Master Thesis

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2024

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1 Graph Data Structure

A *graph* G [Figure 1] is a non-linear data structure consisting of vertices and edges. The vertices are sometimes also referred to as nodes and the edges are arcs that connect any two nodes in the graph. Graphs are used to represent relationships between different entities and have applications in many fields including Computer Science, Physics, Biology, Chemistry, Optimization Theory and many more.

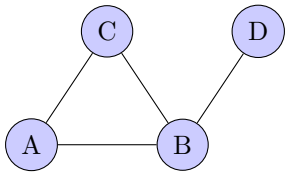


Figure 1: A simple graph

1.1 Formal Definition

A graph is formally defined as a tuple $G = (V, E)$, where:

- V is a finite set of vertices (or nodes).
- E is a set of edges, where each edge is an unordered pair of distinct vertices from V. Thus, $E \subseteq \{\{u, v\} \mid u, v \in V \text{ and } u \neq v\}$.

1.2 Types of Graphs

Graphs can be classified into various types based on their properties, including:

- **Directed Graph** [Figure 2]: A graph in which the edges have a direction, i.e., each edge is an ordered pair of vertices.

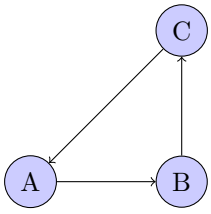


Figure 2: Directed graph example.

- **Undirected Graph** [Figure 3]: A graph in which the edges do not have a direction, i.e., each edge is an unordered pair of vertices.

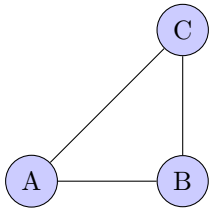


Figure 3: Undirected graph example.

- **Weighted Graph** [Figure 4]: A graph in which a weight (or cost) is associated with each edge.

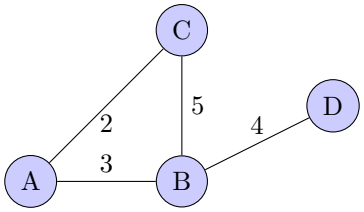


Figure 4: Weighted graph example.

- **Simple Graph** [Figure 5]: A graph with no loops (edges connecting a vertex to itself) and no multiple edges (more than one edge connecting the same pair of vertices).

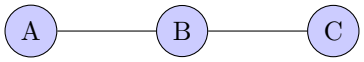


Figure 5: Simple graph example.

- **Complete Graph** [Figure 6]: A graph in which there is exactly one edge between each pair of distinct vertices.

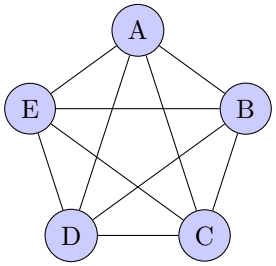


Figure 6: Complete graph example.

- **Bipartite Graph** [Figure 7]: A graph whose vertices can be divided into two disjoint sets U and W such that every edge connects a vertex in U to a vertex in W.

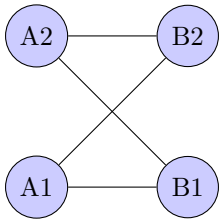


Figure 7: Bipartite graph example.

1.3 Graph Representation

Graphs can be represented in various ways, including:

- **Adjacency Matrix** [Figure 8]: A square matrix A of size $|V| \times |V|$ where $A_{ij} = 1$ if there is an edge between vertices v_i and v_j, and $A_{ij} = 0$ otherwise.

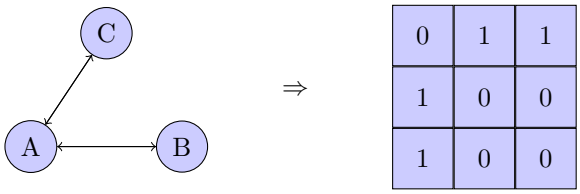
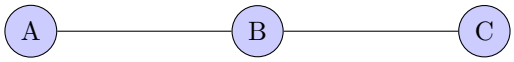


Figure 8: Adjacency Matrix representation.

- **Adjacency List** [Figure 9]: An array of lists. The array contains a list for each vertex, and each list contains the vertices that are adjacent to the corresponding vertex.



$$[\ Adj(A) = [B], \quad Adj(B) = [A, C], \quad Adj(C) = [B]\ ]$$

Figure 9: Adjacency List representation for an undirected graph.

2 Neural Networks

A *neural network* is a computational model that is inspired by the way biological neural networks in the human brain process information. It consists of intercon-

nected units called neurons that work together to solve specific problems. The basic building block of a neural network is the perceptron, which computes a weighted sum of its inputs and passes the result through an activation function.

2.1 Basic Structure of a Neural Network

A simple neural network [Figure 10] consists of three types of layers:

- **Input Layer**: The layer that receives the input data.
- **Hidden Layers**: One or more intermediate layers that process the inputs received from the input layer.
- **Output Layer**: The layer that produces the final output.

The following figure illustrates a basic neural network with one hidden layer:

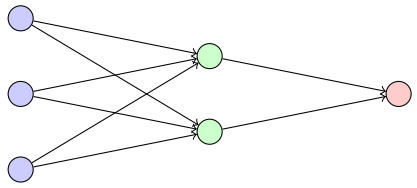


Figure 10: A simple neural network with one hidden layer.

2.2 Training Neural Networks

Training a neural network involves adjusting the weights of the connections to minimize the error between the predicted output and the actual output. This is typically done using a method called *backpropagation* along with an optimization algorithm like *gradient descent*. The training process involves multiple iterations, where in each iteration, the network processes a batch of input data, calculates the output, computes the error, and updates the weights to reduce this error.

2.2.1 Backpropagation

Backpropagation [Figure 11] is an algorithm used to compute the gradient of the loss function with respect to each weight by the chain rule, iterating backward from the last layer to the first layer. During the forward pass, the input data propagates through the network layer by layer until the final output is obtained. The error is then calculated using a loss function, which measures the difference between the predicted output and the actual output. In the backward pass, this error is propagated back through the network, allowing the algorithm to

compute the gradients of the loss function with respect to each weight. These gradients indicate how much the loss would change with a small change in the weights, guiding the weight update process.

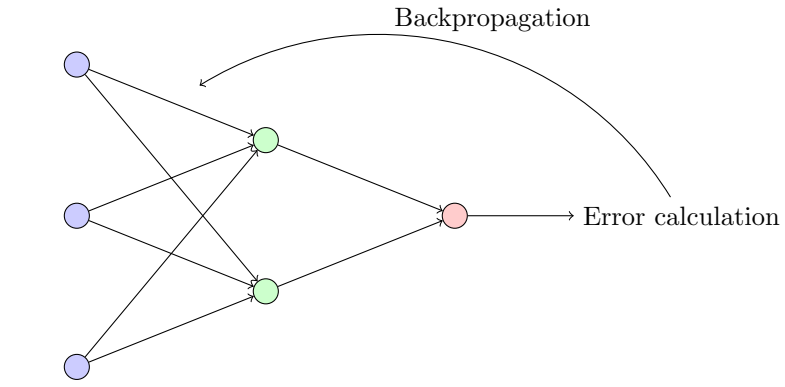


Figure 11: A simple neural network with one hidden layer.

2.2.2 Gradient Descent

Gradient descent [Figure 12] is an optimization algorithm used to minimize the loss function by iteratively moving towards the steepest descent, based on the computed gradients. At each iteration, the algorithm updates the weights by moving them in the opposite direction of the gradient of the loss function with respect to the weights. The size of these steps is determined by the learning rate, a hyperparameter that needs to be carefully chosen. A too large learning rate can cause the algorithm to overshoot the minimum, while a too small learning rate can make the convergence excessively slow.

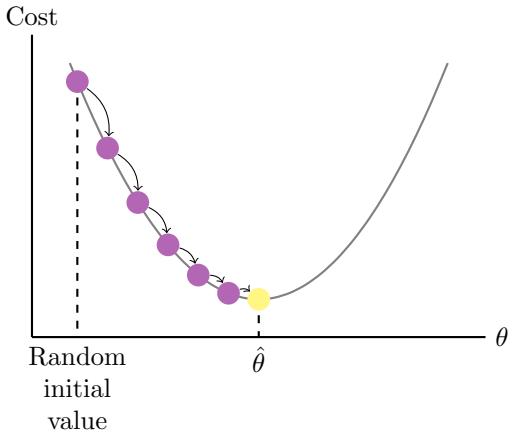


Figure 12: Gradient descent method applied on a simple function.

2.3 Advanced Topics in Neural Networks

2.3.1 Deep Neural Networks

A *deep neural network* (DNN) [Figure 13] is an artificial neural network with multiple hidden layers between the input and output layers. DNNs can model complex patterns and relationships in data, making them powerful tools for tasks such as image and speech recognition. The increased depth allows these networks to learn hierarchical representations of the data, capturing low-level features in the early layers and high-level features in the deeper layers.

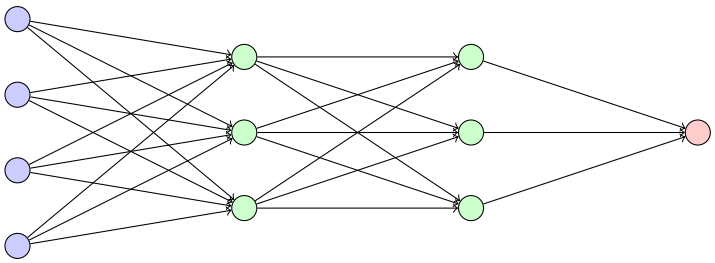


Figure 13: A Deep neural network with two hidden layers.

2.3.2 Convolutional Neural Networks

A *convolutional neural network* (CNN) [Figure 14] is a specialized type of neural network designed for processing structured grid data, like images. CNNs use convolutional layers that apply a series of filters to the input data to extract

features. These filters slide over the input data, performing element-wise multiplications and summing the results, which helps in detecting patterns such as edges, textures, and shapes.

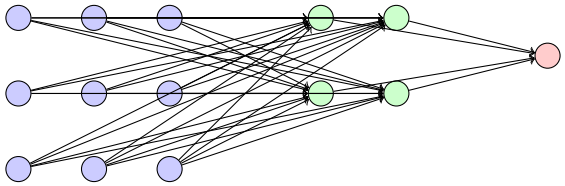


Figure 14: A simple convolutional neural network architecture.

2.3.3 Recurrent Neural Networks

A *recurrent neural network* (RNN) [Figure 15] is a type of neural network that is well-suited for sequential data, such as time series or natural language. RNNs have connections that form directed cycles, allowing information to persist. This cyclic structure enables RNNs to maintain a hidden state that captures information from previous time steps, making them effective for tasks where the context is important, such as language modeling and machine translation.

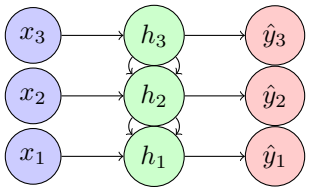


Figure 15: Recurrent Neural Network (RNN) unrolled through time.

2.4 Graph Neural Networks and Attention Mechanisms

2.4.1 Graph Neural Networks

A *graph neural network* (GNN) is a type of neural network designed to handle graph-structured data. GNNs generalize neural networks to work directly on the graph domain by incorporating the graph's structure into the learning process. Nodes in a GNN aggregate feature information from their neighbors through multiple layers, enabling the network to capture the dependencies and relationships inherent in the graph. This message-passing mechanism [Figure 16] allows GNNs to learn rich node representations and can be used for tasks such as node classification, link prediction, and graph classification.

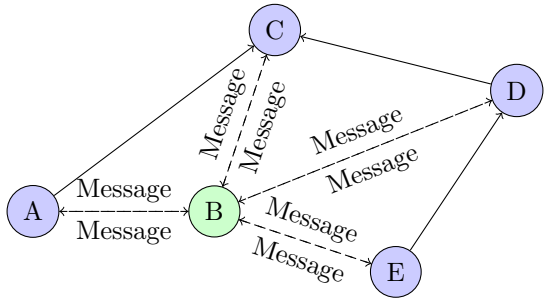


Figure 16: Message passing between node B and its neighbors in a GNN.

2.4.2 Attention Mechanisms

Attention mechanisms are techniques used to enhance the performance of neural networks by dynamically focusing on relevant parts of the input data while processing. The most famous use of attention mechanisms is in the *Transformer* model, which has revolutionized natural language processing tasks. The attention mechanism [Figure 17] computes a weighted sum of values, where the weights are derived from the compatibility of the query with the corresponding keys, allowing the model to selectively focus on important parts of the input. This selective focus helps improve the efficiency and accuracy of the model, especially in tasks involving sequences, such as machine translation and text summarization. The combination of GNNs and attention mechanisms has shown significant promise in various applications.

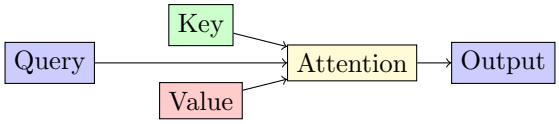


Figure 17: Attention mechanism in neural networks.

3 Graph Similarity Problem

The *graph similarity problem* involves determining the degree of similarity between two graphs. This problem has numerous applications in pattern recognition, computer vision, bioinformatics, and other fields. One common method to quantify graph similarity is through the *graph edit distance* (GED).

3.1 Graph Edit Distance (GED)

The *graph edit distance* between two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is defined as the minimum cost required to transform G_1 into G_2 using a sequence of atomic operations. Formally, let Σ be the set of all possible edit operations,

and let $c : \Sigma \to \mathbb{R}^+$ be a cost function that assigns a positive real number to each operation. The GED is then given by:

$$\text{GED}(G_1, G_2) = \min_{\sigma \in \Sigma^*} \sum_{o \in \sigma} c(o)$$

where Σ^* denotes the set of all finite sequences of operations from Σ, and o represents an individual operation within a sequence σ.

The computation of GED is known to be **NP-HARD**, indicating that finding the exact minimum edit distance between two graphs is computationally intensive.

3.2 Atomic Operations

The basic atomic operations typically includes:

- **Vertex Insertion**: Inserting a new vertex v into the graph.
- **Vertex Deletion**: Deleting an existing vertex v from the graph.
- **Edge Insertion**: Inserting a new edge $e = \{u, v\}$ into the graph.
- **Edge Deletion**: Deleting an existing edge $e = \{u, v\}$ from the graph.

To demonstrate the Graph Edit Distance (GED), consider pair of graphs represented in [Figure 18]:

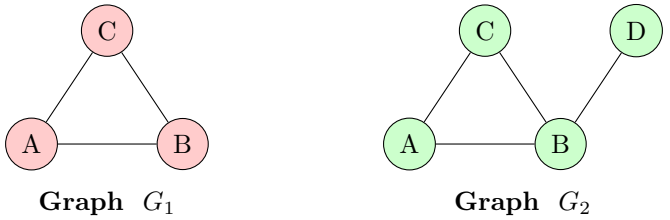


Figure 18: Pair of graphs to demonstre Graph Edit Distance.

In this example, graph G_1 has vertex set $V_1 = \{A, B, C\}$ and edge set $E_1 = \{\{A, B\}, \{A, C\}, \{B, C\}\}$, while graph G_2 has vertex set $V_2 = \{A, B, C, D\}$ and edge set $E_2 = \{\{A, B\}, \{A, C\}, \{B, C\}, \{B, D\}\}$. The transformation (which cost is lowest) from G_1 to G_2 involves: Inserting the vertex D and Inserting the edge $\{B, D\}$. If we assign a cost of 1 to each operation the total cost (GED) is: $1 + 1 = 2$.

4 State of the Art Review

Traditional imperative solutions for solving the graph edit distance (GED) problem do exist and can be quite effective for graphs of modest size. These methods typically involve explicit algorithms that compare graphs node by node and

edge by edge, often using combinatorial techniques. However, as the number of nodes in the graph increases, the complexity of these methods grows exponentially, leading to scalability issues. In such cases, imperative solutions often become impractical, taking an inordinate amount of time to compute the GED.

To address these scalability challenges, recent research has focused on leveraging artificial intelligence (AI) models. These AI-based approaches offer more robust and scalable solutions by learning patterns and features from graph data, significantly reducing computation times and improving accuracy. In this section, we review some of the prominent AI-based models that have advanced the state of the art in GED computation, including SimGNN, GPN, TaGSim, and GedGNN.

4.1 SimGNN

The first innovative model that significantly outperformed the competition is SimGNN [**?**], introduced in 2019. SimGNN serves as a foundational model in the field of graph similarity computation, and subsequent models often inherit its core concepts, making it the starting point of reference for anyone working in this niche field.

SimGNN is an end-to-end neural network-based approach designed to learn a function that maps a pair of graphs to a similarity score. An overview of SimGNN is illustrated in Figure 19. The architecture of SimGNN involves several key stages:

- **Node Embedding Stage**: Each node in the graph is transformed into a vector that encodes its features and structural properties.
- **Graph-Level Embedding Stage**: The node embeddings are aggregated using an attention mechanism to produce a single embedding for each graph.
- **Graph-Graph Interaction Stage**: The graph-level embeddings of the two graphs are interacted to produce interaction scores that represent the similarity between the graphs.
- **Final Similarity Score Computation Stage**: The interaction scores are further processed to compute the final similarity score, which is compared against the ground-truth similarity score for parameter updates.

In addition to the graph-level embedding interaction strategy, SimGNN incorporates a pairwise node comparison strategy:

- **Pairwise Node Comparison**: This strategy involves computing pairwise interaction scores between the node embeddings of the two graphs. For graphs of different sizes, fake nodes with zero embeddings are added to the smaller graph to ensure compatibility. The resulting similarity matrix is used to extract histogram features, which are then combined with graph-level interaction scores to provide a comprehensive view of graph similarity.

The combination of these two strategies allows SimGNN to capture both coarse global comparison information and fine-grained node-level comparison information, resulting in a robust and thorough approach to graph similarity computation.

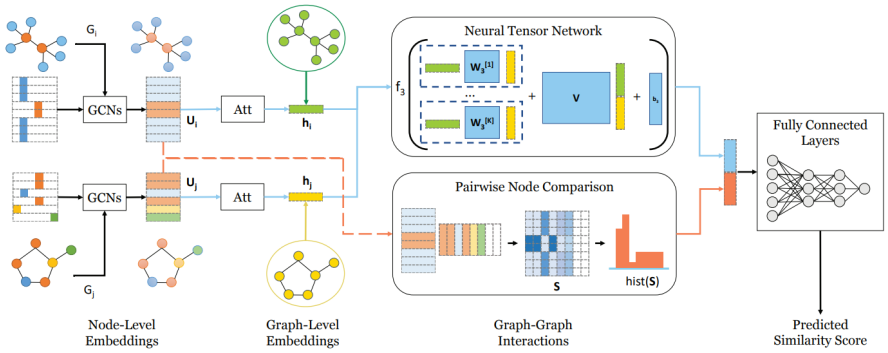


Figure 19: SimGNN architecture overview.

4.2 GedGNN

Very recently (2023), the GedGNN [**?**] model introduced significant advancements in the field of graph similarity computation, demonstrating substantial performance improvements over previous models like SimGNN. An overview of GedGNN is illustrated in Figure 20. The architecture of GedGNN comprises several key components:

- **Node Embedding Generation**: GedGNN employs a Graph Neural Network (GNN) to generate node embeddings for the input graphs. Specifically, it utilizes a three-layer Graph Isomorphism Network (GIN), which is known for its exceptional ability to capture intricate graph structures.
- **Cross Matrix Modules**: GedGNN incorporates two distinct cross matrix modules to capture node-to-node correspondences between the embeddings of the two graphs:
  - One module produces a matching matrix (A_{match}), which predicts the ground-truth matching matrix.
  - The other module generates a cost matrix (A_{cost}), where each element represents the cost of edit operations required to align nodes between the two graphs.
- **Similarity Score Prediction**: The final similarity score, representing the graph edit distance (GED) value, is computed by calculating the weighted sum of costs in the cost matrix, with an additional bias value.

Compared to SimGNN, GedGNN offers several key advancements, including enhanced efficiency, increased accuracy, and greater robustness. Additionally, GedGNN is capable of retrieving an edit path between the two graphs in input. A post-processing algorithm based on k-best matching is employed to derive k potential node matchings from the matching matrix produced by GedGNN, with the best matching leading to a high-quality edit path.

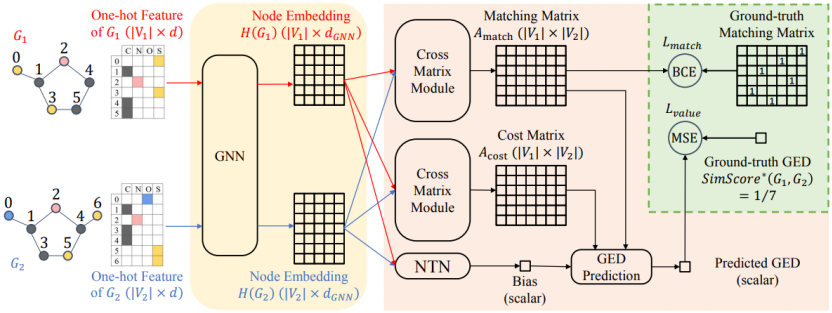


Figure 20: GedGNN architecture overview.

4.3 Other Relevant Mentions

This section highlights additional notable contributions in the field of graph similarity and edit distance computation, showcasing a range of innovative approaches and models.

- **Dynamic Embedding and Edit Path Search** [**?**]: Proposes a hybrid approach integrating dynamic graph embedding with edit path search, enhancing interpretability and cost-efficiency in solving graph edit distance problems.
- **PSimGNN** [**?**]: Describes PSimGNN, which partitions graphs and uses a graph neural network for efficient similarity computation, combining coarse and fine-grained approaches to outperform existing methods.
- **Noah** [**?**]: Introduces Noah, which integrates A* search with Graph Path Networks for approximate GED computation, optimizing search complexity and demonstrating practical effectiveness.
- **HGNN** [**?**]: Presents HGNN, combining GNNs with hash learning for efficient graph-based data retrieval, addressing irregular structures and high computational complexity in graph operations.
- **INFMCS** [**?**]: Introduces INFMCS, an interpretable model inferring Maximum Common Subgraph during graph similarity learning, combining transformers and graph convolution for improved performance.

- **H2MN** [**?**]: Presents H2MN, leveraging hierarchical hypergraph matching for graph similarity learning, employing hyperedge pooling and multi-perspective matching to achieve superior results.
- **Isomorphic Vertex Reduction** [**?**]: Proposes a method to reduce GED computation costs by addressing redundant mappings from isomorphic vertices, aiming for optimization in exact and approximate GED computations.
- **NA-GSL** [**?**]: Proposes NA-GSL, a unified framework incorporating attention mechanisms for graph similarity estimation, achieving improved performance through graph convolution and cross-graph co-attention.
- **DiffAtt** [**?**]: Introduces DiffAtt, a graph-level fusion module leveraging attention mechanisms to compute GED efficiently, outperforming traditional methods in accuracy and speed.
- **GED-CDA** [**?**]: Presents GED-CDA, incorporating context dependency attention modules for GED computation, capturing inter- and intra-graph dependencies effectively, and demonstrating high efficiency.
- **GREED** [**?**]: Describes GREED, a siamese GNN model for GED and Subgraph Edit Distance, preserving metric properties and achieving high accuracy and efficiency for large-scale retrieval tasks.
- **MATA*** [**?**]: Introduces MATA*, a hybrid model combining GNNs and A* algorithms for approximate GED computation, addressing scalability and efficiency issues with promising results.
- **MGMN** [**?**]: Presents MGMN, a multilevel graph matching network capturing cross-level interactions for graph similarity, demonstrating superior performance and robustness with increasing graph size.
- **WWLS** [**?**]: Proposes WWLS, combining Wasserstein distance with L1-approximated tree edit distance to detect subtle structural differences, showing superior performance in graph classification tasks.
- **EUGENE** [**?**]: Introduces EUGENE, an unsupervised method for GED estimation using algebraic representation and rounding, demonstrating competitive performance and potential for broader applications.

5 Bottleneck Loading GPU Problem

6 Dataset Generation

References