BiNE

理论

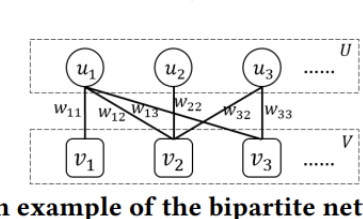

Figure 2: An example of the bipartite network structure

表示法

- **二分网络定义：** 用 $G=(U,V,E)$ 表示二分网络，其中：
  - U 和 V 分别代表两种类型的顶点集合。
  - $E \subseteq U \times V$ 定义了这两组顶点之间的边。
- **顶点表示：**
  - u_i 表示集合 U 中的第 i 个顶点。
  - v_j 表示集合 V 中的第 j 个顶点。
  - 其中 $i=1,2,\ldots,|U|$；$j=1,2,\ldots,|V|$。
- **边的权重：**
  - 每条边 (u_i,v_j) 带有一个非负权重 w_{ij}，描述连接的顶点 u_i 和 v_j 之间的关系强度。
  - 如果 u_i 和 v_j 之间没有连接，则边的权重 w_{ij} 被设置为零。
- **矩阵表示：**
  - 使用一个 $|U| \times |V|$ 的矩阵来表示这种关系，其中矩阵的元素对应于顶点间的边的权重。

1. 模型改进

1-1 两个目标函数关系

1. 显示关系：显示关系捕捉的是上图中的U和V两个集合中的，简单理解就是捕捉二部图的两种不同类型节点之间的关系
2.隐式关系：隐式关系是捕捉上图中U和U集合中的节点关系，以及V和V集合中的关系，这种关系是捕捉同类型的节点之间的关系

1-2 随机游走策略

1. 自适应生成随机游走序列，自适应生成是依据与其节点的重要性来设定的，也就是重要的节点应当进行更多次随机游走
2.随机游走的长度的不同，对比起原始的设定好的随机游走的长度，这部分是通过概率的方式来确定是否停止随机游走，通过这样的方式更加合理

2. 具体阐述模型改进点

2-1 模型显示关系

2-1-1连接概率计算

Now we consider how to estimate the local proximity between two vertices in the embedding space. The effectiveness and prevalence of word2vec inspire many works [4, 8, 20] to use inner product to model the interaction between two entities. We follow this setting, and use sigmoid function to transform the interaction value to the probability space:

$$\hat{P}(i,j) = \frac{1}{1+\exp(-\vec{\mathbf{u}}_i^T \vec{\mathbf{v}}_j)}, \qquad (2)$$

通过两个嵌入后的两个向量之间的转置相乘并且通过sigmod函数来得到两个节点之间连接的概率

2-1-2 KL-Divergence

where $\vec{\mathbf{u}}_i \in \mathbb{R}^d$ and $\vec{\mathbf{v}}_j \in \mathbb{R}^d$ are the embedding vectors of vertices u_i and v_j, respectively.

With the empirical distribution of the co-occurring probability between vertices and the reconstructed distribution, we can learn the embedding vectors by minimizing their difference. We choose the KL-divergence as the difference measure between distributions, which can be defined as:

$$minimize \quad O_1 = KL(P\|\hat{P}) = \sum_{e_{ij}\in E} P(i,j)\log\left(\frac{P(i,j)}{\hat{P}(i,j)}\right) \propto -\sum_{e_{ij}\in E} w_{ij}\log \hat{P}(i,j). \qquad (3)$$

Intuitively, minimizing this objective function will make two vertices that are strongly connected in the original network also close with each other in the embedding space, which preserves the local proximity as desired.

通过最小化顶点共现概率的实证分布和重构分布之间的差异来学习嵌入向量

2-2 模型隐式关系

2-2-1 隐式关系的构建

4.2.1 Constructing Corpus of Vertex Sequences. It is a common way to convert a network into a corpus of vertex sequences by performing random walks on the network, which has been used in some homogeneous network embedding methods [4, 8]. However, directly performing random walks on a bipartite network could fail, since there is no stationary distribution of random walks on bipartite networks due to the periodicity issue [34]. To address this issue, we consider performing random walks on two homogeneous networks that contain the 2nd-order proximity between vertices of the same type. Following the idea of Co-HITS [1], we define the 2nd-order proximity between two vertices as:

$$w_{ij}^U = \sum_{k\in V} w_{ik} w_{jk}; \quad w_{ij}^V = \sum_{k\in U} w_{ki} w_{kj}. \qquad (4)$$

这里使用的方法不是直接在二部图上进行随机游走而去获取训练语料库而是通过转化为两张同构图去进行随机游走的，这种方式主要是捕捉二阶相似性。

2-2-2 两张同构图的表示法

where w_{ij} is the weight of edge e_{ij}. Hence, we can use the $|U| \times |U|$ matrix $\mathbf{W}^U = [w_{ij}^U]$ and the $|V| \times |V|$ matrix $\mathbf{W}^V = [w_{ij}^V]$ to represent the two induced homogeneous networks, respectively.

2-2-3 进行有策略的随机游走

real-world network. To generate a corpus with a high fidelity, we propose a biased and self-adaptive random walk generator, which can preserve the vertex distribution in a bipartite network. We highlight its core designs as follows:

- First, we relate the number of random walks starting from each vertex to be dependent on its importance, which can be measured by its centrality. For a vertex, the greater its centrality is, the more likely a random walk will start from it. As a result, the vertex importance can be preserved to some extent.
- We assign a probability to stop a random walk in each step. In contrast to DeepWalk and other work [14] that apply a fixed length on the random walk, we allow the generated vertex sequences have a variable length, in order to have a close analogy to the variable-length sentences in natural languages.

1. 随机游走次数设定：每个节点发生多少次随机游走是由它的重要性所决定的，该重要性也就是它的中心性。
2.随机游走长度设定：这个随机游走的长度是可变的是通过一个概率值设定随机游走停止是否停止。

2-2-4通过skip-gram来学习顶点嵌入方式

4.2.2 Implicit Relation Modeling. After performing biased random walks on the two homogeneous networks respectively, we obtain two corpora of vertex sequences. Next we employ the Skip-gram model [11] on the two corpora to learn vertex embeddings. The aim is to capture the high-order proximity, which assumes that vertices frequently co-occurred in the same context of a sequence should be assigned to similar embeddings. Given a vertex sequence

使用Skip-gram模型对这两个顶点序列的语料库进行处理，目的是学习顶点嵌入。这个过程的目标是捕捉高阶邻近性，假设在同一个序列上下文中频繁共现的顶点应该被赋予相似的嵌入。

2-2-5 保持高阶邻近性

$\vec{\theta}_c$ (or $\vec{\vartheta}_c$) to denote its role as a context. As there are two types of vertices in a bipartite network, we preserve the high-order proximities separately. Specifically, for the corpus D^U, the conditional probability to maximize is:

$$maximize \quad O_2 = \prod_{u_i\in S \wedge S\in D^U} \prod_{u_c\in C_S(u_i)} P(u_c|u_i). \qquad (5)$$

where $C_S(u_i)$ denotes the context vertices of vertex u_i in sequence S. Similarly, we can get the objective function for corpus D^V:

$$maximize \quad O_3 = \prod_{v_j\in S \wedge S\in D^V} \prod_{v_c\in C_S(v_j)} P(v_c|v_j). \qquad (6)$$

在二部网络中，由于存在两种类型的顶点U和V，分别为这两种顶点保持高阶邻近性，因此需要最大化语料库Du的条件概率P（uc|ui）同理对于Dv也要这样进行

2-2-6 条件概率参数化

Following existing neural embedding methods [4, 8, 20], we parameterize the conditional probability $P(u_c|u_i)$ and $P(v_c|v_j)$ using the inner product kernel with softmax for output:

$$P(u_c|u_i) = \frac{\exp(\vec{\mathbf{u}}_i^T \vec{\theta}_c)}{\sum_{k=1}^{|U|}\exp(\vec{\mathbf{u}}_i^T \vec{\theta}_k)}, \quad P(v_c|v_j) = \frac{\exp(\vec{\mathbf{v}}_j^T \vec{\vartheta}_c)}{\sum_{k=1}^{|V|}\exp(\vec{\mathbf{v}}_j^T \vec{\vartheta}_k)}, \qquad (7)$$

where $P(u_c|u_i)$ denotes how likely u_c is observed in the contexts of u_i; similar meaning applies to $P(v_c|v_j)$. With this definition, achieving the goal defined in Equations (5) and (6) will force the vertices with the similar contexts to be close in the embedding space. Nevertheless, optimizing the objectives is non-trivial, since each evaluation of the softmax function needs to traverse all vertices of a side, which is very time-costing. To reduce the learning complexity, we employ the idea of negative sampling [11].

通过内积核与softmax输出来参数化，这里条件概率是在ui上下文观察到uc的可能性，这种区其最大从而保持同类型系统但之间的高阶邻近性

2-2-7 负采样LSH

2-2-7-1 该部分使用负采样的意义

4.2.3 Negative Sampling. The idea of negative sampling is to approximate the costly denominator term of softmax with some sampled negative instances [36]. Then the learning can be performed by optimizing a point-wise classification loss. For a center

负采样的目的是通过采样一些负实例来近似softmax的代价高昂的分母项。通过这种方式，学习过程可以转化为优化点分类损失

2-2-7-2 如何选择高质量的负样本

formed by optimizing a point-wise classification loss. For a center vertex u_i, high-quality negatives should be the vertices that are dissimilar from u_i. Towards this goal, some heuristics have been applied, such as sampling from popularity-biased non-uniform distribution [11]. Here we propose a more grounded sampling method that caters the network data.

对于中心顶点ui，高质量的负样本应该是与ui不相似的顶点。为了达到这个目标，采用了一些启发式方法，比如从受欢迎程度偏差的非均匀分布中采样。

2-2-7-3 采样的负采样方式（LSH）

First we employ locality sensitive hashing (LSH) [37] to block vertices after shingling each vertex by its ws-hop neighbors with respect to the topological structure in the input bipartite network. Given a center vertex, we then randomly choose the negative samples from the buckets that are different from the bucket contained the center vertex. Through this way, we can obtain high-quality and diverse negative samples, since LSH can guarantee that dissimilar vertices are located in different buckets in a probabilistic way [37].

使用局部敏感哈希（LSH）技术来分块顶点，每个顶点根据其在输入二部网络中的ws-跳邻居进行分块。然后，从包含中心顶点的块中随机选择负样本。因为LSH能够以概率方式保证不相似的顶点位于不同的块中。

2-2-7-4 替换条件概率即对2-2-6去进行替换

Let $N_S^{ns}(u_i)$ denote the ns negative samples for a center vertex u_i in sequence $S \in D^U$, we can then approximate the conditional probability $p(u_c|u_i)$ defined in Equation (7) as:

$$p(u_c, N_S^{ns}(u_i)|u_i) = \prod_{z\in\{u_c\}\cup N_S^{ns}(u_i)} P(z|u_i), \qquad (8)$$

2-2-8 根据正采样和负采样的方式去替换2-2-5

where the probability $P(z|u_j)$ is defined as:

$$P(z|u_i) = \begin{cases} \sigma(\vec{\mathbf{u}}_i^T \vec{\theta}_z), & \text{if } z \text{ is a context of } u_i \\ 1-\sigma(\vec{\mathbf{u}}_i^T \vec{\theta}_z), & z \in N_S^{ns}(u_i) \end{cases},$$

where σ denotes the sigmoid function $1/(1+e^{-x})$. By replacing $p(u_c|u_i)$ in Equation (5) with the definition of $p(u_c, N_S^{ns}(u_i)|u_i)$, we can get the approximated objective function to optimize. The

最大化上下文顶点之间的接近度，同时最小化负样本之间的接近度

3 联合优化

To embed a bipartite network by preserving both explicit and implicit relations simultaneously, we combine their objective functions to form a joint optimization framework.

$$maximize \quad L = \alpha\log O_2 + \beta\log O_3 - \gamma O_1. \qquad (9)$$

where parameters α, β and γ are hyper-parameters to be specified to combine different components in the joint optimization framework.

O2和O3是对于隐式关系的代表，而O1是代表的显示关系。通过设定超参数来对其进行权重调节该部分用的是SGA是随机梯度上升，因为我们需要优化的是目标函数因此选择SGA而不是SGD

代码实现

1. 形参设定

这里直接指定了使用的训练数据是用wiki的数据集，已经处理好的

2. 实验参数设定

3. 数据加载

4. 图加载类

初始化

4-1 construct_training_graph建立训练用图

5 随机游走生成器

之后调用的函数都是在GraphUtils这个类中的，因为是在生成的图上进行随机游走

5-1 计算节点中心性

5-2 开始随机游走

首先先会建立同构图（5-2-1），随后根据同构图进行随机游走（5-2-2）从而为后续隐形关系的捕捉提供基础。
这部分的同构图的构成是通过A.dot(AT)。v的同构图是通过AT.dot(A)形成的

5-2-1 保存同构图

5-2-2 开始随机游走

5-2-2-1 加载图中连接的节点信息

5-2-2-2 获取随机游走的语料

6 基于随机游走采样的语料进行上下文节点（正样本）负采样获取

6-1 进行负采样

6-2 得到上下文节点和负采样节点

7. 对节点embedding进行初始化

8. 正式开始训练

8-1 skip_gram(更新两种隐式关系)

用于更新词嵌入和上下文向量，同时计算损失。它使用负采样方法优化损失函数，通过调整嵌入向量和上下文向量来最大化中心词和上下文词的联合概率，同时最小化中心词和负样本词的联合概率。这种方法在自然语言处理和词嵌入领域非常有效。

8-2 KL_divergence （在两种隐式关系更新后更新两种节点间的显式关系）

这个函数用于在推荐系统或类似的应用中更新用户和项目的嵌入向量。它根据两个节点间的相互作用（通过边权重 e_ij 表示）以及它们当前的嵌入状态，使用 KL 散度作为损失函数来优化嵌入向量。