

Training Course on Graph Neural Networks and Graph Machine Learning

Professional Development Training Course Outline

Category	Data Science	Duration	10 Days
Base Fee	\$3,000 USD	Delivery Mode	Online / On-site Hybrid

Course Introduction

In an increasingly interconnected world, understanding and leveraging **relational data** is paramount for advanced **data science** and **artificial intelligence** applications. Traditional machine learning models often struggle to capture the intricate dependencies and rich contextual information embedded within **graph-structured data**. This is where **Graph Neural Networks (GNNs)** and **Graph Machine Learning** emerge as revolutionary paradigms. GNNs, a powerful class of **deep learning models**, are specifically designed to operate directly on graphs, enabling the extraction of meaningful patterns, predicting connections, and classifying nodes or entire networks with unprecedented accuracy.

Training Course on Graph Neural Networks (GNNs) & Graph Machine Learning dives deep into the theoretical foundations and practical applications of GNNs, equipping participants with the skills to effectively analyze and model complex **network data**. From fundamental **graph theory** concepts and various **GNN architectures** like **Graph Convolutional Networks (GCNs)** and **Graph Attention Networks (GATs)** to advanced topics such as **graph embedding**, **large-scale graph processing**, and **dynamic graphs**, this program covers the entire spectrum. Through hands-on exercises and real-world **case studies** spanning **social network analysis**, **recommendation systems**, **drug discovery**, and **fraud detection**, attendees will gain the expertise to unlock profound insights from their relational datasets and drive innovation within their organizations.

Programme Curriculum

Training Course on Graph Neural Networks (GNNs) & Graph Machine Learning: Analyzing and Modeling Relational Data

Introduction

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Course Objectives

1. Master the foundational concepts of graph theory and network science.
2. Understand the core principles of Graph Neural Networks (GNNs) and their distinction from traditional neural networks.
3. Implement various GNN architectures, including Graph Convolutional Networks (GCNs), Graph Attention Networks (GATs), and GraphSAGE.
4. Apply graph embedding techniques for learning low-dimensional representations of nodes and graphs.
5. Develop skills in node classification, link prediction, and graph classification tasks using GNNs.
6. Explore advanced GNN architectures and their applications in complex scenarios.
7. Learn techniques for handling large-scale graph data and ensuring computational efficiency.
8. Gain proficiency in popular GNN libraries like PyTorch Geometric and Deep Graph Library (DGL).
9. Implement GNNs for real-world problems across diverse industries.
10. Understand model interpretability techniques for GNNs to explain predictions.
11. Explore the latest research trends and future directions in Graph Machine Learning.
12. Design and optimize GNN models for specific relational data challenges.
13. Develop a robust training methodology for GNNs, including hyperparameter tuning and evaluation.

Organizational Benefits

- Transform complex relational data into actionable intelligence, uncovering patterns and relationships invisible to traditional analytical methods.
- Improve the accuracy of predictions in areas like customer behavior, fraud detection, and drug efficacy, leading to better decision-making.

- Leverage GNNs to optimize network routing, supply chain logistics, and resource allocation, driving operational efficiencies.
- Develop highly personalized recommendation systems and customer engagement strategies, boosting satisfaction and loyalty.
- Enhance security by identifying sophisticated fraudulent networks and anomalous activities in real-time.
- Empower R&D teams in areas like drug discovery and material science to accelerate new product development.
- Foster a culture of data-driven innovation by equipping teams with cutting-edge analytical tools for graph data.
- Stay ahead of the curve in an increasingly data-centric landscape by adopting advanced **AI and Machine Learning** techniques.

Target Audience

1. Data Scientists.
2. Machine Learning Engineers.
3. AI Researchers.
4. Software Developers.
5. Analytics Professionals.
6. Bioinformaticians & Chemoinformaticians
7. Financial Analysts & Fraud Investigators
8. Anyone with a strong foundation in Python and Machine Learning

Course Outline

Module 1: Introduction to Graph Theory and Network Science

- Fundamentals of graphs: nodes, edges, types of graphs (directed, undirected, weighted, unweighted).
- Representing graphs: adjacency matrices, adjacency lists, edge lists.
- Key graph properties: degree, paths, cycles, connectivity, centrality measures.
- Introduction to real-world networks: social networks, citation networks, biological networks.
- **Case Study:** Analyzing a small social network dataset to identify central figures and community structures using basic graph metrics.

Module 2: Limitations of Traditional Machine Learning on Graph Data

- Why traditional ML models (CNNs, RNNs, MLPs) struggle with non-Euclidean graph data.
- The concept of permutation invariance and its importance in graph learning.
- Challenges in defining fixed-size input features for nodes and edges.
- The need for models that can capture relational information and propagate messages.
- **Case Study:** Demonstrating the failure of a simple neural network to classify nodes in a graph without considering connectivity.

Module 3: Foundations of Graph Neural Networks (GNNs)

- The message-passing paradigm: aggregate and update functions.
- Node embeddings and graph embeddings.
- Introduction to Graph Convolution (Spectral vs. Spatial approaches).
- The role of aggregation functions (sum, mean, max).
- **Case Study:** Illustrating the message-passing process on a toy graph to understand how node representations are learned.

Module 4: Graph Convolutional Networks (GCNs)

- Detailed explanation of the GCN architecture and its mathematical formulation.
- Implementing GCNs for node classification.
- Understanding the role of regularization and activation functions in GCNs.
- Training GCNs: loss functions, optimizers, and evaluation metrics.
- **Case Study:** Building a GCN model to classify academic papers in a citation network (e.g., Cora dataset).

Module 5: Graph Attention Networks (GATs)

- Introduction to the attention mechanism in GNNs.
- How GATs learn varying importance for neighboring nodes.
- Implementing GATs for enhanced relational learning.
- Multi-head attention and its benefits.
- **Case Study:** Applying GATs to a protein-protein interaction network for improved biological function prediction.

Module 6: Inductive Learning with GraphSAGE

- Understanding the limitations of transductive GNNs.
- GraphSAGE: A framework for learning node embeddings in an inductive setting.
- Sampling strategies for efficient neighborhood aggregation.
- Different aggregation functions in GraphSAGE (mean, LSTM, pooling).
- **Case Study:** Using GraphSAGE to generate embeddings for new users in a dynamic social media platform and predict their interests.

Module 7: Advanced GNN Architectures

- Recap of different GNN variants and their strengths.
- Exploring Heterogeneous Graph Neural Networks (HGNNs).
- Introduction to Relational Graph Convolutional Networks (RGCNs) for multi-relational graphs.
- Graph Autoencoders (GAE) and Variational Graph Autoencoders (VGAE) for graph generation.
- **Case Study:** Modeling a knowledge graph with RGCNs for question answering or entity linking.

Module 8: Graph Embedding Techniques

- Traditional graph embedding methods: Node2Vec, DeepWalk.
- Comparing traditional embeddings with GNN-learned embeddings.
- Utilizing embeddings for downstream tasks: visualization, clustering.
- Evaluating the quality of graph embeddings.
- **Case Study:** Visualizing learned node embeddings from a fraud transaction network to identify suspicious clusters.

Module 9: Training and Optimization of GNNs

- Data preprocessing for graph data: feature engineering, graph normalization.
- Loss functions tailored for graph tasks (e.g., negative sampling for link prediction).
- Hyperparameter tuning strategies for GNNs.
- Regularization techniques to prevent overfitting in graph models.

- **Case Study:** Optimizing a GNN model for a large-scale product recommendation system to improve recommendation accuracy.

Module 10: Handling Large-Scale Graph Data

- Challenges of training GNNs on massive graphs.
- Graph partitioning strategies for distributed training.
- Mini-batch training and sampling techniques for large graphs.
- Introduction to specialized frameworks for scalable GNNs.
- **Case Study:** Discussing approaches for training GNNs on graphs with billions of nodes and edges, such as the Google Maps graph.

Module 11: Real-World Applications: Social Network Analysis

- Community detection: algorithms and GNN-based approaches.
- Influence maximization and viral marketing.
- Sentiment analysis on social graphs.
- User profiling and friend recommendation.
- **Case Study:** Identifying influential users and detecting echo chambers within a Twitter-like social network using GNNs.

Module 12: Real-World Applications: Recommendation Systems

- Collaborative filtering and content-based recommendation.
- Modeling user-item interactions as graphs.
- GNN-based approaches for personalized recommendations.
- Cold-start problem resolution using GNNs.
- **Case Study:** Developing a GNN-powered movie recommendation engine, considering user preferences and movie genres.

Module 13: Real-World Applications: Drug Discovery & Bioinformatics

- Representing molecules as graphs: atoms as nodes, bonds as edges.
- Predicting molecular properties and drug-target interactions.
- Analyzing biological networks: protein-protein interaction networks, gene regulatory networks.
- Drug repurposing and lead optimization using GNNs.
- **Case Study:** Utilizing GNNs to predict the binding affinity of small molecules to a target protein for drug discovery

Module 14: Real-World Applications: Fraud Detection & Financial Networks

- Modeling financial transactions and accounts as graphs.
- Identifying fraudulent patterns and communities.
- Anomaly detection in financial networks.
- Graph-based approaches for anti-money laundering (AML).
- **Case Study:** Detecting credit card fraud rings by analyzing transactional graphs for unusual connectivity patterns.

Module 15: Model Interpretability and Future Trends in GNNs

- Explaining GNN predictions: techniques like GNNExplainer.
- Robustness and adversarial attacks on GNNs.
- Dynamic and temporal graph neural networks.

- Graph Transformers and their potential.
- **Case Study:** Interpreting the decisions of a GNN model in a sensitive application, like medical diagnosis, to build trust and understand biases.

Training Methodology

This course employs a participatory and hands-on approach to ensure practical learning, including:

- Interactive lectures and presentations.
- Group discussions and brainstorming sessions.
- Hands-on exercises using real-world datasets.
- Role-playing and scenario-based simulations.
- Analysis of case studies to bridge theory and practice.
- Peer-to-peer learning and networking.
- Expert-led Q&A sessions.
- Continuous feedback and personalized guidance.

Register as a group from 3 participants for a Discount

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Certification

Upon successful completion of this training, participants will be issued with a globally- recognized certificate.

Tailor-Made Course

We also offer tailor-made courses based on your needs.

Key Notes

- a. The participant must be conversant with English.
- b. Upon completion of training the participant will be issued with an Authorized Training Certificate
- c. Course duration is flexible and the contents can be modified to fit any number of days.
- d. The course fee includes facilitation training materials, 2 coffee breaks, buffet lunch and A Certificate upon successful completion of Training.
- e. One-year post-training support Consultation and Coaching provided after the course.
- f. Payment should be done at least a week before commence of the training, to FINESKILL TRAINING CENTER account, as indicated in the invoice so as to enable us prepare better for you.

Upcoming Scheduled Sessions

Start Date	End Date	Location	Price
07 Sep 2026	18 Sep 2026	Physical	\$3,000
14 Sep 2026	25 Sep 2026	Physical	\$3,000
21 Sep 2026	02 Oct 2026	Physical	\$3,000
28 Sep 2026	09 Oct 2026	Physical	\$3,000
05 Oct 2026	16 Oct 2026	Physical	\$3,000
12 Oct 2026	23 Oct 2026	Physical	\$3,000
19 Oct 2026	30 Oct 2026	Physical	\$3,000
26 Oct 2026	06 Nov 2026	Physical	\$3,000

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