Modern Deep Learning Models

Tong Shu

DL-GPU Workshop 2024
Day 7

05/21/2024

Graph Neural Networks

Graph Learning

- Node classification
  - A task that involves predicting the category (class) of a node in a graph.
- Link prediction
  - A task that involves predicting missing links between pairs of nodes in a graph.
- Graph classification
  - A task that involves categorizing different graphs into predefined categories.
- Graph generation
  - A task that involves generating new graphs based on a set of desired properties.

Graph Measures

- Degree centrality is simply defined as the degree of the node.
  - A high degree centrality significantly influences the network.
- Closeness centrality measures the average length of the shortest path between the target node and all other nodes in the graph.
  - A node with high closeness centrality can quickly reach all other vertices in the network.
- Betweenness centrality measures the number of times a node lies on the shortest path between pairs of other nodes in the graph.
  - A node with high betweenness centrality acts as a bottleneck or bridge between different parts of the graph.
- Density is the ratio between the actual number of edges and the maximum possible number of edges in the graph.
  - The density of a graph is calculated as the number of edges divided by the maximum number of edges.
  - A graph is considered dense if its density is greater than 0.5 and sparse if its density is less than 0.1.

Word2Vec

- Word2Vec translates words into vectors (also known as embeddings) using large datasets of text.
- Example

```
vec(king) = [−2.1, 4.1, 0.6]
vec(queen) = [−1.9, 2.6, 1.5]
vec(man) = [3.0, −1.1, −2]
vec(woman) = [2.8, −2.6, −1.1]
```

  - Euclidian distance
  - Cosine similarity
    - $\text{cosine similarity}(\vec{A}, \vec{B}) = cos(\theta) = \dfrac{\vec{A} \cdot \vec{B}}{||\vec{A}|| \cdot ||\vec{B}||}$
  - Ability to solve analogies
    - vec(king) - vec(man) + vec(woman) ≈ vec(queen)

Continuous Skip-Grams Model

- Feed a single word to the model and predict the words around it.
- Increasing the range of context words leads to better embeddings but also increases the training time.

Skip-gram

Creating Skip-Grams

- Skip-grams are implemented as pairs of words (target word, context word)
  - The target word is the input
  - The context word is the word to predict.
  - The number of skip grams for the same target word depends on a parameter called context size.

Context Size	Text	Skip-grams
1	**the *train*** was late.	('the', 'train')
	the* train *was late	('train', 'the') ('train', 'was')
	the ***train* was *late***	('was', 'train') ('was', 'late')
	the train ***was* late**	('late', 'was')
2	**the *train* *was*** late	('the', 'train') ('the', 'was')
	the* train *was late	('train', 'the') ('train', 'was') ('train', 'late')
	the train* was *late	('was', 'the') ('was', 'train') ('was', 'late')
	the ***train* *was* late**	('late', 'train') ('late', 'was')

The Skip-Gram Model

- Imagine that we have a sequence of N words $w_1, w_2, \cdots, w_N$. The probability of seeing the word w_2 given the word w_1 is written $p(w_2 \mid w_1)$.

- The goal is to maximize the sum of every probability of seeing a context word given a target word in an entire text: $\frac{1}{N}\sum_{n=1}^{N}\sum_{-C\leq j\leq C, j\neq 0}\log p(w_{n+j} \mid w_n)$
  - C is the size of the context vector.

- The basic skip-gram model uses the softmax function to calculate the probability of a context word embedding h_c given a target word embedding h_t: $p(w_x \mid w_t) = \frac{e^{h_c h_t^T}}{\sum_{i=1}^{|V|} e^{h_i h_t^T}}$
  - $|V|$ is the vocabulary of size.

The Skip-Gram Model (Cont.)

- Model structure
  - A projection layer with a weight matrix W_{embed}, takes a one-hot encoded-word vector as an input and returns the corresponding N-dim word embedding.
    - It acts as a simple lookup table that stores embeddings of a predefined dimensionality.
  - A fully connected layer with a weight matrix W_{output}, takes a word embedding as input and outputs $|V|$-dim logits.
    - A softmax function is applied to these predictions to transform logits into probabilities.
  - No activation function: Word2Vec is a linear classifier that models a linear relationship between words.

The Skip-Gram Model (Cont.)

- Let's call x the one-hot encoded-word vector the input.
- The corresponding word embedding can be calculated as a simple projection: $h = W_{\text{embed}}^{\text{T}} \cdot x$
- Using the skip-gram model, we can rewrite the previous probability as follows:

$$p(w_c \mid w_t) = \frac{e^{W_{\text{output}} \cdot h}}{\sum_{i=1}^{|V|} e^{W_{\text{output}_{(i)}} \cdot h}}$$

- The skip-gram model outputs a $|V|$-dim vector, which is the conditional probability of every word in the vocabulary: $\text{word2vec}(w_t) = \begin{bmatrix} p(w_1 \mid w_t) \\ p(w_2 \mid w_t) \\ \vdots \\ p(w_{|V|} \mid w_t) \end{bmatrix}$
- During training, these probabilities are compared to the correct one-hot encoded-target word vectors.
- The difference between these values (calculated by a loss function such as the cross-entropy loss) is backpropagated through the network to update the weights and obtain better predictions.

Word2Vec Architecture

Random Walks

- Random walks are sequences of nodes produced by randomly choosing a neighboring node at every step.

- Using random walks can generate meaningful sequences of nodes that act like sentences.
  - Sentences can be represented as graphs.

- Even if nodes are randomly selected, the fact that they often appear together in a sequence means that they are close to each other.

Random Walks (Cont.)

- Each run
  - Input parameters
    - The starting node (start)
    - The length of the walk (length), i.e., the number of steps
  - Output: a node sequence with the given length
    - E.g., [‘0’, '4', '3', '6', '3', '4', '7', '8', '7', '4', '9']

- Repeated runs
  - If certain nodes are often found together in the same output, they are considered to be similar.

DeepWalk Algorithm

- Goal: produce high-quality feature representations of nodes in an unsupervised way.

- Application: capture the similarity between nodes in a homophilic graph.
  - Core idea: under the network homophily hypothesis, nodes that are close to each other are similar and should have high similarity scores.
  - Process
    - Generate many random walks of a fixed length with uniformly distributed start nodes
    - Train a skip-gram model using the generated random walks to obtain node embeddings
    - Calculate the similarity score between two nodes based on their node embeddings

Defining a Neighborhood

- The exploration process for the neighborhood of a node is called a sampling strategy.
  - Consider the three closest nodes in terms of connections
    - E.g., N(A) = {B, C, D}
    - Breadth-First Search (BFS) focuses on the local network around a node.
  - Select nodes that are not adjacent to previous nodes first.
    - E.g., N(A) = {D, E, F}
    - Depth-First Search (DFS) establishes a more macro view of the graph.

Structural Equivalence v.s. Homophily

- Structural equivalence
  - Nodes are structurally equivalent if they share many of the same neighbors.
  - If nodes share many neighbors, their structural equivalence is higher.
- Homophily
  - Similar nodes are more likely to be connected.

- BFS is ideal to emphasize structural equivalence since this strategy only looks at neighboring nodes.
  - In these random walks, nodes are often repeated and stay close to each other.
- DFS emphasizes the opposite of homophily by creating sequences of distant nodes.
  - These random walks can sample nodes that are far from the source and thus become less representative.

Introducing Biases in Random Walks

- Bias the randomness of these walks in Node2Vec
  - Promoting nodes that are not connected to the previous one (similar to DFS)
  - Promoting nodes that are close to the previous one (similar to BFS)

- Example
  - j: current node
  - i: previous node
  - k: future node
  - π_{jk}: unnormalized transition probability from node j to node k
    - $\pi_{jk} = \alpha(i, k) \cdot \omega_{jk}$
    - ω_{jk}: the weight of the edge from j to k
    - $\alpha(i, k)$: the search bias between nodes i and k

  - In DeepWalk, $\alpha(a, b) = 1$ for any pair of nodes a and b.

Introducing Biases in Random Walks (Cont.)

- In Node2Vec
  - The value of $\alpha(a, b)$ is defined based on the distance between the nodes

$$\alpha(a,b) = \begin{cases} 1/p, & \text{if } d_{ab} = 0 \\ 1, & \text{if } d_{ab} = 1 \\ 1/q, & \text{if } d_{ab} = 2 \end{cases}$$

  - d_{ab} is the shortest path distance between nodes a and b.
  - The return parameter p approximates DFS
    - The walk starts from node i and now arrives at node j. The probability of going back to the previous node is controlled by the return parameter p.
    - The higher it is, the more the random walk will explore new nodes instead of repeating the same ones and looking like DFS.
  - The in-out parameter q approximates BFS.
    - The probability of going to node k_2 is controlled by the in-out parameter q.
    - The higher it is, the more the random walk will focus on nodes that are close to the previous one and look like BFS.
  - The unnormalized probability of going to k_1 is 1
    - Because this node is in the immediate neighborhood of the previous node, i.

Application of Node2Vec

- With biased random walks, the implementation of Node2Vec is very similar to implementing DeepWalk.

- Node classification: classify each node of a graph as part of one of the two groups.
  - Use the node embeddings provided by Node2Vec as input to a machine-learning classifier (e.g., Random Forest).
  - Repeat this process 100 times and take the mean value to limit the randomness of the results.

Parameter Analysis

- For a homophilic network, the homophily property is emphasized by DFS, which is encouraged by increasing the parameter *p*.
- Average accuracy and standard deviation for different values of *p* and *q*

	p=1	p=2	p=3	p=4	p=5	p=6	p=7
q=1	92.95% (± 4.61%)	94.45% (± 4.19%)	96.36% (± 4.69%)	95.41% (± 4.14%)	95.59% (± 4.30%)	95.82% (± 4.67%)	95.41% (± 3.94%)
q=2	93.64% (± 4.36%)	93.95% (± 3.97%)	95.09% (± 4.34%)	95.55% (± 3.80%)	96.27% (± 3.82%)	96.18% (± 3.90%)	97.45% (± 3.60%)
q=3	93.45% (± 3.82%)	94.41% (± 4.11%)	95.77% (± 3.59%)	95.27% (± 3.63%)	96.68% (± 3.90%)	95.64% (± 3.69%)	96.00% (± 3.82%)
q=4	94.14% (± 3.93%)	94.14% (± 3.93%)	95.45% (± 3.40%)	95.05% (± 3.58%)	95.95% (± 3.46%)	96.41% (± 3.71%)	95.59% (± 3.31%)
q=5	94.41% (± 3.68%)	94.18% (± 3.64%)	94.68% (± 3.58%)	95.36% (± 3.75%)	95.64% (± 3.34%)	95.55% (± 3.58%)	95.27% (± 4.01%)
q=6	94.91% (± 3.71%)	94.55% (± 3.08%)	94.59% (± 3.13%)	95.05% (± 3.86%)	95.77% (± 3.23%)	94.55% (± 4.17%)	95.05% (± 3.75%)
q=7	94.64% (± 4.03%)	95.00% (± 3.78%)	93.59% (± 3.97%)	94.86% (± 3.67%)	94.14% (± 3.87%)	95.27% (± 3.74%)	95.82% (± 3.38%)

  - DeepWalk ($p = 1$ and $q = 1$) performs worse than any other combination ($1 \leq p \leq 7$ and $1 \leq q \leq 7$) for this dataset and shows how useful biased random walks can be.
  - High values of *p* lead to better performance, which validates that this is a homophilic network due to the connection between DFS and homophily.

Classifying Nodes

- Classifying nodes with vanilla neural networks (vanilla NNs)
  - A vanilla neural network (also called a multi-layer perceptron) takes the tabular dataset of node features as its input.
- Classifying nodes with vanilla graph neural networks (vanilla GNNs)
  - A neural network layer corresponds to a linear transformation $h_A = x_A W^T$.
    - h_A is the embedding of node A
    - x_A is the input vector (node features) of node A and W is the weight matrix.
  - The graph linear layer can be written as $h_A = \sum_{i \in \mathcal{N}_A} x_i W^T$
    - N_A is the set of neighbors of node A.
    - Equation variants: we could have a weight matrix W_1 dedicated to the central node, and another one W_2 for the neighbors.
  - The equation of the linear layer can be rewritten as $H = XW^T$.
    - X is the input matrix.
  - The graph linear layer can be rewritten as $H = \tilde{A}^T X W^T$.
    - Updated adjacency matrix $\tilde{A} = A + I$, where the adjacency matrix A contains the connections between every node in the graph.

Vanilla NNs v.s. Vanilla GNNs

- Summary of accuracy scores with a standard deviation
  - In order to obtain comparable results, the same experiment is repeated 100 times for each model on each dataset.

	MLP	**GNN**
Cora	53.47% (±1.81%)	74.98% (±1.50%)
Facebook	75.21% (±0.40%)	84.85% (±1.68%)

  - The MLP has poor accuracy on Cora. It performs better on the Facebook Page-Page dataset but is still surpassed by our vanilla GNN in both cases.
  - These results show the importance of including topological information in node features.
  - Instead of a tabular dataset, GNN considers the entire neighborhood of each node, which leads to a 10-20% boost in terms of accuracy in these examples.

Designing the Graph Convolutional Layer

- The vanilla GNN layer does not take into account the difference in the number of neighbors.
  - The embedding of a node i is calculated as $h_i = \sum_{j \in \mathcal{N}_i} x_j W^T$.
  - It consists of a simple sum without any normalization coefficient.

- Simple solution: dividing the embedding by the number of neighbors.
  - New GNN layer: $h_i = \frac{1}{\deg(i)} \sum_{j \in \mathcal{N}_i} x_j W^T$, where $\deg(A)$ is the degree of node A
  - The degree matrix D counts the number of neighbors for each node.
  - The inverse of this matrix D^{-1} directly gives us the normalization coefficients, $\frac{1}{\deg(i)}$.
  - Self-loops are added to the degree matrix $\tilde{D}^{-1} = (D + I)^{-1}$ like self-loops added to the graph by $\tilde{A} = A + I$.

Example

- $$D = \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}, D^{-1} = \begin{bmatrix} \frac{1}{3} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}, \tilde{D}^{-1} = \begin{bmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & \frac{1}{3} \end{bmatrix}$$

- $$\tilde{D}^{-1}\tilde{A} = \begin{bmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & \frac{1}{3} \end{bmatrix} \cdot \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} \end{bmatrix}$$

- $$\tilde{A}\tilde{D}^{-1} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & \frac{1}{3} \end{bmatrix} = \begin{bmatrix} \frac{1}{4} & \frac{1}{2} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{4} & \frac{1}{2} & 0 & 0 \\ \frac{1}{4} & 0 & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{4} & 0 & \frac{1}{3} & \frac{1}{3} \end{bmatrix}$$

Designing the Graph Convolutional Layer (Cont.)

- How to put the matrix of normalization coefficients into the formula $H = \tilde{A}^T X W^T$?
  - $\tilde{D}^{-1}\tilde{A}XW^T$ will normalize every row of features.
  - $\tilde{A}\tilde{D}^{-1}XW^T$ will normalize every column of features.
  - Naturally, the first option looks more appealing because it nicely normalizes neighboring node features.

- Weakness of the first option: features from nodes with many neighbors spread very easily, unlike features from more isolated nodes.

- Solution: a hybrid normalization to counterbalance this effect.
  - Higher weights are assigned to nodes with few neighbors using the formula $H = \tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}XW^T$
  - In terms of individual embeddings, this operation can be written as

$$h_i = \frac{1}{\sqrt{\deg(i)}} \sum_{j \in \mathcal{N}_i} \frac{1}{\sqrt{\deg(j)}} x_j W^T$$

Comparing Graph Convolutional and Graph Linear Layers

- Number of nodes with specific node degrees in the Cora dataset
  - This imbalanced distribution looks exponential with a heavy tail
  - It ranges from 1 neighbor (485 nodes) to 168 neighbors (1 node).
- Number of nodes with specific node degrees in the Facebook Page-Page dataset
  - This distribution of node degrees looks even more skewed, with a number of neighbors that ranges from 1 to 709.

Graph Convolutional v.s. Graph Linear Layers

- Summary of accuracy scores with standard deviation

	MLP	GNN	GCN
Cora	53.47% (±1.81%)	74.98% (±1.50%)	80.17% (±0.61%)
Facebook	75.21% (±0.40%)	84.85% (±1.68%)	91.54% (±0.28%)

  - These high scores are attributed to the wide range of node degrees in these two datasets.
  - By normalizing features and considering the number of neighbors of the central node and its own neighbors, the GCN gains a lot of flexibility.

- Compared to the vanilla GNN, the main feature of the GCN is that it considers node degrees to weigh its features.

Transformer

Attention

- From RNN to Transformer
  - Attention has replaced recurrence functions requiring an increase in the number of parameters as the distance between two words increases.

- Attention mechanism
  - A “word-to-word” (or token-to-token) operation.
  - Determines how each word is related to all other words in a sequence, including the word being analyzed itself.

Model Architecture

- Encoder stack
  - Input embedding
  - Positional encoding (PE)
  - Sublayer 1: Multi-head attention
  - Sublayer 2: Feedforward Network (FFN)

- Decoder stack
  - Output embedding
  - Positional encoding
  - Attention layers
  - FFN sublayer
  - Post-Layer Normalization (Post-LN)
  - Linear layer

Encoder Stack

- Efficient constraint
  - The output of every sublayer of the model has a constant dimension $d_{\text{model}} = 512$, including the embedding layer and the residual connections.

- Input embedding
  - A tokenizer will transform a sentence/word into tokens.
  - The skip-grams model of the word2vec embedding approach
- Positional encoding (PE)
- A multi-headed attention mechanism
  - From layers 1 to 6, each layer learns from the previous layer and explores different ways of associating the tokens in the sequence.
- A fully connected position-wise feedforward network

Positional Encoding

- Tokenizer
  - Use sine and cosine functions to generate different frequencies for the positional encoding for each position and each dimension i of the $d_{\text{model}} = 512$ of the word embedding vector
    - $PE_{(pos,2i)} = \sin \dfrac{pos}{10000^{2i/d}\text{model}}$
    - $PE_{(pos,2i+1)} = \cos \dfrac{pos}{10000^{2i/d}\text{model}}$

- Adding positional encoding to the embedding vector
  - Creating independent positional vectors would have a high cost on the training speed of the Transformer and make attention sublayers overly complex to work with.
  - Idea: add a positional encoding value to the input embedding instead of having additional vectors to describe the position of a token in a sequence.
    - $\text{ie} \cdot d^2_{\text{model}} + \text{pe}$

Multi-Head Attention

- The multi-head attention sublayer contains eight heads and is followed by post-layer normalization, which will add residual connections to the output of the sublayer and normalize it.
- Inside each head h_n of the attention mechanism, the "word" matrices have three representations:
  - A query matrix (Q) that has a dimension of $d_q = 64$, which seeks all the key-value pairs of the other "word" matrices.
  - A key matrix (K) with a dimension of $d_k = 64$.
  - A value matrix (V) with a dimension of $d_v = 64$.
- To obtain Q, K, and V, we must train the model with their respective weight matrices Q_w, K_w, and V_w
  - $Q = x \cdot Q_w$, $K = x \cdot K_w$, $V = x \cdot V_w$
- Attention is defined as scaled dot-product attention, which is represented in the following equation in which we plug Q, K, and V:
  - $$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^{\mathrm{T}}}{\sqrt{d_k}}\right)V$$

Post-Layer Normalization

- The goal of the residual connections is to make sure critical information is not lost.

- Layer normalization is described as LayerNormalization(x + Sublayer(x))
  - Sublayer(x) is the sublayer itself.
  - x is the information available at the input step of Sublayer(x).
- LayerNormalization(v) $= \gamma \dfrac{v - \mu}{\sigma} + \beta$, where $v = x$ + Sublayer(x)
  - μ is the mean of v of dimension d.
  - σ is the standard deviation v of dimension d.
  - γ is a scaling parameter.
  - β is a bias vector.

Feedforward Network (FFN)

- The FFNs in the encoder and decoder are fully connected.

- The FFN is a position-wise network.
  - Each position is processed separately and in an identical way.

- The FFN contains two layers and applies a ReLU activation function.

- The input and output of the FFN layers is $d_{\text{model}} = 512$, but the inner layer is larger with $d_{ff} = 2048$.

- $\text{FFN}(x) = \max(0, xW_1 + b_1)W_2 + b_2$

Decoder Stack

- Output embedding and positional encoding
- Attention layers
- Feedforward network (FFN) sublayer
- Post-Layer Normalization (Post-LN)
- Linear layer
  - The output layer maps the outputs of the model to the size of the vocabulary to produce the raw logits of the prediction.
- The raw logits of the output can go through a softmax function, apply the values obtained to the tokens in the vocabulary, and choose the best probable token for the task requested.

Attention Layers

- The masked multi-head attention sublayer 1 only lets attention apply to the positions up to and including the current position.
  - The future words are hidden from the Transformer, and this forces it to learn how to predict.

- The multi-head attention sublayer 2
  - Only attends to the positions up to the current position the Transformer is predicting to avoid seeing the sequence it must predict.
  - Draws information from the encoder by taking encoder (K, V) into account during the dot-product attention operations.
  - Draws information from the masked multi-head attention sublayer 1 (masked attention) by also taking sublayer 1(Q) into account during the dot-product attention operations.
- The decoder uses the trained information of the encoder.

- The input of the self-attention multi-head sublayer of a decoder
  - Input_Attention=(Output_decoder_sublayer-1(Q),Output_encoder_layer(K,V))

Transformer in PyTorch

- https://pytorch.org/tutorials/beginner/transformer_tutorial.html

Question & Answer