
100,000	100	100	100	100	100		
	n = 100 and r = 2						
1000	0 (100)	100	100	100	100		
5000	0 (100)	100	100	100	100		
10,000	0(100)	100	100	100	100		
100,000	0(100)	100	100	100	100		
n = 100 and $r = 3$							
1000	0 (100)	100	100	100	100		
5000	0(100)	100	100	100	100		
10,000	0 (100)	100	100	100	100		
100,000	0(100)	100	100	100	100		
n = 100 and $r = 4$							
1000	0 (100)	77 (23)	24(76)	100	100		
5000	0(100)	100	100	100	100		
10,000	0(100)	100	100	100	100		
100,000	0(100)	100	100	100	100		
n = 100 and r = 5							
1000	0 (100)	35(52)	40	100	100		
5000	0(100)	96(4)	100	100	100		
10,000	0 (100)	100	100	100	100		
100,000	0(100)	100	100	100	100		

Table S2: Performance of \hat{r} as an estimator of r when n = 100 and $r \in \{1, 2, 3, 4, 5\}$.

k	Binomial	Gamma	NegBin	Normal	Poisson		
	n = 200 and $r = 6$						
1000	0 (100)	59(10)	1	100	100		
5000	0(100)	100	100	100	100		
10,000	0(100)	100	100	100	100		
100,000	0(100)	100	100	100	100		
	n = 200 and r = 8						
1000	0 (100)	0	0	100	100		
5000	0(100)	0	0	100	100		
10,000	0(100)	78	0	100	100		
100,000	0(100)	100	100	100	100		
	n = 200 and r = 10						
1000	0 (100)	0	0	100	100		
5000	0(100)	0	0	100	100		
10,000	0(100)	0	0	100	100		
100,000	0(100)	69	11	100	100		
	n = 200 and r = 12						
1000	0 (100)	0	0	100	100		
5000	0(100)	0	0	100	100		
10,000	0(100)	0	0	100	100		
100,000	0(100)	0	0	100	100		

Table S3: Performance of \hat{r} as an estimator of r when n = 200 and $r \in \{6, 8, 10, 12\}$.

Appendix D. Performance of Estimator of Π_{M}

The following figures show the performance of the nonparametric estimator $\hat{\Pi}_{\mathbf{M}}$ of $\Pi_{\mathbf{M}}$ for several scenarios beyond that shown in Figure 1. The results are given over a range of n and r values as indicated in the figure captions. Column 1: Boxplots of the difference between the row spaces spanned by \mathbf{M} and $\hat{\mathbf{M}}$ as measured by $d(\mathbf{M}, \hat{\mathbf{M}})$ when the true dimension of \mathbf{M} is utilized to form $\hat{\mathbf{M}}$ (i.e., setting $\hat{r} = r$). Column 2: Boxplots of $d(\mathbf{M}, \hat{\mathbf{M}})$ when using the proposed estimator \hat{r} of the row space dimension in forming $\hat{\mathbf{M}}$. Column 3: An assessment of the estimate $\hat{\mathbf{D}}_k$ of \mathbf{D}_k , where the latter term is the average of the column-wise variances of \mathbf{Y} . The difference is measured by $\|\hat{\mathbf{D}}_k - \mathbf{D}_k\| = \max_{1 \le j \le n} |\hat{\delta}_{kj} - \bar{\delta}_{kj}|$.



Figure S1: Performance of $\hat{\Pi}_{\mathbf{M}}$ when n = 15 and r = 1.



Figure S2: Performance of $\hat{\Pi}_{\mathbf{M}}$ when n = 15 and r = 2.



Figure S3: Performance of $\hat{\Pi}_{\mathbf{M}}$ when n = 15 and r = 3.



Figure S4: Performance of $\hat{\Pi}_{\mathbf{M}}$ when n = 15 and r = 4.



Figure S5: Performance of $\hat{\Pi}_{\mathbf{M}}$ when n = 100 and r = 1.



Figure S6: Performance of $\hat{\Pi}_{\mathbf{M}}$ when n = 100 and r = 2.



Figure S7: Performance of $\hat{\Pi}_{\mathbf{M}}$ when n = 100 and r = 3.



Figure S8: Performance of $\hat{\Pi}_{\mathbf{M}}$ when n = 100 and r = 4.



Figure S9: Performance of $\hat{\Pi}_{\mathbf{M}}$ when n = 100 and r = 5.



Figure S10: Performance of $\hat{\Pi}_{\mathbf{M}}$ when n = 200 and r = 6.



Figure S11: Performance of $\hat{\Pi}_{\mathbf{M}}$ when n = 200 and r = 8.



Figure S12: Performance of $\hat{\Pi}_{\mathbf{M}}$ when n = 200 and r = 10.



Figure S13: Performance of $\hat{\Pi}_{\mathbf{M}}$ when n = 200 and r = 12.