Generalization of Probabilistic Latent Semantic Analysis to k-partite Graphs

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Abstract: Many data can be easily modelled as bipartite or k-partite graphs. Among the many computational analyses that can be run on such graphs, link prediction, i.e., the inference of novel links between nodes, is one of the most valuable and has many applications on real world data. While for bipartite graphs many methods exist for this task, only few algorithms are able to perform link prediction on k-partite graphs. The Probabilistic Latent Semantic Analysis (PLSA) is an algorithm based on latent variables, named topics, designed to perform matrix factorisation. As such, it is straightforward to apply PLSA to the task of link prediction on bipartite graphs, simply by decomposing the association matrix. In this work we extend PLSA to k-partite graphs; in particular we designed an algorithm able to perform link prediction on k-partite graphs, by exploiting the information in all the layers of the target graph. Our experiments confirm the capability of the proposed method to effectively perform link prediction on k-partite graphs.

1 INTRODUCTION

Graphs or networks are valuable ways to model and represent particular phenomena, in particular when relationships between the modeled entities exist. For example graphs can be used to represent molecule-to-molecule interactions in bioinformatics or friendships in a social network. Among the many analyses that can be executed on a graph, the prediction of new links (Kumar et al., 2020) (Pham and Dang, 2021) (Daud et al., 2020) is one of the most common. Link prediction involves identifying previously unknown connections between entities of the graph, which can be used as a tool for knowledge discovery (e.g., when applied to a protein-to-protein graph to identify putative new interactions) or with recommendation purposes (e.g., when applied to social network with the aim of suggesting new friendships to the users). Link prediction assumes particular properties when applied to bipartite or k-partite graphs. In general, a k-partite graph, with $k \geq 2$, is a graph whose nodes are divided into k partitions, and edges are allowed only between elements belonging to different partitions. One of the most classical example 2-partite graph is the consumer-product graph. For instance, a streaming platform users and movie as two separated partition and add a link whenever a user watch a movie. So here, the two partitions are the *users* and the *movies*. In many cases data are naturally modeled by k-partite graphs. Because of the importance of this task, many different methods have been developed to for link prediction in particular for bipartite graphs. The Probabilistic Latent Semantic Analysis (PLSA), initially developed for information retrieval within a corpus of documents, is among those methods.

Oftentimes, additional information is available for any of the two entities of bipartite graph. For instance, in the case of the streaming platform, the different genres and actors associated to each movie may be available. This additional information can naturally be incorporated into the graph by adding new independent sets of nodes. The original bipartite graph thus becomes a k-partite graph. The question which naturally arises is: how to use this additional information to improve the quality of the predicted links? While some methods easily adapt to such scenarios (e.g., the Non-Negative Matrix Tri-Factorization), the extension of PLSA to k-partite graphs is not trivial and requires additional generalization.

In this work, we propose an extension of PLSA able to deal with k-partite graph of, potentially, any dimension.

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We highlight the contribution of this manuscript as follows:

- We generalize the Probabilistic Latent Semantic Analysis (PLSA) method from bipartite to k-partite graphs. In particular, we provide a new probabilistic framework which takes into account the additional information in the additional layers of the graph;
- We derive the Expectation Maximization (EM) algorithm to train the generalized PLSA;
- We evaluated experimentally the algorithm on different datasets to test its performance and demonstrate its efficacy.

2 RELATED WORK

Given its relevance, the problem of link prediction in a bipartite graphs has been tackled with various machine learning methods (Benchettara et al., 2010). One common approach consists in using matrix factorization techniques on the association matrix of the graph (Menon and Elkan, 2011). The method which was generalized from bipartite to multipartite graphs was the NMTF algorithm. More recently, more sophisticated methods have been proposed, e.g., based on mutual information (Kumar and Sharma, 2020), community detection (Koptelov et al., 2020), domain knowledge (Zhang et al., 2019) or randomized edge swapping (Pinoli et al., 2021).

For what it regards the analysis and the link prediction for k-partite graphs, the extension of the Non-Negative Matrix Tri-Factorization (Žitnik and Zupan, 2014) to multipartite graph is one of the most common. It has been adopted mainly in bioinformatics for tasks such has drug repurposing (Ceddia et al., 2020), association between genes and diseases (Hwang et al., 2012) or patient stratification for personalized medicine (Gligorijević et al., 2016). Alternative methods are based on graph summarization (Thor et al., 2011) and network embeddings (Liu et al., 2021).

3 BACKGROUND

In this section we introduce the original version of PLSA and in particular how it can be used for the task of link prediction in bipartite graphs.

3.1 Probabilistic Latent Semantic Analysis

Probabilistic Latent Semantic Analysis was initially developed in the context of Information Retrieval for natural language processing of a corpus of documents (Hofmann, 1999). Suppose you are given a set of D documents $\mathcal{D}$ and that these documents are written in a vocabulary $\mathcal{W}$ of W words. Such a corpus can naturally be modeled by a bipartite graph, where each document and word are represented by a node, and the number of occurrences of the word $w \in \mathcal{W}$ in document $d \in \mathcal{D}$ is represented by a weighted edge $(d, w,$ number of occurences of w in d$)$. For example, in the bipartite graph in 1, we have $\mathcal{D} = \{d_1, d_2, d_3\}, \mathcal{W} = \{w_1, w_2, w_3, w_4, w_5, w_6, w_7\}, D = 3, W = 7$. In document d_3, w_6 occurs two times, w_3 only once, and w_2 does not occur. Commonly, a bipartite graph is represented by its corresponding *association matrix*, which has on one dimension that correspond to the *left* partition of nodes and the other to the *right* one; an element on the i-th rows and j-th column is equal to the weight of the link between the i-th element of the first partition and the j-th element of the second. If they are not connected, the weight will be 0. In the case of unweighted graphs, the weight associated to a link is 1. The example of 1 can be represented by the following 3×7 matrix:

$$\begin{bmatrix} 1 & 3 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 & 1 & 2 & 1 \end{bmatrix}$$

The goal of PLSA is to use such matrix to build a probability distribution over the set $\mathcal{D} \times \mathcal{W}$ of potential edges, while extracting meaningful information along the way and returning a probabilistic model for the generation of links in the graph. The probability distribution can then be used to predict novel links. We now start by reviewing the derivation of the probability distribution associated to PLSA in terms of bipartite graphs, as well as how to estimate it. We then derive the generalization to k-partite graphs.

3.2 PLSA for Bipartite Graphs

We here review the PLSA method with a particular focus on its application to the task of link prediction in bipartite matrices. We start by providing the necessary notation and then we describe the method.

3.2.1 Notation

Let us introduce some notations related to k-partite graph. Clearly, such notation encompass also the case

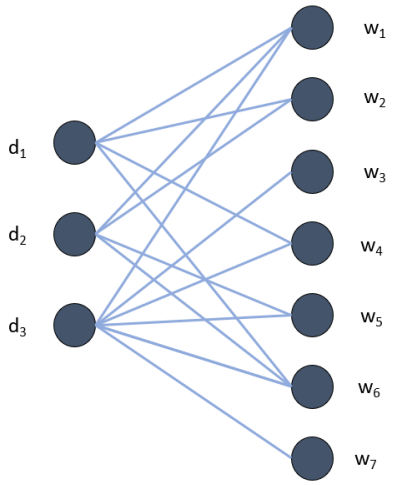


Figure 1: Graph representation of the data.

of bipartite graphs. Let $G = (V,E)$ be a K-partite graph, where V is the set of nodes and E is the set of edges, or links. The partitioning $(V_k)_{k\in[1,...,K]}$ denote the sets of nodes associated to the graph and is such that $V_1 \cup V_2 \cup \cdots \cup V_K = V$ and $\forall i,j \in [1,...,K], i \neq j \implies V_i \cap V_j = \emptyset$. The matrix $R_{1,2}$ is the bipartite association matrix between V_1 and V_2. We can model a k-partite graph as a combination of bipartite graphs, and let $\mathcal{A}$ denote the subset of $[1,...,K]^2$ for which the corresponding association matrices are non-zeros.

3.2.2 Method for Training PLSA for Bipartite Graphs

Let $G = (V_1,V_2,R_{1,2})$ be a bipartite graph. The goal of PLSA is to build a probabilistic framework which estimates from the set of observed edges $E_{1,2}$ a probability distribution on $V_1 \times V_2$. That is, we want to construct a matrix $A \in \mathbb{R}^{|V_1|\times|V_2|}$ such that

$$A(v_1,v_2) = \mathbb{P}(v_1,v_2)$$

$E_{1,2}$, the set of edges present in the original graph, and is treated as a vector of observations. The matrix A is the parameter which must be estimated. The likelihood of the problem is:

$$\begin{aligned}\mathcal{L}(E_{1,2},A) &= \mathbb{P}(E_{1,2}|A)\\ &= \prod_{v_1,v_2\in E_{1,2}} \mathbb{P}(v_1,v_2)\\ &= \prod_{v_1,v_2\in V_1\times V_2} \mathbb{P}(v_1,v_2)^{R_{1,2}(v_1,v_2)}\end{aligned}$$

In the original proposal, the matrix A is computed by maximizing the log-likelihood :

$$l(E_{1,2},A) = \sum_{(v_1,v_2)\in V_1\times V_2} R_{1,2}(v_1,v_2) log(\mathbb{P}(v_1,v_2))$$

The goal in computing A is to extract out of the raw graph G information, so some kind of structure is introduced. This is done through the introduction of the notion of a set of topics $T = \{t_1,t_2,...,t_L\}$, i.e., hidden variables. More specifically, PLSA assumes that edges are generated according to Bayesian network in Figure 2. The network above describes a ran-

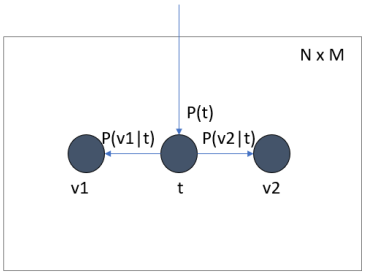


Figure 2: Bayesian network describing PLSA.

dom experiment for generating an edge. First, pick a topic t randomly, according to the probability distribution $(\mathbb{P}(t))_{t\in T}$. Then, choose a node v_1 from the set V_1 and a node v_2 from the set V_2 independently. The choices are made according to the probability distributions $(\mathbb{P}(v_1|t)_{v_1\in V_1}$ and $(\mathbb{P}(v_2|t)_{v_2\in V_2}$ respectively. This generates the edge (v_1,v_2). Repeat this random experiment $N \times M$ times, to generate $N \times M$ edges. More formally, the given two nodes $v_1 \in V_1$ and $v_2 \in V_2$, the probability of a link between the two $\mathbb{P}(v_1,v_2)$, is decomposed as:

$$\mathbb{P}(v_1,v_2) = \sum_{t\in T} \mathbb{P}(t)\mathbb{P}(v_1,v_2|t)$$

Furthermore, PLSA assumes the following independence relation to be true:

$$\mathbb{P}(v_1,v_2|t) = \mathbb{P}(v_1|t)\mathbb{P}(v_2|t)$$

In this scenario, the parameters that must be estimated are: $\mathbb{P}(t),\mathbb{P}(v_1|t),\mathbb{P}(v_2|t)$ for all $t \in T, v_1,v_2 \in V_1 \times V_2$. The way this is done is through the Expectation Maximization algorithm (EM). More specifically, the parameters $\mathbb{P}(t|v_1,v_2)$ are computed during the E step, and these parameters are used in the M step to update $\mathbb{P}(t),\mathbb{P}(v_1|t),P(v_2|t)$. One can show (Hofmann and Puzicha, 1998; Hong, 2012) that the following E-Step and M-Step are:

E-Step:

$$\mathbb{P}(t|v_1,v_2) = \frac{\mathbb{P}(t)\mathbb{P}(v_1|t)\mathbb{P}(v_2|t)}{\sum_{s\in T}\mathbb{P}(s)\mathbb{P}(v_1|s)\mathbb{P}(v_2|s)}$$

M-Step:

$$\mathbb{P}(t) = \frac{\sum_{v_1,v_2 \in V_1 \times V_2} R_{1,2}(v_1,v_2)\mathbb{P}(t|v_1,v_2)}{\sum_{v_1,v_2 \in V_1 \times V_2} R_{1,2}(v_1,v_2)}$$

$$\mathbb{P}(v_1|t) = \frac{\sum_{v_2 \in V_2} R_{1,2}(v_1,v_2)\mathbb{P}(t|v_1,v_2)}{\sum_{v,v_2 \in V_1 \times V_2} R_{1,2}(v,v_2)\mathbb{P}(t|v,v_2)}$$

$$\mathbb{P}(v_2|t) = \frac{\sum_{v_1 \in V_1} R_{1,2}(v_1,v_2)\mathbb{P}(t|v_1,v_2)}{\sum_{v_1,v \in V_1 \times V_2} R_{1,2}(v_1,v)\mathbb{P}(t|v_1,v)}$$

Now that the basic model for bipartite graphs has been introduced, we are ready to extend it to k-partite graph.

4 GENERALIZATION OF PLSA TO K-PARTITE GRAPHS

The original PLSA algorithm allows one to build a probabilistic model able to generate edges in a bipartite graph. First, a topic is chosen randomly, then an edge is generated according to that topic. In order to generalize this to a multi-partite graph, the key idea is to add another layer of randomness. Thus, this generative model starts by picking randomly an association matrix. Then, choose a topic, and finally choose two vertices according to that topic. This random framework can be summarized in the Bayesian network in Figure 3.

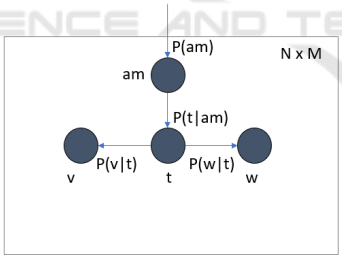


Figure 3: Multi-partite PLSA : The Bayesian network.

We now provide a formal description of the method. Let $(i,j) \in \mathcal{A}$, $(v,w) \in V_i \times V_j$ represents a potential edge between V_i and V_j. The goal is to decompose the probability $\mathbb{P}(v,w)$. We can first write :

$$\mathbb{P}(v,w) = \mathbb{P}((i,j))\mathbb{P}(v,w|(i,j))$$

We then decompose $P(v,w|(i,j))$ using the topics :

$$\mathbb{P}(v,w|(i,j)) = \sum_{t \in T} \mathbb{P}(v,w|t,(i,j))\mathbb{P}(t|(i,j))$$

A first independence hypothesis is introduced, as in bipartite PLSA :

$$\mathbb{P}(v,w|t,(i,j)) = \mathbb{P}(v|t,(i,j))\mathbb{P}(w|t,(i,j))$$

Finally, we introduce a new type of independence relation :

$$\mathbb{P}(v|t,(i,j)) = \mathbb{P}(v|t)$$
$$\mathbb{P}(w|t,(i,j)) = \mathbb{P}(w|t)$$

What this independence relation implies is that, for a given topic t and vertex v, the probability of choosing vertex v given t does not depend on the association matrix chosen in the first place. Indeed, since we consider a multipartite graph, v can be associated to multiple association matrices. The probability of edge (v,w) being generated can be expressed as:

$$\mathbb{P}(v,w) = \mathbb{P}((i,j)) \sum_{t \in T} \mathbb{P}(t|(i,j))\mathbb{P}(v|t)\mathbb{P}(w|t) \quad (1)$$

In this case,the parameters which must be estimated are:

- $\forall (i,j) \in \mathcal{A}, \mathbb{P}((i,j))$, the probability of picking association matrix (i,j);
- $\forall (i,j) \in \mathcal{A}, \forall t \in T, \mathbb{P}(t|(i,j))$ the probability of picking topic t given association matrix (i,j).;
- $\forall k \in [1,...,K], v \in V_k, t \in T, \mathbb{P}(v|t)$ the probability of picking vertex v given topic t.

Note that the number of topics is the same for all the association matrices. Only the probability distribution of choosing a given topic changes from one association matrix to another. Thus, the meaning of the topics changes for each association matrix. The estimation of these parameters can be achieved using maximum likelihood, which is equal to :

$$L = \sum_{(i,j) \in \mathcal{A}} \sum_{(v,w) \in V_i \times V_j} R_{i,j}(v,w) log(\mathbb{P}(v,w)) \quad (2)$$

where $\mathbb{P}(v,w)$ is described in (1). Thus L depends on the parameters $\mathbb{P}(v|t), \mathbb{P}(t), \mathbb{P}((i,j)), \forall k \in [1,...,K], v \in V_k, t \in T, (i,j) \in \mathcal{A}$. The optimization problem to be solved is :

$$\max_{\mathbb{P}(v|t),\mathbb{P}(t),\mathbb{P}((i,j))} L$$

4.1 Decomposing the Optimization Problem

Let us introduce notations so as to be able to write succinct equations: Let $l_{i,j}$ be the log-likelihood of the bipartite graph associated to $V_i \times V_j$:

$$l_{i,j} = \sum_{(v,w) \in V_i \times V_j} R_{i,j}(v,w) log(\sum_{t \in T} \mathbb{P}(t|(i,j))\mathbb{P}(v|t)\mathbb{P}(w|t)))$$

Let then introduce two functions, l and f, defined in the following way :

$$l(\mathbb{P}(t),\mathbb{P}(v|t)) = \sum_{(i,j) \in \mathcal{A}} l_{i,j}$$

$$f(\mathbb{P}((i,j))) = \sum_{(i,j)\in\mathcal{A}} \sum_{(v,w)\in V_i\times V_j} R_{i,j}(v,w) log(\mathbb{P}((i,j)))$$

Recalling the expression of L in (2), and replacing $\mathbb{P}(v,w)$ by its description in (1), and splitting the logarithm in two parts, we can then write the total likelihood according to the following rule:

$$L = f(\mathbb{P}((i,j)) + l(\mathbb{P}(t|(i,j)), \mathbb{P}(v|t))$$

The initial maximum log likelihood problem can thus be split into two:

$$\max_{\mathbb{P}(t),\mathbb{P}(v|t)} l(\mathbb{P}(t), \mathbb{P}(v|t))$$

and

$$\max_{\mathbb{P}((i,j))} f(\mathbb{P}((i,j))$$

While the second problem can be solved analytically, the first one requires the use of the EM algorithm.

4.2 Solving the First Optimization Problem: Introduction of Latent Random Variables

Because of the sum inside the logarithm, the optimization problem described above cannot be solved analytically. The EM framework is used to solve this optimization problem. The latent random variables introduced are z(t, v, w), for all $t \in T, v \in V_i, w \in V_j, (i,j) \in \mathcal{A}$. More specifically, z(t, v, w) equals 1 if and only if topic t is chosen for the edge (v, w). The complete log-likelihood (the likelihood associated to the latent variables) is then:

$$l(x,\theta,z) = \sum_{\substack{(i,j)\in\mathcal{A}\\ v\in V_i\\ w\in V_j\\ t\in T}} R_{i,j}(v,w) z(t,v,w) log(\mathbb{P}(v|t)\mathbb{P}(w|t)\mathbb{P}(t|(i,j)))$$

Where the notations introduced are :

- x : The association matrices $R_{i,j}$;
- z: the indicator variables z(t, v, w), which equals 1 if topic t has been chosen for edge (v, w); 0 otherwise, for each $k \in [1,...,K], (v,t) \in V_k \times T$;
- θ: The probability matrices $\mathbb{P}(v|t), \mathbb{P}(t|(i,j))$, for each $k \in [1,...,K], (v,t) \in V_k \times T$, $(i,j) \in \mathcal{A}$.

4.3 Extension of EM Algorithm to Multipartite Graphs

Now that we have introduced a generalization of PLSA to k-partite graphs, we should derive the E-Step and M-Step of the EM algorithm to train the model. To understand the logic and the notations of this section, please refer to the Appendix at the end of this paper.

4.3.1 E-Step

The Q function can be computed from the complete log likelihood:

$$Q(\theta) = \mathbb{E}(l(x,\theta,z)|x,\theta^{(p)})$$

Leveraging the linearity of expectation, and the fact that $\mathbb{E}(z(t,v,w)|x,\theta^{(p)}) = \mathbb{P}(t|v,w)$, where $\mathbb{P}(t|v,w) = \mathbb{P}(z(t,v,w) = 1|v,w)$ is the probability that topic t has been chosen given the edge (v, w), we then get:

$$Q(\theta) = \sum_{\substack{(i,j)\in\mathcal{A}\\ v\in V_i\\ w\in V_j\\ t\in T}} R_{i,j}(v,w)\mathbb{P}(t|v,w) log(\mathbb{P}(v|t)\mathbb{P}(w|t)\mathbb{P}(t|(i,j)))$$

Let $(i,j) \in \mathcal{A}, (v,w) \in V_i \times V_j$. To compute $Q(\theta)$, one only has to compute $\mathbb{P}(t|v,w)$. This can be achieved through Bayes-Theorem:

$$\begin{aligned}\mathbb{P}(t|v,w) &= \mathbb{P}(t|v,w,(i,j)) \\ &= \frac{\mathbb{P}(t|(i,j))\mathbb{P}(v|t,(i,j))\mathbb{P}(w|t,(i,j))}{\sum_{s\in T}\mathbb{P}(s|(i,j))\mathbb{P}(v|s,(i,j))\mathbb{P}(w|s,(i,j))} \\ &= \frac{\mathbb{P}(t|(i,j))\mathbb{P}(v|t)\mathbb{P}(w|t)}{\sum_{s\in T}\mathbb{P}(s|(i,j))\mathbb{P}(v|s)\mathbb{P}(w|s)}\end{aligned}$$

where we used the two independence relations assumed by the model.

4.3.2 M-Step

Now, the goal is to find θ which maximize Q. This can be done by solving the following optimization problem:

$$\begin{aligned}\max_{\theta} Q(\theta) \\ \text{subject to } \forall (i,j) \in \mathcal{A}, \sum_{t\in T} \mathbb{P}(t|(i,j)) = 1 \\ \forall k \in [1,...,K], \forall t \in T, \sum_{v\in V_k} \mathbb{P}(v|t) = 1 \\ \forall (i,j) \in \mathcal{A}, \forall t \in T, \mathbb{P}(t|(i,j)) \geq 0 \\ \forall t \in T, \forall k \in [1,...,K], \forall v \in V_k, \mathbb{P}(v|t) \geq 0\end{aligned}$$

Since Q is a concave function, and the constraints are linear, this is a convex optimization problem. Furthermore, the constraints are feasible; according to Slater's condition, strong duality holds(Boyd and Vandenberghe, 2004). We can therefore solve this

problem using the Lagrangian:

$$\mathcal{L}(\theta,\lambda,\mu) = Q(\theta) + \sum_{(i,j)\in\mathcal{A}} \lambda_{i,j}(1 - \sum_{t\in T} \mathbb{P}(t|(i,j))) + \sum_{t\in T}\sum_{k\in[1,K]} \lambda_{k,t}(1 - \sum_{v\in V_k} \mathbb{P}(v|t)) - \sum_{t\in T}\sum_{k\in[1,K]}\sum_{v\in V_k} \mu_{v,t}\mathbb{P}(v|t) - \sum_{(i,j)\in\mathcal{A}}\sum_{t\in T} \mu_{t,i,j}\mathbb{P}(t|(i,j))$$

where $\lambda_{i,j}, \lambda_{k,t}, \mu_{v,t}, \mu_{t,i,j}$ are the Lagrange multipliers of the problem, with $\mu_{v,t} \geq 0, \mu_{t,i,j} \geq 0$ since they are associated to inequality constraints. Since all the functions are differentiable, we can write the KKT conditions, which allow us to derive the point (θ,λ,μ) for which the problem is optimal. The KKT conditions, in the general case, correspond to the following system:

$$\begin{cases} \frac{\partial \mathcal{L}}{\partial \theta_i} = 0 \\ \frac{\partial \mathcal{L}}{\partial \lambda_j} = 0 \\ \mu_k \frac{\partial \mathcal{L}}{\partial \mu_k} = 0, \mu_k \geq 0 \end{cases} \quad (KKT)$$

where $\theta_i, \lambda_j, \mu_k$ designates the different components of the vectors θ, λ and μ. We call a KKT point any point (θ,λ,μ) which satisfies (KKT). In particular, we assume in the following derivation of a KKT point that $\mu_{v,t} = 0$ and $\mu_{t,i,j} = 0$, (i.e. we set $\mu = 0$). The third line of the (KKT) system is then automatically satisfied. Hence if we can find θ and λ with $\mu = 0$ such that (θ,λ,μ) is a KKT point, since the problem is convex and strong duality holds, we know that θ is the optimal point of the problem.

$$\frac{\partial \mathcal{L}}{\partial \mathbb{P}(t|(i,j))} = \frac{\sum_{\substack{v\in V_i \\ w\in V_j}} R_{i,j}(v,w)\mathbb{P}(t|v,w)}{\mathbb{P}(t|(i,j))} - \lambda_{i,j} = 0$$

Isolating $\mathbb{P}(t|(i,j))$, we get:

$$\mathbb{P}(t|(i,j)) = \frac{1}{\lambda_{i,j}} \sum_{v\in V_i}\sum_{w\in V_j} R_{i,j}(v,w)\mathbb{P}(t|v,w)$$

In order to satisfy the constraint $\sum_{t\in T} \mathbb{P}(t|(i,j)) = 1$, one finds that $\lambda_{i,j}$ must satisfy:

$$\lambda_{i,j} = \sum_{t\in T}\sum_{v\in V_i}\sum_{w\in V_j} R_{i,j}(v,w)\mathbb{P}(t|v,w)$$

The KKT conditions also tell us that: For a given $k \in [1,...,K], v \in V_k$:

$$\frac{\partial \mathcal{L}}{\partial \mathbb{P}(v|t)} = \sum_{i|(i,k)\in\mathcal{A}}\sum_{y\in V_i} R_{i,k}(y,v)\mathbb{P}(t|y,v)\frac{1}{\mathbb{P}(v|t)} + \sum_{j|(k,j)\in\mathcal{A}}\sum_{w\in V_j} R_{k,j}(v,w)\mathbb{P}(t|v,w)\frac{1}{\mathbb{P}(v|t)} - \lambda_{k,t} = 0$$

where the notations $i|(i,k) \in \mathcal{A}$ means that the sum is performed over all the association matrices which have k as their right independent set (meaning V_k maps onto the columns of $R_{i,k}$). Similarly, $j|(k,j) \in \mathcal{A}$ means summing over all association matrices which have k as their left independent set (meaning the elements of V_k map onto the rows of $R_{k,j}$). Isolating $\mathbb{P}(v|t)$, one gets:

$$\mathbb{P}(v|t) = \frac{1}{\lambda_{k,t}}\Big(\sum_{i|(i,k)\in\mathcal{A}}\sum_{y\in V_i} R_{i,k}(y,v)\mathbb{P}(t|y,v) + \sum_{j|(k,j)\in\mathcal{A}}\sum_{w\in V_j} R_{k,j}(v,w)\mathbb{P}(t|v,w)\Big)$$

In order to satisfy the constraint $\sum_{v\in V_k} \mathbb{P}(v|t) = 1$, one finds that $\lambda_{k,t}$ must satisfy:

$$\lambda_{k,t} = \sum_{i|(i,k)\in\mathcal{A}}\sum_{y\in V_i}\sum_{v\in V_k} R_{i,k}(y,v)\mathbb{P}(t|y,v) + \sum_{j|(k,j)\in\mathcal{A}}\sum_{v\in V_k}\sum_{w\in V_j} R_{k,j}(v,w)\mathbb{P}(t|v,w)$$

4.3.3 Summary

To sum up, the EM-algorithm is composed of two steps:

The E-Step:

$$\mathbb{P}(t|v,w) = \frac{\mathbb{P}(t|(i,j))\mathbb{P}(v|t)\mathbb{P}(w|t)}{\sum_{s\in T}\mathbb{P}(s|(i,j))\mathbb{P}(v|s)\mathbb{P}(w|s)}$$

And, **the M-Step:**

$$\mathbb{P}(t|(i,j)) = \frac{\sum_{\substack{v\in V_i \\ w\in V_j}} R_{i,j}(v,w)\mathbb{P}(t|v,w)}{\sum_{\substack{s\in T \\ v\in V_i \\ w\in V_j}} R_{i,j}(v,w)\mathbb{P}(s|v,w)}$$

$$\mathbb{P}(v|t) = \frac{1}{\lambda_{k,t}}\Big(\sum_{i|(i,k)\in\mathcal{A}}\sum_{y\in V_i} R_{i,k}(y,v)\mathbb{P}(t|y,v) + \sum_{j|(k,j)\in\mathcal{A}}\sum_{w\in V_j} R_{k,j}(v,w)\mathbb{P}(t|v,w)\Big)$$

with $\lambda_{k,t}$ satisfying :

$$\lambda_{k,t} = \sum_{i|(i,k)\in\mathcal{A}}\sum_{y\in V_i}\sum_{v\in V_k} R_{i,k}(y,v)\mathbb{P}(t|y,v) + \sum_{j|(k,j)\in\mathcal{A}}\sum_{v\in V_k}\sum_{w\in V_j} R_{k,j}(v,w)\mathbb{P}(t|v,w)$$

4.4 Solving the Second Optimization Problem

The second problem allows us to determine the probabilities $\mathbb{P}((i,j))$ of choosing a given association ma-

trix. The optimization problem to be solved is :

$$\max_{\mathbb{P}((i,j))} f(\mathbb{P}((i,j)))$$
$$\text{subject to} \sum_{(i,j)\in\mathcal{A}} \mathbb{P}((i,j)) = 1$$
$$\forall (i,j) \in \mathcal{A}, \mathbb{P}((i,j)) \geq 0$$

Using techniques similar to the ones used in the derivation of the M-step, one can show that for a given $(i,j) \in \mathcal{A}$:

$$\mathbb{P}((i,j)) = \frac{\sum_{(v,w)\in V_i\times V_j} R_{i,j}}{\sum_{(i,j)\in\mathcal{A}} \sum_{(v,w)\in V_i\times V_j} R_{i,j}}$$

$$\mathbb{P}((i,j)) = \frac{\text{Number of edges in bipartite graph associated to } R_{i,j}}{\text{Number of edges in the complete graph}}$$

4.5 Initialization Strategies

The EM algorithm only returns a local maximum, thus the starting point of the algorithm have a critical importance for the final result. In particular, the parameters which must be initialized are:

- The probability distributions over the topics : $(\mathbb{P}(t|(i,j)))_{t\in T}$ for each association matrix (i,j);
- The probability distributions over the vertices $(\mathbb{P}(v|t))_{v\in V_k}$ for each set of vertices V_k and each $t \in T$.

In the remainder of this subsection we delineate three different initialization strategies for the probability distributions over the vertices.

Random Initialization: initialize every element with positive random numbers, and normalize properly to get valid probability distributions.

Latent Semantic Analysis Initialization: Latent Semantic Analysis (LSA) is the method from which PLSA is based on. It can therefore put more information in the parameters than the random initialisation does. It has already been used in (Farahat and Chen, 2015) to initialize PLSA. Here we propose a new way to initialize PLSA using LSA. Let $G = (V_1, V_2, R_{1,2})$ be a bipartite graph. LSA performs singular value decomposition on the association matrix, and keeps only the first K singular values as non zeros, where K is a fixed number:

$$\hat{R}_{1,2} = U_1 \Sigma U_2^T$$

and uses the different components to represent the data. (Hofmann, 1999) showed that the results of PLSA can be expressed in a form analogous to LSA. Let A $=(\mathbb{P}(v,w))_{v\in V_1, w\in V_2}$ be the probability matrix associated to the problem of PLSA. By setting $\hat{U}_1 = (\mathbb{P}(v|t)_{v\in V_1, t\in T}$, $\hat{U}_2 = (\mathbb{P}(w|t)_{w\in V_2, t\in T}$, and $\hat{\Sigma} = diag((\mathbb{P}(t))_{t\in T})$, one can write:

$$\hat{A} = \hat{U}_1 \hat{\Sigma} \hat{U}_2^T$$

Thus, the initialization method we implemented is the following: Let $(i,j) \in \mathcal{A}$. We start by decomposing $R_{i,j}$ using LSA, and we keep only the first —T— principal components:

$$R_{i,j} = U \Sigma V^T$$

We then translate the coefficients of U so that they are all positive, we do the same with V, and we finally normalize the columns of U and V so that they each represent a probability distribution. We then set the matrix$(\mathbb{P}(v|t))_{v\in V_i, t\in T}$ to be equal to the modified U, and $(\mathbb{P}(w|t))_{w\in V_j, t\in T}$ to be equal to the modified V. Since the graph is multipartite, there can be more than one association matrix associated to a given independent set, so the final initialization taken is the mean of the initalizations provided by each association matrix.

K-means Initialization: Another way to initialize the vertices is to perform K-means clustering on the rows/columns of the association matrix, as it was done for instance in (Dissez et al., 2019). Again, for a given set V_k, an initialization is produced for each association matrix to which V_k is related. In order to incorporate all the information provided by these association matrices, we sum all the initializations performed, before normalizing to get a probability distribution.

4.6 Stopping Criterion

One issue which must be tackled is when should the EM-algorithm be stopped. In other words, to determine how many iterations should be run. We propose two ways of doing this.

Set Number of Iterations: The first way is to set a fixed number of iterations in advance, and to run the algorithm for this amount of iterations. The number to be put can be chosen during the training phase.

Relative Change of Likelihood: The problem with the stopping criterion defined above is that it doesn't give much meaning to the number of iterations chosen. Since we know the log likelihood function to be concave, we know that that the rate of change of the log likelihood is decreasing. One way to stop the algorithm is thus to look at the relative rate of change of the likelihood function. Let l_n be the value of the loglikelihood function at iteration n. And let ε be a small number determined empirically. The stopping criterion would then be:

$$\frac{l_n - l_{n-1}}{l_{n-1}} \leq \varepsilon$$

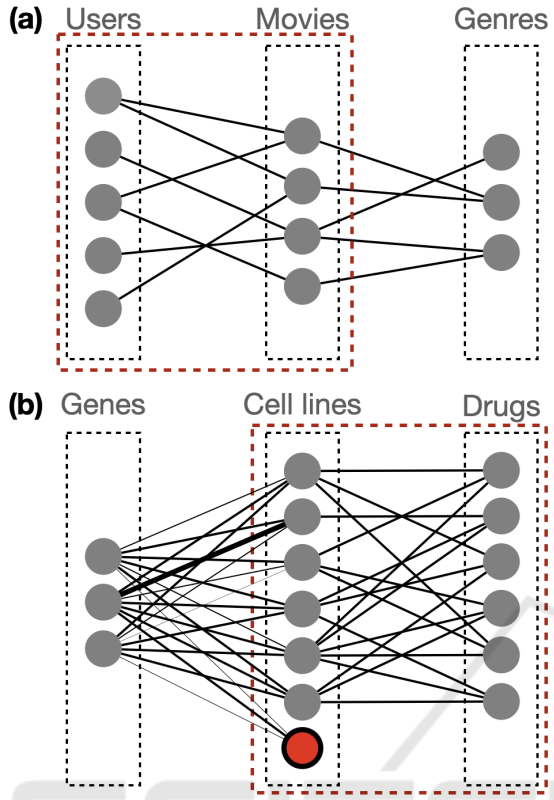


Figure 4: Sketch of the k-partite graphs. **(a)** represents the USER-MOVIE-GENRE; both matrices are non-fully connected and the connections are not weighted. **(b)** represents the GENE-CELL-DRUG; in this case the association matrix between genes and cell lines is dense and weighted. The *cell line* in red, represents the new cell line for which only connections with genes are known. In both sub-figures the graph in the red box is the one on which we want to predict unknown links.

4.7 Choosing the Number of Topics

There is no systematic method to specify the number of topics, and this must be done empirically during the training phase. A method which can be used is to compute the AUROC curve for different numbers of topics, and choose the number of topics which gives the best performance.

5 APPLICATIONS

Here, we evaluate the proposed method on two scenarios. In the first case we have a graph USER-MOVIE-GENRE and we show how the additional information MOVIE-GENRE is beneficial in link prediction between USERS and MOVIES.

In the second case we apply our method to a dataset GENE-CELL-DRUG. Here we simulate a different scenario: we suppose a new element is added to the CELL partition. Moreover, such element does not have any connection with any element in DRUG partition, but only connection with elements in GENE. We prove that the links in the GENE-CELL layer of the graph is enough to effectively predict links in the CELL-DRUG dataset for the newly inserted elements.

5.1 Application to a Movie Dataset

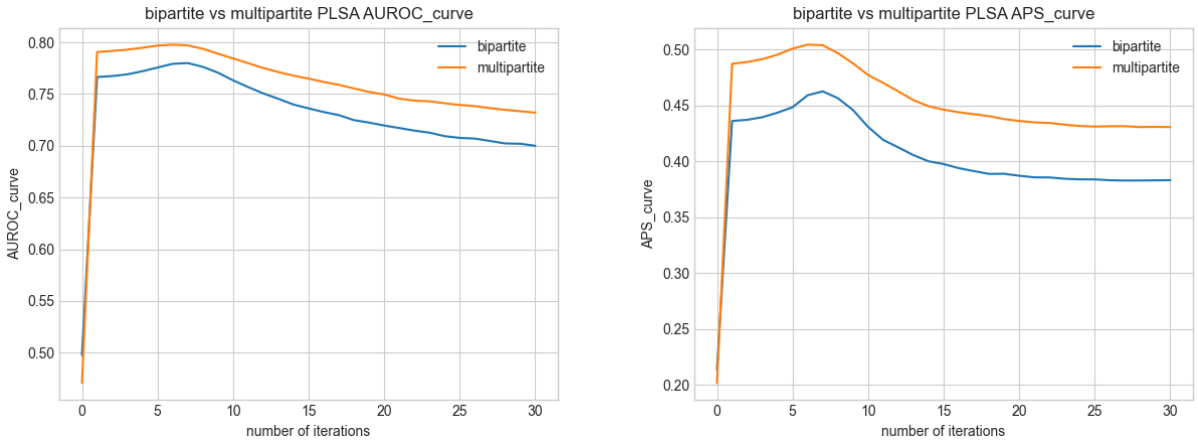
This dataset mimics a classic user-product dataset where the link prediction is performed for recommendation purposes and the additional information are available regarding each of the products.

Dataset: the dataset is sketched in panel(a) of Figure 4. In a crowd sourced research we collected a dataset of **130** users, each of who indicates among a set of **66** movies which ones they have watched at. Each movie is also linked to one or more genre, in a set of **19** possible genres. In the dataset we have a total of **1568** connections between users and movies and **230** connections between movies and genre.

Evaluation: first of all, for the target association matrix R_{UM} between users and movies, we create an associated mask matrix M of the same dimension. A random 5% of the element of M are 0, while the others are ones. Then we compute an association matrix R'_{UM}, equal to the component-wise multiplication of R_{UM} and M. Thus, for any zero-entry of M, the corresponding entry in R'_{UM} will be set to 0. This correspond to the deletion of some edges in the network. Successively, we run PLSA using R'_{UM} and in order to predict novel edges. The predictions made by the system are the probability of edges being generated. On the portion corresponding to the mask coefficients equal to 0 we compute two measures, namely the Average Precision Score (APS) and the Area Under the Receiver Operating Characteristic curve (AUROC). We run this test several times, varying the matrix M. For each run the performance is recorded. The final performance is the mean performance averaged over all the runs.

Number of Topics: To determine the number of topics to use, one should be

In order to evaluate the benefits that can derive from the inclusion of the second graph layer between *movies* and *genres*, we run the algorithm twice: once with the bipartite graph and once with the 3-partite graphs, and we compared the performances. Results are reported in Figure 5. The results demonstrate that our method is effectively able to exploit and propagate the information of the auxiliary graph and, thus,



(a) Area under the ROC curve.

(b) Average Precision score.

Figure 5: Results of the first use case. The plots shows that the addition of the second matrix is able to improve the results of both AUROC and APS of approximately the 10%.

is a valuable method for link prediction in k-partite graphs.

5.2 Application to a Drug Dataset

Here we test our method on a biological dataset about the response of tumoral cell lines (biological model employed in *in vitro* experiments) to anti tumor drugs. **Dataset:** Given a cell line, it can be either *sensitive* or *resistant* to a certain drug. Furthermore, each cell line is also associated with a panel of genes, and for each cell line and each gene the link connecting the two has a weight that represent the expression (level of activity) of the gene in the cell line. The topology of the graph is depicted in Figure 4, panel (b). We have a set of **576** genes, a set of **379** cell lines and a set of **202** drugs. The graph connecting genes to cell lines is dense and weighted, while the other is sparse and unweighted.

Evaluation: on this dataset we performed two types of evaluation. First of all we compared the AUROC accordingly to the type of initialization. We did this test by using a 5% mask on the cell line to drugs matrix, as in the previous experiment. Results are reported on Figure 6. We can observe that the *random* initialization is the worse, while the *k-means* based one performs the best and allows to obtain an AUROC greater than 75% after only 10 iterations.

In second type of experiment, we supposed to add a cell line to the dataset. For the given cell line the gene expression (and thus the *left graph*) is known, while the association to the drugs are not (refer to Figure 4. We simulate this scenario with a leave-one-out validation, where at each iteration we removed all the edges between the selected cell line and the drugs. We measure the calculated the ROC curve for the experiment and we got a AUROC of 0.622. Results are reported in Figure 7. Although a AUROC of 0.622 may not impress, it has to be noted that all the predictive power come from the supplementary graph layer (i.e., the cell to gene association); indeed, as there is no previous information about the relationship between the cell line and any of the drugs, only using the such matrix let to a 0.5 of AUROC, which means that it is not possible to predict anything.

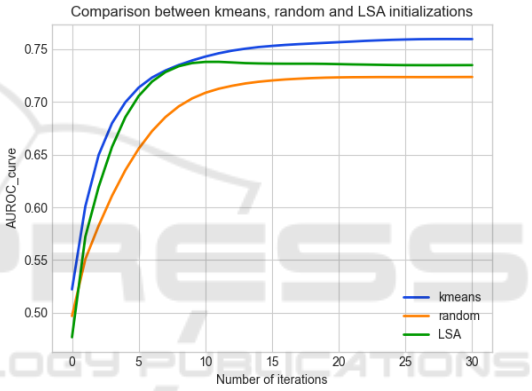


Figure 6: Comparison of the AUROC with different initialization strategies on the k-partite graph.

6 CONCLUSION AND FUTURE WORK

The PLSA is a method designed to work on corpus of documents to extract from them relevant topics. Yet, it can easily extended to work with bipartite graph for the task of link prediction. However, extending PLSA to work with k-partite graph is not trivial and requires

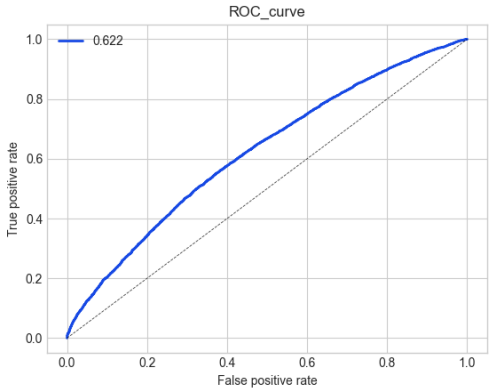


Figure 7: ROC curve of the leave-one-out experiment.

to modify the methods itself. In this work we derived a version of PLSA which is able to work with k-partite graphs as well with bipartite graphs, thus extending the potential of the method. Indeed, k-partite graphs have shown to be valuable model for many different types of data, in particular in bioinformatics, healthcare and recommender systems. In particular, we firstly derived a new bayesian model that extends the classical PLSA to k-partite graphs; then we derived the Expectation-Maximization (EM) algorithm to train the model from the data. Our proposed algorithm is capable to deal with k-partite graphs of any size, without limitation.

Through evaluation on two datasets, we show how the extended PLSA is able to exploit information from auxiliary graph's layer to enhance the link prediction in the main bipartite graph.

Future work comprise better evaluation of the method and in particular of its variants (e.g., different initializations, stop critera) and study on how to identify the best number of topics to guarantee optimal performance. Furthermore we will apply the method to real-world scenarios, such as the problem of drug repurposing.

Finally, we plan to further investigate the probabilistic properties of such method to propose an extension that is able to provide an explanation for each predicted link, thus contributing in the direction of explainable artificial intelligence.

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A THE EM ALGORITHM

In this section, we present the general framework of the EM algorithm (Haugh, 2015), (Dempster et al., 2015). We are given a vector of observation x, as well as a parameter θ which we want to estimate through the maximization of the likelihood function. The initial problem is therefore :

$$\max_{\theta} l(x,\theta)$$

where l is the log likelihood of the problem. The EM algorithm is used when solving this optimization problem is difficult. The way it is built is by introducing a vector z of latent random variables. These random variables provide additional information about the data. The problem is that they are not observed. What the EM-Algorithm does is it computes simultaneously the correct value of θ and of z. Given an estimate of the parameter $\theta^{(p)}$, the way $\theta^{(p+1)}$ is computed is through two steps : The E-Step and the M-Step. the algorithm is given as an entry a first guess of θ. It runs the E-Step, then the M-Step, and does so for a fixed number of iterations.

A.1 The E-Step

The E-Step corresponds to the estimation of the different latent random variables (or rather their probability distribution). The end result of this step is the computation of a function $Q(\theta)$, whose probabilistic expression is:

$$Q(\theta) = \mathbb{E}(l(\theta,x,z)|x,\theta^{(p)})$$

Where $l(\theta,x,z)$ is the log-likelihood of both the set of observed and latent variables. Note that the expression of $l(\theta,x,z)$ is different of $l(x,\theta)$, and this is why the EM algorithm works. Being able to compute Q is usually equivalent to the computation of the following probabilities :

$$\mathbb{P}(z|x,\theta^{(p)})$$

A.2 The M-Step

The M-Step corresponds to the next estimation of the parameter θ. The M-Step computes $\theta^{(p+1)}$ by solving the following optimization problem:

$$\max_{\theta} Q(\theta)$$

This optimization problem is often much simpler than the original problem, and it is often the case that analytical expressions of $\theta^{(p+1)}$ can be found (as in PLSA).

A.3 Link with PLSA

To make matters clearer, we map the variables involved in PLSA with the general framework of the EM-algorithm:

- x : The association matrices $R_{i,j}$
- z: the indicator variables z(t, v, w), which equal 1 if topic t has been chosen for edge (v, w); 0 otherwise, for each $k \in [1,...,K], (v,t) \in V_k \times T$
- θ: The probability matrices $\mathbb{P}(v|t), \mathbb{P}(t|(i,j))$, for each $k \in [1,...,K], (v,t) \in V_k \times T$, $(i,j) \in \mathcal{A}$.