ON TENSORS, SPARSITY, AND NONNEGATIVE FACTORIZATIONS *

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Abstract. Tensors have found application in a variety of fields, ranging from chemometrics to signal processing and beyond. In this paper, we consider the problem of multilinear modeling of sparse count data. Our goal is to develop a descriptive tensor factorization model of such data, along with appropriate algorithms and theory. To do so, we propose that the random variation is best described via a Poisson distribution, which better describes the zeros observed in the data as compared to the typical assumption of a Gaussian distribution. Under a Poisson assumption, we fit a model to observed data using the negative log-likelihood score. We present a new algorithm for Poisson tensor factorization called CANDECOMP—PARAFAC Alternating Poisson Regression (CP-APR) that is based on a majorization-minimization approach. It can be shown that CP-APR is a generalization of the Lee-Seung multiplicative updates. We show how to prevent the algorithm from converging to non-KKT points and prove convergence of CP-APR under mild conditions. We also explain how to implement CP-APR for large-scale sparse tensors and present results on several data sets. both real and simulated.

Key words. Nonnegative tensor factorization, Nonnegative CANDECOMP-PARAFAC, Poisson tensor factorization, Lee-Seung multiplicative updates, majorization-minimization algorithms

1. Introduction. Tensors have found application in a variety of fields, ranging from chemometrics to signal processing and beyond. In this paper, we consider the problem of multilinear modeling of sparse count data. For instance, we may consider the number of papers published by a specific author at a specific conference [9], the number of packets sent from one IP address to another using a specific port [32], or to/from and term counts on emails [1]. Our goal is to develop a descriptive model of such data, along with appropriate algorithms and theory.

Let \mathfrak{X} represent an N-way data tensor of size $I_1 \times I_2 \times \cdots \times I_N$. We are interested in R-component nonnegative CANDECOMP/PARAFAC factor model \mathfrak{M} of the form

$$\mathbf{M} = \sum_{r=1}^{R} \lambda_r \ \mathbf{a}_r^{(1)} \circ \cdots \circ \mathbf{a}_r^{(N)}, \tag{1.1}$$

where $\mathbf{a}_r^{(n)}$ represents the rth column of the nonnegative factor matrix $\mathbf{A}^{(n)}$ of size $I_n \times R$. We refer to each summand as a component. Assuming each factor matrix has been column-normalized to sum to one, we refer to the nonnegative λ_r 's as weights.

In many applications such as chemometrics [31], we fit the model to the data using a least squares criteria, implicitly assuming that the random variation in the tensor data follows a Gaussian distribution. In the case of sparse count data, however, the random variation is better described via a Poisson distribution [23, 30], i.e.,

$$x_i \sim \text{Poisson}(m_i)$$

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rather than $x_i \sim N(m_i, \sigma_i^2)$, where the subscript **i** is shorthand for the multi-index (i_1, i_2, \ldots, i_N) . In fact, a Poisson model is a much better explanation for the zero observations that we encounter in sparse data — these zeros just correspond to events that were very unlikely to be observed. Thus, we propose that rather than using the least squares error function given by $\sum_{\bf i} |x_{\bf i} - m_{\bf i}|^2$, for count data we should instead minimize

$$f(\mathbf{M}) = \sum_{\mathbf{i}} m_{\mathbf{i}} - x_{\mathbf{i}} \log m_{\mathbf{i}}, \tag{1.2}$$

which equals the negative log-likelihood of the observations up to an additive constant. The difficulty of this approach as compared to using a least squares error function is fitting this more complex objective function.

- 1.1. Contributions. Although other authors have considered fitting tensor data using a Poisson likelihood criteria (i.e., KL divergence) [34, 6], we offer the following contributions:
- We develop alternating Poisson regression fitting algorithm for the nonnegative CP model, called CP-APR. The subproblems are solved using a majorization-minimization (MM) approach. If the algorithm is restricted to a single inner iteration per subproblem, it reduces to the standard Lee-Seung multiplicative updates [19, 20, 34]; however, using multiple inner iterations is shown to accelerate the method.
- It is known that the Lee-Seung multiplicative updates may converge to a non-stationary point [13]. We introduce a novel technique for avoiding *inadmissible zeros* (i.e., zeros that violate stationarity conditions) that is only a trivial change to the basic algorithm and prevents convergence to non-stationary points, even in the matrix case.
- Assuming the subproblems can be solved exactly, we prove convergence of the CP-APR algorithm. In particular, we can show convergence even for sparse input data and solutions on the boundary of the nonnegative orthant.
- We explain how to efficiently implement CP-APR for large-scale sparse data. Although it is well-known how to do large-scale sparse calculations for the least squares fitting function [2], the Poisson likelihood fitting algorithm requires new kernels.
- We present experimental results showing the effectiveness of the method on both real and simulated data. In fact, the Poisson assumption leads quite naturally to a generative model for sparse data.
- 1.2. Related Work. Much of the past work in nonnegative matrix and tensor analysis has focused on the least squares error [28, 27, 4, 13, 17, 15, 12], which corresponds to an assumption of normal independently identically distributed (i.i.d.) noise. The focus of this paper is Kullback-Leibler (KL) divergence, which corresponds to maximum likelihood estimation under a independent Poisson assumption; see §2.3. The seminal work in this domain are the papers of Lee and Seung [19, 20], which propose very simple multiplicative update formulas for both least squares and KL divergence, resulting in a very low cost-per-iteration. Welling and Weber [34] were the first to generalize the Lee and Seung algorithms to nonnegative tensor factorization (NTF). Applications of NTF based on KL-divergence include EEG analysis [24] and sound source separation [11]. We note that generalizations of KL divergence have have also been proposed in the literature, including Bregman divergence [7] and beta divergence [6].

Compared with algorithm development, markedly less attention has been given to the global convergence properties of nonnegative factorization algorithms. Lee and Seung's algorithm is guaranteed to decrease the loss function at every step, but this is not a guarantee that the iterates converge to a local minimum or even a stationary point of the loss function. To the contrary, Gonzalez and Zhang [13] empirically showed that, in the case of least squares loss, the Lee and Seung method can converge to non-KKT points; in §6.3, we show a similar example for KL divergence.

This failure to converge to a KKT point is due to finite precision in the calculations. If the solution is strictly positive (on the interior), Finesso and Spreij [10] develop a variant of the Lee-Seung algorithm for KL-divergence and prove that iterates from their modified updates will converge to an interior stationary point, provided the initial iterate has strictly positive entries; Zafeiriou and Petrou [35] develop tensor extensions of [10] using the same proof strategy. A key assumption in the convergence proofs of these variants of Lee-Seung is that iterates initialized in the interior remain in the interior throughout the procedure, but this is generally not the case in finite precision. Our example in §6.3 shows that initializing the iterate sequence to the interior is not sufficient to guarantee convergence to KKT points in finite precision, even for dense data. This should especially be concerning for fitting models to sparse count data where intermediate iterates and limit points are more likely to visit and subsequently get "stuck" at the boundary.

In contrast our convergence proof does not assume that iterates will never visit the boundary of the parameter space on their way to a limit, but instead relies on our fix for avoiding inadmissible zeros to ensure convergence to a KKT point. Additionally, we prove convergence for our generalization of the Lee-Seung algorithm using standard tools from constrained optimization theory, in contrast to employing lifting as in [10, 35].

1.3. Outline. The remainder of this paper is organized as follows. In §2, we describe the notation, common multilinear operations used in this paper, the Poisson model for count data, and review key optimization results we use to prove convergence of CP-APR. We develop CP-APR in stages over the next two sections. In §3, we describe the sequence of alternating minimization problems that comprise the outer loop of CP-APR, as well as the KKT conditions for the global optimization problem. We conclude the section with a convergence proof for the outer iterates. In §4, we describe and prove the convergence of our MM subproblem solver. Important implementation issues, foremost of which are inadmissible zero avoidance and computations for sparse data tensors, are covered in §5. In §6, we present results of numerical experiments for simulated and real data sets. We conclude in §7 with a summary of our work and discussion of future work.

2. Notation and Preliminaries.

2.1. Notation. Throughout, scalars are denoted by lowercase letters (a), vectors are denoted by boldface lowercase letters (\mathbf{v}) , matrices are denoted by boldface capital letters (\mathbf{A}) , and higher-order tensors are denoted by boldface Euler script letters (\mathfrak{X}) . We use the following special notation: \mathbf{e} denotes a vector of all ones and \mathbf{E} denotes the matrix of all ones. The *i*th entry of a vector \mathbf{v} is denoted v_i . The (i,j) entry of a matrix \mathbf{A} is denoted a_{ij} and the *j*th column of a matrix \mathbf{A} is denoted by \mathbf{a}_j . We use multi-index notation so that a boldface \mathbf{i} represents the index (i_1, \ldots, i_N) , thus the (i_1, \ldots, i_N) of a tensor \mathfrak{X} can be written as x_i .

We also use subscripts to denote iteration index for infinite sequences, and the difference between its use for an entry and its use as an iteration index should be clear by context. When there is a conflict, the iteration index is the innermost index. Thus,

the kth vector in a sequence would be denoted \mathbf{v}_k , the ith entry would be denoted v_i , and the ith entry of the kth vector in a sequence would be denoted $(\mathbf{x}_k)_i$.

The notation $\|\cdot\|$ refers to the two-norm or Frobenious norm for matrices, i.e., the sum of the squares of the entries. The notation $\|\cdot\|_1$ refers to the one-norm, i.e., the sum of the absolute values of the entries.

The outer product is denoted by \circ . The symbol * represents elementwise multiplication of two same-sized objects; likewise, the symbol \oslash represents elementwise division. The symbol \odot denotes Khatri-Rao matrix multiplication, i.e., the columnwise Kronecker product. The mode-n matricization or unfolding of a tensor \mathcal{X} is denoted by $\mathbf{X}_{(n)}$ and is of size $I_n \times J_n$ where $J_n \equiv \prod_{m \neq n} I_n$. See Appendix A for further details on these operations.

2.2. Kruskal Tensors. The model in (1.1) is a Kruskal tensor [2] and is generally used to represent CANDECOMP/PARAFAC factorization [5, 14]. We can express (1.1) using the shorthand notation:

$$\mathbf{M} = \left[\mathbf{\lambda}; \mathbf{A}^{(1)}, \dots, \mathbf{A}^{(N)} \right]. \tag{2.1}$$

Elementwise, the model entries are

$$m_{\mathbf{i}} = \sum_{r=1}^{R} \lambda_r \ a_{i_1 r}^{(1)} \ a_{i_2 r}^{(2)} \cdots \ a_{i_N r}^{(N)} \quad \text{for all} \quad 1 \le i_n \le I_n, \ n = 1, \dots, N,$$
 (2.2)

Depending on context, \mathcal{M} either represents the tensor produced by (1.1) or, if we refer to \mathcal{M} as a member of a set, to the constituent parameters appropriately scaled (e.g., so that all the factor matrices are column stochastic). We note that there is scaling ambiguity that allows us to express the same \mathcal{M} in different ways, i.e.,

$$\mathbf{M} = \left[\mathbf{A}^{(1)}, \dots, \mathbf{A}^{(n-1)}, \mathbf{B}^{(n)}, \mathbf{A}^{(n+1)}, \dots, \mathbf{A}^{(N)} \right]$$
(2.3)

where

$$\mathbf{B}^{(n)} = \mathbf{A}^{(n)} \mathbf{\Lambda}$$
 and $\mathbf{\Lambda} = \operatorname{diag}(\mathbf{\lambda})$. (2.4)

Note that the weights in (2.3) are omitted in the shorthand notation because they are all ones. We will frequently switch between representation (2.1) and (2.3). It is known that the matricization of Kruskal tensors have a special form [2], i.e.,

$$\mathbf{M}_{(n)} = \mathbf{B}^{(n)} \left(\mathbf{A}^{(N)} \odot \cdots \odot \mathbf{A}^{(n+1)} \odot \mathbf{A}^{(n-1)} \odot \cdots \odot \mathbf{A}^{(1)} \right)^{\mathsf{T}}.$$

2.3. The Poisson Distribution and KL Divergence. In statistics, count data is often best described as following a Poisson distribution. For a general discussion of the Poisson distribution, see, e.g., [30]. We summarize key facts here.

A random variable X is said to have a Poisson distribution with parameter $\mu > 0$ if it takes integer values $x = 0, 1, 2, \ldots$ with probability

$$P(X = x) = \frac{e^{-\mu}\mu^x}{x!}. (2.5)$$

The mean and variance of X are both μ ; therefore, the variance increases along with the mean, which seems like a reasonable assumption for count data. It is also useful

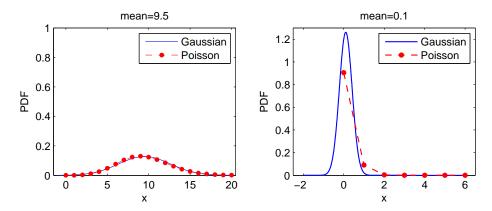


Fig. 2.1: Illustration of Gaussian and Poisson distributions for two parameters. For both examples, we assume that the variance of the Gaussian is equal to the mean m.

to note that the sum of independent Poisson random variables is also Poisson. This is important in our case since each Poisson parameter is a multilinear combination of the model parameters. We contrast Poisson and Gaussian distributions in Figure 2.1. Observe that there is a close match between the Gaussian and Poisson for larger values of the mean, μ . For small values of μ , however, the match is not as strong and the Gaussian random variable can take on negative values.

We can determine the optimal Poisson parameters by maximizing the likelihood of the observed data. Let x_i be a vector of observations and let μ_i be the vector of Poisson parameters. (We assume that μ_i 's are not independent, else the function would entirely decouple in the parameters to be estimated.) Then the negative of the log of the likelihood function for (2.5) is

$$\sum_{i} \mu_i - x_i \log \mu_i, \tag{2.6}$$

excepting the addition of the constant term $\sum_{i} \log(x_{i}!)$, which is omitted. This function is sometimes referred to as the generalized Kullback-Leibler (KL) divergence.

Because we are working with sparse data, there are many instances for which we expect $x_i = 0$, which leads to some ambiguity in (2.6) if $\mu_i = 0$. We assume throughout that

$$0 \cdot \log(\mu) = 0 \quad \text{for all} \quad \mu \ge 0. \tag{2.7}$$

This is for notation convenience; otherwise, we would need to rewrite (2.6) as

$$\sum_{i} \mu_i - \sum_{i: x_i \neq 0} x_i \log \mu_i.$$

2.4. KKT Conditions for Constrained Stationarity. We briefly review the first-order conditions for constrained stationary points; see [26] for further details. Consider the following nonlinear program:

min
$$f(\mathbf{x})$$
 s.t. $c_i(\mathbf{x}) = 0$ for $i \in \mathcal{E}$ and $c_i(\mathbf{x}) \ge 0$ for $i \in \mathcal{I}$. (2.8)

DEFINITION 2.1 (LICQ [26]). Given the point \mathbf{x} and the active set $\mathcal{A}(\mathbf{x}) = \mathcal{E} \cup \{ i \in \mathcal{I} \mid c_i(\mathbf{x}) = 0 \}$ for (2.8), we say that the linear independence constraint qualification (LICQ) holds if the set of active constraint gradients $\{ \nabla c_i(\mathbf{x}) \mid i \in \mathcal{A}(\mathbf{x}) \}$ is linearly independent.

THEOREM 2.2 (First-order necessary conditions [26]). Suppose that \mathbf{x} is a local solution to (2.8) and that LICQ holds at \mathbf{x} . Then there exists a Lagrange multiplier $\boldsymbol{\eta}$ such that the following conditions are satisfied at $(\mathbf{x}, \boldsymbol{\eta})$:

$$\nabla f(\mathbf{x}) - \sum_{i} \eta_{i} \nabla c_{i}(\mathbf{x}) = 0,$$

$$c_{i}(\mathbf{x}) = 0, \text{ for all } i \in \mathcal{E},$$

$$c_{i}(\mathbf{x}) \geq 0, \text{ for all } i \in \mathcal{I},$$

$$\eta_{i} \geq 0, \text{ for all } i \in \mathcal{I},$$

$$\eta_{i} c_{i}(\mathbf{x}) = 0, \text{ for all } i \in \mathcal{I}.$$

$$(2.9)$$

Points that satisfy these conditions (2.9) are constrained stationary points, better known as Karush-Kuhn-Tucker (KKT) points. When (2.8) is a convex program, the first-order necessary conditions in (2.9) are sufficient conditions for global optimality.

THEOREM 2.3 (Proposition 5.4.3 in [18]). Let the functions f and c_i be defined as in (2.8) and assume that f and c_i for $i \in \mathcal{I}$ are convex and c_i for $i \in \mathcal{E}$ are affine. If a point \mathbf{x} satisfies (2.9), then \mathbf{x} is the global minimizer of (2.8).

2.5. Majorization-Minimization Algorithms for Optimization. The basic idea of a majorization-minimization (MM) algorithm is to convert a hard optimization problem (e.g., non-convex and/or non-differentiable) into a series of simpler ones (e.g., smooth convex) that are easy to minimize and that majorize the original function, as follows.

DEFINITION 2.4. Let f and g be real-valued functions on \mathbb{R}^n and $\mathbb{R}^n \times \mathbb{R}^n$, respectively. We say that g majorizes f at $\mathbf{x} \in \mathbb{R}^n$ if $g(\mathbf{y}, \mathbf{x}) \geq f(\mathbf{y})$ for all $\mathbf{y} \in \mathbb{R}^n$ and $g(\mathbf{x}, \mathbf{x}) = f(\mathbf{x})$.

LEMMA 2.5. Let $x \ge 0$ be a scalar and $\pi \ge 0$, $\pi \ne 0$, be a vector of length R. For a vector $\mathbf{c} \ge 0$, $\mathbf{c} \ne 0$, of length R, let the function f be defined by

$$f(\mathbf{c}) = \mathbf{c}^\mathsf{T} \boldsymbol{\pi} - x \log (\mathbf{c}^\mathsf{T} \boldsymbol{\pi}).$$

Then f is majorized at $\bar{\mathbf{c}} \geq 0$ by

$$g(\mathbf{c}, \overline{\mathbf{c}}) = \mathbf{c}^{\mathsf{T}} \boldsymbol{\pi} - x \sum_{r=1}^{R} \alpha_r \log \left(\frac{c_r \pi_r}{\alpha_r} \right) \quad where \quad \alpha_r = \frac{\overline{c}_r \pi_r}{\overline{\mathbf{c}}^{\mathsf{T}} \pi}.$$

Proof. If x = 0, then $g(\mathbf{c}, \overline{\mathbf{c}}) = f(\mathbf{c})$ for all \mathbf{c} , and g trivially majorizes f at $\overline{\mathbf{c}}$. Consider the case when x > 0. It is immediate that $g(\overline{\mathbf{c}}, \overline{\mathbf{c}}) = f(\overline{\mathbf{c}})$. The majorization follows from the fact that log is strictly concave and that we can write $\mathbf{c}^{\mathsf{T}}\boldsymbol{\pi}$ as a convex combination of the elements $c_r\pi_r/\alpha_r$. Note that if any elements $\overline{c}_r\pi_r$ are zero, they do not contribute to the sum since we assume (2.7) and $\alpha_r = 0$. \square

If $f(\mathbf{x})$ is the function to be optimized and $g(\cdot, \mathbf{x})$ majorizes f at \mathbf{x} , the basic MM iteration is

$$\mathbf{x}_{k+1} = \arg\min_{\mathbf{y}} g(\mathbf{y}, \mathbf{x}_k). \tag{2.10}$$

It is easy to see that (2.10) always takes non-increasing steps with respect to f since $f(\mathbf{x}_{k+1}) \leq g(\mathbf{x}_{k+1}, \mathbf{x}_k) \leq g(\mathbf{x}_k, \mathbf{x}_k) = f(\mathbf{x}_k)$, where \mathbf{x}_k is the current iterate and \mathbf{x}_{k+1} is the optimum computed at that iterate.

The convergence theory of MM algorithms relies on characterizing the properties of the map $\psi(\mathbf{x}) \equiv \arg\min_{\mathbf{y}} g(\mathbf{y}, \mathbf{x})$. The following general result for algorithm maps will be used to prove the convergence of the MM algorithm for solving the subproblem, although we do not assume that the map ψ is associated with an MM algorithm.

THEOREM 2.6. Let f be a continuous function on a domain \mathcal{D} , and let ψ be a continuous iterative map from \mathcal{D} into \mathcal{D} such that $f(\psi(\mathbf{x})) < f(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{D}$ with $\psi(\mathbf{x}) \neq \mathbf{x}$. Suppose there is an \mathbf{x}_0 such that the set $\mathcal{L}_f(\mathbf{x}_0) \equiv \{ \mathbf{x} \in \mathcal{D} \mid f(\mathbf{x}) \leq f(\mathbf{x}_0) \}$ is compact. Define $\mathbf{x}_{k+1} = \psi(\mathbf{x}_k)$ for $k = 0, 1, \ldots$ Then (a) the sequence of iterates $\{\mathbf{x}_k\}$ has at least one limit point and all its limit points are fixed points of ψ , and (b) the distance between successive iterates converges to 0, i.e. $\|\mathbf{x}_{k+1} - \mathbf{x}_k\| \to 0$.

Proof. The proof of (a) follows that of Proposition 10.3.2 of [18]. First note that the sequence of iterates must be in $\mathcal{L}_f(\mathbf{x}_0)$ because $f(\mathbf{x}_k) \leq f(\mathbf{x}_0)$ for all k. Since $\mathcal{L}_f(\mathbf{x}_0)$ is compact, $\{\mathbf{x}_k\}$ has a convergent subsequence whose limit is in $\mathcal{L}_f(\mathbf{x}_0)$; denote this as $\mathbf{x}_{k_\ell} \to \mathbf{x}_*$ as $\ell \to \infty$. Since f is assumed to be continuous, $\lim_{k \to \infty} f(\mathbf{x}_k) = f(\mathbf{x}_k)$. Moreover, clearly $f(\mathbf{x}_k) \leq f(\mathbf{x}_{k_\ell})$ for all k_ℓ .

Note that $f(\psi(\mathbf{x}_{k_{\ell}})) \leq f(\mathbf{x}_{k_{\ell}})$. Taking the limit of both sides and applying the continuity of ψ and f, we must have that $f(\psi(\mathbf{x}_*)) \leq f(\mathbf{x}_*)$. But we also have that

$$f(\mathbf{x}_*) \le f(\mathbf{x}_{k_{\ell+1}}) \le f(\mathbf{x}_{k_{\ell}+1}) = f(\psi(\mathbf{x}_{k_{\ell}})).$$

Again taking limits we obtain $f(\mathbf{x}_*) \leq f(\psi(\mathbf{x}_*))$. Therefore $f(\mathbf{x}_*) = f(\psi(\mathbf{x}_*))$. But by assumption, this equality implies that \mathbf{x}_* is a fixed point of ψ , and thus (a) is proven.

We now turn to the proof of (b), which follows the proof of Proposition 10.3.3 in [18]. Recall $\{\mathbf{x}_k\}$ denotes the iterate sequence. Since $f(\mathbf{x}_k)$ is decreasing and f is bounded below on $\mathcal{L}_f(\mathbf{x}_0)$, we can assert that $f(\mathbf{x}_k)$ is a convergent sequence with a limit f_* . Assume the contrary of (b), i.e., that there exists an $\epsilon > 0$ and a subsequence $\{k_\ell\}$ of the indices such that

$$\|\mathbf{x}_{k_{\ell}+1} - \mathbf{x}_{k_{\ell}}\| > \epsilon \text{ for all } k_{\ell}.$$
 (2.11)

Note that this subsequence is different from the one discussed in proving part (a). Since $\mathbf{x}_{k_{\ell}} \in \mathcal{L}_f(\mathbf{x}_0)$, by possibly restricting $\{k_{\ell}\}$ to a further subsequence, we may assume that $\mathbf{x}_{k_{\ell}}$ converges to a limit \mathbf{u} . By possibly restricting $\{k_{\ell}\}$ to yet a further subsequence, we may additionally assume that $\mathbf{x}_{k_{\ell}+1}$ converges to a limit \mathbf{v} . By (2.11), we can conclude $\|\mathbf{v} - \mathbf{u}\| \ge \epsilon$. Note that $\mathbf{x}_{k_{\ell}+1} = \psi(\mathbf{x}_{k_{\ell}})$. Taking the limit of both sides and using the continuity of ψ we obtain $\psi(\mathbf{u}) = \mathbf{v}$. Additionally, using the continuity of f,

$$f(\mathbf{u}) = \lim_{\ell \to \infty} f(\mathbf{x}_{k_{\ell}}) = f_* = \lim_{\ell \to \infty} f(\mathbf{x}_{k_{\ell}+1}) = f(\mathbf{v}).$$

Since $\mathbf{v} = \psi(\mathbf{u})$, we have that $f(\mathbf{u}) = f(\psi(\mathbf{u}))$ which by assumption occurs if and only if $\mathbf{u} = \psi(\mathbf{u})$. This implies that $\mathbf{u} = \mathbf{v}$, and we have arrived at a contradiction.

3. CP-APR: Alternating Poisson Regression. In this section we introduce the CP-APR algorithm for fitting a nonnegative *Poisson tensor decomposition (PTF)* to count data. The algorithm employs an alternating optimization scheme that sequentially optimizes one factor matrix while holding the others fixed; this is also known as nonlinear Gauss-Seidel. The subproblems are solved via a majorization-minimization (MM) algorithm.

3.1. The Optimization Problem. Our optimization problem is defined as

$$\min f(\mathbf{M}) \equiv \sum_{i} m_{i} - x_{i} \log m_{i} \quad \text{s.t. } \mathbf{M} = \left[\mathbf{\lambda}; \mathbf{A}^{(1)}, \dots, \mathbf{A}^{(N)} \right] \in \Omega,$$
 (3.1)

where

$$\Omega = \Omega_{\lambda} \times \Omega_{1} \times \dots \times \Omega_{n} \quad \text{with}$$

$$\Omega_{\lambda} = [0, +\infty)^{R} \quad \text{and} \quad \Omega_{n} = \left\{ \mathbf{A} \in [0, 1]^{I_{n} \times R} \mid \|\mathbf{a}_{r}\|_{1} = 1 \text{ for } r = 1, \dots, R \right\}.$$
(3.2)

In other words, we assume that the factor matrices have stochasticity constraints on the columns, thereby avoiding possible scale ambiguities.

The function f is not finite on all of Ω . For example, if there exists \mathbf{i} such that $m_{\mathbf{i}} = 0$ and $x_{\mathbf{i}} > 0$, then $f(\mathbf{M}) = +\infty$. If $m_{\mathbf{i}} > 0$ for all \mathbf{i} such that $x_{\mathbf{i}} > 0$, however, then we are guaranteed that $f(\mathbf{M})$ is finite. Consequently, we will generally wish to restrict ourselves to a domain for which $f(\mathbf{M})$ is finite. We define

$$\Omega(\zeta) \equiv \operatorname{conv}(\{ \mathcal{M} \in \Omega \mid f(\mathcal{M}) \le \zeta \}), \tag{3.3}$$

where $\operatorname{conv}(\cdot)$ denotes the convex hull. We observe that $\Omega(\zeta) \subset \Omega$ (strict subset) since, for example, the all-zero model is not in $\Omega(\zeta)$. In the following lemma, we show that $\Omega(\zeta)$ is compact for any $\zeta > 0$. The proof is given in Appendix B.

LEMMA 3.1. Let f be as defined in (3.1) and $\Omega(\zeta)$ be as defined in (3.3). For any $\zeta > 0$, $\Omega(\zeta)$ is compact.

3.2. CP-APR Main Loop: Nonlinear Gauss-Seidel. We solve problem (3.1) via an alternating approach, holding all factor matrices constant except one. Consider the problem for the nth factor matrix. Recall that we can express \mathcal{M} as

$$\mathbf{M}_{(n)} = \mathbf{B}^{(n)} \mathbf{\Pi}^{(n)},$$

where $\mathbf{B}^{(n)}$ is defined in (2.4) and

$$\mathbf{\Pi}^{(n)} \equiv \left(\mathbf{A}^{(N)} \odot \cdots \odot \mathbf{A}^{(n+1)} \odot \mathbf{A}^{(n-1)} \odot \cdots \odot \mathbf{A}^{(1)} \right)^{\mathsf{T}}.$$
 (3.4)

Thus, we can rewrite the objective function in (3.1) as

$$f(\mathbf{M}) = \mathbf{e}^\mathsf{T} \left[\mathbf{B}^{(n)} \mathbf{\Pi}^{(n)} - \mathbf{X}_{(n)} * \log \left(\mathbf{B}^{(n)} \mathbf{\Pi}^{(n)} \right) \right] \mathbf{e},$$

where **e** is the vector of all ones, * denotes the elementwise product, and the log function is applied elementwise. We note that it is convenient to update $\mathbf{A}^{(n)}$ and λ simultaneously since the resulting constraint on $\mathbf{B}^{(n)}$ is simply $\mathbf{B}^{(n)} \geq 0$.

Thus, at each inner iteration of the Gauss-Seidel algorithm, we optimize $f(\mathbf{M})$ restricted to the nth block, i.e.,

$$\mathbf{B}^{(n)} = \arg\min_{\mathbf{B} \ge 0} f_n(\mathbf{B}) \equiv \mathbf{e}^{\mathsf{T}} \left[\mathbf{B} \mathbf{\Pi}^{(n)} - \mathbf{X}_{(n)} * \log \left(\mathbf{B} \mathbf{\Pi}^{(n)} \right) \right] \mathbf{e}. \tag{3.5}$$

The updates for λ and $\mathbf{A}^{(n)}$ come directly from $\mathbf{B}^{(n)}$. Note that some care must be taken if an entire column of $\mathbf{B}^{(n)}$ is zero; if the rth column is zero, then we can set $\lambda_r = 0$ and $\mathbf{b}_r^{(n)}$ to an arbitrary nonnegative vector that sums to one. The full

Algorithm 1 CP-APR Algorithm (Ideal Version)

Let \mathfrak{X} be a tensor of size $I_1 \times \cdots \times I_N$. Let $\mathfrak{M} = [\![\boldsymbol{\lambda}; \mathbf{A}^{(1)}, \cdots, \mathbf{A}^{(N)}]\!]$ be an initial guess for an R-component model such that $\mathfrak{M} \in \Omega(\zeta)$ for some $\zeta > 0$.

```
1: repeat
2: for n = 1, ..., N do
3: \Pi \leftarrow \left(\mathbf{A}^{(N)} \odot \cdots \odot \mathbf{A}^{(n+1)} \odot \mathbf{A}^{(n-1)} \odot \cdots \odot \mathbf{A}^{(1)}\right)^{\mathsf{T}}
4: \mathbf{B} \leftarrow \arg\min_{\mathbf{B} \geq 0} \mathbf{e}^{\mathsf{T}} \left[\mathbf{B}\Pi - \mathbf{X}_{(n)} * \log \left(\mathbf{B}\Pi\right)\right] \mathbf{e} \triangleright subproblem
5: \lambda \leftarrow \mathbf{e}^{\mathsf{T}}\mathbf{B}
6: \mathbf{A}^{(n)} \leftarrow \mathbf{B}\Lambda^{-1}
7: end for
8: until convergence
```

procedure is given in Algorithm 1; this is a variant (because of the handling of λ) of nonlinear Gauss-Seidel.

We defer the proof of convergence until §3.3, but we discuss how to check for convergence here. First, we mention an assumption that is important to the theory and also arguably practical. Let

$$\mathcal{S}_i^{(n)} = \left\{ j \mid (\mathbf{X}_{(n)})_{ij} > 0 \right\}$$
(3.6)

denote the set of indices of columns for which the *i*th row of $\mathbf{X}_{(n)}$ is non-zero. If N=3, then $\mathbf{X}_{(1)}(i,:)$ corresponds to a vectorization of the *i*th horizontal slice of \mathbf{X} , $\mathbf{X}_{(2)}(i,:)$ to a vectorization of the *i*th lateral slice, and $\mathbf{X}_{(3)}(i,:)$ to a vectorization of the *i*th frontal slice. More generally, we can think of vectorizing "hyperslices" with respect to each mode.

Assumption 3.2. The rows of the submatrix $\Pi^{(n)}(:, \mathcal{S}_i^{(n)})$ (i.e., only the columns corresponding to nonzero rows in $\mathbf{X}_{(n)}$ are considered) are linearly independent for all $i = 1, \ldots, I_n$ and $n = 1, \ldots, N$.

Assumption 3.2 implies that $|\mathcal{S}_i^{(n)}| \geq R$ for all i. Thus, we need to observe at least $R \cdot \max_n I_n$ counts in the data tensor \mathfrak{X} , and the counts need to be sufficiently distributed across \mathfrak{X} . Consequently, the conditions appeal to our intuition that there are concrete limits on how sparse the data tensor can be with respect to how many parameters we wish to fit. If, for example, we had $\mathbf{X}_{(1)}(i,:) = 0$, it is clear that we can remove element i from the first dimension entirely since it contributes nothing. We are making a stronger requirement: each element in each dimension must have at least R nonzeros in its corresponding hyperslice.

A potential problem is that Assumption 3.2 depends on the current iterate, which we cannot predict in advance. However, we observe that if $\lambda > 0$ and the factor matrices have random uniform [0,1] positive entries and $R \leq \min_n \prod_{m \neq n} I_m$, then this condition is satisfied with probability one¹. This condition can be checked as the iterates progress.

The matrix

$$\mathbf{\Phi}^{(n)} \equiv \left[\mathbf{X}_{(n)} \oslash \left(\mathbf{B}^{(n)} \mathbf{\Pi}^{(n)} \right) \right] \mathbf{\Pi}^{(n)\mathsf{T}}, \tag{3.7}$$

 $^{^{1}}$ We can actually appeal to a weaker assumption; if the entries are drawn from any distribution that is absolutely continuous with respect to the Lebesgue measure on [0,1] then the condition is satisfied with probability one.

with \oslash denoting elementwise division, will come up repeatedly in the remainder of the paper. For instance, we observe that the partial derivative of f with respect to $\mathbf{A}^{(n)}$ is

$$rac{\partial f}{\partial \mathbf{A}^{(n)}} = \left(\mathbf{E} - \mathbf{\Phi}^{(n)}\right) \mathbf{\Lambda},$$

where **E** is the matrix of all ones. Consequently, the matrix $\Phi^{(n)}$ plays a role in checking convergence as follows.

THEOREM 3.3. If $\lambda > 0$ and $\mathbf{M} = [\![\lambda; \mathbf{A}^{(1)}, \dots, \mathbf{A}^{(N)}]\!] \in \Omega(\zeta)$ for some $\zeta > 0$, then \mathbf{M} is a KKT point of (3.1) if and only if

$$\min\left(\mathbf{A}^{(n)}, \mathbf{E} - \mathbf{\Phi}^{(n)}\right) = 0 \text{ for } n = 1, \dots, N.$$
(3.8)

Proof. Since $\lambda > 0$, we can assume that λ has been absorbed into $\mathbf{A}^{(m)}$ for some m. Thus, we can replace the constraints $\lambda \in \Omega_{\lambda}$ and $\mathbf{A}^{(m)} \in \Omega_n$ with $\mathbf{B}^{(m)} \geq 0$. In this case, the partial derivatives are

$$\frac{\partial f}{\partial \mathbf{B}^{(m)}} = \mathbf{E} - \mathbf{\Phi}^{(m)} \quad \text{and} \quad \frac{\partial f}{\partial \mathbf{A}^{(n)}} = \left(\mathbf{E} - \mathbf{\Phi}^{(n)}\right) \mathbf{\Lambda} \text{ for } n \neq m. \tag{3.9}$$

Since $\mathbf{M} \in \Omega(\zeta)$ for some $\zeta > 0$, we know that not all elements of \mathbf{M} are zero; thus, LICQ holds. From Theorem 2.2, the following conditions define a KKT point:

$$\mathbf{E} - \mathbf{\Phi}^{(m)} - \mathbf{\Upsilon}^{(m)} = 0,$$

$$\left(\mathbf{E} - \mathbf{\Phi}^{(n)}\right) \mathbf{\Lambda} - \mathbf{\Upsilon}^{(n)} - \mathbf{e}(\boldsymbol{\eta}^{(n)})^{\mathsf{T}} = 0, \quad \text{for } n \neq m,$$

$$\mathbf{e}^{\mathsf{T}} \mathbf{A}^{(n)} = 1, \quad \text{for } n \neq m,$$

$$\mathbf{A}^{(n)} \geq 0, \quad \text{for } n \neq m,$$

$$\mathbf{B}^{(m)} \geq 0,$$

$$\mathbf{\Upsilon}^{(n)} \geq 0, \quad \text{for all } n,$$

$$\mathbf{\Upsilon}^{(n)} * \mathbf{A}^{(n)} = 0, \quad \text{for all } n \neq m,$$

$$\mathbf{\Upsilon}^{(m)} * \mathbf{B}^{(m)} = 0.$$

$$(3.10)$$

Here $\Upsilon^{(n)}$ are the Lagrange multipliers for the nonnegativity constraints and $\eta^{(n)}$ are the Lagrange multipliers for the stochasticity constraints.

If $\mathbf{M} = \langle \boldsymbol{\lambda}; \mathbf{A}^{(1)}, \dots, \mathbf{A}^{(N)} \rangle$ is a KKT point, then from (3.10), we have that $\mathbf{\Upsilon}^{(m)} = \mathbf{E} - \mathbf{\Phi}^{(m)} \geq 0$, $\mathbf{B}^{(m)} \geq 0$, and $\mathbf{\Upsilon}^{(m)} * \mathbf{B}^{(m)} = 0$. Thus, $\min(\mathbf{A}^{(m)}\boldsymbol{\Lambda}, \mathbf{E} - \mathbf{\Phi}^{(m)}) = 0$. Since $\boldsymbol{\lambda} > 0$ and m is arbitrary, (3.8) follows immediately.

If, on the other hand, (3.8) is satisfied, choosing $\Upsilon^{(m)} = \mathbf{E} - \Phi^{(m)}$, and $\Upsilon^{(n)} = \left(\mathbf{E} - \Phi^{(n)}\right) \Lambda$ and $\eta^{(n)} = 0$ for $n \neq m$ satisfies the KKT conditions in (3.10). Hence, \mathfrak{M} must be a KKT point. \square

Observe that the condition $\lambda > 0$ makes λ moot in the KKT conditions — this reflects the scaling ambiguity that is inherent in the model.

From Theorem 3.3, we can check for convergence by verifying

$$\left| \min \left(\mathbf{A}^{(n)}, \mathbf{E} - \mathbf{\Phi}^{(n)} \right) \right| \le \tau \text{ for } n = 1, \dots, N,$$

where $\tau > 0$ is some specified convergence tolerance.

3.3. Convergence Theory for CP-APR. We require the strict convexity of f in each of the block coordinates. This is ensured under Assumption 3.2.

LEMMA 3.4 (Strict convexity of subproblem). Let $f_n(\cdot)$ be the function f restricted to the nth block as defined in (3.5). If Assumption 3.2 is satisfied, then $f_n(\mathbf{B})$ is strictly convex over $\mathcal{B}_n = \{\mathbf{B} \in [0, +\infty)^{I_n \times R} : \mathbf{B}\Pi^{(n)} \neq \mathbf{0}\}.$

Proof. In the proof, we drop the n's for convenience. First note that \mathcal{B} is convex. Let $\mathbf{C} = \mathbf{B}^{\mathsf{T}}$. Recall that we can rewrite (3.5) as shown in (4.1). Hence, it is sufficient to show that the function

$$\hat{f}(\mathbf{C}) = -\sum_{ij} x_{ij} \log(\mathbf{c}_i^\mathsf{T} \boldsymbol{\pi}_j)$$

is strictly convex over the convex set $C = \{\mathbf{C} \in [0, +\infty)^{R \times I_n} : \mathbf{C}^\mathsf{T} \mathbf{\Pi} \neq \mathbf{0}\}$. Fix $\alpha \in (0, 1)$ and $\bar{\mathbf{C}}, \hat{\mathbf{C}} \in C$ such that $\bar{\mathbf{C}} \neq \hat{\mathbf{C}}$. Since the inner product is affine and log is a strictly concave function, we need only show that there exists some i and j such that $x_{ij} \neq 0$ and $\hat{\mathbf{c}}_i^\mathsf{T} \boldsymbol{\pi}_j \neq \bar{\mathbf{c}}_i^\mathsf{T} \boldsymbol{\pi}_j$. We know at least one column must differ since $\bar{\mathbf{C}} \neq \hat{\mathbf{C}}$; let i correspond to that column and define $\mathbf{d} = \hat{\mathbf{c}}_i - \bar{\mathbf{c}}_i \neq 0$. By Assumption 3.2, we know that $\mathbf{\Pi}(:, S_i)$ has full row rank. Thus, there exists a column j of $\mathbf{\Pi}$ such that $x_{ij} \neq 0$ and $\mathbf{d}^\mathsf{T} \boldsymbol{\pi}_j \neq 0$. Hence, the claim. \square

Here we state our main convergence result. Although this result assumes that the subproblems can be solved exactly (which is not the case in practice), it gives some idea as to the convergence behavior of the method. We follow the reasoning of the proof of convergence of nonlinear Gauss-Seidel [3, Proposition 3.9], adapted here for the way that λ is handled.

THEOREM 3.5 (Convergence of CP-APR). Suppose that $f(\mathbf{M})$ is strictly convex with respect to each block component and that it is minimized exactly for each block component subproblem of CP-APR. Let \mathbf{M}_* be a limit point of the sequence $\{\mathbf{M}_k\}$ such that $\lambda_* > 0$. Then \mathbf{M}_* is a constrained stationary point of (3.1).

Proof. Let $\mathbf{M}_k = \langle \boldsymbol{\lambda}_k, \mathbf{A}_k^{(1)}, \dots, \mathbf{A}_k^{(N)} \rangle$ be the kth iterate produced by the *outer* iterations of Algorithm 1. Define $\mathbf{Z}_k^{(n)}$ to be the nth iterate in the inner loop of outer iteration k with the λ -vector absorbed into the nth factor, i.e.,

$$\mathbf{Z}_k^{(n)} = \langle \mathbf{A}_{k+1}^{(1)}, \dots, \mathbf{A}_{k+1}^{(n-1)}, \mathbf{B}_{k+1}^{(n)}, \mathbf{A}_k^{(n+1)}, \dots, \mathbf{A}_k^{(N)} \rangle,$$

where $\mathbf{B}_{k+1}^{(n)}$ is the solution to the *n*th subproblem at iteration *k* such that $\mathbf{A}_{k+1}^{(n)}$ is the column-normalized version of $\mathbf{B}_{k+1}^{(n)}$, i.e., $\mathbf{A}_{k+1}^{(n)} = \mathbf{B}_{k+1}^{(n)} (\operatorname{diag}(\mathbf{B}_{k+1}^{(n)}\mathbf{e}))^{-1}$. Observe that

$$\mathbf{Z}_k^{(N)} = \langle \mathbf{A}_{k+1}^{(1)}, \dots, \mathbf{A}_{k+1}^{(N-1)}, \mathbf{A}_{k+1}^{(N)} \operatorname{diag}(\boldsymbol{\lambda}_{k+1}) \rangle,$$

so there is a correspondence between $\mathfrak{Z}_k^{(N)}$ and \mathfrak{M}_{k+1} such that $f(\mathfrak{Z}_k^{(N)}) = f(\mathfrak{M}_{k+1})$. For convenience, we define

$$\mathbf{Z}_k^{(0)} = \langle \mathbf{A}_k^{(1)} \operatorname{diag}(\boldsymbol{\lambda}_k), \mathbf{A}_k^{(2)}, \dots, \mathbf{A}_k^{(N)} \rangle,$$

Since we assume the subproblem is solved exactly at each iteration, we have

$$f(\mathbf{M}_k) \ge f(\mathbf{Z}_k^{(1)}) \ge f(\mathbf{Z}_k^{(2)}) \ge \cdots f(\mathbf{Z}_k^{(N-1)}) \ge f(\mathbf{M}_{k+1}) \text{ for all } k.$$
 (3.11)

Recall that $\Omega(\zeta)$ is compact by Lemma 3.1. Since the sequence $\{\mathcal{M}_k\}$ is contained in the set $\Omega(\zeta)$, it must have a convergent subsequence. We let $\{k_\ell\}$ denote the indices

of that convergent subsequence and $\mathbf{M}_* = \langle \mathbf{\lambda}_*, \mathbf{A}_*^{(1)}, \dots, \mathbf{A}_*^{(N)} \rangle$ denote its limit point. By continuity of f,

$$f(\mathbf{M}_{k_{\ell}}) \to f(\mathbf{M}_*).$$

We first show that $\|\mathbf{A}_{k_{\ell}+1}^{(1)} - \mathbf{A}_{k_{\ell}}^{(1)}\| \to 0$. Assume the contrary, i.e., that it does not converge to zero. Let $\gamma_{k_{\ell}} = \|\mathbf{Z}_{k_{\ell}}^{(1)} - \mathbf{Z}_{k_{\ell}}^{(0)}\|$. By possibly restricting to a subsequence of $\{k_{\ell}\}$, we may assume there exists some $\gamma_0 > 0$ such that $\gamma(k_{\ell}) \geq \gamma_0$ for all ℓ . Let $\mathbf{S}_{k_{\ell}}^{(1)} = (\mathbf{Z}_{k_{\ell}}^{(1)} - \mathbf{Z}_{k_{\ell}}^{(0)})/\gamma_{k_{\ell}}$; then $\mathbf{Z}_{k_{\ell}}^{(1)} = \mathbf{Z}_{k_{\ell}}^{(0)} + \gamma_{k_{\ell}}\mathbf{S}_{k_{\ell}}^{(1)}$, $\|\mathbf{S}_{k_{\ell}}^{(1)}\| = 1$, and $\mathbf{S}_{k_{\ell}}^{(1)}$ differs from zero only along the first block component. Notice that $\{\mathbf{S}_{k_{\ell}}^{(1)}\}$ belong to a compact set and therefore has a limit point $\mathbf{S}_{*}^{(1)}$. By restricting to a further subsequence of $\{k_{\ell}\}$, we assume that $\mathbf{S}_{k_{\ell}}^{(1)} \to \mathbf{S}_{*}^{(1)}$

Let us fix some $\epsilon \in [0,1]$. Notice that $0 \leq \epsilon \gamma_0 \leq \gamma_{k_\ell}$. Therefore, $\mathfrak{Z}_{k_\ell}^{(0)} + \epsilon \gamma_0 \mathbf{S}_{k_\ell}^{(1)}$ lies on the line segment joining $\mathfrak{Z}_{k_\ell}^{(0)}$ and $\mathfrak{Z}_{k_\ell}^{(0)} + \gamma_{k_\ell} \mathbf{S}_{k_\ell}^{(1)} = \mathfrak{Z}_{k_\ell}^{(1)}$ and belongs to $\Omega(\zeta)$ because $\Omega(\zeta)$ is convex. Using the convexity of f w.r.t. the first block component and the fact that $\mathfrak{Z}_{k_\ell}^{(1)}$ minimizes f over all \mathfrak{Z} that differ from $\mathfrak{Z}_{k_\ell}^{(1)}$ in the first block component, we obtain

$$f(\mathbf{Z}_{k_{\ell}}^{(1)}) = f(\mathbf{Z}_{k_{\ell}}^{(0)} + \gamma_{k_{\ell}} \mathbf{S}_{k_{\ell}}^{(1)}) \le f(\mathbf{Z}_{k_{\ell}}^{(0)} + \epsilon \gamma_{0} \mathbf{S}_{k_{\ell}}^{(1)}) \le f(\mathbf{Z}_{k_{\ell}}^{(0)}).$$

Since $f(\mathbf{Z}_{k_{\ell}}^{(0)}) = f(\mathbf{M}_{k_{\ell}}) \to f(\mathbf{M}_{*})$, equation (3.11) shows that $f(\mathbf{Z}_{k_{\ell}}^{(1)})$ also converges to $f(\mathbf{M}_{*})$. Taking limits as ℓ tends to infinity, we obtain

$$f(\mathbf{M}_*) < f(\mathbf{Z}_*^{(0)} + \epsilon \gamma_0 \mathbf{S}_*^{(1)}) < f(\mathbf{M}_*),$$

where $\mathfrak{Z}_*^{(0)}$ is just \mathfrak{M}_* with λ_* absorbed into the first component. We conclude that $f(\mathfrak{M}_*) = f(\mathfrak{Z}_*^{(0)} + \epsilon \gamma_0 \mathbf{S}_*^{(1)})$ for every $\epsilon \in [0,1]$. Since $\gamma_0 \mathbf{S}_*^{(1)} \neq 0$, this contradicts the strict convexity of f as a function of the first block component. This contradiction establishes that $\|\mathbf{A}_{k_\ell+1}^{(1)} - \mathbf{A}_{k_\ell}^{(1)}\| \to 0$. In particular, $\mathfrak{Z}_{k_\ell}^{(1)}$ converges to $\mathfrak{Z}_*^{(0)}$.

By definition of $\mathfrak{Z}_{k_{\ell}}^{(1)}$ and the assumption that each subproblem is solved exactly, we have

$$f(\mathbf{Z}_{k_{\ell}}^{(1)}) \leq f(\langle \mathbf{B}, \mathbf{A}_{k_{\ell}}^{(2)}, \dots, \mathbf{A}_{k_{\ell}}^{(N)} \rangle)$$
 for all $\mathbf{B} \geq 0$.

Taking limits as $\ell \to \infty$, we obtain

$$f(\mathbf{M}_*) \le f(\langle \mathbf{B}, \mathbf{A}_*^{(2)}, \dots, \mathbf{A}_*^{(N)} \rangle)$$
 for all $\mathbf{B} \ge 0$.

In other words, $\mathbf{B}_{*}^{(1)} = \mathbf{A}_{*}^{(1)} \operatorname{diag}(\boldsymbol{\lambda}_{*})$ is the minimizer of f with respect to the first block components with the remaining components are fixed at $\mathbf{A}_{*}^{(2)}$ through $\mathbf{A}_{*}^{(N)}$. Using the KKT conditions from Theorem 2.2, we have that

$$\mathbf{B}_{*}^{(1)} \ge 0, \quad \frac{\partial f}{\partial \mathbf{B}^{(1)}}(\mathbf{B}_{*}^{(1)}) \ge 0, \quad \mathbf{B}_{*}^{(1)} * \frac{\partial f}{\partial \mathbf{B}^{(1)}}(\mathbf{B}_{*}^{(1)}) = 0.$$

In turn, since $\lambda_* > 0$, we have

$$\min\left(\mathbf{A}_*^{(1)}, \mathbf{E} - \mathbf{\Phi}_*^{(1)}\right) = 0.$$

Repeating the previous argument shows that $\|\mathbf{A}_{k_{\ell}+1}^{(2)} - \mathbf{A}_{k_{\ell}}^{(2)}\| \to 0$ and that $\min\left(\mathbf{A}_{*}^{(2)}, \mathbf{E} - \mathbf{\Phi}_{*}^{(2)}\right) = 0$. Continuing inductively, we eventually conclude that

$$\min\left(\mathbf{A}_{*}^{(n)}, \mathbf{E} - \mathbf{\Phi}_{*}^{(n)}\right) = 0 \quad \text{for} \quad n = 1, \dots, N.$$

Thus, by Theorem 3.3, \mathcal{M}_* is a KKT point of $f(\mathcal{M})$. \square

4. Solving the CP-APR Subproblem via Majorization-Minimization. Consider the nth subproblem in (3.5). Here we drop the n's for convenience and let $\mathbf{C} = \mathbf{B}^\mathsf{T}$ so that (3.5) reduces to

$$\min_{\mathbf{C} \ge 0} \underbrace{\sum_{ij} \mathbf{c}_i^\mathsf{T} \boldsymbol{\pi}_j - x_{ij} \log \left(\mathbf{c}_i^\mathsf{T} \boldsymbol{\pi}_j \right)}_{f(\mathbf{C}^\mathsf{T})}.$$
(4.1)

Here, dropping the n's, we have that \mathbf{C} is a matrix of size $R \times I$, $\mathbf{\Pi}$ is a matrix of size $R \times J$, and \mathbf{X} is a matrix of size $I \times J$. According to Assumption 3.2, for every i there is at least one j such that $x_{ij} > 0$. Thus, we can assume that we have $\mathbf{\bar{C}} \geq 0$ such that $f(\mathbf{\bar{C}}^{\mathsf{T}})$ is finite. Then by Lemma 2.5, f is majorized at $\mathbf{\bar{C}}^{\mathsf{T}}$ by the function

$$g(\mathbf{C}, \bar{\mathbf{C}}) = \sum_{rij} \left[c_{ri} \pi_{rj} - \alpha_{rij} x_{ij} \log \left(\frac{c_{ri} \pi_{rj}}{\alpha_{rij}} \right) \right] \quad \text{where} \quad \alpha_{rij} = \frac{\bar{c}_{ri} \pi_{rj}}{\bar{\mathbf{c}}_i^\mathsf{T} \pi_j}. \tag{4.2}$$

The advantage of this majorization is that the problem is now completely separable in terms of c_{ri} , i.e., the individual entries of \mathbf{C} . We now show that $g(\cdot, \bar{\mathbf{C}})$ has a unique global minimum and give an analytic expression for it.

LEMMA 4.1. Let f and g be as defined in (4.1) and (4.2), respectively. Then, for all $\bar{\mathbf{C}} \geq \mathbf{0}$ such that $f(\bar{\mathbf{C}}^{\mathsf{T}})$ is finite, the function $g(\cdot, \bar{\mathbf{C}})$ has a unique global minimum \mathbf{C}_* which is given by

$$(\mathbf{C}_*)_{ri} = \sum_j \alpha_{rij} x_{ij}$$
 where $\alpha_{rij} = \frac{\overline{c}_{ri} \pi_{rj}}{\overline{\mathbf{c}}_i^\mathsf{T} \boldsymbol{\pi}_j}$, for all $r = 1, \dots, R, \ i = 1, \dots, I$.

Proof. Because $g(\mathbf{C}, \overline{\mathbf{C}})$ separates in the elements of \mathbf{C} we focus on solving each elementwise minimization problem. Dropping subscripts, the minimization problem with respect to c_{ri} can be rewritten as

$$\min_{c \ge 0} c - \sum_{j} \alpha_j x_j \log \left(\frac{c \pi_j}{\alpha_j} \right), \tag{4.3}$$

where we have used the fact that $\sum_j \pi_j = 1$. It is sufficient to prove that this univariate problem has a unique global minimizer, $c_* = \sum_j \alpha_j x_j$. First, consider the case where the second term is nonzero. Some quick calculus reveals the solution. Moreover, the function is strictly convex and so has a unique global minimum. Second, consider the case where the second term is zero. Then, it is immediate that the unique global minimum is $c_* = 0$. Moreover, the second term can only vanish when $\sum_j \alpha_j x_j = 0$, and so the formula applies. \square

Algorithm 2 CP-APR Algorithm (with Subproblem Solver)

Let \mathfrak{X} be a tensor of size $I_1 \times \cdots \times I_N$. Let $\mathfrak{M} = \langle \lambda; \mathbf{A}^{(1)}, \cdots, \mathbf{A}^{(N)} \rangle$ be an initial guess for an R-component model such that $\mathfrak{M} \in \Omega(\zeta)$ for some $\zeta > 0$.

```
1: repeat
                    for n = 1, \ldots, N do
   2:
  3:
                             \boldsymbol{\Pi} \leftarrow \left( \boldsymbol{\mathbf{A}}^{(N)} \odot \cdots \odot \boldsymbol{\mathbf{A}}^{(n+1)} \odot \boldsymbol{\mathbf{A}}^{(n-1)} \odot \cdots \odot \boldsymbol{\mathbf{A}}^{(1)} \right)^{\mathsf{T}}
repeat
   4:
                                                                                                                                                                                               ⊳ subproblem loop
   5:
                                        oldsymbol{\Phi} \leftarrow \left( \mathbf{X}_{(n)} \oslash \left( \mathbf{B} oldsymbol{\Pi} 
ight) 
ight) oldsymbol{\Pi}^\mathsf{T}
   6:
   7:
   8:
                              until convergence
                              oldsymbol{\lambda} \leftarrow \mathbf{e}^\mathsf{T} \mathbf{B} \\ \mathbf{A}^{(n)} \leftarrow \mathbf{B} \mathbf{\Lambda}^{-1}
  9:
10:
                     end for
11:
12: until convergence
```

Rewriting the results of Lemma 4.1 in terms of **B** yields an MM update of the form:

$$b_{ir} \leftarrow b_{ir} \sum_{j} \frac{x_{ij}}{\sum_{r'} b_{ir'} \pi_{r'j}} \pi_{rj}.$$

In matrix format, the updates can be expressed as

$$\mathbf{B} \leftarrow \mathbf{B} * \mathbf{\Phi},$$

where Φ is as defined in (3.7) and depends on **B**. The next result ensures that if $\mathbf{B} \neq \mathbf{B} * \Phi$, then the update strictly decreases f.

COROLLARY 4.2. Let $\mathbf{B} \geq 0$ such that $f(\mathbf{B})$ is finite and suppose $\mathbf{B} \neq \mathbf{B} * \mathbf{\Phi}$. Then $f(\mathbf{B}) > f(\mathbf{B} * \mathbf{\Phi})$.

Proof. By Lemma 4.1 $(\mathbf{B} * \mathbf{\Phi})^{\mathsf{T}}$ is the unique global minimizer of $g(\cdot, \mathbf{B}^{\mathsf{T}})$ which majorizes f at \mathbf{B}^{T} . Therefore, if $\mathbf{B} \neq \mathbf{B} * \mathbf{\Phi}$, we must have

$$f(\mathbf{B}) = g(\mathbf{B}^\mathsf{T}, \mathbf{B}^\mathsf{T}) > g((\mathbf{B} * \mathbf{\Phi})^\mathsf{T}, \mathbf{B}^\mathsf{T}) \geq f(\mathbf{B} * \mathbf{\Phi}). \quad \Box$$

The CP-APR algorithm using the MM algorithm to solve the Gauss-Seidel subproblem is given in Algorithm 2.

4.1. Convergence of MM Algorithm for Subproblem. We prove the MM Algorithm of $\S 4$ minimizes the subproblem in (3.5). If we are updating the nth factor matrix and drop the n's, we can write the subproblem as

$$\min_{\mathbf{B} > 0} f(\mathbf{B}) \equiv \mathbf{e}^{\mathsf{T}} \left[\mathbf{B} \mathbf{\Pi} - \mathbf{X} * \log(\mathbf{B} \mathbf{\Pi}) \right] \mathbf{e}. \tag{4.4}$$

Recall that **X** is the nonnegative data tensor reshaped to a matrix of size $I \times J$, Π is a nonnegative matrix of size $R \times J$ with rows that sum to 1, and **B** is a nonnegative matrix of size $I \times R$. Recall that the MM algorithm iterations are defined by

$$\mathbf{B}_{k+1} = \psi(\mathbf{B}_k) \equiv \mathbf{B}_k * \Phi(\mathbf{B}_k), \text{ where } \Phi(\mathbf{B}_k) = [\mathbf{X} \oslash (\mathbf{B}_k \mathbf{\Pi})] \mathbf{\Pi}$$
 (4.5)

and **X** and **\Pi** come from (4.4). If $\mathbf{B}_0 \geq 0$, clearly $\mathbf{B}_k \geq 0$ for all k. Observe that

$$\nabla f(\mathbf{B}) = \mathbf{E} - \mathbf{\Phi}(\mathbf{B}). \tag{4.6}$$

We now provide a series of lemmas leading up to a proof that, under mild conditions on the starting point \mathbf{B}_0 , the MM iterates will converge to the unique global minimum of (4.4). For clarity, we restate Assumption 3.2 in terms of the local variables for this section as follows:

ASSUMPTION 4.3. The rows of the submatrix $\Pi(:, \{j \mid \mathbf{X}_{ij} > 0\})$ (i.e., only the columns corresponding to nonzero rows in \mathbf{X} are considered) are linearly independent for all i = 1, ..., I.

LEMMA 4.4. Let f be as defined in (4.4). For any nonnegative matrix \mathbf{B}_0 such that $f(\mathbf{B}_0)$ is finite, the level set $\mathcal{L}_f(\mathbf{B}_0) = \{ \mathbf{B} \geq 0 \mid f(\mathbf{B}) \leq f(\mathbf{B}_0) \}$ is compact.

Proof. The proof follows the same logic as the proof for Lemma B.1. \square

LEMMA 4.5. Let f be as defined in (4.4) and ψ be as defined in (4.5), and suppose Assumption 4.3 is satisfied. For any nonnegative matrix \mathbf{B}_k such that $f(\mathbf{B}_0)$ is finite, the sequence $\mathbf{B}_{k+1} = \psi(\mathbf{B}_k)$ converges.

Proof. Note that all limit points of ψ are fixed points of f by Theorem 2.6.

First, we show that the set of fixed point is finite. Suppose that **B** is a fixed point of ψ . Then we must have $\mathbf{B} * (\mathbf{E} - \Phi(\mathbf{B})) = 0$. By Theorem 2.3 and Lemma 3.4, it can be verified that **B** is the *unique* global minimizer of

min
$$f(\mathbf{U})$$
 s.t. $\mathbf{U} \in \{ \mathbf{U} \ge 0 \mid u_{ir} = 0 \text{ if } b_{ir} = 0 \},$

where f is as defined in (4.4). Therefore, any fixed point that has the same zero pattern of **B** must be equal to **B**. Since there are only a finite number of possible zero patterns, the number of fixed points is finite.

Since every limit point is a fixed point by Theorem 2.6(a), there are only finitely many limit points. Let $\{\mathcal{N}_p\}$ denote a collection of arbitrarily small neighborhoods around each fixed point indexed by p. Only finitely many iterates \mathbf{B}_k are in $\mathcal{L}_f(\mathbf{B}_0) - \cup_p \mathcal{N}_p$. So, all but finitely many iterates \mathbf{B}_k will be in $\cup_p \mathcal{N}_p$. But $\|\mathbf{B}_{k+1} - \mathbf{B}_k\|$ eventually becomes smaller than smallest distance between any two neighborhoods by Theorem 2.6(b). Therefore the sequence \mathbf{B}_k must belong to one of the neighborhoods for all but finitely many k. So, any sequence of iterates must eventually converge to exactly one of the fixed points of ψ . \square

We now argue that it is impossible for the MM iterate sequence to converge to a non-KKT point if it has been appropriately initialized.

LEMMA 4.6. Let f be as defined in (4.4) and suppose Assumption 4.3 is satisfied. Suppose $\mathbf{B}_k \to \mathbf{B}_*$ is a convergent sequence of iterates defined by (4.5) with $\mathbf{B}_0 \geq 0$ and $f(\mathbf{B}_0)$ finite. If $(\mathbf{B}_0)_{ir} > 0$ for all (i,r) such that $(\Phi(\mathbf{B}_*))_{ir} > 1$, then $\nabla f(\mathbf{B}_*) \geq \mathbf{0}$.

Proof. We give a proof by contradiction. Suppose there exists (i, r) such that $(\mathbf{B}_0)_{ir} > 0$ but $(\nabla f(\mathbf{B}_*))_{ir} < 0$. Since \mathbf{B}_* is a fixed point of ψ , we must have $[1 - (\Phi(\mathbf{B}_*))_{ir}](\mathbf{B}_*)_{ir} = 0$. By our assumption, however $(\nabla f(\mathbf{B}_*))_{ir} = [1 - (\Phi(\mathbf{B}_*))_{ir}] < 0$. Thus, we must have $(\mathbf{B}_*)_{ir} = 0$. On the other hand, $(\mathbf{B}_k)_{ir} > 0$ for all k (proof left to reader). Since $\Phi(\cdot)$ is a continuous function of \mathbf{B} on $\mathcal{L}_f(\mathbf{B}_0)$, we know that there exists some K such that k > K implies \mathbf{B}_k is close enough to \mathbf{B}_* such that $(\nabla f(\mathbf{B}_k))_{ir} = [1 - (\Phi(\mathbf{B}_k))_{ir}] < 0$. Since $(\mathbf{B}_k)_{ir} > 0$, we have $[1 - (\Phi(\mathbf{B}_k))_{ir}](\mathbf{B}_k)_{ir} < 0$, which implies $(\mathbf{B}_k)_{ir} < (\mathbf{B}_{k+1})_{ir}$ for all k > K. But this contradicts $\lim_{k \to \infty} (\mathbf{B}_k)_{ir} = (\mathbf{B}_*)_{ir} = 0$. Hence, the claim. \square

THEOREM 4.7 (Convergence of MM algorithm). Let f be as defined in (4.4) and assume Assumption 4.3 holds, let \mathbf{B}_0 be a nonnegative matrix such that $f(\mathbf{B}_0)$ is finite

and $(\mathbf{B}_0)_{ir} > 0$ for all (i,r) such that $(\mathbf{\Phi}(\mathbf{B}_*))_{ir} > 1$, and let the sequence $\{\mathbf{B}_k\}$ be defined as in (4.5). Then $\{\mathbf{B}_k\}$ converges to the global minimizer of f.

Proof. By Lemma 4.5, the sequence $\{\mathbf{B}_k\}$ converges; we call the limit point \mathbf{B}_* . At this limit point, we have: (a) $\mathbf{B}_* \geq 0$, (b) $\nabla f(\mathbf{B}_*) \geq 0$ by Lemma 4.6, (c) and $\mathbf{B}_* * \nabla f(\mathbf{B}_*) = 0$ by virtue of \mathbf{B}_* being a fixed point of ψ . Thus, the point \mathbf{B}_* satisfies the conditions in (2.9) with respect to (4.4). Furthermore, since f is convex by Lemma 3.4, we can conclude that \mathbf{B}_* is the global minimum of f. \square

Observe that the condition that $(\mathbf{B}_0)_{ir} > 0$ for all (i, r) such that $(\mathbf{\Phi}(\mathbf{B}_*))_{ir} > 1$ is easily satisfied by simply choosing \mathbf{B}_0 strictly positive.

5. CP-APR Implementation Details. Algorithm 2 omits many details and numerical checks that are needed in any practical implementation. Thus, Algorithm 3 provides a detailed version that can be directly implemented. A highlight of this implementation is the "inadmissible zero" avoidance, which fixes a long-standing problem with multiplicative updates.

Algorithm 3 Detailed CP-APR Algorithm

Let \mathfrak{X} be a tensor of size $I_1 \times \cdots \times I_N$. Let $\mathfrak{M} = \langle \boldsymbol{\lambda}; \mathbf{A}^{(1)}, \cdots, \mathbf{A}^{(N)} \rangle$ be an initial guess for an R-component model such that $\mathfrak{M} \in \Omega(\zeta)$ for some $\zeta > 0$. Choose the following parameters:

```
• k_{\text{max}} = \text{Maximum number of outer iterations}
```

- $\ell_{\text{max}} = \text{Maximum number of inner iterations}$ (per outer iteration)
- τ = Convergence tolerance on KKT conditions (e.g., 10^{-4})
- $\kappa = \text{Inadmissible structural zero avoidance adjustment (e.g., 0.01)}$
- κ_{tol} = Tolerance for identifying a potential structural nonzero (e.g., 10^{-10})

```
• \epsilon = \text{Minimum divisor to prevent divide-by-zero (e.g., 10^{-10})}
  1: for k = 1, 2, ..., k_{\text{max}} do
  2:
                 isConverged \leftarrow true
  3:
                for n=1,\ldots,N do
                       \mathbf{S}(i,r) \leftarrow \begin{cases} \kappa, & \text{if } k > 1, \mathbf{A}^{(n)}(i,r) < \kappa_{\text{tol}}, \text{ and } \mathbf{\Phi}^{(n)}(i,r) > 1, \\ 0, & \text{otherwise} \end{cases}
  4:
                        \mathbf{B} \leftarrow (\mathbf{A}^{(n)} + \mathbf{S})\mathbf{\Lambda}
  5:
                        \Pi \leftarrow \left(\mathbf{A}^{(N)} \odot \cdots \odot \mathbf{A}^{(n+1)} \odot \mathbf{A}^{(n-1)} \odot \cdots \odot \mathbf{A}^{(1)}\right)^{\mathsf{T}}
  6:
                        \begin{array}{l} \mathbf{for}\ \ell \stackrel{\cdot}{=} 1, 2, \dots, \ell_{\max}\ \mathbf{do} \\ \boldsymbol{\Phi}^{(n)} \leftarrow \left(\mathbf{X}_{(n)} \oslash \left(\max(\mathbf{B}\boldsymbol{\Pi}, \epsilon)\right)\right) \boldsymbol{\Pi}^\mathsf{T} \end{array}
                                                                                                                                                         7:
  8:
                                if |\min(\mathbf{B}, \mathbf{E} - \mathbf{\Phi}^{(n)})| < \tau then
  9:
                                        break
10:
                                end if
11:
                                isConverged \leftarrow false
12:
                                \mathbf{B} \leftarrow \mathbf{B} * \mathbf{\Phi}^{(n)}
13:
14:
                        end for
                        oldsymbol{\lambda} \leftarrow \mathbf{e}^\mathsf{T} \mathbf{B}
15:
                        \mathbf{A}^{(n)} \leftarrow \mathbf{B} \mathbf{\Lambda}^{-1}
16:
                end for
17:
                if isConverged = true then
18:
19:
                        break
                 end if
20:
21: end for
```

5.1. Divide-by-Zero Avoidance. In line 6 of Algorithm 2, if $(\mathbf{B}\Pi)_{ij} = 0$ for some (i,j) such that $x_{ij} \neq 0$, then we will have a division by zero. Although our theory guarantees that we will never have an exact zero, very small divisors can be equally problematic. In order to avoid this complication, we force every entry of the divisor to be at least ϵ , i.e., we can change the divisor to

$$\max(\mathbf{B}\mathbf{\Pi}, \epsilon),$$

where the max is computed elementwise and ϵ is some user-specified parameter. This is a common adjustment in multiplicative updates.

5.2. Inadmissible Zero Avoidance. A long-standing problem with multiplicative updates is that some elements may get "stuck" at zero. For example, if $a_{ir}^{(n)} = 0$, then the multiplicative updates in line 7 of Algorithm 2 will never change it. In many cases, a zero entry may be the correct answer, so we want to allow it. In other cases, though, the zero entry may be incorrect in the sense that it does not satisfy the KKT conditions, i.e., $a_{ir}^{(n)} = 0$ but

$$1 - \Phi_{ir}^{(n)} < 0.$$

We refer to these values as *inadmissible zeros*. We can correct this problem before we enter into the multiplicative update phase of the algorithm, i.e., when we initialize **B** in line 3 of Algorithm 2. In the detailed version of the algorithm, any inadmissible zeros (or near-zeros) are "schooched" away from zero and into the interior in lines 4–5 of Algorithm 3. The amount of the schooch is controlled by the user-defined parameter κ . We will later show that this adjustment prevents convergence to non-KKT points.

The convergence conditions on the subproblem require that

$$\min\left(\mathbf{B}^{(n)}, \mathbf{E} - \mathbf{\Phi}^{(n)}\right) = 0,$$

which we check in line 9 of Algorithm 3. We do not require the value to be exactly zero but instead check that it is smaller in magnitude than the user-defined parameter τ . We break out of the subproblem loop as soon as this condition is satisfied.

From Theorem 3.3, we can check for overall convergence by verifying (3.8). We do not want to calculate this at the end of every n-loop because it is expensive. Instead, we know that the iterates will stop changing once we have converged and so we can validate the convergence of all factor matrices by checking that no factor matrix has been modified and every subproblem has converged. This is done via the Boolean variable isConverged in Algorithm 3.

- **5.4.** Lee-Seung is a special case of CP-APR. If we only take one iteration of the subproblem loop (i.e., setting $\ell_{\rm max}=1$), then CP-APR is the Lee-Seung multiplicative update algorithm for the generalized KL divergence. Thus, we can view the Lee-Seung algorithm as a special case of our algorithm where we do not solve the subproblems exactly; quite the contrary, we only take one step towards the subproblem solution. The fix for the inadmissible zeros can also be used for the standard Lee-Seung algorithm.
- **5.5. Sparse Tensor Implementation.** Consider a large-scale sparse tensor that is too large enough to be stored as a dense tensor requiring $\prod_n I_n$ memory. In this case, we can store the tensor as a sparse tensor as described in [2], requiring only $(N+1) \cdot \operatorname{nnz}(\mathfrak{X})$ memory.

The elementwise division in the update of Φ in line 6 of Algorithm 2 requires that we divide the tensor (in matricized form) \mathbf{X} by the current model estimate (in matricized form) $\mathbf{M} = \mathbf{B}\mathbf{\Pi}$. Unfortunately, we cannot afford to store \mathbf{M} explicitly as a dense tensor because it is the same size as \mathbf{X} . In fact, we generally cannot even form $\mathbf{\Pi}$ explicitly because it requires almost as much storage as the product. We observe, however, that we need only calculate the values of \mathbf{M} that correspond to nonzeros in \mathbf{X} .

Let $P = \operatorname{nnz}(\mathfrak{X})$. Then we can store the sparse tensor \mathfrak{X} as a set of values and multi-indices, $(v^{(p)}, \mathbf{i}^{(p)})$ for $p = 1, \ldots, P$. In order to avoid forming the current model estimate, \mathfrak{M} , as a dense object, we will store only selected rows of Π , one per nonzero in \mathfrak{X} ; we denote these rows by $\mathbf{w}^{(p)}$ for $p = 1, \ldots, P$. The pth vector is given by the elementwise product of rows of the factor matrices, i.e.,

$$\mathbf{w}^{(p)} = \mathbf{A}^{(1)}(i_1^{(p)},:) * \cdots * \mathbf{A}^{(n-1)}(i_{n-1}^{(p)},:) * \mathbf{A}^{(n+1)}(i_{n+1}^{(p)},:) * \cdots * \mathbf{A}^{(N)}(i_N^{(p)},:).$$

In order to determine $\hat{\mathbf{X}} = \mathbf{X} \oslash \mathbf{M}$ in the calculation of $\mathbf{\Phi}$, we proceed as follows. The tensor $\hat{\mathbf{X}}$ will have the same nonzero pattern as \mathbf{X} , and we let $\hat{v}^{(p)}$ denote its values. It can be determined that

$$\hat{v}^{(p)} = x^{(p)} / \left\langle \mathbf{w}^{(p)}, \mathbf{A}^{(n)}(i_n^{(p)},:) \right\rangle.$$

To calculate $\Phi = \hat{\mathbf{X}}\Pi$, we simply have

$$\Phi(i',r) = \sum_{p: i_n^{(p)} = i'} \hat{v}^{(p)} \mathbf{w}^{(p)}(r).$$

The storage of the $\mathbf{w}^{(p)}$ for $p=1,\ldots,P$ vectors and the entries $\hat{v}^{(p)}$ requires (R+1)P additional storage.

- 6. Numerical Results for CP-APR.
- **6.1.** Comparison of Objective Functions for Sparse Count Data. We contend that, for sparse count data, (1.2) is a better objective function than least squares. To support our claim, we consider simulated data where we know the correct answer. We compare CP-APR (our method) with CP-ALS.

We consider a 3-way tensor (N=3) of size $1000 \times 800 \times 600$ and R=10 factors. It will be generated from a model $\mathbf{M} = [\![\boldsymbol{\lambda}; \mathbf{A}^{(1)}, \dots, \mathbf{A}^{(N)}]\!]$. The entries of the vector $\boldsymbol{\lambda}$ are selected uniformly at random from [0,1]. Each factor matrix $\mathbf{A}^{(n)}$ is generated as follows: (1) For each column in $\mathbf{A}^{(n)}$, randomly select 10% (i.e., 1/R)

of the entries to be selected uniformly at random from the interval [0, 100]. (2) The remaining entries are selected uniformly at random from [0, 1]. (3) Each column is scaled so that its 1-norm is 1 (i.e., its sum is 1). An "observed" tensor can be thought of as the outcome of tossing $\nu \ll \prod I_n$ balls into $\prod I_n$ empty urns where each entry of the tensor corresponds to an urn. For each ball, we first draw a factor r with probability $\lambda_r / \sum \lambda_r$. The indices (i, j, k) are selected randomly proportional to $\mathbf{a}_r^{(n)}$ for n = 1, 2, 3. In other words, the ball is then tossed into the (i, j, k)th urn with probability $a_{ir}^{(1)} a_{jr}^{(2)} a_{kr}^{(3)}$. In this manner, the balls are allocated across the urns independently of each other. This procedure generates entries x_i that are each distributed as Poisson (m_i) . We adjust the final λ so that the scale matches that of \mathfrak{X} , i.e., $\lambda \leftarrow \nu \lambda / \|\lambda\|$.

The CP-APR method uses the following parameters: $k_{\rm max}=200$ (maxiters), $\ell_{\rm max}=10$ (maxinneriters), $\tau=10^{-4}$ (tol), $\kappa=10^{-2}$ (kappa), $\kappa_{\rm tol}=100 \cdot \epsilon_{\rm mach}$ (kappatol), $\epsilon=0$ (epsilon). We use CP-ALS implementation in the Tensor Toolbox for Matlab, Version 2.4; we use its default parameter settings except that we set the maximum number iterations (maxiters) to 200 and the convergence tolerance (tol) to 10^{-8} . This relatively small tolerance ensures that it does not stop prematurely.

We compare CP-APR and CP-ALS in terms of their "factor match score," defined as follows. Let $\mathbf{M} = [\![\boldsymbol{\lambda}; \mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(N)}]\!]$ be the true model and let $\bar{\mathbf{M}} = [\![\bar{\boldsymbol{\lambda}}; \bar{\mathbf{A}}^{(1)}, \ldots, \bar{\mathbf{A}}^{(N)}]\!]$ be the computed solution. The score of $\bar{\mathbf{M}}$ is computed as

$$\operatorname{score}(\bar{\mathbf{M}}) = \frac{1}{R} \sum_{r} \left(1 - \frac{|\xi_r - \bar{\xi}_r|}{\max\{\xi_r, \bar{\xi}_r\}} \right) \prod_{n} \frac{\mathbf{a}_r^{(n)\mathsf{T}} \bar{\mathbf{a}}_r^{(n)}}{\|\mathbf{a}_r^{(n)}\| \|\bar{\mathbf{a}}_r^{(n)}\|},$$

where

$$\xi_r = \lambda_r \prod_n \|\mathbf{a}_r^{(n)}\|$$
 and $\bar{\xi}_r = \bar{\lambda}_r \prod_n \|\bar{\mathbf{a}}_r^{(n)}\|$.

The FMS is a rather abstract measure, so we also give results for the number of columns in $\mathbf{A}^{(1)}$ that are correctly identified. In other words, we count the number of times that the cosine of the angle between the true solution and the computed solution is greater than 0.95, mathematically,

$$\frac{\mathbf{a}_r^{(1)\mathsf{T}}\bar{\mathbf{a}}_r^{(1)}}{\|\mathbf{a}_r^{(1)}\|\|\bar{\mathbf{a}}_r^{(1)}\|} \ge 0.95.$$

We use the first mode, but the results are representative of the other modes.

Results that are averages of 10 problems are shown in Table 6.1. We compare the factor match score of CP-APR and CP-ALS for observations ranging 480,000 (0.1%) down to 24,000 (0.005%). Recall that Assumption 3.2 implies that the absolute minimum number of observations is $R \cdot \max_n I_n = 10,000$. We consider both the factor match score and the number of columns correctly identified, as described above. We have used very few observations data as real problems do indeed tend to be this sparse. Nonetheless, both CP-APR and CP-ALS are able to correctly identify many of the components in the data. Overall, CP-APR gets better FMS scores and correctly identifies more columns; moreover, this is consistent for every single problem. CP-ALS does indeed find some correct information, but CP-APR finds more.

6.2. The Benefit of Extra Inner Iterations. We next show that varying the maximum number of inner iterations ℓ_{max} can accelerate the convergence. Recall

| | | CP-APR | | CP-ALS | | |
|--------------|----------|--------|--------|--------|--------|--|
| Observations | | FMS | # Cols | FMS | # Cols | |
| 480,000 | (0.100%) | 0.96 | 9.5 | 0.71 | 7.3 | |
| $240,\!000$ | (0.050%) | 0.91 | 9.2 | 0.72 | 7.4 | |
| 48,000 | (0.010%) | 0.80 | 7.9 | 0.59 | 6.3 | |
| 24,000 | (0.005%) | 0.74 | 6.9 | 0.51 | 5.7 | |

Table 6.1: Accuracy comparison of CP-APR and CP-ALS for sparse count data (mean of 10 trials). The factor match score (FMS) is in the range [0,1] with one being optimal. The number of columns correctly identified ranges from 1 to 10, with 10 being ideal.

that $\ell_{\rm max}=1$ corresponds to the Lee-Seung algorithm. We consider a 3-way tensor (N=3) of size $500\times 400\times 300$ and R=5 factors. We generate 100 problem instances from 100 randomly generated models $\mathbf{M}=[\![\lambda;\mathbf{A}^{(1)},\ldots,\mathbf{A}^{(N)}]\!]$ as described in §6.1 with 0.1% observations. We compare CP-APR with $\ell_{\rm max}=1,5,$ and 10. We track both the number of times line 8 of Algorithm 3 is executed and the CPU time using the MATLAB command cputime. The experiments were performed on an iMac computer with a 3.4 GHz Intel Core i7 processor and 8 GB of RAM. The mean and median factor match scores as compared to the true generative factors are shown in Table 6.2. We see that the value of $\ell_{\rm max}$ does not significantly impact accuracy. The high scores (near 1) indicate that CP-APR iterates typically converged to the true model, regardless of the setting of $\ell_{\rm max}$.

| $\ell_{ m max}$ | 1 | 5 | 10 |
|-----------------|--------|--------|--------|
| Median | 0.9858 | 0.9858 | 0.9862 |
| Mean | 0.9483 | 0.9514 | 0.9603 |

Table 6.2: Median and mean factor match scores for 100 simulated problems, varying the number of inner iterations.

Table 6.3a and Table 6.3b present summary statistics tally of multiplicative updates and total run times respectively. The distribution of updates and times was highly skewed as some problems required a substantial number of iterations. Nonetheless, we generally see a monotonic decrease in the number of updates and time as $\ell_{\rm max}$ increases. The differences are more substantial when comparing wall clock time. The reason for the disproportionate decrease in wall-clock time compared to the tally of updates is that the cost of the calculation of Π in line 6 of Algorithm 3 is amortized over all the subproblem iterations.

6.3. Fixing Misconvergence of Lee-Seung. We demonstrate the effectiveness of our simple fix for avoiding inadmissible zeros, as described in §5.2. Gonzalez and Zhang [13] have a well known example that demonstrates this problem but does not provide a solution. Here we produce similar results and show how our technique corrects the problem. As in [13], we consider fitting a rank-10 bilinear model for a 25×15 dense positive matrix with entries drawn independently and uniformly from [0, 1]. We apply CP-APR using $\ell_{\text{max}} = 1, \tau = 10^{-15}, \epsilon = 0, \kappa_{\text{tol}} = 100 \cdot \epsilon_{\text{mach}}$. We do two runs: one with $\kappa = 0$, corresponding to the standard Lee-Seung algorithm,

| ℓ_{max} | 1 | 5 | 10 | | ℓ_{max} | 1 | 5 | 10 |
|-----------------------|--------|-------|-------|---|-----------------------|---------|--------|--------|
| Mean | 16370 | 11710 | 11660 | | Mean | 299.60 | 106.10 | 87.92 |
| Min | 1641 | 1930 | 2748 | | Min | 27.33 | 16.84 | 20.16 |
| 1Q | 6320 | 5016 | 5192 | | 1Q | 106.40 | 44.94 | 38.68 |
| 2Q | 9819 | 7655 | 7290 | | 2Q | 168.70 | 68.98 | 55.00 |
| 3Q | 17760 | 14020 | 11860 | | 3Q | 323.00 | 124.20 | 92.35 |
| Max | 161100 | 88390 | 81240 | _ | Max | 3122.00 | 739.40 | 579.70 |

(a) Number of multiplicative updates

(b) Time (seconds)

Table 6.3: Comparing CP-APR with different values of ℓ_{max} for sparse count data over 100 trials. We report the mean, minimum, maximum, and the quartiles.

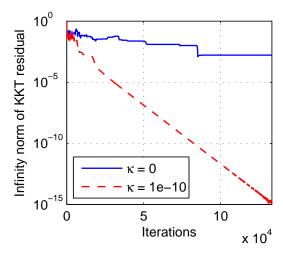


Fig. 6.1: Lee-Seung permitting inadmissible zeros (blue solid line) and avoiding inadmissible zeros (red dashed line).

and the other with $\kappa=10^{-10}$ to move away from inadmissible zeros. In both runs we use the same strictly positive initial guess. Figure 6.1 shows the magnitude of the KKT residual over more than 10^5 iterations. When $\kappa>0$, the sequence clearly convergences. On the other hand when $\kappa=0$ the iterates appear to get stuck at a non-KKT point. Closer inspection of the factor matrix iterates reveals a single offending inadmissible zero in the second factor matrix. We recognize that we have an inadmissible zero because its partial derivative is -0.0016 but should be nonnegative.

6.4. Enron Data. We consider the application of CP-APR to email data from the infamous Federal Energy Regulatory Commission (FERC) investigation of Enron Corporation. We use the version of the dataset prepared by Zhou et al. [37] and further processed by Perry and Wolfe [29], which includes detailed profiles on the employees. The data is arranged as a three-way tensor $\mathfrak X$ arranged as sender \times receiver \times month, where entry (i,j,k) indicates the number of messages from employee i to employee j in month k. The original data set had 38,388 messages (technically, there were only 21,635 messages but some messages were sent to multiple recipients and so are counted

multiple times) exchanged between 156 employees over 44 months (November 1998 – June 2002). We preprocessed the data, removing months that had less than 300 messages and removing any employees that did not send and receive an average of at least one message per month. Ultimately, our data set spanned 28 months (December 1999 – March 2002), involved 105 employees, and a total of 33,079 messages. The data is arranged so that the senders are sorted by frequency (greatest to least). The tensor representation has a total of 8,540 nonzeros (many of the messages occur between the same sender/receiver pair in the same time period). The tensor is 2.7% dense.

We apply CP-APR to find a model for the data. There is no ideal method for choosing the number of components. Typically, this value is selected through trial and error, trading off accuracy (as the number of components grows) and model simplicity. Here we show results for R=10 components. We use the default settings for the method, with $\ell_{\rm max}=10$ and $k_{\rm max}=200$.

Figure 6.2 illustrates six components in the resulting factorization. For each component, the top two plots shows the activity of senders and receivers, with the employees ordered from left to right by frequency of sending emails. Each employee has a symbol indicating their seniority (junior or senior), gender (male or female), and department (legal, trading, other). The sender and receiver factors have been normalized to sum to one, so the height of the marker indicates each employee's relative activity within the component. The third component (in the time dimension) is scaled so that it indicates total message volume explained by that component. The light gray line shows the total message volume. It is interesting to observe how the components break down into specific subgroups. For instance, component 1 in Figure 6.2a consists of nearly all "legal" and is majority female. This can be contrasted to component 5 in Figure 6.2d, which is nearly all "other" and also majority female. Component 3 in Figure 6.2b is a conversation among "senior" staff and mostly male: on the other hand, "junior" staff are more prominent in Component 4 in Figure 6.2c. Component 8 in Figure 6.2e seems to be a conversation among "senior" staff after the SEC investigation has begun. Component 10 in Figure 6.2f indicates that a couple of "legal" staff are communicating with many "other" staff immediately after the SEC investigation is announced, perhaps advising the "other" staff on appropriate responses to investigators.

6.5. SIAM Data. As another example, we consider five years (1999-2004) of SIAM publication metadata that has previously been used by Dunlavy et al. [8]. Here, we build a three-way sparse tensor based on title terms (ignoring common stop words), authors, and journals. The author names have been normalized to last name plus initial(s). The resulting tensor is of size 4,952 (terms) \times 6,955 (authors) \times 11 (journals) and has 64,133 nonzeros (0.017% dense). The highest count is 17 for the triad ('education', 'Schnabel B', 'SIAM Rev.'), which is a result of Prof. Schnabel's writing brief introductions to the education column for *SIAM Review*. In fact, the next 4 highest counts correspond to the terms 'problems', 'review', 'survey', and 'techniques', and to authors 'Flaherty J' and 'Trefethen N'.

Computing a ten-component factorization yields the results shown in Table 6.4. We use the default settings for the method, with $\ell_{\text{max}} = 10$ and $k_{\text{max}} = 200$. In the table, for the term and author modes, we list any entry whose factor score is greater than $10^{-7} \cdot I_n$, where I_n is the size of the *n*th mode; in the journal mode, we list any entry greater than 0.01. The 10th component corresponds to introductions written by section editors for SIAM Review. The 1st component shows that there is overlap in both authors and title keyword between the SIAM J. Computing and the SIAM

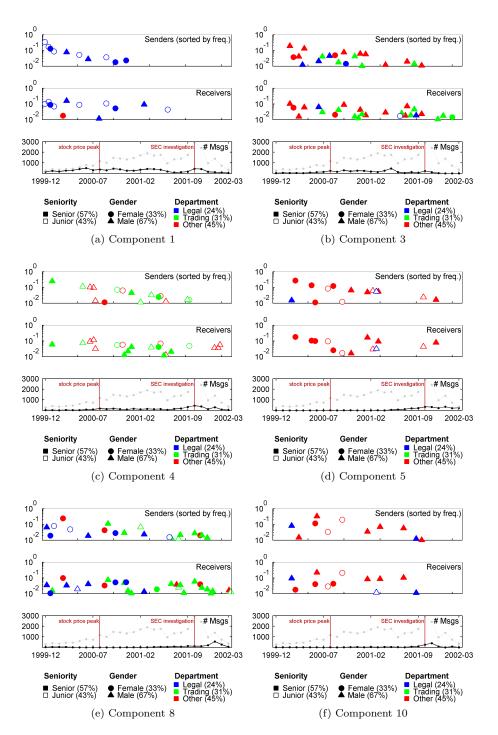


Fig. 6.2: Components from factorizing the Enron data.

| # | Terms | Authors | Journals |
|----|--------------------------------|---------------------------------|--------------------|
| 1 | graphs, problem, algorithms, | Kao MY, Peleg D, Motwani R, | SIAM J Comput, |
| | approximation, algorithm, | Cole R, Devroye L, Goldberg | SIAM J Discrete |
| | complexity, optimal, trees, | LA, Buhrman H, Makino K, He | Math |
| | problems, bounds | X, Even G | |
| 2 | method, equations, methods, | Chan TF, Saad Y, Golub GH, | SIAM J Sci Comput |
| | problems, numerical, | Vassilevski PS, Manteuffel TA, | |
| | multigrid, finite, element, | Tuma M, Mccormick SF, Russo | |
| | solution, systems | G, Puppo G, Benzi M | |
| 3 | finite, methods, equations, | Du Q, Shen J, Ainsworth M, | SIAM J Numer Anal |
| | method, element, problems, | Mccormick SF, Wang JP, | |
| | numerical, error, analysis, | Manteuffel TA, Schwab C, | |
| | equation | Ewing RE, Widlund OB, | |
| | | Babuska I | |
| 4 | control, systems, optimal, | Zhou XY, Kushner HJ, Kunisch | SIAM J Control |
| | problems, stochastic, linear, | K, Ito K, Tang SJ, Raymond | Optim |
| | nonlinear, stabilization, | JP, Ulbrich S, Borkar VS, | |
| | equations, equation | Altman E, Budhiraja A | |
| 5 | equations, solutions, problem, | Wei JC, Chen XF, Frid H, Yang | SIAM J Math Anal |
| | equation, boundary, | T, Krauskopf B, Hohage T, Seo | |
| | nonlinear, system, stability, | JK, Krylov NV, Nishihara K, | |
| | model, systems | Friedman A | |
| 6 | matrices, matrix, problems, | Higham NJ, Guo CH, Tisseur | SIAM J Matrix Anal |
| | systems, algorithm, linear, | F, Zhang ZY, Johnson CR, Lin | A |
| | method, symmetric, problem, | WW, Mehrmann V, Gu M, Zha | |
| | sparse | HY, Golub GH | |
| 7 | optimization, problems, | Qi LQ, Tseng P, Roos C, Sun | SIAM J Optimiz |
| | programming, methods, | DF, Kunisch K, Ng KF, | |
| | method, algorithm, nonlinear, | Jeyakumar V, Qi HD, | |
| | point, semidefinite, | Fukushima M, Kojima M | |
| | convergence | | |
| 8 | model, nonlinear, equations, | Venakides S, Knessl C, Sherratt | SIAM J Appl Math |
| | solutions, dynamics, waves, | JA, Ermentrout GB, Scherzer | |
| | diffusion, system, analysis, | O, Haider MA, Kaper TJ, Ward | |
| | phase | MJ, Tier C, Warne DP | 27.13.5.7.1 |
| 9 | equations, flow, model, | Klar A, Ammari H, Wegener R, | SIAM J Appl Math |
| | problem, theory, asymptotic, | Schuss Z, Stevens A, Velazquez | |
| | models, method, analysis, | JJL, Miura RM, Movchan AB, | |
| 10 | singular | Fannjiang A, Ryzhik L | GT43.CP |
| 10 | education, introduction, | Flaherty J, Trefethen N, | SIAM Rev |
| | health, analysis, problems, | Schnabel B, [None], Moon G, | |
| | matrix, method, methods, | Shor PW, Babuska IM, Sauter | |
| | control, programming | SA, Van Dooren P, Adjei S | |

Table 6.4: Highest-scoring items in a 10-term factorization of the term \times author \times journal tensor from five years of SIAM publication data.

- J. Discrete Math. The 2nd and 3rd components have some overlap in topic and two overlapping authors, but different journals. Both components 8 and 9 correspond to the same journal but reveal two subgroups of authors writing on slightly different topics.
- 7. Conclusions & Future Work. We have developed an alternating Poisson regression fitting algorithm, CP-APR, for PTF. While the specific loss function has been studied before, our development focuses on issues related to sparse count data. When tensor data is dense, CP fits based on minimizing least squares (CP-ALS) and maximizing the Poisson likelihood (CP-APR) tend to be very similar. In the case of

sparse count data, however, we have shown in simulations that CP-APR recovers a true CP model more reliably than CP-ALS. Indeed, in classical statistics, it is well known that the randomness observed in sparse count data is better explained and analyzed by the Poisson model than a Gaussian one.

Our algorithm is simple to implement and analyze theoretically. Specifically, CP-APR admits an easily verifiable stopping rule based on KKT conditions instead of heuristics, and can also exploit data sparsity to minimize computational and storage requirements. CP-APR uses an MM algorithm to update each factor matrix in turn, holding all others fixed. When only one step of the MM algorithm is performed, CP-APR corresponds to the Lee and Seung algorithm. Allowing for multiple steps in the MM subproblem solver, however, has the benefit of generally accelerating convergence. More importantly, we show how to fix the well-known problem in the Lee and Seung algorithm of getting stuck at non-KKT points by introducing a "schooch" to avoid inadmissible zeros. We provide a numerical example verifying that this trivial change remedies a non-trivial problem of misconvergence. With the benefits of the "schooch" in hand, we use standard optimization theory to prove the convergence of CP-APR to constrained stationary points. The regularity conditions imposed in our proofs make rigorous and concrete our intuition that in the context of sparse count data, CP-APR will converge provided that the data tensor meets a minimal density and that counts are sufficiently spread throughout the data tensor with respect to the size of the factor matrices being fit.

Finally, we present two real-data examples that demonstrate CP-APR's ability to find meaningful latent structure in very sparse count data. Nonetheless, as promising as these results are, there remains much room for future work. Foremost among practical considerations is speed of convergence. Although iterate updates are relatively simple to compute, CP-APR can require many iterates. One approach to accelerating convergence would be to replace the MM algorithm subproblem solver. For example, Kim et al. [16] present fast quasi-Newton methods for minimizing box-constrained convex functions that can be used to solve a nonnegative least squares or minimum KL-divergence subproblem in a nonlinear Gauss-Seidel solver. An added benefit of CP-APR is that our convergence results are agnostic to the method used to solve each subproblem. Provided that the subproblem is solved to optimality, the Gauss-Seidel part of our algorithm is guaranteed to converge. A second approach is to focus on the sequence of outer iterates. Zhou et al. [36] provide a general quasi-Newton acceleration scheme for iterative methods based on a quadratic approximation of the iteration map instead of the loss.

There has also been significant work in finding sparse factors via ℓ_1 -penalization for matrices [22] and tensors [25, 33, 12, 21]. Sparse factors often provide more easily interpreted models, and penalization may also accelerate the convergence. While the factor matrices generated by CP-APR are often sparse even without imposing an ℓ_1 -penalty, the degree of sparsity is not currently tunable.

Perhaps most challenging, however, are open questions related to rank and inference. Questions about how to choose rank are not new. But given the context of sparse count data, might that structure be exploited to derive a sensible heuristic or even rigorous criterion for choosing the rank? We already see that Assumption 3.2 imposes an upper bound on the rank to ensure algorithmic convergence. Regarding inference, our focus in this work was in thoroughly developing the algorithmic groundwork for fitting a PTF model for sparse count data. CP-APR can be used to estimate latent structure. Once an estimate is in hand, however, it is natural to ask

how much uncertainty there is in that estimate. For example, is it possible to put a confidence interval around the entries in the fitted factor matrices, especially zero or near zero entries? Given that inference for the related but simpler case of Poisson regression has been worked out, we suspect that a sensible solution is waiting to be found. The benefits of answering these questions warrant further investigation. We highlight them as important topics for future research.

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Appendix A. Notation Details.

Outer product. The outer product of N vectors is an N-way tensor. For example, $(\mathbf{a} \circ \mathbf{b} \circ \mathbf{c})_{ijk} = a_i b_j c_k$.

Elementwise multiplication and division. Let \mathcal{A} and \mathcal{B} be two same-sized tensors (or matrices). Then $\mathcal{C} = \mathcal{A} * \mathcal{B}$ yields a tensor that is the same size as \mathcal{A} (and \mathcal{B}) such that $c_{\mathbf{i}} = a_{\mathbf{i}}b_{\mathbf{i}}$ for all \mathbf{i} . Likewise, $\mathcal{C} = \mathcal{A} \otimes \mathcal{B}$ yields a tensor that is the same size as \mathcal{A} (and \mathcal{B}) such that $c_{\mathbf{i}} = a_{\mathbf{i}}/b_{\mathbf{i}}$ for all \mathbf{i} .

Khatri-Rao product. Give two matrices **A** and **B** of sizes $I_1 \times R$ and $I_2 \times R$, then $\mathbf{C} = \mathbf{A} \odot \mathbf{B}$ is a matrix of size $I_1 I_2 \times R$ such that

$$\mathbf{C} = \begin{bmatrix} \mathbf{a}_1 \otimes \mathbf{b}_1 & \mathbf{a}_2 \otimes \mathbf{b}_2 & \cdots & \mathbf{a}_R \otimes \mathbf{b}_R \end{bmatrix}$$

where the Kronecker product of two vectors of size I_1 and I_2 is a vector of length I_1I_2 given by

$$\mathbf{a} \otimes \mathbf{b} = \begin{bmatrix} a_1 \mathbf{b} \\ a_2 \mathbf{b} \\ \vdots \\ a_{I_1} \mathbf{b} \end{bmatrix}.$$

matricization of a tensor. The mode-n matricization or unfolding of a tensor \mathfrak{X} is denoted by $\mathbf{X}_{(n)}$ and is of size $I_n \times J_n$ where $J_n \equiv \prod_{m \neq n} I_n$. In this case, tensor element \mathbf{i} maps to matrix element (i,j) where

$$i = i_n$$
 and $j = 1 + \sum_{\substack{k=1 \ k \neq n}}^{N} (i_k - 1) \left(\prod_{\substack{m=1 \ m \neq n}}^{k-1} I_m \right).$

Appendix B. Proof of Lemma 3.1. In this section, we provide a proof for Lemma 3.1. We first establish two useful lemmas.

LEMMA B.1. Let f and \mathfrak{M} be as in (3.1). If $f(\mathfrak{M}) \leq \zeta$, then $\mathbf{e}^{\mathsf{T}} \lambda \in [e^{-\zeta/\xi}, \zeta]$ for some $\xi > 0$.

Proof. Because the factor matrices are column stochastic, we can observe that

$$f(\mathbf{M}) = \mathbf{e}^{\mathsf{T}} \boldsymbol{\lambda} - \sum_{\mathbf{i}} x_{\mathbf{i}} \log \left(\sum_{r} \lambda_{r} \ a_{i_{1}r}^{(n)} \cdots a_{i_{N}r}^{(n)} \right),$$

$$\geq \mathbf{e}^{\mathsf{T}} \boldsymbol{\lambda} - \xi \log \left(\mathbf{e}^{\mathsf{T}} \boldsymbol{\lambda} \right) \quad \text{where} \quad \xi = \left(\prod_{n=1}^{N} I_{n} \right) \max_{\mathbf{i}} x_{\mathbf{i}}. \quad \Box$$
(B.1)

LEMMA B.2. Let f be as defined in (3.1) and $\Omega(\zeta)$ be as defined in (3.3). The function $f(\mathbf{M})$ is bounded for all $\mathbf{M} \in \Omega(\zeta)$.

Proof. Let $\bar{\mathcal{M}}, \hat{\mathcal{M}} \in \{ \mathcal{M} \mid f(\mathcal{M}) \leq \zeta \}$. Define $\bar{\mathcal{M}}$ to be the convex combination

$$\tilde{\mathbf{M}} = \alpha \bar{\mathbf{M}} + (1 - \alpha) \hat{\mathbf{M}}$$
 where $\alpha \in [0.5, 1)$.

Note that the restriction on α is arbitrary but makes the proof simpler later on. Observe that

$$\tilde{m}_{\mathbf{i}} = \sum_{r} \left\{ \left(\alpha \bar{\lambda}_{r} + (1 - \alpha) \hat{\lambda}_{r} \right) \prod_{n} \left(\alpha \bar{a}_{i_{n}r}^{(n)} + (1 - \alpha) \hat{a}_{i_{n}r}^{(n)} \right) \right\}$$

On the one hand, by Lemma B.1,

$$\tilde{m}_{\mathbf{i}} \leq \sum_{r} \left(\alpha \bar{\lambda}_r + (1 - \alpha) \hat{\lambda}_r \right) = \alpha \sum_{r} \bar{\lambda}_r + (1 - \alpha) \sum_{r} \hat{\lambda}_r \leq \alpha \zeta + (1 - \alpha) \zeta = \zeta.$$

On the other hand,

$$\tilde{m}_{\mathbf{i}} \ge \sum_{r} \left\{ \alpha \bar{\lambda}_{r} \prod_{n} \alpha \bar{a}_{i_{n}r}^{(n)} \right\} = \alpha^{N+1} \bar{m}_{\mathbf{i}}$$

Thus,

$$\alpha^{N+1}\bar{m}_{\mathbf{i}} \leq \tilde{m}_{\mathbf{i}} \leq \bar{m}_{\mathbf{i}} + \zeta$$

Now consider

$$\tilde{m}_{\mathbf{i}} - x_{\mathbf{i}} \log \tilde{m}_{\mathbf{i}} \leq \bar{m}_{\mathbf{i}} + \zeta - x_{\mathbf{i}} \log \alpha^{N+1} \bar{m}_{\mathbf{i}}
= (\bar{m}_{\mathbf{i}} - x_{\mathbf{i}} \log \bar{m}_{\mathbf{i}}) + \zeta - (N+1)x_{\mathbf{i}} \log \alpha
< (\bar{m}_{\mathbf{i}} - x_{\mathbf{i}} \log \bar{m}_{\mathbf{i}}) + \zeta + (N+1)x_{\mathbf{i}} \log 2.$$

Thus,

$$f(\tilde{\mathbf{M}}) \le f(\bar{\mathbf{M}}) + \zeta \prod_{n} I_n + (N+1) \log 2 \sum_{i} x_i \le \zeta \left(1 + \prod_{n} I_n \right) + (N+1) \log 2 \sum_{i} x_i. \quad \Box$$

Given these two lemmas, we are finally ready to provide the proof of Lemma 3.1.

Proof. [of Lemma 3.1] Fix ζ . If $\{ \mathbf{M} \in \Omega \mid f(\mathbf{M}) \leq \zeta \}$ is empty, then $\Omega(\zeta)$ is empty and there is nothing left to do. Thus, assume $\{ \mathbf{M} \in \Omega \mid f(\mathbf{M}) \leq \zeta \}$ is nonempty. Since f is continuous at all $\mathbf{M} \in \Omega$ for which $f(\mathbf{M})$ is finite, f is obviously continuous on $\Omega(\zeta)$ by Lemma B.2. Since f is continuous, $\{ \mathbf{M} \in \Omega \mid f(\mathbf{M}) \leq \zeta \}$ is closed because it is the preimage of the closed set $(-\infty, \zeta]$ under f; thus, $\Omega(\zeta)$ is closed because it is a convex combination of closed sets. Consequently, we only need to show that $\Omega(\zeta)$ is bounded. Assume the contrary. Then there exists a sequence of models $\mathbf{M}_k = \left[\mathbf{\lambda}_k; \mathbf{A}_k^{(1)}, \dots, \mathbf{A}_k^{(N)} \right] \in \Omega(\zeta)$ such that $\mathbf{e}^\mathsf{T} \mathbf{\lambda}_k \to \infty$. By Lemma B.2, $f(\mathbf{M})$ is finite on $\Omega(\zeta)$, but this contradicts Lemma B.1. Hence, the claim. \square

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