

MORPHOLOGY, PHYSIOLOGY AND PATHOPHYSIOLOGY

COMPARATIVE ANALYSIS OF THE RESULTS OF PREDICTING DIAMETERS OF DAUGHTER SEGMENTS OF CORONARY ARTERY BIFURCATIONS UNDER NORMAL CONDITIONS, OBTAINED USING GRAPH NEURAL NETWORKS AND KNOWN NUMERICAL MODELING METHODS

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ABSTRACT

Background. The accurate determination of human coronary artery (HCA) diameters plays a pivotal role in the diagnosis, risk assessment, and treatment planning of ischemic heart disease. Given that vascular networks possess a fractal structure and consist of arterial bifurcations (AB), a critical task is the prediction of the diameters of daughter (distal) arterial segments (AS) based on the known diameter of the mother (proximal) AS. Existing numerical modeling methods (ENMM) for predicting arterial diameters rely on approximate analytical dependencies derived empirically.

Aim. To conduct a comparative analysis of the results of predicting diameters of daughter segments (bifurcation components) obtained using Graph Neural Networks and known numerical modeling methods based on morphometric data of real healthy human coronary arteries.

Methods. To achieve this objective, various GNN architectures were implemented and tested: GCN, GraphSAGE, GAT, and TransformerConv. Additionally, ENMM and a Multilayer Perceptron (MLP) were evaluated. A comparative statistical analysis of the results was conducted. The study utilized previously obtained morphometric data on the internal diameters of AS comprising 30 corrosion cast graphs of healthy HCAs.

Results. This study proposes the use of GNNs for this specific task for the first time. Comparative analysis demonstrated that all GNN models surpassed both ENMM and the Multilayer Perceptron in accuracy when predicting the diameters of smaller-caliber daughter AS. The TransformerConv architecture demonstrated the best performance, achieving a coefficient of determination $R^2 = 0.96$ and RMSE = 0.199 for predicting the larger daughter segment diameter, and $R^2 = 0.76$ and RMSE = 0.221 for the smaller segment.

Conclusion. The developed models may serve as the foundation for creating clinical decision support systems, enabling more precise assessments of the structural status of human coronary arteries.

Keywords: human heart, coronary arteries, graph neural networks, diameter prediction, arterial bifurcation, medical diagnostics

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СРАВНИТЕЛЬНЫЙ АНАЛИЗ РЕЗУЛЬТАТОВ ПРОГНОЗИРОВАНИЯ ДИАМЕТРОВ ДОЧЕРНИХ СЕГМЕНТОВ БИФУРКАЦИЙ ВЕНЕЧНЫХ АРТЕРИЙ В НОРМЕ, ПОЛУЧЕННЫХ С ИСПОЛЬЗОВАНИЕМ ГРАФОВЫХ НЕЙРОННЫХ СЕТЕЙ И ИЗВЕСТНЫХ МЕТОДОВ ЧИСЛЕННОГО МОДЕЛИРОВАНИЯ

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РЕЗЮМЕ

Обоснование. Точное определение диаметров венечных артерий сердца человека (ВАСЧ) играет ключевую роль в диагностике, оценке рисков и планировании лечения ишемической болезни сердца. Поскольку сосудистые сети имеют фрактальную структуру и состоят из артериальных бифуркаций (АБ), важной задачей является прогнозирование диаметров дочерних (дистальных) артериальных сегментов (АС) на основе известной величины диаметра материнского (проксимального) АС. Известные методы численного моделирования – прогнозирования диаметров артерий используют приближенные аналитические зависимости, полученные эмпирически.

Цель. Провести сравнительный анализ результатов прогнозирования диаметров дочерних сегментов (составных частей бифуркации), полученных с использованием графовых нейронных сетей и известных методов численного моделирования (ИМЧМ), основанных на данных морфометрии реальных венечных артерий сердца человека в норме.

Методы. Для достижения поставленной цели были реализованы и протестированы различные архитектуры GNN: GCN, GraphSAGE, GAT и TransformerConv. А также ИМЧМ и многослойный перцептрон. Проведен сравнительный статистический анализ результатов. Использовали ранее полученные данные морфометрии величин внутренних диаметров АС, составляющих 30 графов коррозионных препаратов ВАСЧ в норме.

Результаты. Впервые предложено использовать GNN для решения данной задачи. Сравнительный анализ результатов показал, что все GNN-модели превосходили по точности ИМЧМ и многослойный перцептрон, в прогнозировании величин диаметров дочерних АС меньшего калибра. Наилучшие результаты продемонстрировала TransformerConv, достигнув коэффициента детерминации $R^2 = 0,96$ и $RMSE = 0,199$ для прогноза большего дочернего диаметра и $R^2 = 0,76$ и $RMSE = 0,221$ — для меньшего.

Заключение. Разработанные модели могут стать основой для создания клинических систем поддержки принятия решений, позволяющих более точно оценивать состояние структуры ВАСЧ.

Ключевые слова: сердце человека, венечные артерии, графовые нейронные сети, прогнозирование диаметров, артериальная бифуркация, медицинская диагностика

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BACKGROUND

The importance of predicting diameters of human coronary arteries (HCA) in modern cardiology is immense. The accurate determination of these parameters is crucial for the diagnosis, prevention, and treatment of ischemic heart disease. This includes the detection of stenosis, assessment of hemodynamic risk, and planning for revascularization procedures.

From a morphological perspective, intraorgan arterial networks can be considered as fractal systems [1, 2]. Their primary structural component is the arterial bifurcation (AB), which consists of a parent (proximal) arterial segment (AS) with diameter D and two daughter (distal) ASs with diameters d_{max} and d_{min} . These daughter segments differ in their internal diameter. Therefore, it is of practical interest to predict the diameter of these daughter segments based on the diameter of the parent segment. To address this challenge, existing numerical modelling methods have been proposed [3, 4]. However, modern machine learning techniques, such as neural networks, have not yet been applied in this field.

The vascular network structure can be represented as a graph, specifically a binary tree. A specialized class of algorithms, Graph Neural Networks (GNNs), has been developed to process data with this structure [5]. Typical GNN applications include classification and link prediction, but this study proposes using GNNs for regression, specifically predicting the diameter of daughter ASs based on the parent AS diameter.

AIM

To conduct a comparative analysis of the results of predicting diameters of daughter segments (bifurcation components) obtained using graph neural networks and known numerical modeling methods based on morphometric data from real healthy human coronary arteries.

METHODS

Study Design. The study was based on the results of a morphometric analysis of 30 human coronary arteries, obtained through corrosion casting [6]. The initial data were provided in Excel format. From the entire set of features, the following variables were selected for model training and validation: parent AS diameter (D , mm); sex (1 – male, 2 – female); age group (1 – second period of mature age (males 36–60 years, females 36–55 years); 2 – elderly age (males 61–75 years, females 56–75 years) (Classification of the Academy of Medical Sciences of the USSR, 1965); and branching level – the newly formed AB series, ranging from 1 to 20. The target variables to be predicted were the diameters of the two daughter ASs: d_{max} (mm) – diameter of the larger AS, and d_{min} (mm) – diameter of the smaller AS. The sample

size included 30 specimens, each containing more than 100 measured ASs. The data were structured as 30 graphs. Branching level and all diameter values were considered as numerical variables, whereas sex and age were considered categorical. A preliminary statistical analysis using the Pandas and NumPy libraries revealed that the distribution of AS diameters deviated from normal and contained outliers.

Data Preprocessing and Graph Construction. The PyTorch Geometric (PyG) framework was used to implement GNNs [7]. Tabular data from Excel were preprocessed using the Pandas library and converted to PyTorch tensors. Anatomical connections (for constructing the graph data structure) between ASs were determined using the NetworkX library [8]. To avoid data leakage, the split into training and test sets was performed at the level of entire HCA trees (graphs). The training set consisted of 22 HCA trees (graphs) (73 %), and the test set contained 8 (27 %). This approach ensures that the model does not use information about the structure of trees (graphs) from the test set during training. Training data were normalized using RobustScaler from the scikit-learn library [9], which is robust to outliers. Normalization parameters were saved for subsequent application to test data and during inference.

GNN Architectures. Four key GNN architectures were implemented: GCN (Graph Convolutional Network), GraphSAGE (Sample and Aggregate), GAT (Graph Attention Network), and TransformerConv (Graph Transformer). To compare the effectiveness of the GNN approach, a Multilayer Perceptron (MLP) trained on the same input features but without considering the graph structure, as well as the results of ENMM, were also used.

Hardware and Training Process. All experiments were conducted using a PC with Windows 11 and WSL2 subsystem and Ubuntu 24.04 distribution. Hardware configuration: Intel Core i7-14700KF processor, 64 GB RAM, Nvidia GPU with 32 GB video memory. Library versions used: PyTorch 2.7.0+cu128 and PyTorch Geometric 2.6.1. The AdamW optimizer [10] with L2 regularization (weight decay) was used to train the models to prevent overfitting; the Huber loss function [11] was employed, which combines the advantages of MSE (for small errors) and MAE (for large errors), making it robust to outliers. Dropout technique and early stopping (with no improvement in loss for 50 epochs) were used for regularization. Automated hyperparameter search was performed using the Optuna library [12] over 200 trials. All experiments were logged in the MLflow environment.

ENMM – Baseline Models for Comparison. To verify the results of neural network predictions, ENMM were used [3, 4]. The model based on [3] utilizes the relationship between the parent AS diameter (D), the larger and smaller daughter AS diameters (d_{max} and d_{min}), and the asymmetry ratio (*ratio*):

$$D^{\frac{7}{3}} = d_{max}^{\frac{7}{3}} + d_{min}^{\frac{7}{3}} \quad (1)$$

where D is the parent AS diameter, d_{max} is the diameter of the larger daughter AS, and d_{min} is the diameter of the smaller daughter AS. The authors also express branching asymmetry as the ratio of daughter diameters:

$$ratio = \frac{d_{min}}{d_{max}}. \quad (2)$$

From (1) and (2), the diameters of the daughter ASs can be calculated:

$$d_{max} = D \cdot \left(\frac{1}{1+ratio^{\frac{7}{3}}} \right)^{\frac{3}{7}}, \quad (3)$$

$$d_{min} = ratio \cdot d_{max}. \quad (4)$$

where $ratio=0.625$

The model based on [4] relates the diameters of the daughter ASs (d_{max} and d_{min}) to the parent AS diameter (D) and the asymmetry parameters (α, β):

$$d_{max} = \alpha D, \quad d_{min} = \beta D. \quad (5)$$

where $\alpha \approx 0.9, \beta \approx 0.6$.

Comparative analysis of the modeling results. Two metrics were used to assess prediction accuracy: R^2 (coefficient of determination) and RMSE (root mean square error). Prediction quality was evaluated on the test set using the coefficient of determination (R^2). This metric determines what proportion of the variance in the dependent variable is explained by the regression model. The coefficient of determination (R^2) was calculated using the formula presented below:

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (6),$$

where y_i is the actual value, $\hat{y}_i$ is the model prediction, $\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$ is the mean value, and n is the number of samples in the test set. The closer R^2 is to 1, the better the model performance. A negative value indicates that the model performs worse than simply predicting the mean value. The Root Mean Squared Error (RMSE) was also used as a metric – a standard error measure in regression tasks. It preserves the same units as the original data (mm), making it convenient for interpretation:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (7).$$

The closer the RMSE is to 0, the better. Five state-of-the-art GNN architectures were compared, along with two classical analytical models from the scientific literature.

RESULTS

Preliminary analysis of the results (Table 1) shows that predicting d_{min} is significantly more challenging than predicting d_{max} . The calculated R^2 and RMSE values for various MLP and GNN architectures, as well as for the numerical modeling methods described in the literature [3, 4], indicate that for all models except TransformerConv, the R^2 value for the smaller daughter AS is substantially lower, while the RMSE is higher. This is logical, as the diameter of the smaller daughter AS may be more strongly influenced by hemodynamic and topological factors.

The results of predicting two key parameters of HCA ASs are presented: d_{max} is the diameter of the larger daughter AS of the AB, and d_{min} is the diameter of the smaller daughter AS of the AB. The Multilayer Perceptron (MLP) demonstrates satisfactory results, particularly for predicting d_{max} . This performance is notably better than that of GCN and GraphSAGE, suggesting that even without explicitly accounting for the graph structure, the network is able to capture the underlying patterns.

However, its inferiority to the best GNN models confirms the importance of considering structural connections. The results obtained using GCN and GraphSAGE showed moderate, rather modest results for d_{max} . Their simple mechanisms for aggregating information from neighboring nodes seem insufficient for accurately modeling the HCA structure. It should be noted that GraphSAGE performs slightly better at predicting d_{min} than MLP and GCN architectures.

GAT (Graph Attention Network) demonstrates selectivity. For d_{max} it ranks second in accuracy after TransformerConv ($R^2 = 0.71$), while for d_{min} it shows the highest RMSE among the networks studied. It is possible that the attention mechanism of GAT helps to identify key “parent” features for the larger daughter AS (d_{max}), but proves less effective for the smaller AS (d_{min}).

TransformerConv demonstrates exceptional accuracy for both parameters: R^2 values close to ideal (0.95 and 0.76), and RMSE values minimal (0.199 mm and 0.221 mm). This indicates that the attention mechanism underlying this GNN architecture is ideally suited for capturing complex, non-local dependencies in HCA structure. All GNN architectures showed positive and significant R^2 values. The numerical modeling methods [3, 4], based on physical principles, showed unsatisfactory or even extremely poor results, particularly for ($R^2 = -0.79$ and -0.51). This indicates that real HCA bifurcations are more complex than

TABLE 1

R² AND RMSE VALUES FOR VARIOUS MLP AND GNN ARCHITECTURES, AS WELL AS ENMM, DESCRIBED IN THE LITERATURE

Model	Prediction results			
	d_{max}		d_{min}	
	R^2	RMSE (mm)	R^2	RMSE (mm)
MLP	0.59	0.566	0.37	0.359
GCN	0.51	0.625	0.37	0.359
GraphSAGE	0.53	0.612	0.43	0.341
GAT	0.71	0.479	0.28	0.385
TransformerConv	0.95	0.199	0.76	0.221
Model by Olufsen M.S. et al. [12]	0.42	0.675	-0.79	0.609
Model by Huo Y. & Kassab G. [3]	0.46	0.653	-0.51	0.559

Note. d_{max} – diameter of the larger daughter arterial segment (AS); d_{min} – diameter of the smaller daughter AS; R^2 – coefficient of determination; RMSE – root mean square error; MLP – Multilayer Perceptron; GCN (Graph Convolutional Network) – graph convolutional network; GraphSAGE (Sample and Aggregate) – graph sampling and aggregation network; GAT (Graph Attention Network) – graph attention network; TransformerConv (Graph Transformer) – graph transformer.

described by the analytical laws traditionally used for this purpose.

DISCUSSION

Unlike traditional neural networks designed for processing isolated objects such as tables or images, GNNs operate on structured systems composed of interconnected graph nodes. These networks extract information not only from the individual components (nodes), but also from the topology (connections) between them (edges). The operating principle of GNNs is based on the message-passing mechanism. Each node collects features from its nearest neighbors. The collected messages are then aggregated using a permutation-invariant function (e.g., sum, mean, max). The aggregated information is then combined with the node's current features to update its state. This multi-layer architecture allows nodes to incorporate information from nodes that are increasingly distant from it.

In this study, key GNN architectures were implemented. GCN (Graph Convolutional Network) [5] aggregates the features of neighboring nodes, taking into account the degree (number of connections). This architecture is highly efficient, but it does not differentiate between the importance of each neighbor. GraphSAGE (Sample and Aggregate) [13] uses fixed-size sampling method instead of considering all neighbors, making it scalable for large graphs. GAT (Graph Attention Network) [14] assigns a weighting coefficient to each neighboring node, determining its relevance to the central node using an attention mechanism. TransformerConv (Graph Transformer) [15] employs an advanced attention mechanism inspired by the transformer architecture [16], allowing it to capture more complex global dependencies in the graph. Its superiority is explained by global attention. Unlike GAT, which

only looks at nearest neighbors, the transformer can evaluate the importance of any node in the graph. This allows the model to take into account the complex influence of remote regions of the vascular network on the local AB geometry, resulting in high accuracy.

A comparison of model performance has established a clear correlation between modeling outcomes and AS diameter. Numerical modeling techniques [3, 4] exhibit limited accuracy in forecasting the parameter for ASs with greater diameters. This suggests that the models establish an explicit link between the daughter AS diameter and the parent AS diameter. At the same time, all neural network architectures show clear superiority over numerical modeling methods [3, 4].

For smaller-diameter daughter ASs, this trend continues: all investigated neural networks outperform numerical modeling methods. This advantage is explained by the ability of neural networks to identify complex, non-obvious connections between the values of studied parameters, while numerical modeling methods [3, 4], based on simplified mathematical formulations, does not account for the individual phenotypic characteristics of HCAs.

For smaller-diameter daughter ASs, the situation is similar: all investigated neural networks outperform numerical modeling methods. This advantage is explained by the ability of neural networks to identify complex and non-obvious relationships between the values of the studied parameters, whereas numerical modeling methods [3, 4], based on simplified mathematical representations, do not take into account the individual phenotypic characteristics of HCAs.

Interestingly, despite the natural structure of blood flow, only one graph network, the transformer (TransformerConv), was able to extract sufficient information from this structure to exceed the 70 % R^2 threshold for predicting the diameter of the smaller daughter AS.

This achievement is due to the attention mechanism, which takes into account both local and global connections within the HCA network. Analysis of the prediction results of the numerical modeling methods [3, 4] shows that they perform poorly in predicting d_{min} , with a negative R^2 indicating that their predictions are not only inaccurate, but also systematically biased. This raises questions about the universality of underlying physical principles, such as minimum energy or shear stress laws. Their relatively better performance (though still poor) in predicting d_{max} may indicate that the larger daughter AS diameter may follow some generally accepted empirical rules.

The significant superiority of neural network models, especially graph neural networks, compared to numerical modeling methods in predicting the diameters of smaller daughter ASs confirms their potential for addressing theoretical and practical (clinical) biomedical challenges. The high R^2 values for all models studied in the context of the larger daughter AS indicates a strong correlation between the diameters of this daughter branch and the parent AS, which is also confirmed by the high accuracy of hydrodynamic models.

CONCLUSION

Neural network models have shown promising results in predicting the diameters of daughter arterial segments within coronary artery bifurcations. This indicates the potential of the proposed approach. GNNs, especially TransformerConv, are a powerful tool for predicting bifurcation geometry and significantly outperform conventional numerical modeling methods. However, these models should not be applied to predict the diameter of the smaller daughter AS (d_{min}) in the studied dataset as their use may lead to significant errors. The prediction of d_{min} is a more challenging task that requires the use of advanced architectures such as TransformerConv or the development of novel specialized approaches.

The primary limitation of this research is the relatively small size of the training dataset, which has a negative impact on prediction accuracy. In order to enhance model performance, it would be beneficial to enlarge and refine the training data set, minimizing the occurrence of outliers.

For practical applications, such as medical modeling or surgical planning, graph transformers (TransformerConv) are recommended, as they demonstrate maximum accuracy and reliability.

Researchers in the field of hemodynamics are advised to reconsider or significantly supplement the existing branching laws based on data collected through machine learning methods. Further research in this area should focus on expanding model functionality by simultaneously predicting not only the diameters but also the lengths of daughter ASs and bifurcation angles. This would significantly improve the accuracy of HCA models and greatly enhance their potential for widespread use in theoretical and practical medical applications.

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Conflicts of interest

The authors declare no conflicts of interest.

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