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Graph machine learning for flight delay prediction due to holding manouver

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"Without education, we are in a horrible and deadly danger of taking educated people seriously."

G.K. Chesterton

ABSTRACT

FRANCO, J. L. **Graph ML for Flight Delay Prediction due to Holding Manouver**. 2024. 20p. Monografia (Trabalho de Conclusão de Curso) - Instituto de Ciências Matemáticas e de Computação, Universidade de São Paulo, São Carlos, 2024.

The growing demand for efficient last-mile delivery solutions, driven by the rise of e-commerce and urbanization, necessitates innovative approaches to manage the complexities of urban logistics. This study investigates the use of drones for last-mile delivery through a graph-based approach, focusing on the Multi-Agent Pathfinding (MAPF) problem, which involves routing multiple drones to deliver packages efficiently. Most algorithms proposed for the Last Mile Delivery Drones (LMDD) problem tend to overlook the inherent complexities of the MAPF problem. This research adopts a graph-based representation of the delivery area, transforming the problem into a network flow optimization. The proposed graph-based heuristic method is evaluated against a purely Mixed Integer Linear Programming (MILP)-based solution. Experimental results demonstrate that the heuristic approach not only enhances computational efficiency but also maintains high solution quality. Specifically, the heuristic outperforms MILP in terms of runtime while achieving comparable accuracy in path optimization. Additionally, a hybrid implementation combining heuristic and MILP is proposed. The exact MILP model has exponential complexity time as the number of drones is increased, which is expected since the MAPF paradigm is NP-Complete. The complexity of the heuristic is bounded by $\mathcal{O}(N^3 K \max(\log N, \log K))$, where K is the number of drones and N is the dimension, if the grid is square. The study highlights the potential of centralized control systems for managing a fleet of delivery drones. The findings from extensive simulations indicate that the graph-based heuristic effectively balances computational efficiency and operational reliability, making it a viable solution for real-world last-mile delivery applications. This research contributes to the broader field of drone logistics by offering a scalable and robust method for optimizing drone delivery paths, thereby supporting the integration of drones into commercial delivery systems.

Keywords: Optimization. Graphs. Last Mile Delivery Drones.

RESUMO

FRANCO, J. L. **Graph ML for Flight Delay Prediction due to Holding Manouver**. 2024. 20p. Monografia (Trabalho de Conclusão de Curso) - Instituto de Ciências Matemáticas e de Computação, Universidade de São Paulo, São Carlos, 2024.

A crescente demanda por soluções eficientes de entrega de última milha, impulsionada pelo crescimento do comércio eletrônico e urbanização, exige abordagens inovadoras para gerenciar as complexidades da logística urbana. Este estudo investiga o uso de drones para entrega de última milha por meio de uma abordagem baseada em grafos, focando no problema de Multi-Agent Pathfinding (MAPF), que envolve o roteamento de múltiplos drones para entregar pacotes de forma eficiente. A maioria dos algoritmos propostos para o problema de Drones de Entrega de Última Milha (LMDD, em inglês) tendem a ignorar as complexidades inerentes do problema MAPF. Esta pesquisa adota uma representação baseada em grafos da área de entrega, transformando o problema em uma otimização de fluxo de rede. O método heurístico baseado em grafos proposto é avaliado em comparação com uma solução puramente baseada em Programação Linear Inteira Mista (MILP, em inglês). Os resultados experimentais demonstram que a abordagem heurística não apenas melhora a eficiência computacional, mas também mantém alta qualidade nas soluções. Especificamente, a heurística supera a MILP em termos de tempo de execução, enquanto alcança uma precisão comparável na otimização de caminhos. Além disso, é proposta uma implementação híbrida combinando heurística e MILP. O modelo MILP exato tem complexidade exponencial conforme o número de drones aumenta, o que é esperado, uma vez que o paradigma MAPF é NP-Completo. A complexidade da heurística é limitada por $\mathcal{O}(N^3 K \max(\log N, \log K))$, onde K é o número de drones e N é a dimensão, se a grade for quadrada. O estudo destaca o potencial de sistemas de controle centralizados para gerenciar uma frota de drones de entrega. Os resultados de simulações extensivas indicam que a heurística baseada em grafos equilibra a eficiência computacional e a confiabilidade operacional de forma eficaz, tornando-a uma solução viável para aplicações de entrega de última milha do mundo real. Esta pesquisa contribui para o campo mais amplo da logística de drones oferecendo um método escalável e robusto para otimizar os caminhos de entrega de drones, apoiando assim a integração de drones em sistemas de entrega comerciais. Este trabalho também sugere avanços com agentes inteligentes usando Aprendizado por Reforço (RL, em inglês) e Redes Neurais de Grafos (GNNs, em inglês) para melhorar o paradigma descentralizado, o qual nós provamos ser inferior à nossa metodologia centralizada, uma vez que utiliza uma otimização local em contraste com nossa otimização global.

Palavras-chave: Otimização. Grafos. Drones de Entrega de Última Milha.

LIST OF FIGURES

LIST OF TABLES

LIST OF ABBREVIATIONS AND ACRONYMS

LMDD	Last Mile Delivery Drones
MAPF	Multi-Agent Pathfinding
BFS	Breadth First Search
MILP	Mixed Integer Linear Programming
MOEA	Multiobjective Evolutionary Algorithm
UAV	Unmanned aerial vehicle
NSGA-I	Non-dominated Sorting Genetic Algorithm
PLS	Pareto Local Search
MIP	Mixed Integer Programming
TSP	Traveling Salesman Problem
TS	Tabu Seach
GVNS	General Variable Neighborhood Search
ALNS	Adaptive Large Neighborhood Search
SA	Simulated Annealing
UTM	Unmanned Aircraft System Traffic Management
FAA	Federal Aviation Administration
BVLOS	Beyond Visual Line of Sight
NASA	National Aeronautics and Space Administration
RL	Reinforcement Learning
GNN	Graph Neural Network

CONTENTS

1 INTRODUCTION

2 THEORETICAL FRAMEWORK AND RELATED WORKS

Graph machine learning can be tracked backwards to the problem of 'learning' on data that is inherently a graph (SILVA; ZHAO, 2016; CHAMI *et al.*, 2022) or can be modeled as a graph (VERRI; ZHAO, 2013; YOU *et al.*, 2020). This field encompasses a variety of tasks, including node/edge classification, network construction, link prediction, graph classification, graph cut/partitioning, network embeddings, graph coarsening/reduction, which rely on learning representations from graph-structured data. Over the last decades, researchers have developed numerous approaches to tackle these challenges, initially these techniques were most developed by complex networks researchers. However, in the last decade with the advancements in deep learning, the field has seen a significant shift towards the merging of three main communities: graph signal processing, deep learning and complex nets.

As described, defining the field of graph machine learning is not straightforward, as it encompasses a broad range of methods and applications. The tasks mentioned above are just a few examples of the many challenges that can be addressed through graph-based learning techniques. For clarity, these tasks can be categorized into three main learning paradigms: supervised, unsupervised, and semi-supervised learning. In this study, we are interested on the (semi-)supervised learning paradigm, which encompasses a variety of techniques designed to leverage learning to (partially-)labeled data (VERRI; URIO; ZHAO, 2018; AMANCIO *et al.*, 2014). But we can refine even more, in fact, this work will focus in the subset of graph elements prediction(classification/regression) methods.

In this chapter, we provide an overview of the theoretical framework of graph machine learning for node/edge prediction. Here we consider the division of the field into `classical` graph learning and `deep` graph learning, where here 'classical' refers to the machine learning techniques applied to graphs before the advent of graph neural networks, where standard ML algorithms were applied to graph data and the topological information measures were encoded as features together with the tabular data (COSTA, 2007; SILVA; ZHAO, 2016). This bipartition is what will pave the way of our explanation, since the last decade has seen a complex interplay between these two approaches. The field's evolution can be traced back to when Bruna *et al.* (2013) introduced one of the first GNN architectures leaned on the theory of graph signal processing. Concurrently, researchers were developing node embedding techniques like DeepWalk (PEROZZI; AL-RFOU; SKIENA, 2014) and node2vec (GROVER; LESKOVEC, 2016), which bridged classical and deep approaches while remaining using complex networks concepts. The subsequent years saw a surge in GNN architectures, including Graph Convolutional Networks (KIPF; WELLING, 2016) and GraphSAGE (HAMILTON; YING; LESKOVEC, 2017), marking a shift towards more

sophisticated deep learning approaches for graphs and the unification of the field.

In the following sections, we explain each subset, their theory and applications, and how they have evolved over time. We also discuss the challenges and limitations of these methods.

2.1 Classical graph learning

These early efforts focused on shallow learning techniques such as feature engineering, graph traversal algorithms, and spectral methods, which laid the foundation for understanding graph structure and dynamics. Methods like community detection, centrality measures, and link prediction became key tools for analyzing large-scale networks in areas such as social science, biology, and infrastructure systems. By modeling relationships as graphs, these approaches enabled researchers to capture both local and global properties, leading to significant insights in network theory and real-world applications.

2.2 Deep graph learning

The rise of deep learning has revolutionized the field of graph machine learning, enabling the development of more powerful and scalable models for graph data. Graph neural networks can be divide in two main categories: spectral-based and spatial-based. Here is a trick thing, the GCN architecture (KIPF; WELLING, 2016) is commonly divulgated as a spatial-based method, since it is more intuitive talking about the convolution operation in the spatial domain, where we simply aggregate information from the immediate neighbors. However, the GCN is a spectral-based method, in fact, it can be thought as a simplification of the first spectral GNN (BRUNA *et al.*, 2013) proposed and that builds the math behind GCNs. That said, first we introduce the spectral-based GNNs and then the spatial-based ones.

2.2.1 Spectral-based GNNs

Spectral methods are rooted in graph signal processing. The core idea is that a signal on a graph can be represented as node features, where each feature vector at a node corresponds to a 'signal' defined over the graph. In this context, the graph Laplacian $\mathcal{L} = D - A$, where D is the degree matrix and A is the adjacency matrix, plays a crucial role. It captures the structure of the graph and can be used to perform operations analogous to Fourier transforms in classical signal processing. Spectral methods can be categorized into two types: eigenvalue-based, where the focus is on creating a graph filter in the Fourier domain, and eigenvector-based, where the goal is to use a spectral basis to decompose the signal (BO *et al.*, 2023).

Bruna *et al.* (2013) introduced the first spectral Graph Neural Network (GNN), termed the Spectral CNN (SCNN), which aimed to translate ideas from standard Con-

volutional Neural Networks for images to graphs. The SCNN leverages the spectral decomposition of the graph Laplacian $\mathcal{L} = U\Lambda U^T$ to define a filter convolution operation in the Fourier domain. In this framework, the graph Fourier transform of a signal f is represented as $\hat{f} = U^T f$, and the convolution operation ($\star$) is defined as $g_\theta \star f = U g_\theta U^T f$, where g_θ is a learnable filter parameterized by θ. While powerful, the SCNN faces significant challenges: it requires $\mathcal{O}(n^3)$ computational complexity to calculate the entire graph spectrum, which is prohibitively expensive for large graphs. Moreover, the non-localized nature of eigenvectors means global information can overshadow local structural details, leading suboptimal balance between local and global information aligned with a huge parameter complexity (CHEN, 2020).

To address these limitations, Defferrard, Bresson and Vandergheynst (2016) introduces Chebyshev polynomials to approximate spectral filters, effectively reducing computational complexity while preserving the ability to capture localized patterns in the graph structure. The main ideia is to redefine our previous filtering operation to $g_\theta(\mathcal{L})f = \sum_{k=0}^{K-1} \theta_k T_k(\widetilde{\mathcal{L}})f$, where $T_k(\widetilde{\mathcal{L}}) =$ is the Chebyshev polinomial of order k evaluated at the scaled Laplacian $\widetilde{\mathcal{L}} = 2\frac{\mathcal{L}}{\lambda_{\max}} - I_n$. This innovation not only makes spectral GNNs more scalable to larger graphs but also enhances their ability to balance local and global information processing. By doing so, Defferrard et al.'s work paved the way for more efficient and effective graph neural network architectures, bridging the gap between theoretical spectral approaches and practical applications in various domains such as social network analysis, molecular property prediction, and recommendation systems. This advancement marked a crucial step in the evolution of GNNs, enabling their application to larger and more complex graph-structured data while maintaining computational efficiency.

3 PROBLEM DESCRIPTION

4 MATERIALS AND METHODS

Our data is a lot imbalanced, but there is little work on imbalanced data in the literature for graph machine learning and most of the work is based on oversampling ((**??**) GRAPH SMOTE), however current literature shows that oversampling can lead to overfitting and poor generalization. In this work, we will deal with class imbalancing using undersampling for the GAT.

5 RESULTS

6 CONCLUSION

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