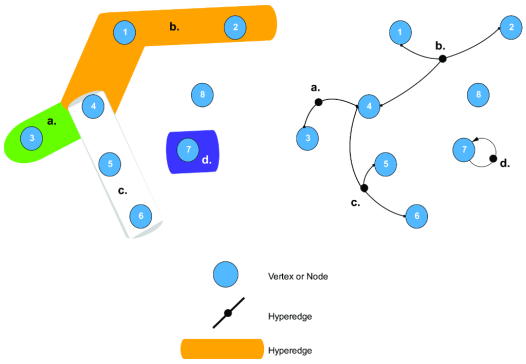
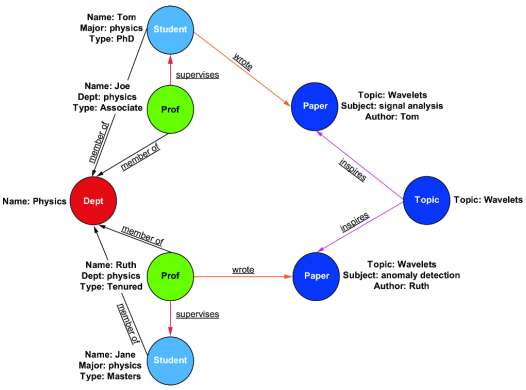
Graph Machine Learning



hypergraph



knowledge graph

Introduction

Machine Learning as Optimization: A Simple Summary

Machine learning is fundamentally an **optimization problem** where we search for the best possible model to perform a specific task.

The Core Process

Goal: Find a mathematical model that achieves optimal performance on a given task

Key Components:

1. **Performance Metric** (Loss Function/Cost Function)
2. Quantifies how well the model is performing
3. Lower loss = better performance
4. **Data-Driven Learning**
5. Algorithm receives data (often large amounts)
6. Uses this data to make iterative improvements
7. **The Learning Cycle** (Training):

```
Make Decision/Prediction
    ↓
Evaluate with Loss Function
    ↓
Calculate Error
    ↓
Update Model Parameters
    ↓
(Repeat until performance is satisfactory)
```

The Essence: At each iteration, the model makes predictions, measures how wrong it is, and adjusts its internal parameters to do better next time. Through repeated cycles, the model progressively improves its performance.

This iterative process of **learning from mistakes** is what we call **training -** it's how machines get "smarter" at their tasks over time.

🎓 Supervised Learning in Graph ML

<x, y>

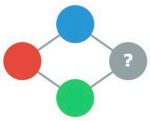
x = Input (graph, node features, network structure)
y = Known output (labels we want to predict)

↓

Goal: Learn from labeled examples, then predict on new data

Node Classification

Discrete Labels

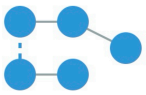


Predict: Node Category

- 📱 Social Network: User interests
- 🧬 Biology: Protein function
- 📄 Citation: Paper topic

Link Prediction

Edge Exists?



Predict: Will edge exist?

- 👥 Social: Friend suggestions
- 🛒 E-commerce: Product recommendations
- 💊 Drug: Protein interactions

Graph Classification

Discrete Labels

Predict: Graph Property

- ⚗️ Chemistry: Molecule toxicity
- 📱 Social: Community type
- 🧠 Neuroscience: Brain state

Key Differences from Traditional ML

Traditional ML:

- Independent samples
- Fixed features
- No relationships

Graph ML:

- Connected samples
- Relational features
- Network structure matters

Supervised Learning

<x, y>

Goal: Learn from labeled examples
We know: Inputs AND outputs

All labels known

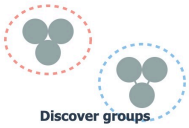
Graph ML Tasks:

- Node classification
- Link prediction
- Graph classification

Unsupervised Learning

<x>

Goal: Find patterns and structure
We know: Only inputs (no labels)



Discover groups

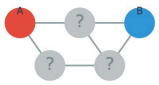
Graph ML Tasks:

- Community detection
- Node clustering
- Graph embedding

Semi-Supervised

<x, y> + <x>

Goal: Use few labels to guide learning
We know: Few labels + many unlabeled



Few labels guide learning

Graph ML Tasks:

- Label propagation
- Few-shot node classification
- Graph SSL methods

Reinforcement Learning

State → Action → Reward/Penalty

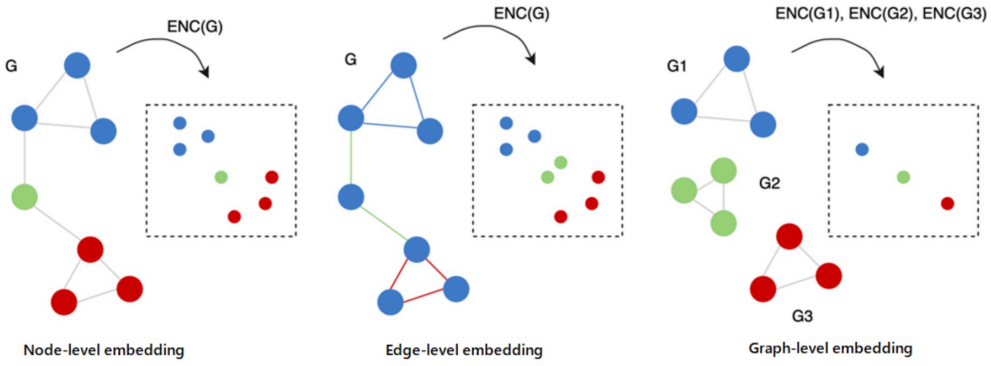
Goal: Learn sequence of decisions
Method: Trial and error with feedback
Objective: Maximize rewards, minimize penalties

Graph ML Tasks:

- Graph navigation/path finding
- Molecule generation
- Network optimization

Learn best path through rewards/penalties

Graph Learning Tasks



Node-level embedding | Edge-level embedding | Graph-level embedding

Graph Machine Learning levels

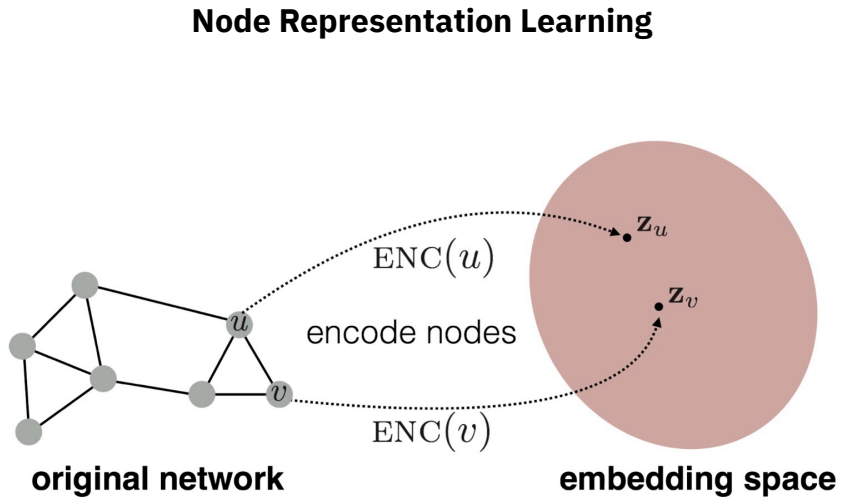


Figure 3.1: Illustration of the node embedding problem. Our goal is to learn an encoder (ENC), which maps nodes to a low-dimensional embedding space. These embeddings are optimized so that distances in the embedding space reflect the relative positions of the nodes in the original graph.

$$\text{ENC} : \mathcal{V} \rightarrow \mathbb{R}^d,$$

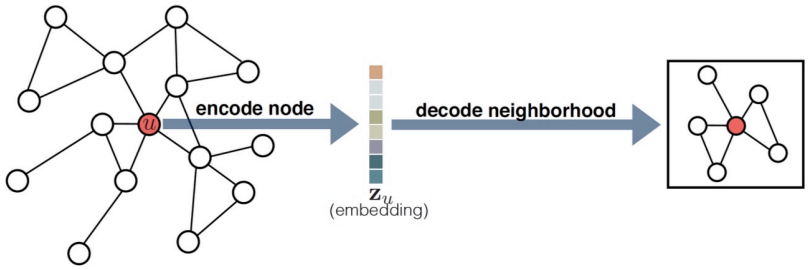


Figure 3.2: Overview of the encoder-decoder approach. The encoder maps the node u to a low-dimensional embedding $\mathbf{z}_u$. The decoder then uses $\mathbf{z}_u$ to reconstruct u's local neighborhood information.

$$\text{DEC} : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^+.$$

$$\text{DEC}(\text{ENC}(u), \text{ENC}(v)) = \text{DEC}(\mathbf{z}_u, \mathbf{z}_v) \approx \mathbf{S}[u, v].$$

To achieve the reconstruction this objective, the standard practice is to minimize an empirical reconstruction loss Lover a set of training node pairs D:

$$\mathcal{L} = \sum_{(u,v)\in\mathcal{D}} \ell\big(\mathrm{DEC}(\mathbf{z}_u, \mathbf{z}_v), \mathbf{S}[u,v]\big),$$

Method	Decoder	Similarity measure	Loss function
Lap. Eigenmaps	$\|\mathbf{z}_u - \mathbf{z}_v\|_2^2$	general	$\mathrm{DEC}(\mathbf{z}_u, \mathbf{z}_v) \cdot \mathbf{S}[u,v]$
Graph Fact.	$\mathbf{z}_u^\top \mathbf{z}_v$	$\mathbf{A}[u,v]$	$\|\mathrm{DEC}(\mathbf{z}_u, \mathbf{z}_v) - \mathbf{S}[u,v]\|_2^2$
GraRep	$\mathbf{z}_u^\top \mathbf{z}_v$	$\mathbf{A}[u,v], \ldots, \mathbf{A}^k[u,v]$	$\|\mathrm{DEC}(\mathbf{z}_u, \mathbf{z}_v) - \mathbf{S}[u,v]\|_2^2$
HOPE	$\mathbf{z}_u^\top \mathbf{z}_v$	general	$\|\mathrm{DEC}(\mathbf{z}_u, \mathbf{z}_v) - \mathbf{S}[u,v]\|_2^2$
DeepWalk	$\frac{e^{\mathbf{z}_u^\top \mathbf{z}_v}}{\sum_{k\in\mathcal{V}} e^{\mathbf{z}_u^\top \mathbf{z}_k}}$	$p_{\mathcal{G}}(v\|u)$	$-\mathbf{S}[u,v] \log(\mathrm{DEC}(\mathbf{z}_u, \mathbf{z}_v))$
node2vec	$\frac{e^{\mathbf{z}_u^\top \mathbf{z}_v}}{\sum_{k\in\mathcal{V}} e^{\mathbf{z}_u^\top \mathbf{z}_k}}$	$p_{\mathcal{G}}(v\|u)$ (biased)	$-\mathbf{S}[u,v] \log(\mathrm{DEC}(\mathbf{z}_u, \mathbf{z}_v))$

Shallow embedding approaches face three major drawbacks:

```
1.  No Parameter Sharing:
Each node has its own independent embedding vector, leading to
poor statistical efficiency and high computational cost. The
number of parameters grows linearly with the number of nodes
O(|V|), making the method unscalable for large graphs.

2.  No Use of Node Features:
These methods ignore rich node attribute information that could
improve the quality and generalizability of learned
representations.

3.  Transductive Limitation:
Shallow embeddings can only represent nodes seen during training.
They cannot generalize to unseen nodes without retraining,
preventing their use in inductive settings.
```

DeepWalk Architecture

DeepWalk is a two-step approach for learning node representations:

1. **Random Walk Generation**: Generate random walks from the graph (similar to sequences of words)
2. **SkipGram Training**: Use SkipGram to learn node representations

Word2Vec and SkipGram

SkipGram Model: Predicts context words given a target word.

Mathematical Formulation: For a vocabulary of N words: $w_1, w_2, ..., w_N$

The goal is to maximize the probability of context words given the target word:

$$ P(w_{i+j}|w_i) = \frac{exp(v_{w_{i+j}}^T v_{w_i})}{\sum_{w=1}^N exp(v_w^T v_{w_i})} $$

where v_w is the vector representation of word w.

Objective Function:

$$\frac{1}{N}\sum_{n=1}^{N}\sum_{-c\leq j\leq c, j\neq 0}\log p(W_{n+j}|W_n)$$

where c is the context window size.

Node2Vec

Extension of DeepWalk with biased random walks:

- **p parameter**: Controls return to previous node
- **q parameter**: Controls exploration vs exploitation

Random Walk Strategy:

- **BFS-like**: Explores local neighborhood (homophily)

- **DFS-like**: Explores distant nodes (structural roles)

node2vec: Scalable Feature Learning for Networks

A Comprehensive Tutorial with Examples

Table of Contents

Introduction and Motivation

What is node2vec?

node2vec is an algorithmic framework for learning continuous feature representations (embeddings) for nodes in networks. It was introduced by Grover & Leskovec in 2016 and extends the earlier DeepWalk algorithm.

The Big Idea

Analogy: If words that appear in similar contexts should have similar embeddings (Word2Vec), then **nodes that appear in similar "graph contexts" should have similar embeddings**.

Key Innovation

node2vec introduces **flexible, biased random walks** that can smoothly interpolate between:

- **Breadth-First Search (BFS)**: Local neighborhood exploration
- **Depth-First Search (DFS)**: Exploring farther nodes

This flexibility allows node2vec to capture both:

1. **Homophily**: Nodes in the same community (nearby nodes)
2. **Structural equivalence**: Nodes with similar roles (e.g., both are hubs)

Background: From Word2Vec to node2vec

Word2Vec: The Inspiration

Skip-gram model learns word embeddings by:

1. Taking a sentence: "the quick brown fox jumps"
2. Creating pairs: (quick, the), (quick, brown), (brown, quick), (brown, fox), ...
3. Learning embeddings where: P(context_word | center_word) is high

Mathematical objective: ``` maximize: Σ log P(w_context | w_center)

where: P(w_c | w_center) = exp(z_c^{T} · z_center) / Σ_w exp(z_w^{T} · z_center) ```

Adapting to Graphs

The mapping:

- Sentences → **Random walks** on the graph
- Words → **Nodes**
- Context window → **Nodes appearing together in walks**

Example: Walk: 1 → 3 → 5 → 7 → 9

- Creates pairs: (1,3), (1,5), (3,1), (3,5), (3,7), (5,3), (5,7), (5,9), ...

Random Walks on Graphs

What is a Random Walk?

A **random walk** is a path through the graph where at each step, we randomly choose one of the current node's neighbors.

Example Graph:

```
    1 --- 2
    |     |
    3 --- 4 --- 5
          |
          6
```

Random walk starting from node 1:

```
Step 0: At node 1
Step 1: Randomly pick neighbor → go to 2 or 3
Step 2: From there, randomly pick a neighbor
...
Continue for k steps
```

Example walk: 1 → 3 → 4 → 5 → 4 → 6

Uniform Random Walk (DeepWalk)

In **DeepWalk**, the probability of moving to a neighbor is uniform:

```
P(next = v | current = u) = 1/degree(u)  if (u,v) is an edge
                            0             otherwise
```

Problem: Uniform walks may not capture all graph properties equally well.

Biased Random Walks

The Problem with Uniform Walks

Consider these two graph properties:

1. **Homophily** (Community): Nodes 1, 2, 3 form a tight cluster
2. **Structural Role**: Node 1 and Node 10 are both "hub" nodes

Uniform random walks might not capture both equally well!

The node2vec Solution: Bias the Walk!

node2vec introduces **two parameters** to control the walk:

1. **p** (return parameter): Controls likelihood of revisiting a node
2. **q** (in-out parameter): Controls exploration vs. exploitation

The Biased Random Walk Mechanism

Setup: Currently at node **v**, came from node **t**, deciding where to go next.

Neighbors of v:

- **t**: The previous node (where we came from)
- $\mathbf{x_1}$: Neighbor at distance 1 from t (same distance as v)
- $\mathbf{x_2}$: Neighbor at distance 2 from t (farther than v)

Transition probabilities (unnormalized):

```
α(t, x) = 1/p    if x = t        (returning to previous node)
          1      if d(t,x) = 1    (staying at same distance)
          1/q    if d(t,x) = 2    (moving away)
```

where `d(t,x)` is the shortest path distance between t and x.

Visual Example

```
        t (previous)
        |
        v (current)
       /|\
      / | \
     /  |  \
    x₁  x₂  x₃

where:
- x₁ is also neighbor of t (distance 1 from t)
- x₂ is not neighbor of t (distance 2 from t)
- x₃ = t (distance 0, returning)
```

Transition probabilities:

`P(x₃ | v, came from t) ∝ 1/p  (return to t)`

`P(x₁ | v, came from t) ∝ 1    (explore at same level)`

`P(x₂ | v, came from t) ∝ 1/q  (go farther)`

Understanding Parameters p and q

Parameter p (Return Parameter)

Controls: Likelihood of immediately returning to the previous node

```
p < 1: High probability of returning → more "backtracking"
p = 1: No bias
p > 1: Low probability of returning → more "forward moving"
```

Use case:

- **Low p**: Keeps walk local, good for community detection
- **High p**: Encourages exploration, prevents getting stuck

Parameter q (In-Out Parameter)

Controls: Balance between BFS and DFS

```
q < 1: DFS-like behavior (explore far)
       → Good for capturing structural equivalence
       → Nodes with similar "roles" get similar embeddings

q = 1: No bias (similar to unbiased walk)

q > 1: BFS-like behavior (stay local)
       → Good for capturing homophily
       → Nodes in same community get similar embeddings
```

Example Settings

Setting 1: Community Detection (capture homophily)

`p = 1`

`q = 2`

→ BFS-like: Explores local neighborhood thoroughly

Setting 2: Structural Equivalence (capture roles)

`p = 1`

`q = 0.5`

→ DFS-like: Explores farther, finds nodes with similar structural patterns

Setting 3: Balanced

`p = 1`

`q = 1`

→ Unbiased (like DeepWalk)

The node2vec Algorithm

High-Level Algorithm

```
Algorithm: node2vec

Input:
  - Graph G = (V, E)
  - Dimensions d
  - Walk length l
  - Walks per node r
  - Context window size k
  - Parameters p, q

Output:
  - Embeddings Z ∈ R^(|V| × d)

Steps:
1. Precompute transition probabilities for biased walks
2. Generate walks:
   For each node u ∈ V:
     For i = 1 to r:
       Generate biased random walk of length l starting from u
3. Learn embeddings using Skip-gram:
   Optimize embeddings to predict context nodes from center nodes
4. Return learned embeddings Z
```

Step-by-Step Detailed Algorithm

Step 1: Precompute Transition Probabilities

For computational efficiency, we precompute all transition probabilities:

```
def precompute_transition_probs(G, p, q):
    """
    For each edge (t, v) in the graph, compute
    probabilities for the next step from v.
    """
    transition_probs = {}

    for edge in G.edges():
```

```
        t, v = edge  # came from t, currently at v
        probs = {}

        for neighbor in G.neighbors(v):
            if neighbor == t:
                # Returning to previous node
                probs[neighbor] = 1/p
            elif G.has_edge(neighbor, t):
                # Distance 1 from t
                probs[neighbor] = 1
            else:
                # Distance 2 from t
                probs[neighbor] = 1/q

        # Normalize
        norm = sum(probs.values())
        for neighbor in probs:
            probs[neighbor] /= norm

        transition_probs[(t, v)] = probs

    return transition_probs
```

Step 2: Generate Biased Random Walks

```
def generate_walk(G, start_node, walk_length, transition_probs):
    """
    Generate a single biased random walk.
    """
    walk = [start_node]

    for i in range(walk_length - 1):
        current = walk[-1]
        neighbors = list(G.neighbors(current))

        if len(neighbors) == 0:
            break

        if len(walk) == 1:
            # First step: uniform random choice
            next_node = random.choice(neighbors)
```

```
        else:
            # Use biased probabilities
            previous = walk[-2]
            probs = transition_probs[(previous, current)]
            next_node = random.choices(neighbors,
                                       weights=[probs[n] for n in
neighbors])[0]

        walk.append(next_node)

    return walk
```

Step 3: Train Skip-gram Model

```
def train_skipgram(walks, d, window_size, num_epochs):
    """
    Learn embeddings using skip-gram objective.
    Uses negative sampling for efficiency.
    """
    # Initialize embeddings
    vocab_size = max(max(walk) for walk in walks) + 1
    Z = np.random.randn(vocab_size, d) * 0.01

    for epoch in range(num_epochs):
        for walk in walks:
            # Generate training pairs
            for i, center_node in enumerate(walk):
                # Context window
                start = max(0, i - window_size)
                end = min(len(walk), i + window_size + 1)

                for j in range(start, end):
                    if i != j:
                        context_node = walk[j]

                        # Positive pair: (center_node,
context_node)
                        # Negative samples: (center_node,
random_node)

                        # Update embeddings using gradient descent
```

```
                        # [Implementation details omitted for
brevity]

    return Z
```

Mathematical Formulation

Objective Function

node2vec maximizes the log-probability of observing network neighborhoods:

```
maximize: Σ_{u ∈ V} log P(N_S(u) | z_u)
```

Where:

- `N_S(u)` is the network neighborhood of node u generated by strategy S
- `z_u` is the embedding of node u

Skip-gram Formulation

Using the skip-gram assumption (independence):

```
P(N_S(u) | z_u) = Π_{v ∈ N_S(u)} P(v | z_u)
```

Prediction Probability

```
P(v | z_u) = exp(z_u^T · z_v) / Σ_{w ∈ V} exp(z_u^T · z_w)
```

This is expensive to compute (O(|V|) for each pair)!

Negative Sampling (Optimization Trick)

To make training efficient, node2vec uses **negative sampling**:

```
log P(v | z_u) ≈ log σ(z_u^T · z_v) + Σ_{i=1}^k E_{v_i ~ P_n} [log
σ(-z_u^T · z_{v_i})]
```

Where:

- σ is the sigmoid function
- P_n is the negative sampling distribution (usually uniform)
- k is the number of negative samples (typically 5-20)

Final Loss Function:

```
L = Σ_{(u,v)∈D} [-log σ(z_u^T · z_v) - γ Σ_{v_n ~ P_n} log σ(-
z_u^T · z_{v_n})]
```

Where D is the set of (center, context) pairs from random walks.

Complete Worked Example

Let's work through node2vec on a small graph!

The Graph

```
    1 --- 2 --- 3
    |     |     |
    4 --- 5 --- 6
```

Adjacency:

- 1: [2, 4]
- 2: [1, 3, 5]
- 3: [2, 6]
- 4: [1, 5]
- 5: [2, 4, 6]
- 6: [3, 5]

Parameters

```
p = 1      (no return bias)
q = 0.5    (DFS-like: prefer exploring far)
l = 5      (walk length)
r = 3      (walks per node)
d = 3      (embedding dimension)
k = 2      (context window)
```

Step 1: Compute Transition Probabilities

Example: Currently at node 5, came from node 2

Neighbors of 5: {2, 4, 6}

Distances from node 2 (where we came from):

- Node 2: distance 0 (it's where we came from) → probability $\propto$ 1/p = 1
- Node 4: distance 2 (not neighbor of 2) → probability $\propto$ 1/q = 2
- Node 6: distance 2 (not neighbor of 2) → probability $\propto$ 1/q = 2

Unnormalized weights: {2: 1, 4: 2, 6: 2}

Normalized probabilities:

```
P(2 | at 5, from 2) = 1/5 = 0.20
P(4 | at 5, from 2) = 2/5 = 0.40
P(6 | at 5, from 2) = 2/5 = 0.40
```

Interpretation: With q = 0.5 (DFS-like), we're more likely to explore farther (nodes 4, 6) than return to 2.

Step 2: Generate Random Walks

Walk 1 from node 1: ``` Start: 1 Step 1: 1 → 2 (random choice from neighbors) Step 2: 2 → 5 (using transition probs based on coming from 1) Step 3: 5 → 6 (using transition probs based on coming from 2) Step 4: 6 → 3 (using transition probs based on coming from 5)

Walk: [1, 2, 5, 6, 3] ```

Walk 2 from node 1:
`Walk: [1, 4, 5, 2, 3]`

Walk 3 from node 1:
`Walk: [1, 2, 3, 6, 5]`

Similar walks from all other nodes (2, 3, 4, 5, 6)...

Total walks: 6 nodes × 3 walks/node = **18 walks**

Step 3: Extract Training Pairs

From walk `[1, 2, 5, 6, 3]` with window size k=2:

Center = 1 (position 0):

- Context: {2, 5}
- Pairs: (1,2), (1,5)

Center = 2 (position 1):

- Context: {1, 5, 6}
- Pairs: (2,1), (2,5), (2,6)

Center = 5 (position 2):

- Context: {1, 2, 6, 3}
- Pairs: (5,1), (5,2), (5,6), (5,3)

Center = 6 (position 3):

- Context: {2, 5, 3}
- Pairs: (6,2), (6,5), (6,3)

Center = 3 (position 4):

- Context: {5, 6}
- Pairs: (3,5), (3,6)

Step 4: Train Skip-gram

Initialize embeddings randomly:

```
z_1 = [0.12, -0.34, 0.56]
z_2 = [-0.23, 0.45, 0.12]
z_3 = [0.34, 0.22, -0.11]
z_4 = [-0.45, 0.13, 0.28]
z_5 = [0.21, -0.12, 0.33]
z_6 = [0.33, 0.24, -0.15]
```

Training pair example: (5, 6) (node 5 predicts node 6)

Forward pass: ``` score = $z\_5^T \cdot z\_6$ = 0.21×0.33 + (-0.12)×0.24 + 0.33×(-0.15) = 0.0693 + (-0.0288) + (-0.0495) = -0.009

P(6 | 5) = exp(-0.009) / Σ_w exp($z\_5^T \cdot z\_w$) ```

Negative sampling: Sample negative nodes (say nodes 1, 4)

Loss:

```
loss = -log σ(z_5^T · z_6) - log σ(-z_5^T · z_1) - log σ(-z_5^T · z_4)
```

Gradient descent: Update embeddings to minimize loss

After training (many iterations over all pairs):

```
Learned embeddings (example):
z_1 = [0.67, 0.45, -0.12]
z_2 = [0.71, 0.52, -0.08]  ← similar to z_1 (neighbors)
```

```
z_3 = [0.69, 0.48, -0.15]  ← similar to z_2, z_6
z_4 = [0.64, 0.43, -0.18]  ← similar to z_1 (neighbors)
z_5 = [0.70, 0.49, -0.10]  ← central node, similar to all
z_6 = [0.68, 0.47, -0.14]  ← similar to z_3, z_5
```

Observation: Nodes in the same cluster have similar embeddings!

Implementation Guide

Pseudocode

```
import numpy as np
import random
from collections import defaultdict

class Node2Vec:
    def __init__(self, G, dimensions=128, walk_length=80,
                 num_walks=10, p=1, q=1, window_size=10):
        self.G = G
        self.d = dimensions
        self.walk_length = walk_length
        self.num_walks = num_walks
        self.p = p
        self.q = q
        self.window_size = window_size

    def fit(self):
        # Step 1: Precompute probabilities
        self.transition_probs = self.precompute_transition_probs()

        # Step 2: Generate walks
        walks = self.generate_walks()

        # Step 3: Train skip-gram
        self.embeddings = self.train_skipgram(walks)

        return self.embeddings
```

```
    def precompute_transition_probs(self):
        # Implementation as shown earlier
        pass

    def generate_walks(self):
        walks = []
        nodes = list(self.G.nodes())

        for _ in range(self.num_walks):
            random.shuffle(nodes)
            for node in nodes:
                walk = self.generate_walk(node)
                walks.append(walk)

        return walks

    def generate_walk(self, start_node):
        # Implementation as shown earlier
        pass

    def train_skipgram(self, walks):
        # Can use existing libraries like gensim.Word2Vec
        from gensim.models import Word2Vec

        # Convert walks to strings for gensim
        walks_str = [[str(node) for node in walk] for walk in
walks]

        model = Word2Vec(walks_str,
                         vector_size=self.d,
                         window=self.window_size,
                         min_count=0,
                         sg=1,  # skip-gram
                         workers=4,
                         epochs=5)

        # Extract embeddings
        embeddings = {}
        for node in self.G.nodes():
            embeddings[node] = model.wv[str(node)]
```

```
        return embeddings
```

Using Existing Implementation

The easiest way is to use existing libraries:

```
# Install: pip install node2vec

from node2vec import Node2Vec
import networkx as nx

# Create graph
G = nx.karate_club_graph()

# Generate walks and learn embeddings
node2vec = Node2Vec(G,
                    dimensions=64,     # embedding dimension
                    walk_length=30,    # length of each walk
                    num_walks=200,     # walks per node
                    p=1,               # return parameter
                    q=1,               # in-out parameter
                    workers=4)

# Train
model = node2vec.fit(window=10,       # context window
                     min_count=1,
                     batch_words=4)

# Get embeddings
embeddings = model.wv
```

Comparison with Other Methods

node2vec vs DeepWalk

Aspect	DeepWalk	node2vec
Random walks	Uniform	Biased (p, q parameters)
Flexibility	Less flexible	More flexible
Captures	Mixed properties	Can target specific properties
Speed	Faster	Slightly slower (precomputation)

node2vec vs Graph Factorization

Aspect	Graph Factorization	node2vec
Approach	Matrix factorization	Random walks
Similarity	Deterministic	Stochastic
Scalability	$O(\|V\|^2)$	$O(\|E\|)$
Flexibility	Limited	High (via p, q)

When to Use node2vec?

Use node2vec when:

- You need flexible embeddings
- Graph is large (millions of nodes)
- You want to tune homophily vs structural equivalence
- You need state-of-the-art performance

Consider alternatives when:

- Graph is very small (< 100 nodes) → matrix methods may be simpler
- You need interpretable embeddings → spectral methods
- You have rich node features → GNNs

Applications and Use Cases

1. Link Prediction

Task: Predict missing edges

Setup:

- Train node2vec on partial graph
- For candidate edge (u,v), compute similarity: $z_u^T \cdot z_v$
- High similarity → likely edge

Hyperparameters: p=1, q=1 (balanced)

2. Node Classification

Task: Classify nodes into categories

Setup:

- Learn embeddings with node2vec
- Use embeddings as features in classifier (SVM, Logistic Regression)

Hyperparameters: p=1, q=0.5 (DFS-like, captures roles)

3. Community Detection

Task: Find tightly connected groups

Setup:

- Learn embeddings with BFS-like walks
- Cluster embeddings (K-means)

Hyperparameters: p=1, q=2 (BFS-like, captures homophily)

4. Recommendation Systems

Task: Recommend items to users

Setup:

- Build user-item graph
- Learn embeddings
- Recommend items with high similarity to user's embedding

Real-World Examples

Bioinformatics: Protein-protein interaction networks

- p=1, q=0.5 (find proteins with similar functions)

Social Networks: Friend recommendation

- p=1, q=2 (find people in same community)

Knowledge Graphs: Entity linking

- p=0.5, q=2 (explore local neighborhood)

Advantages and Limitations

Advantages

1. **Scalable**: Linear in number of edges O(|E|)
2. **Flexible**: Parameters p, q control embedding properties
3. **General**: Works on any graph (directed, weighted, etc.)
4. **Proven**: Strong empirical performance
5. **Unsupervised**: No labels needed

Limitations

1. **Transductive**: Can't embed new nodes without retraining
2. **No features**: Ignores node attributes
3. **Hyperparameters**: Need to tune p, q
4. **Memory**: Stores many random walks

5. **Static**: Doesn't handle dynamic graphs well

Solutions to Limitations

For new nodes:

- Retrain (expensive)
- Or use inductive methods (GraphSAGE)

For node features:

- Concatenate node2vec embeddings with features
- Or use GNNs

For dynamic graphs:

- Incremental training
- Or use temporal GNN methods

Tips and Best Practices

Hyperparameter Tuning

Walk length (l):

- Short walks (10-40): Faster, local structure
- Long walks (80-100): Slower, global structure
- **Typical**: 80

Walks per node (r):

- Few walks (10): Faster, less stable
- Many walks (100+): Slower, more stable
- **Typical**: 10-20

Dimensions (d):

- Low (32-64): Faster, less expressive
- High (128-256): Slower, more expressive
- **Typical**: 128

Parameters p and q:

- Start with p=1, q=1 (unbiased)
- For communities: increase q (q=2)
- For roles: decrease q (q=0.5)
- Grid search over {0.5, 1, 2, 4}

Computational Tips

1. **Precompute transition probabilities** once
2. **Parallelize** walk generation
3. **Use existing Word2Vec implementations** (gensim)
4. **Sample fewer walks** for initial experiments
5. **Cache** random walks for multiple experiments

Summary

The node2vec Algorithm in Three Steps

1. **Generate biased random walks** using parameters p and q
2. **Extract (center, context) pairs** from walks
3. **Learn embeddings** using skip-gram with negative sampling

Key Takeaways

- node2vec = **Flexible random walks** + **Skip-gram**
- Parameter **p** controls return probability
- Parameter **q** controls BFS vs DFS behavior
- Captures both **homophily** and **structural equivalence**
- **Scalable** to millions of nodes
- **State-of-the-art** performance on many tasks

When You've Mastered node2vec

You understand:

- ✓ How random walks capture graph structure
- ✓ How p and q parameters control exploration
- ✓ How skip-gram learns from walks
- ✓ How to tune hyperparameters for your task
- ✓ When to use node2vec vs alternatives

References

Original Paper:

- Grover, A., & Leskovec, J. (2016). node2vec: Scalable Feature Learning for Networks. KDD.

Related Methods:

- Perozzi, B., et al. (2014). DeepWalk: Online Learning of Social Representations. KDD.
- Mikolov, T., et al. (2013). Efficient Estimation of Word Representations. ICLR.

Implementations:

- Official: https://github.com/aditya-grover/node2vec
- Python library: https://github.com/eliorc/node2vec

GRL Book: Hamilton, W. L. (2020). Graph Representation Learning. Morgan & Claypool.

Exercises

Exercise 1: Parameter Effects

Try different (p, q) combinations on the Karate Club graph. How do embeddings change?

Exercise 2: Implementation

Implement the biased random walk from scratch.

Exercise 3: Application

Use node2vec for link prediction on a dataset of your choice.

Exercise 4: Comparison

Compare node2vec with DeepWalk and graph factorization on the same task.

illustration here

```
The node embedding approaches we discussed used a shallow
embedding approach to generate representations of nodes, where we
simply optimized a unique embedding vector for each node.

  The key idea is that we want togenerate representations of nodes
that actually depend on the structure of the graph, as well as any
feature information we might have.
```

$$f(\mathbf{P}\mathbf{A}\mathbf{P}^\top) = f(\mathbf{A})$$

$$f(\mathbf{P}\mathbf{A}\mathbf{P}^\top) = \mathbf{P}f(\mathbf{A})$$

The shallow encoders are an example of permutation equivariant functions.)

Graph Neural Networks (GNNs)

Regardless of the motivation, the defining feature of a GNN is that it uses a form of neural message passing in which vector messages are exchanged between nodes and updated using neural networks [Gilmer et al., 2017].

We will describe how we can take an input graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, along with a set of node features $\mathbf{X} \in \mathbb{R}^{d \times |\mathcal{V}|}$, and use this information to generate node embeddings $\mathbf{z}_u, \ \forall u \in \mathcal{V}$.

Message Passing Framework

Core Idea: Update node representations by aggregating information from neighbors.

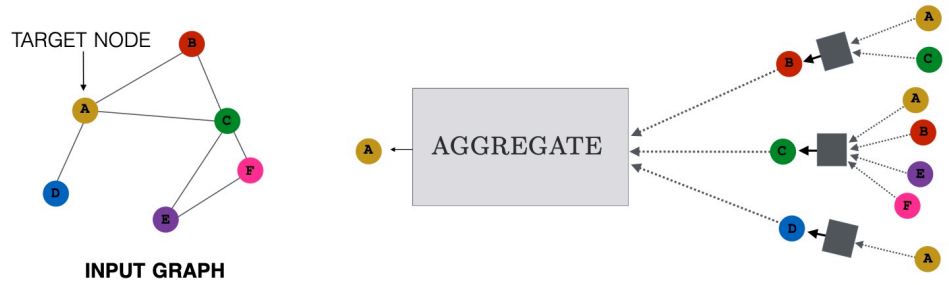


Figure 5.1: Overview of how a single node aggregates messages from its local neighborhood. The model aggregates messages from A's local graph neighbors (i.e., B, C, and D), and in turn, the messages coming from these neighbors are based on information aggregated from their respective neighborhoods, and so on. This visualization shows a two-layer version of a message-passing model. Notice that the computation graph of the GNN forms a tree structure by unfolding the neighborhood around the target node.

$$\mathbf{h}_u^{(k+1)} = \text{UPDATE}^{(k)}\left(\mathbf{h}_u^{(k)}, \text{AGGREGATE}^{(k)}\left(\{\mathbf{h}_v^{(k)}, \forall v \in \mathcal{N}(u)\}\right)\right)$$

$$= \text{UPDATE}^{(k)}\left(\mathbf{h}_u^{(k)}, \mathbf{m}_{\mathcal{N}(u)}^{(k)}\right),$$

where UPDATE and AGGREGATE are arbitrary differentiable functions (i.e., neural networks), and $\mathbf{m}_{\mathcal{N}(u)}$ is the "message" that is aggregated from u's graph neighborhood $\mathcal{N}(u)$. We use superscripts to distinguish the embeddings and functions at different iterations of message passing.\footnote{For example, $\mathbf{h}_u^{(k)}$ and $\text{UPDATE}^{(k)}$ refer to the embedding and update function at the k-th iteration.}

Mathematical Formulation:

$$h_v^{(l+1)} = \sigma(W^{(l)} \cdot \mathrm{AGGREGATE}^{(l)}(\{h_u^{(l)} : u \in \mathcal{N}(v)\}))$$

where:

- $h_v^{(l)}$ is the representation of node v at layer l
- $\mathcal{N}(v)$ is the neighborhood of node v
- $\mathrm{AGGREGATE}$ is an aggregation function
- σ is an activation function

$$\begin{aligned}
\text{Step } 1: \quad & \mathbf{h}^{(1)} = \mathbf{A}[1] \\
\text{Step } 2: \quad & \mathbf{h}^{(2)} = \mathbf{A}[1] \oplus \mathbf{A}[2] \\
\text{Step } 3: \quad & \mathbf{h}^{(3)} = \mathbf{A}[1] \oplus \mathbf{A}[2] \oplus \mathbf{A}[3] \\
\text{Step } 4: \quad & \mathbf{h}^{(4)} = \mathbf{A}[1] \oplus \mathbf{A}[2] \oplus \mathbf{A}[3] \oplus \mathbf{A}[4] \\
& \vdots \\
\text{Step } n: \quad & \mathbf{h}^{(n)} = \mathbf{A}[1] \oplus \mathbf{A}[2] \oplus \cdots \oplus \mathbf{A}[n] \\
\text{Final:} \quad & \mathbf{z_G} = \mathrm{MLP}(\mathbf{h}^{(|\mathcal{V}|)}) \\
& \quad = \mathrm{MLP}(\mathbf{A}[1] \oplus \mathbf{A}[2] \oplus \cdots \oplus \mathbf{A}[|\mathcal{V}|])
\end{aligned}$$

Node Features (not really but similar)

$$\mathbf{A}[1], \mathbf{A}[2], \ldots, \mathbf{A}[|\mathcal{V}|]$$

Aggregate them

Apply an operation like summation:

$$\mathbf{h_G} = \mathbf{A}[1] \oplus \mathbf{A}[2] \oplus \cdots \oplus \mathbf{A}[|\mathcal{V}|]$$

$$If \oplus = \sum, then : \mathbf{h_G} = \sum_{i=1}^{|\mathcal{V}|} \mathbf{A}[I]$$

Feed the aggregated representation into an MLP

$$\mathbf{z_G} = \mathrm{MLP}(\mathbf{h_G})$$

Example

Suppose your graph has 3 nodes with features:

$$\mathbf{A}[1] = [1, 0], \quad \mathbf{A}[2] = [0, 1], \quad \mathbf{A}[3] = [1, 1]$$

Aggregation by summation:

$$\mathbf{h_G} = [1, 0] + [0, 1] + [1, 1] = [2, 2]$$

$$\mathbf{z_G} = \mathrm{MLP}([2, 2])$$

$$\mathbf{z_G} = \sigma(\mathbf{W}_2\, \mathrm{ReLU}(\mathbf{W}_1 [2, 2]^\top + \mathbf{b}_1) + \mathbf{b}_2)$$

If each node feature vector $\mathbf{A}[i]$ has dimension d, and your graph has $|\mathcal{V}|$ nodes, then concatenating them gives:

$$\mathbf{h_G} = \mathbf{A}[1] \oplus \mathbf{A}[2] \oplus \cdots \oplus \mathbf{A}[|\mathcal{V}|] \Rightarrow \mathbf{h_G} \in \mathbb{R}^{d \times |\mathcal{V}|}$$

—or as a single long vector of size $d|\mathcal{V}|$.

So if each $\mathbf{A}[i] = [a_{1i}, a_{2i}, a_{3i}]$ (3 features per node), and you have 4 nodes, then:

$$\mathbf{h_G} = [a_{11}, a_{21}, a_{31}, a_{12}, a_{22}, a_{32}, a_{13}, a_{23}, a_{33}, a_{14}, a_{24}, a_{34}]$$

That is permutation variant!

```
A = torch.tensor([[1,2,3],
                  [4,5,6],
                  [7,8,9],
                  [10,11,12]])
h_G = torch.cat([A[0], A[1], A[2], A[3]])  #
[1,2,3,4,5,6,7,8,9,10,11,12]
z_G = mlp(h_G)
```

Shallow encoders are equavariant functions:

Adjacency (path 1–2–3):

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \qquad \mathbf{X} = \begin{bmatrix} 2 \\ -1 \\ 3 \end{bmatrix}$$

Shallow encoder:

$$f(\mathbf{A}, \mathbf{X}) = \mathbf{A}\mathbf{X}.$$

Permutation (relabel to order 2,3,1):

$$\mathbf{P} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

Original output

$$\mathbf{A}\mathbf{X} = \begin{bmatrix} -1 \\ 5 \\ -1 \end{bmatrix}$$

Permuted inputs

$$\mathbf{X}' = \mathbf{P}\mathbf{X} = \begin{bmatrix} -1 \\ 3 \\ 2 \end{bmatrix}, \qquad \mathbf{A}' = \mathbf{P}\mathbf{A}\mathbf{P}^\top = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

Output after permutation

$$\mathbf{A'X'} = \begin{bmatrix} 5 \\ -1 \\ -1 \end{bmatrix}$$

Compare with permuted original output

$$\mathbf{P}(\mathbf{AX}) = \mathbf{P} \begin{bmatrix} -1 \\ 5 \\ -1 \end{bmatrix}$$

$$\begin{bmatrix} 5 \\ -1 \\ -1 \end{bmatrix}$$

They match, so

$f(\mathbf{PAP}^\top, \mathbf{PX}) = \mathbf{P}\, f(\mathbf{A}, \mathbf{X})$, which demonstrates permutation equivariance for the shallow encoder $f(\mathbf{A}, \mathbf{X}) = \mathbf{AX}$.

Message Passing

Neural message passing in GNNs: nodes exchange vector “messages” with neighbors and update their states using neural networks.

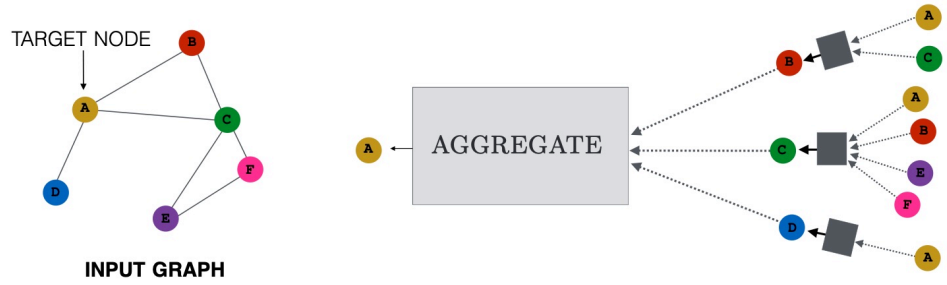


Figure 5.1: Overview of how a single node aggregates messages from its local neighborhood. The model aggregates messages from A's local graph neighbors (i.e., B, C, and D), and in turn, the messages coming from these neighbors are based on information aggregated from their respective neighborhoods, and so on. This visualization shows a two-layer version of a message-passing model. Notice that the computation graph of the GNN forms a tree structure by unfolding the neighborhood around the target node.

At each iteration k:

$$\mathbf{h}_u^{(k+1)} = \text{UPDATE}^{(k)}\left(\mathbf{h}_u^{(k)}, \text{AGGREGATE}^{(k)}(\{\mathbf{h}_v^{(k)} \mid v \in \mathcal{N}(u)\})\right)$$

• $\mathbf{h}_u^{(k)}$ — current embedding (feature) of node u

• $\mathcal{N}(u)$ — neighbors of node u

• AGGREGATE — combines messages from neighbors (permutation-invariant)

• UPDATE — updates node u's representation using its previous embedding and the aggregated message

At the end (after K iterations):

$$\mathbf{z}_u = \mathbf{h}_u^{(K)} \forall u$$

Example

1 — 2 — 3

Adjacency list: • 1’s neighbors: {2} • 2’s neighbors: {1, 3} • 3’s neighbors: {2}

———

Step 1: Initialize features

At iteration k = 0:

$$\mathbf{h}_1^{(0)} = 1, \quad \mathbf{h}_2^{(0)} = 2, \quad \mathbf{h}_3^{(0)} = 3$$

———

Step 2: Define AGGREGATE and UPDATE

For simplicity: $\mathrm{AGGREGATE}^{(k)}(\{\, \mathbf{h}v^{(k)} \,\}) = \sum_{v \in \mathcal{N}(u)} \mathbf{h}_v^{(k)}$

$$\mathrm{UPDATE}^{(k)}(x, y) = x + y$$

———

Step 3: Compute iteration k=1

Node 1:

$$\mathrm{AGGREGATE} = \mathbf{h}_2^{(0)} = 2$$

$$\mathrm{UPDATE} : \mathbf{h}_1^{(1)} = 1 + 2 = 3$$

Node 2:

$$\mathrm{AGGREGATE} = \mathbf{h}_1^{(0)} + \mathbf{h}_3^{(0)} = 1 + 3 = 4$$

$$\mathrm{UPDATE} : \mathbf{h}_2^{(1)} = 2 + 4 = 6$$

Node 3:

$$\text{AGGREGATE} = \mathbf{h}_2^{(0)} = 2$$

$$\text{UPDATE} : \mathbf{h}_3^{(1)} = 3 + 2 = 5$$

Step 4: Output after one iteration

$$\mathbf{h}_1^{(1)} = 3, \quad \mathbf{h}_2^{(1)} = 6, \quad \mathbf{h}_3^{(1)} = 5$$

Step 5: Next iteration k=2

Node 1:

$$\text{AGGREGATE} = \mathbf{h}_2^{(1)} = 6$$

$$\text{UPDATE} : \mathbf{h}_1^{(2)} = 3 + 6 = 9$$

Node 2:

$$\text{AGGREGATE} = \mathbf{h}_1^{(1)} + \mathbf{h}_3^{(1)} = 3 + 5 = 8$$

$$\text{UPDATE} : \mathbf{h}_2^{(2)} = 6 + 8 = 14$$

Node 3:

$$\text{AGGREGATE} = \mathbf{h}_2^{(1)} = 6$$

$$\text{UPDATE} : \mathbf{h}_3^{(2)} = 5 + 6 = 11$$

Step 6: Final embeddings (after K=2)

$$\mathbf{z}_1 = 9, \quad \mathbf{z}_2 = 14, \quad \mathbf{z}_3 = 11$$

Term	Meaning	In our example
$\mathbf{h}_u^{(0)}$	Node's initial features	1, 2, 3
$\mathrm{AGGREGATE}$	Gathers neighbor info	Sum of neighbor values
UPDATE	Combines own info + neighbor info	Simple addition
Permutation equivariance	Node reordering yields permuted results	True here (aggregation uses a **set**)

```
▪ After the first iteration (k = 1), each node's embedding
contains information from its 1-hop neighborhood — i.e., its
immediate neighbors.
▪ After the second iteration (k = 2), each node's embedding
includes information from its 2-hop neighborhood (neighbors of
neighbors).
▪ In general, after k iterations, every node embedding encodes
information from its k-hop neighborhood.
```

The information captured by GNNs comes in two main forms:

```
1.  Structural information – the topology of the graph, such as
node degrees or local motifs (e.g., molecular substructures like
benzene rings).
2.  Feature-based information – aggregated attributes or features
of neighboring nodes, similar to how CNNs gather information from
spatially nearby pixels.
```

GNNs stand out because they can integrate the embedding process directly into the learning algorithm itself... As the network processes inputs through its layers, the embeddings are refined and updated, making the learning phase and the embedding phase inseparable. This means that GNNs learn the most informative representation of the graph data during training time.

```
import NetworkX as nx
from Node2Vec import Node2Vec
books_graph = nx.read_gml('PATH_TO_GML_FILE')
node2vec = Node2Vec(books_graph, dimensions=64,
 walk_length=30, num_walks=200, workers=4)
model = node2vec.fit(window=10, min_count=1,\
batch_words=4)
embeddings = {str(node): model.wv[str(node)]\
 for node in gml_graph.nodes()}
```

```
 node_embedding = model.wv['Losing Bin Laden']
 print(node_embedding)
```

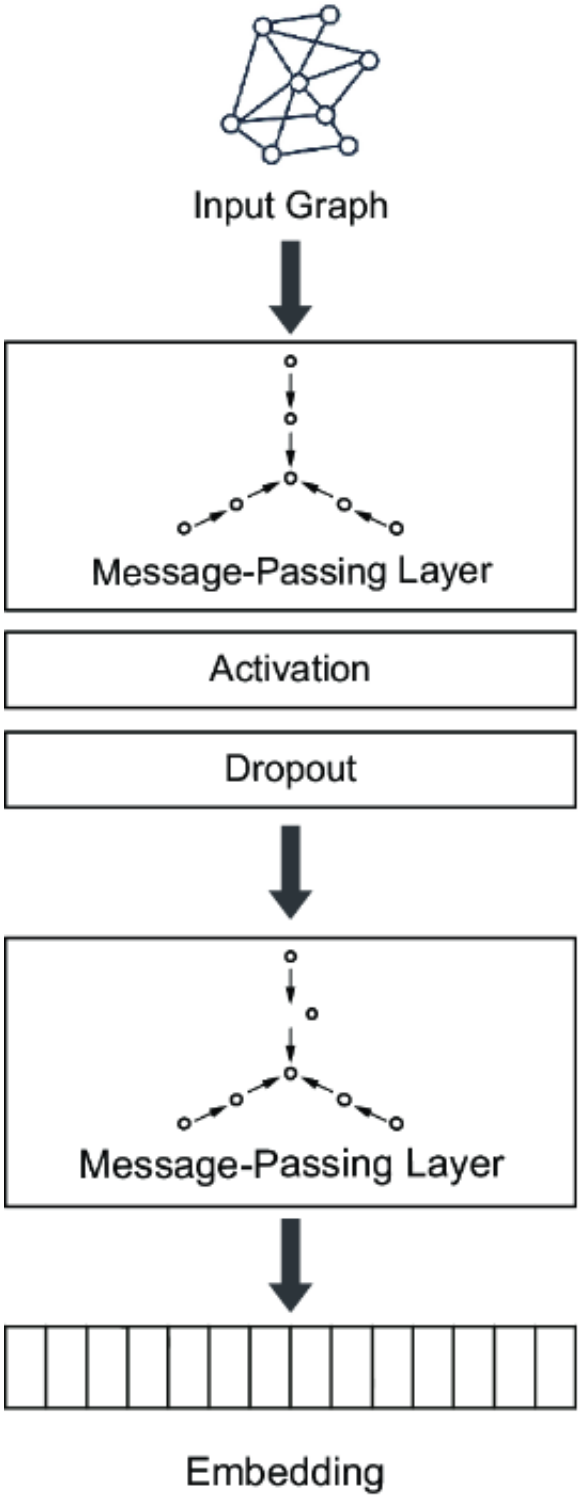
```
node_embeddings = [embeddings[str(node)] \
for node in gml_graph.nodes()]
node_embeddings_array = np.array(node_embeddings)

umap_model = umap.UMAP(n_neighbors=15, min_dist=0.1,
n_components=2, \
random_state=42)
umap_features = umap_model.fit_transform\
(node_embeddings_array)

plt.scatter(umap_features[:, 0], \
umap_features[:, 1], color=node_colors, alpha=0.7)
```

Our SimpleGNN class inherits from torch.nn.Module and is composed of two GCNConv layers, which are the building blocks of our GNN. This architecture is shown in figure 2.7, consisting of the first layer, a message passing layer

(self.conv1), an activation (torch.relu), a dropout layer (torch.dropout), and a second message passing layer.




```
import torch
```

```
import torch.nn.functional as F
from torch_geometric.nn import GCNConv

class SimpleGNN_embeddings(torch.nn.Module):
    def __init__(self, num_features, hidden_channels):
        super(SimpleGNN_embeddings, self).__init__()
        self.conv1 = GCNConv(num_features, hidden_channels)
        self.conv2 = GCNConv(hidden_channels, hidden_channels)

    def forward(self, x, edge_index):
        x = self.conv1(x, edge_index)
        x = torch.relu(x)
        x = F.dropout(x, p=0.5, training=self.training)
        x = self.conv2(x, edge_index)
        return x
```

```
import torch
import torch.nn as nn
import torch.nn.functional as F

class SimpleMLP(nn.Module):
    def __init__(self, in_dim, hidden=64, out_dim=NUM_CLASSES):
        super().__init__()
        self.fc1 = nn.Linear(in_dim, hidden)
        self.fc2 = nn.Linear(hidden, hidden)
        self.fc3 = nn.Linear(hidden, out_dim)
        self.dropout = nn.Dropout(p=0.5)

    def forward(self, x):
        # x: [num_nodes, in_dim]  (or [batch, in_dim] for non-graph data)
        x = F.relu(self.fc1(x))
        x = self.dropout(x)
        x = F.relu(self.fc2(x))
        x = self.fc3(x)     # logits
        return x
```

```
import torch
import torch.nn as nn
import torch.nn.functional as F
from torch_geometric.nn import GCNConv

class SimpleGCN(nn.Module):
    def __init__(self, in_dim, hidden=64, out_dim=NUM_CLASSES):
        super().__init__()
        self.conv1 = GCNConv(in_dim, hidden)
        self.conv2 = GCNConv(hidden, hidden)
        self.conv3 = GCNConv(hidden, out_dim)
        self.dropout = nn.Dropout(p=0.5)

    def forward(self, x, edge_index):
        # x: [num_nodes, in_dim]
        # edge_index: [2, num_edges] (COO format)
        x = F.relu(self.conv1(x, edge_index))
        x = self.dropout(x)
        x = F.relu(self.conv2(x, edge_index))
        x = self.conv3(x, edge_index)  # logits
        return x
```

GCNs act as message-passing layers that are critical in constructing embeddings.

```
data = from_NetworkX(gml_graph)
```

Method from_NetworkX specifically translates the edge lists and node/edge attributes into PyTorch tensors.

When no node features are available or they aren't informative,.... Xavier initialization, which sets the initial node features with values drawn from a distribution that keeps the variety of activations consistent across layers.

This technique ensures that the model starts with a balanced representation, preventing problems such as vanishing or exploding gradients.

```
 data.x = torch.randn((data.num_nodes, 64), dtype=torch.float)
'nn.init.xavier_uniform_(data.x) '
```

```
model = SimpleGNN(num_features=data.x.shape[1],
hidden_channels=64)
```

Specifically, model.eval() turns off certain behaviors specific to training, such as dropout, which randomly deactivates some neurons to prevent overfitting, and batch normalization, which normalizes inputs across a mini-batch. By disabling these features, the model provides consistent and deterministic outputs, ensuring that the evaluation accurately reflects its true performance on unseen data.

we employ torch.no_grad(), which ensures that the computational graph that records operations for backpropagation isn't constructed, preventing us from accidentally changing performance.

```
model.eval()
with torch.no_grad():
    gnn_embeddings = model(data.x, data.edge_index)
```

```
gnn_embeddings_np = gnn_embeddings.detach().cpu().numpy()
```

Semi-supervised learning

```
labels = []
for node, data in gml_graph.nodes(data=True):
    if data['value'] == 'c':
        labels.append('right')
    elif data['value'] == 'l':
        labels.append('left')
    else:
        labels.append('neutral')
labels = np.array(labels)

random.seed(52)

indices = list(range(len(labels)))
```

```
labelled_percentage = 0.2

labelled_indices = random.sample(indices, \
int(labelled_percentage * len(labels)))

labelled_mask = np.zeros(len(labels), dtype=bool)
unlabelled_mask = np.ones(len(labels), dtype=bool)

labelled_mask[labelled_indices] = True
unlabelled_mask[labelled_indices] = False

labelled_labels = labels[labelled_mask]
unlabelled_labels = labels[unlabelled_mask]

label_mapping = {'left': 0, 'right': 1, 'neutral': 2}
numeric_labels = np.array([label_mapping[label] for label in
labels])
```

```
X_train_gnn = gnn_embeddings[labelled_mask]
Y_train_gnn = numeric_labels[labelled_mask]

X_n2v = np.array([embeddings[str(node)] \
for node in gml_graph.nodes()])
X_train_n2v = X_n2v[labelled_mask]
y_train_n2v = numeric_labels[labelled_mask]
```

Random Forest

```
clf_gnn = RandomForestClassifier()
clf_gnn.fit(X_train_gnn, y_train_gnn)

clf_n2v = RandomForestClassifier()
clf_n2v.fit(X_train_n2v, y_train_n2v)
```

Emb	Acc	F1
GNN	83%	82%

N2V	85%	81%

End to End

```
class SimpleGNN_inference(torch.nn.Module):
    def __init__(self, num_features, hidden_channels):
        super(SimpleGNN, self).__init__()
        self.conv1 = GCNConv(num_features, hidden_channels)
        self.conv2 = GCNConv(hidden_channels, hidden_channels)

    def forward(self, x, edge_index):
        # First Graph Convolutional layer
        x = self.conv1(x, edge_index)
        x = F.relu(x)
        x = F.dropout(x, training=self.training)

        # Second Graph Convolutional layer
        x = self.conv2(x, edge_index)
        predictions = F.log_softmax(x, dim=1)

        return x, predictions
```

```
for epoch in range(3000):
    optimizer.zero_grad()

    _, out = model(data.x, data.edge_index)

    out_masked = out[data.train_mask]

    loss = loss_fn(out_masked, train_labels)
    loss.backward()
    optimizer.step()

    if epoch % 10 == 0:
        print(f'Epoch {epoch}, Log Loss: {loss.item()}')
```

Model	GNN Accuracy	GNN F1 Score
Two-layer, randomized features	82.27%	82.14%
Two-layer, N2V features	87.79%	88.10%
Four-layer, randomized features	86.58%	86.90%
Four-layer, N2V features	88.99%	89.29%

Model	Data Input	Accuracy	F1 Score
Random forest	Embedding from GNN	83.33%	82.01%
Random forest	Embedding from N2V	84.52%	80.72%
Two-layer simple GNN	Graph with randomized node features	82.27%	82.14%
Two-layer simple GNN	Graph with n2v embeddings as node features	87.79%	88.10%
Four-layer simple GNN	Graph with randomized node features	86.58%	86.90%
Four-layer simple GNN	Graph with n2v embeddings as node features	88.99%	89.29%

References

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