Abstract

The design of algorithms that solve Combinatorial Optimization problems is a challenging task due to their intractable nature. One of the fundamental and most studied problem in the area is the Graph Partitioning problem. In recent years, several Deep Learning strategies have shown to be successful when dealing with this problem. One of the famous ones is the Generalizable Approximate Partitioning (GAP) framework. The present work is aimed to present an extension to this framework that works for non-attributed graphs and generalizes well to large ones.

One of the first observations made by the authors of this work is that in GAP, they used an architecture based on Graph Convolutional Networks (GCN) which tends to be slow for big graphs. Here, it is presented a modification, still inspired on GCN, that reduces the computation time.

In addition, it was noted that GAP requires graphs with node features due to the model architecture chosen by its authors. That dependency was eliminated used a random walk approach to generate node features. This was an important modification because the algorithm now relies purely on the graph's structure which is Graph Partitioning problem.

In the last part of the written, it is shown how to use a negative sampling technique to accelerate the process of finding balanced partitions without sacrificing the quality of those partitions. The proposed algorithm shows results comparable with widely used partitioning algorithms like METIS.

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CHAPTER 1

INTRODUCTION

This chapter provides to the reader the necessary information to get familiar with the present work. It intends to contextualize the reader with the topics in the subsequent chapters and show them the path that should be followed.

1.1 Presentation

The computational complexity behind solving Combinatorial Optimization problems is a very well known concern. Combinatorial Optimization problems ... On one hand, it is necessary to keep researching for new theoretical results limitations and to more asumptions and use this knowledge to influence the way we approach that kind of problems. On the other hand, there is a need to solve those problems in real life and come up with practical and efficient solutions in a considerably small amount of time. The theoretical and practical are tied To deal with the computational complexity in solving problems of the Combinatorial Optimization type, different techniques have been proposed which are based on optimization strategies like Heuristic Methods or Integer Programming, just to mention a few.

The ability to address the underlying issues that arise in this kind of problems has been improved drastically during the last years. Those huge steps forward towards need for fast approximations for

In terms of mathematical results and computing power, the technological progress that has taken place during the last decade has given rise to new ways to find algorithms that provide efficient solutions, particularly for graph-related Combinatorial Optimization problems.

Some recent approaches are being designed to take advantage of Machine Learning capabilities. In particular, Deep Learning strategies are providing alternative ways to deal with some of the underlying issues that arise with those kinds of problems. For determined problems, those approaches have shown to be the most successful in terms of running time efficiency, less human intervention, and the quality of the solutions.

Balanced graph partitioning is one of the fundamental Combinatorial Optimization problems and one of those who has gotten the best from Deep Learning.

application to solve time consuming and computationally too expensive to get solutions

1.2 Objectives

1.2.1 General objective

- To develop an machine learning algorithm that solves the graph partitioning problem that works for large-scale graph instances.

1.2.2 Particular objective

- To understand and analyze the Generalizable Approximate Partitioning (GAP) framework and to use it for solving the graph partitioning problem.

- Based on GAP, design an algorithm that works for general graphs (non-attributed graphs) that relies completely on their structure.

- To build a framework that is easy to modify in order to use different objective functions in the partitioning stage.

- To explore different types of sampling and study the impact they have in the efficiency of the algorithm.

1.3 Justification

Graphs are mathematical representations of what is colloquially known as networks. They are used to describe the relationships between objects which is adopted as a similitude measure and allows to model an extensive amount of real life problems. Due to their modeling capacity and their power of abstraction, they are widely studied in different areas of mathematics and computer science.

Applications of graph partitioning to real life:

Graph partitioning plays an essential role in paralleling computations and the design of new algorithms on large graphs. For example device placement problem where one aims to distribute work accross multiple devices and have applications in Deep Learning to train Neural Networks accross multiple devices [7]

Intentional Islanding in Power Systems Considering Load-Generation Balance problem of intentional islanding in power systems considering load generation balance [12]

Image segmentation [5] Applications of graph partitioning to solve graph-related problems:

Graph partitioning it is used as a subrutine in tasks as graph compression [1]

1.4 Limitations and project scope

- The sizes of the datasets
- Values based on previous work
- What assumptions do I make?
- not distributed work which could improve
- It only accepts a certain format SCOTCH and Networkx

1.5 Research Problem

Graph partitioning algorithms based on DL

https://arxiv.org/pdf/2104.03546.pdf

1.6 Hypothesis

1.7 Project organization

Future work extend to different problem statements, such as balanced graph partitioning with tolerance or weighted graph partitioning. Study the real impact on choosing the way to extract the features and try different algorithms look for new ways the algorithm relies only on topological graph's structure To generalize the algorithm and code to construct graphs from the features

CHAPTER 2

THEORY AND CONCEPTUAL FRAMEWORK

2.1 Preliminaries

Description of concepts

Definition 2.1.1. *orthogonal complement*

Theorem 2.1.1. *For every $n \times n$ symmetric real matrix, the eigenvalues are real and the eigenvectors can be chosen real and orthonormal.*

Theorem 2.1.2 (Courant-Fisher Formula)**.** *Let A be an $n \times n$ real symmetric matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ and corresponding eigenvectors $v_1, v_2, ..., v_n$. Then*

$$\lambda_1 = \min_{\|x\|=1} x^T A x = \min_{x \neq 0} \frac{x^T A x}{x^T x},$$

$$\lambda_2 = \min_{\substack{\|x\|=1 \\ x \perp v_1}} x^T A x = \min_{x \neq 0} \frac{x^T A x}{x^T x},$$

$$\lambda_n = \lambda_{max} = \max_{\substack{\|x\|=1 \\ x \perp v_1}} x^T A x = \max_{\substack{x \neq 0 \\ x \perp v_1}} \frac{x^T A x}{x^T x}.$$

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

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

2.2 Graphs and Laplacian Matrices

For the rest of the chapter, let $G = (V, E)$ be a graph, where $V = \{v_1, v_2, ..., v_n\}$ 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 $d_1, d_2, ..., d_n$ on the diagonal.

2.2.1 The Unnormalized Laplacian

The unnormalized graph *Laplacian matrix* L is defined as

$$L = D - A$$

Proposition 2.2.1 (Some properties of L)**.** *The matrix L, as defined above, satisfies the following properties:*

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

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

2. *L is symmetric and positive semi-definite*

3. *L has n non-negative, real-valued, eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$*

4. *The smallest eigenvalue of L is 0, the corresponding eigenvector is the constant one vector $\mathbb{1}$.*

2.2.2 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

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

2.2.3 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 2.2.1. *Given a graph $G = (V, E)$ and an integer K, a partition of G is a collection of K subsets $P_1, P_2, ..., P_K \subset V$ such that:*

1. *$P_i \cap P_j = \emptyset$ for $i \neq j$, where $i, j \in \{1, 2, ..., K\}$*

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 $P_1, P_2, ..., P_K$ such that minimizes the *cut value* of the partition, usually called just *cut*, which is defined as

$$\textsc{Cut}(P_1, P_2, ..., P_K) := \frac{1}{2} \sum_{k=1}^{K} |\partial(P_k)| \tag{2.1}$$

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

$$\textsc{Vol}(S) := \sum_{v_i \in S} d_i$$

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

$$\begin{aligned}\textsc{RatioCut}(P_1, P_2, ..., P_K) &:= \frac{1}{2} \sum_{k=1}^{K} \frac{|\partial(P_k)|}{|P_k|} \\ &= \sum_{k=1}^{K} \frac{\textsc{Cut}(P_k, \overline{P_k})}{|P_k|}\end{aligned}$$

$$\begin{aligned}\textsc{NormCut}(P_1, P_2, ..., P_K) &:= \frac{1}{2} \sum_{k=1}^{K} \frac{|\partial(P_k)|}{\textsc{Vol}(P_k)} \\ &= \sum_{k=1}^{K} \frac{\textsc{Cut}(P_k, \overline{P_k})}{\textsc{Vol}(P_k)}\end{aligned}$$

2.2.4 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

2.3 Literature review

2.3.1 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 [4].

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. [8], 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 $V = \{v_1, v_2, ..., v_n\}$, 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.

2.3.1.1 Expected Normalized Cut Loss Function

Recall the normalized cut given by

$$\textsc{NormCut}(P_1, P_2, ..., P_K) = \sum_{k=1}^{K} \frac{\textsc{Cut}(P_k, \overline{P_k})}{\textsc{Vol}(P_k)} \tag{2.2}$$

In order to calculate the normalized cut expected value, one needs to compute the expected value of $\textsc{Cut}(P_k, \overline{P_k})$ and $\textsc{Vol}(P_k)$ from Equation 2.2. For the deduction of those quantities, an approach similar to the one presented in [2] 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

$$\mathbb{E}[\textsc{Cut}(P_k, \overline{P_k})] = \sum_{i=1}^{|V|} \sum_{v_j \in \mathcal{N}(v_i)} Y_{ik}(1 - Y_{jk}) \tag{2.3}$$

Due to the fact that for a given node the adjacent nodes can be retrieved from the adjacency matrix A, Equation 2.3 can be rewritten as follows:

$$\mathbb{E}[\textsc{Cut}(P_k, \overline{P_k})] = \sum_{i=1}^{|V|} \sum_{j=1}^{|V|} Y_{ik}(1 - Y_{kj}^T) A_{ij} \tag{2.4}$$

Keeping in mind that $\textsc{Vol}(P_k)$ 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 $\textsc{Vol}(P_k)$ as follows:

$$\begin{aligned} \Gamma &= Y^T \Delta \\ \mathbb{E}[\textsc{Vol}(P_k)] &= \Gamma_k \end{aligned} \tag{2.5}$$

From the results obtained in Equation 2.4 and Equation 2.5, a way to calculate the expected value of $\text{NORMCUT}(P_1, P_2, ..., P_K)$ is given by:

$$\mathbb{E}[\text{NORMCUT}(P_1, P_2, ..., P_K)] = \sum_{k=1}^{K} \sum_{i=1}^{|V|} \sum_{j=1}^{|V|} \frac{Y_{ik}(1 - Y_{kj}^T) A_{ij}}{\Gamma_k} \tag{2.6}$$

Nazi et al. [8] 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 2.6. 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:

$$\mathscr{L} = \sum_{k=1}^{K} \sum_{i=1}^{|V|} \sum_{j=1}^{|V|} \frac{Y_{ik}(1 - Y_{kj}^T) A_{ij}}{\Gamma_k} + \sum_{k=1}^{K} \left(\sum_{i=1}^{|V|} Y_{ik} - \frac{|V|}{K} \right)^2 \tag{2.7}$$

2.3.1.2 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 [3]

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

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 $\boldsymbol{W}^{(l)}$ is a learnable parameter matrix.

2.3.1.3 The Partitioning Module

The second module of GAP is composed of a fully connected layer that takes as input a node embedding vector $\boldsymbol{z}_u$ 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 2.7.

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 $P_1, P_2, ..., P_K$. At the same time, it ensures that for a given node, the sum of the probabilities of belonging each of the partitions is 1

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

2.3.2 PinSAGE and Markov Chain Negative Sampling (MCNS)

CHAPTER 3

PROPOSED SOLUTION (GRAPH PARTITIONING FOR LARGE GRAPHS)

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

3.1 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 Grpah Convolutional Neural Networks (GCN) and its limitations. Emphasize in how GraphSAGE solve those limitations and how it extends the GCN capabilities

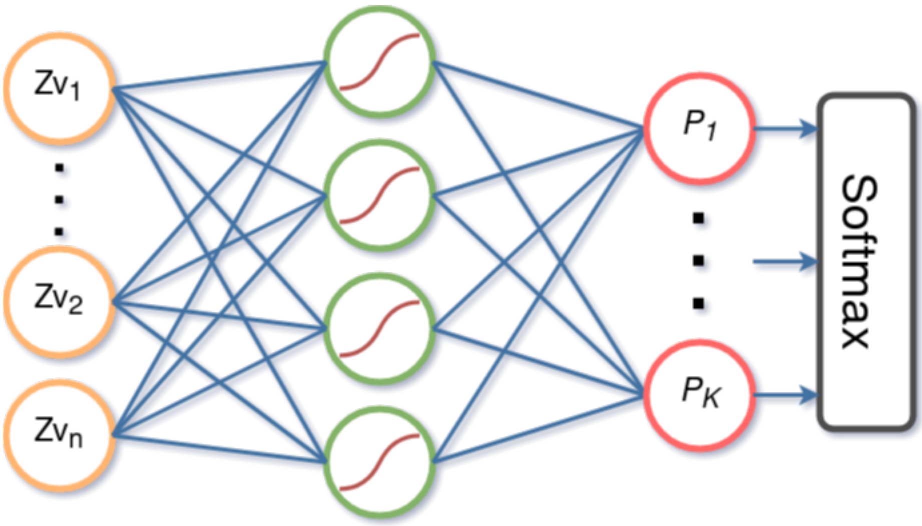
3.2 Node Features

One of the main limitations of GAP is that it requires node features. Due to the nature of the GCNs that make use of the symmetrically normalized graph Laplacian 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 net- works," arXiv preprint arXiv:2010.13993, 2020.

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



and after playing a little bit

although GCN have been shown to extract very useful information about graph topology we need to find a different way to get that information

Some work on using Graph Neural Networks without features has been made. Use one hot representation or Initialize random feature matrices (Those methods have been shown to be equivalents and they do not generalize as mention in [6]. Other methods propose using applying methods as PCA to the adjacency matrix to extract the top k-eigenvalues but those approaches are computationaly very expensive, which is infeasible for large graphs and only and does not To help capturing local information related to the graph's structure a random walk approach was chosen, have been shown efficient representation learning techniques for graphs https://arxiv.org/pdf/1901.01346.pdf, random walk kernels to produce high quality graph representations https://proceedings.neurips.cc/paper/2020/file/ba95d78a7c942571185308775a97 Paper.pdf

in particular Deep Walk to extract features about the topology of the network

According to the original paper [9], 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 γ is reached.

As specified by Perozzi et. al. [9], 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 [13], and the computational needs of the problem to be solved, it was found convenient to set $\gamma = 60$, $d = 64$, $w = 15$, and $t = 80$.

For the algorithm that is proposed here, the implementation by the Karate Club API [10] was used.

Traditional approaches like METIS or SCOTCH implements different versions of the algorithm according to the balancedness measure, either the cardinality or the volume of the partitions. One of the great innovations presented in [8] is the introduction of a loss function derived from the expectation of the normalized cut. Even though they

Ratio cut it is still used and relevant to modern research cite here https://proceedings.neurips.cc/paper/202
Paper.pdf

or here https://www.springerprofessional.de/en/metaheuristic-approaches-for-ratio-cut-and-normalized-cut-graph-/20360832

the authors of [2] proposed some modifications to GAP so it can be used for graphs without features. However the presented

for future - Study the weighted problem Study better features related to the problem other ways to extract useful features for non-attributed graphs

METIS was used from the networkx interface

Computation Graphs		
Name	**Nodes**	**Edges**
add20	2395	7462
data	2851	15093
3elt	4720	13722
uk	4824	6837
add32	4960	9462
bcsstk33	8738	291583
whitaker3	9800	28989
crack	10240	30380
fe_body	45087	163734
t60k	60005	89440
wing	62032	121544
finan512	74752	261120
fe_rotor	99617	662431
598a	110971	741934
m14b	214765	1679018
auto	448695	3314611

Table 3.1: Summary of the graphs characteristics. Taken from "The Graph Partitioning Archive [11]"

CHAPTER 4

Experimental Results

The number of partitions was set to three

For the dataset used to train and test the algorithm "The Graph Partitioning Archive" [11]

CHAPTER 5

CONCLUSION

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

5.1 Contributions

5.2 Recommendations and future work

APPENDIX A

ANALISIS

El apéndice inicia aquí.

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