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()}
```

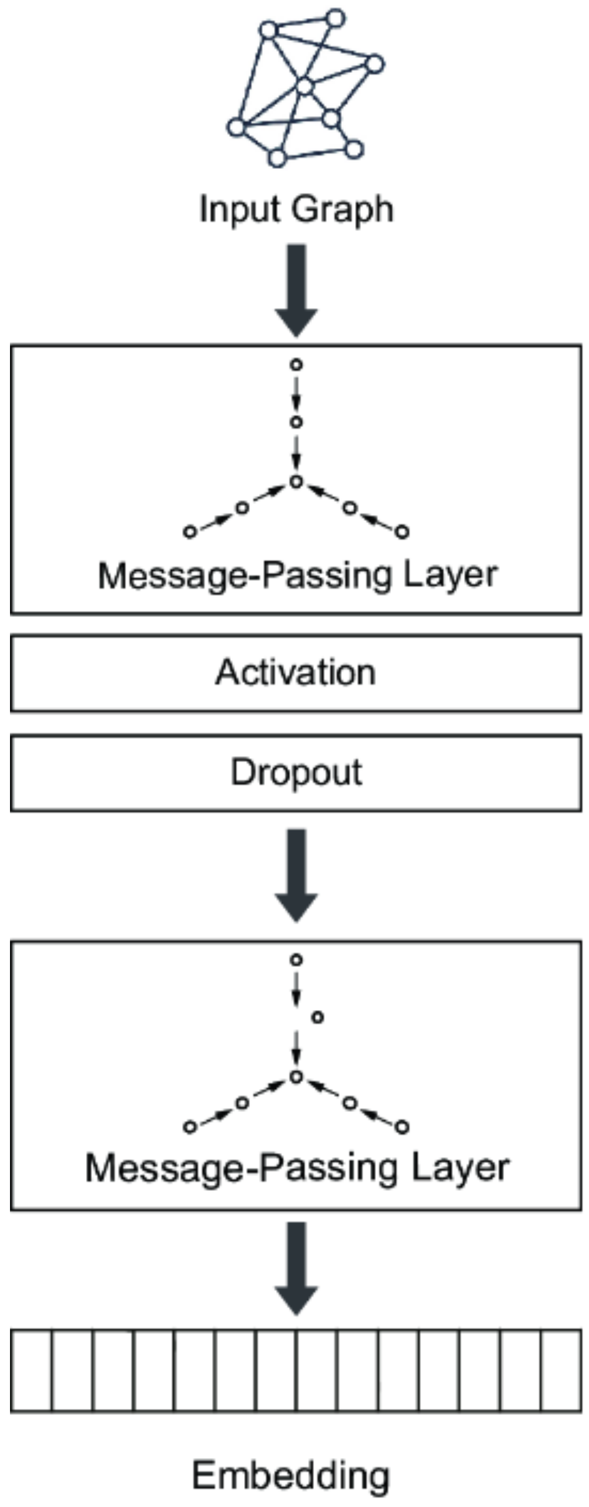
```
 node_embedding = model.wv['Losing Bin Laden']
 print(node_embedding)
```

```
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%

Distance and similarity concepts for graphs

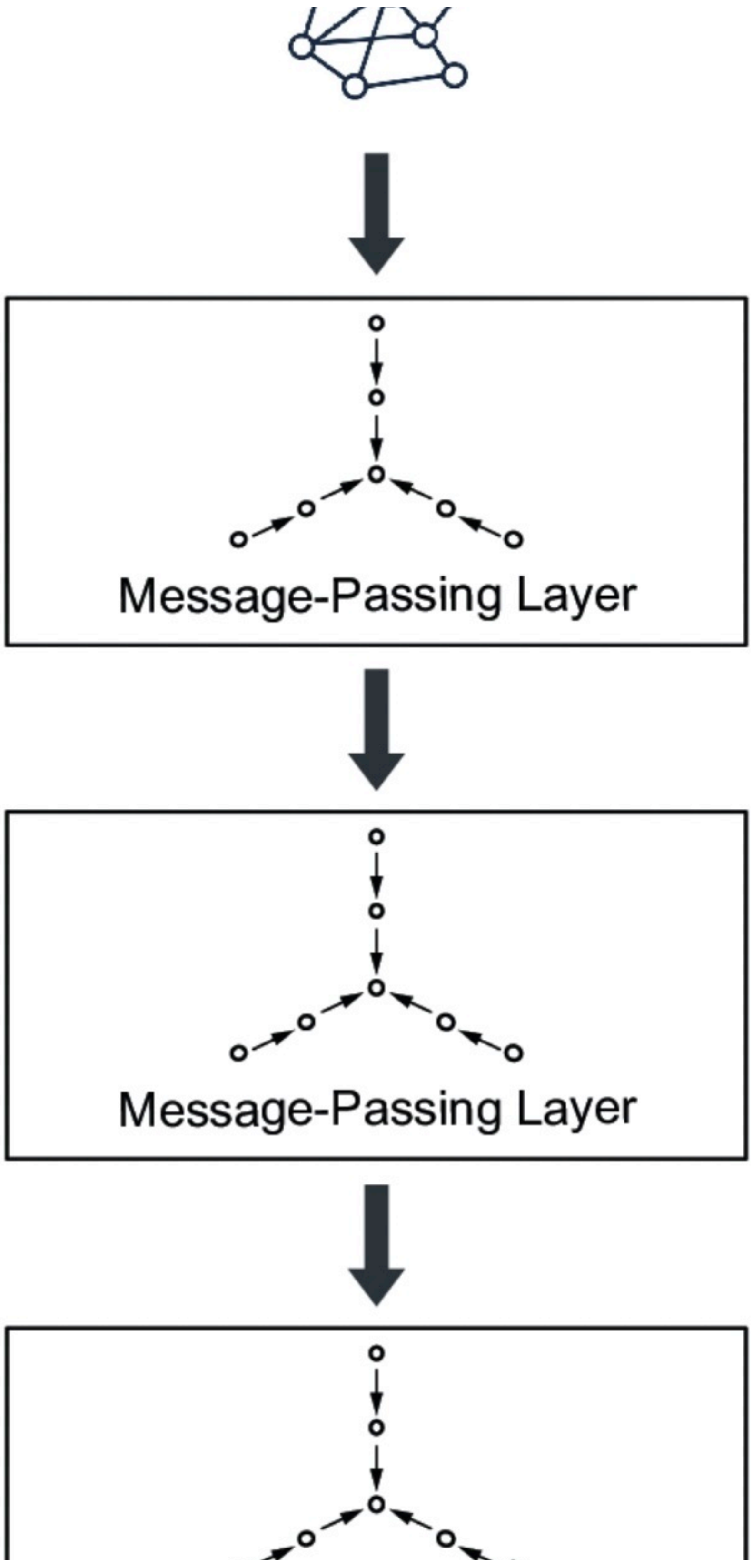
- k-hop
- probability of visiting a node in k-hobs
- many more...

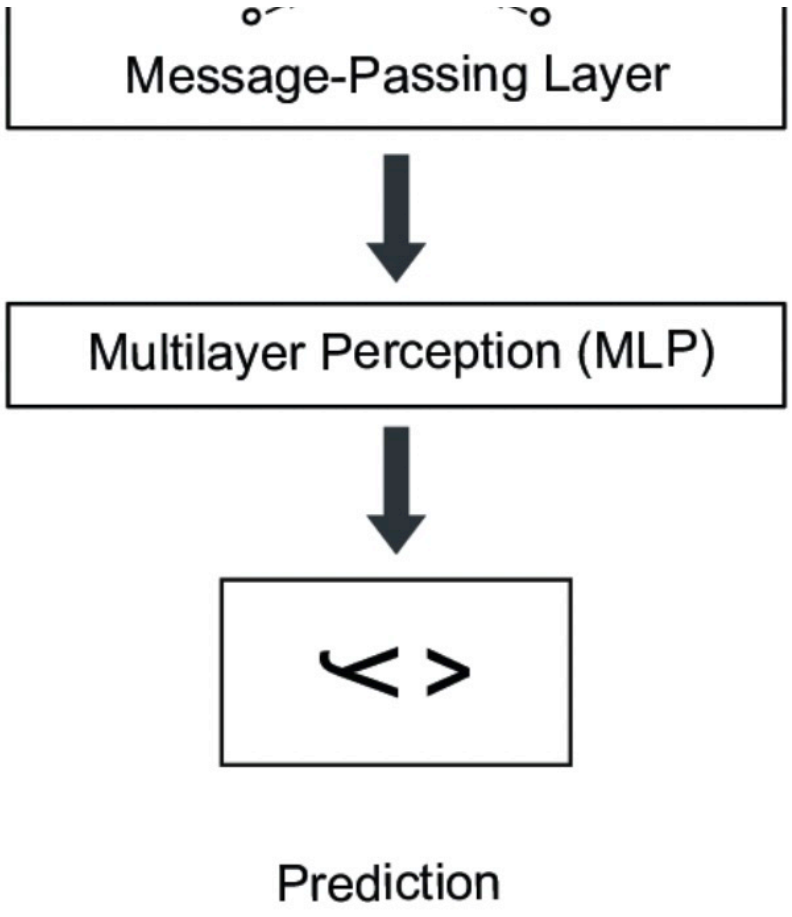
Inductive methods excel in generalizing to accommodate new, unseen data, enabling models to adapt and learn beyond their initial training set. Conversely, transductive methods specialize in optimizing embeddings *specifically for the training data itself, making them highly effective within their learned context but less flexible when introduced to new data.*

Transductive wouldn't be better in spam detection because models would require retraining with every new batch of emails, making them computationally expensive and impractical for real-time spam detection.

Inductive models wouldn't take full advantage of the specific network structure and node interconnections because they only process part of the data—the training set. This isn't enough information for accurate community detection.

Representation	**Description**	**Examples**
Basic data representations	• Great for analytical methods that involve network traversal • Useful for some node classification algorithms • Information provided: Node and edge neighbors	• Adjacency list • Edge list • Adjacency matrix
Transductive (shallow) embeddings	• Useless for data not trained on • Difficult to scale	• DeepWalk • N2V • TransE • RESCAL • Graph factorization • Spectral techniques
Inductive embeddings	• Models can be generalized to new and structurally different graphs • Represents data as vectors in continuous space • Learns a mapping from data (new and old) to positions within the continuous space	• GNNs can be used to inductively generate embeddings • Transformers • N2V with feature concatenation


Message-Passing Layer
Message-Passing Layer



Each step in the message-passing layer of our GNNs, we'll be passing information from nodes to another node one hop away. Importantly, a neural network then takes the data from the one-hop neighbors and applies a nonlinear transformation. This is the beauty of GNNs; we're applying many small neural networks at the level of individual nodes and/or edges to build embeddings of the graph features.

Message Passing Layer in GNN

At each step, node v updates its embedding by aggregating information from one-hop neighbors $\mathcal{N}(v)$:

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

A simple instantiation:

$$\mathbf{h}_v^{(k)} = \sigma\left(\mathbf{W}_1 \mathbf{h}_v^{(k-1)} + \sum_{u \in \mathcal{N}(v)} \mathbf{W}_2 \mathbf{h}_u^{(k-1)}\right)$$