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Research paper

Diagnosis knowledge constrained network based on first-order logic for syndrome differentiation

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ABSTRACT

Traditional Chinese medicine (TCM) has been recognized worldwide as a valuable asset of human medicine. The procedure of TCM is to treatment based on syndrome differentiation. However, the effect of TCM syndrome differentiation relies heavily on the experience of doctors. The gratifying progress of machine learning research in recent years has brought new ideas for TCM syndrome differentiation. In this paper, we propose a deep network model for TCM syndrome differentiation, which improves network performance by injecting TCM syndrome differentiation knowledge in the form of first-order logic into the deep network. Experimental results show that the accuracy of our proposed model reaches 89%, which is significantly better than the deep learning model MLP and other traditional machine learning models. In addition, we present the collected and formatted TCM syndrome differentiation (TSD) dataset, which contains more than 40,000 TCM clinical records. Moreover, 45 symptoms ("证"), 322 patterns("候"), and more than 500 symptoms are labeled in TSD respectively. To the best of our knowledge, this is the first TCM syndrome differentiation dataset labeling diseases, syndromes and pattern. Such detailed labeling is helpful to explore the relationship between various elements of syndrome differentiation.

1. Introduction

Traditional Chinese Medicine (TCM) is the experience and theoretical knowledge summed up by the ancient Chinese people in their struggle against diseases, and it is the crystallization of human medical science [1]. Generally, the diagnosis and treatment process of TCM includes syndrome differentiation and treatment. In detail, a doctor must first identify a patient's symptoms and then proceed with treatment based on them [2]. In other words, syndrome differentiation is one of the most important processes in TCM. The traditional method of syndrome differentiation is that a doctor obtain the basic situation of the disease by observing and analyzing the symptoms of a patient. Considering the human body as a black box, the causes, locations and layers of disease can be represented by a spherical black box model, as shown in Fig. 1. Obviously, the symptom is the outward appearance of the disease, which reflects the current disease cause and disease location. However, as the human body is a complex organic whole, the relationship between symptoms and diseases is complicated, which makes the differentiation of symptoms very difficult [3]. In addition, the wide variety of symptoms and various combinations further increase the difficulty of differentiate syndromes. Particularly, TCM syndrome differentiation requires accurate identification of disease, syndrome ("证") and pattern (" 候") (detailed in Section 3) [4]. However, the lack of a unified standard in the development of TCM over thousands of years makes it difficult to distinguish these three elements. These are the problems that TCM needs to solve urgently.

Syndrome differentiation is essentially a classification problem, and some scholars have tried to solve it with machine learning (ML) methods [5]. Some traditional ML algorithms such as DecisionTree (DT) [6], Support Vector Machines (SVM) [7], K-Nearest Neighbor (KNN) [8] and other algorithms have been designed to classify TCM diseases [9]. They have achieved good results, but their studies are all focused on a certain disease or a syndrome, and their performance is limited in data containing a large number of features, and they cannot be used as a general method of syndrome differentiation. In recent years, some scholars have used deep learning algorithms such as Topic Model [10], GCN [11], and DBN [12] to simulate the process of TCM diagnosis and treatment [13–15]. They obtained prescription recommendation results by designing their algorithm and training it with a dataset containing symptoms and prescriptions. However, they do not clarify the relationship between symptoms and syndromes, which is not in line with the idea of "treatment based on syndrome differentiation"

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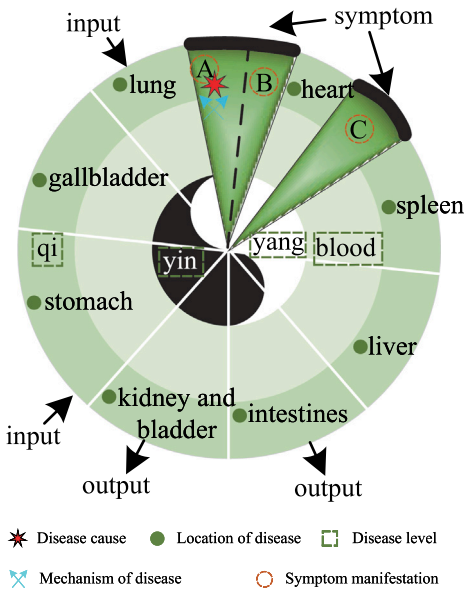

Fig. 1. Diagram of human spherical black box. Symptoms are the external manifestations of a disease, which can reflect information such as the cause, location, pathogenesis, and process of the disease.

in TCM [16]. Simultaneously, the lack of support for diagnostic knowledge also makes the results of these models questionable by doctors. Moreover, as the models designed in these studies are very complex and lack the support of TCM syndrome differentiation knowledge, a large number of data are needed to ensure the training effect. Chen et al. [17–19] used traditional machine learning and deep learning model combined with TCM property theory to study the classification of TCM property, which provides a new idea for the combination of TCM theory and artificial intelligence.

The lack of TCM electronic data has been a constant concern in recent years. Some scholars have made contributions to the collection of TCM clinical data [14,20]. They have achieved very good results in terms of quantity and standardization. However, they did not annotate details in the data, such as precise pulse diagnosis information, syndrome and pattern, which brought challenges to the task of using data to learn syndrome differentiation. In response to the above-mentioned problems, we propose an innovative TCM syndrome differentiation model, which improves the reliability of the results by injecting TCM diagnostic knowledge into the deep network. In this paper, we use diagnosis knowledge based on disease cause, disease of location and symptoms, which is the essence of holistic syndrome differentiation in TCM (detailed background is presented in Section 3). Furthermore, we present the constructed TCM syndrome differentiation dataset. Our main contributions are as follows:

- We represent TCM diagnostic knowledge by devising first-order logic rules, which is the first introduced in TCM syndrome differentiation to our knowledge. Moreover, we construct a professional TCM diagnostic knowledge base, which provides logical reasoning basis for intelligent syndrome differentiation.
- We propose a novel TCM syndrome differentiation model called DL-TCM, which can realize efficient syndrome classification by injecting diagnostic knowledge into the deep network. To this end, we transform non-differentiable first-order logic into differentiable functions by designing mapping relations.
- We construct a TCM syndrome differentiation dataset, referred to as TSD, which consists of more than 40,000 TCM clinical records. Moreover, diseases, syndromes, and patterns are respectively labeled in TSD. Besides, experimental results show that the performance of DL-TCM is better than the state-of-the-art syndrome differentiation models on TSD.

The rest of this paper is organized as follows. Section 2 provides an overview of related works with respect to TCM syndrome differentiation and Dataset. Our proposed model is presented in Section 3. The detailed implementation and the experimental results are provided in Section 4. We discuss this research in depth in Section 5. Finally, Section 6 summarizes this paper.

2. Related work

2.1. ML in syndrome differentiation

Syndrome differentiation is a very important part in the process of TCM diagnosis and treatment, which lays the foundation for the subsequent treatment effect [1]. Zhang et al. [16,21]proposed a deep transfer learning model applied to TCM tongue diagnosis, by using a deep squeeze-and-excitation convolutional network to learn the clinical classification of tongue syndrome to make symptom diagnosis for patients. Alice et al. [22] summarized and analyzed the current application status of artificial neural network and deep learning technology in the field of TCM pulse diagnosis, and believed that the integration of TCM pulse diagnosis theory and modern science is of great significance. At the same time, they pointed out that there are still some bottlenecks in the development of TCM pulse diagnosis and artificial intelligence technology. Dai et al. [23] have proposed a new deep learning framework for diagnosing patients by fusing diagnostic information across multiple modalities, which includes simulating the vision, listen, smell, inquiry, and touch of a TCM doctor. Xu et al. [24] took chronic obstructive pulmonary disease as an example, and analyzed the data set composed of 18,471 real clinical records by establishing a neural network to study the intelligent syndrome differentiation of TCM based on artificial neural network. Ma et al. [25] proposed a supervised probabilistic topic model SSTM with a three-layer Bayesian structure for TCM syndrome differentiation. They treat symptoms as hashtags and then differentiate potential symptoms based on disease location. Experiments show that their proposed SSTM model is more effective than other models in dialectics.

The above studies have made positive contributions to TCM syndrome differentiation, but lack of knowledge support in the field of TCM syndrome differentiation leads to lack of reliability in the results. Furthermore, the datasets on dialectics are less researched and labeled insufficiently, making it difficult to adapt to some deep learning networks.

2.2. TCM syndrome differentiation dataset

Some scholars have noticed the lack of TCM syndrome differentiation datasets and have started researches. Some high-quality TCM syndrome differentiation datasets have been collected and established. Ren et al. [20] introduced the first publicly available TCM syndrome differentiation dataset containing 54,152 real clinical records covering 148 syndromes. Meanwhile, they propose a pre-trained model ZYBERT based on the unlabeled text corpus collected in the field of Chinese medicine. Jiang et al. [26] collected 436 TCM clinical records containing symptoms, diagnoses, and prescriptions, which they then evaluated using fuzzy mathematical algorithms to identify sub-health states such as qi deficiency, yin deficiency, yang deficiency, and phlegm-dampness. Compared with similar studies, the data items they collected are more complete, and the algorithm has higher accuracy, which can already be used to assist the detection of traditional Chinese medicine. Weng et al. [27] constructed a dataset of 832 cases containing 239 symptoms, and then used the SVM classifier to classify common syndromes such as heart yin deficiency, heart yang deficiency, and blood stasis, and the accuracy rate of syndrome differentiation reached 89.69%. Wen

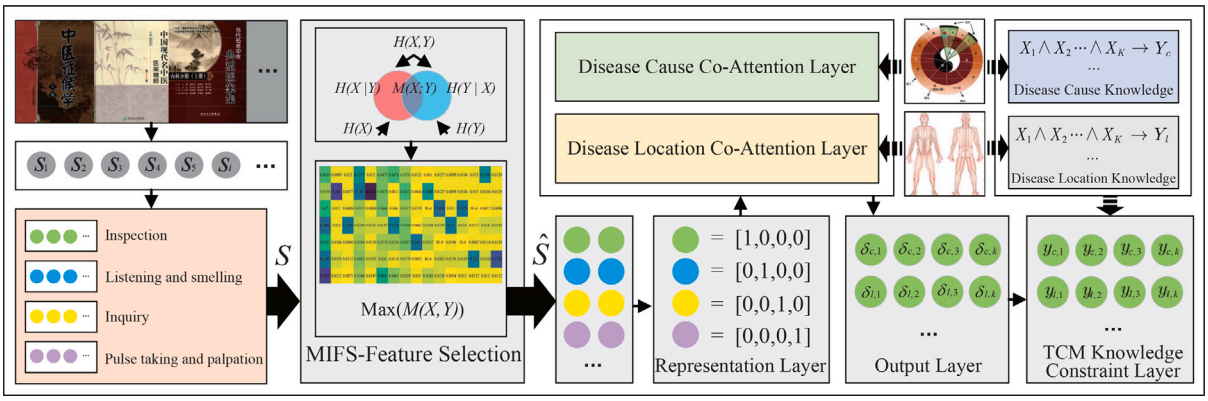

Fig. 2. The overall frame. The data comes from the published medical records of modern Chinese medicine, and we use mutual information to perform feature screening and then perform deep network training. The deep network includes the Disease Cause Co-Attention Layer and the Disease Location Co-Attention Layer, and the output layer result is corrected by the TCM knowledge constraint layer in the form of first-order logic to get the final result.

et al. [28] collected a TCM dataset containing 80,000 data, and they localized the inquiry text into three entity types: symptoms, symptom descriptions, and body parts, while proposing a cross-domain adversarial learning model based on Chinese named entity recognition for TCM online consultation services. The experimental results show that the overall accuracy of their method exceeds 70%. Hu et al. [29] collected 7326 TCM medical records containing two syndromes of yin deficiency and yang deficiency, and proposed an end-to-end model based on convolutional neural network to identify syndromes. The experimental results showed that the accuracy of the method was 92.55%. Liu et al. [30] collected clinical records of 1206 patients diagnosed with non-small cell lung cancer, which consisted of chief complaint, medical records, medical history, laboratory test results, four TCM test results, and syndrome differentiation results. At the same time, they propose a model for syndrome classification of unstructured medical records using deep learning. The experimental results showed that the F1-score of the model was 0.8884%, indicating that the study played a positive role in TCM diagnosis. Xie et al. [31] collected clinical medical records of 1713 patients with rheumatoid arthritis, including four TCM syndromes: damp-heat resistance syndrome, phlegm stasis and blood stagnation syndrome, liver and kidney deficiency syndrome, and wind-cold resistance syndrome. They used 6 models to classify TCM syndromes, and the results showed that neural networks had the highest accuracy for the task of syndrome classification.

The datasets constructed in the above studies have greatly promoted the research on TCM syndrome differentiation, but these datasets do not reflect the difference between syndrome and pattern. At the same time, how to combine TCM clinical data with diagnostic knowledge is still a research field that needs to be explored.

3. The proposed method

In this section, we describe our proposed method in detail. First of all, we introduce the relevant background knowledge of TCM involved in this paper. Then, we introduce the notations and formulas used in this paper. Finally, our modeling process and network architecture are introduced.

3.1. Background knowledge of TCM

Diseases, syndrome (“证 ”) and pattern (“候”) in TCM are three different concepts and contain strict connotations [4]. Among them, disease is a generalization of a series of pathogenic processes caused by a certain disease cause acting on a certain disease location. Syndrome is a statement of stages in each period of the disease process, and it will keep changing with the development of the disease. The content of the syndrome includes disease cause, disease location and pathogenesis, the most important of which are the first two. So the disease cause and disease location are also used to name a syndrome. The pattern is the embodiment of the different mechanism of disease of the syndrome in the change. Therefore, the syndrome plays a central role in the above three, it not only expresses the nature of the disease of a certain disease, but also plays the role of commander when it expresses the special disease state.

Syndrome enables doctors to examine the development and changes of the disease as a whole, and provides ideas for guiding clinical treatment. For example, “deficiency-cold of spleen and stomach” from its syndrome name suggests that deficiency-cold exists in the spleen and stomach, which has become a sign of current treatment. Then, whether choosing therapeutic methods, classical formula or medicines, this sign is inseparable. Therefore, only correct identification can guarantee the effectiveness of subsequent treatment. In this paper, we focus on solving the important and complex problem of syndrome differentiation by using deep learning techniques.

Since TCM contains many complex terminology, in order to clearly express the thoughts of our paper, the terminology of TCM used in this paper is basically from the *International Standard Chinese-English Basic Nomenclature of Chinese Medicine* edited by the World Federation of Chinese Medicine Societies [32].

3.2. Problem statement

Let $\mathcal{S} = \{s_1, s_2, \ldots, s_n\}$ denotes the symptom set of a patient, where $s_i \in \mathcal{S}$ represents one of the symptoms of the patient. Given the symptom set $\mathcal{S}$, the aim is to predict the syndrome $y \in \mathcal{Y}$ of the patient. Simultaneously, we inject the knowledge of disease cause $\mathbf{c_{know}}$ and disease location $\mathbf{l_{know}}$ used in TCM diagnosis into the neural network to improve the prediction accuracy. The overall architecture of the proposed method is shown in Fig. 2. We first collected published TCM medical records using a self-developed medical record collection system. These data are then sorted and formatted according to the categories of Inspection, Listening and smelling, Inquiry, and Pulse taking and palpation, respectively. Then we use the MIFS feature selection method based on mutual information to filter out the potentially important features and then send them to the DL-TCM syndrome differentiation network according to the classification target. DL-TCM consists of a deep learning module that fuses a network of two attention layers based on etiology and disease location and a symbolic TCM diagnostic knowledge module. We first input a set of symptoms into the neural network containing two attention layers based on disease cause and disease location, and obtained preliminary results of syndrome differentiation. Then, the final prediction result is obtained by re-weighting the preliminary prediction result using the first-order logic rules in the symbol module. The details of each part are detailed below.

3.3. MIFS-feature selection

Since the data may contain a large number of features that affect model performance, we first supervised feature selection before conducting experiments. We use statistical methods to calculate the degree of association between features and target labels. Specifically, we use mutual information to measure the association between features and labels. Mutual information is expressed by the following formula:

$$M(S;Y) = \sum_{s,y} p(s,y) \log \frac{p(s,y)}{p(s)p(y)}.$$

Mutual information can be easily transformed into the form of KL divergence:

$$\begin{aligned} M(S;Y) &= \sum_{s,y} p(s,y) \log \frac{p(s,y)}{p(s)p(y)} \\ &= D_{KL}(p(s,y) \parallel p(s)p(y)). \end{aligned} \tag{1}$$

KL divergence is often used to measure the difference between two probability distributions, and if s and y are independent random variables, then $p(s,y) = p(s)p(y)$ and Eq. (1) is equal to 0. Therefore, the larger the value of $M(S;Y)$, the greater the correlation between the two variables, so mutual information can be used to filter features. Then we input the feature set $\hat{S}$ filtered by the MIFS-Feature Selection method and label set $\mathcal{Y}$ into the Syndrome Differentiation Network.

3.4. Syndrome differentiation network

In diagnosis, the doctor first determines the disease cause and disease location according to the symptoms presented by the patient, and then give the syndrome differentiation result after comprehensive consideration. Inspired by this, the disease cause and disease location attention layers are designed to enhance the representation of symptoms.

3.4.1. Symptom representation layer

In this Layer, we represent a set of symptoms s as follows:

$$x_i = F(S) \in \mathbb{R}^d,$$

where $F(\cdot)$ is the embedding layer. We use the One-hot method to encode the embedding of S, and d is the number of symptoms. Then we use $\mathbf{X} \in \mathbb{R}^{N \times d}$ to represent the matrix formed by stacking all medical record data x_i, where N represents the number of samples.

3.4.2. Disease cause attention layer

We use the disease cause attention mechanism at this layer to enhance the representation of the relationship between symptoms and disease cause. Specifically, we first soft-align the symptoms with the disease cause diagnosis knowledge, and use the dot product to calculate the similarity between $\mathbf{X}$ and $\mathbf{c}_{\mathbf{know}}$ as follows:

$$\mathbf{A}_{\mathbf{c}} = \mathbf{X} \cdot \mathbf{c}_{\mathbf{know}} \in \mathbb{R}^N,$$

where $\mathbf{c}_{\mathbf{know}} = (c_{\mathbf{know},1}, c_{\mathbf{know},2}, \ldots, c_{\mathbf{know},d})$ is a row vector, which expresses the symptoms that can determine the disease cause. The value of $c_{\mathbf{know},i}$ equal to 1 indicates that the item is related to the disease cause, otherwise 0. It is designed according to the research of [4] on TCM syndromes and is recognized by the industry as TCM knowledge.

Then, we apply a softmax function on $\mathbf{A}_{\mathbf{c}}$ to weight the important symptom features with the knowledge of disease cause, as follows:

$$\alpha_{\mathbf{c},i} = \mathbf{softmax}(\mathbf{A}_{\mathbf{c}}).$$

As shown below, each row in the disease cause knowledge-aware and symptom representation $\widetilde{\mathbf{X}}_{\mathbf{c}}$ is the weighted sum of the rows in the symptom representation:

$$\widetilde{\mathbf{X}}_{\mathbf{c}} = \sum_i \alpha_{\mathbf{c},i} \mathbf{X} \in \mathbb{R}^N.$$

3.4.3. Disease location attention layer

Similarly, we use the disease location knowledge $\mathbf{A}_{\mathbf{l}}$ to obtain symptoms that are significant for disease location representation, as follows:

$$\mathbf{A}_{\mathbf{l}} = \mathbf{X} \cdot \mathbf{l}_{\mathbf{know}} \in \mathbb{R}^N,$$

where $\mathbf{l}_{\mathbf{know}} = (l_{\mathbf{know},1}, l_{\mathbf{know},2}, \ldots, l_{\mathbf{know},d})$ expresses the symptoms that can determine the disease location. Let the value of the symptom $l_{\mathbf{know},i}$ that can represent the disease location in $\mathcal{Y}$ be 1, and 0 otherwise. Then we apply a softmax function as follow:

$$\alpha_{\mathbf{l},i} = \mathbf{softmax}(\mathbf{A}_{\mathbf{l}}).$$

Similarly, each row in the disease location knowledge-aware and symptom representation $\widetilde{\mathbf{X}}_{\mathbf{l}}$ is the weighted sum of the rows in the symptom representation:

$$\widetilde{\mathbf{X}}_{\mathbf{l}} = \sum_i \alpha_{\mathbf{l},i} \mathbf{X} \in \mathbb{R}^N,$$

where $\widetilde{\mathbf{X}}_{\mathbf{l}}$ is the disease location knowledge-aware representation. In order to take full advantage of the disease cause and location attention information, we fuse $\mathbf{X}, \widetilde{\mathbf{X}}_{\mathbf{c}}, \widetilde{\mathbf{X}}_{\mathbf{l}}$ by concatenation operation as follow:

$$\mathbf{Z} = [\mathbf{X}, \widetilde{\mathbf{X}}_{\mathbf{c}}, \widetilde{\mathbf{X}}_{\mathbf{l}}].$$

3.4.4. Output layer

In this Layer, we feed the fused representation $\mathbf{Z}$ to an output layer with a softmax activation function, which computes the probability distribution:

$$\delta = \mathbf{softmax}(\mathbf{W}_\theta \mathbf{Z}), \tag{2}$$

where $\mathbf{W}_\theta$ is the trainable parameter.

3.5. TCM knowledge constraint layer

In this Layer, we let the output of the syndrome differentiation network enter the TCM knowledge constraint layer to adjust it. In general, we rectify the final result by re-weighting the output δ of the syndrome differentiation network. When the symptom S meets the TCM diagnosis conditions, the associated value of y increases, otherwise the value of y decreases. Specifically, we use a first-order logical constraint function $d(\cdot)$ guided by TCM knowledge to revise the output layer result δ. The function $d(\cdot)$ enhances or weakens y by judging whether the current diagnosis result violates the principles of TCM diagnosis. Given the output result δ of Eq. (2) and a TCM diagnosis rule $M \rightarrow Y$, we combine first-order logic with deep networks by the following formula:

$$y = \mathbf{softmax}(\delta + \beta d(M)),$$

where β is a hyperparameter representing the importance of diagnostic knowledge. Details of $d(\cdot)$ are provided in Table 1.

3.6. Training

Given a set of symptoms from TCM medical records $D = \{s_1, s_2, \ldots, s_n\}$, the model predicted values $\mathcal{Y} = \{y_1, y_2, \ldots, y_n\}$, and the true labels of the data $\hat{\mathcal{Y}} = \{\hat{y}_1, \hat{y}_2, \ldots, \hat{y}_n\}$. Suppose the label has k categories, we denote the predicted value of the ith sample as $y_i = (y_1^i, y_2^i, \ldots, y_k^i)$, the true label as $\hat{y}_i = (\hat{y}_1^i, \hat{y}_2^i, \ldots, \hat{y}_k^i)$. We train the model with the cross-entropy loss as shown below:

$$J(\mathcal{Y}, \hat{\mathcal{Y}}) = -\frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{k} \hat{y}_j^i \log(y_j^i).$$

3.7. First-order logic and TCM knowledge

In this section, we will detail how to allow a positive reaction between first-order logic and TCM knowledge to influence the training results of deep networks.

Table 1
Mapping functions for first-order logic.

$d(M_i) = m_i$,
$d\left(\bigwedge_i M_i\right) = \max\left(0, \sum_i m_i - \mid M \mid +1\right)$,
$d\left(\bigvee_i M_i\right) = \min\left(1, \sum_i m_i\right)$,
$d\left(\bigwedge_i M_i \left(\bigvee_j M_j\right)\right)$ $= \max\left(0, \max\left(\sum_i m_i - \mid M_i \mid +1, \sum_j m_j\right)\right)$,
$d\left(\left(\bigvee_i M_i\right) \wedge \left(\bigvee_j M_j\right)\right)$ $= \max\left(0, \max\left(\sum_i m_i - \mid M_i \mid, \sum_j m_j - \mid M_j \mid\right) + 1\right)$,
$d\left(\neg \bigwedge_i M_i\right) = \min\left(0, N - \sum_i m_i\right)$.

3.7.1. First-order logic

First-order logic consists of propositions composed of individuals, functions, quantifiers, and connectives, and inference relationships between these propositions. Importantly, first-order logic allows formulas to be quantified, an indispensable tool for many fields that require quantification rules. Formally, a simple logic rule is usually represented by $M \rightarrow Y$, where M is called the precondition and Y is called the consequent. Preconditions can also consist of multiple variables and connectives, e.g., $M_1 \wedge M_2 \vee M_3 \vee \cdots \vee M_n \rightarrow Y$. However, the consequent Y of these first-order logic rules is non-differentiable and cannot directly participate in the computation of the neural network. Therefore, we transform the Boolean operations of first-order logic into probabilistic logic, represented on a continuous real-valued space, following the method of Gan et al. [33]. Specifically, we associate the variable M in the precondition with the corresponding neuron output x. Then, the logic rules were transformed into softened versions using Łukasiewicz Tnorm and T-conorm [34]. We find functions that can map first-order logic to real values by using the method of Li et al. [35]. In addition, we also design a mapping function for negation predicates. The mapping function $d(\cdot)$ as shown in Table 1, where M_i is defined as the ith variable of first-order logic and m_i as the associate neuron in the neural network. In the next subsection we will introduce in detail how to use first-order logic to represent TCM knowledge.

3.7.2. TCM knowledge

In this section, we will show the results of compiling some typical TCM cold syndrome differentiation knowledge into first-order logic rules, which are important basis for clinical diagnosis.

The first rule of syndrome differentiation is: If the patient simultaneously has symptoms of aversion to cold and liking for warmth, clear water and liquid, and a clear smell, it can be determined that the patient suffers from cold syndrome. We formulate this TCM diagnostic knowledge with first-order logic and denote it as TK_1:

$$M_{AC} \wedge M_{CW} \wedge M_{CS} \rightarrow Y,$$

where M_{AC} indicates whether the patient has symptoms of aversion to cold and preference for warmth. M_{CW} indicates whether the patient's vomit, excrement and blood are clear. M_{CS} represents whether the patient's sputum, vomit, excrement and other odors are clear and fishy. This rule will add support to the results of the syndrome differentiation with distinct cold syndrome features.

The second rule of dialectical syndrome is: if the patient has symptoms of turbid water and odor, that is, the patient's vomit or excrement is turbid and sour, it can be determined that it is not a cold syndrome. We formulate this TCM diagnostic knowledge with first-order logic and denote it as TK_2:

$$\neg M_{CW} \wedge \neg M_{CS} \rightarrow \neg Y.$$

This rule penalizes the results of wrong dialectics.

The third rule of dialectical syndrome is: when a patient has symptoms such as contraction, urgency, and inability to stretch, it can be identified as a cold syndrome. That is, the patient will experience contractions, like pressure, like warmth, no sweat, and a tight pulse. We formulate this TCM diagnostic knowledge with first-order logic and denote it as TK_3:

$$M_{AC} \wedge (M_{EC} \vee M_{PR} \vee M_{WA} \vee M_{SW} \vee M_{PT}) \rightarrow Y,$$

where M_{EC} means whether the patient has a sense of contraction, M_{PR} means whether he likes pressing, M_{WA} means whether he likes warmth, M_{SW} means whether he sweats, and M_{PT} means whether the pulse is tight or not. This rule adds support for the dialectical element of "contraction".

The fourth rule of dialectical syndrome is: if the patient's body is black, such as black complexion, black nails, or black disease, and the pulse is tight or slow, it can be diagnosed as cold syndrome. We formulate this TCM diagnostic knowledge with first-order logic and denote it as TK_4:

$$(M_{BF} \vee M_{BN} \vee M_{BD}) \wedge (M_{PT} \vee M_{PS}) \rightarrow Y,$$

where M_{BF}, M_{BN}, and M_{BD} indicate whether the patient has symptoms of black complexion, black nails or black disease, respectively. M_{PS} represents whether the pulse is slow. This rule emphasizes the importance of color diagnosis.

The core idea of this paper is to use the above first-order logic rules to constrain the training process, so as to achieve the purpose of correctly identifying syndrome. That is, the joint action of the medical case sample data and the TCM diagnosis knowledge, a reliable dialectical result y is finally obtained.

4. Experiments

In this section, we present the implementation details of our proposed algorithm and the results compared with other state-of-the-art classification algorithms. Our experiments use the self-built TCM syndrome differentiation (TSD) dataset, which is still in a state of continuous completion.

4.1. Dataset description

Before starting, we first introduce the collected TSD dataset. TSD is derived from real-world TCM clinical records. We have compiled more than 50 published TCM medical case books, such as *A Collection of Extracts of Famous Modern TCM Medical Cases in China* [36], and collected more than 40,000 labeled TCM data. Each piece of data includes the patient's four diagnostic information and diagnosis results, and Table 3 shows some of the features. The diagnosis result includes information on the syndrome, pattern, disease name, disease cause, and disease location. For example, the following TCM clinical medical record: "夏突腹泻, 继即呕吐, 精神疲倦, 四肢无力, 口渴小便全无, 脉沉微, 苔白滑, 肌肤微热, 声微气促, 脾肾虚寒, 调中土温脾肾, 振阳救阴, 投附子理中汤, 吐泻大减, 四肢温暖, 加猪苓、茯苓各15g, 洋泻、陈皮各3g", the content we recorded consisted of three parts: (a) The entire text. (b) The following symptoms: diarrhea, vomiting, mental fatigue, weakness of limbs, thirst, anuria, deep pulse, faint pulse, slippery coating, white coating, mild fever, faint low voice, short breath. (c) Syndrome differentiation label: disease: diarrhea, syndrome: Spleen and kidney Yin cold, pattern: Yang stagnation.

We select 6 cold syndromes and 1 non-cold syndrome to conduct the experiments in this paper, which contains 790 pieces of data and 7 classification labels. We select 6 types of cold syndromes based on the theory of TCM, that is, the 6 most basic types of cold syndromes, not other complex syndromes that change with the development of the disease. They are Spleen and stomach yin cold, Spleen and kidney yin cold, Liver and kidney yin cold, Spleen and stomach deficiency cold, Liver and kidney deficiency cold, Lung cold and heat. For ease of presentation we use the abbreviations in Table 2 instead.

The number and proportion of the 7 categories of data are shown in Fig. 4. In addition, the disease cause and disease location labels included in the TSD are shown in Fig. 3, where the dark labels indicate that they are included in the 790 pieces of data we select.

Table 2
Abbreviation for the syndrome.

Abbreviation	Full name
SSYC	Spleen and stomach yin cold
SKYC	Spleen and kidney yin cold
LKYC	Liver and kidney yin cold
SSDC	Spleen and stomach deficiency cold
LKDC	Liver and kidney deficiency cold
LCH	Lung cold and heat

4.2. Feature selection

We finally screen 190 features using the MIFS feature selection method. Fig. 5 shows the heat map of the association between some features and labels. Fig. 5 shows that features such as Complexion, Nasal congestion, and Phlegm are highly correlated with the syndrome differentiation labels of cold syndrome, indicating that they may play an important role in the results of cold syndrome differentiation.

4.3. Experiment setup

The proposed algorithm is implemented in Python (The version is 3.8.2.) and runs on a computer with an AMD Ryzen 7 3700X 3.60 GHz 8-Core processor and 16G of memory. Since there are almost no end-to-end studies using deep learning methods for TCM syndrome identification, we try to compare with the generic deep learning classification algorithms Multilayer Perceptron (MLP) and traditional ML classification algorithms DecisionTree, SVM, K-Nearest and Adaboost.

In the experiment, we use a deep network structure of three-layer MLP + disease cause and disease location attention layer + TCM knowledge constraint layer. The size of hidden states of MLP is 80. The hyperparameter δ is set to 1 and the learning rate is set to 0.01. The Adam optimizer is used in the experiment. Five-fold cross-validation method is used to divide the dataset randomly and equally into 5 parts, and then use the calculated average as the final result. To evaluate the classification performance of the proposed algorithm, we use the accepted metrics for classification algorithm evaluation: Precision, Recall, F1-score and Accuracy. Since our objective is a multi-classification problem, this paper we use Macros-Precision, Macros-Recall, Macros-F1 and Macro-Recall, as follows.

4.3.1. Precision

Precision is used to measure the correctness of the classification results, which is defined as the ratio of the number of samples that are correctly classified into a certain category to the total number of samples that are actually classified into this category. It is formulated as follows:

$$\text{Macro-precision} = \frac{1}{n}\sum_{i=1}^{n} Precision_i,$$

where $Precision_i$ represents the precision of class i and is given as:

$$Precision_i = \frac{TruePositive_i}{TruePositive_i + FalsePositive_i}.$$

4.3.2. Recall

Recall measures the completeness of the classification results and is defined as the ratio of the number of samples correctly classified into that class to the number of samples actually classified into that class. It is formulated as follows:

$$\text{Macro-Recall} = \frac{1}{n}\sum_{i=1}^{n} Recall_i,$$

where $Recall_i$ represents the recall of class i and is given as:

$$Recall_i = \frac{TruePositive_i}{TruePositive_i + FalseNegative_i}.$$

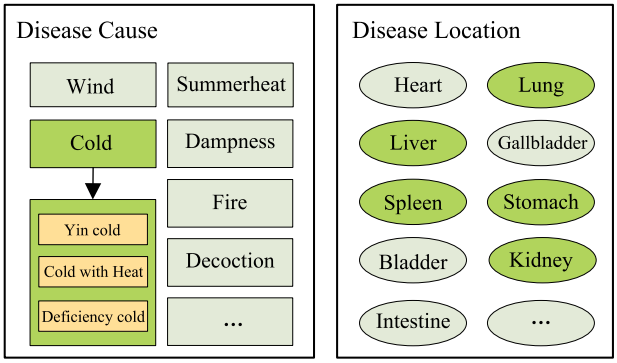

Fig. 3. Part of the disease cause and disease location labels included in the TSD.

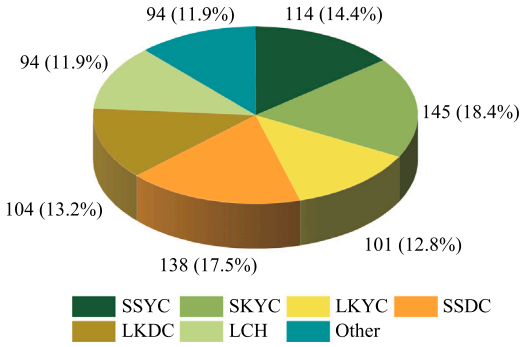

Fig. 4. Pie chart of the different categories of data contained in the cold symptoms dataset.

4.3.3. F1-score

The F1-score is the harmonic mean of precision and recall. It is formulated as follows:

$$\text{Macro-F1} = \frac{1}{n}\sum_{i=1}^{n} F1_i,$$

where $F1_i$ represents the f1-score of class i and is given as:

$$F1_i = \frac{2 * Precision_i * Recall_i}{Precision_i + Recall_i}.$$

4.3.4. Accuracy

Accuracy is the proportion of correctly classified samples. It is formulated as follows:

$$\text{Accuracy} = \frac{1}{n}\sum_{i=1}^{n} Accuracy_i,$$

where $Accuracy_i$ represents the accuracy of class i and is given as:

$$Accuracy_i = \frac{TruePositive_i + TrueNegative_i}{TotalSamples_i}.$$

The value of precision, recall, F1-score, and accuracy are between [0,1], with 1 indicating good and 0 indicating poor.

4.4. Results

4.4.1. Comparative experiments

In the experiments, we compare the classification results with the deep learning method MLP and the traditional ML methods DT, SVM, KNN and Adaboost. The comparison models are implemented using the Scikit-learn module, and we take average of 20 runs of each model.

Table 3
Partial symptom display of the syndrome differentiation dataset TSD.

Diagnostic type	Symptoms and types included in the syndrome differentiation dataset			
Inspection	Inspection of vitality (presence of vitality, unconsciousness, ...)	Inspection of physique (cachexia with withering bones, obesity, ...)	Tongue inspection (light red tongue, enlarged tongue, ...)	...
Listening and smelling	Listen to voice (faint low voice, hoarseness, ...)	Listen to language (delirious speech, stuttering, ...)	Smelling (delicious taste in mouth, fetid mouth odor, ...)	...
Inquiry	Inquiry about cold and heat (aversion to cold, fever, ...)	Inquiry about sweating (great dripping sweating, without sweating, ...)	Inquiry about pain (abdominal pain, headache, ...)	...
Pulse taking and palpation	Pulse position (floating pulse, deep pulse, ...)	Pulse rate (rapid pulse, slow pulse, ...)	Pulse shape (surging pulse, thready pulse, ...)	...

Table 4
Classification algorithm comparison results.

Model	Precision(%)	Recall(%)	F1-score(%)	Accuracy(%)
KNN [8]	60.12 ± 6.28	58.20 ± 5.96	59.16 ± 5.84	59.62 ± 5.98
Adaboost [9]	62.46 ± 6.55	6084 ± 6.98	6120 ± 6.23	62.14 ± 6.24
DT [6]	64.14 ± 6.44	63.58 ± 6.32	63.86 ± 6.42	64.10 ± 6.50
SVM [7]	65.30 ± 6.22	63.82 ± 5.98	64.68 ± 5.96	65.28 ± 6.04
MLP [7]	72.24 ± 5.63	70.44 ± 5.42	71.20 ± 5.34	72.32 ± 5.60
DL-TCM	**89.62 ± 5.20**	**87.42 ± 5.05**	**88.40 ± 5.14**	**89.24 ± 5.19**

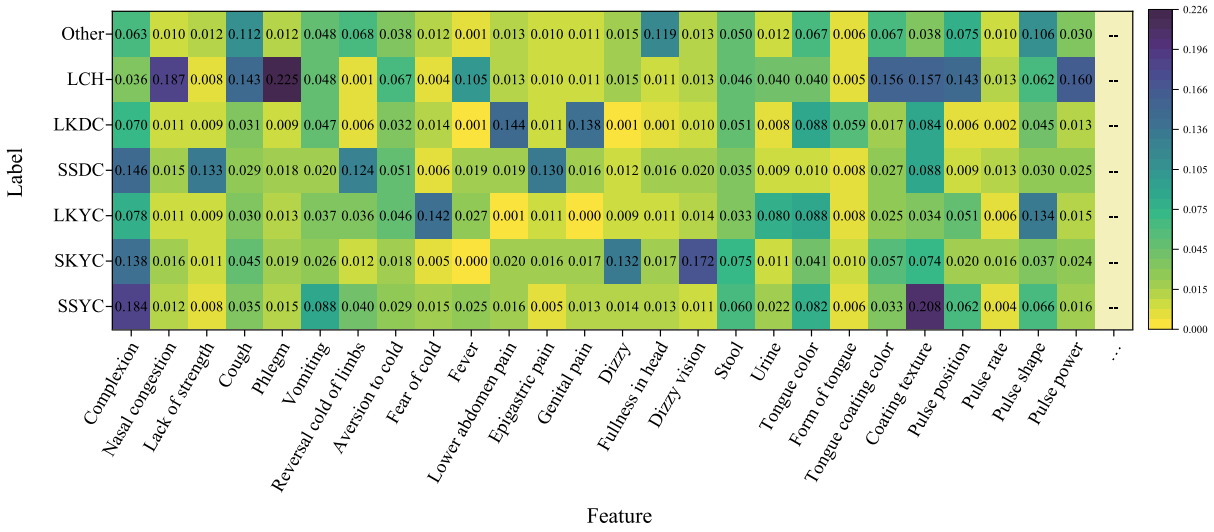

Fig. 5. Heat map of the association between symptoms and syndromes.

Table 4 shows the numerical results of the proposed model and the comparison models for classification.

From the results in Table 4, the DL-TCM model is significantly better than the other five models in terms of classification of syndrome differentiation. A three-layer perceptron model is used for our comparison, and DL-TCM outperform it by 16.92% in terms of accuracy. At the same time, we see that traditional ML methods are not competitive. The large number of features and limited samples lead to mediocre performance of both deep learning models and ML models.

Fig. 6 depicts the training and testing accuracy of DL-TCM over 4000 epochs. As the number of epochs increases DL-TCM achieves competitive training accuracy, i.e., 0.8988, and validation accuracy, i.e., 0.8922. The initial accuracy values start at 0.0725 at epoch 1 and do not change significantly after epoch 1600, eventually stabilizing around 0.89.

Subsequently, we plot the loss function for the training and test datasets for 4000 epochs, as shown in Fig. 7. This learning curve shows the decay of the cross-entropy loss function relative to the number of epochs, which helps predict whether our model is fit, underfitted or overfitted for both the test and training datasets. From Fig. 7 we see that both the training and test loss functions decay as the number of epoch increases, with 1.1735 for the training dataset and 1.1680 for the test dataset at epoch 4000. After 3200 epochs, the training and test losses stabilize at the same point. Thus, the model successfully captures the classification pattern.

Finally, Fig. 8 depicts the combined performance metrics of the 4000 epochs. In epoch 4000 compared to the other two performance metrics, the precision value is high, i.e., 0.8956. Our model shows no significant change after 3200 rounds. It can also be seen in Fig. 8 that the recall at epoch 4000 is lower than the precision and F1 score, i.e., 0.8745. meanwhile, it stabilizes to a value after epoch 4200. Also, regarding the F1-score, the value at epoch 4000 is 0.8838 and it does not show any significant change after epoch 3200.

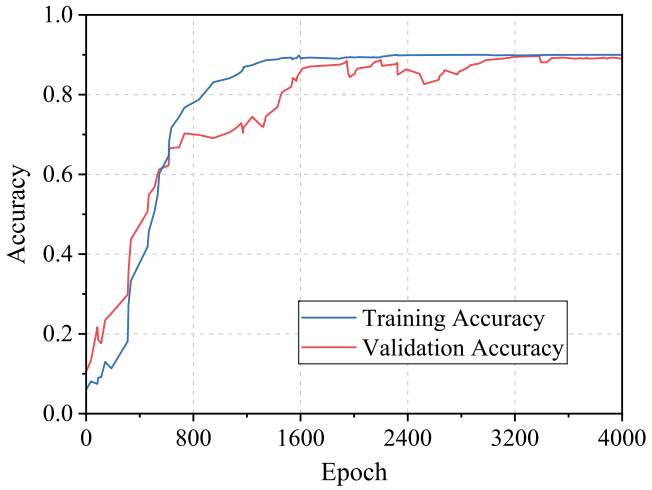

Fig. 6. Training vs. validation accuracy of DL-TCM for 4000 epochs.

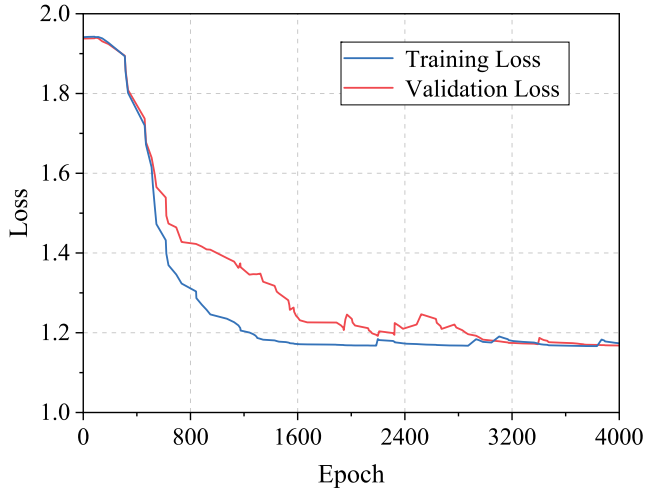

Fig. 7. Training vs. Testing loss functions of DL-TCM.

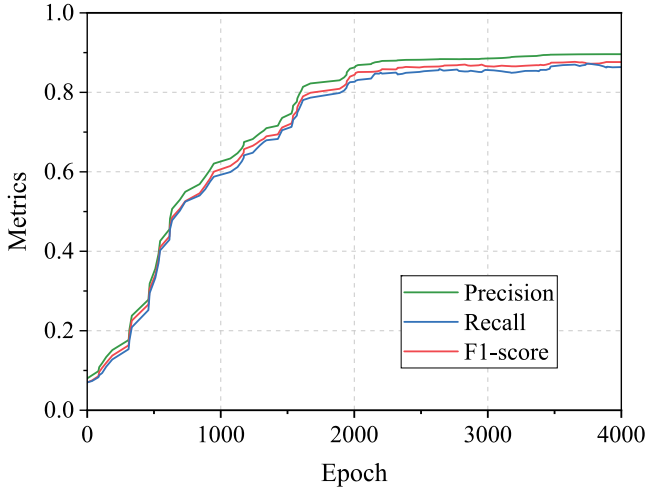

Fig. 8. Comparison of performance metrics of DL-TCM over 4000 epochs.

4.4.2. Ablation experiment

We perform the ablation experiment on DLTCM. The influence of the disease cause, the disease location attention layer (DAL) and TCM knowledge constraint layer (TCL) on the model effect is observed by removing them respectively. We try to keep the experimental setup the same in the ablation experiment except for module additions and subtractions. Experimental results are used to assess their importance to the overall model performance and thus to understand their contribution or role.

As shown in Table 5, we first experiment with a baseline model, a three-layer MLP without any additional module, which has an accuracy of 72.32%. We then add the disease cause, the disease location attention layers to the baseline model. Since these two layers need to be spliced in the calculation, it is impossible to remove one of the modules separately. So we combine the disease cause, the disease location attention layers together for the experiment denoted by TCL. Experimental results show that the overall performance of the model has been improved after the addition of TCL module, and the accuracy rate has reached 79.28%, which is 6.96% higher than the baseline model. This indicates that etiology and locus attention mechanism play a positive role in the performance of the model. Similarly, we add a TCM knowledge constraint layer module called TCL to the baseline model and get results that improve model's performance. Specifically, the model accuracy reaches 80.16% after the addition of TCL module, an increase of 7.84% compares to the baseline model.

In conclusion, the disease cause, the disease location attention layers and TCM knowledge constraint layer all play a positive role in the performance of the model. Moreover, the performance is optimal when the two are combined into the DL-TCM model.

5. Discussion

This study proposed a deep-network TCM syndrome differentiation method called DL-TCM based on first-order logical constraints. By embedding the attention mechanism based on domain knowledge of disease cause and disease location into deep network, and combining domain knowledge of first-order logical form with deep network, the accuracy of TCM syndrome classification is greatly improved.

In the experiment, we respectively compared with traditional machine learning methods (KNN, Adaboost, DT, SVM) and deep learning methods (MLP), and the results showed that our proposed DL-TCM had outstanding performance in syndrome classification. For traditional machine learning methods, due to insufficient amount of TCM clinical data and too many symptoms of patients in each piece of data, that is, the number of data samples is small but the data dimension is large, which leads to poor performance of traditional machine learning in this task. For deep learning methods, the sparse feature matrix and insufficient sample size also fail to get good classification results. We design a disease cause and disease location attention mechanism for DL-TCM, which can enhance the feature representation conducive to syndrome differentiation, while using first-order logic rules to constrain the network. In order to verify the effect of the designed two deep network layers on the overall model enhancement, we conducted ablation experiments. The experimental results show that the first-order logical constraint layer plays a stronger role in the performance improvement of the model, but on the whole, the two modules we designed play a positive role in the performance improvement of the model.

In general, it is the first time to use first-order logic rules to express the knowledge of TCM syndrome differentiation. The TCM diagnosis knowledge base constructed by us provides theoretical basis for the intelligent syndrome differentiation of TCM. At the same time, we design a set of mapping functions to combine the non-differentiable first-order logic with the deep network to improve the classification effect of the model. In addition, the TCM syndrome differentiation dataset constructed by us has detailed labels including diseases, syndromes and patterns, which provides a data basis for the modernization of TCM. However, this study is only limited to the identification of syndromes, and the further understanding of the disease, such as pattern recognition, is not supported. In addition, we should use data on more types of disease to train the generality of the model. We will carry out the next step to address the above limitations of this work.

Table 5
Ablation experiment results.

Module	DAL	TCL	Precision(%)	Recall(%)	F1-score(%)	Accuracy(%)
MLP	✗	✗	72.24 ± 5.63	70.44 ± 5.42	71.20 ± 5.34	72.32 ± 5.60
Model 1	✓	✗	79.21 ± 5.56	79.15 ± 5.38	79.19 ± 5.43	79.28 ± 5.61
Model 2	✗	✓	80.16 ± 5.33	80.16 ± 5.30	80.16 ± 5.41	80.16 ± 5.45
DL-TCM	✓	✓	89.62 ± 5.20	87.42 ± 5.05	88.40 ± 5.14	89.24 ± 5.19

6. Conclusion

In this paper, we propose a TCM syndrome differentiation model based on a deep learning approach. We tried to combine TCM diagnostic knowledge in the form of first-order logic with deep neural networks to improve network performance. The knowledge of TCM diagnosis we use is based on disease cause and disease location, which has positive significance for the reliability of the field of smart TCM. We conducted comparison experiment and ablation experiment, and the experimental results show that our proposed DL-TCM algorithm is competitive. At the same time, we present the collected data of 40,000 formatted TCM medical records, which few researchers have done so far. In future work, we will use more types of syndromes to increase the generality of our proposed model. At the same time, try to further identify the degree of disease development on the basis of syndromes, such as pattern differentiation. In addition, the TCM syndrome differentiation dataset TSD will be continuously improved.

Declaration of competing interest

We declare that we have no financial and personal relationships with other people or organizations that can inappropriately influence our work, there is no professional or other personal interest of any nature or kind in any product, service and/or company that could be construed as influencing the position presented in, or the review of, the manuscript.

Data availability

Data will be made available on request.

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