INNOVATION PARTNERSHIPS
UNIVERSITY OF MICHIGAN

Unified Complex Networks – Calibration of Graph Neural Networks and Classification Tasks

TECHNOLOGY NUMBER: 2024-251

Technology ID
2024-251

Category
Software
MOSS - Michigan Open Source Support

Inventor
Danai Koutra
Puja Trivedi
Rushil Anirudh
Jayaraman Thiagarajan
Mark Heimann

Further information
Ashwathi Iyer
ashwathi@umich.edu

View online

OVERVIEW

Novel, flexible method improves calibration and uncertainty estimates in graph neural networks

- Addresses GNNs' poor calibration and unreliable uncertainty quantification using a generalizable approach
- Drug discovery, social network analysis, fraud detection, and recommender systems

BACKGROUND

Graph Neural Networks (GNNs) have become a critical tool for analyzing structured data in fields such as biology, chemistry, social sciences, and recommendation systems. Traditionally, GNNs are used for classifying nodes or entire graphs by learning complex relationships within networked data. However, while GNNs excel in prediction accuracy, ensuring reliable calibration—meaning that predicted probabilities reflect true uncertainties—remains a challenge. Poor calibration can result in misleading confidence scores, which reduces trust in model predictions, particularly in safety-critical domains like healthcare or finance. Existing methods for uncertainty estimation, such as Bayesian neural networks or post-hoc calibration techniques, often struggle with scalability, integration complexity, or lack generality, necessitating a more effective and adaptable solution for real-world deployments.

INNOVATION

The innovation presents a novel, flexible method specifically designed to enhance the calibration and uncertainty quantification of Graph Neural Networks during both node and graph classification tasks. Technically, the approach integrates advanced regularization and output calibration strategies seamlessly within existing GNN architectures, without significant computational overhead. This flexibility makes the method broadly adaptable across different GNN frameworks and datasets. The planned code release will further empower researchers and practitioners by providing accessible tools to deploy better calibrated and more trustworthy GNNs. Potential real-world applications include risk assessment in financial transaction networks, identifying reliable biomarkers in biological graphs, robust drug discovery pipelines, and safer recommender systems. By addressing calibration shortcomings, the method enables GNN-based models to deliver actionable and dependable uncertainty insights in mission-critical settings.

ADDITIONAL INFORMATION

PROJECT LINKS:

DEPARTMENT/LAB:

- Danai Koutra, Electrical Engineering and Computer Science (EECS)

LICENSE: