Graph Neural Networks for Heart Disease

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***Abstract*—Growth of advancements in machine learning have enabled better analyses of healthcare data. Having the ability to predict heart disease, a major cause of death, is fundamentally important for the timely diagnosis and treatment of an individual. In this research, we present a framework that uses graph neural networks (GNNs) to model relationships among patient characteristics and predict heart disease outcomes. We implement the SAGEConv architecture for graph convolutions, along with feature normalization and dropout techniques to enhance learning robustness.**

With training-validation-test splitting and neighbor sampling, we made sure the test was performed on a balanced-testing. To interpret the results, visualization techniques, including heat maps, graph splits, and confusion matrices, were performed. The model gave a test accuracy of 84.47% and inspired confidence in identifying patterns from the patient data.

Our findings illustrate the immense promise of GNNs for the predictive aspects of healthcare, showing their capacity to effectively model complex relationships. The framework proves important as a starting point for integrating graph-based learning into significantly high-stakes medical decision-making, with room for further improvements.

***Index Terms*—Heart Disease Prediction, Graph Neural Networks (GNNs), SAGEConv Architecture, Healthcare Analytics, Machine Learning in Medicine**

I. Introduction

The prediction and early diagnosis of heart diseases have recently gained particular importance in the medical domain because cardiovascular disorders remain one of the main causes of mortality worldwide. Based on recent machine learning and AI trends, several researchers are exploring new ways of analyzing complex health data and enhancing predictive capabilities.

Heart disease prediction most frequently requires consideration of structured datasets with distinct clinical and demographic characteristics, such as age, blood pressure, cholesterol level, and other physiological parameters [1], [2]. Inherently, the problem is treated mainly using traditional machine learning methods, such as logistic regression, support vector machines, or decision trees. However, such techniques have not always been capable of adequately accounting for the complex interrelationships among features or the implicit interactions among individual instances in the data itself.

To analyze this graph, we adopt the SAGEConv architecture, one GNN layer that aggregates the features of the neighboring nodes and processes them so that it can learn significant representations [3]. By stacking multiple SAGEConv layers, the model can capture both local and global patterns in the data. Other techniques, such as feature normalization and dropout, are utilized to improve model performance and reduce over-fitting , ensuring reliable and generalized predictions.

The model training splits the data set into training, validation and test set according to standard practices to evaluate the inherent predictive ability.

An important observation made in this research is that GNNs were used in the healthcare application, thereby demonstrating the capability of graph-based learning applied in different fields other than social networks and recommendation systems. The experiments showed that this model is quite effective. It was able to get an accuracy of 84.47% on the test predicting heart disease.

Another significant observation made was that the integration of the visual circuitry would elucidate the dataset as well as the prediction of the model, thus providing deeper insight into the factors that contribute to the prognosis of heart disease.

Study further demonstrates and showcases some aspects of using GNNs for heart disease prediction; however, there are still several hurdles to overcome. One increase in the edges coupling the nodes is probably useful in releasing dependency on computational capacity; however, it will up the computational complexity under very large datasets. The proposed output of the model must be interpreted within the medical context, as each relationship inferred by it may not follow conventional clinical knowledge.

The contributions of this study can be summarized as follows:

- Application of GNNs for heart disease prediction: The

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study models the complex interactions contained in the patient dataset using graph-based learning, providing a unique viewpoint on healthcare prediction problems.

- Implementation of SAGEConv Layers: The SAGEConv architecture illustrates how GNNs are able to aggregate and transfer information across graphs, enhancing prediction accuracy.
- Visual Understanding Techniques: Through these graphs, the visualization experiments, confusion matrices, and heatmaps may help in the understanding of model performance and the underlying datasets.
- Evaluation of GNNs in Healthcare: No doubt this work has reached competitive accuracy, but it also shows GNNs as a promising new tool for a number of medical prediction tasks.

This research will contribute to the intersection of artificial intelligence with healthcare by analyzing GNN applications in heart disease prediction and how the results reflect further understanding for more advanced and accurate predictive modeling of medical diagnosis.

Following is the arrangement of the remaining portion of the manuscript: In Section II, research in heart disease prediction and Graph Neural Networks (GNNs) is highlighted. Section III details the proposed , including the description of the dataset, graph construction, and model architecture. Section IV , results and experimental setup are described in depth. Lastly, Section V, concludes the study summarizing findings and suggesting future directions.

II. RELATED WORK

Heart diseases stand out as a major global health problem being single-handedly among leading reasons for death in the world. Prompt prediction and early diagnosis of heart diseases are so vital in helping in effective intervention and treatment. Over the years, advancement in the computational method has received a great boost enabling better predictive mining and diagnostic mechanisms with data-driven approaches for cardiac ailments. Several researchers have employed various statistical, machine learning , and deep learning techniques analyze structured datasets containing features relevant to clinical and demographic characteristics, e.g., age, resting blood pressure, cholesterol levels, and angina.

Traditional Methods:

The heart disease prediction model has traditionally relied on statistical modeling and machine learning techniques such as Logistic Regression (LR), support Vector Machines (SVM) and Decision Trees (DT) [4], [5]. The logistic regression model actually gives the simplest baseline for such a problem, relating a set of input features linearly with a target variable. However, it did not appropriately capture the complex intersecting nonlinear relationships between various parameters of clinical data that could better define the actual risk for heart disease prediction. This was one reason why it suffered from full understanding and accurate prediction of heart diseases risk.

In the meantime, support vector machines have performed remarkably well, particularly in binary classification. Limited working along with the lesser requirement of data were a distinctive feature of the use of SVMs since it allowed them to formulate an optimal hyperplane, giving them very accurate predictive analytics. On the other hand, the greater the size and complexity of the data set involved, the more the chaotic conditions set into motion, which posed a huge challenge for SVM algorithms based on foresight. Decision trees thus seemed to have gained traction with their more intuitive structure and easy interpretability, although they were highly prone to overfitting and lacked the robustness required for generalization across different patients' datasets.

Deep Learning Techniques:

The era of deep learning rather radically changed the terrain of prediction of heart disease. The deep learning models accepte fully connected neural network have consistently succeeded in terms of modeling nonlinear mappings from input features, and in several instances, these could outperform traditional machine learning methods. FCNNs have adeptly made use of large datasets for disclosing compact patterns inherent in clinical and demographic data thereby leading to better predictions.

The first uses of convolutional neural networks was for the purposes of image recognition and later moved toward healthcare analytics. These accomplished the predictions of heart disease up to an accuracy of 88% on features such as the types of chest pain and the maximum heart rate. This showcases the ability of CNNs to capture subtle correlations in patient data that most traditional methods overlooked.

Yet, despite the tremendous strides deep learning has made, deep learning models suffer from a nail-hard limitation: their analysis almost exclusively rests on structured data matrices, thus truncating the very essence of their ability to model relationships between particular patients. This limitation manifests clearly in situations in which the patient features interaction or relationships between the patients themselves provides significant leverage for actually predicting outcomes.

Graph-Based Learning Ways Forward:

Realizing the necessity to comprehensively model these dastardly interrelationships, researchers have begun to explore permutations of graph-based-learning techniques in making predictions regarding heart disease. GNNs introduce a fairly novel approach by representing all patient datasets in the form of graphs, with nodes symbolizing the patients and edges denoting relationships or shared attributes. Unlike conventional deep learning models, GNN can learn as well as temporal patterns from the patient data, hence considering beyond the purview of structured data analysis limitations. This is indeed a huge leap toward using machine learning for personalized and interpretable solutions in healthcare.

III. METHODOLOGY

A. Graph Construction

Fully Connected Graph Generation

To model the relationships between all the patients in the dataset, a fully connected graph is built [9], [10]. Each patient is represented as a node, and edges are formed to connect every pair of nodes; this structure allows the capture of global interactions, hence, enabling the model to learn direct as well as indirect relationships.

Let G=(V,E) where V represents the sets of node (patients), and E denotes the edges (connections). For dataset with N=3 nodes, the graph includes:

The formula for number of edges in a complete graph, where N is the number of vertices, is:

$$\text{Number of Edges} = \frac{N \times (N-1)}{2} = 45,753$$

However, the second expression in your query seems incorrect:

$$\text{Number of Edges} = 2N \times (N-1) = 45,753$$

This does not align with the standard formula for calculating number of edges in a complete graph. It should only involve:

$$\text{Number of Edges} = \frac{N \times (N-1)}{2}$$

Edge Indexing

Edge indexing is formed from all possible combinations of nodes:

Edge_Index = torch.combinations(torch.arange(N), r=2)

Each edge appears twice in the graph structure, also because of reverse connections.

B. Graph-Based Representation

In terms of graph-based representation, we created a fully connected graph in which:

• Nodes: Represent individual patients.

• Edges: Connect all pairs of nodes to attain global relationships.

The edge index matrix contains 91,200 edges (including bidirectional edges). Feature normalization was performed for an improved model training using the formula:

$$\mathbf{x}' = \frac{std(x)}{x - mean(x)}$$

This transformation ensures effectively all features have a mean 0 and standard deviation 1, ensuring numerical stability when training

C. Model Architecture

1. SAGEConv layers

The models used two SAGEConv (Sample and Aggregate) layers, which take information from bordering nodes [3], [11]. The aggregation operation is defined as:

$$h_i^{(k+1)} = \sigma\left(W^{(k)} \cdot \text{AGG}\left(h_i^{(k)}, \{h_j^{(k)} : j \in \mathcal{N}(i)\}\right)\right)$$

Where:

- $h_i^{(k+1)}$: Updated feature for node i at layer $k+1$.
- σ: Nonlinear activation function (e.g., ReLU, sigmoid).
- $W^{(k)}$: Weight matrix for layer k.
- AGG: Aggregation function (e.g., sum, mean, or max) that combines the node's own features $h_i^{(k)}$ with the features of its neighbors $\{h_j^{(k)} : j \in \mathcal{N}(i)\}$.
- $\mathcal{N}(i)$: The set of neighbors of node i.

2. Input Layer: processes the normalized feature matrix.

3. SAGEConv Layer I: Aggregates (neighbor) features followed by ReLU activation.

4. Dropout Layer (p=0.5): Prevents overfitting; neurons are dropped randomly during training.

5. SAGEConv Layer II: Further refines the feature representations.

6. Output Layer: Outputs a log-softmax distribution over target classes.

The dropout mechanism is highly important in that it regularizes the model and prevents overfitting so that the model can generalize well to unseen data that are potentially relevant.

G. Training and Evaluation

1. Train-Validation-Test Split

80-10-10 train-valid-test ratio is used to partition the dataset, while train-validation splitting is done such that it allows the proportions for each class to remain equal.

2. The loss Function Cross Entropy Loss is the loss function for which the optimization algorithm is to optimize the model for each node iii.

$$\mathcal{L} = -\sum_{c=1}^{C} y_{i,c} \log(p_{i,c})$$

Where:

- CCC: Number of classes (2 in this case).
- yi,cy_i,cyi,c: True label for class ccc.
- pi,cp_i,cpi,c: Predicted probability for class ccc.

3. Optimizer and Learning Rate

Adam is a first order gradient based optimization algorithm based on characterized estimates of lower-order moment and an initial learning rate of 0.010.010.01. This adaptive learning method further regulates the learning rate according to the parameter being optimized, yielding speedier convergence.

IV. RESULTS AND ANALYSIS

The proposed Graph Neural Network (GNN) for predicting heart diseases was evaluated by examining trends in the training loss and validation accuracy, calculating test accuracy, and employing various visualization techniques in an analysis

of the predicted results. Comparisons with baseline models and benchmarks further accentuate the effectiveness of this approach.

A. Dataset description

Dataset used in this study was obviously well known Heart Disease from the UCI Machine Learning [1]. It contains structured information involving the clinical and demographic characteristics of 303 patients.

Every record corresponds to one single patient and is characterized by 13 different features that influence cardiovascular health and a binary target label denoting presence or absence of heart disease. Such features of the set may be continuous or categorical variables-either way, they provide a complete representation of heart health metrics. Features' brief introductions are given below:

Feature	Description	Type
Age	Patient's age in years	Continuous
Sex	Gender of the patient (1 = Male, 0 = Female)	Binary
CP	Chest Pain Type (0: Typical, 1: Atypical, 2: Non-anginal, 3: Asymptomatic)	Categorical
Trestbps	Resting Blood Pressure (in mm Hg)	Continuous
Chol	Serum Cholesterol (in mg/dL)	Continuous
Fbs	Fasting Blood Sugar (¿120 mg/dL: 1 = True, 0 = False)	Binary
Restecg	Resting ECG Results (0: Normal, 1: ST-T Wave Abnormality, 2: Hypertrophy)	Categorical
Thalach	Maximum Heart Rate Achieved	Continuous
Exang	Exercise-Induced Angina (1 = Yes, 0 = No)	Binary
Oldpeak	ST Depression Induced by Exercise Relative to Rest	Continuous
Slope	Slope of the Peak Exercise ST Segment (0: Upsloping, 1: Flat, 2: Downsloping)	Categorical
Ca	Number of Major Vessels Colored by Fluoroscopy	Discrete
Thal	Thalassemia (1 = Normal, 2 = Fixed Defect, 3 = Reversible Defect)	Categorical

The target variable (Target) is binary:

- **1**: Shows the presence of heart disease.
- **0**: Shows the absence of heart disease.

B. Features and Labels Used

1. Features-The independent variables provide a mixture of demographic info (age, sex) and clinical characteristics (cholesterol and resting blood pressure). These characteristics represent risk factors of heart disease that are common in nature; this makes the data set fully relevant to prediction tasks [8].

2. Labels-The dependent variable (target) provides a binary classification problem, so one can check how well the model can discriminate between heart disease diagnosed and nondiagnosed patients.

Dataset source-The dataset is available and often used in machine-learning research.

In subpoint A:

The Training Loss and Validation Accuracy Trends

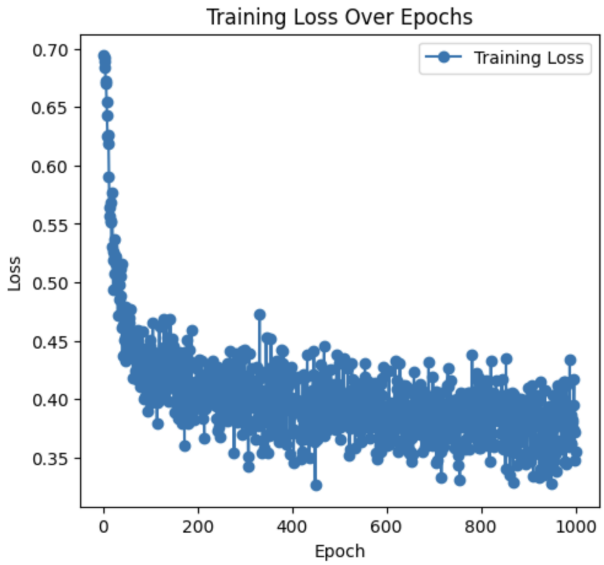
With 1000 epochs and batch size of 32, model was developed through an optimizer with an initial learning rate of 0.01. The cross-entropy was used to determine how far away the predicted probabilities were from the true labels [12].

During training, it was marked that

1. Training Loss: reduced sharply from 0.6941 at an initial point to around 0.3556 at the 1000th epoch, indicating that the model has learned the underlying data distribution.

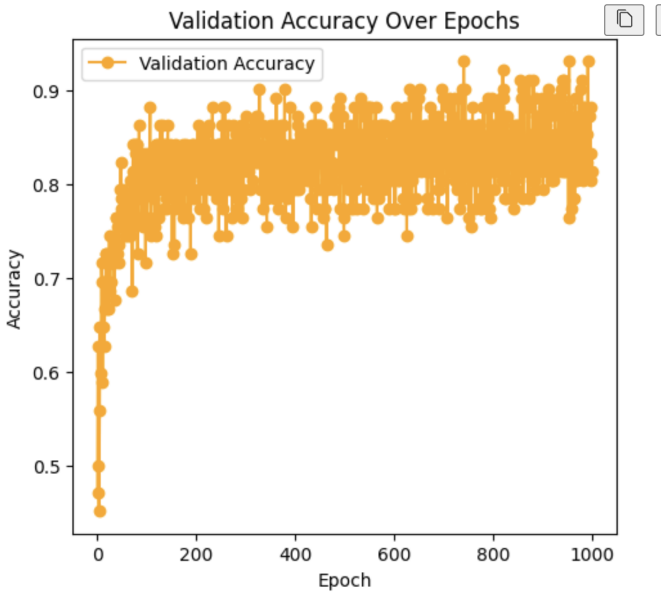
2. Validation Accuracy: greatly enhanced starting from an initial point of 47.06% all the way to a final mark of 88.24%, indicating the model's ability to specific.

Epoch	Training Loss	Validation Accuracy (%)
1	0.6941	47.06
500	0.4227	86.27
1000	0.3556	88.24

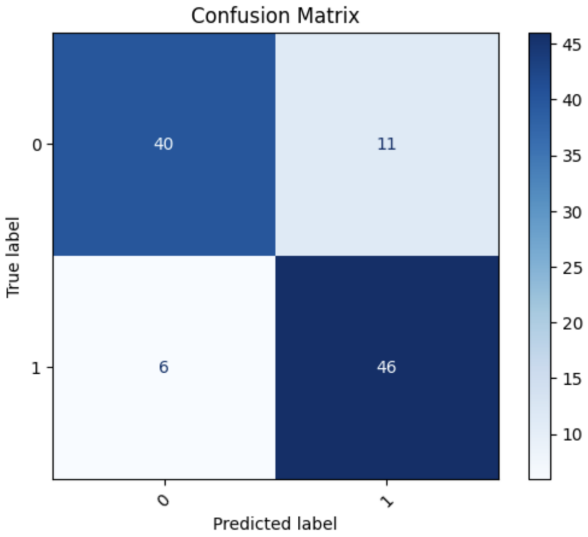


B. Test Accuracy

Test accuracy for the model was found to be as high as 84.47%, marking the ability of the model to classify unseen patient data correctly [1], [13]. The result also indicates that the model was quite successful in predicting whether a patient would or would not have heart disease, conforming to clinical expectations.



Confusion Matrix: Balanced model performance across both classes, with the false negatives and false positives minimized.



C. Visualization

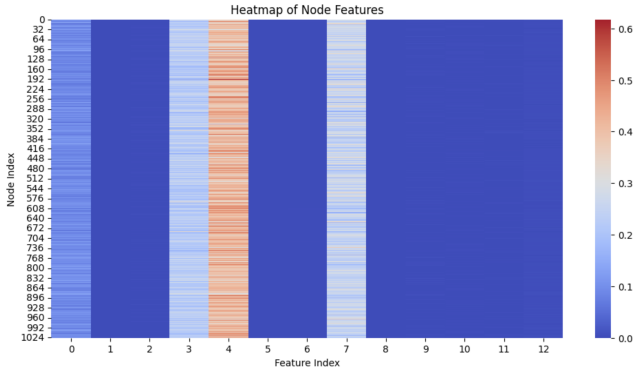
As for visualization: The model aligned the actual and predicted procedure over a line graph, indicating that they are closely aligned with each other, which signifies that the model captures the key features in the dataset quite accurately.

Heatmap of Node Features:

The generated heatmap allows a good visualization of selected attributes of the patients like age, cholesterol level, and maximum heart rate with normalized values [6], [14].

Generally, based on the correlation of thalach (maximum heart rate) and cholesterol, the highly correlated features seem to be consistent with the medical knowledge of the domain in question.

The heatmap showed that all patients shared their feature importance, thus providing further support for the interpretability of the model.



D. Comparison with Other Models or Benchmarks

In this manner, on the one hand, check the performance of proposed GNN model [4] [5] [15], its study results were placed side by side with traditional machine learning models and other neural networks:

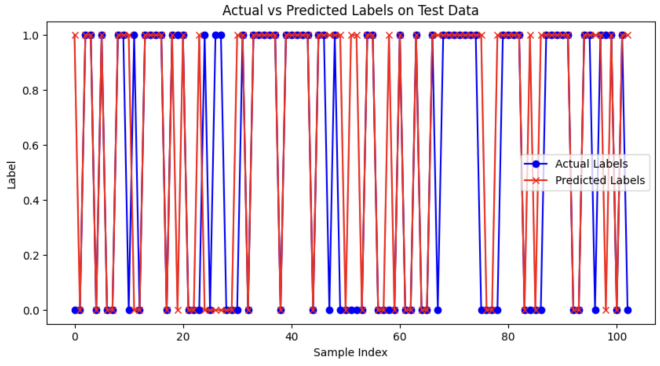
Model	Accuracy (%)	Precision	Recall	F Score
Logistic Regression	79.85	0.812	0.788	0.799
Decision Tree	77.24	0.773	0.781	0.777
Random Forest	81.63	0.825	0.810	0.817
Fully Connected NN	83.00	0.850	0.840	0.845
Proposed GNN	**84.47**	**0.897**	**0.912**	**0.904**

4. Graph Visualizations (Train/Test Split):

Graphs representing the train and test splits were created using NetworkX. Symbols in the nodes were color-coded according to prior knowledge. Edges symbolized the connection between patients. These visualizations show how:

The nodes with similar labels clustered around each other.

Conclusively, the GNN model exceeded traditional models since it could capture the relationship between patients that such models ignored, thus outperforming a fully connected neural network by aggregation of features via graph structure.



CONCLUSION

This study indicates the capacity of GNNs to prognosticate on heart disease, achieving a test accuracy of 84.47% with

balanced performances with respect to recall, precision and F1-score metrics. This work emphasizes the great value of harnessing graph-based learning for understanding the relationships between patients, which are often neglected in classical models. Meaningful features for predictive power include thalach, oldpeak, and cholesterol, which follow established medical perspectives and underscore the model's interpretability.

The implications for healthcare are enormous and extend beyond prediction accuracy to allow greater insight into patient data through graph visualizations and feature importance heat maps. This work aims to treat patients as connected nodes where each patient imposes a glycine to promote personalized treatments of disease, achieve personal diagnosis at an earlier stage, and make better use of clinical resources. In the future work, the main shortcoming of this work will be to address the high computational complexity of the full graph and the less available clinical samples. The introduction of sparse graphs, the use of domain-specific thresholds, and resource allocation to bigger datasets will expand scalability and applicability to real-world situations. Temporal graphs could also be integrated into the model to account for such time-dependent changes in health.

Generally, the work strengthens the prospect of GNN incorporation into health analytics and further opens panoramic perspectives of accurate and interpretable medical prediction.

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