Message Passing Neural Networks

(MPNNs)

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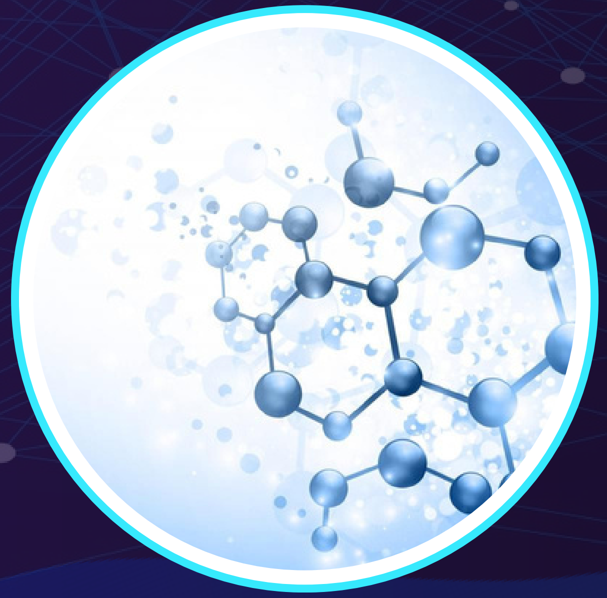
Why Graphs?

Many real-world problems are graphs.

- Social networks → People as nodes, friendships as edges
- Molecules → Atoms as nodes, bonds as edges
- Transport → Intersections as nodes, roads as edges

Graphs are irregular — every node can have a different number of neighbors.
That's why we need specialized models.



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What are GNNs?

A Graph Neural Network is a neural network that works directly on graphs.

- Nodes: The basic entities in the graph. Each node can have features (describing properties)
- Edges: The relationships or connections between nodes.
- Input: Nodes, edges, and features
- Output: Node, edge, or graph-level predictions

Nodes learn by aggregating info from neighbors

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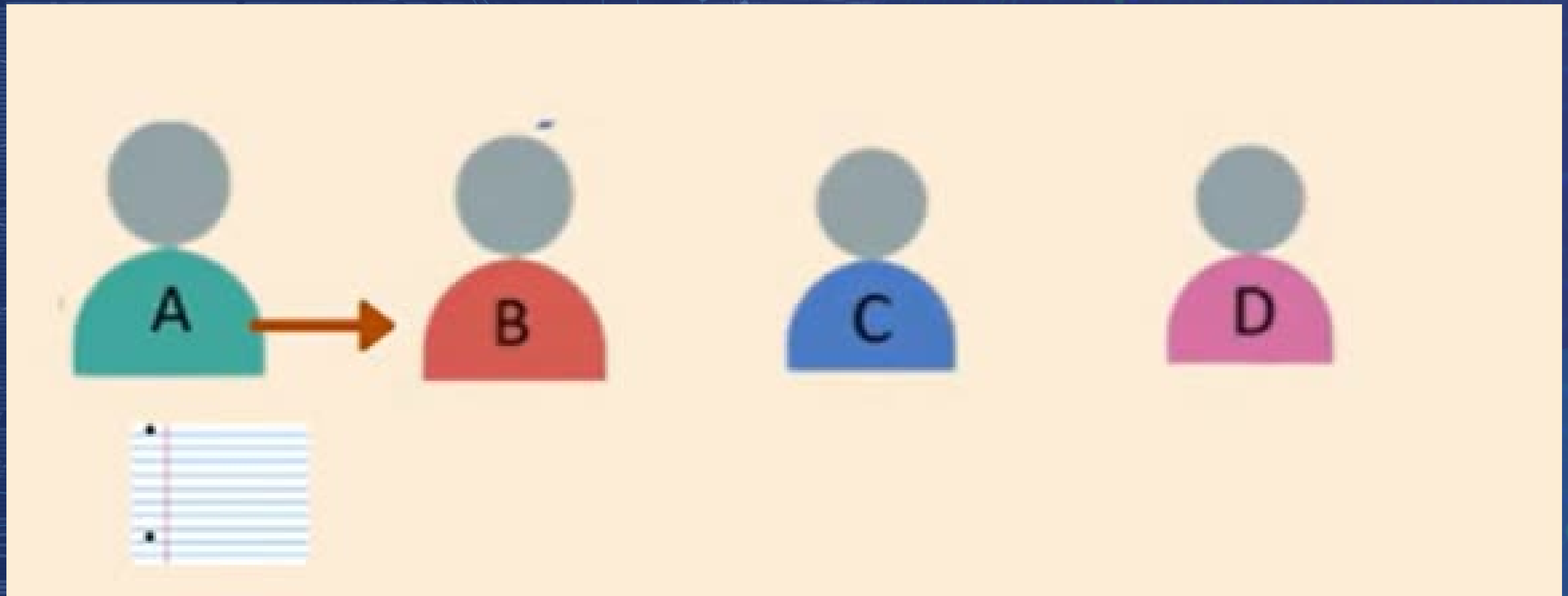
Message Passing Intuition

Think of a gossip network:

- Each node sends a message to its neighbors
- Each node collects incoming messages
- Each node updates its state based on neighbors

After 1 round → knows neighbors,
After 2 → neighbors-of-neighbors

Gossip spreading step by step



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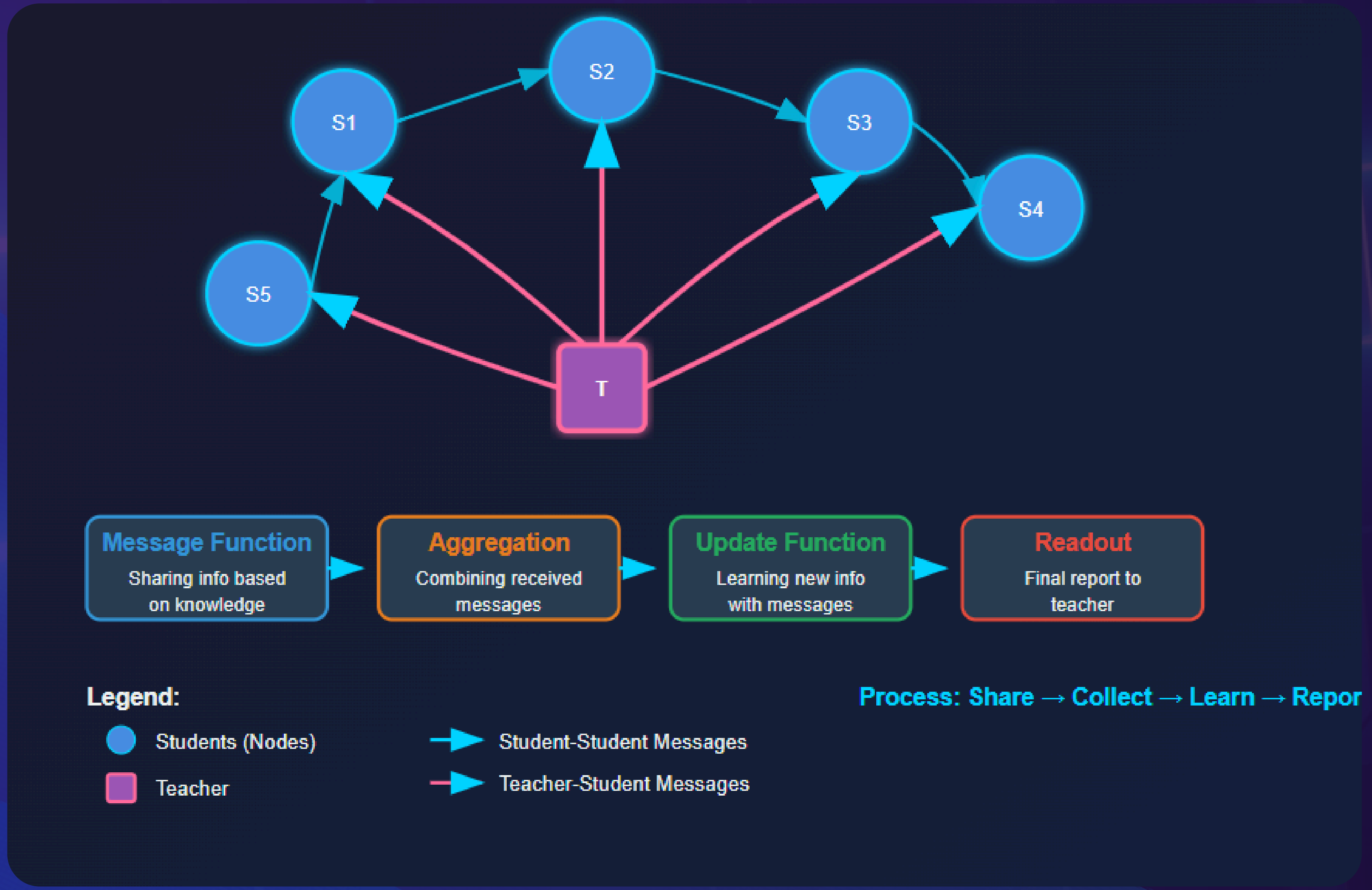
Formal MPNN Framework



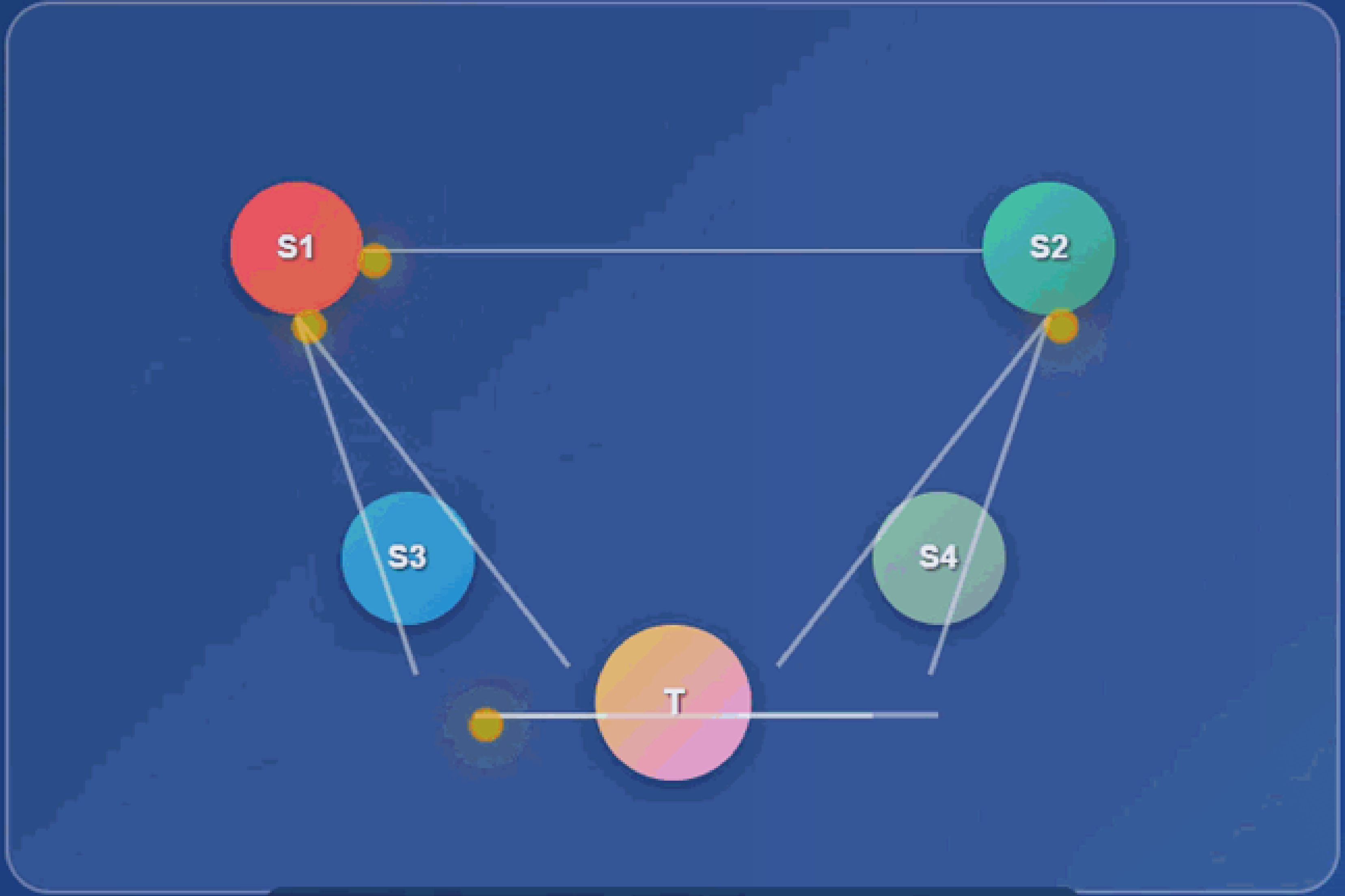
Think of a classroom of students (nodes). Each student learns not only from the teacher but also from talking to their friends (neighbors).

- Message Function → Sharing info: Each student sends a message to their friends (depends on own knowledge, friend's knowledge, relationship).
- Aggregation → Collecting info: Students combine all received messages (sum, mean, or max).
- Update Function → Learning new info: Mix old knowledge with new messages.
- Readout → Final report: Collect knowledge from all students for the teacher.

So MPNN = Share → Collect → Learn → Report.

Phase 2: Message Passing

MPNN: Share → Collect → Learn → Report



Messages flow between connected students (neighbors)

07 Toy Example – How Information Spreads

Imagine 4 students in a group, each starts with score = 1.

- Student A has 2 friends. Each sends their '1'. → A's new score = 3.
- Student B has 3 friends. Each sends their '1'. → B's new score = 4.

More friends = more knowledge spread.

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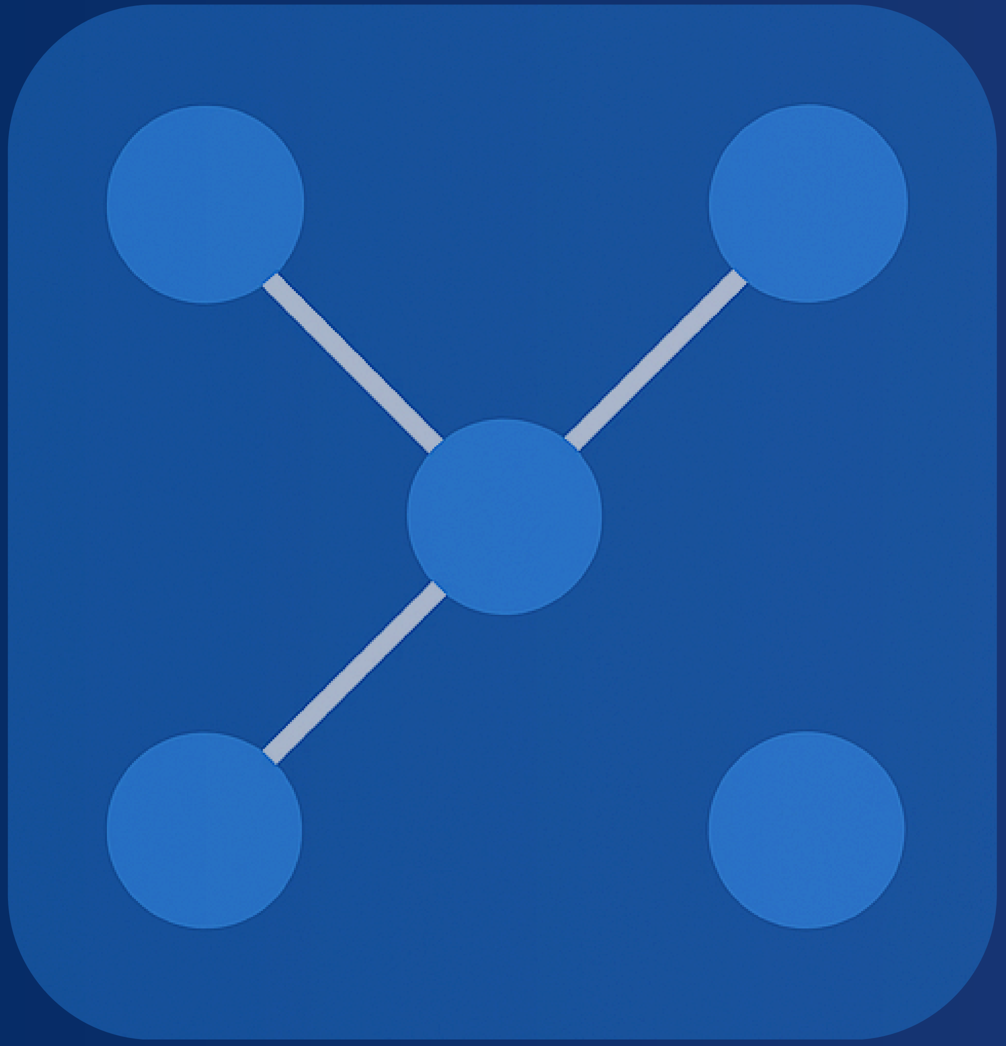
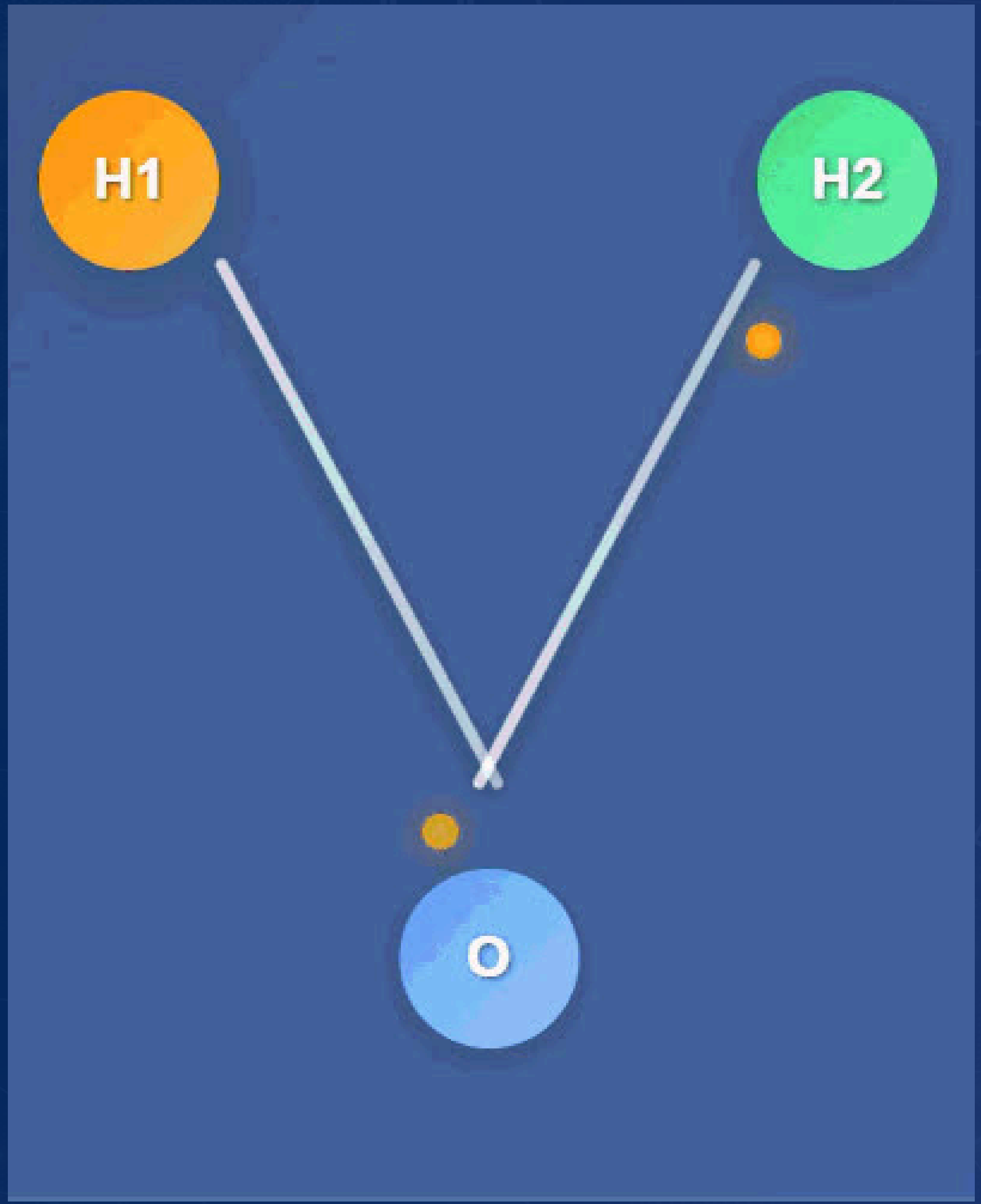
Design Choices In MPNNs



- How to share info (Message): Simple notes OR attention (important friends).
- How to collect info (Aggregator): Sum (total marks), Mean (average), Max (strongest idea).
- How to learn new info (Update): Simple math OR advanced memory (GRU).
- How to report (Readout): Collect all students' scores → final class report.

Different choices = different kinds of Graph Neural Networks.



Applications of MPNNs

- Chemistry & Drug Discovery – Predict molecular properties (toxicity, solubility, drug efficacy)
- Traffic & Transportation – Forecast congestion, optimize routes (smart cities, maps)
- Social Networks – Link prediction, fraud detection, friend recommendations
- Recommendation Systems – Users ↔ Items as a graph → personalized suggestions
- Knowledge Graphs / NLP – Question answering, semantic search

MPNNs for Molecular Property Prediction In Applications

MPNN Application Working:

MPNNs operate on graph data (e.g., molecules). Nodes (atoms) send and receive messages from neighbors to update their states. After several message-passing rounds, node features are aggregated to form a graph representation, which is used to predict properties like solubility or toxicity.

Popular Variants of MPNNs

Graph Convolutional Network (GCN)

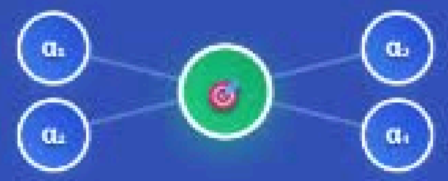
Spectral approach with normalized adjacency matrix. Simple aggregation via averaging neighbor features.

GraphSAGE

Sampling and aggregating from node neighborhoods. Uses different aggregators (mean, max, LSTM).

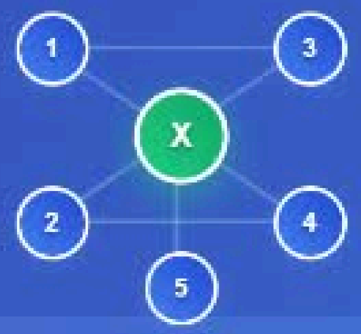
Graph Attention Network (GAT)

Attention mechanism to weight neighbor contributions. Learns importance of different neighbors dynamically.



Graph Isomorphism Network (GIN)

Maximally powerful GNN for distinguishing graph structures. Uses injective aggregation functions.



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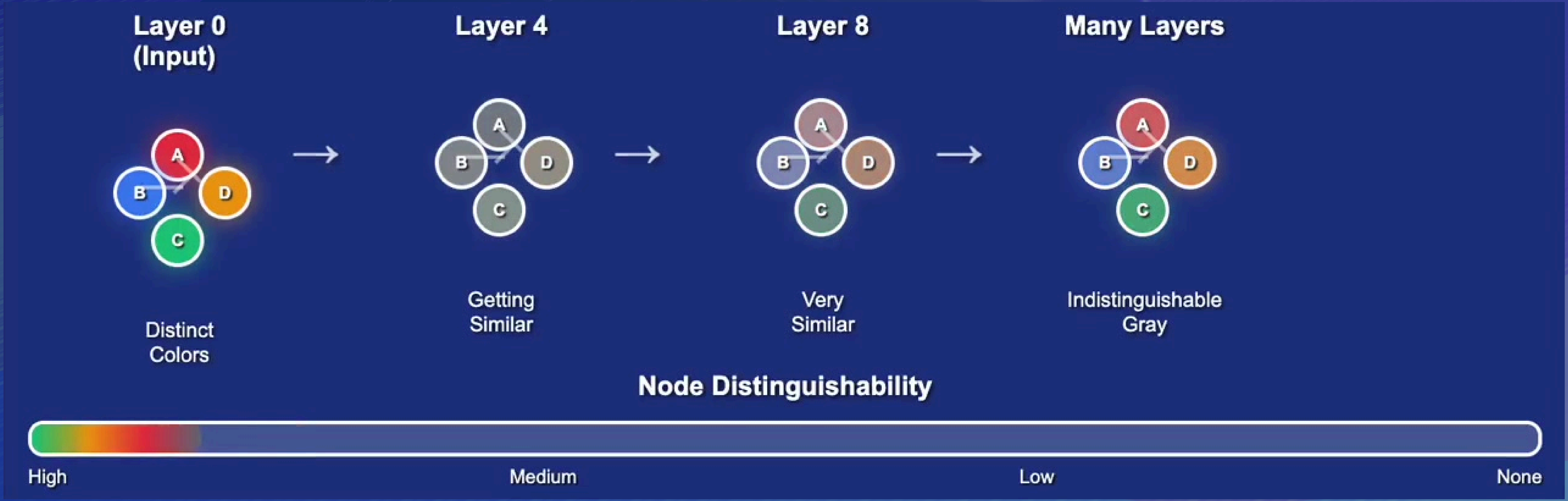
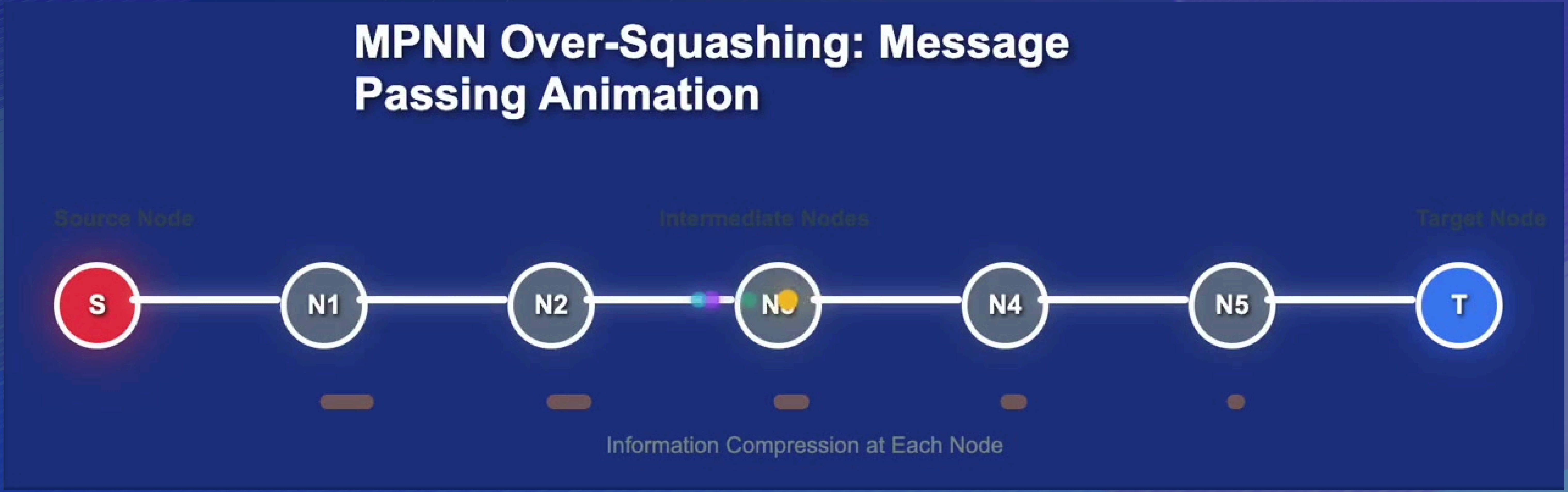
Limitations and Challenges of MPNNs

- **Over-Smoothing -** Too many layers make node features indistinguishable



Limitations and Challenges of MPNN s

- **Over-Squashing –** Long-range information gets compressed



Limitations and Challenges of MPNN s

- **Scalability Issues –** Large graphs consume excessive memory
- **Expressiveness Limitations –** WL-test constraints
- **Training Challenges –** Irregular graph structures hinder batching
- **Data and Label Limitations –** Small, domain-specific datasets

Future Opportunities in MPNNs

- Scalability to Large Graphs
- Integration with Transformers
- Dynamic & Temporal Graph Learning
- Cross-Domain Applications
- Explainability & Data Efficiency

Summary

- Message Passing Neural Networks (MPNNs) are a type of Graph Neural Network

- That learn by exchanging information between connected nodes. They capture

- Both local and global graph patterns, and are applied in chemistry, traffic

- Forecasting, and social networks. However, they face challenges such as oversmoothing, scalability, and limited datasets.

THANK YOU....