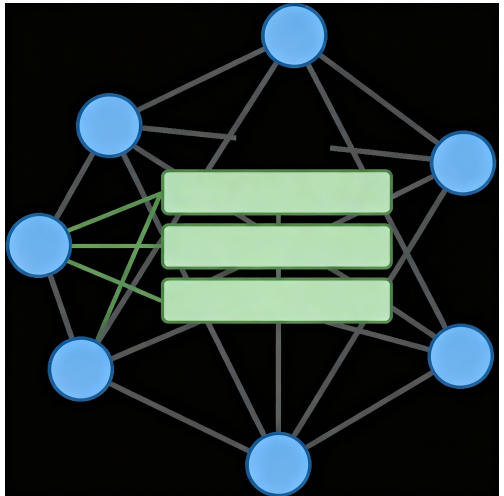
Understanding Key Challenges in Graph Neural Networks

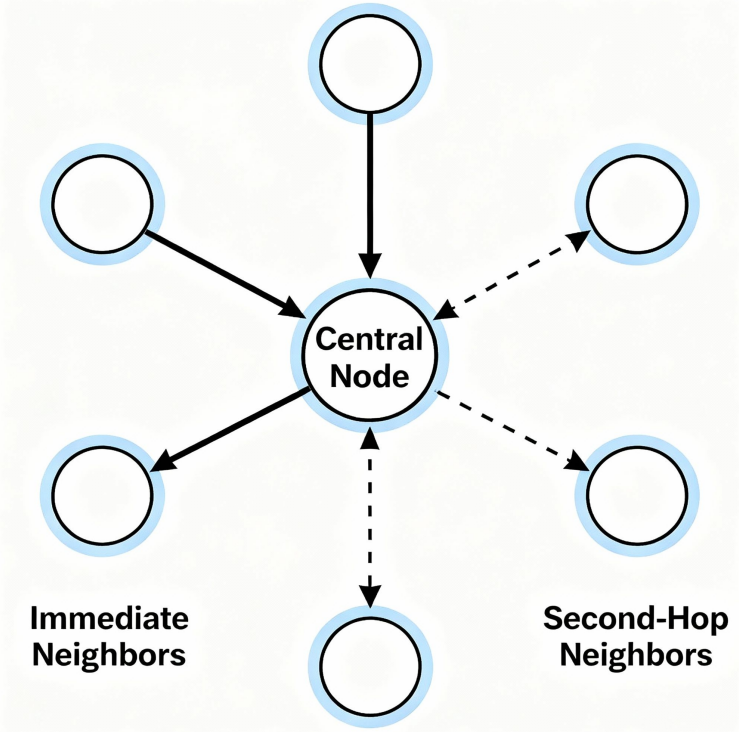


Intuition Behind Graph Neural Networks

GNNs learn node representations by **aggregating features** from neighbors.

Combine information from multiple hops to capture graph structure.

Effective for social networks, molecules, recommendation systems.

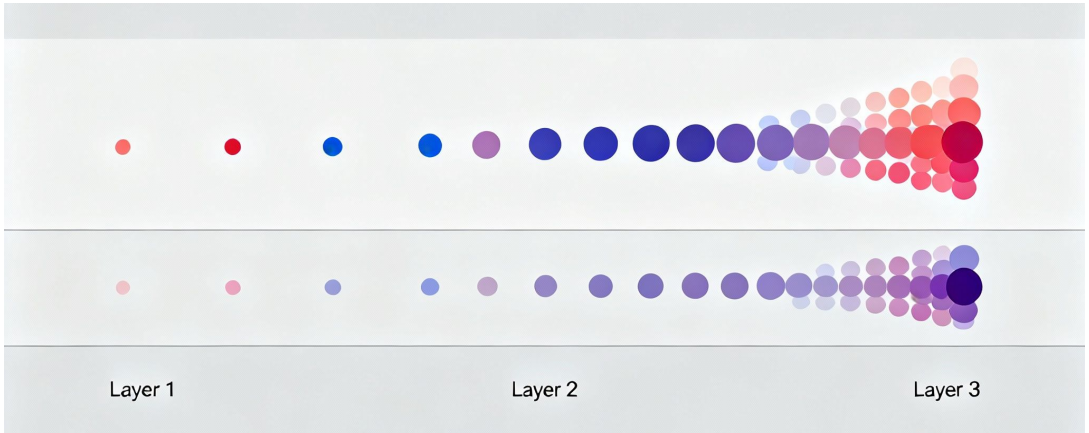


Over-smoothing Problem in GNNs

Definition: Node representations become indistinguishable as layers increase.

Causes: Repeated aggregation blurs unique node features.

Impact: Loss of discriminative power, hurting performance in deep GNNs.

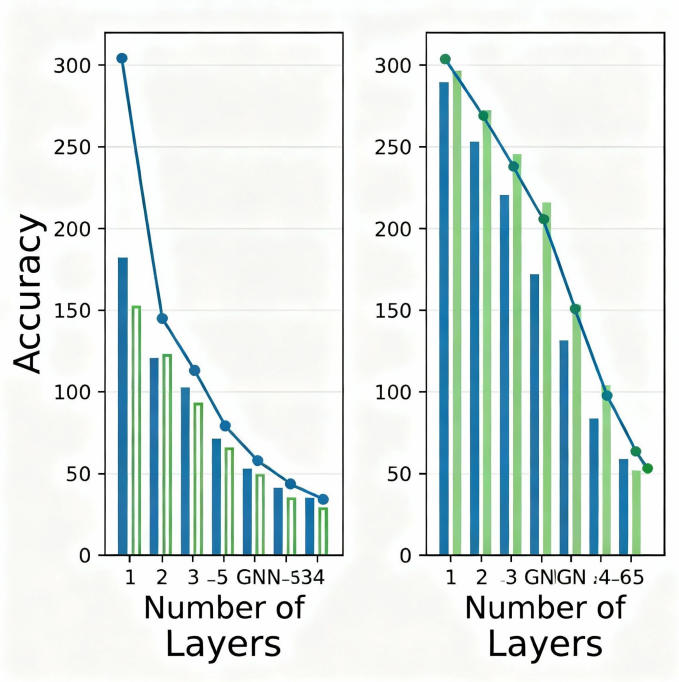


Real-world Example of Over-smoothing

Scenario: Classifying nodes in a social network with many layers.

Early layers: Clear differentiation of user interests.

Deep layers: Personalized info gets lost, users appear same.

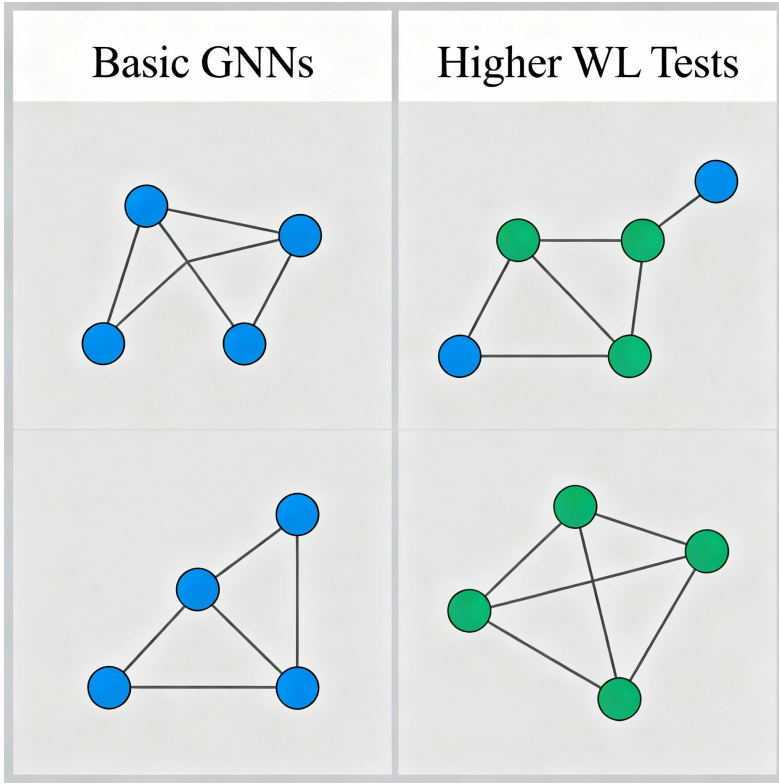


Expressive Power of Graph Neural Networks

Expressive power: Ability to distinguish different graph structures.

Weisfeiler-Lehman (WL) test connection: GNNs as graph isomorphism testers.

Standard GNNs ≈ 1-WL test, limits capturing complex structures.

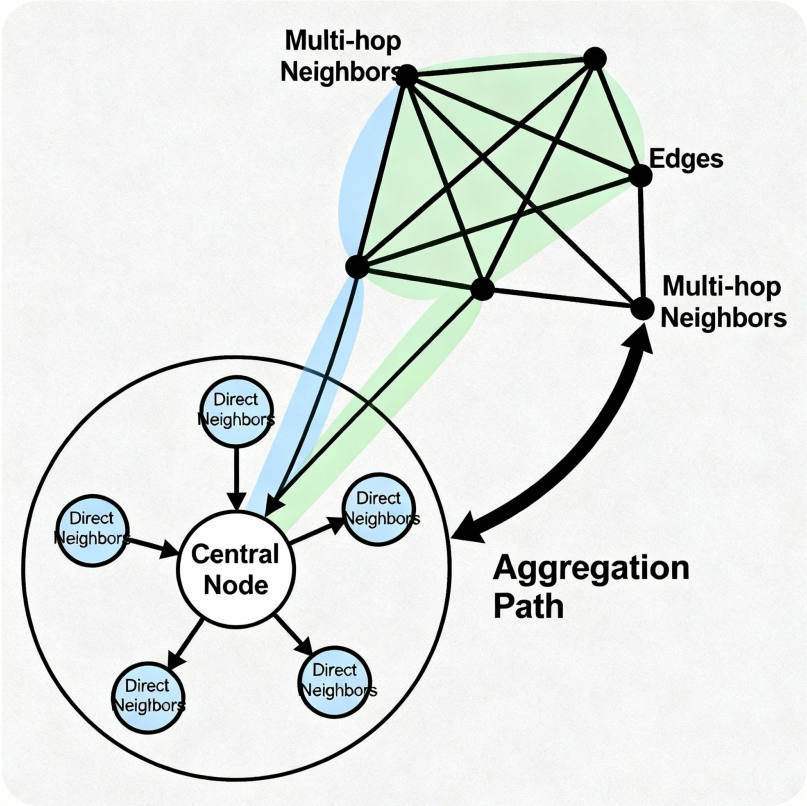


Enhancing Expressive Power

Higher-order GNNs (k-WL inspired).

Incorporating subgraph or edge features.

Using attention mechanisms.



Scalability Challenges in GNNs

Graph sizes grow large: millions or billions of nodes.

Computing multi-hop neighbors is **costly**.

Memory and computation **bottlenecks** in training and inference.

Solutions for Scalability

Sampling methods: GraphSAGE, Cluster-GCN.

Mini-batch training on subgraphs.

Approximate algorithms and graph partitioning.

Interpretability of GNNs

Why interpretability matters: Trust, debugging, regulatory compliance.

Challenges: Complex neighbor aggregation; opaque learned features.

Methods: Node/edge importance, subgraph pattern explanations.

Adversarial Robustness in GNNs

GNNs vulnerable to adversarial attacks: **maliciously** altered nodes or edges.

Effects: Misclassification, disruption of learned patterns.

Defenses: Robust training, graph sanitization, detection mechanisms.

Summary and Takeaways

Over-smoothing limits deep GNN layers—balance depth carefully.

Expressive power tied to graph isomorphism tests—look beyond 1-WL for complex tasks.

Scalability addressed via sampling and partitioning.

Interpretability crucial for trust—use explanation tools.

Adversarial robustness: ongoing challenge with emerging defenses.