Unifying Spectral and Spatial Graph Neural Networks

Zhiqian Chen
Mississippi State University
Starkville, MS, USA
zchen@cse.msstate.edu

Lei Zhang
Northern Illinois University
Dekalb, IL, USA
zhanglei@niu.edu

Liang Zhao
Emory University
Atlanta, GA, USA
liang.zhao@emory.edu

Abstract

In recent years, Graph Neural Networks (GNNs) have attracted considerable attention. However, the rapid emergence of diverse GNN models, each grounded in different theoretical foundations, complicates the model selection process, as these models are not easily understood within a unified framework. Initial GNNs were constructed using spectral theory, while others were developed based on spatial theory. This theoretical divergence makes direct comparisons difficult. Furthermore, the variety of models within each theoretical domain further complicates their evaluation. In this tutorial, we explore state-of-the-art GNNs and present a comprehensive framework that bridges the spatial and spectral domains, clarifying their interrelationship. This framework deepens our understanding of GNN operations. The tutorial delves into key paradigms, such as spatial and spectral methods, through a synthesis of spectral graph theory and approximation theory. We conduct an in-depth analysis of recent research advancements, addressing emerging issues like over-smoothing, using well-established GNN models to illustrate the universality of our framework.

CCS Concepts

• **Computing methodologies → Spectral methods**; • **Theory of computation → Numeric approximation algorithms**.

Keywords

Graph Machine Learning, Spectral Graph Theory, Approximation Theory

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1 Target audience, Prerequisites, and Benefits

Our target audience includes all levels of researchers and practitioners in machine learning over graphs. The prerequisites for this tutorial are basic calculus, linear algebra, machine learning, and graph theory. We plan to cover half of the materials for beginners (estimated 30+) and the rest for intermediate and experts (estimated 30+). We expect the audience to come away with an overview of the state-of-the-art models of spectral graph neural networks. While knowledge in spectral graph theory, approximation theory will facilitate a deeper understanding of the proposed framework, the tutorial can be digested without knowledge of specific GNN models. For beginners, this tutorial offers a foundational understanding through a spectral perspective, allowing them to grasp the basic concepts and behaviors of graph neural networks. It aids those applying graph neural networks by providing insights from both spectral and spatial perspectives, thereby enhancing their comprehension and effective use of these networks.

2 Materials/Resources to be distributed

This tutorial has been delivered at CVPR 2024 (June 18, 2 pm), and we shared materials at https://xgraph.team/course/cvpr24/. The CIKM version will be adapted from a focus on computer vision to a concentration on data mining methodologies by adding popular applications. This tutorial is mainly based on our survey and research papers in spectral graph neural networks [6, 7, 9] We have a set of previous tutorial slides for 1-hour talk https://imczq.com/csur.pdf, which will be extended to a 3-hour tutorial. We have been maintaining a collection of related sources at https://github.com/XGraph-Team/Spectral-Graph-Survey. Beyond that, we will develop an interactive code demo based on existing code in https://github.com/XGraph-Team/Spectral-Graph-Survey/code.

3 Tutorial description

The total duration comprises 165 minutes for the tutorial and 15 minutes for a break.

Part 1: Background: Unified GNNs (30 min)

GNNs can be bifurcated into two primary categories based on their underlying computational mechanisms: spectral and spatial approaches. Spectral GNNs, grounded in graph signal processing, hinge upon the eigen-decomposition of the graph Laplacian, with foundational contributions such as ChebNet. These networks furnish a theoretically robust framework for articulating convolution operations on graphs, albeit potentially exacting in terms of computational resources. In contrast, spatial GNNs operate within the vertex domain, aggregating information from neighboring nodes, exemplified by GraphSAGE and GCN. This tutorial provides an extensive overview of the recent advancements in both spectral- and spatial-based GNNs, and embarks on a detailed analysis of the evolutionary trajectories of these two GNN paradigms from a technical perspective. Within each category of GNNs, there exists a multitude of theoretical underpinnings guiding their design. This diversity presents challenges in conducting a unified analysis across disparate GNN frameworks. To surmount this barrier, we will investigate a novel perspective we propose, which could potentially harmonize the treatment of both types within a singular framework, and subsequently discuss its merits and demerits.

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- Current research of graph neural network (5 min)
- Overview of spatial-based GNN (5 min)
- Overview of spectral-based GNN (5 min)
- The challenge, benefit of study the connection between spatial and spectral GNN, and existing unified frameworks (15 min)

Part 2: Preliminary: Graph convolution (40 min)

In this section, we will elucidate the proposed unified perspective through case studies and comprehensive theoretical explanations. For instance, as a fundamental operation, graph matrix normalization will be examined from both spectral and spatial viewpoints, thoroughly justifying the necessity of normalization. Furthermore, we will delve into graph convolution from both perspectives: Spectral graph theory is committed to the analysis of graph structures via the eigenvectors and eigenvalues of matrices associated with the graph, notably the adjacency or Laplacian matrices. Approximation theory, which focuses on identifying the optimal approximation for a function within a designated class of functions, plays a pivotal role in revealing the expressiveness in terms of function of eigenvalues. By leveraging the spectral domain in conjunction with approximation methods, we can categorize all GNNs into linear, polynomial, and rational functions. Correspondingly, the spatial approach can be segregated into first-order, higher-order, and skip-connection strategies among neighbors. These two sets of three-tier categorizations precisely correspond, providing an additional layer of insights, rendering our proposed perspective both unified and conducive to elucidating a broader spectrum of GNNs.

- Spectral graph theory (15 min)
- Approximation theory for GNNs (15 min)
- A new unified framework to bridge spatial and spectral GNNs (10 min)

Part 3: Theoretical study: viewpoints of uncertainty, sampling oversmoothing, and inverse (60 min)

This section offers a profound and innovative theoretical perspective on prevalent topics within the domain of Graph Neural Networks (GNNs), exploring areas such as uncertainty, sampling, oversmoothing, and inverse problems to furnish a comprehensive framework for analyzing and comprehending various phenomena in GNNs. Moreover, these new insights can be interpreted through both spectral and spatial lenses. The uncertainty principle is employed to understand the distinct global and local effects observable in the spectral and spatial domains, respectively. The examination of sampling theory in the context of graphs is facilitated by a unified framework that integrates explicit closed-form solutions. The phenomenon of oversmoothing in GNNs, characterized by the diminution of node feature distinctiveness as successive layers are applied, can be interpreted within the same conceptual framework. The realm of inverse problems, focusing on resolving edge-related challenges in graphs, presents an alternate viewpoint for understanding GNNs.

- Uncertainty principle: Global v.s. Local views (10 min)
- Theoretical views on spatial and spectral methods (10 min)
- Sampling Point of View (15 min)
- Over-smoothing Point of View (15 min)
- Inverse Problem Point of View (10 min)

Part 4: Future Directions (20 min)

Recent advancements in using Partial Differential Equations (PDEs) for graph analysis have shown promise. Specifically, the behavior of polynomial and rational functions in this context bears resemblance to diffusion and wave functions, offering innovative tools to study GNNs leveraging these functions. However, current spectral graph theories predominantly cater to simple graphs. Extending these theories to encompass signed, directed, and hypergraphs remains an underdeveloped area. While there has been progress, a comprehensive theoretical framework integrating these graph types is still in development. Future research endeavors will explore the feasibility of formulating a unified spectral theory. This theory would not only encompass various graph types, including simple, signed, directed, and hypergraphs, but also address the dynamics intrinsic to these graphs. The aim is to create a holistic and integrated theoretical understanding of graph behaviors and properties across a diverse range of graph types and their dynamics.

- PDE on graphs (10 min)
- Spectral Graph Theories for Non-simple graphs (5 min)
- Graph Dynamics (5 min)

Part 5: Conclusion and Q&A (15 min)

Similar Tutorials

This tutorial stands out due to its novelty as the inaugural lesson exploring the theoretical capabilities of GNN in the ***spectral*** *domain, while also addressing the integration of spectral and spatial-based GNN approaches which cover most GNN.* Over the past three years, several most pertinent tutorials have been identified: In CVPR 2021: *Learning Representations via Graph-structured Networks.* The principal distinction lies in the fact that these tutorials concentrate on applications in computer vision, whereas our tutorial will be centered on spectral graph theory. In KDD 2022, *Trustworthy Graph Learning: Reliability, Explainability, and Privacy Protection* focuses on explainability and ethics issues, while *Graph Neural Networks: Foundation, Frontiers, and Applications* provides a comprehensive overview of topics in graph neural networks but lacks the perspective from spectral views. In past CIKM, there are several approaches that emphasize different applications or aspects rather than delving into the theoretical nature of graph neural networks, particularly from spectral perspectives: *Reasoning beyond Triples: Recent Advances in Knowledge Graph Embeddings*, *Leveraging Graph Neural Networks for User Profiling: Recent Advances and Open Challenges*, and *Fair Graph Mining.*

Whereas extant tutorials [1–3] and surveys predominantly aim to provide an exhaustive compilation of topics, the present tutorial prioritizes a profound comprehension buttressed by rigorous theoretical underpinnings. A distinct strand of related literature attempts to classify works into disparate categories, or approaches them from varied theoretical stances, including attention mechanisms, matrix factorization, network embedding methodologies, message-passing frameworks, and natural language processing insights. Notwithstanding, these investigations often restrict themselves to specific segments of the GNN spectrum, potentially foregoing a holistic viewpoint. In contrast, the analysis in this tutorial encompasses a broad swath of the GNN landscape. Concurrently, while a significant portion of GNN surveys gravitate towards the realm of black-box explainability, the focal point of this tutorial remains anchored in interpretable graph neural networks buttressed by a solid theoretical framework. Recent survey papers, particularly [4], explore polynomial and linear spectral graph theories, elucidating new insights from an eigenvector standpoint, inclusive of topics such as graph wavelets and conjugate bases. In contrast, [5] centers on the spectral domain but neglects developments from the past five years, an oversight our study rectifies by introducing a novel approach grounded in approximation theory. Moreover, [8] predominantly examines the transferability of spectral graph neural networks, whereas our investigation presents a groundbreaking framework that integrates a majority of GNN architectures under a single umbrella. Additionally, [10] represents the most comparable survey paper, yet their emphasis is primarily on analyzing low-pass filtering behaviors. We aim to incorporate selected analyses from the latest survey papers into our tutorials.

4 Brief Bio Sketches

Dr. Zhiqian Chen is an Assistant Professor in the Department of Computer Science and Engineering at Mississippi State University. Specializing in graph machine learning and its applications, Dr. Chen's research endeavors have garnered support from the National Science Foundation (NSF) and the United States Department of Agriculture (USDA). His accolades include an Outstanding Contribution Award from Toyota Research North America in 2016 and a Best Paper Award from ACM SIGSPATIAL. Dr. Chen has an impressive portfolio of research published in esteemed journals and conferences such as AAAI, IJCAI, IEEE ICDM, EMNLP, ACM Computing Surveys, and Nature Communication. Beyond his scholarly contributions, he has been an active reviewer for prestigious academic platforms including AAAI, ICML, ICLR, NeuralPS, and SIGKDD.

Dr. Lei Zhang is an Assistant Professor of Computer Science at Northern Illinois University. His research interests span the expansive domains of machine learning and data mining, with a specific emphasis on graph neural networks, graph structure learning, bilevel optimization, neural architecture search, and social network mining. He has published papers in top-tier conferences such as AAAI, ICDM, and IJCAI. He was awarded the Cunningham Fellowship from Virginia Tech in summer 2023.

Dr. Liang Zhao is an associate professor at the Department of Computer Science at Emory University. His research interests include data mining, artificial intelligence, and machine learning, with special interests in spatiotemporal and network data mining, deep learning on graphs, nonconvex optimization, and interpretable machine learning. He has published over a hundred papers in top-tier conferences and journals such as KDD, ICDM, TKDE, NeurIPS, Proceedings of the IEEE, TKDD, TSAS, IJCAI, AAAI, WWW, CIKM, SIGSPATIAL, and SDM. He won NSF CAREER Award in 2020. He has also won Cisco Faculty Research Award in 2023, Meta Research Award in 2022, Amazon Research Award in 2020, and Jeffress Trust Award in 2019, , and was ranked as one of the "Top 20 Rising Star in Data Mining" by Microsoft Search in 2016. He has won best paper award in ICDM 2022, best poster runner-up in ACM SIGSPATIAL 2022, Best Paper Award Shortlist in WWW 2021, Best Paper Candidate in ACM SIGSPATIAL 2022, Best Paper Award in ICDM 2019, and best paper candidate in ICDM 2021. He is recognized as "Computing Innovative Fellow Mentor" in 2021 by Computing Research Association. He is a senior member of IEEE.

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