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Graph Neural Network Graph Embedding Optimization Method for Vascular Stress Prediction

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Abstract: This study focuses on the accurate prediction of vascular stress by using graph neural network, and innovatively proposes a graph embedding method adapted to vascular structure. By comparing with the traditional finite element vertex diagram representation, and deeply analyzing various key factors affecting vascular stress, the efficiency and accuracy of this method are fully verified, which provides potential technical support for vascular mechanics research and related disease diagnosis. In biomedical engineering, vascular stress analysis is very important for the diagnosis and treatment of cardiovascular diseases. Although the traditional finite element analysis is accurate, it has high calculation cost and poor adaptability in the face of complex vascular geometry, material nonlinearity and diverse loads. In this study, an innovative vascular graph embedding method is proposed, and different segments of blood vessels are regarded as vertices to build models, which effectively reduces complexity. GraphSAGE algorithm is used to predict stress, and compared with the traditional finite element vertex graph representation, research is carried out. Comprehensively consider the geometric changes of blood vessels, curvature, uneven pipe diameter and branch structure; Simulating the nonlinearity of materials under physiological and pathological conditions; Set boundary conditions such as vascular end fixation, elastic support and freedom; Covers uniform, concentrated and dynamic blood flow loads. Experiments show that the new method has obvious advantages, the memory occupation of GPU is reduced to about 2%, and the training time is reduced to 4%. Its GraphSAGE model is accurate in stress prediction, and the average accuracy of the maximum von Mises stress is 92.3%. This achievement shows the potential of graph neural network and new graph embedding method in vascular stress analysis, which can provide key support for the research and treatment of vascular diseases and strongly promote the development of biomechanics and medical engineering.

Keywords: Graph Neural Network; Prediction of Vascular Stress; Graph Embedding; Reduced Order Model.

1. Introduction

Blood vessels play a core role in human physiological functions, and their mechanical properties are closely related to the occurrence and development of cardiovascular diseases. Accurate prediction of vascular stress distribution is of great significance for deeply understanding the physiological and pathological process of blood vessels and optimizing the diagnosis and treatment strategy of cardiovascular diseases. Finite element analysis, the traditional method of vascular stress analysis, can provide accurate results, but when dealing with complex vascular models and large-scale data, it faces difficulties such as soaring calculation cost and low calculation efficiency. With the rapid development of machine learning technology, especially graph neural network, it is possible to construct an efficient reduced-order model for vascular stress prediction, which is also the core goal of this study.

2. The Graph Neural Network Foundation

2.1. Figure Neural Network Principle

Graph neural network, as a neural network architecture specialized in processing graph structure data, is essentially different from convolutional neural network commonly used in regular grid data processing. In the framework of graph neural network, graph is defined as G= (V, E, A), where v is a set of vertices, representing the key structural units or characteristic points of blood vessels; E is an edge set connecting vertices, which reflects the relationship between structural units; A is the adjacency matrix, which is used to accurately describe the topological structure of the graph. For vertices vi and vj, edge eij=(vi, vj) indicates the connection relationship between them. In an undirected graph, eij is equivalent to eji and Aij=Aji. At the same time, each vertex is accompanied by an input feature RN×D, where d is the input feature dimension of each vertex, covering key information such as vascular wall thickness, elastic modulus and vascular radius.[1]

2.2. Graph Volume Product Operation Mechanism

In the aspect of graph convolution operation, there are two main types: graph method and graph space method. The atlas method constructs the graph volume product with the help of the eigenvalues and eigenvectors of Laplacian matrix, such as Spectral CNN and Chebyshev Spectral CNN, etc. However, when dealing with large-scale graph data, the memory overhead of this method is too large, which limits its application scope. Graph space method realizes convolution operation, original graph neural network, graph sampling and aggregation, graph isomorphism network and so on based on the spatial proximity relationship between vertices and their adjacent vertices. GraphSAGE network is selected in this study, which follows the framework of message-passing neural network and iteratively optimizes vertex features through three closely connected stages: aggregation, propagation and update. Specifically, in the aggregation stage, vertices use differentiable and permutation invariant functions to collect information from neighboring vertices; In the propagation stage, the aggregated information is organically integrated with the inherent characteristics of vertices to generate a brand-new feature representation; In the updating stage, the vertex embedding is updated with the help of differentiable functions. σ Update vertex embedding. [2] In this study, "sum" is selected as the aggregation function, and the corresponding GraphSAGE operator is defined as, where hvl-1 and hlv represent the embedding of vertex V in l-1 layer and L layer respectively, Wl is the trainable parameter of the current layer, message propagation is realized by vector splicing, and message update adopts tanh activation function.

$h_v^l = \sigma\left(W^l\left(h_v^{l-1} + sum_{u\in N(v)} h_u^{l-1}\right)\right)$, among h σ 。

2.3. Loss Function and Superparameter Setting

In this study, the mean square error is used as the loss function, and its expression is, where n is the total number of data points, and yi and Yi respectively represent the true value and predicted value of the ith data point. Through the quasi-random search strategy, the hyperparameters of the model are finely adjusted, and the number of hidden layers is determined to be 32, the number of hidden neurons in each layer is 64, the activation function is tanh, the optimizer is Adam, the learning rate is set to 0.02, the batch size is 512, and the L2 regularization factor is le-4, and these hyperparameters are kept constant throughout the study.

$MSE = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{y}_i\right)^2$, among n Total number of data points, y $\hat{y}_i$ Respectively representing the true value and the predicted value of the ith data point. Through the quasi-random search strategy, the super parameters of the model are finely adjusted, and the number of hidden layers is determined to be 32, the number of hidden neurons in each layer is 64, the activation function is tanh, the optimizer is Adam, the learning rate is set to 0.02, the batch size is 512, and the L2 regularization factor is.

3. The Graph Embedding Method of Blood Vessels

3.1. Disadvantages of Traditional Finite Element Vertex Graph Representation

The traditional finite element vertex graph represents that in vascular modeling, each finite element is mapped to a vertex, and the connections between elements correspond to edges. However, with the refinement of the vascular model, the scale of the graph will expand rapidly. Theoretically, it is assumed that the GNN architecture is fixed (the depth is L, and the embedding size of the I-layer converted graph is Fi), and the average neighbor number k of vertices in graphs of different scales is roughly the same, and the time complexity of feature transformation and aggregation operations occupies a dominant position in the overall computational complexity. At this time, the time complexity of feature transformation is, the time complexity of aggregation operation is, and the total training complexity can be obtained by combining the two, which is further simplified as. It can be seen that the training time complexity is linearly and positively correlated with the number of vertices n of the graph, which will inevitably lead to an exponential increase in the demand for computing resources, which seriously limits its feasibility in practical applications.

$O\left(N\times\sum_{i=1}^{L}F_{i-1}\times F_i\right)$ The time complexity of aggregation operation is $O\left(N\times k\times\sum_{i=1}^{L}F_i\right)$ Combining them, the total training complexity is $O\left(N\times\sum_{i=1}^{L}F_{i-1}\times F_i\right)+O\left(N\times k\times\sum_{i=1}^{L}F_i\right)$ $O\left(N\times\left(C_1+C_2\right)\right)$ .It can be seen that the training time complexity is linearly and positively correlated with the number of vertices n of the graph, which will inevitably lead to an exponential increase in the demand for computing resources, which seriously limits its feasibility in practical applications.

3.2. The Embedding Method of Vascular Map Proposed in this Paper

In order to overcome the limitations of traditional methods, this study proposes a brand-new strategy for embedding vascular maps. The blood vessels are divided into several key structural units, and the branch points of blood vessels and the connection points of different elastic modulus areas are the vertices in the diagram. Each vertex not only contains its own geometric information, including the length, diameter and wall thickness of the local vascular segment, but also includes biomechanical information, elastic coefficient, Poisson's ratio, hemodynamic information, local blood flow velocity and pressure. In this way, compared with the traditional method, the number of vertices is effectively reduced and the complexity of the graph is greatly reduced. In the process of graph construction, the connection relations between structural units are accurately encoded by adjacency matrix, but these connection relations are not directly reflected in the input embedding of vertices, thus further optimizing the efficiency of data storage and calculation. For stress prediction, the detailed structure and mechanical information of blood vessels are obtained by means of high-precision medical imaging technology and computational fluid dynamics simulation, and the advanced data processing algorithm is used to convert it into unified input data to meet the input requirements of GNN model and ensure that the model can accurately learn the stress distribution law of blood vessels.

4. Data Preparation

4.1. Parameter Setting of Vascular Models

In this study, the common blood vessels in human body, such as coronary artery and carotid artery, are selected as the research objects. The length of blood vessels is set according to the actual physiological situation, with the diameter ranging from 2 to 10 mm and the thickness of blood vessel wall fluctuating from 0.1 to 1 mm. Considering the changes of blood vessels in different physiological States, the elastic modulus is set between 0.1 and 10 MPa, and Poisson's ratio is between 0.4 and 0.5. At the same time, in order to simulate the real vascular environment, different degrees of vascular stenosis are introduced, among which the degree of stenosis is between 0-70%, the blood vessel is curved, the bending radius is between 5-50mm, the blood flow velocity changes, and the flow velocity is between 0.1-1m/s, which comprehensively covers the physiological and pathological characteristics of blood vessels.

4.2. Experimental Case Design

In order to explore the influence of various factors on vascular stress prediction, a series of experimental cases were designed:

A case study on the change of vascular geometric characteristics

Focus on the influence of vascular diameter change, keep other parameters, including vascular wall thickness, elastic modulus and blood flow velocity constant, gradually change the vascular diameter, and construct multiple data sets, each of which corresponds to a different diameter size, so as to analyze the internal relationship between vascular diameter change and stress distribution.

Focus on the study of the influence of blood vessel bending degree, fix other geometric and physical parameters of blood vessels, generate blood vessel model data sets with different bending degrees by adjusting the bending radius and bending angle of blood vessels, and then investigate the mechanism of bending on blood vessel stress.

Case of material property change

This paper discusses the influence of the change of vascular elastic modulus, changes the elastic modulus of vascular wall under the premise of other conditions unchanged, simulates the change of vascular elasticity under different physiological and pathological conditions, and studies the correlation between elastic modulus and vascular stress distribution in the process of vascular hardening or softening.

Analyze the influence of the change of blood vessel wall thickness, keep the diameter, elastic modulus and other parameters of blood vessel stable, change the blood vessel wall thickness, and construct the corresponding data set to reveal the role of blood vessel wall thickness in stress distribution.

Cases of hemodynamic factors

Investigate the influence of blood flow velocity change, keep the vascular structure and material characteristics unchanged, set different blood flow velocity scenes, generate data sets, and study the dynamic relationship between blood flow velocity and vascular stress, as well as the difference of the influence of high-speed blood flow or low-speed blood flow on vascular wall stress.

To study the comprehensive influence of vascular stenosis on hemodynamics and stress distribution, introduce stenosis lesions of different degrees and positions into blood vessels, and combine with the change of blood flow velocity to construct a complex data set to analyze the influence mechanism of blood flow disorder caused by stenosis on vascular wall stress.

Comprehensive case

A comprehensive model evaluation is carried out, taking into account the changes of geometric characteristics, material characteristics and hemodynamic factors of blood vessels at the same time, and constructing a highly complex data set to simulate the complex state of real blood vessels in the physiological and pathological process, so as to test the prediction ability and stability of the model in complex environment.

For each experimental case, an independent data set is carefully prepared and scientifically divided according to the proportion of 80% for training, 10% for verification and 10% for testing. The data set is generated with the help of advanced medical image processing software, computational fluid dynamics simulation software and biomechanical modeling tools, and the accuracy and reliability of the data are ensured through multi-modal data fusion and parametric modeling technology. In the process of data processing, the original data are strictly normalized and standardized to meet the input requirements of GNN model. At the same time, data enhancement technology is used to expand the data set and improve the generalization ability of the model. The training of GNN model is carried out efficiently on a computing platform equipped with high-performance GPU, using Python programming language and deep learning framework.

5. Results and Discussion

5.1. Impact of Graph Representation on GNN Computing Resources

Through a typical simplified blood vessel model test case, the embedding method of blood vessel diagram proposed in this study is compared with the traditional finite element vertex diagram representation. The experimental results show that the two methods have similar performance in predicting vascular stress distribution, but there is a world of difference in computing resource consumption. Under the same GraphSAGE architecture, hyperparameter setting and data set conditions, this research method only needs 0.3s to train each epoch, while the traditional finite element vertex graph representation takes up to 8s, which is about 27 times that of this research method. In terms of GPU memory occupation, this research method only needs 0.6GB when processing data of the same size, while the traditional method is as high as 25GB. This fully proves that the graph embedding method proposed in this study significantly improves the training efficiency and greatly reduces the dependence on computing resources, which makes it possible to realize large-scale vascular stress prediction on ordinary computing equipment and effectively expands the application scope of this technology.

5.2. Prediction Results of Vascular Stress Under Different Factors

Influence of geometric characteristics of blood vessels

According to the change of blood vessel diameter, the GraphSAGE model using the graph embedding method in this study can accurately capture the change of stress distribution caused by the change of diameter. When the diameter of blood vessel increases from 4mm to 6mm, the model accurately predicts the distribution of stress in the circumferential and axial directions, and the prediction error in the high stress area of blood vessel inner wall is controlled within 5%, which is highly consistent with the actual physical law.

The model also performs well in the case of vascular curvature. Taking a curved branch of coronary artery as an example, when the bending radius is reduced from 20mm to 10mm, the model successfully predicts that the stress on the lateral vascular wall at the bending part increases significantly and the stress on the medial side decreases, and the stress change trend is consistent with the results of clinical research and theoretical analysis, and the prediction accuracy is over 95%.

Influence of material characteristic factors

GraphSAGE model effectively reflects the relationship between elastic modulus and stress when studying the changes of elastic modulus of blood vessels. When the elastic modulus increases from 2MPa to 8MPa in the process of simulating vascular sclerosis, the model predicts that the stress of vascular wall will increase obviously under the same blood pressure, and the average error of stress prediction under different elastic modulus is about 6%.

For the change of vascular wall thickness, the model can also accurately predict its influence on stress. When the thickness of carotid artery wall increases from 0.5mm to 0.8mm, the model correctly predicts that the stress of vascular wall decreases accordingly, especially in the high stress concentration area, the prediction results are highly consistent with the actual situation, and the prediction accuracy is over 94%.

Influence of hemodynamic factors

When investigating the influence of blood flow velocity change, the model clearly shows the dynamic correlation between blood flow velocity and vascular stress. When the blood flow velocity increases from 0.3m/s to 0.8m/s, the model accurately predicts the increasing trend of shear stress and circumferential stress of blood vessel wall, and the stress prediction error at different flow velocities is controlled within 8% [3]

In view of vascular stenosis, the model successfully captures the complex changes of stress in the stenosis site and its upstream and downstream vascular walls. If the coronary artery is stenotic, when the degree of stenosis reaches 50%, the model accurately predicts that the stress on the upstream blood vessel wall of the stenosis increases, while the stress on the downstream blood vessel wall decreases and complex eddy stress distribution appears, which is highly consistent with the hemodynamic theory and clinical observation results, and the prediction accuracy is over 92%.

Comprehensive factor influence

Considering various factors comprehensively, although the vascular model is extremely complex, the GraphSAGE model can still maintain a high prediction accuracy. In the complex scene of simulating coronary atherosclerosis with vascular curvature and blood flow velocity changes, the prediction results of the model for stress distribution in vascular wall are in good agreement with the actual situation, and the prediction errors in high stress areas and areas with large stress gradient are controlled within 10%, which shows that the model has strong reliability and stability in dealing with complex vascular physiological and pathological conditions.

5.3. Analysis and Discussion of Results

Through the in-depth analysis of the above experimental results, it can be seen that the embedding method of vascular graph based on graph neural network proposed in this study has obvious advantages in dealing with the problem of vascular stress prediction. Compared with the high consumption of traditional methods, the high efficiency of this method provides the possibility for the rapid analysis of large-scale vascular models, which is helpful to promote the rapid transformation of vascular mechanics research from theory to clinical practice. In terms of prediction accuracy, the model can accurately capture the variation law of vascular stress whether it is a single factor change or a combination of multiple factors, which is due to its unique graph embedding design, which can effectively integrate multi-source information such as geometry, material and hemodynamics of blood vessels, so that the model can learn more comprehensive and in-depth representation of vascular mechanical characteristics. However, the study also found that the model still has some room for improvement in dealing with extremely complex vascular diseases and stress prediction under rare physiological conditions. The prediction error will increase slightly when simulating the rare cases of severe stenosis of multiple vessels with sharp changes in vascular wall elasticity. Future research can further optimize the graph embedding method, introduce more complex network structure or multi-modal data fusion strategy, enhance the adaptability and generalization ability of the model to extreme situations, and combine more clinical data for training and verification to improve the application value of the model in actual clinical diagnosis and treatment decision.

6. Conclusion and Prospect

In this study, an efficient graph embedding method for vascular stress prediction based on graph neural network is successfully proposed. Through the comparative experiment with the traditional finite element vertex graph representation and the comprehensive analysis of various vascular related factors, the excellent performance of this method in calculation efficiency and prediction accuracy is fully verified. Compared with the traditional method, the calculation resource consumption is greatly reduced, which provides technical support for the wide application of vascular stress analysis in clinical and scientific research. In terms of prediction accuracy, the prediction of stress distribution under different vascular conditions is highly consistent with the actual situation, which provides a powerful tool support for the pathogenesis research, early diagnosis and personalized treatment of cardiovascular diseases. Future research can be further expanded in the following directions, further optimizing the graph neural network architecture and graph embedding algorithm, exploring the model design more suitable for the complex structure and physiological and pathological characteristics of blood vessels, and improving the prediction accuracy and generalization ability of the model; Strengthen the deep integration with clinical image data and biomechanical experimental data, realize real-time prediction and dynamic monitoring of vascular stress based on real patient data, and promote the development of precision medical care for cardiovascular diseases; Expand the application field, and apply this method to the simulation of vascular interventional therapy and the optimization of artificial blood vessel design, so as to contribute to the innovative development of cardiovascular medical engineering.

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