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Neural Network-Based Prescription of Chinese Herbal Medicines

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Abstract —**Objective: To develop a neural network model that recommends traditional Chinese medicine (TCM) herbal prescriptions. Methods: We constructed a new dataset of diagnosis and treatment knowledge from the *Treatise on Febrile Diseases*. Based on TCM's logical principles of "syndrome differentiation" and "state recognition", a back-propagation neural network model is proposed that simulates clinical diagnosis and treatment. Results: The proposed model is a four-layer BP neural network. Experiments on the constructed dataset show that the proposed method achieved the best precision, recall, and F1-scores. Conclusion: The proposed method provides much more accurate herbal prescription recommendations than logistic regression.**

Keywords* — *TCM assisted diagnosis and treatment; BP neural network; prescription recommendation

I. INTRODUCTION

During clinical diagnosis and treatment, young and experienced doctors might prescribe different herbs [1] to the same patient, which is not ideal for patient treatment and the development of TCM. Recently, researchers have tried to simulate the diagnosis and treatment process of doctors using machine learning algorithms [2] and artificial neural networks [3], which have provided several reference schemes for doctors to use when prescribing Chinese herbal medicines in clinical practice.

This paper proposes a neural network-based recommendation model to automate the Chinese herbal prescription process. Specifically, we first studied the Treatise on Febrile Diseases, which is an open-access and widely accepted TCM dataset. Second, we used TCM's logical principles of syndrome differentiation [4] and state identification [5] to label the dataset. Finally, we used a back-propagation (BP) neural network [6], to establish a recommendation model for Chinese herbal prescriptions. In addition, we compared the proposed model with logistic regression [7], and validated its effectiveness and application value from both quantitative and qualitative perspectives.

II. RELATED WORK

With the continuous development of deep learning [8] and other technologies, BP neural networks have been applied in the field of TCM automation. For example, Guo et al. [9] used a neural network to explore the relationships between the properties and efficacy of Chinese herbal prescriptions, and achieved effective prediction of the efficacy of single-type prescriptions. Chen et al. [10] used the hierarchical feature extraction characteristic of neural networks to simulate the dialectical thinking process of the human brain and designed an artificial neural network for TCM syndrome differentiation based on dominant diseases.

In the TCM field, "syndrome differentiation" is the most representative diagnostic and treatment logic. In addition, the diagnostic and treatment logic of "state recognition" [11] has attracted widespread attention and has been extensively studied in the field of TCM. This logic not only introduces many state elements (e.g., "location", "nature", and "degree") but also combines computer technology with statistical methods, thus simplifying the process of TCM diagnosis and treatment. Logistic regression is a type of linear regression analysis model. In the medical field, logistic regression has been extensively applied to medical diagnosis problems. The BP neural network is a type of artificial neural network. This algorithm has capabilities beyond those of traditional statistical methods in terms of adaptation, fault tolerance, and self-organization.

III. PROPOSED METHOD

A. Dataset and preprocessing

In this work, we collected experimental data from the *Treatise on Febrile Diseases*. The final dataset was composed of 358 diagnosis and treatment examples gained from the experimental dataset. The structure and content of the new dataset are illustrated for a specific case in Table I; which depicts information on diagnosis and treatment data items relating to the ephedra decoction.

To conveniently process the diagnosis and treatment data by computer, the symptoms and herbs for each diagnosis and treatment case were encoded using multi-hot encoding

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technology. In other words, binarization processing ("0" and "1") was performed for each symptom and herb.

TABLE I. A case from the *Treatise on Febrile Diseases*.

Symptoms	State element	TCM syndrome	Herbs	Prescrip -tion
发热(fever), 无汗 (adiapneustia), 身痛(pantalgia)	外风 (wind), 热(hot), 表(surface)	太阳伤寒证 (Solar typhoid syndrome)	麻黄(ephedra), 桂枝(cassia twig), 炙甘草(fried licorice), 杏仁(almond)	麻黄汤 (ephedra decoction)

B. Model construction

According to the logical principles of "syndrome differentiation" and "state recognition", a four-layer BP neural network model was designed to achieve automatic recommendations for Chinese herbal prescriptions. The proposed model is composed of one input layer, two hidden layers, and one output layer, as shown in Fig. 1. Specifically, the input layer is the entrance of the whole model, which corresponds to the 158 symptoms in the dataset. Therefore, the number of neurons in the first layer was set to 158. The first hidden layer corresponds to the 53 state elements in the dataset (hence, neurons in this layer = 53). The second hidden layer corresponds to 200 TCM syndromes (neurons = 200). The output layer represents 76 herbs (neurons = 76).

Propagation between different layers in a neural network is a process of mapping from the nodes in the previous layer to the nodes in the next layer. Training of a neural network involves learning how to fit the mapping relations among different layers. Therefore, propagation from the input layer to the first hidden layer simulates the summary process from the symptom set to the state element set. Propagation from the hidden layer to the second hidden layer simulates the summary process from the state element set to the syndrome set. Propagation from the second hidden layer to the output layer simulates the process of recommending Chinese herbal prescriptions. The structural design of the proposed model simulates the logical thinking process of "syndrome differentiation" and "state recognition" in TCM.

C. Model training

The training process used for the proposed model can be divided into forward propagation, loss calculation, and back-propagation. The propagation operation is defined as:

$$Q_{\mathrm{i}}^{L+1} = \sigma(\sum_{k} W_{ki}^{L} Q_{k}^{L}). \quad (1)$$

Where Q_{i}^{L+1} is the i^{th} neuron in the $L+1$ layer, $\sigma()$ is a nonlinear activation function, and W_{ki}^{L} is the weight. According to Eq. (1), the proposed model's process of propagation from the input layer to the output layer can be defined as:

$$\mathrm{y_h} = \mathrm{sigmoid}(\sum_{j} W_{jh}^{3}\, \mathrm{ReLU}(\sum_{i} W_{ij}^{2}\, \mathrm{ReLU}(\sum_{s} W_{si}^{1} x_{s}))). \quad (2)$$

The two activation functions are defined as:

$$\mathrm{ReLU}(x) = \max(0, x). \quad (3)$$

$$\mathrm{sigmoid}(x) = \frac{1}{1 + e^{-x}}. \quad (4)$$

Since the proposed model prescribes a group of herbs, it will output multiple predicted labels. Therefore, the proposed model is considered a multi-label classification model and, thus, a multi-label cross-entropy loss function is used as the loss function of our model; i.e.,

$$L = -\frac{1}{H}\sum_{h\in H}(t_{h}\log y_{h} + (1-t_{h})\log(1-y_{h})) \quad (5)$$

Where H is the number of neurons in the output layer, which is equal to the total number of herbs. The symbols $t_{h}(t_{h} \in \{0, 1\})$ and $y_{h}(0 \le y_{h} \le 1)$ denote the practical labels and predicted label, respectively. Finally,since the aim is to optimize the network weight, we used the BP algorithm [9].

IV. EXPERIMENTAL RESULTS AND ANALYSIS

To validate the effectiveness of the proposed model for making Chinese herbal prescriptions, we used a new dataset containing diagnosis and treatment knowledge from the *Treatise on Febrile Diseases*. The proposed model was compared with logistic regression [2]. The performance of the different methods in making Chinese herbal prescriptions was evaluated according to the metrics of precision, recall, and F1-score.

A. Quantitative analysis

Table II compares the quantitative results of the two methods (proposed model and logistic regression). From Table II, it can be seen that the precision, recall, and F1-score of the proposed model were best. These are better than logistic regression, indicating that the proposed model provides superior recommendation performance. Specifically, the more sufficient the training data, the more significant the performance of the proposed model.

B. Qualitative analysis

Table III provides examples of the Chinese herbal prescriptions recommended by different methods when K = 5. The underlined herbs were correctly predicted by the corresponding model.When K = 5, all five Chinese herbs predicted by the proposed model could be found in the labels and all of them were correctly recommended. However, the logistic regression model only predicted four of them correctly, and gave one wrong recommendation. In summary, the proposed model performed better than the logistic regression model in terms of prescribing Chinese herbs.

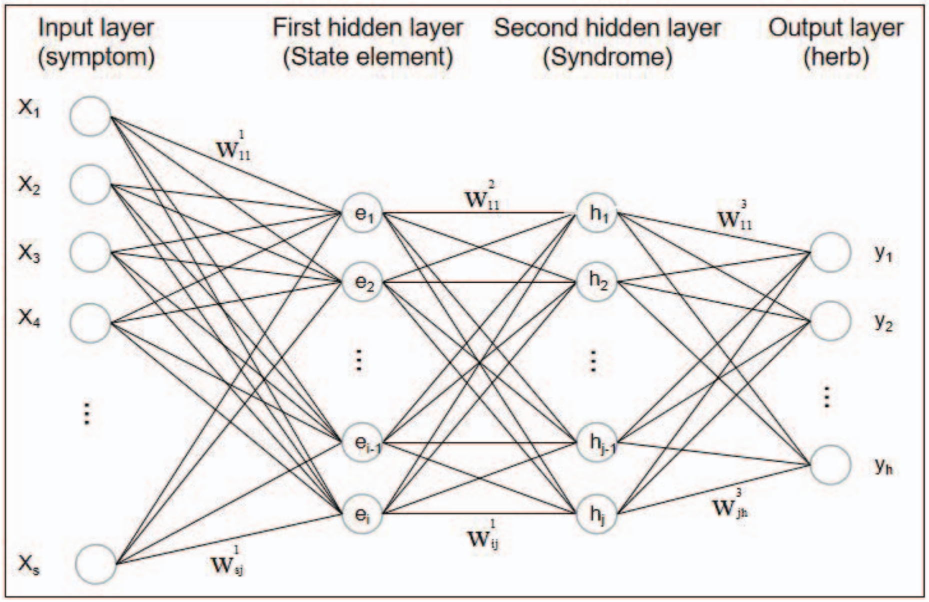

Figure 1. Framework of the four-layer BP neural network model.

TABLE II. Comparative performance of different algorithms on different experimental datasets.

Group	Algorithm	Precision @5	Precision @10	Recall @5	Recall @10	F1-score@5	F1-score@10
1	Proposed model	**0.6857**	**0.4045**	**0.8455**	**0.9591**	**0.7569**	**0.5689**
	Logistic regression	0.6400	0.3800	0.7733	0.8948	0.7003	0.5334
2	Proposed model	**0.5622**	**0.3608**	**0.6518**	**0.7849**	**0.6034**	**0.4941**
	Logistic regression	0.5211	0.3507	0.5598	0.7362	0.5397	0.4750
3	Proposed model	**0.4919**	**0.3233**	**0.6327**	**0.7773**	**0.5534**	**0.4550**
	Logistic regression	0.4878	0.3177	0.5899	0.7508	0.5340	0.4465
4	Proposed model	**0.5398**	0.3516	**0.6173**	**0.7702**	**0.5756**	**0.4826**
	Logistic regression	0.5328	**0.3517**	0.5775	0.7539	0.5543	0.4796
5	Proposed model	**0.4920**	0.3222	**0.5813**	**0.7335**	**0.5322**	0.4474
	Logistic regression	0.4793	**0.3273**	0.5513	0.7319	0.5128	**0.4524**

TABLE III. Herbal prescription recommendation cases based on different algorithms.

Symptom set	Set of Chinese herbal prescriptions		
Symptoms	Predicted results of the proposed model	Predicted results of logistic regression	Labels
小便不利 (Difficult urination) 头汗出 (Head sweat out) 胸胁满 (Chest and rib-side fullness) 口渴 (Thirst) 心烦 (Distracted)	炙甘草 (Fried licorice) 柴胡 (Radix bupleuri) 桂枝 (Cassia twig) 牡蛎 (Concha ostreae) 黄芩 (Scutellaria baicalensis)	柴胡 (Radix bupleuri) 黄芩 (Scutellaria baicalensis) 炙甘草 (Fried licorice) 牡蛎 (Concha ostreae) 茯苓 (Poria cocos)	桂枝 (Cassia twig) 柴胡 (Radix bupleuri) 炙甘草(Fried licorice) 牡蛎 (Concha ostreae) 黄芩 (Scutellaria baicalensis) 瓜蒌根 (Trichosanthes root) 干姜 (Rhizoma zingiberis)

V. CONCLUSION AND FUTURE WORK

This paper presented a Chinese herbal prescription model based on a BP neural network. Unlike existing neural network-based prescription methods, the proposed model learns from the TCM principles of "syndrome differentiation" and "state recognition" to construct a four-layer BP neural network. The unique design helps in exploring the internal matching relationships between TCM symptom groups and Chinese herbal medicines and better simulates the logical process of TCM clinical diagnosis and treatment.

We conducted experiments on a diagnosis and treatment knowledge dataset from the *Treatise on Febrile Diseases*. The experimental results show that the proposed model provides superior recommendation performance compared with the logistic regression model. In future work, we will introduce more advanced algorithms (e.g., graph neural networks) to further improve the accuracy of Chinese herbal prescriptions.

CONFLICT OF INTEREST STATEMENT

The authors declare that there is no conflict of interests regarding the publication of this article.

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