Probabilistic Clustering using Maximal Matrix Norm Couplings

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Abstract

In this paper, we present a local information theoretic approach to explicitly learn probabilistic clustering of a discrete random variable. Our formulation yields a convex maximization problem for which it is NP-hard to find the global optimum. In order to algorithmically solve this optimization problem, we propose two relaxations that are solved via gradient ascent and alternating maximization. Experiments on the MSR Sentence Completion Challenge, MovieLens 100K, and Reuters21578 datasets demonstrate that our approach is competitive with existing techniques and worthy of further investigation.

I. INTRODUCTION

Clustering is one of many important techniques in unsupervised learning that finds structure in unlabeled data. One important class of clustering algorithms is metric based, where each row of the data matrix corresponds an item’s vector representation in \( \mathbb{R}^n \). The most well known example of metric based clustering is \( k \)-means clustering (or Lloyd-Max algorithm [1], [2]).

In this paper, we instead focus on probabilistic clustering, where the data matrix is usually viewed as the joint co-occurrences (or affinities) between two discrete sets, \( \mathcal{X} \) and \( \mathcal{Y} \), of items and users, respectively. The co-occurrence matrix can be normalized to sum to 1 to represent a joint probability matrix. Much like [3], we want to maximize the “cluster-to-item” mutual information over the set of “user-to-cluster” assignment matrices. Our main contributions include relaxing this mutual information optimization into a Frobenius norm optimization over “DTM” matrices (to be defined later), relating such matrices to graph Laplacians in spectral graph theory, and proposing an alternating maximization algorithm to approximately solve this matrix optimization. Moreover, unlike spectral methods, we directly learn a transition kernel for soft clustering as opposed to following the usual two-step procedure of learning an embedding and then applying \( k \)-means clustering.

A. Outline

This paper is organized as follows: Section II defines the divergence transition matrix and derives the relationship between its Frobenius norm and mutual information. Section III discusses the Frobenius maximization problem for probabilistic clustering and analyzes its convexity and complexity. Section IV relaxes the optimization problem and presents two algorithms based on gradient ascent and alternating maximization, respectively. Section V presents some experimental results that validate our model.

II. BACKGROUND

A. Notation

We let \( \mathcal{X}, \mathcal{Y}, \) and \( \mathcal{Z} \) denote the non-empty, finite alphabet sets corresponding to the random variables \( X, Y, \) and \( Z \), respectively. For a set \( \mathcal{X} \), we let \( \mathcal{P}_\mathcal{X} \subseteq \mathbb{R}^{\mathcal{X}} \) denote the probability simplex of probability mass functions (pmfs) on \( \mathcal{X} \), and \( \mathcal{P}_\mathcal{X}^\circ \) denote the relative interior of \( \mathcal{P}_\mathcal{X} \). Furthermore, for any two sets \( \mathcal{X} \) and \( \mathcal{Y} \), we let \( \mathcal{P}_{\mathcal{Y}|\mathcal{X}} \subseteq \mathbb{R}^{\mathcal{Y} \times \mathcal{X}} \) denote the set of all column stochastic matrices (channels or transition probability kernels) from \( \mathcal{X} \) to \( \mathcal{Y} \). For convenience, we perceive joint pmfs of any two random variables as matrices, e.g. \( \mathcal{P}_{\mathcal{Y} \times \mathcal{X}} \subseteq \mathbb{R}^{\mathcal{Y} \times \mathcal{X}} \), and for any (marginal) pmf \( P_X \in \mathcal{P}_\mathcal{X} \), we let \( [P_X] \in \mathbb{R}^{\mathcal{X} \times \mathcal{X}} \) denote the diagonal matrix with \( P_X \) along the principal diagonal.

For any \( m \times n \) real matrix \( A \in \mathbb{R}^{m \times n} \), we let \( \sigma_1(A) \geq \sigma_2(A) \geq \cdots \geq \sigma_{\min(m,n)}(A) \) denote the ordered singular values of \( A \), and \( \text{tr}(A) \) denote the trace of \( A \). Furthermore, we will use the notation:

\[
\|A\|_p \triangleq \left( \sum_{i=1}^{\min(m,n)} \sigma_i(A)^p \right)^{\frac{1}{p}}
\]
to represent the Schatten $\ell^p$-norm of $A$ with $1 \leq p \leq \infty$. Two pertinent specializations of the Schatten $\ell^p$-norm are:

$$\|A\|_{p,\ast} \triangleq \|A\|_1 = \text{tr}\left((A^T A)^{1/2}\right) \tag{2}$$

$$\|A\|_{p,2} \triangleq \|A\|_2 = \text{tr}\left((A^T A)^{1/2}\right) \tag{3}$$

which denote the nuclear norm and Frobenius norm of $A$, respectively. (Note that in (2), $(A^T A)^{1/2}$ is the unique positive semidefinite square root matrix of $A^T A$.) Finally, we will use $A \geq 0$ to imply that $A$ is entry-wise non-negative.

For any two vectors $x, y \in \mathbb{R}^n$, we let $\sqrt{x}$ denote the entry-wise square root of $x$, $\|x\|_2$ denote the Euclidean $\ell^2$-norm of $x$, and $xy \in \mathbb{R}^n$ denote the (entry-wise) Hadamard product of $x$ and $y$.

**B. Information Theoretic Motivation**

Suppose we are given training data $(Y_1, X_1), \ldots, (Y_n, X_n)$ that is drawn i.i.d. from a joint pmf $P_{Y,X} \in \mathcal{P}_{\mathcal{Y} \times \mathcal{X}}$ such that $P_X \in \mathcal{P}_\mathcal{X}$ and $P_X \in \mathcal{P}_\mathcal{X}$. Our goal is to perform clustering on $\mathcal{Y}$ by learning the transition probability kernel $P_{Z|Y} \in \mathcal{P}_{\mathcal{Y} \times \mathcal{Y}}$, where $Z$ is the set of cluster labels with $|Z| \ll |\mathcal{Y}|$, and $P_{Z|Y=y} \in \mathcal{P}_Z$ represents a soft assignment of $y \in \mathcal{Y}$. Since our training data is “unlabeled,” we assume that $X \rightarrow Y \rightarrow Z$ form a Markov chain to extract information about the clusters from our training data. From hereon, we assume that $P_{Y,X}$ is known as it can be empirically estimated from the data, and $P_{Z} \in \mathcal{P}_Z$ is known from some prior domain knowledge. For example, when clustering readers of political blogs, $\mathcal{X}$ is the set of blogs, $\mathcal{Y}$ is the set of readers, and $P_Z$ can be set using priors on the distribution of liberals and conservatives in the country.

The following information theoretic problem can be used to perform probabilistic clustering:

$$\sup_{P_{Z|Y} \in \mathcal{P}_{Z|Y}: P_{Z|Y} P_Y = P_Z} I(X; Z) \tag{4}$$

where $P_{X,Y}$ and $P_Z$ are fixed, $X \rightarrow Y \rightarrow Z$ form a Markov chain, and $I(X; Z)$ denotes the mutual information between $X$ and $Z$ (see [4, Section 2.3] for a definition). In the sections that follow, we will refer to $P_{Z|Y} P_Y = P_Z$ as the constraint on the marginal. Intuitively, the formulation in (4) finds soft clusters by maximizing $I(X; Z)$ and thereby exploiting the information that $X$ contains about $Y$. Note that $I(X; Z) \leq I(X; Y)$ by the data processing inequality [4, Section 2.8], but $P_{Z|Y} = I_{|Z|}$ (which denotes the $|Z| \times |Z|$ identity matrix) is not a solution because $|Z| \ll |\mathcal{Y}|$.

It is worth mentioning that the formulation in (4) is related to the information bottleneck method developed in [5] (which is useful for lossy source compression and clustering), as well as the linear information coupling problem introduced in [6] (which provides intuition about network information theory problems).

**C. Local Approximations**

Since the mutual information objective in the probabilistic clustering formulation in (4) has no inherent operational meaning, we will use local approximations, much like [6], to transform (4) into a simpler Frobenius norm maximization problem (which is a non-convex quadratic program as shown in section III). To this end, for a fixed reference pmf $P_Z \in \mathcal{P}_Z$, we define a locally perturbed pmf $Q_Z \in \mathcal{P}_Z$ of $P_Z$ as follows:

$$Q_Z = P_Z + \epsilon \sqrt{P_Z} \phi \tag{5}$$

where $\phi \in \mathbb{R}^{|\mathcal{Y}|}$ is a spherical perturbation vector such that $\phi^T \sqrt{P_Z} = 0$ [7, Equation (14)], and $\epsilon \neq 0$ is a scalar that is small enough to ensure that $Q_Z \in \mathcal{P}_Z$. For such perturbed pmfs $Q_Z$, we can locally approximate the Kullback-Leibler (KL) divergence between $Q_Z$ and $P_Z$ as a scaled Euclidean $\ell^2$-norm of $\phi$. Indeed, as shown in [6], a straightforward calculation using Taylor’s theorem yields:

$$D(Q_Z || P_Z) = \frac{1}{2} \epsilon^2 \|\phi\|_2^2 + o(\epsilon^2) \tag{6}$$

where $D(\cdot || \cdot)$ denotes KL divergence (see [4, Section 2.3] for a definition), and $o(\epsilon^2)$ represents a function satisfying $\lim_{\epsilon \rightarrow 0} o(\epsilon^2)/\epsilon^2 = 0$.

Now consider the following local perturbation relations that we will use to locally approximate (4):

$$\forall y \in \mathcal{Y}, \ P_{Z|Y=y} = P_Z + \epsilon \sqrt{P_Z} \phi_y \tag{7}$$
where \( \{ \phi_y \in \mathbb{R}^{|Y|} : y \in \mathcal{Y}, \phi_y^T \sqrt{P_Z} = 0, \|\phi_y\|_2 = 1 \} \) are unit norm spherical perturbation vectors, and \( \epsilon \neq 0 \) is small enough to ensure that \( P_{Z|Y=y} \in P_Z \) for every \( y \in \mathcal{Y} \). Due to the Markov relation \( X \rightarrow Y \rightarrow Z \), the conditions in (7) imply after some straightforward computation that:
\[
\forall x \in \mathcal{X}, \quad P_{Z|X=x} = P_Z + \epsilon \sqrt{P_Z} \psi_x
\]
where the spherical perturbation vectors \( \{ \psi_x \in \mathbb{R}^{|Z|} : x \in \mathcal{X}, \psi_x^T \sqrt{P_Z} = 0 \} \) are given by:
\[
\forall x \in \mathcal{X}, \forall z \in \mathcal{Z}, \quad \psi_x(z) = \sum_{y \in \mathcal{Y}} P_{Y|X}(y|x) \phi_y(z).
\]

To succinctly describe the local approximation of the objective function of (4) that stems from (8), we introduce the so-called divergence transition matrices.

**Definition 1 (Divergence Transition Matrix [6]).** Given a joint pmf \( P_{Y,X} \in \mathcal{P}_{\mathcal{Y} \times \mathcal{X}} \), with conditional pmfs \( P_{Y|X} \in \mathcal{P}_{\mathcal{Y}|\mathcal{X}} \) and marginal pmfs satisfying \( P_X \in \mathcal{P}_X \) and \( P_Y \in \mathcal{P}_Y \), the divergence transition matrix (DTM) of \( P_{Y,X} \) is defined as:
\[
B_{Y,X} = B(P_{Y,X}) \triangleq [P_Y]^{-\frac{1}{2}} P_{Y|X} [P_X]^{-\frac{1}{2}} = [P_Y]^{-\frac{1}{2}} P_{Y|X} [P_X]^{\frac{1}{2}}.
\]

It is well-known that the largest singular value of \( B_{Y,X} \) is \( \sigma_1(B_{Y,X}) = 1 \) with corresponding right and left singular vectors \( \sqrt{P_X} \) and \( \sqrt{P_Y} \), respectively (see e.g. [6], [7, Appendix A]):
\[
B_{Y,X} \sqrt{P_X} = \sigma_1(B_{Y,X}) \sqrt{P_Y} = 1 \sqrt{P_Y},
\]
\[
B_{Y,X}^T \sqrt{P_Y} = \sigma_1(B_{Y,X}) \sqrt{P_X} = 1 \sqrt{P_X}.
\]

Moreover, the next proposition decomposes the DTM of random variables in a Markov chain.

**Proposition 1 (Composed DTM).** If \( X \rightarrow Y \rightarrow Z \) form a Markov chain, then \( B_{Z,X} = B_{Z,Y} B_{Y,X} \).

**Proof.** Observe using Definition 1 that:
\[
B_{Z,X} = [P_Z]^{-\frac{1}{2}} P_{Z|X} [P_X]^{\frac{1}{2}} = [P_Z]^{-\frac{1}{2}} P_{Z|Y} P_{Y|X} [P_X]^{\frac{1}{2}} = [P_Z]^{-\frac{1}{2}} P_{Z|Y} [P_Y]^{\frac{1}{2}} [P_Y]^{-\frac{1}{2}} P_{Y|X} [P_X]^{\frac{1}{2}}
\]
where the second equality uses the Markov property.

Finally, we locally approximate \( I(X; Z) \) using (8).

**Proposition 2 (Local Approximation of Mutual Information).** Under the local perturbation conditions in (8), we have:
\[
I(X; Z) = \frac{1}{2} \left( \| B_{Z,X} \|_F^2 - 1 \right) + o(\epsilon^2).
\]

**Proof.** Observe that:
\[
I(X; Z) = \sum_{x \in \mathcal{X}} P_X(x) D(P_{Z|X=x} || P_Z)
\]
\[
= \frac{1}{2} \epsilon^2 \sum_{x \in \mathcal{X}} P_X(x) \| \psi_x \|_2^2 + o(\epsilon^2)
\]
\[
= \frac{1}{2} \epsilon^2 \sum_{x,z} P_X(x) \left( \frac{P_{Z|X}(z|x) - P_{Z}(z)}{\epsilon \sqrt{P_Z(z)}} \right)^2 + o(\epsilon^2)
\]
\[
= \frac{1}{2} \sum_{x,z} \left( \frac{P_{Z,X}(z,x) - P_{Z}(z)P_X(x)}{\sqrt{P_Z(z)P_X(x)}} \right)^2 + o(\epsilon^2)
\]
\[
= \frac{1}{2} \left\| B_{Z,X} - \sqrt{P_Z / P_X} \right\|_F^2 + o(\epsilon^2)
\]
where the first equality follows from a straightforward calculation, the second equality follows from (8) and (6), the fifth equality follows from Definition 1, and the final equality holds due to (12).

We will present the Frobenius norm maximization formulation that follows from applying this local approximation result to (4) in section III.

D. Connections to Spectral Graph Theory

In the case of $\mathcal{X} = \mathcal{Y}$, if we view $P_{Y|X}$ as a matrix of Markov transition probabilities, (11) is the matrix being factorized in diffusion maps [8]. If we view $P_{Y,X}$ as a weighted adjacency matrix, (10) is almost identical to the symmetric normalized graph Laplacian [9], [10]. Similar to the Laplacian, the DTM carries an important property that we will use later.

Proposition 3. The multiplicity of the singular value at 1 of $B(P_{Y,X})$ is equivalent to the number of connected components in a bipartite graph that has weighted adjacency matrix $P_{Y,X}$.

For a proof, we refer readers to [11, Theorem 3.1.1], which relates the eigenvalues of the identity minus the Laplacian to the singular values of the (corresponding) DTM.

III. MAXIMAL FROBENIUS NORM COUPLING

Inspired by Proposition 2, we will learn the $P_{Z|Y} \in \mathcal{P}_{Z|Y}$ that probabilistically clusters each $y \in \mathcal{Y}$ by maximizing $\|B_{Z,X}\|_F^2$ instead of $I(X;Z)$. This Frobenius norm formulation of probabilistic clustering is presented in the next definition.

Definition 2 (Frobenius Norm Formulation). Given a joint pmf $P_{Y,X} \in \mathcal{P}_{Y \times X}$ so that the marginal pmfs satisfy $P_X \in \mathcal{P}_X$ and $P_Y \in \mathcal{P}_Y$, and a target pmf $P_Z \in \mathcal{P}_Z$, we seek to solve the following extremal problem:

$$
\max_{P_{Z|Y} \in \mathcal{P}_{Z|Y} : P_{Z|Y} P_Y = P_Z} \|B_{Z,X}\|_F^2
$$

(13)

where $X \rightarrow Y \rightarrow Z$ form a Markov chain. We will refer to an optimal argument $P_{Z|Y}^*$ of this problem, which represents a desirable soft clustering assignment, as a maximal Frobenius norm coupling.

We make some pertinent remarks about Definition 2. Firstly, a “coupling” of two marginal pmfs $P_Y$ and $P_Z$ is generally defined as a joint pmf $P_{Z,Y}$ that is consistent with these marginals (and often has additional desirable properties)—see e.g. [12, Section 4.2]. However, since the maximizing conditional pmf $P_{Z|Y}^*$ implicitly defines a joint pmf $P_{Z,Y}^* = P_{Z|Y}^*[P_Y]$, we refer to $P_{Z|Y}^*$ itself as a coupling. Secondly, although the Frobenius norm formulation in (13) can be perceived as a local approximation of (4) (which nicely connects the two problems), we will not actually require $P_{Z|Y}^*$ to be close to $P_Z$ as in (7) (i.e. weak dependence between $Z$ and $Y$) when using this formulation. Thirdly, the formulation in (13) is intuitively well-founded because [13] and [14] illustrate that the singular values of the DTM $B_{Z,X}$ capture how informative or correlated mutually orthogonal embeddings of $Z$ and $X$ are. Hence, maximizing the sum of all squared singular values maximizes the relevant dependencies between $Z$ and $X$. Naturally, there are various other reasonable formulations of probabilistic clustering that use singular values of the DTM. We present one such class of formulations in (14) in the next subsection.

A. Theoretical Discussion

Consider the following generalization of (13) that also intuitively captures some notion of probabilistic clustering:

$$
\max_{P_{Z|Y} \in \mathcal{P}_{Z|Y} : P_{Z|Y} P_Y = P_Z} \|B_{Z,X}\|_F^p
$$

(14)

where $P_Z \in \mathcal{P}_Z$ and $P_{Y,X} \in \mathcal{P}_{Y \times X}$ are fixed such that $P_X \in \mathcal{P}_X$ and $P_Y \in \mathcal{P}_Y$. Using Proposition 1, we may rewrite the objective function of (14) as $\|B_{Z,X}\|_F^p = \|P_Z\|^{-\frac{1}{2}} \|P_{Z|Y} P_Y\|_{F} \|B_{Y,X}\|_F^p$. Since the quantity inside the norm is linear in $P_{Z|Y}$, and the $p$th power of a Schatten $p$-norm is convex, the objective function is convex. Moreover, the constraints on $P_{Z|Y}$ in (14) define a compact and convex set in $\mathbb{R}^{\left|Z\right| \times \left|Y\right|}$. (As a result, the maximum in (14) can indeed be achieved due to the extreme value theorem.) Hence, (14) is a maximization of a convex function over a convex set. While convex functions can be easily minimized over convex sets, non-convex problems like (14) are often computationally hard (see e.g. [15]).
To illustrate this, consider the notable special case of (14) with \( p = 2 \) which yields the problem in (13):

\[
\max_{P_{Z|Y} \in \mathbb{R}^{[|Y|]}} \| B_{Z,Y} B_{Y,X} \|_F^2
\]

subject to (s.t.) \( P_{Z|Y} P_Y = P_Z, \ I_{|Z|}^T P_{Z|Y} = I_{|Y|}^T \),

\[
P_{Z|Y} \geq 0
\]

where \( I_k \equiv [1 \cdots 1]^T \in \mathbb{R}^k \), the second and third constraints ensure that \( P_{Z|Y} \in \mathcal{P}_{|Y|} \), and we use Proposition 1 to rewrite the objective function. Letting \( A = B_{Z,Y} \) and \( B = B_{Y,X} \), we can straightforwardly rewrite this problem as follows:

\[
\max_{A \in \mathbb{R}^{[|Y|]}} \| AB \|_F^2
\]

s.t. \( A \sqrt{P_Y} = \sqrt{P_Z}, A^T \sqrt{P_Z} = \sqrt{P_Y}, \)

\[
A \geq 0.
\]

This is clearly a non-convex quadratic program (QP). Indeed, letting \( a = \text{vec}(A) \in \mathbb{R}^{[|Y|]} \) (which stacks the columns of \( A \) to form a vector), \( M_1 = (B \otimes I_{|Z|})(B^T \otimes I_{|Z|}), M_2 = \sqrt{P_Y}^T \otimes I_{|Z|}, \) and \( M_3 = I_{|Y|} \otimes \sqrt{P_Z}^T \), the preceding problem is equivalent to:

\[
\max_{a \in \mathbb{R}^{[|Z||Y|]}} a^T M_1 a
\]

s.t. \( M_2 a = \sqrt{P_Z}, \ M_3 a = \sqrt{P_Y}, \ a \geq 0 \)

where \( \otimes \) denotes the Kronecker product, and we use the fact that \( \text{vec}(ABC) = (C^T \otimes A) \text{vec}(B) \) for any matrices \( A, B, \) and \( C \) with valid dimensions. The QP in (17) is non-convex because \( M_1 \) is positive semidefinite and we are maximizing the associated convex quadratic form. It is proved in [16] that such QPs are NP-hard (also see [17], [18] and the references therein). Therefore, there are no known efficient algorithms to exactly solve (13), and we will resort to relaxations and other heuristics in the ensuing sections.

Finally, we provide some brief intuition for the NP-hardness of (15). The feasible set of (15) is the convex polytope \( \mathcal{P}_{Z|Y} \cap \mathcal{H}, \) where \( \mathcal{H} \equiv \{ M \in \mathbb{R}^{[|Z||Y|]} : MP_Y = P_Z \} \) is a \( |Z| (|Y| - 1) \)-dimensional affine subspace of \( \mathbb{R}^{[|Z||Y|]} \). In general, this convex polytope has super-exponentially many extreme points. To see this, consider the special case where \( m = |Y| = |Z| \) and \( P_Y = P_Z \) are the uniform pmf. Then, \( \mathcal{P}_{Z|Y} \cap \mathcal{H} \) is the set of all doubly stochastic matrices, and its extreme points are the \( m! \) different \( m \times m \) permutation matrices by the Birkhoff-von Neumann theorem [19, Theorem 8.7.2]. For general \( |Y|, |Z|, P_Y, \) and \( P_Z \), the extreme points of \( \mathcal{P}_{Z|Y} \cap \mathcal{H} \) have more complex structure (see e.g. [20], which studies the uniform \( P_Y \) and arbitrary \( P_Z \) case). When we maximize a convex function over \( \mathcal{P}_{Z|Y} \cap \mathcal{H} \) as in (15), the optimum is achieved at an extreme point of \( \mathcal{P}_{Z|Y} \cap \mathcal{H} \). So, we have to search over all super-exponentially many extreme points to find this optimal point. This is computationally very inefficient.

**B. Comparison to Formulations that Directly Modify Co-occurrences**

A key feature of formulations in (13) is that it clusters using a transition kernel \( P_{Z|Y} \) and keeps the original data distribution \( P_{Y,X} \) intact. For comparison, let consider a different optimization problem that clusters by modifying the non-negative co-occurrence matrix \( P \in \mathbb{R}^{[|Y||X|]} \) directly:

\[
\min_{Q \in \mathbb{R}^{[|Y||X|]}, \|Q - P\|_F^2 - \lambda \sum_{i=1}^{|Z|} \sigma_i(B(Q))}
\]

where \( \lambda > 0 \) is a hyperparameter that should be set high enough to emphasize the second term in the objective function, \( B(Q) \) denotes the DTM corresponding to the joint pmf obtained after normalizing \( Q \), and \( |Z| \) represents the ideal number of clusters we want (note that the set \( Z \) is inconsequential in this formulation). Because (18) does not learn a transition kernel, in this subsection we do not normalize the data \( P \) to be a valid pmf in order to simplify the presentation.

Intuitively, (18) tries to find the closest non-negative matrix \( Q \) that has the top \( |Z| \) singular values as 1 (i.e. has \( |Z| \) connected components—see Proposition 3). This is closely related to the model in [21] and one drawback of this kind of formulation is that it has \( |Y||X| \) parameters to learn. Since the number of clusters is typically much smaller than the number of items, i.e. \( |Z| \ll |Y| \), our formulation in (14) has a much lower number \( |Z||Y| \) of parameters to learn.
A more important drawback of (18) is that sometimes, the intuitively correct clustering is not the globally optimal solution. We demonstrate this phenomenon via an example. Let \( \mathcal{X} = \mathcal{X}_1 \cup \mathcal{X}_2 \) for disjoint sets \( \mathcal{X}_1 \) and \( \mathcal{X}_2 \), \( \mathcal{Y} = \mathcal{Y}_1 \cup \mathcal{Y}_2 \) for disjoint sets \( \mathcal{Y}_1 \) and \( \mathcal{Y}_2 \), \( |\mathcal{X}_1| = |\mathcal{X}_2| = n \), \( |\mathcal{Y}_1| = |\mathcal{Y}_2| = m \), and the number of clusters \( |\mathcal{Z}| = 2 \). Furthermore, let the data matrix \( P \) have the following structure:

\[
P = \begin{bmatrix}
s \mathbf{1} & \mathbf{1} \\
\mathbf{1} & s \mathbf{1}
\end{bmatrix}
\]  

where \( \mathbf{1} \) is a matrix of all 1’s of appropriate dimension, and \( s > 1 \) is some scale factor. Clearly, there are two distinct communities, and the intuitive result with two clusters is:

\[
Q_1 = \begin{bmatrix}
s \mathbf{1} & \mathbf{0} \\
\mathbf{0} & s \mathbf{1}
\end{bmatrix}
\]  

where \( \mathbf{0} \) is a matrix of all 0’s of appropriate dimension. Since \( Q_1 \)’s structure creates two connected components, \( \mathcal{X}_1 \cup \mathcal{Y}_1 \) and \( \mathcal{X}_2 \cup \mathcal{Y}_2 \), the largest two singular values of \( B(Q_1) \) are both 1. Moreover, the objective function has value \( 2mn - 2\lambda \).
Now consider a different $Q$ that also creates two connected components by only disconnecting one item from $X$ and one item from $Y$ from the rest of the items:

$$Q_2 = \begin{bmatrix} s1 & 1 & 0 \\ 1 & s1 & 0 \\ 0 & 0 & s \end{bmatrix} \begin{cases} m \\ m-1 \\ 1 \end{cases}$$

(21)

where the disconnected item forms the bottom $1 \times 1$ block. The largest two singular values of $B(Q_2)$ are still 1 because of the two connected components. However, the objective function now equals $m+n+s^2(m+n-2)-2\lambda$. Thus, when $s < \sqrt{(2mn-m-n)/(m+n-2)}$, the intuitively correct answer $Q_1$ is not the global optimum of (18).

In contrast, our maximum Frobenius norm formulation in (13) (without the constraint on the marginal) easily obtains the two intuitive clusters encoded in $P$. For example, let $m = n = 50$, $Z = \{0, 1\}$ denote the cluster labels, and consider the transition kernels $P_{Z|Y}$ corresponding to the intuitive clustering shown in (20) (defined by $P_{Z|Y}^1(0|y) = 1$ for $y \in Y_1$ and $P_{Z|Y}^1(1|y) = 1$ for $y \in Y_2$), and $P_{Z|Y}^2$ corresponding to the clustering shown in (21) (defined by $P_{Z|Y}^2(0|y) = 1$ for $y \neq y_0$ and $P_{Z|Y}^2(1|y_0) = 1$ for some $y_0 \in Y_2$). Then, the plots in Figure 1 illustrate that the intuitive clustering of $P_{Z|Y}^1$ is greatly preferred by the maximum Frobenius norm formulation. Therefore, our formulation does not exhibit the drawbacks of formulations like (18).

IV. OPTIMIZATION ALGORITHMS

To solve the non-convex QP given by the Frobenius norm formulation of probabilistic clustering in (13), we will use a heuristic gradient ascent algorithm (subsection IV-A) as well as a nuclear norm relaxation (subsection IV-B). Although one approach to finding approximate solutions to an NP-hard problem like (13) is via semidefinite programming (SDP) relaxations, we do not explore SDP based algorithms in this paper. Moreover, many of the simpler SDP relaxations for non-convex QPs do not accurately capture our setting because they only appear to be tight when at least one of the constraints is also quadratic [22].

A. Heuristic Gradient Ascent Algorithm

We now present a gradient-based algorithm for approximating the maximal Frobenius norm coupling defined by the formulation of probabilistic clustering in (13), or equivalently, in (16). For computational efficiency, we move the first constraint in (16) to the objective function to obtain:

$$\max_{A \in \mathbb{R}^{(|X| \times |Y|)}} \|AB\|_F^2 - \lambda \|A\sqrt{P_Y} - \sqrt{P_Z}\|_2^2 \quad \text{s.t.} \quad A^T \sqrt{P_Z} = \sqrt{P_Y}, \quad A \geq 0$$

(22)

where $\lambda > 0$ is a hyperparameter that controls how strictly the $A\sqrt{P_Y} = \sqrt{P_Z}$ constraint is imposed. In other words, the solution no longer has to induce clusters with exactly $P_Z$ as their marginal pmf, but it incurs a penalty proportional to the squared $\ell^2$-norm of the difference $A\sqrt{P_Y} - \sqrt{P_Z}$. Note that any other differentiable distance between distributions can be substituted here.

The gradients of the components in the objective function of (22) are:

$$\frac{\partial}{\partial A} \|AB\|_F^2 = \frac{\partial}{\partial A} \text{tr}(ABB^T A^T) = 2ABB^T$$

$$\frac{\partial}{\partial A} \|Av - w\|_2^2 = 2(Av^T - wv^T)$$

(23)

(24)

where $v = \sqrt{P_Y}$, $w = \sqrt{P_Z}$, and we use denominator layout notation (or Hessian formulation).
Furthermore, since there is an equivalence between (15) and (16), the remaining constraints in (22) correspond exactly to the second and third constraints in (15) which are just enforcing $P_{Z|Y}$ to be a valid column stochastic matrix. Thus, we can either use any existing algorithms (e.g. [23], [24]) for projection back onto the simplex and apply them column-wise to $P_{Z|Y}$ or revise them to operate on $A$ directly. Algorithm 1 describes the entire optimization procedure for problem (22).

**Algorithm 1** Gradient Ascent Algorithm for Frobenius Norm Formulation

**Input:** Joint distribution $P_{Y,X}$, target marginal $P_Z$, marginal penalty multiplier $\lambda > 0$, step size $\alpha > 0$

**Output:** Soft clusters induced by $P_{Z|Y}$

1: Initialize $A_0 \in \mathbb{R}^{|Z| \times |Y|}$ to be an entry-wise positive matrix
2: $B \leftarrow [P_Y]^{-\frac{1}{2}} P_{Y,X} [P_X]^{-\frac{1}{2}}$
3: $M_1 \leftarrow BB^T$
4: $M_2 \leftarrow \lambda \sqrt{P_Y T Y}$
5: $M_3 \leftarrow \lambda \sqrt{P_Z T Z}$
6: while $A_t$ not converged do
7: $A_t \leftarrow A_{t-1} (I_{|Y|} + \alpha (M_1 - M_2)) + \alpha M_3$
8: if $A_t$ violates constraint above tolerance then
9: $A_t \leftarrow \text{proj}(A_t)$
10: end if
11: end while
12: return $P_{Z|Y} \leftarrow [P_Z]^{\frac{1}{2}} A_t [P_Y]^{-\frac{1}{2}}$

**B. Nuclear Norm Relaxation**

Let us consider a modified problem where we approximate the Frobenius norm in (13) using a nuclear norm. This yields the problem in (14) specialized to the $p = 1$ case. We further relax this problem by completely disregarding the constraint on the marginal to obtain:

$$\max_{P_{Z|Y} \in \mathcal{P}_{Z|Y}} \|B_{Z,X}\|_*$$

(25)

which defines a “maximal nuclear norm coupling” representing a desirable clustering assignment. To derive some intuition about this problem, we recall a well-known result from the literature. For any fixed channel $P_{Z|X} \in \mathcal{P}_{Z|X}$, the second largest singular value $\sigma_2(B_{Z,X})$ of $B_{Z,X}$ is the Hirschfeld-Gebelein-Rényi maximal correlation between $Z$ and $X$, which is given by:

$$\sigma_2(B_{Z,X}) = \max_{f: Z \rightarrow \mathbb{R}, g: X \rightarrow \mathbb{R}} \mathbb{E}[f(Z)g(X)]$$

(26)

$$= \max_{f \in \mathbb{R}^{|Z|}, g \in \mathbb{R}^{|X|}, f^T P_{Z,X} g = 0} f^T P_{Z,X} g$$

(27)

where the equality can be easily justified using the Courant-Fischer variational characterization of singular values (cf. [25], [7, Definition 3, Proposition 2], and the references therein). In particular, the optimal $f^*$ and $g^*$ can be obtained in terms of singular vectors of $B_{Z,X}$ corresponding to the singular value $\sigma_2(B_{Z,X})$, and they serve as useful features that capture the maximal correlation between $Z$ and $X$ [11], [14]. From this perspective, (25) maximizes the statistical dependence between $Z$ and $X$ as measured by the sum of maximal correlations (or singular values) subject to the Markov constraint $X \rightarrow Y \rightarrow Z$ for the purposes of probabilistic clustering.

To derive an algorithm for (25) that also uses SVD structure, we consider a generalization of (27). Using Ky Fan’s extremum principle, cf. [26, Theorem 3.4.1], we obtain the relation:

$$\|B_{Z,X}\|_* = \max_{F \in \mathbb{R}^{|Z| \times r}, G \in \mathbb{R}^{|X| \times r}, F^T P_{Z,X} G = I_r} \text{tr}(F^T P_{Z,X} G)$$

(28)

where $r = \min(|X|, |Z|)$. The proof of [26, Theorem 3.4.1] also shows that the optimal solutions of (28) are:

$$F^* = [P_Z]^{-\frac{1}{2}} U \quad \text{and} \quad G^* = [P_X]^{-\frac{1}{2}} V$$

(29)
where $U \in \mathbb{R}^{|Z| \times r}$ and $V \in \mathbb{R}^{|X| \times r}$ are matrices with orthonormal columns that correspond to the left and right singular vector bases of the DTM $B_{Z,X}$, respectively. Thus, since $P_{Z,X} = P_{Z|Y} P_{Y,X}$ by the Markov property, we can rewrite (25) as:

$$\max_{F \in \mathbb{R}^{|Z| \times r}, \ G \in \mathbb{R}^{|X| \times r}, \ F^T[P_Z] = G^T[P_X]} \text{tr}(F^T P_{Z|Y} P_{Y,X} G).$$

(30)

Inspired by [21], we also use alternating maximization to solve this problem. With $P_{Z|Y}$ fixed, the optimal $F$ and $G$ are given by (29). With $F$ and $G$ fixed, the objective function in (30) is linear in the entries of $P_{Z|Y}$ and can be solved using any linear programming (LP) packages. Algorithm 2 describes the entire optimization procedure.

Algorithm 2 Alternating Maximization Algorithm for Nuclear Norm Formulation

**Input:** Joint distribution $P_{Y,X}$

**Output:** Clusters induced by $P_{Z|Y}$

1: Initialize $P_{Z|Y}$ to be a $|Z| \times |Y|$ column stochastic matrix
2: $P_X \leftarrow 1_{|Y|}^T P_{Y,X}$
3: while $P_{Z|Y}$ not converged do
4: $P_{Z,X} \leftarrow P_{Z|Y} P_{Y,X}$
5: $P_Z \leftarrow P_{Z,X} 1_{|X|}$
6: $B \leftarrow [P_Z]^{-\frac{1}{2}} P_{Z,X} [P_X]^{-\frac{1}{2}}$
7: $U, \Sigma, V \leftarrow \text{SVD}(B)$
8: $F \leftarrow [P_Z]^{-\frac{1}{2}} U$
9: $G \leftarrow [P_X]^{-\frac{1}{2}} V$
10: $P_{Z|Y} \leftarrow \arg \max_{P_{Z|Y} \in \mathbb{P}_{Z|Y}} \text{tr}(F^T P_{Z|Y} P_{Y,X} G)$
11: end while
12: return $P_{Z|Y}$

We remark that this algorithm does not require any prior knowledge of $P_Z$. This is one potential advantage of the relaxed nuclear norm formulation in (25) over the original Frobenius norm formulation in (13). On the other hand, problem (30) has the uncommon feature that the constraint on $F$ depends on $P_{Z|Y}$ (or more precisely, on $P_Z$, which is derived from $P_{Z|Y}$). In typical instances of alternating maximization problems, the feasible sets of the variables (over which we alternate) are “independent” of each other (see e.g. [27]). One way to “decouple” the feasible set of $F$ from $P_{Z|Y}$ is to fix some $P_Z$ (when we have prior knowledge). This imposes an additional linear constraint on $P_{Z|Y}$ which is easily handled by an LP. In our experiments, we do not impose this additional constraint because Algorithm 2 converges to a reasonable solution without the constraint.

V. EXPERIMENTS

A. Word Embedding for MSR Sentence Completion Challenge

Though this paper is about clustering, we first want to validate that the DTM is an informative matrix for large scale unsupervised learning. To do this, we use it to learn word embeddings for the MSR Sentence Completion Challenge [29]. The dataset consists of a training corpus of raw text taken from classic English literature and 1040 Scholastic Aptitude Test (SAT) style sentence completion questions.
This is conceptually different from a co-occurrence matrix since a set of these cases, the extra documents from the smallest clusters are still present in the data, acting as noise. Overall accuracy counts all documents from those smallest clusters as incorrectly classified, and $k$-accuracy disregards those documents and only reports accuracy of documents from the top $k$ clusters. In both of these cases, the extra documents from the smallest clusters are still present in the data, acting as noise.

**TABLE II**

Examples from the top 100 most rated movies divided into the clusters found by Algorithm 2. Note that cluster 2 is empty because it only contains movies outside the top 100 most rated movies.

| Cluster 1            | Cluster 2     | Cluster 3          | Cluster 4     | Cluster 5     |
|----------------------|---------------|--------------------|---------------|---------------|
| RAIDERS OF THE LOST ARK | N/A           | THE TERMINATOR      | STAR WARS     | CONTACT       |
| THE GODFATHER        | N/A           | TERMINATOR 2       | RETURN OF THE JEDI | LIAR LIAR    |
| PULP FICTION         | N/A           | BRAVEHEART         | FARGO         | THE ENGLISH PATIENT |
| SILENCE OF THE LAMBS | N/A           | THE FUGITIVE       | TOY STORY     | SCREAM        |

**TABLE III**

Clustering accuracy on Reuters21578 for Algorithm 2. The nuclear norm increases more slowly when $k \geq 8$, which implies that $k = 8$ or 10 is the “right” number of clusters.

| $k$ | Coverage | Overall acc. | $k$-acc. | $\| \cdot \|_a$ |
|-----|----------|--------------|----------|----------------|
| 2   | 69.55%   | 65.15%       | 93.67%   | 1.71           |
| 3   | 73.42%   | 65.51%       | 89.22%   | 2.33           |
| 4   | 77.01%   | 62.25%       | 80.83%   | 2.85           |
| 6   | 82.35%   | 57.43%       | 69.74%   | 3.72           |
| 8   | 85.43%   | 54.11%       | 63.34%   | 4.49           |
| 10  | 87.85%   | 48.52%       | 55.23%   | 5.14           |

Let $P_{Y,X}$ be the normalized word-word co-occurrence matrix and let $U\Sigma V^T \approx [P_Y]^{-\frac{1}{2}}P_{Y,X}[P_X]^{-\frac{1}{2}}$ be the 640-dimensional truncated SVD of the DTM. We use the alternating conditional expectations (ACE) algorithm [14], [30] to approximate $[P_Y]^{-\frac{1}{2}}U$, and use that as the word embedding.

We use various functions of cosine similarity between the candidate word and the surrounding words to select the most probable answer. Table I shows that our method is competitive with popular single architecture word embedding techniques. This is not entirely surprising as there are other papers such as [31], [32], and [33] that advocate approximately factorizing various versions of the co-occurrence matrix. However, it provides empirical evidence that our method is valid and worth investigating more (on embedding as well as clustering).

**B. MovieLens 100K**

For qualitative validation, we use Algorithm 2 to find 5 clusters using the MovieLens 100K dataset. The data is in the form of a movie-user rating matrix, where each entry can be blank to denote unrated, or in the range $\{1, \ldots, 5\}$. This is conceptually different from a co-occurrence matrix since a 5-rated movie does not mean a user watched that movie 5 times more frequently compared to a 1-rated movie.

For preprocessing, we replace all blank entries with 0 to denote no co-occurrence. We assume each unit increment in rating corresponds to tripling of a user’s affinity toward a movie. Thus, we map each valid rating using the function $r \mapsto 3^{r-1} - 1$. Then, we row normalize such that each row (corresponding to one movie) sums to 1.

From Table II, we can see an approximate division of genres among clusters 1, 3, 4, and 5. Cluster 2 captures many of the less popular movies and does not contain any one from the set of 100 movies with the most ratings. Since MovieLens 100K does not contain ground truth cluster labels, we do not experiment further beyond this qualitative example.

**C. Reuters21578**

The Reuters21578 dataset contains 8293 documents and their frequencies on 18933 terms. Although the ground truth shows 65 topic clusters, the largest 10 clusters include 87.9% of all documents while the smallest 8 clusters each has 1 document. Thus, we argue that a good algorithm needs to provide a metric to infer a meaningful number of clusters.

For this experiment, we do not perform any data preprocessing and classify all documents into $k \in \{2, 3, 4, 6, 8, 10\}$ clusters. Because we do not have clusters devoted to the 65−$k$ smallest clusters, in Table III, we report the classification accuracy in two ways. Overall accuracy counts all documents from those smallest clusters as incorrectly classified, and $k$-accuracy disregards those documents and only reports accuracy of documents from the top $k$ clusters. In both of these cases, the extra documents from the smallest clusters are still present in the data, acting as noise.
Similar to spectral clustering [34], we can plot the norm given by Algorithm 2 against $k$ to identify the $k$ that strikes a balance between document coverage and classification accuracy. At the cost of disregarding the smallest clusters, we achieve improved overall accuracy compared to the best algorithm (43.94%) reported in [21, Table 2].

Alternatively, we have access to the ground truth cluster marginal pmf, we can use Algorithm 1. Table IV shows that this prior information offers significant improvements in accuracy as $k$ gets large.

### VI. Conclusion and Future Work

In this paper, we reviewed the mutual information formulation for probabilistic clustering (4). Then, to convert (4) into a matrix optimization (13), we locally approximated mutual information as the Frobenius norm of the DTM in Proposition 2. This allowed us to explicitly learn a maximal matrix norm coupling $P_{Z|Y}$ for clustering as opposed to the standard procedure (embedding and $k$-means). Learning $P_{Z|Y}$ also lets us encode prior information. We saw one example of this with the predefined $P_Z$ in (13). We can also add constraints that fix certain columns of $P_{Z|Y}$ if a subset of the data is labeled to perform semi-supervised learning.

There are two aspects of our approach that can be improved in future. Firstly, we can implement more efficient non-convex optimization algorithms that converge to solutions closer to the global optimum. Secondly, we can improve our model’s robustness to noise. Currently, we treat the observed noisy co-occurrence matrix as a good estimate of the true distribution while matrix factorization (MF) approaches treat the noise as entry-wise Gaussian perturbations of a low rank model [35]. In our experience, MF tends to perform well on data with high entry-wise noise while our approach performs well on data with complex community structures and lower noise.

Another future direction is to probabilistically cluster $X$ in addition to $Y$. The optimization problem for this is:

$$\max_{A \in \mathbb{R}^{|Z| \times |Y|}, C \in \mathbb{R}^{|W| \times |X|}} \|ABC^T\|_F^2$$

subject to

$$A\sqrt{P_Y} = \sqrt{P_Z}, A^T\sqrt{P_Z} = \sqrt{P_Y},$$

$$C\sqrt{P_X} = \sqrt{P_W}, C^T\sqrt{P_W} = \sqrt{P_X},$$

$$A \geq 0, C \geq 0.$$

where $C$ obtains the clusters of $X$, cf. (16). This parallels the notion of co-clustering in the literature [3], and is a topic worthy of further investigation.

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