Università della Calabria

Department of Mathematics and Computer Science

Master's Degree Course in
Artificial Intelligence and Computer Science

Master's Thesis

Approximating Graph Edit Distance through Graph Neural Networks: Methods, Limitations, and Proposals

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1 Introduction

Graphs are fundamental structures in computer science and mathematics that model relationships between entities. They consist of vertices (or nodes) and edges (or links) that connect pairs of vertices. This simple yet powerful representation can capture a wide variety of real-world scenarios, providing a versatile tool for analyzing complex systems. For instance, social networks can be represented as graphs where nodes denote individuals, and edges represent their connections or interactions, enabling the study of social dynamics, influence, and community formation. In biology, protein-protein interaction networks, neural networks of the brain, and ecological networks can all be modeled as graphs, facilitating the understanding of biological processes, brain functionality, and ecosystem interdependencies. Similarly, in transportation, cities can be nodes and roads or flights can be edges, creating a network that facilitates route optimization, urban planning, and logistical efficiency. Graphs can also model communication networks, where devices are nodes and connections are edges, allowing for analysis of data flow, network robustness, and optimization of resource allocation.

Graph theory provides a rich framework for analyzing these structures, with properties such as connectivity, centrality, and clustering coefficient helping to understand the underlying patterns and behaviors within the network. Connectivity measures how well the nodes are connected, centrality identifies the most important nodes within the graph, and clustering coefficient gives insight into the degree to which nodes tend to cluster together. Additionally, other important graph properties include graph diameter, which measures the longest shortest path between any two nodes, and graph density, which indicates the level of interconnectedness in the network. These properties help in uncovering critical information about the structure and function of the graph, enabling more effective analysis and decision-making.

The Graph Edit Distance (GED) problem is a critical measure in graph theory, providing a similarity metric between two graphs. GED quantifies how many operations (such as insertions, deletions, and substitutions of nodes and edges) are required to transform one graph into another. This measure is invaluable for various applications, including bioinformatics, where it can compare molecular structures to identify potential drug candidates or understand evolutionary relationships. In computer vision, GED is crucial for object recognition, where the structural similarity between graphical representations of different objects must be assessed to identify and classify them accurately. Other graph similarity measures include graph isomorphism, which checks for exact structural similarity, and subgraph isomorphism, which identifies if one graph is a subgraph of another, useful for pattern matching and searching within larger networks.

Knowing the exact GED between two graphs can provide profound insights. For example, in bioinformatics, understanding the similarity between different molecular structures can lead to the discovery of new drugs and therapeutic targets by revealing structural patterns that correlate with biological activity.

In social network analysis, GED can help detect communities or clusters of users with similar interaction patterns, aiding in the identification of influential individuals, the spread of information, or the formation of social groups. Moreover, in pattern recognition and image analysis, GED can assist in identifying objects and understanding their structural relationships, enhancing the accuracy and reliability of automated systems. The ability to quantify the similarity between graphs allows for more precise and meaningful comparisons, driving innovations and improvements across these fields.

However, computing the exact GED is notoriously difficult due to its high computational complexity. The problem is NP-hard, meaning that the time required to solve it grows exponentially with the size of the graphs, making it computationally prohibitive for large graphs. This involves an exhaustive search over all possible edit paths, which is impractical for real-world applications. Various heuristics and approximation algorithms have been proposed, but they often struggle to balance accuracy and computational efficiency, leading to trade-offs that can impact the reliability of the results. The NP-hard class encompasses problems that are at least as hard as the hardest problems in NP, and no known polynomial-time algorithm can solve them. This inherent difficulty underscores the challenge of computing GED and the necessity for developing efficient approximation methods that can provide accurate results within reasonable timeframes.

Neural networks, a cornerstone of modern machine learning, have revolutionized numerous fields by providing robust methods for handling complex, high-dimensional data. A neural network is a series of algorithms that attempt to recognize underlying relationships in a set of data through a process that mimics the way the human brain operates. They consist of interconnected layers of nodes, or neurons, each capable of processing inputs and producing outputs. Neural networks are trained using large datasets where they adjust their internal parameters based on the error between the predicted outputs and the actual outputs. This training process involves forward propagation, where inputs are passed through the network to generate outputs, and backpropagation, where the error is propagated back through the network to update the weights, thereby improving the model's accuracy. Neural networks have been successfully applied to a wide range of tasks, including image and speech recognition, natural language processing, and more recently, graph-structured data analysis, demonstrating their versatility and effectiveness.

Graph Neural Networks (GNNs) are a specialized type of neural network designed to work directly with graph-structured data. GNNs aim to leverage the graph's inherent structure by performing convolution operations over the nodes and edges, capturing both local and global graph properties. This makes them well-suited for various tasks, including node classification, link prediction, and graph classification. Given their ability to learn complex patterns and representations, GNNs hold promise for approximating the GED. GNNs operate by iteratively updating the representation of each node based on its neighbors, effectively capturing the dependencies and relationships within the graph. This iterative process enables GNNs to learn hierarchical representations that are cru-

cial for understanding and analyzing graph-structured data, allowing for more accurate and meaningful predictions in various applications.

This thesis reviews a range of key articles to explore the current state-of-the-art methods in GED computation, encompassing both neural network-based approaches and traditional methods. The reviewed works span various innovative strategies, each attempting to tackle the challenges of GED computation from different angles. By critically analyzing these methods, this review aims to identify their strengths and limitations, offering insights into potential improvements. The seminal paper on SimGNN [2] serves as a foundation for many subsequent works, introducing a neural network-based approach to GED computation that has inspired numerous advancements. More recent works, such as GedGNN [11], continue to push the boundaries of what is possible, integrating novel techniques and improving upon previous methods.

Improving GED computation methods is crucial for enhancing the performance of numerous applications that rely on graph similarity measures. For instance, more efficient and accurate GED computation can lead to breakthroughs in drug discovery by enabling faster and more precise comparison of molecular structures, facilitating the identification of new compounds with therapeutic potential. In social network analysis, it can facilitate the detection of more accurate community structures, leading to better understanding and management of social dynamics, improving the effectiveness of interventions and policy decisions. In computer vision, improved methods can enhance object recognition systems, making them more reliable and efficient, which is vital for applications ranging from autonomous vehicles to security systems. The implications of better GED computation extend to numerous domains, highlighting the importance of continued research and development in this area to unlock new possibilities and advancements.

As we delve into the review of these articles, the goal is to provide a comprehensive overview of the advancements in GED computation. By highlighting innovative strategies and pinpointing areas for further research, this thesis aims to contribute to the ongoing efforts to refine and enhance GED computation methods. We will reproduce the results of key recent papers, such as the one proposing GedGNN, to validate their findings. Additionally, this thesis will offer critical and constructive advice on aspects such as code quality, the fairness of presented results, and the limitations of the datasets used. We will discuss issues like poor dataset quality and propose solutions, including artificial dataset generation and the development of neural networks that can be tested on any dataset, ensuring a fairer evaluation. This comprehensive review aims to bridge the gap between existing methods and the potential for new, more effective techniques, ultimately contributing to the broader field of graph theory and its myriad applications. By providing a thorough analysis and constructive feedback, this thesis seeks to guide future research and development efforts, paving the way for advancements that will enhance the accuracy, efficiency, and applicability of GED computation methods in various fields.

2 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, Social Sciences, and many more. They are fundamental in modeling networks such as social networks, communication networks, biological networks, and transportation systems, making them indispensable tools for analyzing and solving complex problems. In everyday tasks, graphs can represent relationships in recommendation systems, routing algorithms in GPS navigation, workflow optimization, and resource allocation in various industries.

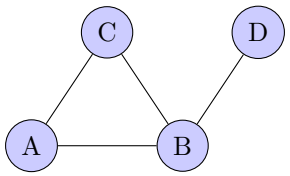


Figure 1: Simple undirected graph example.

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

- V is a finite set of vertices (or nodes). Each vertex represents an entity or a data point, and the set of vertices V is often denoted as $V = \{v_1, v_2, \ldots, v_n\}$ where n is the number of vertices.
- E is a set of edges, where each edge is an unordered pair of distinct vertices from V. Thus, $E \subseteq \{\{u, v\} \mid u, v \in V \text{ and } u \neq v\}$. Each edge signifies a relationship or connection between the pair of vertices it links.

For instance The graph depicted in Figure 1 can be formally defined as a tuple $G = (V, E)$, where:

- V is the set of vertices, $V = \{A, B, C, D\}$
- E is the set of edges, $E = \{(A, B), (A, C), (B, C), (B, D)\}$

2.1 Types of Graphs

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

- **Directed Graph** [Figure 2]: A directed graph (or digraph) is a graph in which every edge has a direction, represented as an ordered pair (u, v) where $u, v \in V$ and $u \neq v$. It is used in various applications such as web page ranking, where links from one page to another have a specific direction, and citation networks, where one paper cites another.

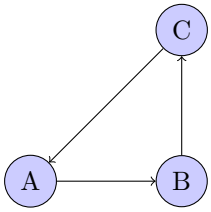


Figure 2: Directed graph where edges have directions indicated by arrows.

- **Undirected Graph** [Figure 3]: An undirected graph is a graph in which the edges do not have a direction, represented as an unordered pair $\{u, v\}$ where $u, v \in V$ and $u \neq v$. This type of graph is commonly used to model social networks where the connections (friendships) are mutual, indicating that if one person is friends with another, the reverse is also true.

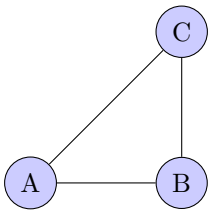


Figure 3: Undirected graph example where edges are bidirectional (there are no arrows).

- **Weighted Graph** [Figure 4]: A weighted graph is a graph in which each edge has an associated weight or cost, represented as a function $w : E \to \mathbb{R}$ where $w(e)$ is the weight of edge $e \in E$. This is particularly useful in transportation networks where the weights can represent distances, travel times, or costs associated with traveling between locations.

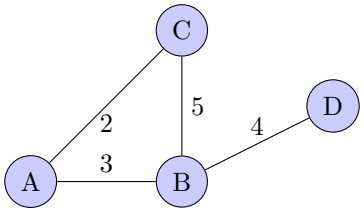


Figure 4: Weighted graph example where each edge is labeled with a weight.

- **Simple Graph** [Figure 5]: A simple graph is a graph that has no loops (edges connecting a vertex to itself) and no multiple edges (more than one edge connecting the same pair of vertices). Simple graphs are the most basic type of graph, with straightforward structures that make them easy

to analyze. They are used in many basic network models to simplify the analysis and understand the fundamental properties of the network.

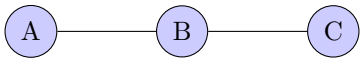


Figure 5: Simple graph example with a linear connection between vertices A, B, and C, with no loops or multiple edges.

- **Complete Graph** [Figure 6]: A complete graph is a graph in which there is exactly one edge between each pair of distinct vertices. Formally, a complete graph on n vertices, denoted as K_n, has $E = \{\{u, v\} \mid u, v \in V, u \neq v\}$. Complete graphs are used in scenarios where maximum connectivity is required, such as in certain network topologies and in combinatorial optimization problems.

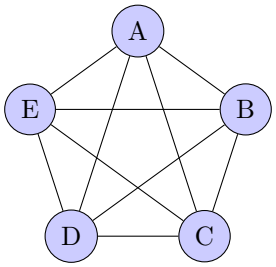


Figure 6: Complete graph example where each node is connected to each other.

- **Bipartite Graph** [Figure 7]: A bipartite graph is 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. Bipartite graphs are used to model relationships between two different classes of objects. For example, in job assignments, vertices in U can represent jobs, and vertices in W can represent workers, with edges indicating which workers are assigned to which jobs.

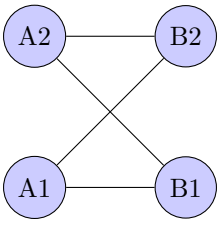


Figure 7: Bipartite graph example with two distinct sets of vertices with edges connecting vertices across the sets but not within them.

- **Multigraph** [Figure 8]: A multigraph is a graph which allows multiple edges between the same pair of vertices. Formally, $G = (V, E)$ where E is a multiset of unordered pairs of vertices. Multigraphs are used to model scenarios where multiple relationships or interactions can exist between entities. For example, in transportation networks, multiple routes or connections can exist between the same pair of locations, and these multiple edges can represent different routes or modes of transport.

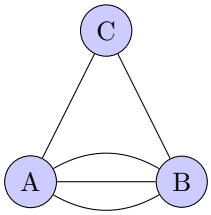


Figure 8: Multigraph example with multiple edges between vertices A and B.

- **Cyclic Graph** [Figure 9]: A cyclic graph is a graph that contains at least one cycle, where a cycle is a path of edges and vertices wherein a vertex is reachable from itself. Cyclic graphs are used to model processes or systems where feedback loops are present. For example, in certain biological systems or in recurrent neural networks, cycles can represent the feedback mechanisms or recurrent connections.

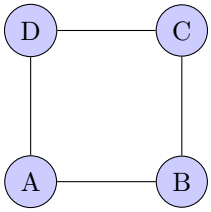


Figure 9: Cyclic graph example with a cycle A-B-C-D-A.

- **Acyclic Graph** [Figure 10]: An acyclic graph is a graph with no cycles. A directed acyclic graph (DAG) is a directed graph with no directed cycles. Acyclic graphs, especially directed acyclic graphs (DAGs), are used in scenarios such as scheduling tasks, where dependencies must not form cycles. In such cases, a task can only start once all its prerequisite tasks are completed, and the absence of cycles ensures that there are no circular dependencies.

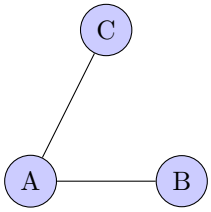


Figure 10: Acyclic graph example with no cycles.

2.2 Graph Representation

Graphs can be represented in various ways, including:

- **Adjacency Matrix** [Figure 11]: An adjacency matrix A for a graph $G = (V, E)$ is a square matrix of size $|V| \times |V|$. The entry A_{ij} is 1 if there is an edge between vertices v_i and v_j, and 0 otherwise. This representation is particularly useful for dense graphs, where the number of edges is close to the maximum possible number of edges. It allows for efficient querying of edge existence and is easy to implement for algorithms that require frequent checks of edge presence. However, the space complexity is $O(|V|^2)$, which can be prohibitive for large graphs with many vertices.

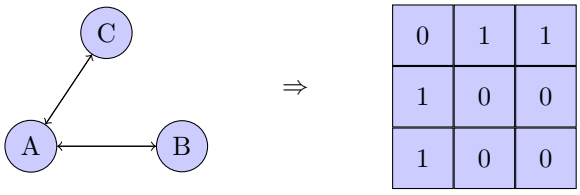
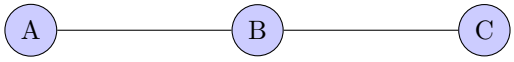


Figure 11: Adjacency Matrix example.

- **Adjacency List** [Figure 12]: An adjacency list is a collection of lists or arrays where each list corresponds to a vertex and contains all the vertices adjacent to that vertex. For a graph $G = (V, E)$, the adjacency list can be represented as an array of lists $\{L_1, L_2, \ldots, L_n\}$, where each L_i contains the neighbors of vertex v_i. This representation is more space-efficient for sparse graphs, where the number of edges is much smaller than the number of possible edges. It facilitates efficient traversal operations such as breadth-first search (BFS) and depth-first search (DFS), where only the relevant neighbors of each vertex need to be examined.



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

Figure 12: Adjacency List example.

2.3 Properties of Graphs

Graphs possess various properties that help in their analysis and application. Some of these properties include:

- **Degree** [Figure 13]: The degree of a vertex is the number of edges incident to it. For a vertex v in a graph $G = (V, E)$, the degree $\deg(v)$ is the count of edges connected to v. In directed graphs, the in-degree represents the number of incoming edges and the out-degree represents the number of outgoing edges. High-degree vertices often play a crucial role in the graph, indicating significant or highly connected nodes.

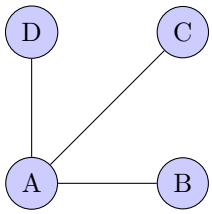


Figure 13: Degree example showing vertex A with degree 3.

- **Connectivity** [Figure 14]: Connectivity refers to how well nodes are interconnected within a graph. A graph is said to be connected if there is a path between every pair of vertices. This property is vital for understanding network reliability and robustness, as it ensures that all nodes can communicate or reach each other directly or indirectly.

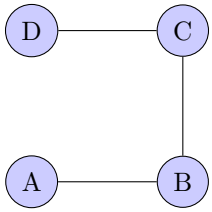


Figure 14: Connectivity example showing a connected graph.

- **Centrality** [Figure 15]: Centrality measures are used to identify the most important vertices within a graph. Different types of centrality include

degree centrality, which counts the number of direct connections a vertex has; closeness centrality, which measures how quickly a vertex can access other vertices; and betweenness centrality, which quantifies how often a vertex acts as a bridge along the shortest path between other vertices. These measures provide various insights into the roles and influence of vertices in a network.

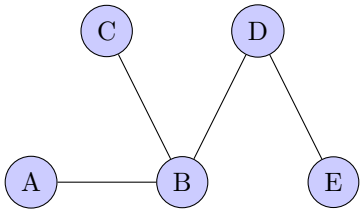


Figure 15: Centrality example showing vertex B as a central node with high degree centrality.

- **Clustering Coefficient** [Figure 16]: The clustering coefficient of a vertex measures the extent to which neighbors of the vertex are also connected to each other. A high clustering coefficient indicates a tightly-knit community within the graph. In mathematical terms, it is calculated as the ratio of the number of actual edges to the number of possible edges among the neighbors of a vertex.

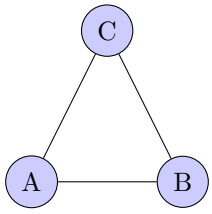


Figure 16: Clustering coefficient example showing a triangle, indicating a high clustering coefficient.

- **Graph Diameter** [Figure 17]: The diameter of a graph is the length of the longest shortest path between any pair of vertices. This metric provides an indication of the "spread" of the graph and helps in understanding how far apart vertices can be in terms of the shortest path distance.

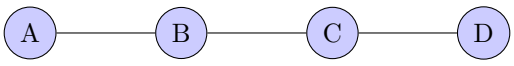


Figure 17: Graph diameter example showing the longest shortest path A-B-C-D with diameter 3.

- **Graph Density** [Figure 18]: Graph density is defined as the ratio of the number of edges in the graph to the number of possible edges between vertices. For a graph with n vertices, the maximum number of edges is $\frac{n(n-1)}{2}$ in an undirected graph. Density provides a measure of how close the graph is to being a complete graph, where all possible edges are present.

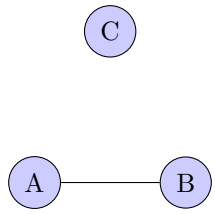


Figure 18: Graph density example showing a sparse graph with few edges relative to the number of vertices.

3 Neural Networks

A *neural network* is a complex computational model inspired by anatomy of the human brain. These models are designed to learn and particularly to recognize patterns in a given data by imitating the functionalities of biological neurons. In fact, the building blocks of every existing neural network are called neurons or nodes. Each of these unit performs simple computations that when combined together allow to tackle a wide range of tasks in a sort of magical way.

3.1 Basic Structure of a Neural Network

Neurons in a neural networks are organized in *layers* which determine the structure and the capability of the net it self. There is a plenitude of way to organize models, but the simplest we can think of [Figure 19] consists only of three layers.

- **Input Layer**: The first layer of every net. It consists of input neurons that receive the initial data. Usually, each neuron in the input layer corresponds to a feature or example in the input dataset. For instance if we are working with an image recognition model, each neuron might represent a pixel value of the input image.
- **Hidden Layer**: Intermediate layer where the actual computation and learning is performed. In the simplest case we only have one hidden layer, but as we will see there can be many more. Each hidden layer consists of neurons that apply *weights* and *activations functions* to the inputs received from the previous layer.
- **Output Layer**: The last layer in the network, which produces the actual output. For example if we are building a regression task model the output

layer could consist of a single neuron which will produce a numeric value as prediction.

The following figure represents a basic neural network with one hidden layer, showing how data flows from the input layer, through the hidden layer, to the output layer:

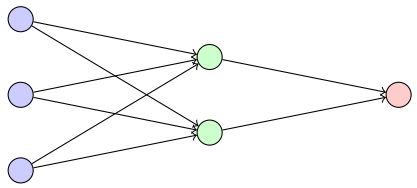


Figure 19: A simple neural network with one hidden layer.

3.1.1 Activation Functions

As already said, in a neural network, each neuron is connected to one or more neurons in the next layer (with exception of the output layer) through *activation functions*. These functions are crucial because they introduce non-linearity into the model, allowing it to capture and learn complex relationships within the data. Without activation functions, we could build a net with thousands of hidden layers but it would still be limited to "linear predictions". Some commonly used activation functions include:

- **Sigmoid**: This function maps any real number into the range (0, 1). It is often used in the output layer for binary classification problems where a probability is needed as output.

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

- **Tanh (Hyperbolic Tangent)**: This function maps any real number into the range (-1, 1). It is zero-centered, which helps in having a more balanced output.

$$\tanh(x) = \frac{2}{1 + e^{-2x}} - 1$$

- **ReLU (Rectified Linear Unit)**: This function is the most commonly used because simple yet effective. It outputs the input directly if it is positive; otherwise, it outputs zero.

$$\text{ReLU}(x) = \max(0, x)$$

3.2 Training Neural Networks

In supervised learning data used is said to *labeled* meaning that for each *example* its *class* is known. Unsupervised and Semi-supervised learning also exist but we are going to deal with these. Weights are numerical values associated with the connections between neurons, usually being in the range [0, 1] when the data is normalized. Training a neural networks means to find the optimal weights values for each connection so to minimize the error between model's prediction and the actual target values. This is usually achieved through the employment of a technique known as *backpropagation* and the usage of an optimization algorithm such as *gradient descent*. The training process is conducted iteratively until net's performance start to degrade or simply it stops learning. This is done with the usage of a dataset usually split in three parts:

- **Training Set**: This subset is used to adjust the weights of the network when performing the actual training. The model learns and updates its weights based on this data to minimize the error between its predictions and the actual values. Usually it constitutes about the 80% of the whole dataset and if it isn't enough big then techniques to generate artifical data are used.
- **Validation Set**: This small subset is used to tune *hyperparameters*, which are the parameters set before the training process begins. Common hyperparameters include the learning rate, the number of hidden layers, the optimization algorithm, the number of neurons in each layer and so on and so forth. Hyperparameters thus could influence the model's architecture significantly and hence finding the right values is crucial for achieving optimal performance. Hyperparameters are usually tested within a space and the best one are then selected. It's especially important to prevent a phenomenon known as *overfitting*.
- **Test Set**: This small to medium sized subset is used to evaluate the model's performance on data it has not seen before. By testing the model on never seen data we obtain unbiased measures metrics to evaluate the model in a fair way.

Overfitting occurs when a model learns the training data too well, capturing noise and details. This leads to high accuracy on the training set but poor performance on the test set. To mitigate and prevent overfitting, techniques such as regularization, dropout, and early stopping are employed to ensure the model generalizes well to unseen data. The end goal is to have a model that generalize well with the respect to any input and the secret to achieve this is to have good data as first thing.

3.2.1 Backpropagation

Learning for a neural networks means to iteratively apply a forward and a backward pass. In the forward pass, the input data is propagated through the

network layer by layer until the output layer is reached. Then the error with respect to the prediction is calculated using a *loss function*, such as mean squared error or mean absolute error. The *gradient* of a function is a fundamental concept in the field of optimization theory because it indicates the direction in which the function maximize. This concept is used in the backward pass, where the gradient of the loss function with respect to each weight of the network is calculated by using the technique note as backpropagation [Figure 20] and backpropagated by applying the chain rule. By exploiting this mechanism over and over weights are adjusted in a manner to minimize the error.

The loss function $L(\mathbf{y}, \hat{\mathbf{y}})$ measures the difference between the predicted output $\hat{\mathbf{y}}$ and the actual output $\mathbf{y}$. For example, in a regression task, the mean squared error (MSE) can be used:

$$L(\mathbf{y}, \hat{\mathbf{y}}) = \frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

Backpropagation uses the chain rule to compute the gradient of the loss function with respect to each weight. The chain rule is a fundamental theorem in calculus used to compute the derivative of the composition of two or more functions. If a variable z depends on y, and y depends on x, then the chain rule states the following:

$$\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx}$$

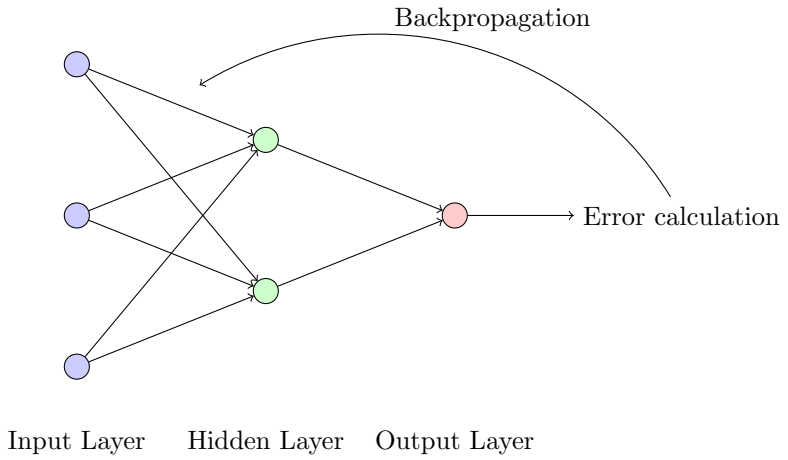


Figure 20: Backpropagation in action within a simple neural network.

3.2.2 Gradient Descent

Once the gradient of the loss function is calculated, an optimization algorithm such as Gradient descent [Figure 21] is used to iteratively update the weights by shifting them in the opposite direction of the gradient. How much to move them corresponds to the learning rate hyperparameter and is where an optimization algorithm often differs from another. The learning rate needs to be carefully chosen because it might prevent the finding of a minima thus avoiding the convergence of the model. The weight update rule for a weight w can generally be expressed as:

$$w \leftarrow w - \eta \frac{\partial L}{\partial w}$$

where η is the learning rate. There is a plenitude of optimization algorithms, such as the stochastic gradient descent (SGD), Adam and RMSprop. Each offering different trade-offs between computation time and convergence stability. It is worth saying that many modern and more complex methods also are capable of dynamically adjusting the learning rate value during the training process.

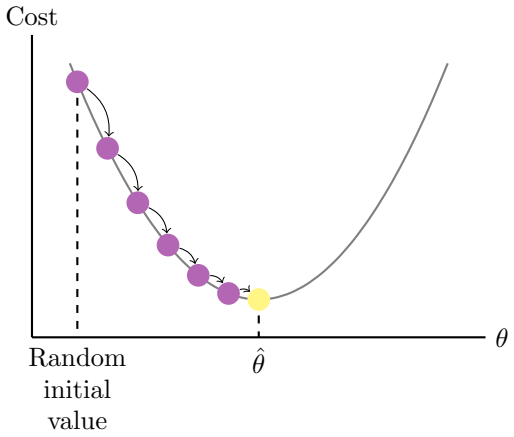


Figure 21: Gradient descent method applied on a concave function.

3.3 Advanced Topics in Neural Networks

3.3.1 Deep Neural Networks

Deep neural networks (DNN) [Figure 22] differ from simple one for having multiple hidden layers between the input and output layers. The increased depth allows DNNs to model data of higher order of complexity with respect to simple nets, often allowing for better performances. Each (hidden) layer in a DNN can be thought as learning at a different level of abstraction, with the early layers capturing low-level features and deeper layers capturing high-level features. For instance in a recognizing image system first edges and textures are recognized to

later form shapes and objects. This hierarchical learning feature makes DNNs extremely powerful for tasks such as image and speech recognition, natural language processing, and even playing strategic games. Training DNNs, however, requires large amounts of data and computational power, and often employs many different techniques such as dropout and batch normalization to improve performance and prevent overfitting.

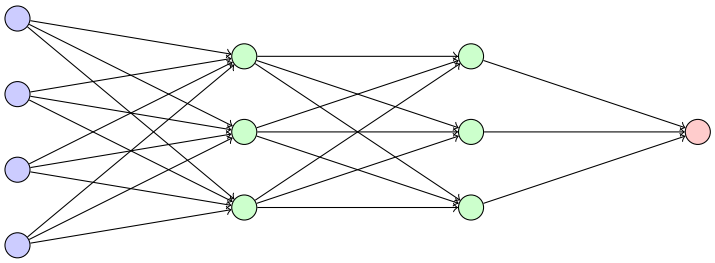


Figure 22: A Deep neural network with two hidden layers.

3.3.2 Convolutional Neural Networks

A *convolutional neural network* (CNN) [Figure 23] is a specialized type of deep neural network designed to process structured grid data, like images. At the core of CNNs there is the convolution operation which consists in sliding a set of filters over the input grid spatial data and consists in integrating two functions to produce a third one which expresses how the shape of one is modified by the other. Convolutions are performed in each position the filter slides on and typically involves a dot product followed by a summation in order to extract features. Mathematically, the convolution operation for a single filter K applied to an input I can be expressed as:

$$S(i,j) = (I * K)(i,j) = \sum_m \sum_n I(i-m, j-n)K(m,n)$$

Convolutional layers are typically followed by pooling layers, which are used to reduce the spatial dimensions of the data by typically halving it at each pass. Even tho it might seems deleterious it has been shown that applying pooling does not reduce performance while decrease computational complexity. CNNs have revolutionized computer vision tasks, achieving state-of-the-art results in image classification, object detection, and segmentation.

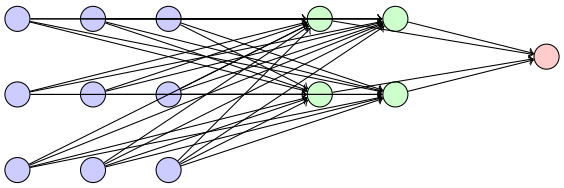


Figure 23: A simple convolutional neural network architecture.

3.3.3 Recurrent Neural Networks

A *recurrent neural network* (RNN) [Figure 24] is a is a specialized type of deep neural network that is particularly well-suited for sequential data, such as time series or natural language. Usually, when dealing with data in which the order does matter RNNs are used because they have connections that form directed cycles between its neurons, allowing information to persist. The hidden state h_t at time step t is computed based on the input x_t and the previous hidden state h_{t-1}:

$$h_t = \sigma(W_h h_{t-1} + W_x x_t + b)$$

where W_h and W_x are weight matrices, b is a bias vector, and σ is an activation function. A common problem with RNNs is the *vanishing gradient problem* which occurs when the calculated gradients become too small as they are backpropagated through long sequences. Variants of RNNs, such as Long Short-Term Memory (LSTM) and Gated Recurrent Unit (GRU) networks, try to mitigate this kind of issue while still allowing for learn long-term dependencies to be learned.

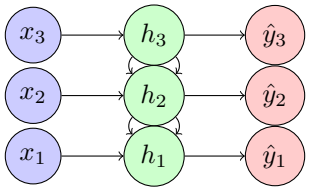


Figure 24: Recurrent Neural Network (RNN) unrolled through time.

3.3.4 Attention Mechanisms

In many contexts, it might be useful to focus more on specific input's parts than others and this is achieved through the usage of attention mechanisms which where firstly introduced in 2017 with the paper *Attention is all you need* [15]. Let's say we are dealing with text, then each word in the input text is associated with a *key* and the element we are focusing on is called *query*; then the attention mechanism [Figure 25] is assigning a *value* (weight) to each key with respect to the query. This allows the model to focus on important parts of the input in a dynamic manner and is especially useful for in tasks involving sequences,

such as machine translation and text summarization. The attention score for a query vector q and a set of key vectors $\{k_1, k_2, \ldots, k_n\}$ is computed as:

$$\text{Attention}(q, K, V) = \text{softmax}\left(\frac{qK^T}{\sqrt{d_k}}\right)V$$

where K is the matrix of keys, V is the matrix of values, and d_k is the dimension of the keys. Also worth to say, is that attention mechanism can be pretty much be integrated with any type of neural network even though that's not always necessary.

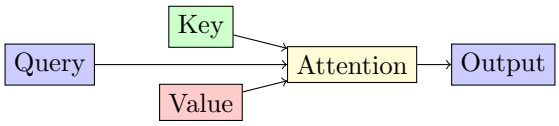


Figure 25: Attention mechanism in neural networks.

3.3.5 Graph Neural Networks

A *graph neural network* (GNN) is an advanced type of deep neural network designed to handle graph-structured data [section 2]. From social networks to molecules, from images to text manipulation, almost anything can be modelled as graphs. Hence, GNNs can be considered as one of the most powerful types of neural network architectures. The core concepts behind GNNs are the neighborhood aggregation and the message passing. The first is used to make a node aware of its neighborhood properties and the second to pass these informations through each node in the graph allowing GNNs to learn rich node representations which can be used for various tasks such as node classification, link prediction, and graph classification. The message-passing step for a node v can be mathematically expressed as:

$$h_v^{(k+1)} = \sigma\left(\sum_{u \in \mathcal{N}(v)} W h_u^{(k)} + b\right)$$

where $h_v^{(k+1)}$ is the node feature vector at layer $k+1$, $\mathcal{N}(v)$ denotes the neighbors of node v, W is a weight matrix, b is a bias vector, and σ is an activation function. There exists many variants of GNNs each leveraging different strategies on how to aggregate and update nodes informations such as Graph Convolutional Networks (GCNs), Graph Attention Networks (GATs), and Graph Recurrent Networks (GNRs).

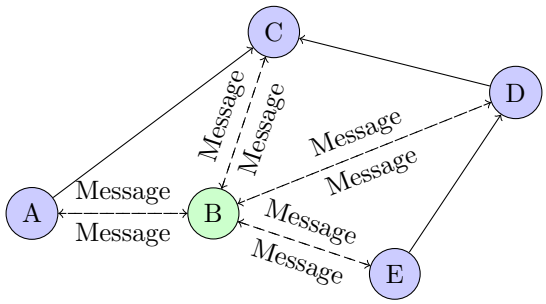


Figure 26: Message passing between node B and its neighbors in a GNN.

We are specifically going to focus on GNNs since every state of the art model trying to address the graph edit distance problem [section 4] which make use of artificial neural networks do use this particular architecture with a Siamese layout.

4 Graph Similarity Problem

Of particular interest is to understand whether two given graphs are similar or not, this question takes the name of *graph similarity problem*. This problem could be of help in numerous domains and real world problems including pattern recognition, computer vision, bioinformatics, social network analysis, and chemical informatics. In such fields, common problems can be modelled as graphs and comparing the structure properties of pair of those could be very beneficial. For instance, in bioinformatics, comparing protein interaction networks can reveal functional similarities between different proteins, while in social network analysis, it can help identify similar community structures within different social groups. Since graph similarity is very important, numerous metrics have been developed to measure graph similarity, each with its own strengths and limitations to take into account. In the following sections, we are going to explore several metrics commonly used to measure graph similarity: Graph Isomorphism, Graph Kernels, and Graph Edit Distance (GED). Each method will be discussed in terms of its fundamental concepts, applications, and limitations, with a focus the latter. Also, it is often desirable to retrieve the edit path from one graph to another in a straightforward manner to understand the specific transformations involved. However, we will focus solely on the similarity metrics and will not address the retrieval of edit paths.

4.1 Graph Isomorphism

In graph theory, graph isomorphism is one of the fundamental concepts used to determine if two graphs are structurally identical. Two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic if there is a bijection $f : V_1 \to V_2$ such that any two vertices u and v in G_1 are adjacent if and only if $f(u)$ and $f(v)$ are

adjacent in G_2. Formally, G_1 and G_2 are isomorphic if:

$$(u, v) \in E_1 \Leftrightarrow (f(u), f(v)) \in E_2$$

Graph isomorphism metric provides in the a binary metric whether two graphs are identical in structure or not. Hence, it is limited because it does not quantify the degree of similarity at all. It is useful in scenarios where a binary outcome is desired. However, it is less useful in all the other cases where graphs are similar but not identical, as it cannot measure partial similarity or small structural differences.

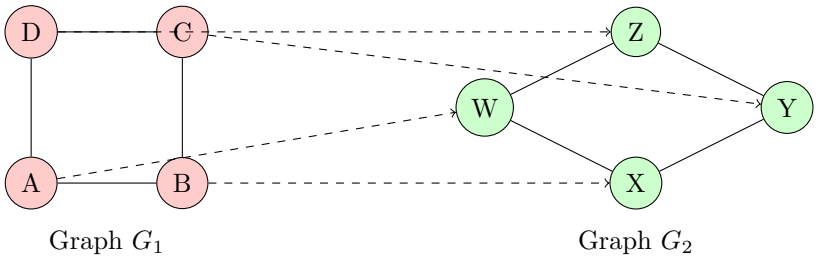


Figure 27: Graph Isomorphism: G_1 (Square) and G_2 (Rhombus).

4.2 Graph Kernels

A common solution in optimization theory when trying to separate two given dataset is to artificially increase their spatial dimension by using kernel tricks [10]. In the same way graph kernels transforms graphs into high-dimensional vectors where it is easier to compare them and exploit this mechanism to compute a similarity metric based on their structural attributes and properties. Common types of graph kernels include:

- **Random Walk Kernels**: Measure the similarity based on the number of matching random walks in both graphs.
- **Shortest Path Kernels**: Measure the similarity based on the distribution of shortest paths between pairs of nodes in each graph.
- **Weisfeiler-Lehman Kernels**: Measure the similarity utilizing an iterative node labeling algorithm to capture the neighborhood structure around each node.

Thus, structural information can be recovered in several different ways by utilizing graph kernels which can then be considered well-suited for use in machine learning algorithms where kernel tricks are commonly used to create algorithmic classificators. However, they can be computationally intensive if not carefully handled and also require careful tuning of parameters.

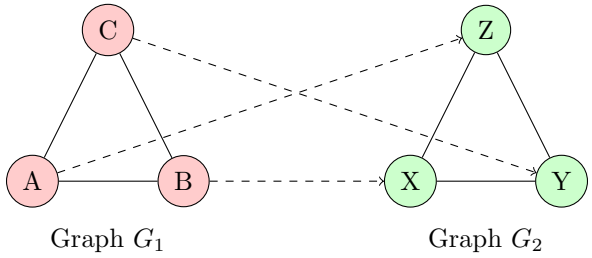


Figure 28: Graph Kernels: Example Graphs with Similar Structures.

4.3 Graph Edit Distance (GED)

One of the most flexible and informative metric that measure the similarity between two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is the *graph edit distance* (GED). GED quantifies similarity by determining the minimum cost required to transform G_1 into G_2 by means of a series of atomic operations. These operations include but are not limited to vertex and edge insertions, deletions, and substitutions. The cost of each operation is determined by a predefined cost function which is usually 1.

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, which falls in the range [0, inf), 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.

However, the computation of GED is known to be *NP-HARD*, which means that finding the exact minimum edit distance between two graphs is computationally intensive. Despite this, GED is preferred over other similarity metrics due to its flexibility and ability to provide a good measure of similarity even when the graphs are not identical.

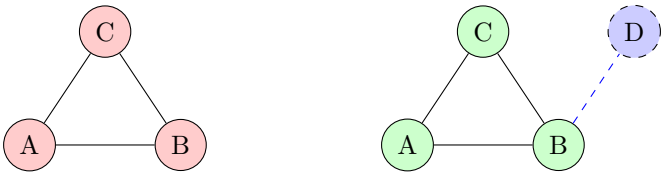
4.3.1 Atomic Operations

The basic atomic operations in GED typically include:

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

- **Edge Deletion**: Deleting an existing edge $e = \{u, v\}$ from the graph.
- **Edge Substitution**: Replacing an existing edge $e = \{u, v\}$ with another edge $e' = \{u', v'\}$.
- **Node Relabelling**: Replacing the label l of a vertex v with another label l'.

To illustrate the concept of Graph Edit Distance (GED), consider the pair of graphs represented in [Figure 29]:



Graph G_1 **Graph** G_2

Figure 29: Graph Edit Distance: Transforming G_1 to G_2 by adding vertex D and edge (B,D).

In this example, graph G_1 has a vertex set $V_1 = \{A, B, C\}$ and an edge set $E_1 = \{\{A, B\}, \{A, C\}, \{B, C\}\}$, while graph G_2 has a vertex set $V_2 = \{A, B, C, D\}$ and an edge set $E_2 = \{\{A, B\}, \{A, C\}, \{B, C\}, \{B, D\}\}$. The transformation with the lowest cost 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: $1 + 1 = 2$.

5 State of the Art Review

Traditional imperative solutions for solving the graph edit distance (GED) problem have been effective for graphs of modest size, utilizing explicit algorithms that compare graphs node by node and edge by edge through combinatorial techniques. However, as the number of nodes in the graph increases, the complexity of these methods grows exponentially, leading to significant scalability issues. In such scenarios, imperative solutions often become impractical, requiring an inordinate amount of time to compute the GED. This challenge is particularly critical in domains like bioinformatics, social network analysis, and cheminformatics, where large-scale graphs are common.

To address these scalability challenges, recent research has pivoted towards leveraging artificial intelligence (AI) models. AI-based approaches offer more robust and scalable solutions by learning patterns and features from graph data, significantly reducing computation times and improving accuracy. This section reviews some of the prominent AI-based models that have advanced the state of the art in GED computation.

The timeline of notable advancements in this field starts with *SimGNN* in 2019 [2], the first approach to utilize neural networks for computing GED. Subsequent models have built upon this foundation, progressively enhancing the accuracy and efficiency of GED computation. This review covers developments from SimGNN to the latest contributions in 2023, culminating in the VLDB paper introducing *GedGNN* [11]. These models collectively represent significant strides in utilizing AI to overcome the limitations of traditional GED computation methods.

5.1 Timeline

2019, *SimGNN: A Neural Network Approach to Fast Graph Similarity Computation* [2]: Introduces SimGNN, addressing graph similarity computation using neural networks. It features a learnable embedding function, an attention mechanism to emphasize important nodes, and a pairwise node comparison method, achieving better generalization and computational efficiency compared to baselines.

2020, *Learning Graph Edit Distance by Graph Neural Networks* [13]: Introduces a framework combining deep metric learning with traditional approximations of graph edit distance using geometric deep learning. The approach employs a message passing neural network (MPNN) to capture graph structure and compute graph distances efficiently, showing superior performance in graph retrieval and competitive results in graph similarity learning.

2020, *Combinatorial Learning of Graph Edit Distance via Dynamic Embedding* [17]: Introduces a hybrid approach for solving the GED problem by integrating a dynamic graph embedding network with an edit path search procedure, enhancing interpretability and cost-efficiency. The learning-based A* algorithm reduces search tree size and saves time with minimal accuracy loss.

2021, *Graph Partitioning and Graph Neural Network-Based Hierarchical Graph Matching for Graph Similarity Computation* [18]: Introduces PSimGNN, which partitions input graphs into subgraphs to extract local structural features, then uses a novel GNN with attention to map subgraphs to embeddings, combining coarse-grained interaction among subgraphs with fine-grained node-level comparison to predict similarity scores.

2021, *Noah: Neural Optimized A* Search Algorithm for Graph Edit Distance Computation* [19]: Introduces Noah, combining A* search algorithm and Graph Path Networks (GPN) for approximate GED computation. Noah learns an estimated cost function using GPN, incorporates pre-training with attention-based information, and adapts an elastic beam size to reduce search complexity.

2021, *Learning Efficient Hash Codes for Fast Graph-Based Data Similarity Retrieval* [16]: Introduces HGNN (Hash Graph Neural Network), a model designed for efficient graph-based data retrieval by leveraging GNNs and hash learning algorithms. HGNN learns a similarity-preserving graph representation and computes compact hash codes for fast retrieval and classification tasks.

2021, *More Interpretable Graph Similarity Computation via Maximum Common Subgraph Inference* [6]: Introduces INFMCS, an interpretable end-to-end

paradigm for graph similarity learning, leveraging the correlation between similarity score and Maximum Common Subgraph (MCS), combining transformer encoder layers with graph convolution for superior performance and interpretability.

2021, *H2MN: Graph Similarity Learning with Hierarchical Hypergraph Matching Networks* [20]: Introduces H2MN, which measures similarities between graph-structured objects by transforming graphs into hypergraphs and performing subgraph matching at the hyperedge level, followed by a multi-perspective cross-graph matching layer.

2022, *TaGSim: Type-aware Graph Similarity Learning and Computation* [1]: Proposes TaGSim, a framework that addresses the limitations of traditional GED methods by incorporating type-specific graph edit operations. TaGSim models the transformative impacts of different graph edits (node and edge insertions, deletions, and relabelings) separately, creating type-aware embeddings and using these embeddings for accurate GED estimation. The framework demonstrates superior performance on real-world datasets compared to existing GED solutions.

2023, *Efficient Graph Edit Distance Computation Using Isomorphic Vertices* [5]: Proposes a novel approach for reducing the search space of GED computation by leveraging isomorphic vertices, targeting redundant vertex mappings and significantly cutting computation costs for exact GED.

2023, *Exploring Attention Mechanism for Graph Similarity Learning* [14]: Proposes a unified framework with attention mechanisms, combining graph convolution and self-attention for node embedding, cross-graph co-attention for interaction modeling, and graph similarity matrix learning for score prediction, showing superior performance on benchmark datasets.

2023, *Graph Edit Distance Learning via Different Attention* [9]: Introduces DiffAtt, a novel graph-level fusion module for GNNs to compute GED efficiently by leveraging graph structural differences using attention mechanisms, incorporated into the GSC model REDRAFT, achieving state-of-the-art performance on benchmark datasets.

2023, *Graph-Graph Context Dependency Attention for Graph Edit Distance* [4]: Introduces GED-CDA, a deep network architecture for GED computation that incorporates a graph-graph context dependency attention module, leveraging cross-attention and self-attention layers to capture inter-graph and intra-graph dependencies.

2023, *GREED: A Neural Framework for Learning Graph Distance Functions* [12]: Introduces GREED, a siamese GNN designed to learn GED and Subgraph Edit Distance (SED) in a property-preserving manner, achieving superior accuracy and efficiency compared to state-of-the-art methods.

2023, *MATA*: Combining Learnable Node Matching with A* Algorithm for Approximate Graph Edit Distance* [8]: Introduces MATA*, a hybrid approach for approximate GED computation leveraging GNNs and A* algorithms, focusing on learning to match nodes rather than directly regressing GED.

2023, *Multilevel Graph Matching Networks for Deep Graph Similarity Learning* [7]: Proposes MGMN, a multilevel graph matching network capturing cross-

level interactions, comprising a Node-Graph Matching Network (NGMN) and a siamese GNN for global-level interactions, demonstrating superior performance as graph sizes increase.

2023, *Wasserstein Graph Distance Based on L1-Approximated Tree Edit Distance Between Weisfeiler-Lehman Subtrees* [3]: Proposes the WWLS distance, combining WL subtrees with L1-approximated tree edit distance (L1-TED), capable of detecting subtle structural variations in graphs, demonstrating superiority in metric validation and graph classification tasks.

2023, *Computing Graph Edit Distance via Neural Graph Matching* [11]: Introduces GEDGNN, a deep learning framework for computing GED by focusing on graph conversion rather than GED value prediction alone. GEDGNN predicts GED values and a matching matrix, followed by a post-processing algorithm for extracting high-quality node matchings.

5.2 SimGNN

The first innovative model that significantly outperformed the competition is SimGNN [2], 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 30. 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. This stage leverages a graph convolutional network to capture local structural information.
- **Graph-Level Embedding Stage**: The node embeddings are aggregated using an attention mechanism to produce a single embedding for each graph. The attention mechanism helps to emphasize more important nodes, improving the overall representation of the 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. This interaction is performed through a neural network that learns the relationship between the embeddings.
- **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.

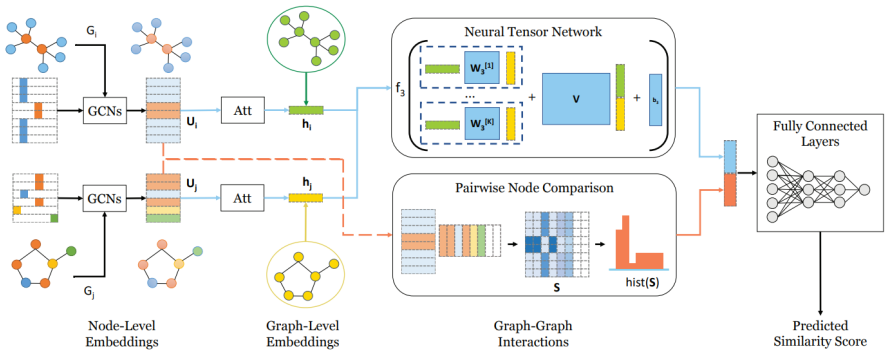


Figure 30: SimGNN architecture overview.

5.3 GPN

The Graph Path Networks (GPN) model, proposed in 2022 within the *NOAH Framework* [19], introduces a novel approach to computing approximate Graph Edit Distance (GED) by leveraging the A* search algorithm optimized through neural networks. This method addresses several limitations found in previous models, including SimGNN, by improving both the search direction and search space optimization.

An overview of GPN is illustrated in Figure 31. The architecture of GPN comprises several key components:

- **Pre-training Module**: This module computes pre-training information such as exact GEDs and graph edit paths. It generates (sub)graph pairs used in training, enriching the model's understanding of graph transformations.

- **Graph Embedding Module**: Utilizing the Graph Isomorphism Network (GIN), this module transforms each node into a vector encoding its

features and structural properties. It incorporates cross-graph information and employs an attention mechanism to obtain the final graph-level embeddings.

- **Learning Module**: This component focuses on optimizing the A* search algorithm by learning an estimated cost function and an elastic beam size. The estimated cost function helps guide the search direction, while the beam size adapts to various user settings, improving the search space optimization.

GPN's enhancements over SimGNN include improved search efficiency and accuracy in GED computation. It also facilitates tasks such as graph similarity search and graph classification, demonstrating its versatility and robustness. Notably, GPN is capable of finding an edit path between graphs, utilizing a combination of pre-training information and adaptive search strategies to achieve high performance across different datasets.

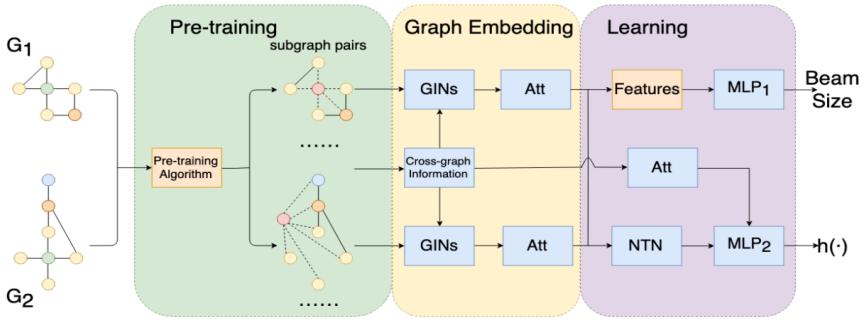


Figure 31: GPN architecture overview.

5.4 TaGSim

TaGSim (Type-aware Graph Similarity) [1], introduced in 2022, represents a significant advancement in the computation of Graph Edit Distance (GED) by addressing the limitations of previous approaches, including those that treat GED as a single global measure. TaGSim refines GED computation by considering the distinct impacts of various types of graph edit operations.

An overview of TaGSim is illustrated in Figure 32. The TaGSim framework operates through the following key components:

- **Type-Aware Graph Embeddings**: TaGSim models the transformative impacts of four specific graph edit operations—node insertion/deletion (NR), node relabeling (NID), edge insertion/deletion (ER), and edge relabeling (EID). Each type of operation is handled separately to capture its localized effects on the graph.

- **Graph Edit Value (GEV) Dimensions**: GED is decoupled into four dimensions corresponding to the different types of graph edits. TaGSim estimates each dimension individually, providing a more granular and accurate representation of graph similarity.
- **Type-Aware Neural Networks**: The framework uses neural networks that are specifically designed to process and learn from the type-aware embeddings. This allows TaGSim to achieve high accuracy in GED estimation by incorporating the distinct impacts of different edit types.

TaGSim's approach offers several advantages over traditional GED computation methods and previous AI-based models. By decoupling the GED into different dimensions, it avoids the pitfalls of treating GED as a single undifferentiated metric. This granularity enhances both the accuracy and interpretability of the similarity scores, making TaGSim a robust solution for various graph analysis tasks.

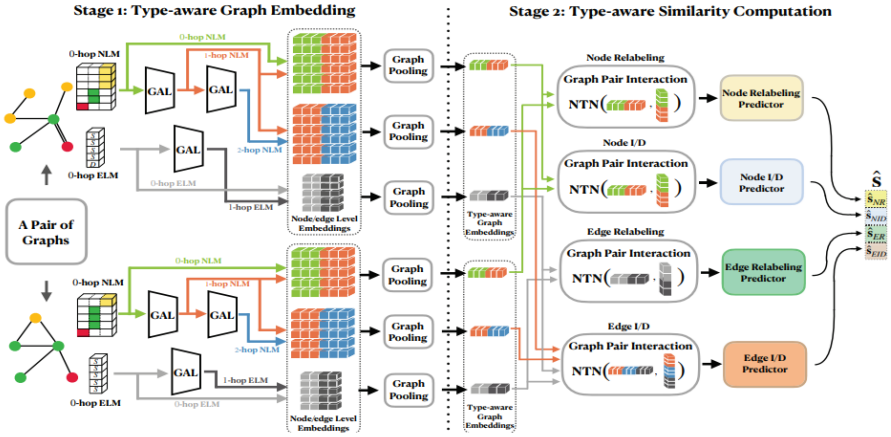


Figure 32: TaGSim architecture overview.

5.5 GedGNN

GedGNN (Graph Edit Distance via Neural Graph Matching) [11], introduced in 2023, represents the latest advancement in the field of Graph Edit Distance (GED) computation. This model addresses the challenge of capturing both node and edge matching effectively through a sophisticated neural network architecture.

An overview of GedGNN is illustrated in Figure 33. The GedGNN architecture comprises several innovative components:

- **Graph Neural Network (GNN) Encoder**: This component uses a GNN to encode the structural and attribute information of the input

graphs. The encoder generates embeddings for nodes and edges, preserving their relational information.

- **Node and Edge Matching Module**: This module performs node and edge matching between the two graphs. It uses an iterative matching algorithm to refine the matches, improving accuracy over multiple iterations.
- **k-Best Matching Post-Processing Algorithm**: To further enhance the matching accuracy, GedGNN incorporates a k-best matching algorithm. This algorithm selects the best k matching solutions from the initial matches, refining the final GED computation.

GedGNN's comprehensive approach ensures high accuracy in GED estimation by combining robust embedding techniques with advanced matching algorithms. This model not only outperforms previous methods but also provides a flexible framework that can adapt to various types of graph structures and similarity measures.

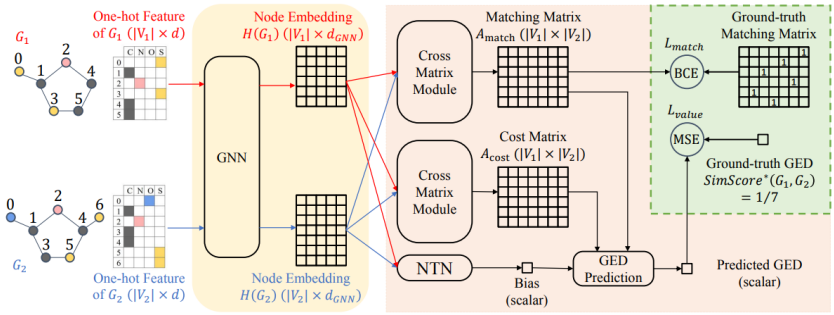


Figure 33: GedGNN architecture overview.

5.6 Encountered Gaps

In working with the codebase provided in the paper presenting GedGNN, several critical gaps have become evident, extending beyond just the implementation of GedGNN to also include other models such as TaGSim, SimGNN, and GPN. These gaps significantly hinder both the usability of the code and the reliability of the results obtained from these models. A primary issue is the lack of clear and well-defined parameters, which severely impacts the reproducibility of results. Instructions regarding key hyperparameters, such as learning rates, regularization factors, and model configurations, are often vague, poorly documented, or entirely omitted. This makes it challenging to replicate experiments accurately and to achieve the reported performance across different environments.

The quality of the codebase itself presents another significant challenge. The overall code is poorly documented, lacking the necessary clarity and organization that would make it easier to read, understand, and refactor. This lack of

structure is evident across the different models included in the codebase, making attempts to extend or modify the code particularly difficult. The absence of best practices in software development, such as modular design and comprehensive commenting, further complicates efforts to ensure that modifications do not introduce new issues or degrade performance.

Scalability is another area where the codebase falls short. Although the code is designed to run on GPUs, it does not scale well, failing to deliver the significant speedups that one might expect, especially for large-scale problems. This inefficiency severely limits the practical application of these models, particularly in scenarios where computational efficiency and the ability to handle larger graphs are crucial. Additionally, the training and testing procedures are generally restricted to graphs with fewer than 10 nodes, which is a major limitation. This restriction prevents the models from learning and scaling effectively when applied to larger and more complex graphs, which are common in real-world applications.

Another critical concern is the fairness of the model evaluations. The benchmarks used in evaluating these models may not fully capture their true performance, as they often do not represent real-world scenarios or test the robustness of the models across diverse graph types and sizes. This raises questions about whether the models are genuinely being tested for their effectiveness or if the evaluations are biased towards specific datasets or problem formulations that favor the models under consideration. Such limitations can lead to inflated performance claims that do not generalize well to other, more varied graph datasets.

Lastly, the quality of the data used for training and evaluating these models is problematic. The datasets employed often contain approximate GED values rather than the true edit distances, introducing inaccuracies that can mislead the training process. Moreover, these datasets are typically small and specialized, focusing on a single type of graph application, such as chemical compounds or social networks. Consequently, the models tend to perform poorly when applied to different types of graphs that were not represented in the training data, indicating a lack of generalizability.

In summary, the codebase for the paper presenting GedGNN and related models such as TaGSim, SimGNN, and GPN presents several significant challenges that hinder their practical utility and broader adoption. These include issues with reproducibility due to unclear parameters, poor code quality that complicates refactoring and extension, limited scalability, unfair model evaluations, and reliance on low-quality, non-generalizable datasets. Additionally, the restriction to small graphs further limits the learning capacity and scalability of these models. Addressing these issues is crucial for advancing the field and ensuring that GED models can be reliably and effectively applied in diverse real-world scenarios.

6 Methodology and Experimentation

7 Discussion and Conclusions

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