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Research on Traditional Chinese Medicine Prescription Recommendation Method Based on Multi-Graph Convolutional Neural Networks

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Abstract: *To improve the recommendation performance of Traditional Chinese Medicine (TCM) prescriptions, a recommendation method based on multi-graph convolutional neural networks is proposed. First, the relationships between herbs and symptoms are represented by constructing homogeneous and heterogeneous graphs. Then, information from high-order neighboring nodes is recursively propagated to update the representation of each node. Finally, the syndrome representation of the patient is obtained through feature fusion and induction, which is used to recommend appropriate TCM prescriptions. Experimental results show that the recommendation method based on multi-graph convolutional neural networks significantly outperforms topic recommendation models and the general neural network models in terms of precision and recall.*

Keywords: *Graph Convolutional Neural Network; TCM prescriptions; Recommendation model; Heterogeneous graph*

1. Introduction

TCM has played an important role in China's healthcare sector for thousands of years [1]. It represents the accumulated experience and theoretical summary of the Chinese people's fight against diseases. TCM typically prescribes prescriptions composed of several herbs based on the patient's symptoms, such as "stomach pain," "feverish head," or "dry vomiting." With the development of information technology, data mining and artificial intelligence technologies have gradually been applied to the field of TCM [2].Traditional recommendation techniques typically rely on the interaction relationships between users and items to recommend other items that users might be interested in. When applied to the field of TCM prescriptions, these techniques can leverage large amounts of historical interaction data between symptoms and herbs to recommend appropriate herbs for patients' treatment. This approach not only assists TCM practitioners in formulating accurate treatment plans but also contributes to the inheritance and development of TCM.

This paper proposes a multi-graph convolutional neural network model (MGCN). The main contributions of this work are as follows: First, a herb-herb homogeneous graph and a herb-symptom heterogeneous graph are constructed based on a large volume of records linking symptoms to TCM prescriptions. Traditional recommendation techniques generally rely solely on heterogeneous graphs, as in reference [3]. However, in the context of TCM prescription recommendations, relying only on heterogeneous graphs overlooks the synergistic effects of hreb combinations. Second, high-order propagation: When applying graph convolutional neural networks to update node representations [4], the model not only aggregates information from directly adjacent nodes but also incorporates information propagated from the neighbors of these adjacent nodes. Third, feature induction: A multilayer perceptron (MLP) is applied to better inductively represent patient symptoms, thereby improving the accuracy of TCM prescription recommendations.

2. MGCN

2.1. Multi-graph Construction Layer

The multi-graph construction layer represents the relationships between herbs and symptoms by

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constructing a herb-herb homogeneous graph and a herb-symptom heterogeneous graph [5] from a TCM prescription $P=\{S,H\}$, where $S=\{s_1,s_2,...,s_n\}$ is the set of symptoms and $H=\{h_1,h_2,...,h_m\}$ is the set of herbs.

First, the construction of the herb-herb homogeneous graph: Generally, TCM prescriptions consist of several herbs. The synergistic relationships between herbs can be reflected by their co-occurrence frequency in prescriptions. When the frequency is greater than or equal to α, an edge is created between the two herb nodes, and the corresponding entry in the interaction matrix is set to 1; otherwise, it is set to 0. We define the construction expression as:

$$HH_{i,j}, HH_{j,i} = \begin{cases} 1, \text{the frequency of cooccurrence of i and j is greater than that of } \alpha \\ 0, \text{otherwie} \end{cases} \tag{1}$$

where $HH \in \mathbb{R}^{m\times m}$ represents the herb-herb interaction matrix, and α denotes the threshold.

Second, the construction of the herb-symptom heterogeneous graph: herbs and symptoms in the same prescription are correlated. Thus, an edge is created between the herb node and the symptom node, with the corresponding matrix entry set to 1; otherwise, it is set to 0. The construction expression is given as follows:

$$HS_{i,l}, HS_{l,i} = \begin{cases} 1, \text{i and j cooccur in the same prescription} \\ 0, \text{otherwise} \end{cases} \tag{2}$$

where $HS \in \mathbb{R}^{n\times m}$ represents the herb-herb interaction matrix.

2.2. Propagation Layer

The full text of the article must be typeset in single column. The information propagation layer is designed to recursively propagate information from high-order neighboring nodes to update the representations of each node in the homogeneous and heterogeneous graphs.

Taking the herb-symptom heterogeneous graph as an example: First, the information from several nodes directly connected to the central node needs to be propagated to the central node. The information of the directly adjacent nodes is represented as follows:

$$m_r = e_i \cdot w_i \tag{3}$$

where e_i is the initial representation of the node, and $e_i \in \mathbb{R}^{1\times d}$, where d represents the initialization dimension; $w_i \in \mathbb{R}^{d\times d_l}$ is weight matrix.

After the central node receives information from all directly adjacent nodes, an averaging operation is applied to aggregate all the information. We define the aggregation function as:

$$m_{N_r} = \tanh\left(\frac{1}{|N_r|}\sum_{i\in N_r} m_i\right) \tag{4}$$

After obtaining the aggregated information from all directly adjacent nodes, the information of the central node itself can be updated. Here, a GCN aggregator is used, which first sums the central node's information and the aggregated information, followed by a nonlinear activation. The updated representation of the central node is formulated as:

$$m_{HS} = \text{Leaky ReLU}(W(e_i + m_{N_r})) \tag{5}$$

where $e_i + m_{N_r}$ denotes the sum of two vectors, W denotes the weight matrix, and Leaky ReLU denotes the activation function.

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After obtaining the information propagated from directly adjacent nodes, it is possible to further acquire the information propagated from high-order nodes to the central node. Assuming the information propagates through k layers in total, the aggregated information is recursively formulated as:

$$m_{N_r}^{k-1} = \tanh\left(\frac{1}{|N_r|}\sum_{i\in N_r} e_i^{k-1} \bullet w_i^k\right) \tag{6}$$

where w_i^k represents the weight matrix of the k-th layer, e_i^{k-1} represents the neighboring node information of the k-th layer, and $\tanh$ represents the activation function. The expression for the central node after aggregating information from the k-th layer is as follows:

$$m_{HS}^k = \mathrm{Leaky\,ReLU}(W^k(e_i^{k-1} + m_{N_r}^{k-1})) \tag{7}$$

where W^k denotes the weight matrix, and $\mathrm{Leaky\,ReLU}$ denotes the activation function.

Similarly, the representation of each node in the herb-herb homogeneous graph can be obtained.

2.3. Inductive Prediction Layer

The feature fusion and prediction layer obtains the final representations of herbs and symptoms through summation. It derives an overall representation of the patient's symptoms using multi-hot encoding, average pooling, and a MLP. The overall representation of the patient's symptoms is then interacted with the final representation of the herbs to predict a score for each herb, indicating its suitability for treating the patient's symptoms.

After obtaining the representation of each node in the multi-graph, the final representation of the herbs can be obtained through summation as:

$$e_H = m_{HS}^k + m_{HH}^k \tag{8}$$

where e_H is the final representation of herbs, m_{HS}^k and m_{HH}^k represent the node representations in the herb-symptom heterogeneous graph and the herb-herb homogeneous graph, respectively. k represents the number of information propagation layers. And the final representation of the symptoms e_S is equal to m_{HS}^k.

The model takes the patient's symptom set as input and outputs a TCM prescription. First, the patient's symptoms ps are represented using a multi-hot encoding, where the corresponding dimension is set to 1 if ps contains symptom s, and 0 otherwise. In the second step, all symptoms s in ps are embedded into their final representations e_S to obtain the matrix $e'_{ps} \in \mathbb{R}^{|ps|\times d}$, where d represents the initialization dimension. Finally, e'_{ps} is processed through average pooling and a MLP to obtain the overall representation of the patient's symptoms, expressed as:

$$e_{ps} = \mathrm{ReLU}(W_{mlp} \bullet \mathrm{Mean}(e'_{ps}) + b_{mlp}) \tag{9}$$

where W_{mlp} denotes the weight matrix in the multilayer perceptron, and b_{mlp} denotes the bias settings.

At this point, the overall representation of the patient's symptoms and the final representations of all herbs have been obtained. The interaction between the two can be used to predict the probability of each herb being suitable for treating the patient's symptoms, the prediction function is as follow:

$$f(ps, H) = e_{ps} \bullet e_H^T \tag{10}$$

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2.4. Multi-graph Construction Layer

The model is designed to output appropriate TCM prescriptions based on the patient's symptom set. Therefore, during the training phase, it is necessary to calculate the difference between the model's output and the actual prescription. This difference is then used to update the weights in the model through backpropagation, enabling the model's output TCM prescriptions to increasingly approximate the actual TCM prescriptions.

Given the symptom set ps, the actual prescription is represented by a multi-hot vector rh, whose dimension equals the number of herb types in the training set. If a herb exists in the actual prescription, the corresponding dimension is set to 1; otherwise, it is set to 0. The weighted mean squared error is used to calculate the difference between rh and the model-recommended prescription $f(ps,H)$, which is formulated as:

$$WMSE(rh, f(ps,H)) = \sum_{i=1}^{|H|} \omega_i (rh_i - f(ps,H)_i)^2 \tag{11}$$

where rh_i represents the value of the i-th dimension in the multi-hot vector, $f(ps,H)_i$ represents the probability of the i-th herb being recommended in the model-recommended prescription, and both have the same dimension, equal to the number of herb types in the training set. ω_i is the weight of the i-th herb.

Finally, the objective function is formulated as :

$$Loss = \arg\min_{\Theta} \sum_{(ps,rh)\in P} WMSE(rh, f(ps,H)) + \|\lambda_\Theta\|_2^2 \tag{12}$$

where λ is the hyperparameter that controls L2 regularization, and θ is the set of all trainable parameters in the model.

3. Experiments and Results

3.1. Evaluation Metrics and Comparison Methods

The above models recommend TCM escriptions based on the patient's symptom set. Therefore, the performance of the model can be evaluated by calculating the difference between the recommended prescription and the actual prescription. Two evaluation metrics are used here: Precision@N and Recall@N. The specific expressions are as follows:

$$Precision@N = \frac{|\{Top(S,N)\} \cap \{H\}|}{|\{N\}|}, Recall@N = \frac{|\{Top(S,N)\} \cap \{H\}|}{|\{H\}|} \tag{13}$$

In the test set, each actual prescription is represented as $P = \{S, H\}$, where S is the symptom set and H is the herb set. $Top(S,N)$ represents the top N herbs with the highest probabilities recommended by the model for the given symptom set S.

To better evaluate the proposed model, the following two classic models are used as baselines for comparison:

PTM [6] is a topic model that treats TCM prescriptions as documents, symptoms and herbs as elements, and treatment methods as topics. This model is trained on 33,765 TCM prescriptions and can reflect the methodology of TCM prescription formulation.

AGREE [7] is a neural network-based group recommendation model that, for the first time, utilizes an attention mechanism to dynamically adjust the weights of group members when facing different items.

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3.2. Experimental Settings and Datasets

All experiments were conducted on a cloud platform with the Ubuntu operating system and an NVIDIA GeForce RTX 2080 Ti GPU. The relevant software configurations are shown in Table 1.

Table 1: Software version

python	tensorflow	nvidia-cuda	numpy	scipy
3.8.10	1.15.1	11.4	1.19.5	1.10.1

For MGCN, the initial dimension dd for herbs and symptoms is set to 64, the order of high-order propagation is 2, the learning rate is 0.0001, the dropout rate is 0.0, and the regularization hyperparameter is 0.007. The topic model PTM has four modes, and the PTM(d) mode, which achieves the best performance, is selected here with the number of topics set to 40, $\alpha = 1$, $\beta = 0.1$, $\beta' = 0.1$, $\eta = 1$.

The dataset consists of 26,360 TCM prescriptions extracted from reference [8]. 90% of the data is randomly selected for model training, while the remaining 10% is used for testing.

3.3. Results

The MGCN model and other comparison models were each tested 10 times, and the final results were averaged. The experimental results are shown in Table 2.

Table 2: Experimental results

	Precision@5	Precision@10	Precision@20	Recall@5	Recall@10	Recall@20
PTM	0.2530	0.2062	0.1535	0.1770	0.2861	0.4231
AGREE	0.2534	0.2163	0.1531	0.1895	0.3081	0.4401
MGCN	0.2812	0.2263	0.1639	0.2001	0.3141	0.4543

Figure 1 shows the performance improvements of MGCN over PTM and AGREE in the evaluation metrics Precision@N and Recall@N:

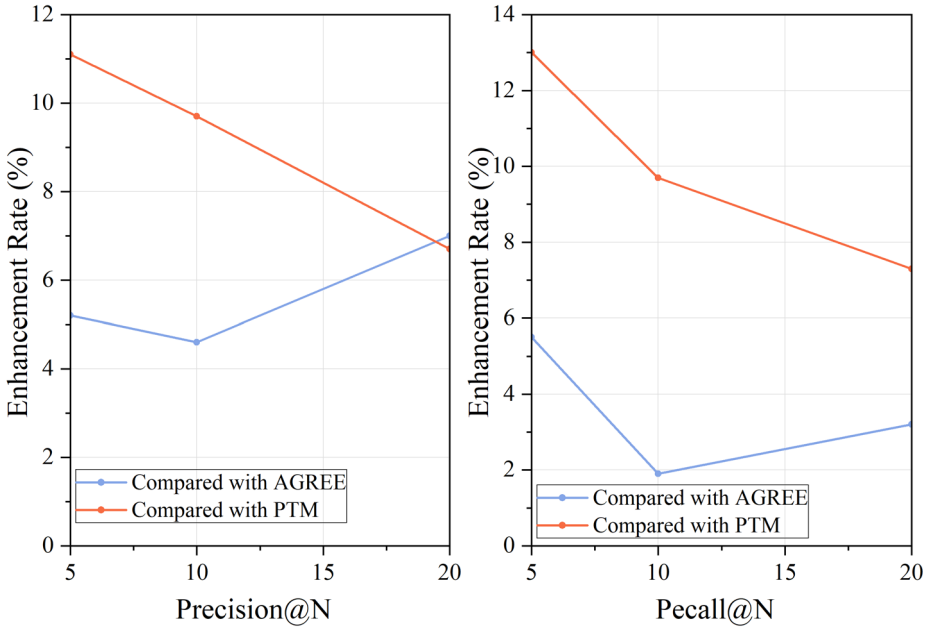

Figure 1: The performance improvements of MGCN over PTM and AGREE in the evaluation metrics Precision@N and Recall@N

4. Conclusions

This paper proposes a Traditional TCM recommendation method based on multi-graph convolutional neural networks through the study of graph neural networks. The method constructs multiple graphs, propagates high-order information, and integrates and induces features to obtain the patient's syndrome representation, which is then used to recommend suitable prescriptions. Comparative experiments

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demonstrate that this method achieves higher recommendation performance.

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