



RECENT ADVANCES AND FUTURE DIRECTIONS

APPLICATIONS AND RESEARCH DIRECTIONS



AGENDA

Introduction & Overview

Core GNN Architectures

Key Applications & Use Cases

Challenges & Research
Directions

1. INTRODUCTION & OVERVIEW

Why Graphs?

- Relational data in numerous fields: social networks, molecular structures, traffic systems, etc.
- Complex dependencies not captured by standard neural networks.

What Are GNNs?

- Neural architectures that operate on graph-structured data.
- Use message passing or neighborhood aggregation to learn node and/or graph-level representations.

2. CORE GNN ARCHITECTURES

Graph Convolutional Networks (GCN)

- Spectral-based approach (Kipf & Welling, 2017).
- Aggregates normalized neighbor features in a single matrix operation. Often used as a baseline in node classification tasks.

Message Passing Neural Networks (MPNN)

- General framework where nodes exchange “messages” with neighbors. Update step merges incoming messages with node’s current state.
- Flexible: sum, mean, max, attention-based aggregations, etc.

Graph Attention Networks (GAT)

- Applies attention over neighbors, learning importance weights. Well-suited for graphs with noisy or heterogeneous connections. Scales to large graphs with multi-head attention variants.

2. CORE GNN ARCHITECTURES

Gated Graph Neural Networks (GGNN)

- Incorporates Gated Recurrent Units (GRUs) or LSTMs in the update step. Enables iterative message passing to capture long-range dependencies. Often used in program analysis, chemistry (molecules with multiple passes).

GraphSAGE

- Introduces neighbor sampling for large-scale (billion-edge) graphs. Aggregators (mean, LSTM, pool) reduce neighbor features into a single vector.
- Can generate embeddings for previously unseen nodes in an inductive manner.

Graph Isomorphism Network (GIN)

- Proposed to be as powerful as the Weisfeiler-Lehman (WL) isomorphism test.
- Uses a learnable “ ϵ ” in the aggregation function to distinguish certain graph structures.
- Often outperforms GCNs on graph classification benchmarks.

2. CORE GNN ARCHITECTURES

Expressive Power:

- GIN aims to match WL-test expressiveness, while GCN is often less powerful but easier to train.

Scalability:

- GraphSAGE & Cluster-GCN address large-scale graphs via sampling/partitioning.

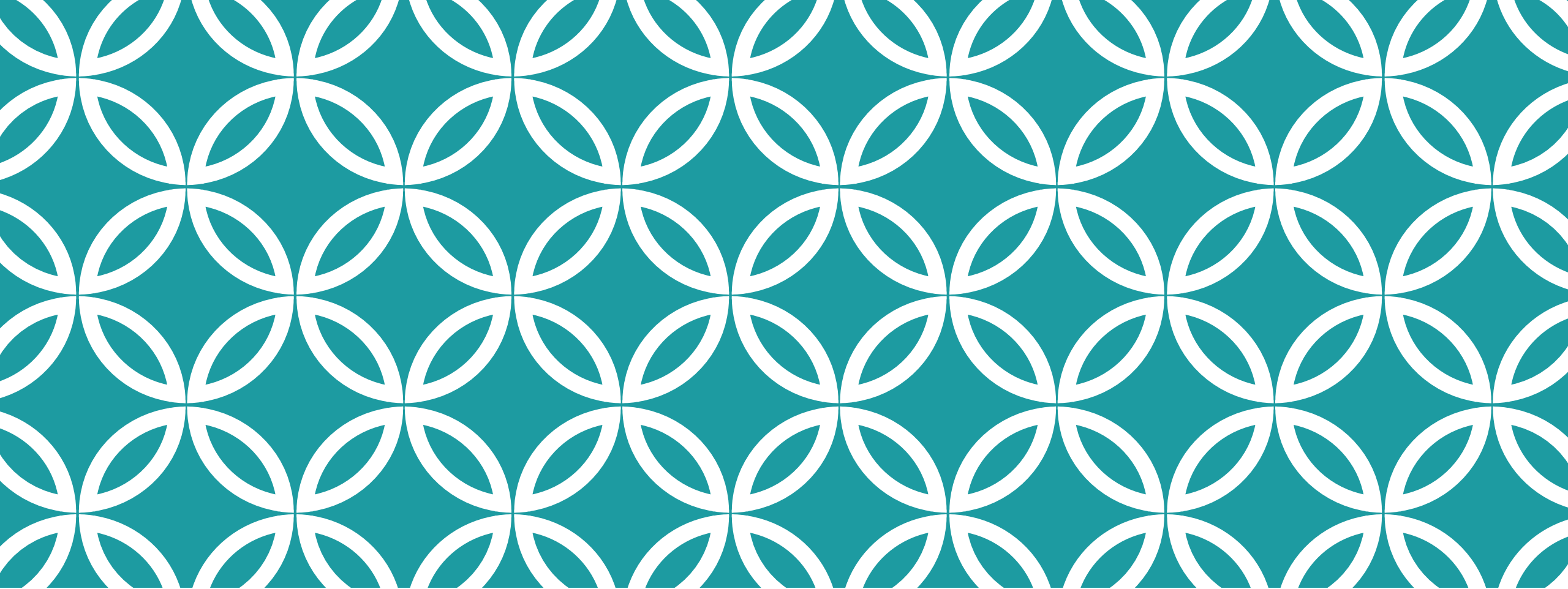
Iterative Updates vs. Single Convolution:

- GGNN uses multiple “timestep” updates vs. GCN’s single-shot layer update.

Attention Mechanisms:

- GAT uses attention over neighbors; MPNN can incorporate different attention schemes (e.g., dot-product attention).

Many real-world GNNs combine these ideas or extend them with custom layers or domain-specific tweaks.



3. KEY APPLICATIONS & USE CASES

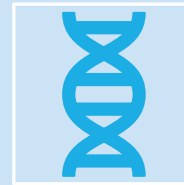
Technical highlights from various domains where GNNs are highly effective.

3.1 DRUG DISCOVERY & MATERIAL SCIENCE

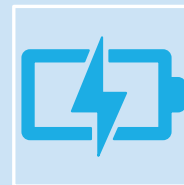
Example Reference:

Chemprop: Chemical Property Prediction

Machine learning of reaction properties via learned representations of the condensed graph of reaction



Predicting molecular properties, binding affinity, or toxicity. Modeling protein–protein interactions and novel compound generation.



Designing advanced materials (e.g., battery cathodes) using GNN property predictions.

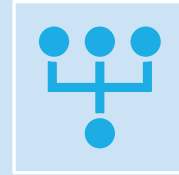
3.2 PHYSICS & SIMULATION

Example Reference:

, *Message Passing Neural PDE Solvers*



Particle physics: jet tagging, anomaly detection.



Physical simulations: GNN-based PDE solvers for fluid and structural mechanics.



Climate modeling: spatio-temporal forecasting.

3.3 COMBINATORIAL OPTIMIZATION

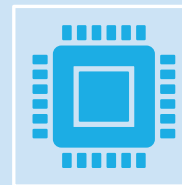
Example Reference:

[A Graph Pointer Network-Based Multi-Objective Deep Reinforcement Learning Algorithm for Solving the Traveling Salesman Problem](#)

[ST-GRAT: A Spatio-Temporal Graph Attention Network](#)



TSP, routing, scheduling:
learning heuristics with
GNNs.



Electronic design automation
(EDA): placement, routing in
VLSI design.

3.5 NEUROSCIENCE & BRAIN CONNECTIVITY

Example Reference:

Pooling Regularized Graph

Neural Network for fMRI

Biomarker Analysis

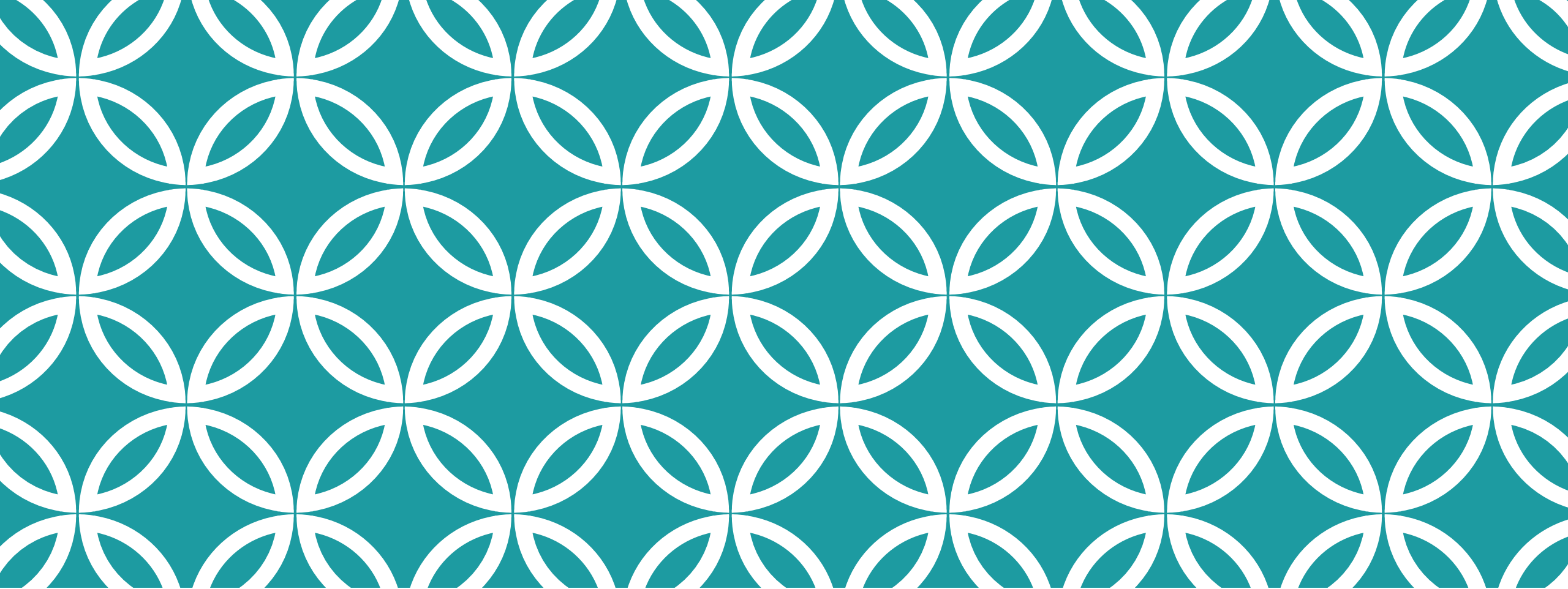
Revealing gene regulation-
based neural network
computing in bacteria



Studying structural/functional brain networks (connectomics).



BCI: classifying EEG signals as graphs of electrode correlations.



4. CHALLENGES & RESEARCH DIRECTIONS

Key technical issues and open areas for deeper exploration.

4.1 SCALABILITY & LARGE-SCALE GRAPHS

Sampling-based methods (GraphSAGE), cluster approaches (Cluster-GCN).

Distributed training frameworks for billion-edge graphs. Memory constraints and efficiency gains (e.g., mini-batch subgraphs).

4.2 DYNAMIC / STREAMING GRAPHS



Constantly evolving topologies (e.g., social networks, sensor data).



Temporal GNNs: EvolveGCN, TGAT, etc. Online inference and incremental updates.

4.3 HETEROGENEOUS & MULTI-MODAL GRAPHS

Different node/edge types, or multi-modal features (image, text, etc.).

Knowledge Graphs, domain-specific ontologies.

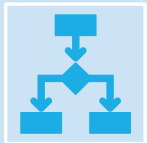
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Metapath aggregation (MAGNN) and attention-based methods.

4.4 INTERPRETABILITY & FAIRNESS



- Explaining GNN outputs: subgraph extraction, saliency maps. Detecting biases (e.g., social networks)
- GraphExplainer



Ensuring fairness :

Frameworks: GraphLIME, FairGNN.

4.5 HYBRID ARCHITECTURES & GRAPH TRANSFORMERS



Combining GNNs with Transformers for attention-based neighbor weighting.

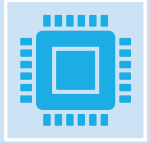


Cross-domain synergy: LLMs + GNNs for knowledge-intensive tasks.



Performance vs. complexity trade-offs.

4.6 AUTOMATED GNN ARCHITECTURE SEARCH



NAS for GNNs (GraphNAS, Auto-GNN).



- Auto-optimized layer stacking, attention mechanisms. Balancing
- performance, interpretability, and scalability.