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 crucial 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 [3] 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 [12], 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 nonlinear data structure consisting of a set of vertices and arcs, where arcs connect pairs of vertices in the set. Graphs are widely used to represent relationships between entities and play a significant role in the development of fields like Computer Science, Optimization, Chemistry and others. They are a pillar in network-based systems modeling such as social media, biological networks, and transportation systems, being a crucial tool for analyzing and solving complex problems. Use cases of graphs can be found in the actual world, for example in recommendation systems, routing and navigation algorithms like GPS, optimization problems and resource allocation (also known as transportation problems).

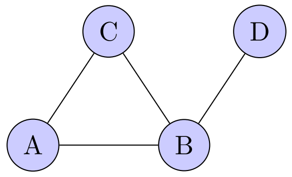


Figure 1: Simple undirected graph example.

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

- V is a finite set of vertices where each represents an entity or a data point. The set 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, $E \subseteq \{\{u, v\} \mid u, v \in V \text{ and } u \neq v\}$. Edges represents the existing relationship between two vertices in the set.

For instance, 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

There exist different categories of graphs depending on their properties, including:

- **Directed Graph** [Figure 2]: also known as digraph, is the case where the direction is indicated on the edges, representing G as an ordered pair (u, v) where $u, v \in V$ and $u \neq v$. It's applied in a range of areas, including web page ranking, where links between pages have a set direction, and citation networks, where one paper references another.

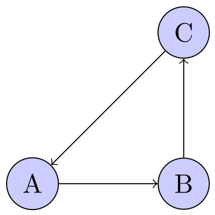


Figure 2: Directed graph where edges have directions indicated by arrows.

- **Undirected Graph** [Figure 3]: the edges do not have a direction, represented as an unordered pair $\{u, v\}$ where $u, v \in V$ and $u \neq v$. This kind of graph is commonly used to model networks where the connections of two nodes are mutual, indicating that relationship is valid in both senses.

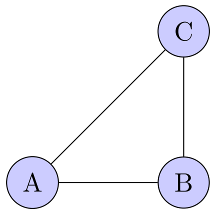


Figure 3: Undirected graph example where edges are bidirectional (there are no arrows).

- **Weighted Graph** [Figure 4]: in this graph edges have a weight (or cost) related, 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 express distances, the time spent traveling from one point to another, or costs associated with the displacement.

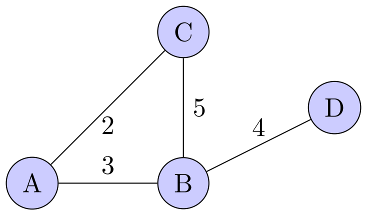


Figure 4: Weighted graph example where each edge is labeled with a weight.

- **Simple Graph** [Figure 5]: is a graph without loops (there doesn't exist a path from a vertex to itself) and has no multiple edges (the same pair of vertices is not connected more than once). Simple graphs are the most basic type of graph existing, with straightforward structures that make them easy to handle. They are often used for modeling basic networks to maintain a clear design and facilitate the analysis of the structure and the understanding of network properties.

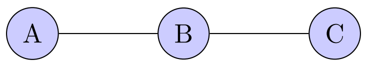


Figure 5: Simple graph example with a linear connection between vertices A, B, and C, with no loops or multiple edges.

- **Complete Graph** [Figure 6]: is a graph in which every vertex is connected with all the other vertices in the set. Formally, a complete graph on n vertices, denoted as K_n, has $E = \{\{u, v\} \mid u, v \in V, u \neq v\}$. They are widely used in cases where is necessary maximum connectivity, such as some network topologies and combinatorial optimization problems.

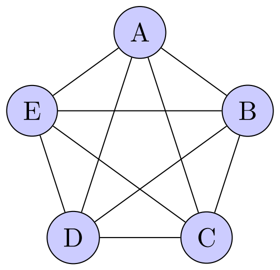


Figure 6: Complete graph example where each node is connected to each other.

- **Bipartite Graph** [Figure 7]: a graph whose vertices are separable into two disjoint sets U and W in a way that an edge only connects a vertex from U with a vertex from W. Bipartite graphs are useful for modeling relationships between objects from two different classes. For example, in the context of job assignment, vertices in U can symbolize jobs and vertices in W workers. Edges will indicate which job is assigned to each worker.

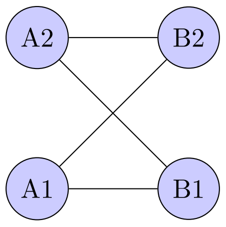


Figure 7: Bipartite graph example with two distinct sets of vertices with edges connecting vertices across the sets but not within them.

- **Multigraph** [Figure 8]: it is a graph where multiple edges occur between the same pair of vertices. Formally, $G = (V, E)$ where E is a multiset of unordered pairs of vertices. Multigraphs are often used for modeling networks where multiple relationships or interactions exist for the same pair of vertices. For example, it is known that in transportation networks exists multiple routes or connections between two locations.

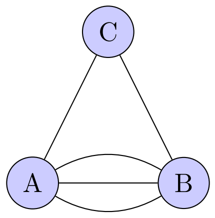


Figure 8: Multigraph example with multiple edges between vertices A and B.

- **Cyclic Graph** [Figure 9]: is the one that contains at least a cycle, being a cycle a path where every vertex on it is reachable from itself. Cyclic graphs are employed to model processes or systems where feedback loops are present. For example, it could be said that in certain biological systems or recurrent neural networks, loops represent the actions or the recurrent connections respectively.

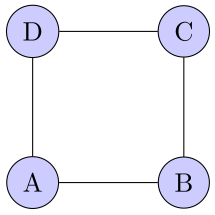


Figure 9: Cyclic graph example with a cycle A-B-C-D-A.

- **Acyclic Graph** [Figure 10]: An acyclic graph is a graph without loops. A direct acyclic graph (DAG) is a directed graph without loops. Acyclic graphs, specially DAGs, are mainly used for modeling cases as task scheduling, where dependencies should not form cycles. In this kind of situation, a task will start only if all its prerequisites are completed. The absence of loops ensures that there aren't circular dependencies.

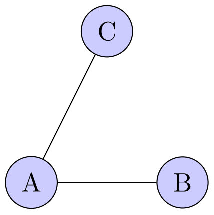


Figure 10: Acyclic graph example with no cycles.

2.2 Graph Representation

There are several manners to represent a graph, including:

- **Adjacency Matrix** [Figure 11]: An adjacency matrix A corresponding to a graph $G = (V, E)$ is a binary square matrix of size $|V| \times |V|$ that expresses the existence of a relationship between a pair of vertices. The value of A_{ij} is 1 if there is an edge connecting vertices v_i and v_j, and 0 otherwise. This structure is particularly convenient for dense graphs where the number of edges is nearest to the limit of possible edges. It facilitates efficiency in the querying process to know if an edge exists and is easy to implement for algorithms that require constant monitoring of the edge's presence. Even so, the space complexity is $O(|V|^2)$, which is a problem for large graphs with many vertices.

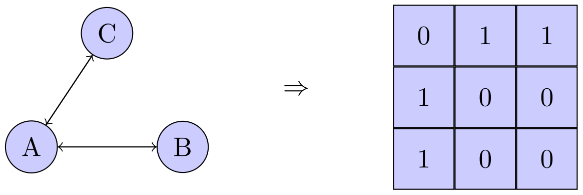
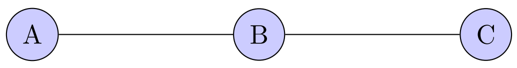


Figure 11: Adjacency Matrix example.

- **Adjacency List** [Figure 12]: An adjacency list is a collection of lists where each one corresponds to a vertex and contains all the adjacent vertices. Having a graph $G = (V, E)$, the adjacency list could be implemented as a list array $\{L_1, L_2, \ldots, L_n\}$ and every L_i will include all v_i's neighbors. These structures are more efficient for sparse graphs due to the number of edges is much smaller than the number of possible edges. The use of an adjacency list facilitates the work of graph algorithms such as breadth-first search (BFS) and depth-first search (DFS), where only the more important neighbors need to be visited.



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

Figure 12: Adjacency List example.

2.3 Properties of Graphs

Graphs have some outstanding properties that help to analyze them and determine the best application for each type, including:

- **Degree** [Figure 13]: The degree of a vertex is the number of vertices in the graph that incident on it. Formally, for a vertex v in a graph $G = (V, E)$, the degree $\deg(v)$ is the number of vertices connected to it. In the case of direct graphs, the in-degree stands for the number of incoming edges, and the out-degree stands for the number of outgoing edges. Vertices with high degrees generally play a crucial role in a graph, indicating significant or highly connected nodes.

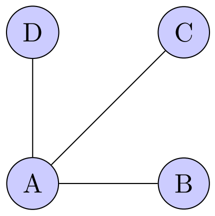


Figure 13: Degree example showing vertex A with degree 3.

- **Connectivity** [Figure 14]: Connectivity refers to the way nodes are connected within the graph. A graph is called connected if there exists a path between every pair of vertices, in other words, each vertex is reachable from any other vertex in the graph. This is a key property for understanding reliability and network robustness and ensures that all nodes can communicate directly or indirectly between them.

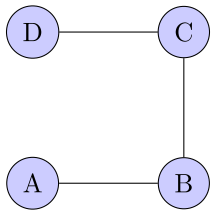


Figure 14: Connectivity example showing a connected graph.

- **Centrality** [Figure 15]: The centrality measures are employed to identify the most significant vertices in a graph. Some of the most important metrics are degree centrality, which quantifies the direct connections to a vertex; closeness centrality, which evaluates the velocity of a node to reach another; and betweenness centrality, which assesses how many times a vertex acts as a bridge in the closeth path between a pair of vertices. These metrics offer distinct points of view about the importance and influence of a node in the net.

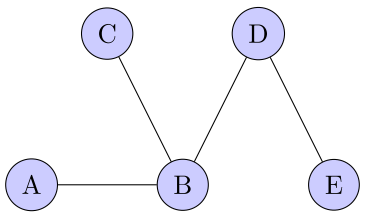


Figure 15: Centrality example showing vertex B as a central node with high degree centrality.

- **Clustering Coefficient** [Figure 16]: The clustering coefficient of a vertex measures how connected the neighbors of that vertex are to each other. A high clustering coefficient suggests a community closely linked in the graph. In mathematics terms, it is defined as the proportion between the real edges and the possible edges among the vertex neighbors.

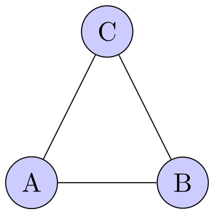


Figure 16: Clustering coefficient example showing a triangle, indicating a high clustering coefficient.

- **Graph Diameter** [Figure 17]: The diameter of a graph is the length of the longest shortest paths between any pair of vertices. This metric indicates the "spread" of the graph and helps to understand how distant the vertices are, considering the minimum distance that connects them.

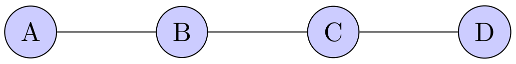


Figure 17: Graph diameter example showing the longest shortest path A-B-C-D with diameter 3.

- **Graph Density** [Figure 18]: The density of a graph is defined as the proportion between the number of existing edges and the maximum possible edges among the vertices. In an undirected graph with n vertices, the total of possible edges is $\frac{n(n-1)}{2}$. The density indicates how close the graph is to completeness, it means, how close it is to having all possible edges.

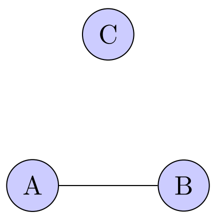


Figure 18: Graph density example showing a sparse graph with few edges relative to the number of vertices.

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:

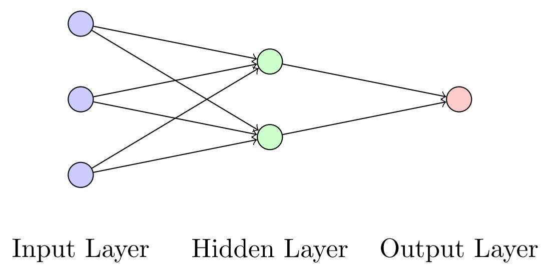


Figure 19: A simple neural network with one hidden layer.

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:

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

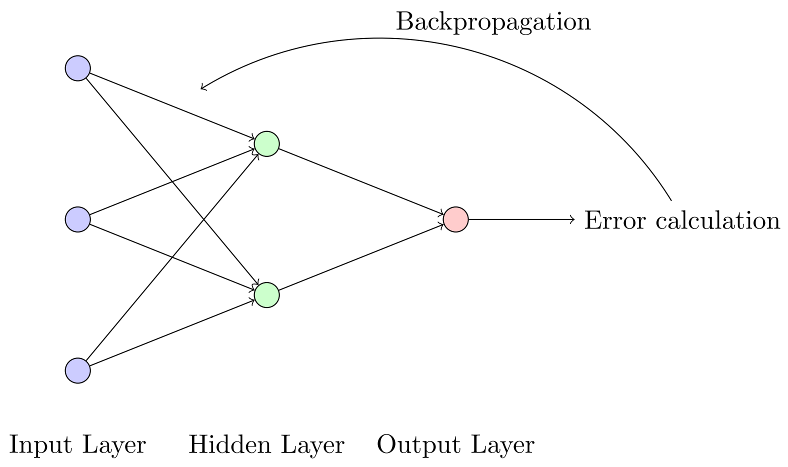


Figure 20: Backpropagation in action within a simple neural network.

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.

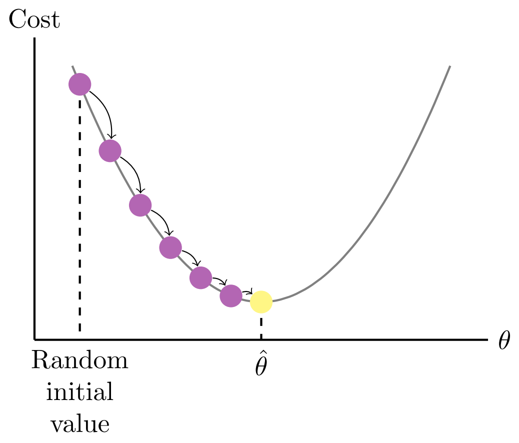


Figure 21: Gradient descent method applied on a concave function.

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.

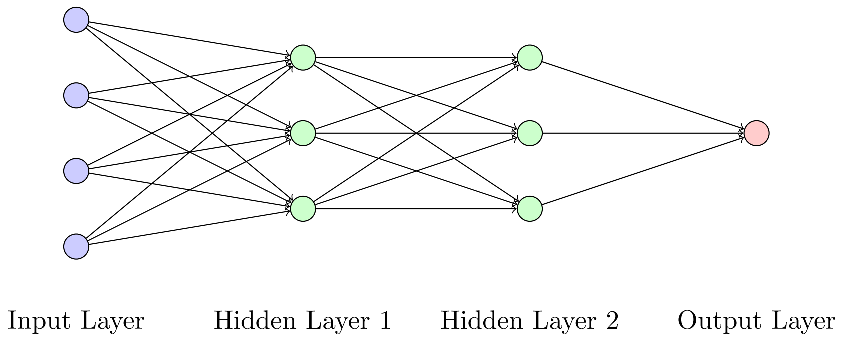


Figure 22: A Deep neural network with two hidden layers.

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.

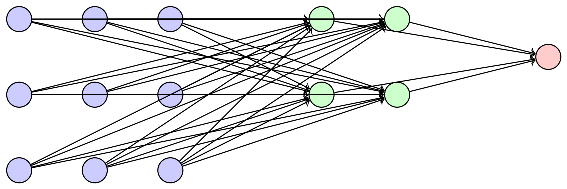


Figure 23: A simple convolutional neural network architecture.

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.

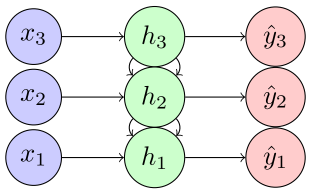


Figure 24: Recurrent Neural Network (RNN) unrolled through time.

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* [16]. 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.

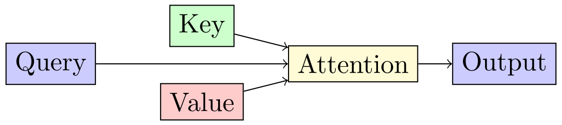


Figure 25: Attention mechanism in neural networks.

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).

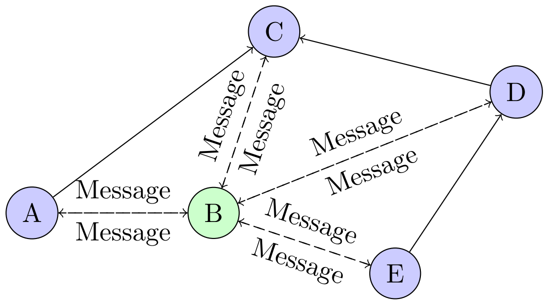


Figure 26: Message passing between node B and its neighbors in a GNN.

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.

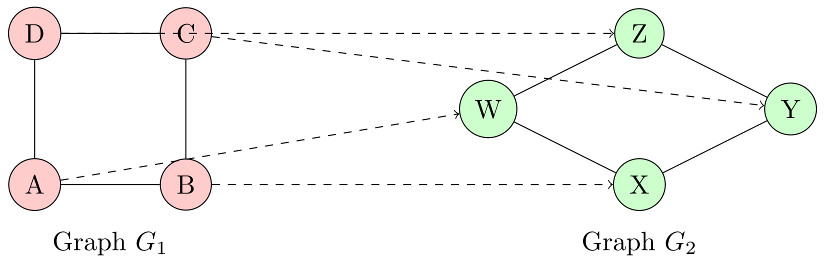


Figure 27: Graph Isomorphism: G_1 (Square) and G_2 (Rhombus).

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 [11]. 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.

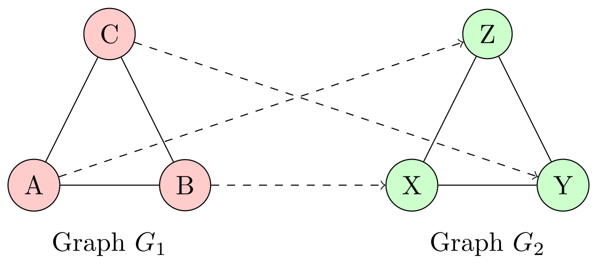


Figure 28: Graph Kernels: Example Graphs with Similar Structures.

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* [1], 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.

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]:

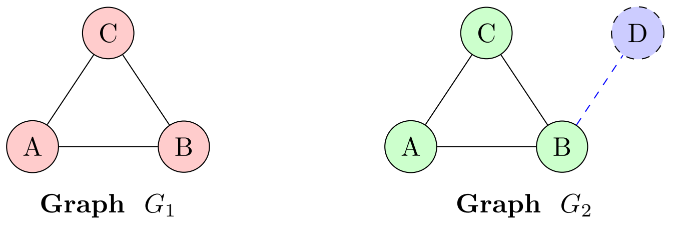


Figure 29: Graph Edit Distance: Transforming G_1 to G_2 by adding vertex D and edge (B,D).

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

Calculating the GED with traditional imperative algorithm is possible but feasible for graphs of modest size. GED is a NP-HARD problems and for traditional solutions there is no way except to compare graphs node by node and edge by edge through combinatorial techniques to find a solution. However, as the number of nodes in the graphs increase, the complexity of these methods grows exponentially, leading to scalability issues thus infeasibility. To overcome these limitations recent works involve the use of artificial intelligence techniques such as neural networks to predict the GED between two graphs. AI-based approaches usually offer more robust and scalable solutions by learning patterns and features from graphs, significantly reducing computation times. This section reviews some of the most important papers dealing with GED calculation from 2019 to the time of writing this (2024).

The timeline we are going to explore starts with *SimGNN* in 2019 [3], the first prominent approach to utilize neural networks for computing GED. After that many other models have been built mostly on SimGNN's foundation each time trying to perform a little better. Finally the timeline ends with most recent and promising work introducing *GedGNN* [12]. All these models try to effectively predict the GED between two graphs, but as we will see, everything seems still to be in early stage of development.

5.1 Timeline

2019, *SimGNN: A Neural Network Approach to Fast Graph Similarity Computation* [3]: Introduces SimGNN, addressing graph similarity computation using neural networks. It features a learnable embedding function, an attention mechanism to focus on 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* [14]: 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* [18]: 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* [19]: 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* [20]: 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* [17]: 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* [7]: 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* [21]: 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* [2]: 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* [6]: 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* [15]: 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* [10]: 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* [5]: 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* [13]: 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* [9]: 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* [8]: 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* [4]: 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* [12]: 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 used neural networks is SimGNN [3], introduced in 2019. SimGNN serves as a foundational model in the field of graph similarity computation, in fact future models will often inherit its core concepts (such as the siamese layout architecture), making it the starting point of reference for anyone dealing with GED computation.

The architecture of SimGNN [Figure 30] is composed by several stages:

- **Node Embedding Stage**: This stage makes use of a graph convolutional network to capture local structural information that transforms each node in the graph into a vector that encodes its features and structural properties.
- **Graph-Level Embedding Stage**: This stage produces a single embedding representing the whole graphs starting from the previously produced nodes embeddings by also using attention mechanisms to focus on important nodes.
- **Graph-Graph Interaction Stage**: This stage puts in communication the two graphs embedding previously produced and produces a matrix of similarity interaction scores.
- **Final Similarity Score Computation Stage**: This stage process the previously produced similarity matrix to compute the final similarity score.

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

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

The combination of these two strategies should allow the model to capture both global and local informations which should result in a robust approach to graph similarity computation.

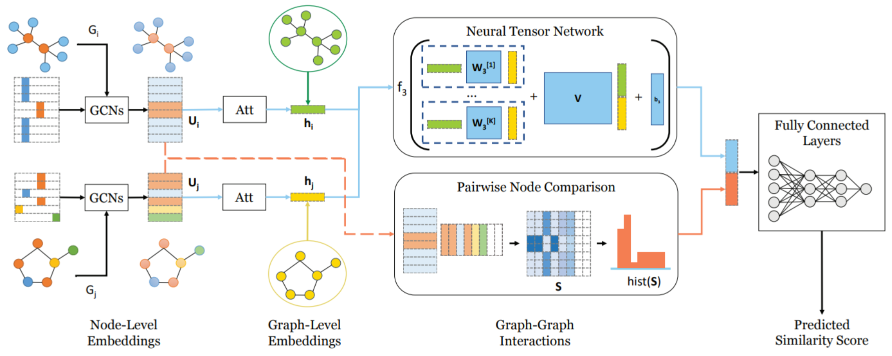


Figure 30: SimGNN architecture overview.

5.3 GPN

In 2022, an innovative hybrid approach for computing GED was released. The Graph Path Networks (GPN) model, proposed within the *NOAH Framework* [20], introduces the GED computation by exploiting the A* search algorithm optimized through neural networks. This method tries to address several previously found limitations trying to improve both the search direction and search space optimization.

The architecture of GPN [Figure 31] is composed by several modules:

- **Pre-training Module**: This module computes pre-training information about the graphs that will be exploited by the next modules.
- **Graph Embedding Module**: This module utilizes layers of Graph Isomorphism Network (GIN) to transform each node into a vector. Then these embeddings are combined into a single graph level embedding by using different attention mechanisms.
- **Learning Module**: This module focuses on optimizing the A* search algorithm by learning an estimated cost function and an elastic beam size. The tradition algorithm is then used for the final prediction.

The main advantage of GPN over SimGNN is that it is capable of finding an edit path between graphs (roughly accurate) between graphs in a short amount of time.

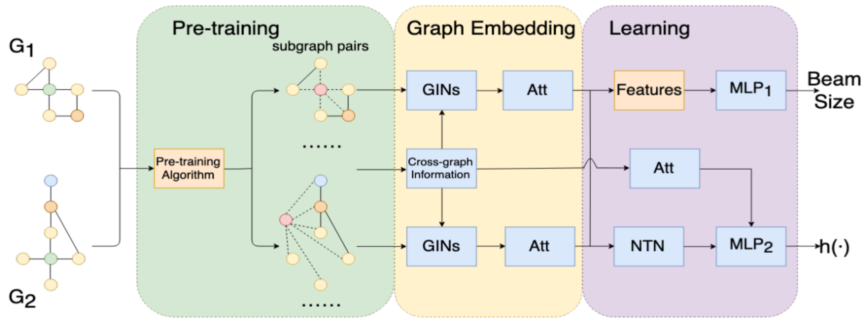


Figure 31: GPN architecture overview.

5.4 TaGSim

In 2022, another innovative approach was released with TaGSim (Type-aware Graph Similarity) [2]. The idea behind GED as a single value has been revaluated and it is now thought as the summation of three different values: ged_nc the number of node relabelling, ged_in the number of node insertions/deletions, ged_ie the number of edges insertions/deletions.

The architecture of TaGSim [Figure 32] is composed by several components:

- **Type-Aware Graph Embeddings**: This component takes into account the different impacts that different atomic operations could have when predicting the GED producing a type-aware graph level embedding. Namely the operations taken into accounts are: 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.

- **Type-Aware Neural Networks**: This component takes advantage of specific 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 and outputs them all.

The main advantage of TaGSim over predecessors is that by decoupling the GED into different dimensions, there is the potential for more granular control and learnability.

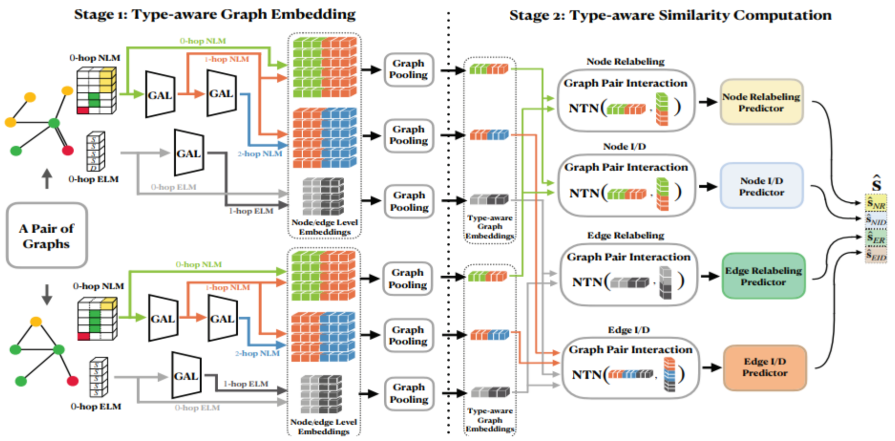


Figure 32: TaGSim architecture overview.

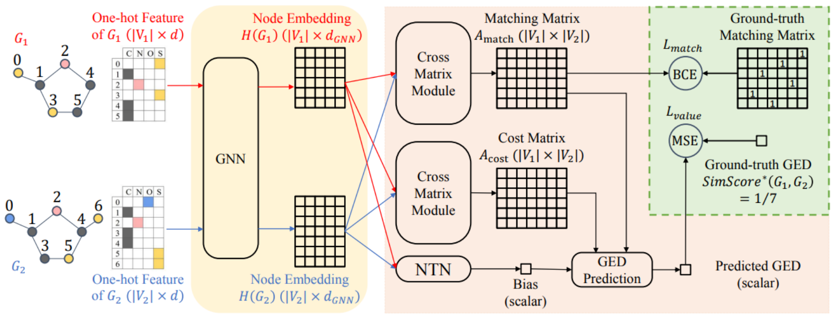
5.5 GedGNN

In 2023, the model that is considered the state of the art at the time of writing this (2024) is released with GedGNN (Graph Edit Distance via Neural Graph Matching) [12]. The idea behind this model is to try to put together all the best ideas from past's models including the basic siamese layout of SimGNN, the use of more advanced convolutional layers of GPN and the split of the GED metric from TaGSim while still allowing for the retrieval of an edit paths by taking inspiration from NOAH framework.

The architecture of GedGNN [Figure 33] is composed by several components:

- **Graph Neural Network (GNN) Encoder**: This component produces the encodings for nodes and edges while preserving their relational information. This is done through the employment of an advanced GNN encoder.
- **Node and Edge Matching Module**: This component performs the node and edge matching between the pair of graphs producing a matching matrix and a cost matrix.
- **k-Best Matching Post-Processing Algorithm**: After predicting the GED value a k-best post-processing algorithm is used trying to retrieve a good edit path.

GedGNN's results state to not only outperforms previous methods but also provides a flexible framework that can adapt to various types of graph structures and similarity measures.



G_1
One-hot Feature of G_1 ($|V_1| \times d$)
Node Embedding $H(G_1)$ ($|V_1| \times d_{GNN}$)
GNN
G_2
One-hot Feature of G_2 ($|V_2| \times d$)
Node Embedding $H(G_2)$ ($|V_2| \times d_{GNN}$)
Cross Matrix Module
Matching Matrix A_{match} ($|V_1| \times |V_2|$)
Cross Matrix Module
Cost Matrix A_{cost} ($|V_1| \times |V_2|$)
NTN
Bias (scalar)
GED Prediction
Predicted GED (scalar)
L_{match}
BCE
Ground-truth Matching Matrix
L_{value}
MSE
Ground-truth GED $SimScore^*(G_1, G_2) = 1/7$

Figure 33: GedGNN architecture overview.

5.6 Encountered Gaps

When studying GedGNN's codebase a lot of problems and concerns have become evident. Perhaps most of these gaps are due to the intrinsic nature of copy pasting from paper to paper over time and to the lack of researcher's ability to extensively testing theyr work.

A primary issue is the quality of the codebase itself, there is a lack of standardization and employments of best practices, lots of similar methods that all seem to do the same thing, lots of classes, lots of confusion, lots of unhandled errors. Code almost seem hardcoded here and there, not allowing for customization and manipulation. The code is not easy to read and the documentation, although written, is very poor.

Strictly correlated to code quality and testing scenarios is the scalability issues on GPUs. When trying to run for the first time the code as is on a GPU some errors also raised up, but apart from this, the models do not scale well on GPU hardware and this is an issue. Training on small datasets is feasible on CPUs but as soon as a bigger dataset are used for test-training new models, problems have become evident with long training times per epoch.

It is not clear why the codebase as is does restrict the usage of graphs for those with only 10 nodes or less in both training, testing and validation scenarios. Perhaps due to the presence of many imperative algorithm with high computational time such as the k-best post processing algorithm that retrieves edit paths; also code as is does break (at least for me) when testing on the IMDB dataset (with any model). Additionally, there is no use of artificial dataset generation, despite being present in the code, creating more confusion and several if statements that will never be reached.

Data used for training is also an issue persisting from SimGNN's times. Datasets used are always the same but the issue (which is not an issue but rather a constructive critic), is that approximate GEDs are used as labels instead of real ones. Datasets are mostly small (with graphs with less than 10 nodes in general) and with modern hardware GED wouldn't take much time to compute exactly. Also, in almost any codebase seen till date, training is structured in such a way that for each pair of graph present in the training set the corresponding GED is required.

But the most important thing that has been shown up is that testing has not been performed in a fair way. It is not clear why, but when dealing with the codebase as is, it is not possible to test a model that has been trained on a specific dataset on a different dataset. Perhaps to not show the evident lack of generalization emersed after doing modifications to the code to perform fair testing [section 6].

In summary, the analysed codebase which presents GedGNN, TaGSim, SimGNN and GPN presents several significant challenges to overcome. These include problems with the reproducibility of the results, fair evaluations, scalability issues, poor code quality, unclear parameters and more. Clearly, resolving many of this issues would lead to a significant advancement in this field.

6 Methodology and Experimentation

Working with high quality dataset is key to obtain performant models, but data, and in particular GED labelling within [12] is just an approximation of the real value, thus influencing model training worsening performances.

6.1 Artificial Dataset Generation

The proposed code is publicly available on GitHub and is meant as a starting point for generating an high quality dataset composed of exact (TaGSim like) GED values along with randomly generated graphs at fixed distances. When working with Python programming language it is often not needed to reinvent the wheel because a package that suits requirements probably already exists and within this context a large use of NetworkX (nx) is made to handle graphs data structures.

Listing 1: Random Graph Generator

```python
class RandomGraphGenerator():
    def generate_random_ER_graph(self, nmin=2, nmax=10, pmin=0.2, pmax=1):
        """Erdos-Renyi graph generation"""
        n  = randint(nmin, nmax)
        p = uniform(pmin, pmax)
        G = nx.gnp_random_graph(n, p, seed=None, directed=False)
        return self._make_connected(G)

    def generate_random_BA_graph(self, nmin=2, nmax=10):
        """Barabasi Albert graph generation"""
        n  = randint(nmin, nmax)
        m = randint(1, n-1)
        if not (m >= 1 and m < n):
            raise Exception(f"m >= 1 and m < n", f"m={m}", f"n={n}")
        G = nx.barabasi_albert_graph(n, m)
        return self._make_connected(G)

    def _make_connected(self, G : nx.Graph):
        for node in list(nx.isolates(G)):
        target_node = choice([n for n in G.nodes() if n != node])
        G.add_edge(node, target_node)
        return G
```

RandomGraphGenerator [Listing 1] is a class that provides two public methods for generating random graphs by reusing *nx* package. Specifically two methods for generating different variants of graphs are provided: one for Erdős-Rényi's types of graphs (or binomial graph) and one for Barabási–Albert's ones. Additionally, we want to make sure the graphs are connected (there are no isolates nodes) to prevent errors during future computations.

Listing 2: Abstract Consecutor

```
class Consecutor(ABC):
    def next(self, G : nx.Graph) -> HistoryValue:
        """Return a tuple with a new graph G' and the distance from G (can
            be 0)"""
        if not self._is_processable(G):
            raise UnprocessableError()
        copy = deepcopy(G)
        rand = random()
        return self._next(copy, rand)

    @abstractmethod
    def _next(self, G : nx.Graph, rand : float) -> HistoryValue:
        """Actual next logic from concrete classes"""
        raise NotImplementedError()

    def _is_processable(self, G : nx.Graph) -> bool:
        """Whether you can make a 'next' on graph G"""
        return len(self._nodes(G)) > 0 and len(self._edges(G)) > 0

    def _nodes(self, G : nx.Graph) -> List[int]:
        """Return the list of nodes of the graph G"""
        return list(G.nodes)

    def _edges(self, G : nx.Graph) -> List[Tuple[int, int]]:
        """Return the list of edges of the graph G"""
        return list(G.edges)

    def _rand_obj_list(self, l : List):
        """Return a random object in list if not empty else None"""
        return l[randint(0, len(l) - 1)] if len(l) > 0 else None

    def _new_node(self, G : nx.Graph):
        """Return a new node for the graph G (biggest indexed node + 1)"""
        return (self._nodes(G)[-1] + 1) if len(self._nodes(G)) > 0 else 0

    def _rand_node(self, G : nx.Graph):
        """Return a random existing node of G if any else None"""
        return self._rand_obj_list(self._nodes(G))

    def _new_edge(self, G : nx.Graph):
        """Return a new edgre for the graph G if not fully-connected else
            None"""
        return self._rand_obj_list(list(nx.non_edges(G)))

    def _rand_edge(self, G : nx.Graph):
        """Return a random existing edge of G if any else None"""
        return self._rand_obj_list(self._edges(G))
```

The *Consecutor* class is what will handle the generation of a graph G' starting from G at a fixed known GED distance. In [Listing 2] is showed the abstract *Consecutor* class that provides common methods for managing graphs modifications.

Listing 3: Incremental Consecutor

```
class IncrementalConsecutor(Consecutor):
    """IncrementalConsecutor add nodes and edges. The way it does so
        ensures there are no isolates at any moment."""
    def _next(self, G : nx.Graph, rand : float) -> HistoryValue:
        if rand <= 0.7:
            return self.__add_edge(G)
        else:
            return self.__add_node_and_edges(G)

    def __add_node_and_edges(self, G : nx.Graph) -> HistoryValue:
        """Add a new node and k edges from the new node to random nodes"""
        new_node = super()._new_node(G)
        G.add_node(new_node)
        nodes = super()._nodes(G)
        k = randint(1, len(nodes) - 1)
        choices = list(filter(lambda n : n != new_node, nodes))
        for _ in range(0, k):
            target = super()._rand_obj_list(choices)
            G.add_edge(new_node, target)
            choices.remove(target)
        return G, (1+k, 0, 1, k)

    def __add_edge(self, G : nx.Graph) -> HistoryValue:
        """Add a new edge if not fully connected"""
        new_edge = super()._new_edge(G)
        if new_edge is None:
            return G, (0, 0, 0, 0)
        G.add_edge(*new_edge)
    return G, (1, 0, 0, 1)
```

The *IncrementalConsecutor* [Listing 3] is the class responsible for creating a graph G' from G in an additive way. If a graph G_1 is at distance d_1 from G_2 and G_3 is generated by solely adding edges or nodes with distance d_2 from G_2 then it is demonstrable that G_1 is distant $|d_1 + d_2|$ from G_3.

Listing 4: Decremental Consecutor

```
class DecrementalConsecutor(Consecutor):
"""DecrementalConsecutor removes nodes and edges, after any atomic
    operation it also removes isolated nodes."""
  def _next(self, G : nx.Graph, rand : float) -> HistoryValue:
    if rand <= 1:
      return self._remove_edge(G)
    else:
      return self._remove_node_and_edges(G)

  def _remove_node_and_edges(self, G : nx.Graph) -> HistoryValue:
    """Remove a random node along with its edges, if this causes a
       node to be isolated it is removed aswell"""
    rvm_node = self._rand_node(G)
    if rvm_node is None:
      return G, (0, 0, 0, 0)
    degree = G.degree(rvm_node)
    G.remove_node(rvm_node)
    isolated = list(nx.isolates(G))
    G.remove_nodes_from(isolated)
    return G, (1+degree+len(isolated), 0, 1+len(isolated), degree)

  def _remove_edge(self, G : nx.Graph) -> HistoryValue:
    """Remove a random edge if there are any, if this causes a node to
       be isolated it is removed aswell"""
    rvm_edge = self._rand_edge(G)
    if rvm_edge is None:
      return G, (0, 0, 0, 0)
    G.remove_edge(*rvm_edge)
    isolated = list(nx.isolates(G))
    G.remove_nodes_from(isolated)
    return G, (1+len(isolated), 0, len(isolated), 1)
```

At the contrary, *DecrementalConsecutor* [Listing 4] is the class responsible for creating a graph G' from G in an subtractive way. If a graph G_1 is at distance d_1 from G_2 and G_3 is generated by solely removing edges or nodes with distance d_2 from G_2 then it is demonstrable that G_1 is distant $|d_1 + d_2|$ from G_3.

Listing 5: Consecutor Executor

```
class ConsecutorExecutor():
  """ConsecutorExecutor can be used to execute steps consecutions
```

```
        starting from a graph G"""
    def __init__(self, consecutor: Consecutor):
        self.consecutor = consecutor

    def execute(self,
        G : nx.Graph,
        steps = 100,
        stopper : Callable[[nx.Graph], bool] = None,
        skip_zero_ged = True) -> History :
        """Perform steps attempts to modify graph G.
        Parameters:
        1. G, the graph where to start from
        2. steps, the number of atomic modifications
        3. stopper, an early custom stopping function on newly generated
            graph
        4. skip_zero_ged, a Consecutor may return a G' with ged 0 w.r.t. G
        Returns a dict representing the history of graph generations with
            edit distance from previous graph.
        """
        history = {}
        history[0] = (G, (0, 0, 0, 0))
        for i in tqdm(range(1, steps+1), total=steps+1, desc="History
            Generation"):
            try:
                # Generation and update G
                G, taged = self.consecutor.next(G)
            except UnprocessableError:
                break
        # Custom stopping condition on newly generated graph
        if stopper is not None and stopper(G):
            break
        # Save only when necessary
        if taged[0] != 0 or not skip_zero_ged:
            history[i] = (G, taged)
        return history
```

ConsecutorExecutor [Listing 5] is the class that handles the *generatio* of *steps* sequential graphs by applying the *next* method from either the *IncrementalConsecutor* or *DecrementalConsecutor*. It is not possible to apply both in the same sequence as the GED value will be invalidated between pairs of graphs: a drawback of this approach is the unfeasibility of building dense and very large datasets.

Listing 6: History Utilities

```
class HistoryUtilities():
    """HistoryUtilities is responsible for providing common history
        utilities functions."""
    def build_ged_combination(self, history : History) ->
        List[MappingGed]:
```

```
    """Function that builds the ged pickle file from the combination
        of every pair of graphs in history"""
    mapping_list = []
    entries = list(history.items())
    all_combs = list(combinations(entries, 2))
    for comb in tqdm(all_combs, total=len(all_combs), desc="Ged Dict
        Generation"):
        id1, id2 = comb[0][0], comb[1][0]
        value = self.calculate_ged_comb(history, id1, id2)
        mapping_list.append(value)
    return mapping_list

def calculate_ged_comb(self, history : History, id1 : HistoryKey,
     id2: HistoryKey) -> MappingGed:
    """Returns the artificial ged distance given an entry
        combination"""
    delimiters = [id1, id2]
    delimiters.sort()
    min, max = delimiters[0], delimiters[1]
    ged = ged_nc = ged_in = ged_ie = 0
    for entry in history.items():
        key = entry[0]
        value = entry[1]
        if min < key <= max:
            TaGED = value[1]
            ged += TaGED[0]
            ged_nc += TaGED[1]
            ged_in += TaGED[2]
            ged_ie += TaGED[3]
        if key > max:
            break
    return (id1, id2, ged, ged_nc, ged_in, ged_ie, [])

def split_by_fractions(self, history: History, train=0.8, test=0.2):
    """Split history in two dicts according to proportions"""
    assert train+test==1.0, 'fractions sum is not 1.0'
    keys = list(history.keys())
    shuffle(keys)
    split_point = int(train * len(keys))
    dict_train = {key: history[key] for key in keys[:split_point]}
    dict_test = {key: history[key] for key in keys[split_point:]}
    return dict_train, dict_test


def save_to_sparse_jsons(self, history : History, outfolder : str):
    """Create/Clean outfolder than save all history as jsons files"""
    if not os.path.exists(outfolder):
        os.makedirs(outfolder)
    file_list = os.listdir(outfolder)
    jsons_files = [file for file in file_list if
```

```
            file.endswith('.json')]
        for file in jsons_files:
            file_path = os.path.join(outfolder, file)
            os.remove(file_path)
        for key, value in tqdm(history.items(),
            total=len(history.items()), desc=f"Saving to {outfolder}"):
            filename = os.path.join(outfolder, f'{key}.json')
            with open(filename, 'w') as f:
                graph = {}
                graph['n'] = value[0].number_of_nodes()
                graph['m'] = value[0].number_of_edges()
                graph['labels'] = None
                graph['graph'] = list(list(map(lambda t: list(t),
                    value[0].edges)))
                json.dump(graph, f)
```

HistoryUtilities [Listing 6] is the final piece of utility to generate and save to disk the dataset consisting of all possible combinations of a given list of sequentially generated graphs along with their TaGED.

Listing 7: Dataset Generation Example

```
generator = RandomGraphGenerator()
hist_utils = HistoryUtilities()
stop_on_empty = lambda G: len(list(G.nodes))==0

start = generator.generate_random_ER_graph(3, 6, 0.5, 1)
# start = generator.generate_random_BA_graph(2, 5)

consecutor = IncrementalConsecutor()
# consecutor = DecrementalConsecutor()

exc_consecutor = ConsecutorExecutor(consecutor)

# Change the parameter to generate more consecutio steps
history = exc_consecutor.execute(start, steps=1000,
    stopper=stop_on_empty, skip_zero_ged=True)

ged = hist_utils.build_ged_combination(history)
train, test = hist_utils.split_by_fractions(history, train=0.8, test=0.2)

NAME = "Medium"
hist_utils.save_to_sparse_jsons(train, f'json_data/{NAME}/train/')
hist_utils.save_to_sparse_jsons(test, f'json_data/{NAME}/test/')
json.dump(ged, open(f'json_data/{NAME}/TaGED.json', 'w'))
```

With [Listing 7] is an example of how to put all the pieces together to actually create a custom dataset and save it to disk in a format suitable GedGNN.

6.2 Experiments and Results

For experimenting and conducting a fair evaluation of the models, two well known datasets, IMDB and Linux, as well as two artificially generated datasets, *1000g_100n* and *Medium* have been employed:

- **Linux**: A dataset that consists of graphs representing function calls within the Linux kernel: a node represent a statement and edges represent the dependency between two statements. The dataset is composed of 1000 graphs and each of them does not have more than 10 nodes, making data specialized and dense.
- **IMDB**: A dataset that consists of movie-related graphs: a node represents an actor, while edges connects two actors if they appear in the same movie. The dataset is composed of 1500 graphs and some of them have more than 10 nodes, making data less dense with respect to *Linux*.
- **1000g_100n**: An artificially generated dataset with 1000 graphs, each containing 100 nodes and a progressively less number of edges. *1000g_100n* does not represent any real scenario in particular and has been generated solely for testing purposes.
- **Medium**: Another artificially generated dataset with 1000 heterogeneous graphs. The variety is big, starting from 3 nodes and 3 edges in the firstly generated graph up to 297 nodes and 21457 edges in the last one, making data very sparse.

Each model presented in the VLDB paper [12], namely SimGNN [subsection 5.2], GPN [subsection 5.3], TaGSim [subsection 5.4] and GedGNN [subsection 5.5] has been trained for 10 epochs with default parameters from the codebase as is for each of the aforementioned dataset. Then each of trained model has been tested, trying to reproduce [12] results on the respective test-set and **on all the other datasets as well** for a total of 64 combinations. In the next tables, results are presented with key metrics:

- **Mean Squared Error (mse)**: Measures the average of the squares of the differences between the predicted GED values and real GED values.
- **Mean Absolute Error (mae)**: Measures the average differences between the predicted GED values and the reak GED values.
- **Accuracy (acc)**: Measures the proportion of correct GED predictions over the total predicted GEDs.

Since predicting GED 100% accurately is very hard for a neural network, the most relevant metric in this context will be the MAE: it is important that the net is very close to the real value.

trainset	**testset**	**mse**	**mae**	**acc**
IMDB	IMDB	4532	**1.28**	0.475
IMDB	Linux	105097	6506	0.008
IMDB	1000g_100n	725792	327867	0.005
IMDB	Medium	362746	5527745	0.004
Linux	IMDB	119051	7414	0.202
Linux	Linux	2547	**0.423**	0.64
Linux	1000g_100n	725792	327867	0.005
Linux	Medium	390191	5996899	0.004
1000g_100n	IMDB	123898	5104	0.043
1000g_100n	Linux	135375	5938	0.027
1000g_100n	1000g_100n	66845	219972	0.002
1000g_100n	Medium	40.19	6938538	0.0
Medium	IMDB	81696	**5.25**	0.057
Medium	Linux	62777	5075	0.079
Medium	1000g_100n	531549	314.44	0.002
Medium	Medium	2436	2724294	0.001

Table 1: Results for SimGNN models

As show in [Table 1], SimGNN works well if it gets trained on a specific dataset and tested on the same type of data; unfortunately there are no significant results for artificial generated datasets, but clearly the model does not generalize. *SimGNN* trained on *Medium* seems to show positive outcomes on *IMDB* but it might due to the fact that few identical already seen graphs could have been feed to the net.

trainset	**testset**	**mse**	**mae**	**acc**
IMDB	IMDB	106.09	**10645**	0.211
IMDB	Linux	41.77	2762	0.089
IMDB	1000g_100n	6936	327867	0.005
IMDB	Medium	502857	7301305	0.005
Linux	IMDB	44103	5777	0.117
Linux	Linux	57506	**3306**	0.065
Linux	1000g_100n	101895	1476.37	0.0
Linux	Medium	155102	3926197	0.0
1000g_100n	IMDB	80138	8048	0.118
1000g_100n	Linux	62778	3251	0.052
1000g_100n	1000g_100n	180992	1979288	0.0
1000g_100n	Medium	110796	3312005	0.0
Medium	IMDB	85028	8398	0.061
Medium	Linux	60467	3275	0.052
Medium	1000g_100n	340701	2184379	0.0
Medium	Medium	276667	5131201	0.001

Table 2: Results for GPN models

GPN seems to be an outlier, since reproducing its original performance has not been possible. As shown in [Table 2], the model does perform bad in every associated scenario.

trainset	**testset**	**mse**	**mae**	**acc**
IMDB	IMDB	**5.2**	2743	0.183
IMDB	Linux	55426	6.42	0.006
IMDB	1000g_100n	34168	250498	0.002
IMDB	Medium	109842	6867463	0.0
Linux	IMDB	104002	185839	0.0
Linux	Linux	1408	**0.427**	0.642
Linux	1000g_100n	33935	671133	0.0
Linux	Medium	89117	6445506	0.0
1000g_100n	IMDB	179554	12471	0.001
1000g_100n	Linux	193506	16509	0.0
1000g_100n	1000g_100n	22926	225854	0.002
1000g_100n	Medium	94807	7074655	0.0
Medium	IMDB	101271	7366	0.155
Medium	Linux	114007	11265	0.0
Medium	1000g_100n	64129	671133	0.0
Medium	Medium	5757	6446658	0.0

Table 3: Results for TaGSim models

TaGSim seems to show the same behaviour as *SimGNN* performing good only when tested on the same type of graphs on which it got trained. A Lack of generalization capability is shown here as well.

trainset	**testset**	**mse**	**mae**	**acc**
IMDB	IMDB	0.816	**0.634**	0.58
IMDB	Linux	9399	1.27	0.221
IMDB	1000g_100n	13861	363687	0.005
IMDB	Medium	201372	4106777	0.005
Linux	IMDB	13153	3539	0.075
Linux	Linux	1161	**0.315**	0.735
Linux	1000g_100n	869809	4367593	0.0
Linux	Medium	212754	3801531	0.0
1000g_100n	IMDB	47711	**5.86**	0.033
1000g_100n	Linux	28688	2126	0.105
1000g_100n	1000g_100n	0.708	78892	0.013
1000g_100n	Medium	411299	6885001	0.003
Medium	IMDB	65417	7611	0.103
Medium	Linux	9204	**1.17**	0.261
Medium	1000g_100n	4651	259151	0.003
Medium	Medium	0.718	267837	0.003

Table 4: Results for GedGNN models

GedGNN seems to be the most promising model for artificial dataset testing. When training on *1000g_100n* and *Medium*, *GedGNN* showed positive results while getting tested on both *IMDB* and *Linux*. A clear sign that if a much bigger and denser dataset were to be used it could have outperformed others specialized types of datasets.

7 Discussion and Conclusions

The results presented in this study provide a comprehensive understanding of the effects of **[specific factor or variable]** on **[outcome or dependent variable]**. The findings demonstrate that **[briefly summarize the main findings]**. This is consistent with previous research indicating **[mention any consistency with previous studies]**. However, the observed **[specific result or observation]** contradicts **[any conflicting results or hypotheses]**, suggesting that **[potential reasons for discrepancies]**.

One notable aspect is the **[highlight any unexpected results or significant observations]**, which could be attributed to **[explain possible reasons or mechanisms]**. The analysis indicates that **[discuss any patterns or trends observed]**, reinforcing the importance of **[mention any theoretical or practical implications]**.

In conclusion, this study highlights the **[main takeaway or insight]** regarding **[specific factor or variable]** and its impact on **[outcome or dependent variable]**. The evidence supports **[restate key findings]**, providing valuable insights into **[broader implications or applications]**. The **[significance of results]** underscores the need for **[mention any key implications or recommendations]**.

The contribution of this study is significant as it **[describe how the study advances understanding or fills a gap in knowledge]**. This provides a foundation for **[mention how the results could be applied or used]**, advancing the field of **[mention the relevant field or discipline]**.

7.1 Future Works

Future research should address the limitations identified in this study, such as **[mention specific limitations]**. To further explore the observed effects, it would be beneficial to **[suggest specific methods or approaches]**. Additionally, investigating **[mention any other variables or factors]** could provide a more comprehensive understanding of **[specific topic or area]**.

Expanding the scope of this study to include **[suggest any new contexts, populations, or settings]** could yield additional insights and validate the findings in different scenarios. Longitudinal studies and experimental designs are recommended to assess the long-term effects and causality of **[specific factor or variable]** on **[outcome or dependent variable]**.

Incorporating advanced analytical techniques and interdisciplinary approaches may also enhance the robustness of future research. Overall, these directions will contribute to a deeper and more nuanced understanding of **[specific topic or area]**, paving the way for **[mention any potential future applications or impacts]**.

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