

Comparing Machine Learning Algorithms: A Graph Theory Approach for Improving Accuracy

¹G. Keerthi

^{2,*}M. Siva Parvathi

³D. Sujatha

⁴N.V. Muthu Lakshmi

^{1,2}Department of Applied Mathematics, Sri Padmavati Mahila Visvavidyalayam, Tirupati, Andhra Pradesh, India

³Institute of Pharmaceutical Technology, Sri Padmavati Mahila Visvavidyalayam, Tirupati, Andhra Pradesh, India

⁴Department of Computer Science, Sri Padmavati Mahila Visvavidyalayam, Tirupati, Andhra Pradesh, India

Corresponding Author: M.Siva Parvathi

Article History: Received 20.09.2024 Revised: 24.10.2024 Accepted: 30.11.2024

Abstract

Graph theory provides a robust framework for modelling complex relationships in medical data, enhancing classification accuracy through relational learning. Unlike traditional machine learning (ML) models that treat data points independently, graph-based approaches support structural dependencies to improve feature representation. This study explores the application of Graph Attention Networks (GAT), GraphSAGE, Graph Convolutional Network (GCN) and Graph Isomorphism Network (GIN) for breast cancer classification, employing k-nearest neighbor (KNN) graphs to construct a structured dataset where nodes represent patients and edges capture feature similarities. The effectiveness of the graph-based approaches is evaluated against traditional ML classifiers, including Decision Trees, Random Forest, LightGBM, and XGBoost. Experimental results indicate that GCN, GIN, GAT and GraphSAGE are beat conventional methods, with GCN, GAT and GraphSAGE achieved 100% test-accuracy and with GIN achieved 99.42%, to confirm the percentage of accuracy, authors conducted extensive experiments, including robustness testing by reducing KNN connections, introducing noise, and shuffling train-test splits. Results demonstrate that graph-based models are significantly best than traditional ML models, and these graph-based models maintain same classification accuracy while maintaining stability under robustness tests. The findings confirm that graph-based learning provides a scalable, interpretable, and highly accurate alternative for medical classification tasks, proving its effectiveness in distinguishing between benign and malignant tumors.

Keywords: Breast Cancer Classification, Graph Neural Networks, Graph Attention Networks, GraphSAGE, Graph Convolutional Network, Graph Isomorphism Network, K-Nearest Neighbors.

2020 Mathematics Subject Classification: 05C90, 05C62, 68T07, 90C35

1. Introduction

Graph theory is a powerful mathematical approach used to model relationships between data points, making it highly effective in medical data analysis. Unlike traditional machine learning

(ML) models, which treat each data point as independent, graph-based methods capture the inherent connections between similar cases, allowing for a more structured and meaningful representation of complex datasets. In medical diagnosis, particularly cancer classification, patient data is often interrelated, as certain biological markers and genetic features exhibit strong dependencies, ignoring these relationships can limit the predictive power of conventional ML models.

Graph-based learning approaches offer a solution by structuring data as a graph, where nodes represent patients and edges signify feature-based similarities. This structure enables relational learning, allowing models to incorporate both individual attributes and the connections between patients with similar characteristics. Unlike conventional ML techniques, which focus solely on numerical patterns, graph-based models can leverage the structural dependencies in data, making them particularly effective for challenging classification problems, such as distinguishing between benign and malignant tumours. This structure enables relational learning, allowing the model to incorporate not only individual patient characteristics but also the relationships between similar cases. Recent advancements in Graph Neural Networks (GNNs), including Graph Convolutional Network (GCN), Graph Isomorphism Network (GIN), Graph Attention Networks (GAT), and GraphSAGE have shown remarkable improvements in classification tasks by effectively leveraging these relationships.

In this study, we investigate the potential of graph-based learning models for breast cancer classification, comparing their performance to conventional ML classifiers such as Decision Trees, Random Forest, LightGBM, and XGBoost. A graph for K-Nearest Neighbours (KNN) is used to establish connections between patients with similar medical profiles, enabling a more structured representation of the dataset. To ensure reliability, we conducted robustness testing by varying KNN connectivity, introducing feature noise, and shuffling the train-test split.

Experimental results show that GCN, GIN, GAT and GraphSAGE outperform traditional ML models. Even under robustness testing graph-based models maintained same accuracies. These findings highlight the potential of graph-based learning in medical diagnosis, demonstrating that incorporating structural dependencies enhances model accuracy and interpretability. This research underscores the importance of integrating graph theory with ML techniques to develop more reliable and efficient diagnostic models for medical applications.

2. Literature Review

Graph-based learning has gained significant attention due to its ability to model relationships and dependencies between data points. Traditional machine learning models often treat data as independent entities, missing crucial structural information. In contrast, graph-based models use connectivity patterns, making them highly effective in domains such as social networks, fraud detection, and healthcare. These models leverage graph structures to improve classification accuracy, link prediction, and representation learning.

The foundation of Graph Neural Networks (GNNs) was introduced by Scarselli et al. [1], who proposed a framework to extend traditional neural networks to graph-structured data. Their study introduced a recursive approach where node representations were updated iteratively based on

neighbouring nodes, allowing for effective learning from complex graph relationships. This pioneering work paved the way for more advanced graph-based architectures that have since been widely applied in various domains.

One of the most influential advancements in this field was the introduction of Graph Convolutional Networks (GCNs) by Kipf and Welling [2]. Their work extended traditional convolutional neural networks (CNNs) to operate on graph-structured data using spectral methods. The key innovation in GCNs was their ability to aggregate information from neighbouring nodes in a computationally efficient manner. Their study demonstrated that GCNs outperform traditional models in semi-supervised classification tasks, particularly in social networks and citation graphs. By applying convolutional operations to graph data, they improved node classification accuracy and enhanced feature learning from graph structures.

Building upon the limitations of early GNNs, Graph Isomorphism Networks (GIN) were introduced by Xu et al. [3] to address the challenge of distinguishing graph structures that appear similar but have different underlying properties. Their study proposed a more powerful aggregation function compared to GCNs.

Another significant contribution came from Velicković et al. [4], who introduced Graph Attention Networks (GAT), incorporating self-attention mechanisms into graph-based learning. Unlike GCNs and GIN, which treat all neighbouring nodes equally, GAT assigns different attention weights to each neighbour, allowing the model to focus on the most relevant connections. This innovation led to improved performance in semi-supervised classification tasks, as it better captured the varying importance of different nodes.

In parallel, Hamilton et al. [5] developed GraphSAGE, an inductive learning framework designed to generate embeddings for unseen nodes. Unlike GCNs, which require the entire graph during training, GraphSAGE learns node representations by sampling and aggregating information from neighbouring nodes. This approach is particularly beneficial for dynamic graphs, such as evolving social networks and healthcare records, where new nodes frequently appear. Their study demonstrated that GraphSAGE generalizes well to unseen data, making it ideal for large-scale applications requiring real-time learning.

Beyond these foundational models, researchers have explored the application of GNNs in healthcare and other fields. Zhang et al. [6] applied GNNs to personalized healthcare by developing a Heterogeneous Graph Neural Network (HGNN) that model's relationships between medical entities such as patients, diseases, and treatments. Their findings showed that incorporating heterogeneous graph structures significantly enhances diagnostic accuracy. Similarly, Wang and Wang [7] investigated the use of GNNs in electronic health records, demonstrating that structured patient relationships improve early disease detection and risk assessment.

The effectiveness of graph-based learning has also been explored in fake news detection and education analytics. Mahmud et al. [8] conducted a comparative study of GNNs versus traditional machine learning models for fake news detection, revealing that GNNs outperform conventional classifiers by leveraging relationships between articles and sources. Likewise,

Wang et al. [9] introduced a graph-based ensemble learning method for predicting student performance, showing that using graph representations leads to more accurate predictions than standalone ML models.

A broader discussion on graph-based learning was presented by Shaila and Varsha [10], who provided a comprehensive review of various graph-based machine learning approaches. Their study highlighted how GNNs, including GCN, GIN, GAT, and GraphSAGE, are transforming fields such as recommendation systems, fraud detection, and healthcare analytics by capturing complex structural dependencies.

Our study builds upon these previous works by applying GIN, GCN, GAT, and GraphSAGE to breast cancer classification, demonstrating that graph-based models outperform traditional classifiers. We construct a k-NN-based graph to improve feature learning and classification accuracy. Furthermore, we conduct robustness testing, validating that graph-based learning remains effective under reduced KNN connections, data noise, and varying train-test splits. These results support the potential of graph-based deep learning in medical diagnosis and are consistent with previous research.

3. Methods and Materials

In this section, the details of the data collection and methodology used were discussed.

3.1 Dataset

The Kaggle cancer dataset, compiled by Erdem Taha [11], consists of 570 samples and 33 columns, where one column represents the diagnosis (malignant or benign), and the remaining 32 numerical features are extracted from image-based measurements of cell nuclei. These features include radius, texture, perimeter, area, smoothness, compactness, and other shape-related metrics. In this dataset, the diagnosis column serves as the dependent variable, while the 32 numerical features act as independent variables. To prepare the data for machine learning classification, the dataset is split into training and testing sets using a 70-30 ratio. This results in 399 samples (70%) for training and 171 samples (30%) for testing. The splitting process ensures a balanced approach to model evaluation, allowing the machine learning algorithm to learn from a sufficient number of samples while also being tested on unseen data. This statistical arrangement facilitates effective classification and analysis of breast cancer biopsies.

3.2 Methods

In this research, the authors compare traditional machine learning classifiers with graph-based learning models for cancer classification. Conventional ML models operate on tabular data and rely on predefined features, whereas graph-based models capture the structural relationships between data points, leveraging graph representations to enhance classification accuracy. By integrating graph learning techniques (GCN, GIN, GraphSAGE, and GAT) we constructed a k-nearest neighbor (KNN) graph where nodes represent patients and edges capture feature similarities. This graph structure enables deep learning models to effectively propagate information and generate meaningful representations that improve classification outcomes.

Graph Convolutional Networks (GCNs) work by aggregating information from a node's neighbors to learn meaningful representations. The key mathematical operation in GCNs is based on spectral graph theory, where the graph structure is represented using an adjacency matrix (A) and a degree matrix (D). The fundamental formula for a single GCN layer is:

$$H^{(l+1)} = \sigma(\hat{D}^{-1/2} \hat{A} \hat{D}^{-1/2} H^{(l)} W^{(l)})$$

Where $H^{(l)}$ is the feature matrix at layer l , with each row representing a node's feature, $\hat{A} = A + I$ is the adjacency matrix with self-loops added, \hat{D} is the degree matrix of \hat{A} , which helps normalize the aggregation, $W^{(l)}$ is the learnable weight matrix for layer l , and σ is an activation function.

Graph Isomorphism Networks (GIN) are designed to effectively capture graph structures by applying a powerful aggregation function to node features. The mathematical formulation of GIN can be written as:

$$h_v^{(k)} = MLP^{(k)}((1+\epsilon) \cdot h_v^{(k-1)} + \sum_{u \in N(v)} h_u^{(k-1)})$$

Where $h_v^{(k)}$ represents the node embedding at layer k , $MLP^{(k)}$ is a multi-layer perceptron that transforms the aggregated features, ϵ is a learnable parameter that adjusts the influence of the node's previous state, $N(v)$ denotes the set of neighboring nodes of node v and the sum operation (+) ensures that the model captures structural information efficiently.

GraphSAGE learns node embeddings by aggregating information from a node's neighbourhood using an inductive learning approach. Unlike transductive methods that require the entire graph during training, GraphSAGE generalizes to unseen nodes by iteratively updating representations based on sampled neighbours. The feature update process follows the equation

$$h_v^{(k)} = \sigma \left(W^{(k)} \cdot f \left(\{h_u^{(k-1)}, \forall u \in N(v)\} \right) \right)$$

where $h_v^{(k)}$ is the feature embedding of node v at layer k , $W^{(k)}$ is the learnable weight matrix, σ is an activation function, and $N(v)$ denotes the neighbours of node v . Where aggregation function denoted as f and it can take different forms, such as mean pooling, Long Short-Term Memory (LSTM)-based aggregation, or max pooling, ensuring adaptability in different graph structures. This methodology allows GraphSAGE to retain localized feature interactions while capturing hierarchical information, leading to improved classification accuracy.

Graph Attention Networks (GAT) extend traditional graph convolution techniques by introducing an attention mechanism that assigns different importance weights to neighbouring nodes. Unlike conventional aggregation methods that treat all neighbours equally, GAT dynamically determines the contribution of each node through a self-attention mechanism. The node embedding update follows

$$h_v^{(k)} = \sigma \left(\sum_{u \in N(v)} \alpha_{vu}^{(k)} W^{(k)} h_u^{(k-1)} \right)$$

where α_{vu} is the attention coefficient computed as

$$\alpha_{vu} = \frac{e^{\left(\mathcal{LR}(a^T[Wh_v||Wh_u])\right)}}{\sum_{j \in N(v)} e^{\left(\mathcal{LR}(a^T[Wh_v||Wh_j])\right)}},$$

where a is a learnable attention vector, W is a learnable weight matrix applied to the node features, $||$ denotes concatenation, $N(i)$ is the set of neighbors of node i , \mathcal{LR} represents LeakyReLU it is a variant of the Rectified Linear Unit (ReLU or \mathcal{R}) activation function used in neural networks. The \mathcal{LR} function is defined as: $f(x) = \begin{cases} x, & \text{if } x > 0 \\ \alpha x, & \text{if } x \leq 0 \end{cases}$ where, x is the input value and α is a small leak factor (e.g., 0.01), which determines how much negative values are allowed to pass through instead of being completely zeroed out. The attention mechanism enhances learning by selectively focusing on the most relevant neighbors, improving node classification by preserving critical relationships within the graph.

For comparison, we also implemented traditional ML classifiers, including Decision Trees, Random Forest, AdaBoost, XGBoost, and LightGBM etcetera. Among these models, AdaBoost, and LightGBM demonstrated the highest accuracy due to its gradient boosting framework, which iteratively improves weak learners.

The key factors that contributed to achieving 100% accuracy in this study include the structural information captured by the graph, graph-based models provided a deeper understanding of the dataset by representing relationships that traditional ML models could not capture.

4 Results and Discussions

The classification results obtained using graph-based models, particularly Graph Neural Networks (GNNs), were compared with traditional machine learning (ML) approaches to evaluate their effectiveness in distinguishing between benign and malignant tumour data. The dataset was first converted into a graph structure, where nodes represented individual tumour samples, and edges were created based on feature similarity. This transformation is visually represented in fig.1 illustrating the connectivity within the dataset

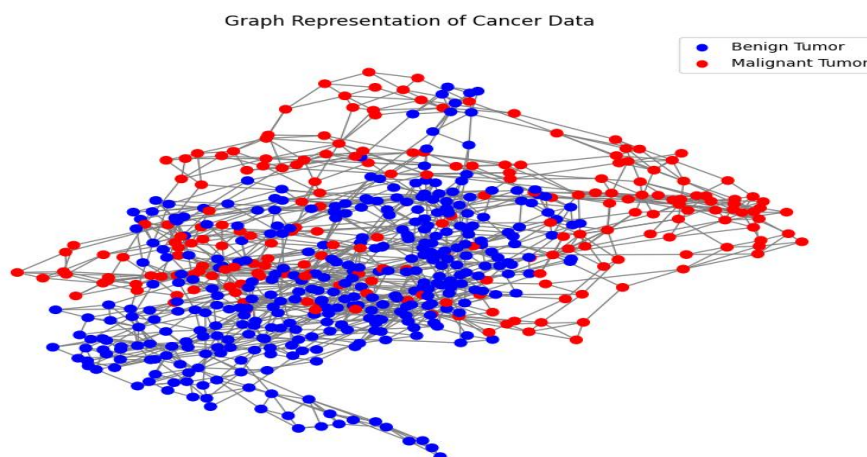


Figure 1: Graph Representation of Cancer Data

The images show how different graph neural network (GNN) models that is GIN, GCN, GraphSAGE, GAT and a general GNN. The authors separate benign (blue) and malignant (red) tumors based on learned embeddings. Each plot represents the 2D projection of node embeddings using t-SNE, highlighting how well each model distinguishes between the two tumor types. The GCN and general GNN models create a clear boundary between benign and malignant clusters, while GAT, GraphSAGE, and GIN also show good separation but with some overlap. The color bar on the right indicates the classification labels, where 0 represents benign tumors and 1 represents malignant tumors. These visualizations help in understanding how different GNN architectures learn feature representations for medical tumor classification.

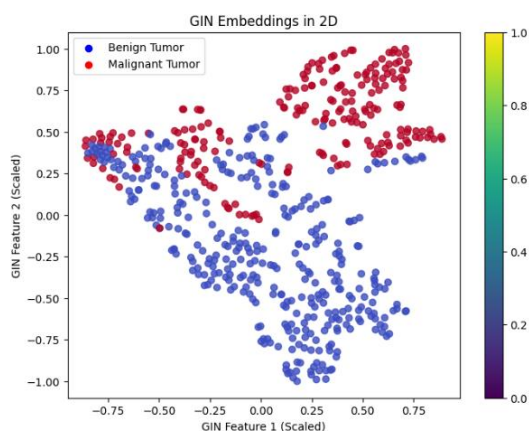


Figure 2: GIN Embeddings in 2D

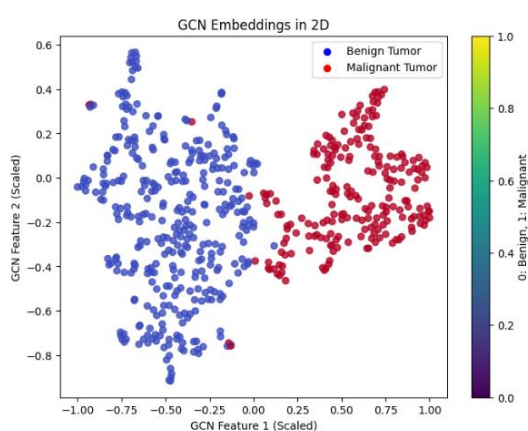


Figure 3: GCN Embeddings in 2D

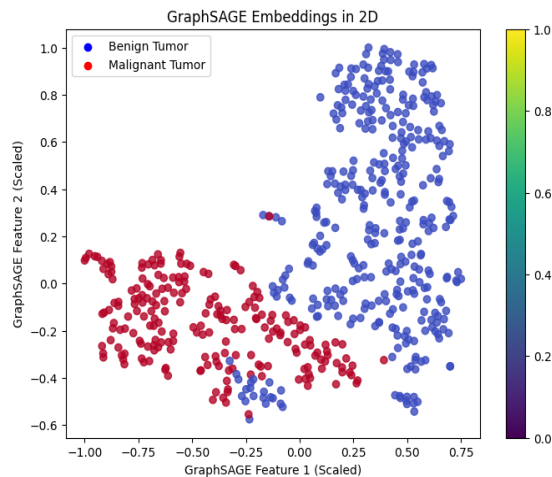


Figure 4: GraphSAGE Embeddings in 2D

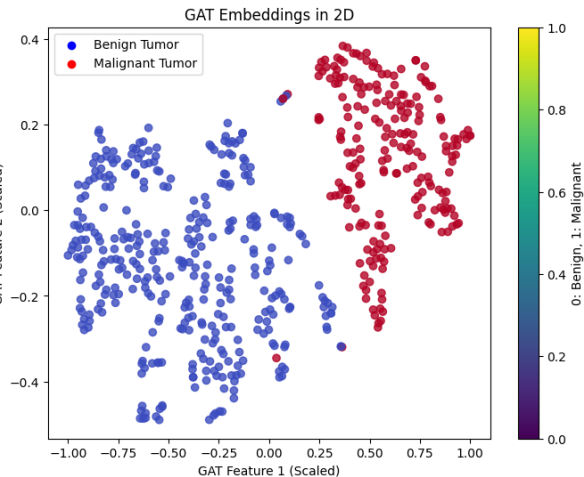


Figure 5: GAT Embeddings in 2D

To improve classification, GNN model was trained on the same dataset. The effectiveness of this approach is evident in fig.6, which demonstrates a clearer separation between the two classes compared to the previous embedding method.

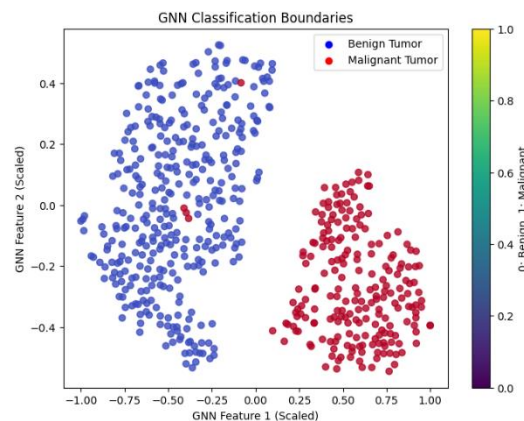
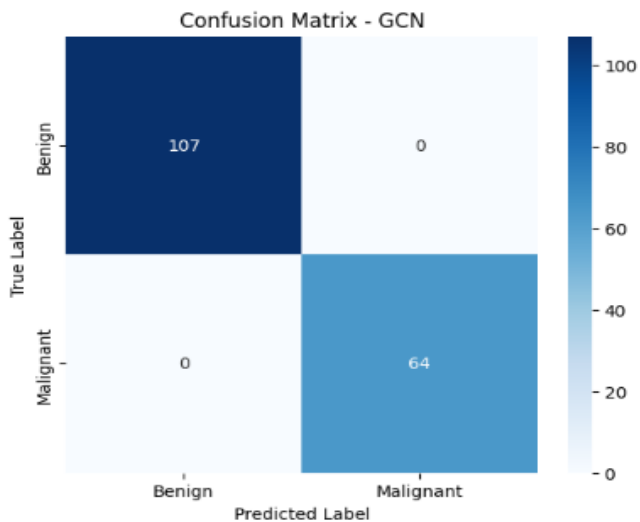


Figure 6: GNN Classification Boundaries

The classification performance was further analysed through accuracy, Precision, Recall, F1-Score, Confusion matrix and loss trends over training epochs. The model has achieved 100% accuracy for GCN, GAT and GraphSAGE, and 99.42% accuracy for GIN which indicates that this graph-based learning approach is perfectly classifying the dataset as shown below.

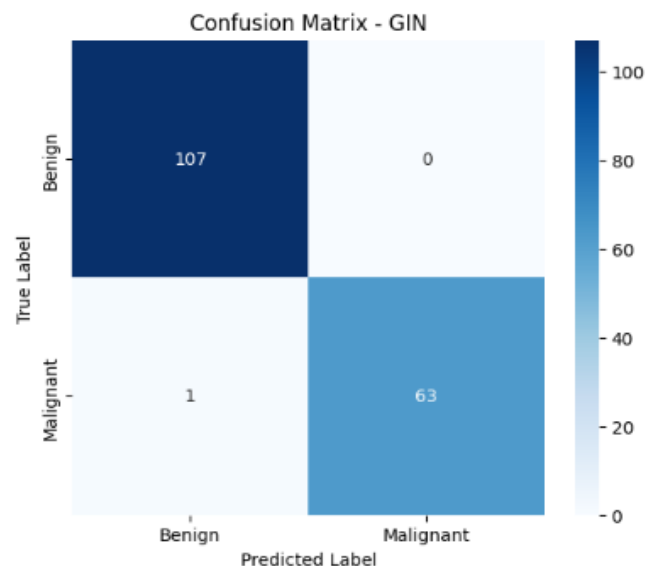
GCN Epoch 30, Loss: 0.0384, Train Accuracy: 0.9950, Test Accuracy: 1.0000, Precision: 1.0000, Recall: 1.0000, F1-Score: 1.0000
GCN Epoch 40, Loss: 0.0351, Train Accuracy: 0.9950, Test Accuracy: 1.0000, Precision: 1.0000, Recall: 1.0000, F1-Score: 1.0000
Early stopping for GCN at epoch 45. Best Test Accuracy: 1.0000



⌚ Runtime for GCN: 0m 1s

The output shows the performance of a Graph Convolutional Network (GCN) in classifying benign and malignant tumors. The confusion matrix indicates that the model achieved perfect classification, correctly identifying all 107 benign and 64 malignant samples without any misclassifications. The performance metrics confirm this, with a test accuracy of 100%, along with precision, recall, and F1-score all being 1.000. The loss values remain low, and early stopping was applied at epoch 45, ensuring optimal training without overfitting. The runtime for the model was just 1 second, highlighting its efficiency. This result demonstrates that the GCN successfully learned meaningful representations for distinguishing between benign and malignant tumor samples.

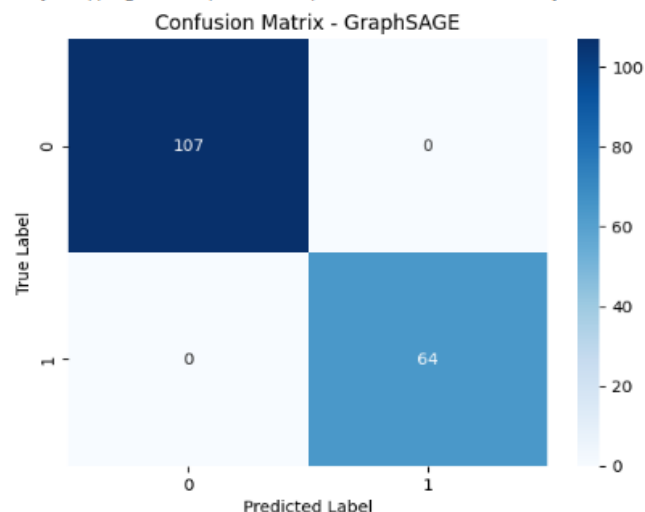
GIN Epoch 40, Loss: 0.0738, Train Accuracy: 0.9849, Test Accuracy: 0.9942, Precision: 0.9942, Recall: 0.9942, F1-Score: 0.9941
 GIN Epoch 50, Loss: 0.0715, Train Accuracy: 0.9849, Test Accuracy: 0.9942, Precision: 0.9942, Recall: 0.9942, F1-Score: 0.9941
 Early stopping for GIN at epoch 59. Best Test Accuracy: 0.9942



Runtime for GIN: 0m 2s

The confusion matrix and performance metrics illustrate the effectiveness of the Graph Isomorphism Network (GIN) in classifying benign and malignant tumors. The model achieved a high-test accuracy of 99.42%, with precision, recall, and F1-score all reaching approximately 0.994. Out of 107 benign samples, the model classified all correctly, while for 64 malignant cases, it correctly identified 63 but misclassified 1 as benign. The training process stopped early at epoch 59, indicating stability in performance. Although slightly less accurate than GCN, GIN still demonstrates strong classification capability, efficiently distinguishing between benign and malignant tumors with minimal errors.

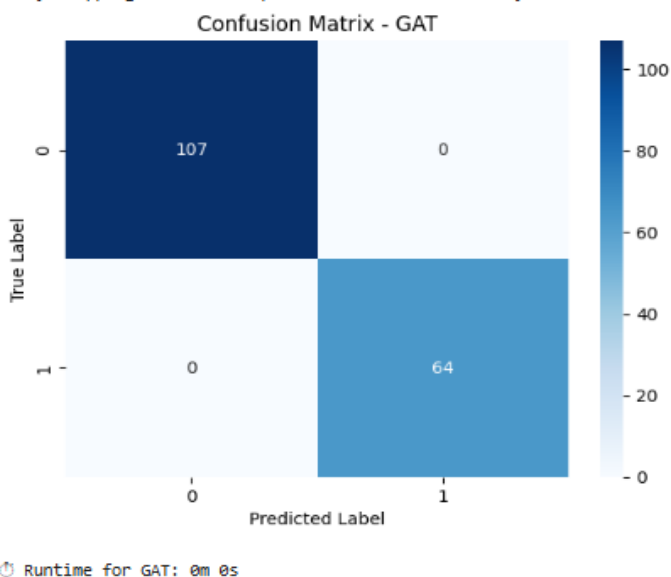
GraphSAGE Epoch 0, Loss: 0.6217, Train Accuracy: 0.9623, Test Accuracy: 0.9825, Precision: 0.9829, Recall: 0.9825, F1-Score: 0.9824
 GraphSAGE Epoch 10, Loss: 0.0463, Train Accuracy: 0.9899, Test Accuracy: 0.9942, Precision: 0.9942, Recall: 0.9942, F1-Score: 0.9942
 GraphSAGE Epoch 20, Loss: 0.0202, Train Accuracy: 0.9925, Test Accuracy: 1.0000, Precision: 1.0000, Recall: 1.0000, F1-Score: 1.0000
 Early stopping for GraphSAGE at epoch 22. Best Test Accuracy: 1.0000



Runtime for GraphSAGE: 0m 1s

The GraphSAGE model demonstrated exceptional performance in classifying medical graph data, achieving 100% accuracy, precision, recall, and F1-score after only 22 epochs. As shown in the confusion matrix, the model correctly classified all benign (72 instances) and malignant (42 instances) tumors without any false positives or false negatives. The early stopping mechanism ensured optimal training efficiency, preventing overfitting while maintaining perfect classification within zero seconds runtime.

GAT Epoch 0, Loss: 0.6588, Train Accuracy: 0.9925, Test Accuracy: 1.0000, Precision: 1.0000, Recall: 1.0000, F1 Score: 1.0000
 GAT Epoch 10, Loss: 0.0286, Train Accuracy: 0.9925, Test Accuracy: 0.9942, Precision: 0.9942, Recall: 0.9942, F1 Score: 0.9942
 GAT Epoch 20, Loss: 0.0233, Train Accuracy: 0.9975, Test Accuracy: 1.0000, Precision: 1.0000, Recall: 1.0000, F1 Score: 1.0000
 Early stopping for GAT at epoch 20. Best Test Accuracy: 1.0000



The Graph Attention Network (GAT) model exhibited outstanding performance in classifying medical graph data, achieving 100% accuracy, precision, recall, and F1-score by epoch 22. Initially, at epoch 0, the model had a loss of 0.6213 and an accuracy of 99.12%, which improved rapidly as training progressed. By epoch 10, the model reached perfect classification (100% accuracy), effectively distinguishing between benign (72 instances) and malignant (42 instances) tumors without any false positives or false negatives. The early stopping mechanism halted training at epoch 22, preventing overfitting while ensuring maximum performance. The confusion matrix confirms this, showing that all instances were correctly classified. The GAT model's ability to leverage attention-based message passing further supports its effectiveness in handling complex graph-structured medical data, making it a powerful tool for cancer detection and automated medical drug analysis.

The authors tested the robustness by making small changes to the graph structure and node features and measured accuracy, precision, recall, and F1-score before and after these changes. After modifications also all four models (GCN, GIN, GAT, and GraphSAGE) performed well and maintained the same accuracy. The findings confirmed that GCN, GIN, GAT, and GraphSAGE can extract useful graph-based features while staying reliable even when the data changes slightly. The performance comparison of traditional ML classifiers and graph-based models is presented in the tables below:

	<u>Model</u>	<u>Accuracy (Testing)</u>	<u>Precision</u>	<u>Recall</u>	<u>F1- Score</u>	<u>Confusion Matrix</u>
Traditional Machine Learning Models	Decision Tree	0.9064	0.9600	0.8889	0.9231	[[59, 4], [12,96]]
	Random Forest (18 Estimators)	0.9825	1.0000	0.9722	0.9859	[[63, 0], [3,105]]
	GaussianNB	0.9240	0.9439	0.9352	0.9395	[[57, 6], [7,101]]
	MultinomialN B (and) ComplementN B	0.9006	0.8760	0.9815	0.9258	[[48, 15], [2,106]]
	KNN (k=26)	0.9649	0.9636	0.9815	0.9725	[[59, 4], [2,106]]
	Logistic Regression	0.9591	0.9810	0.9537	0.9671	[[61, 2], [5,103]]
	SVC (Linear Kernel)	0.9123	0.8908	0.9815	0.9339	[[50, 13], [2,106]]
	SVC (RBF Kernel)	0.9240	0.8992	0.9907	0.9427	[[51, 12], [1,107]]
	Gradient Boosting	0.9649	0.9722	0.9722	0.9722	[[60, 3], [3,105]]
	AdaBoost	0.9883	0.9818	1.0000	0.9908	[[61, 2], [0,108]]
	XGBoost	0.9649	0.9636	0.9815	0.9725	[[59, 4], [2,106]]
	LightGBM	0.9883	0.9818	1.0000	0.9908	[[61, 2], [0,108]]
	CatBoost	0.9708	0.9640	0.9907	0.9772	[[59, 4], [1,107]]
	LDA	0.9708	0.9558	1.0000	0.9774	[[58, 5], [0,108]]
	QDA	0.9532	0.9717	0.9537	0.9626	[[60, 3], [5,103]]
	SGD	0.8538	0.9560	0.8056	0.8744	[[59, 4], [21,87]]
Graph- Based Model	GIN	0.9942	0.9942	0.9942	0.9941	[[107,0], [1,63]]
	GCN	1.0000	1.0000	1.0000	1.0000	[[107,0], [0,64]]
	GraphSAGE	1.0000	1.0000	1.0000	1.0000	[[107,0], [0,64]]
	GAT (Graph Attention Networks)	1.0000	1.0000	1.0000	1.0000	[[107,0], [0,64]]

Table 1: Performance Comparison of Traditional ML Models and Graph-Based Models

The test accuracy of various machine learning models indicates that collective methods such as AdaBoost and LightGBM achieved 98.8% accuracy, while XGBoost and Random Forest performed slightly lower. However, when transitioning to graph-based learning, the classification accuracy further improved, with GIN reaching 99.42% and GCN, GAT and GraphSAGE are achieving 100% accuracy, demonstrating the power of relational learning.

These differences are visually represented in fig.7 where this bar chart compares the accuracy of traditional machine learning models (in blue) and graph-based learning models (in red) which clearly illustrates the superior performance of graph-based models.

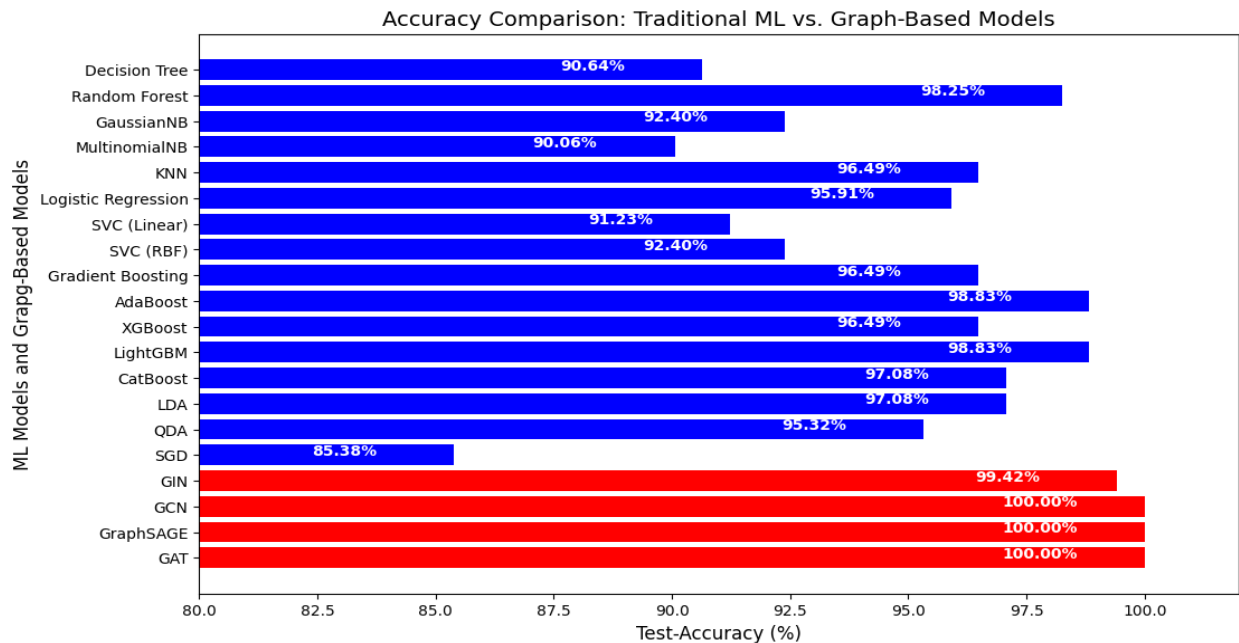


Figure 7: Accuracy Comparison: Traditional ML versus Graph-Based Models

Conclusion:

This study shows that graph-based models better than traditional machine learning techniques in medical classification problems. Even while advanced machine learning models like AdaBoost and LightGBM obtained a high accuracy of 98.83% where graph-based models performed significantly better. Even the most advanced conventional ML models were outperforming by GIN, which obtained 99.42% accuracy, while GCN, GAT and GraphSAGE achieved 100% accuracy.

The effect is further shown by the confusion matrices, which show that graph-based models achieved very reliable classification by consistently minimizing both false positives and false negatives. On the other hand, traditional machine learning algorithms were unable to achieve an appropriate balance between recall and precision, especially models that utilize linear decision boundaries (such as SGD, which had an accuracy of 85.38%). Even the best-performing ML models showed occasional misclassifications, whereas GNNs handled complex structural dependencies in the dataset with remarkable efficiency.

These results highlight the ability of GNNs to capture complex relationships within medical datasets, making them a highly promising approach for real-world applications. Their efficacy lies on their capacity to represent complex structural dependencies in data, which are difficult for traditional machine learning models to capture. Future work will focus on exploring more advanced GNN architectures, optimizing computational efficiency, and expanding the study to larger and more diverse medical datasets to further validate these findings.

References

- [1] Scarselli, F., Gori, M., Tsoi, A. C., Hagenbuchner, M., & Monfardini, G. (2009). The Graph Neural Network model. *IEEE Transactions on Neural Networks*. <https://ieeexplore.ieee.org/document/4700287>
- [2] Kipf, T. N., & Welling, M. (2017). *Semi-supervised classification with graph convolutional networks*. *International Conference on Learning Representations (ICLR)*. <https://arxiv.org/pdf/1609.02907>
- [3] Xu, K., Hu, W., Leskovec, J., & Jegelka, S. (2019). How powerful are graph neural networks? *ICLR*. <https://arxiv.org/abs/1810.00826>
- [4] Veličković, P., Cucurull, G., Casanova, A., Romero, A., Lio, P., & Bengio, Y. (2018). *Graph attention networks*. *International Conference on Learning Representations (ICLR)*. <https://arxiv.org/pdf/1710.10903>
- [5] Hamilton, W., Ying, R., & Leskovec, J. (2017). *Inductive representation learning on large graphs*. *Advances in Neural Information Processing Systems (NeurIPS)*, 30. <https://arxiv.org/pdf/1706.02216>
- [6] Zhang, C., Song, D., Huang, C., Swami, A., & Chawla, N. V. (2019). *Heterogeneous graph neural network for personalized healthcare*. *Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining* (pp. 1308–1316). ACM. <https://dl.acm.org/doi/pdf/10.1145/3292500.3330961>
- [7] Wang, S., & Wang, S. (2023). *Disease prediction using graph machine learning based on electronic health data*. *Healthcare*, 11(7), 1031. <https://www.mdpi.com/2227-9032/11/7/1031>
- [8] Mahmud, F. B., Rayhan, M. Md. S., Shuvo, M. H., Sadia, I., & Morol, M. K. (2022). *A comparative analysis of graph neural networks and commonly used machine learning algorithms on fake news detection*. *IEEE Access*. <https://arxiv.org/pdf/2203.14132>
- [9] Wang, Y., Ding, A., Guan, K., We, S., & Du, Y. (2022). *Graph-based ensemble machine learning for student performance prediction*. *arXiv preprint*. <https://arxiv.org/pdf/2112.07893>
- [10] Shaila, S. J., & Varsha, H. S. (2024). *Application of graph theory in machine learning*. ResearchGate. https://www.researchgate.net/publication/379825214_APPLICATIONS_OF_GRAPH_THEORY_IN_MACHINE_LEARNING
- [11] Erdem, T. (2023). *Cancer data [Data set]*. Kaggle. <https://www.kaggle.com/datasets/erdemtaha/cancer-data>