

RESUMEN

Aquí va el resumen...

ABSTRACT

A

quí inicia el abstract...

AGRADECIMIENTOS

Aquí van los agradecimientos...

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INTRODUCTION

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1.1 Presentation

1.2 Objectives

1.2.1 General objective

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chapter Theory and conceptual framework

1.8 Preliminaries

Description of concepts

Definition 1.8.1. *orthogonal complement*

Theorem 1.8.1. *For every $n \times n$ symmetric real matrix, the eigenvalues are real and the eigenvectors can be chosen real and orthonormal.*

Theorem 1.8.2 (Courant-Fisher Formula). *Let A be an $n \times n$ real symmetric matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ and corresponding eigenvectors v_1, v_2, \dots, v_n . Then*

$$\begin{aligned}\lambda_1 &= \min_{\|x\|=1} x^T A x = \min_{x \neq 0} \frac{x^T A x}{x^T x}, \\ \lambda_2 &= \min_{\substack{\|x\|=1 \\ x \perp v_1}} x^T A x = \min_{x \neq 0} \frac{x^T A x}{x^T x}, \\ \lambda_n &= \lambda_{\max} = \max_{\substack{\|x\|=1 \\ x \perp v_1}} x^T A x = \max_{x \neq 0} \frac{x^T A x}{x^T x}.\end{aligned}$$

In general, for $1 \leq k \leq n$, let S_k denote the span of v_1, v_2, \dots, v_k (with $S_0 = \{0\}$). Then

$$\lambda_k = \min_{\substack{\|x\|=1 \\ x \in S_{k-1}^\perp}} x^T A x = \min_{x \neq 0} \frac{x^T A x}{x^T x}.$$

1.9 Graphs and Laplacian Matrices

For the rest of the chapter, let $G = (V, E)$ be a graph, where $V = \{v_1, v_2, \dots, v_n\}$ is the non-empty set of nodes (or vertices) and E is the set of edges, composed by pairs of the form (v_i, v_j) , where $v_i, v_j \in V$.

It is assumed that all graphs are undirected, meaning that if $(v_i, v_j) \in E$, then $(v_j, v_i) \in E$, for every $v_i, v_j \in V$. For that reason, the edge (v_i, v_j) will be represented as the unordered set $\{v_i, v_j\}$.

A convenient way to represent a graph is through an *adjacency matrix* $A \in \mathbb{R}^{|V| \times |V|}$. Giving a specific order to the graph nodes, one can represent the edges as binary entries in this matrix:

$$A[v_i, v_j] = \begin{cases} 1 & \text{if } \{v_i, v_j\} \in E \\ 0 & \text{otherwise} \end{cases}$$

Let $\mathcal{N}(v_i)$ denote the neighborhood of node v_i , i.e., the set of the adjacent nodes to it. The quantity that represents the number of nodes in $\mathcal{N}(v_i)$ is called the *degree of the vertex* v_i . This is one of the most obvious and informative feature for the structure of the graph and is denoted by

$$d_i = \sum_{j=1}^n A[v_j, v_i].$$

Finally, we can summarize that graph's information in the *degree matrix* D which is defined as the diagonal matrix with the degrees d_1, d_2, \dots, d_n on the diagonal.

1.9.1 The Unnormalized Laplacian

The unnormalized graph *Laplacian matrix* L is defined as

$$L = D - A$$

Proposition 1.9.1 (Some properties of L). *The matrix L , as defined above, satisfies the following properties:*

1. *For every vector $x = (x_1, x_2, \dots, x_n) \in \mathbb{R}$ we have*

$$x^T L x = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n (x_i - x_j)^2$$

2. *L is symmetric and positive semi-definite*
3. *L has n non-negative, real-valued, eigenvalues $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$*
4. *The smallest eigenvalue of L is 0, the corresponding eigenvector is the constant one vector $\mathbb{1}$.*

1.9.2 Normalized Laplacians

The *symmetric normalized Laplacian matrix* L_{sym} is defined as

$$L_{sym} = D^{-\frac{1}{2}} L D^{-\frac{1}{2}}$$

while the *random walk Laplacian* is defined as

$$L_{rw} = D^{-1} L$$

1.9.3 The graph partitioning problem

In order to introduce the graph partitioning problem in its different settings, the mathematical definition of the concepts involved are presented below.

Definition 1.9.1. *Given a graph $G = (V, E)$ and an integer K , a partition of G is a collection of K subsets $P_1, P_2, \dots, P_K \subset V$ such that:*

1. $P_i \cap P_j = \emptyset$ for $i \neq j$, where $i, j \in \{1, 2, \dots, K\}$
2. $\cup_{k=1}^K P_k = V$

A partition of a graph can be seen as simply removing edges from the original graph in such way the obtained partitions are subgraphs. There are many ways a graph can be partitioned into subgraphs and the way it gets done depends completely on the application of interest. However, independently of the problem to solve, the objective relies on minimizing the connections between the partitions in the original graph. The following concepts provides a useful notation to turn the problem into an optimization one.

For a collection $S \subset V$ of vertices, we define the *edge boundary* $\partial(S)$ to consist of all edges in E with exactly one endpoint in S , that is,

$$\partial(S) := \{\{u, v\} \in E \mid u \notin S \text{ and } v \in S\}$$

Now the problem turns into finding a partition P_1, P_2, \dots, P_K such that minimizes the *cut value* of the partition, usually called just *cut*, which is defined as

$$\text{CUT}(P_1, P_2, \dots, P_K) := \frac{1}{2} \sum_{k=1}^K |\partial(P_k)| \quad (1.1)$$

The notion of cut allows to measure the quality of any partition, nevertheless solving the min cut problem ...

For a collection of vertices $S \subset V$, consider the following quantities related to the edges of

$$\text{VOL}(S) := \sum_{v_i \in S} d_i$$

we want to agroupe by similarity so its natural to Cut value of that partition
solve the mincut problem

The next consider two different ways of measuring the size of the partitions

$$\begin{aligned} \text{RATIOCUT}(P_1, P_2, \dots, P_K) &:= \frac{1}{2} \sum_{k=1}^K \frac{|\partial(P_k)|}{|P_k|} \\ &= \sum_{k=1}^K \frac{\text{CUT}(P_k, \overline{P_k})}{|P_k|} \end{aligned}$$

$$\begin{aligned} \text{NORMCUT}(P_1, P_2, \dots, P_K) &:= \frac{1}{2} \sum_{k=1}^K \frac{|\partial(P_k)|}{\text{VOL}(P_k)} \\ &= \sum_{k=1}^K \frac{\text{CUT}(P_k, \overline{P_k})}{\text{VOL}(P_k)} \end{aligned}$$

1.9.4 Spectral partitioning and Normalized Cut

Here will be presented the derivation of the normalized cut as relaxation of the problem to solve the spectral partitioning problem

1.10 Literature review

Mention all the approaches that use Graph Neural Networks and its importance in solving graph related tasks achieving superior performance on many graph-related tasks

1.10.1 Graph Convolutional Neural Networks and GraphSAGE

Talk a little bit about traditional node embeddings approaches and its delimitations. Embeddings: dense vector representations Talk about the message passing framework Start with Graph Convolutional Neural Networks (GCN) and its limitations. Emphasize in how GraphSAGE solve those limitations and how it extends the GCN capabilities

1.10.2 Generalizable Approximate Graph Partitioning (GAP)

Framework

From all the Deep Learning approaches that solve the Graph Partitioning problem, one of the most notorious not only for its simplicity but for its exceptional results, is the *Generalizable Approximate Graph Partitioning* framework better known as GAP [3].

GAP is a Graph Neural Network approach that proposes a continuous relaxation of the problem using a differentiable loss function that is based on the normalized cut. According

to Nazi et al. [4], it is an unsupervised learning algorithm that is capable of generalization, meaning that it can be trained in small graphs, which allows it to generalize into unseen much larger ones. This section describes the model described in the original paper which consists of two modules: the Graph Embedding Module and the Graph Partitioning Module.

In the following subsections, it is assumed that the framework takes a graph $G = (V, E)$ as input, where $V = \{v_1, v_2, \dots, v_n\}$, and outputs the probabilities tensor $Y \in \mathbb{R}^{n \times K}$, where Y_{ik} represents the probability that node v_i belongs to partition P_k . Before going into the model description, the deduction of the loss function is as follows.

1.10.2.1 Expected Normalized Cut Loss Function

Recall the normalized cut given by

$$\text{NORMCUT}(P_1, P_2, \dots, P_K) = \sum_{k=1}^K \frac{\text{CUT}(P_k, \overline{P_k})}{\text{VOL}(P_k)} \quad (1.2)$$

In order to calculate the normalized cut expected value, one needs to compute the expected value of $\text{CUT}(P_k, \overline{P_k})$ and $\text{VOL}(P_k)$ from Equation 1.2. For the deduction of those quantities, an approach similar to the one presented in [1] will be followed.

Since Y_{ik} represents the probability that node $v_i \in P_k$, $1 - Y_{ik}$ is the probability that $v_i \notin P_k$, hence

$$\mathbb{E}[\text{CUT}(P_k, \overline{P_k})] = \sum_{i=1}^{|V|} \sum_{v_j \in \mathcal{N}(v_i)} Y_{ik}(1 - Y_{jk}) \quad (1.3)$$

Due to the fact that for a given node the adjacent nodes can be retrieved from the adjacency matrix A , Equation 1.3 can be rewritten as follows:

$$\mathbb{E}[\text{CUT}(P_k, \overline{P_k})] = \sum_{i=1}^{|V|} \sum_{j=1}^{|V|} Y_{ik}(1 - Y_{kj}^T) A_{ij} \quad (1.4)$$

Keeping in mind that $\text{VOL}(P_k)$ is the sum of the degrees of the nodes in P_k , Δ is defined to be the column tensor where Δ_i is the degree of the node $v_i \in V$. Then, given Y , one can calculate the expected value of $\text{VOL}(P_k)$ as follows:

$$\begin{aligned} \Gamma &= Y^T \Delta \\ \mathbb{E}[\text{VOL}(P_k)] &= \Gamma_k \end{aligned} \quad (1.5)$$

From the results obtained in Equation 1.4 and Equation 1.5, a way to calculate the expected value of $\text{NORMCUT}(P_1, P_2, \dots, P_K)$ is given by:

$$\mathbb{E}[\text{NORMCUT}(P_1, P_2, \dots, P_K)] = \sum_{k=1}^K \sum_{i=1}^{|V|} \sum_{j=1}^{|V|} \frac{Y_{ik}(1 - Y_{kj}^T) A_{ij}}{\Gamma_k} \quad (1.6)$$

Nazi et al. [4] also showed that given the probability tensor Y , one can evaluate how balanced those partitions are. Note that the sum of the columns in Y is the expected number of nodes in each partition, i.e., $\mathbb{E}[|P_k|] = \sum_{i=1}^{|V|} Y_{ik}$. On the other hand, in order to have balanced partitions, the number of nodes in each one should be $\frac{|V|}{K}$. As a consequence, the quantity $\left| \sum_{i=1}^{|V|} Y_{ik} - \frac{|V|}{K} \right|$ measures how balanced the partition P_k is.

Using the last result, and replacing the absolute value by the squared function, one can derive the loss function from Equation 1.6. This is the one originally used in GAP that intends to minimize the expected value of the normalized cut and at the same time balances the cardinalities of the partitions:

$$\mathcal{L} = \sum_{k=1}^K \sum_{i=1}^{|V|} \sum_{j=1}^{|V|} \frac{Y_{ik}(1 - Y_{kj}^T)A_{ij}}{\Gamma_k} + \sum_{k=1}^K \left(\sum_{i=1}^{|V|} Y_{ik} - \frac{|V|}{K} \right)^2 \quad (1.7)$$

1.10.2.2 The Embedding Module

In the graph embedding module, the algorithm learns node embeddings by encoding local structure information and the node features. The embeddings are calculated using Graph Neural Networks (GNN) which have become very popular during the recent years. To ensure generalization, the GAP authors opted for an inductive GNN approach by leveraging GraphSAGE with a Graph Convolutional Network (GCN) based approach.

In the paper where GAP was presented, the authors used a 3-layer GCN using Xavier initialization that can be found in [2]

$$Z = \tanh(\hat{A} \tanh(\hat{A} \tanh(\hat{A} X \mathbf{W}^{(0)}) \mathbf{W}^{(1)}) \mathbf{W}^{(2)})$$

where $\hat{A} = (D + I)^{-\frac{1}{2}}(A + I)(D + I)^{-\frac{1}{2}}$ is a normalized variant of the adjacency matrix with self loops, X is the feature matrix, and $\mathbf{W}^{(l)}$ is a learnable parameter matrix.

1.10.2.3 The Partitioning Module

The second module of GAP is composed of a fully connected layer that takes as input a node embedding vector \mathbf{z}_u generated in the embedding module. This fully connected layer is then followed by a softmax layer trained to minimize the expected normalized loss function given by Equation 1.7.

This module is the responsible for partitioning the graph by returning $Y \in \mathbb{R}^{|V| \times K}$, the probabilities matrix that each node belongs to each of the partitions P_1, P_2, \dots, P_K . At the same time, it ensures that for a given node, the sum of the probabilities of belonging each of

the partitions is 1

$$\sum_{k=0}^K Y_{ik} = 1$$

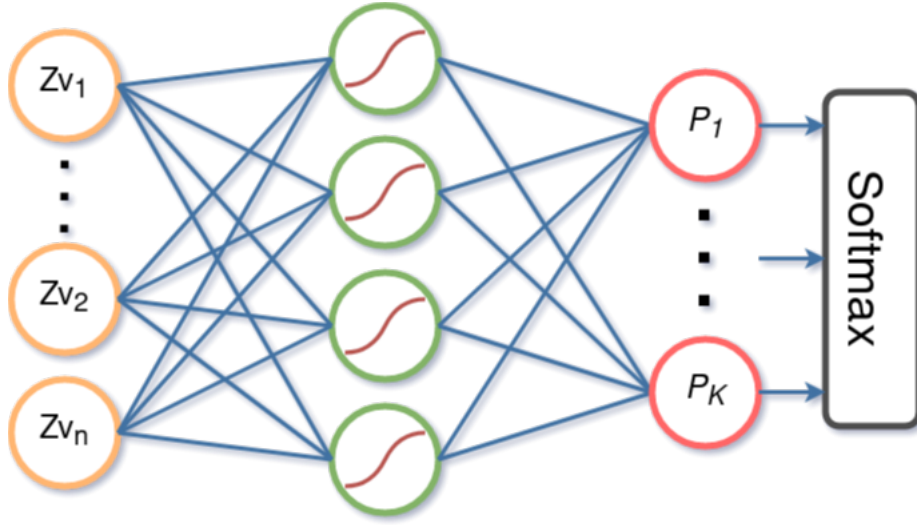
1.10.3 PinSAGE and Markov Chain Negative Sampling (MCNS)

PROPOSED SOLUTION (GRAPH PARTITIONING FOR LARGE GRAPHS)

GNNs aim at learning node representations by learning the similarities shared between connected nodes. However, the expressive ability of a GNN is highly dependent on the quality of node features. Mention here: Deep Fraud Detection on Non-attributed Graph <https://arxiv.org/pdf/2110.01171.pdf> but cited here C. T. Duong, T. D. Hoang, H. T. H. Dang, Q. V. H. Nguyen, and K. Aberer, “On node features for graph neural networks,” arXiv preprint arXiv:1911.08795, 2019. [11] H. Cui, Z. Lu, P. Li, and C. Yang, “On positional and structural node features for graph neural networks on non-attributed graphs,” arXiv preprint arXiv:2107.01495, 2021

Eigendecomposition and top-k-eigenvalues are the k-dimensional feature vector Q . Huang, H. He, A. Singh, S.-N. Lim, and A. R. Benson, “Combining label propagation and simple models out-performs graph neural networks,” arXiv preprint arXiv:2010.13993, 2020.

Different feature initializations <http://www.cs.emory.edu/~jyang71/files/gnnfeature.pdf>



One of the principal limitations that GAP has is that it requires

According to the original paper [5], the DeepWalk algorithm consists of two main components: a random walk generator and an update procedure.

In the first component, a random node v_i is taken uniformly at random to be the root of a random walk \mathcal{W}_{v_i} which in its turn samples recursively from the neighbors of the last visited vertex until the maximum length is reached.

As specified by Perozzi et. al. [5], their experiments suggest that the number of walks started per vertex should be greater or equal than $\gamma = 30$, the latent dimension greater or equal than $d = 64$, and they fixed the sensible values of $w = 10$ for the window size, and $t = 40$ for the walk length. Based on those recommendations, in the experiments carried out in [8], and the computational needs of the problem to be solved, it was found convenient to set $\gamma = 60$, $d = 64$, $w = 10$ (good results with 15), and $t = 60$ (good results with 80).

For the algorithm that is proposed here, the implementation by the Karate Club API [6] was used.

CHAPTER 3

EXPERIMENTAL RESULTS

The number of partitions was set to three

For the dataset used to train and test the algorithm "The Graph Partitioning Archive" [7]

CONCLUSION

Las conclusiones y el trabajo a futuro inicia aquí...

4.1 Contributions**4.2 Recommendations and future work**

APPENDIX



ANALISIS

El apéndice inicia aquí.

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