A Novel Maximum-Entropy-Driven Technique for Low-Rank Orthogonal Nonnegative Matrix Factorization with \( \ell_0 \)-Norm sparsity Constraint*

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Abstract—In data-driven control and machine learning, a common requirement involves breaking down large matrices into smaller, low-rank factors that possess specific levels of sparsity. This paper introduces an innovative solution to the orthogonal nonnegative matrix factorization (ONMF) problem. The objective is to approximate input data by using two low-rank nonnegative matrices, adhering to both orthogonality and \( \ell_0 \)-norm sparsity constraints. The proposed maximum-entropy-principle based framework ensures orthogonality and sparsity of features or the mixing matrix, while maintaining nonnegativity in both. Additionally, the methodology offers a quantitative determination of the “true” number of underlying features, a crucial hyperparameter for ONMF. Experimental evaluation on synthetic and a standard datasets highlights the method’s superiority in terms of sparsity, orthogonality, and computational speed compared to existing approaches. Notably, the proposed method achieves comparable or improved reconstruction errors in line with the literature.

I. INTRODUCTION

In many machine learning, data science and data-driven control applications, where large datasets contain records of many member elements, there is a need for identifying common features across the members and quantify the weight of these features in each member. In many applications, the underlying data is represented by nonnegative real numbers, and often for deriving semantic sense from the decomposed data, it is required that features and extents too are represented by nonnegative real numbers. These problems are modeled as nonnegative matrix factorization (NMF) problems. NMF is a low-rank approximation method that takes a nonnegative data matrix as input and returns a set of nonnegative features that when linearly combined together approximate the original data. More precisely, given a large data matrix \( X \in \mathbb{R}^d_{+}^{n \times m} \), the goal of NMF is to approximate it by a product of low-rank, nonnegative matrices \( W, H \) where \( W \in \mathbb{R}^d_{+}^{d \times k} \) is the features matrix and \( H \in \mathbb{R}^{k \times n} \) is the mixing matrix; Here \( k \ll \min(n, d) \) is the inner dimension that determines the number of features. Each column of \( W \) is a feature that has the same dimension as of the original data, and each column of \( H \) represents the weight of each feature in the corresponding data point. The nonnegativity constraint on \( W \) and \( H \) often leads to a more interpretable and semantic representation of the original data points, and is suitable to decompose data that are inherently nonnegative.

A variety of additional constraints have been imposed on the \( W \) and \( H \) matrix in the literature; One of which is the orthogonality constraint, that in the single-orthogonality case requires \( W \) or \( H \) to be orthogonal matrices and in the double-orthogonality case both matrices have to be orthogonal. There is a class of applications that require orthogonal features [1], [2]. Another commonly posed constraint is the sparsity constraint that requires either of the features or the mixing matrix to be sparse [3]. In this case, NMF produces a small number of localized and compact features, and the relevance of non-significant elements of each feature is diminished.

In our approach, we re-interpret the ONMF problem as a seemingly unrelated capacity-constrained facility location problem (FLP). FLP is an NP-hard combinatorial optimization problem that aims to allocate a set of facilities to a large set of consumer nodes such that the weighted average distance between the nodes and their assigned facility is minimized. The deterministic annealing (DA) is an algorithm that successfully addresses FLPs arising in areas such as data compression and pattern recognition tasks [4]. The DA assigns a probability distribution over all nodes that quantifies the association of each node to each facility, and employs the maximum-entropy-principle (MEP) to determine the probability distribution in an iterative scheme.

Different algorithms have been developed in the literature to solve the ONMF problem, including methods based on iterative projection update rule [5], [6], [7], gradient descent [8], multiplicative gradient projections [9], [10], and other methods that view ONMF as a clustering problem [11] or propose an EM-like algorithm [12] . In the context of NMF, promoting sparsity has led to the incorporation of diverse penalty functions into the overall cost function. The literature extensively covers NMF techniques employing \( \ell_1 \) or \( \ell_2 \)-norm constraints to induce sparsity [13], [14], while comparatively less attention has been given to leveraging the intrinsic \( \ell_0 \)-norm measure [15].

To our knowledge, no existing literature addresses the combined application of NMF with both \( \ell_0 \)-sparsity and orthogonality constraints. Among the mentioned approaches, only a small subset ensures orthogonality/sparsity, but typically at the expense of factors like reconstruction accuracy, sparsity, or computational efficiency. Moreover, these methods are highly reliant on the initial factor matrix setup. Additionally, they often assume or restrict a predetermined number of features. However, the resulting solution attributes, encompassing computational time, reconstruction errors, and their interplay, hinge on the chosen feature count.

In this paper, we introduce a mathematical framework to solve the ONMF problem with forced \( \ell_0 \)-norm sparsity. We assert that our method for solving orthogonal NMF
problems provides several advantages over the state-of-the-art algorithms: (a) invariance to initialization: the proposed iterative algorithm evolves hierarchically, where the number of distinct features increases from one to \( k \). Here the solution from the previous iteration serves as a *an improved guess solution* to the subsequent iteration. (b) orthogonality guarantee: the result of our solution is deterministic where in the features (mixing) matrix each row (column) eventually has exactly one non-zero element. (c) detecting the true number of features: Our approach facilitates a notion for characterizing the “true” number of underlying features. To every possible reconstruction error value, the minimum number of features that guarantees the reconstruction error is determined. The “true” number of features is defined as the number that persists for the largest range of reconstruction values.

In most simulations on synthetic and standard datasets, our algorithm outperformed nine other ONMF methodologies in terms of sparsity, orthogonality, and computational efficiency, achieving at least the same, if not better, reconstruction error.

II. Problem Formulation
Consider the data matrix \( X \in \mathbb{R}^{d \times n} \) that we want to approximate by the product of two nonnegative matrices \( W \in \mathbb{R}^{d \times k} \) and \( H \in \mathbb{R}^{k \times n} \). Since there are no additional constraints on the problem, if a solution \( (W^*, H^*) \) exists, any other pair of the form \((W'B, B^{-1}H^*)\) is also a solution to the problem, for any invertible matrix \( B \). Therefore, the solution is not unique. The orthogonal NMF (ONMF) requires one of the matrices \( W \) (or \( H \)) to be orthogonal. Thus, the ONMF poses the following problem:

\[
\min_{W,H} D(X,WH) \text{ s.t. } HH^T = I \text{ with } H_{ij} \geq 0, \forall i,j \tag{1}
\]

where \( D(X,W) \) is the distance function between the two matrices \( X \) and \( WH \) (representing the reconstruction error), and is often chosen to be the squared Frobenius norm \( ||X - WH||_F^2 \). The orthogonality constraint may be replaced by \( W^TW = I \).

Note that the nonnegativity and orthogonality constraints imply that matrices can have only one non-zero element in each row (column) when \( W \) (or \( H \)) is orthogonal. For instance, when \( W \) is orthogonal, for all \( i \neq j \), we have \( W^TW_{ij} = 0 \iff \sum_k W_{ki}W_{kj} = 0 \Rightarrow W_{ki}W_{kj} = 0 \) for each \( k \). This is possible only when at most one term in each \( k \)-th row is not zero. In the ONMF case, the solution pair \((W^*, H^*)\) is unique, since the matrix \( B \) can only be the different permutations of rows/columns of \( I \), the identity matrix. Any \( W^*B \) and \( B^TH^* \) where \( BB^T = I \) is also a solution to the ONMF problem as \( W^*BB^TH^* = W^*H^* \). However, if \( B \neq I \) or the permutation matrix (which is simply re-ordering rows/columns of \( I \)) then the orthogonality of \( B \) mandates having at least one off-diagonal negative element in it. This negative element, when multiplied by orthogonal \( W^* \) or orthogonal \( H^* \), produces at least one negative element in them that contradicts the nonnegativity condition. Thus, the only possible candidate for \( B \) is different permutations of the identity matrix.

III. Maximum-Entropy-Principle (MEP) Approach to Solve ONMF
Using the notations \( X = [x_1 \ x_2 \ \cdots \ x_n] \in \mathbb{R}^{d \times n} \), \( W = [w_1 \ w_2 \ \cdots \ w_k] \in \mathbb{R}^{d \times k} \), and \( X = [x_{ij}] \in \{0,1\}^{k \times n} \), where the binary variable \( x_{ij} \in \{0,1\} \) is 1 only when \( i \)-th data point is assigned the \( j \)-th feature, the \( \ell_0 \)-sparsity constrained ONMF optimization problem can be re-written as

\[
\min_{Y,X} D(X,YX^T) \text{ s.t. } XX^T = I, \sum_i p_i x_{ij} = c_j \forall j
\]

where \( c_j \in \{0,1\} \) denotes the relative pre-defined \( \ell_0 \)-norm (capacity) of each feature, with \( \sum_j c_j = 1 \) and \( p_i \in [0,1] \) is a priori known weight that gives the relative importance of the \( i \)-th node \((\sum_i p_i = 1, p_i = 1/n \) when all the nodes are of equal importance).

ONMF can be interpreted as an FLP where the goal is to allocate a set of \( k \) facilities \( y_j \) to a large set of \( n \) consumer nodes \( x_i \) such that the weighted average distance between the nodes and their assigned facility is minimized. For any given nonnegative matrix \( X \in \mathbb{R}^{d \times n} \), we can view the columns of \( X \) as the nodes locations, hence the resulting facility-location matrix \( Y \in \mathbb{R}^{k \times n} \) and the assignment matrix \( \chi \in \{0,1\}^{k \times n} \) are both nonnegative, \( \chi \) is an orthogonal matrix, and \( X = Y\chi \). Here \( D(X,Y\chi) = \sum_{j=1}^n d(x_j, y_j) \chi_{ij} \) where \( d(x_j, y_j) \) is a function of \( x_j \) and \( y_j \) that represents the distance between the \( i \)-th node and \( j \)-th facility, and \( \chi^T = I \) enforces the condition that only one facility is assigned to each node. Therefore, this case is equivalent to the ONMF problem with \( H \)-orthogonal constraint, taking \( W \rightarrow Y \) and \( H \rightarrow \chi \). For the \( W \)-orthogonal case, we just need to transpose the data matrix \( X \rightarrow X^T \). Following the same reasoning, \( W^TW = I \) putting \( W \rightarrow \chi^T \) and \( H \rightarrow Y^T \).

A. MEP-based Solution
Note that FLP (and therefore ONMF) problems are optimization problems, where a great deal of complexity arises from the constraint on decision variables \( \chi_{ij} \) to be binary variables. Here, these hard assignments \( \chi_{ij} \) are relaxed by soft assignments \( p_{ij} \in [0,1] \) and the probability mass function (PMF) \( p_{ij} \) associates \( i \)-th data point \( x_i \) to the feature \( w_j \). Hence, according to (1), we can formulate the \( \ell_0 \)-sparsity ONMF as

\[
\min_{\{p_{ij}\},\{w_j\}} \mathcal{F} = D\{\{p_{ij}\},\{w_j\}\} - \frac{1}{\beta} \mathcal{H}\{\{p_{ij}\}\}, \tag{2}
\]

\[s.t. \sum_j p_{ij} = 1 \forall i, \sum_i p_{ij} = c_j \forall j, 0 \leq p_{ij} \leq 1 \forall i,j \]

where \( D\{\{p_{ij}\},\{w_j\}\} = \sum_{i=1}^n p_i \sum_{j=1}^k p_{ij} d(x_i, w_j) \) is the expected value of the cost function in (1), while the Shannon entropy \( \mathcal{H}\{\{p_{ij}\}\} = -\sum_{i=1}^n p_i \sum_{j=1}^k p_{ij} \log p_{ij} \) is a measure of randomness (uncertainty) of the associated PMF \( \{p_{ij}\} \). \( 1/\beta \) characterizes the relative importance of the target cost function and the extent of randomness introduced in the formulation due to the PMF. We can form the
Lagrangian $\mathcal{L}$,
\[
\mathcal{L} = \mathcal{F} + \sum_i \lambda_i \left[ \sum_j p_{ji} - 1 \right] + \sum_j \phi_j \left[ \sum_i p_{ji} - c_j \right]
\]
where $\lambda_i, \phi_j$ are the Lagrangian variables. Note that for a fixed $\beta$, $\mathcal{F}$ is convex with respect to $\{p_{ji}\}$; and the optimal solutions for the PMF are obtained by setting $\frac{\partial \mathcal{L}}{\partial p_{ji}} = 0$:
\[
p_{ji} = e^{-\beta \frac{1}{m} - 1 - \beta \phi_j - \beta d_{ij}}
\]
where $d(x_i, w_j)$ is replaced with $d_{ij}$ for notation simplicity. To ensure primal feasibility, we apply the constraints in (2) as
\[
\phi_j = \frac{1}{\beta} \log \left[ \sum_i \frac{p_{i} e^{-\beta d_{ij}}}{\sum_m e^{-\beta \phi_m - \beta d_{im}}} \right] - \frac{1}{\beta} \log c_j
\]
Defining $e^{-\beta \phi_j} = \alpha_j$ and assuming squared Euclidean distance for $d(\cdot, \cdot)$, the optimal PMF is given by
\[
p_{ji} = \frac{\alpha_j e^{-\beta \|x_i - w_j\|^2}}{\sum_m \alpha_m e^{-\beta \|x_i - w_m\|^2}}
\]
\[
\alpha_j = \frac{c_j}{\sum_i \sum_m \alpha_m e^{-\beta \|x_i - w_m\|^2}}
\]
By re-interpreting this PMF as $\alpha_j$ units of features at each feature vector, we can write the modified free energy function at (3) as
\[
\tilde{\mathcal{F}} = -\frac{1}{\beta} \sum_{i=1}^{n} \sum_{j=1}^{k} \alpha_j e^{-\beta \|x_i - w_j\|^2}
\]
If we remove the requirement to pre-determine the capacities $c_j$, we can treat $\mathcal{F}$ as a dual optimization problem over the equivalent Lagrangian parameter $\alpha_j$ and form a new objective
\[
\min_{\{w_j\}, \{\alpha_j\}} \tilde{\mathcal{F}} = \tilde{\mathcal{F}} + \mu \left( \sum_{j=1}^{k} \alpha_j - 1 \right)
\]
where the second term imposes the constraint that $\sum_{j=1}^{k} \alpha_j = 1$. From now onward, we call this version of our algorithm the "optimally-weighted" MEP-ONMF. The locally optimal values of $\{w_j\}, \{\alpha_j\}$ are determined by setting $\frac{\partial \tilde{\mathcal{F}}}{\partial \alpha_j} = 0$ and $\frac{\partial \tilde{\mathcal{F}}}{\partial w_j} = 0$; which yield
\[
w_j = \sum_{i=1}^{n} p_{ij} x_i \text{ and } \alpha_j = \sum_{i=1}^{n} p_{ij} p_{ji}
\]
where $p_{ij} = p_{ij}/\alpha_j$. Thus, we get optimal (local) solutions for $\{p_{ij}\}$ and $\{w_j\}$ at a fixed $\beta$, and we can form the matrices $W$ and $H$ simply by putting $W_{ij} = w_j$ and $H_{ij} = p_{ji}$. This results in a mixing matrix $H$ that the nonnegative numbers are always one, as each data point is assigned to exactly one feature. Let us take $w_j$ be the feature that has a non-zero value for the $i^{th}$ data point (it is unique since each data point is assigned to exactly one facility). Then, minimizing $E = \sum_{i=1}^{n} \|x_i - \theta_i w_j\|^2$ with respect to $\theta_i$ yields:
\[
\theta_i = \frac{x_i^\top w_j}{\|w_j\|^2}
\]
and we replace ones in the $i^{th}$ columns of $H$ with $(\theta_i)$s. Therefore, our MEP-based algorithm for Orthogonal NMF (MEP-ONMF) is shown in Algorithm [1].

B. Phase Transitions and True Number of Features

The proposed method in section 3.2 evolves hierarchically with respect to $\beta$, as $\beta$ is increased from small ($\approx 0$) to a high ($\approx \infty$) value; at each iteration the solutions from the previous iteration are used for initialization. Note that at initial iterations (when $\beta \approx 0$), higher emphasis is given to the randomness of associations (characterized by $H$ in (2)); hence the ensuing solutions are uniform PMF $p_{ji} \approx \frac{1}{k}$; and all $w_j$ are coincident at the centroid of data points $x_i$. This is evident by looking at equations (6) and (10) at $\beta \approx 0$. Therefore all the $k$ features are coincident at the centroid when $\beta \approx 0$. This can be also explained since the term $\sum_j e^{-\beta \|x_i - w_j\|^2}$ in $\tilde{\mathcal{F}}$ cannot distinguish different summands since $\|x_i - w_j\|^2 \ll \frac{1}{\beta}$ for all $j$ at each $i$. Thus $1/\beta$ acts as a resolution measure on reconstruction error (cost value in (11)); and when this resolution yardstick is too large, one feature is enough to achieve that resolution in reconstruction error. As $\beta$ is increased, this resolution yardstick becomes smaller (finer); whereby $\|x_i - w_j\|^2$ for different $j$s are more distinguishable. As $\beta$ is increased from 0, there is a critical value $\beta_{cr}$, beyond which it is not possible to achieve the now smaller resolution on reconstruction error by a single distinct value of $w_j$ but requires at least two distinct features. Thus as the resolution $(1/\beta)$ or reconstruction error bound is decreased; more number of distinct features appear in the optimal solutions at successive values of $\beta_{cr}$.

In the context of NMF and ONMF algorithms, it is common to assume that the number of features is known a priori, or to constrain it in some way. However, we can utilize the phase transition concept to identify the true number of features present in a dataset. We adapt the notions developed in [16] in the context of the clustering problem to our problem. Based on the phase transitions at successive critical temperatures, we define a measure $\Delta(m) = \frac{\Delta_{m}}{\Delta_{m+1}}$ that quantifies persistence of $m$ distinct features - Here $\Delta(m)$ quantifies the range of reconstruction error bounds (characterized by $1/\beta$) for which $m$ is the smallest number of distinct features necessary (and enough) to guarantee those bounds. The true number of features is then defined as one that persists for the largest range of reconstruction errors. More precisely, true number $m^*$ of features is one that satisfies $m^* = \arg \max \Delta(m)$. See Fig. [1] for a visual illustration.

[1]The dataset and an implementation of the algorithm are available on a Github repository at https://github.com/salar96/MEP-Orthogonal-NMF.
Hence, the iterative scheme between \( p_{ij} \) and \( w_j \) is:

\[
\frac{1}{2} \frac{\partial F}{\partial w_j} = \sum_{i=1}^{n} p_{ij} \alpha_j e^{-\beta d_{ij}} (w_j - x_i) - \sum_{i=1}^{n} p_{ij} w_j = P(j)w_j - \sum_{i=1}^{n} p_{ij} w_j = P(j)(w_j - w_j^+) \tag{12}
\]

where \( P(j) = \sum_{i=1}^{n} p_{ij} \) is the updated \( w_j \) at the next iteration. Hence, we can see that \( W^+ = W - \frac{1}{2} P^{-1} \nabla F \) where \( P = \text{diag}\{P(1), \ldots, P(k)\} \) and \( W = \{w_j, j \in \mathbb{N}_{[1,k]}\} \). Hence, the iterative scheme between \( p_{ij} \) and \( w_j \) forms a descent method on the free energy function where the descent direction \( \mathcal{D} = - P^{-1} \nabla F \) satisfies \( \mathcal{D}^T \nabla F \leq 0 \) with the equality true only when \( \nabla F = 0 \). Note that the nature of this optimization problem is scale-invariant, i.e., if we multiply each \( x_i \) and \( w_j \) by a factor of \( 1/\sigma \), it is equivalent to minimizing the free energy function at a new temperature \( \beta_1 \sigma^2 \). We can take advantage of this fact to increase the convergence rate of our algorithm at each \( \beta_t \), which in this case the descent direction is \( \mathcal{D} = - \sigma^2 P^{-1} \nabla F \). The overall convergence rate of our algorithm also depends on the iterations on \( \beta \), where in this algorithm \( \beta \) is increased geometrically up to a maximum value, i.e., \( \beta_{t+1} = \beta_t \Gamma, \Gamma > 1 \).

### IV. Evaluation Setup

To evaluate our algorithm and compare it with other existing algorithms, we use the following four metrics:

(a) **Reconstruction error**: given by \( E = \frac{\|X - WH\|_F}{\|X\|_F} \) where \( \| \cdot \|_F \) denotes the Frobenius norm.

(b) **Orthogonality**: calculated as \( O = 1 - \frac{\|GG^T - GG^T \otimes I\|_F}{\|GG^T\|_F} \) where \( \otimes \) denotes the Hadamard product and \( I \) is the identity matrix.

(c) **Sparsity**: defined as \( S(A) = 1 - \frac{1}{k} \sum_{j=1}^{k} |A_{ij}|_0 \)

(d) **Execution time (T)**: The total time elapsed in seconds.

The evaluation is done in two scenarios. In scenario one, we ran the algorithms on random synthetic matrices. Specifically, the columns of the data matrix \( X \) were sampled from a Gamma distribution, with the probability density function defined as \( P(x) = x^{\alpha-1} e^{-x/\beta} \Gamma(\alpha) \) where \( \Gamma(\cdot) \) is the Gamma function. Here we have chosen \( \alpha = 10 \) and \( \beta = 1 \). Additionally, a uniform random noise was incorporated into the matrix to further increase the diversity of the data. In this scenario, we use \( k = 20 \) as the inner dimension (rank of the factors) in all of the datasets. In scenario two, we used a Standard bioinformatics dataset [17] that contains microarrays of patients over different periods of time. Microarrays consist of nonnegative numerical data used to obtain information about gene expression patterns across different conditions. These data are usually presented in the form of gene-sample or gene-time matrices [2]. The state of the art works using this dataset have used different orthogonal NMF approaches to extract the features (here called metagenes) that together describe the whole microarray when linearly combined, and yet are non-overlapping, i.e. each gene only belongs to a single metagene.

### V. Results and Discussion

#### A. Synthetic data

The results for synthetic matrices are reported in Table 1a-d. In Table 1a, the underlying dataset is relatively low dimensional. Our proposed method demonstrates the fastest performance time, as well as the highest levels of orthogonality and sparsity when compared to other methods. The HALS method exhibits a lower reconstruction error, but 2All of the algorithms are executed using an Intel® Core™ i7-4790 CPU (@ 3.60 GHz) and each is run 5 times. The reported values for all the metrics are the average values over all runs.
TABLE I
RESULTS OF THE SIMULATION FOR 4 RANDOMLY GENERATED $d \times n$ DATASETS USING METRICS OF SECTION IV.

| $a) = 10$ | $n = 1000$ |
|-----------|------------|
|           | $E(\%)$ | $O(\%)$ | $S(\%)$ | $T(s)$ |
| MEP_ONMF   | 0.026   | 100    | 95     | 0.040 |
| ONMF_apx  | 0.028   | 100    | 95     | 0.133 |
| ONMF_Ding | 2.520   | 85     | 78     | 19.193|
| ONMF_A    | 4.235   | 74     | 66     | 1.789 |
| PNMF      | 4.305   | 81     | 79     | 31.185|
| NHL       | 5.166   | 82     | 80     | 27.051|
| ONMF_EM   | 9.522   | 100    | 95     | 0.086 |
| HALS      | 0.006   | 13     | 24     | 2.099 |
| IONMF     | 1.917   | 10     | 0      | 0.071 |
| NMF       | 0.028   | 10     | 0      | 0.348 |
|           |          |        |        |        |

| $b) = 20$ | $n = 2000$ |
|-----------|------------|
|           | $E(\%)$ | $O(\%)$ | $S(\%)$ | $T(s)$ |
| MEP_ONMF   | 0.027   | 100    | 95     | 0.085 |
| ONMF_apx  | 0.028   | 100    | 95     | 0.264 |
| ONMF_Ding | 1.017   | 97     | 78     | 46.584|
| ONMF_A    | 4.846   | 81     | 66     | 5.930 |
| PNMF      | 4.975   | 86     | 82     | $\approx130$ |
| NHL       | 6.324   | 84     | 85     | $\approx190$ |
| ONMF_EM   | 8.782   | 100    | 95     | 0.201 |
| HALS      | 0.483   | 13     | 29     | 2.783 |
| IONMF     | 5.006   | 11     | 0      | 0.139 |
| NMF       | 0.091   | 14     | 0      | 4.788 |
|           |          |        |        |        |

| $c) = 50$ | $n = 4000$ |
|-----------|------------|
|           | $E(\%)$ | $O(\%)$ | $S(\%)$ | $T(s)$ |
| MEP_ONMF   | 0.028   | 100    | 95     | 0.252 |
| ONMF_apx  | 0.028   | 100    | 95     | 0.420 |
| ONMF_Ding | 3.092   | 90     | 86     | $\approx500$ |
| ONMF_A    | 2.130   | 90     | 61     | 17.181|
| PNMF      | 7.345   | 82     | 82     | $\approx530$ |
| NHL       | 6.538   | 88     | 86     | $\approx550$ |
| ONMF_EM   | 9.839   | 100    | 95     | 0.666 |
| HALS      | 1.042   | 26     | 52     | 26.565|
| IONMF     | 7.028   | 14     | 0      | 0.314 |
| NMF       | 0.210   | 28     | 16     | 30.208|
|           |          |        |        |        |

| $d) = 100$ | $n = 10000$ |
|------------|------------|
|            | $E(\%)$ | $O(\%)$ | $S(\%)$ | $T(s)$ |
| MEP_ONMF   | 0.028   | 100    | 95     | 0.965 |
| ONMF_apx  | 0.028   | 100    | 95     | 1.239 |
| ONMF_Ding | 5.375   | 87     | 87     | $\approx1400$ |
| ONMF_A    | 4.062   | 88     | 69     | 93.992 |
| PNMF      | 6.341   | 90     | 87     | $\approx3600$ |
| NHL       | 7.718   | 86     | 89     | $\approx3560$ |
| ONMF_EM   | 9.491   | 100    | 95     | 3.133 |
| HALS      | 0.049   | 46     | 56     | 90.312 |
| IONMF     | 8.947   | 17     | 0      | 1.269 |
| NMF       | 0.528   | 46     | 37     | $\approx300$ |

Figure 2. The logarithm of the fraction between successive critical $\beta$ over all time periods. The $k^{th}$ value on the x-axis represents the number of features, while the y-axis shows $\log(\frac{\beta_k}{\beta_{k-1}})$ where $\beta_k$ is the critical $\beta$ value at which the $k^{th}$ feature split happens.

at the cost of compromised orthogonality and sparsity. Our method not only guarantees orthogonality and sparsity, but also yields a smaller reconstruction error in comparison to the original NMF method which does not have a guarantee of orthogonality or sparsity. This pattern is also observed in Tables II b and II c, where the dimensions of the datasets have increased significantly. In these cases, our method achieves the lowest reconstruction error among all methods. The ONMF-EM also yields orthogonality and high sparsity, however, it results in a higher reconstruction error. Finally, in Table II d, the dataset is significantly large, and our method is demonstrated to scale well, as the performance time remains efficient in comparison to ONMF-ding, PNMF, and NHL. Our method achieves the best reconstruction error with full orthogonality, the highest sparsity, and the fastest run-time.

B. Standard Bioinformatics Dataset

In this scenario, we have used MEP-ONMF to extract the main features (i.e., metagenes) and compare our results with other methods. The first step was to determine the number of metagenes that we want to calculate. As explained in section III-B, the methodology of MEP-ONMF provides a feasible way to determine the true number of features in a dataset. Simply by looking at the critical $\beta$s diagram ($\beta$s at which a feature split has happened), we can determine the true number of features, and that is when a large gap is seen between two consecutive values. The logarithmic difference between successive critical $\beta$ values for all time periods is depicted in Fig. 3. If a significant spike is observed at the $k^{th}$ split, indicating a transition from $k$ features to $k + 1$ features, it can be concluded that selecting $k$ features yields the most persistent factorization and can thus be considered as the true number of features in the dataset. In almost all time periods, there is a large spike at the third split, except for one ($T_4$) where this gap happens at the fourth. Therefore, we can conclude that the true number of metagenes in this dataset is 3, which approves the number used in previous works. Table II shows the results of the simulation on the dataset, averaged over all the 7 time period and 5 runs for each algorithm in total. The results of this table indicate that our proposed algorithm is able to generate perfectly orthogonal metagenes that exhibit a sparsity of 66%. Additionally, the algorithm results in a smaller reconstruction error but slightly slower performance time in comparison to other methods that do not enforce the constraint of orthogonality.

Figure 3 visually depicts the metagenes computed using MEP-ONMF for individual time periods. The upper plot enforces equal $\ell_0$-norm ($c_1 = c_2 = c_3 = 1/3$) among the three metagenes. The algorithm effectively adheres to
while preserving nonnegativity. Evaluation on synthetic and phase transition points in future research.

Nevertheless, there are avenues to improve, particularly in fine-tuning hyperparameters like $\beta$ for improvement, particularly in fine-tuning hyperparameters like $\beta$ and establishing precise mathematical expressions for phase transition points in future research.

VI. CONCLUSION

This study introduces an innovative approach to address the ONMF problem under an $\ell_0$-sparsity constraint, utilizing a maximum-entropy-principle-based framework to ensure orthogonality and sparsity in the features or mixing matrix while preserving nonnegativity. Evaluation on synthetic and genetic microarray datasets demonstrates the method’s superiority over comparable techniques, offering enhanced sparsity, orthogonality, and performance speed with comparable or improved reconstruction errors. Nevertheless, there are avenues for improvement, particularly in fine-tuning hyperparameters like $\beta$ and establishing precise mathematical expressions for phase transition points in future research.

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