



## Visualized study on formulation regularities of decoctions in traditional Chinese medicine

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### ABSTRACT

Decoctions have been always playing an important role in Traditional Chinese Medicine (TCM). In this paper, we presented a discovery method of the knowledge of traditional classical prescription (TCP) in TCM. This work was based on the theory of formal concept analysis (FCA), and by the construction and study of an attribute partial order graph of the context of Cassia twig decoction and its derivatives that was chosen from Zhongjing Zhang's "Treatise on Febrile Diseases", a historical masterpiece in TCM. The visualized results indicated that we can obtain complete hierarchical structure and find knowledge from the partial-order attribute diagram constructed from the context of TCPs.

**Key words:** Traditional Chinese Medicine (TCM), Cassia twig decoction, knowledge discovery, partial-order attribute diagram, formal concept analysis (FCA)

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### INTRODUCTION

In clinic, herbs or decoctions of herbs play an important role in traditional Chinese Medicine (TCM). Based on four ways of diagnoses (looking, listening, questioning and feeling the pulse), prescription is given to a specific patient by a doctor of TCM. Generally, a number of herbs are combined to form a formulation that used to make a kind of decoctions for treatment. The prescription mainly depends upon the doctor's own experience and knowledge of other experts. It is an important research topics in TCM that how to inherit and develop this kind of experts' knowledge. To solve this problem, we must firstly find and study the knowledge discovery method of traditional classical prescription (TCP) in TCM [1-2].

In recent years, researchers and scholars in the world have done lots of researches in this domain. For example: Jinhua Tao etc. using the frequent pattern mining algorithm for knowledge discovery and comparison of high frequency in prescription medication of Chinese prescription database and obtained a series of experimental results [1]. Zhang, Nevin L etc. studied the regularities in the use of drugs in traditional Chinese medicine prescriptions [3]. Chen Hua-Jun discussed the national semantic infrastructure for traditional Chinese medicine [4]. Rui Jin etc. studied the principle of Chinese medicinal property theory learned from strong association rules using many-to-one mapping method [5]. Dettner Dion etc. studied a co-evolving memetic wrapper for herb-herb interaction analysis in TCM informatics [6]. Stranieri etc. did data mining work in TCM also [7]. Zhou, X etc. studied the development of traditional Chinese medicine clinical data warehouse for medical knowledge discovery and decision support [8]. Shaojie Qiao etc. studied about the knowledge discovery system for traditional Chinese medicine [9]. Though progresses have been made, we are still far from the aimed destination because of the complexity of pharmacology knowledge in TCM. In recent years, some new algorithms have attracted the attention of researchers, such as rough set and neural network [10]. Hong wenxue

etc. introduced the theory of formal concept analysis (FCA) [11] into the knowledge discovery in TCM and achieved some good results [12-13]. Partial order structure has the advantages of concise concept hierarchy, no cross connection, clear category meaning and distinct hierarchical relationship. So it is meaningful to study on TCP knowledge discovery basing on FCA theory method mentioned above.

In this paper, we presented a text mining and knowledge discovery method of the context of formulations of decoctions in TCM. This work was based on the theory of formal concept analysis (FCA), and by the construction and visualization of an attribute partial order graph of the context of Cassia twig decoction and its derivatives that was chosen from Zhongjing Zhang's "Treatise on Febrile Diseases", a historical masterpiece which still has important instructive significance in clinic practice now.

## EXPERIMENTAL SECTION

### CONTEXT (DATA) PREPARING AND PROCESSING DIAGRAM

The process of this study is shown in Figure 1: firstly, determine the keywords to obtain the raw data, and then the data was standardized. Second step is to establish the form background of Cassia twig decoction and its derivatives. Third step: optimization, reduction on the form background constructed. And then, we calculated and generated the partial-ordered attribute diagram (chart of prescription group) basing on the FCA theory. Finally, we discussed the regularities and rules obtained from the partial-ordered attribute diagram. Concepts and knowledge discovered here can be used to find important factors related to efficacy in clinic treatment.

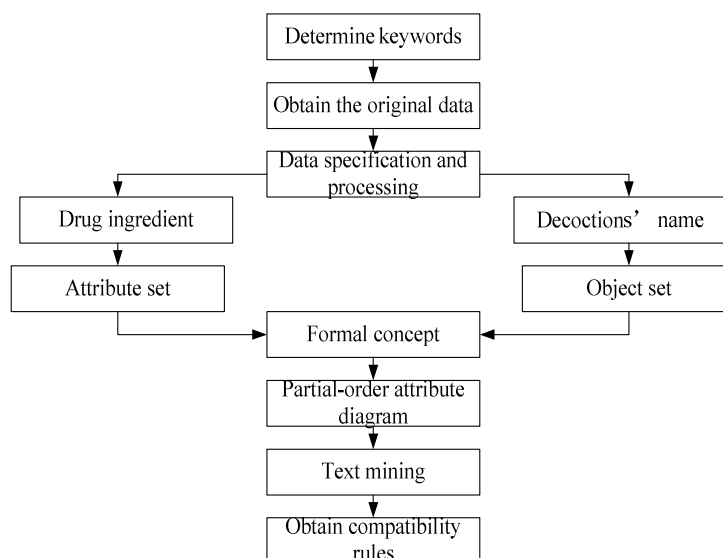


Fig.1 Flow chart of this study

### FORMAL CONCEPT ANALYSIS (FCA) THEORY FOR DATA PROCESSING

The formal concept analysis data is expressed by context, the definition is given formally as follows.

**Definition1 Formal context:** A formal context  $K=(U, M, I)$  consists of two sets  $U=\{u_1, u_2, \dots, u_n\}$  and  $M=\{m_1, m_2, \dots, m_k\}$  and a relation  $I$  between  $U$  and  $M$ . The elements of  $U$  are called the objects and the elements of  $M$  are called the context. Suppose  $m \in M$ , we define  $g(m)=\{u \in U \mid (u, m) \in I\}$  which denotes the object set of attribute  $m$ , meanwhile, suppose  $u \in U$ , we define  $f(u)=\{m \in M \mid (u, m) \in I\}$  which denotes the attribute set of object.

#### ATTRIBUTE DEFINITION

**Definition 2 common attribute:** Suppose there is a formal context  $K=(U, M, I)$ , if the attribute  $m \in M$  satisfies the following conditions:

- (1)  $\{g(m) \mid m \in M\} \neq U$ , and
- (2)  $m_i \in M - m$ , such that  $g(m) \not\subset g(m_i)$ ,  $i=1, 2, 3, \dots, n$ , and
- (3)  $m_i, m_j \in M$ , such that  $g(m_i) \cup g(m_j) \subset g(m)$ ,  $i, j=1, 2, \dots, n$ , then we call  $m$  the common attribute.

**Definition3 derivative attribute:** Suppose there is a formal context  $K=(U, M, I)$ , if the attributes  $m_i, m_j \in M$  and satisfy the condition that  $g(m_i) \in g(m_j)$ , then we call  $m_i$  the derivative attribute of  $m_j$ .

**Definition4 unique attribute:** Suppose there is a formal context  $K=(U, M, I)$ , if the attributes  $m \in M$  satisfy the following conditions:  $|g(m)|=1$ , then we call  $m$  the unique attribute.

#### STANDARDIZATION AND CONSTRUCTION OF FORMAL CONTEXT

There are two difficulties in prescribing decoctions in clinic in TCM, one is to determine the formulation of a decoction, that means how many herbs will be included. Another is the quantity of each herb in a decoction. For the cassia twig decoction is one of Zhongjing's "the most famous Prescription", we select his cassia twig decoction and its derivatives as the original data (the context) for study. We aimed at finding and visualizing the regularities of this group of decoctions when Zhongjing used them to cure one kind of disease. Follow the procedure showed in Fig.1, we obtained the optimized form background as Fig.2, the horizontal direction from a1 to a19 representing the attributes and the vertical direction from o1 to o19 are objectives.

	a1	a2	a3	a4	a5	a6	a7	a8	a9	a10	a11	a12	a13	a14	a15	a16	a17	a18	a19
o10	●	●	●	●	●														
o14	●	●	●		●								●	●		●			
o6	●	●	●	●							●								
o15	●	●	●		●														
o13	●	●	●		●	●													
o18	●	●																	
o7	●	●	●	●	●										●				
o11	●	●	●	●	●														
o12	●	●	●	●	●														
o17	●	●	●											●		●			
o3	●	●	●	●	●		●	●											
o5	●	●	●	●	●	●													
o9	●	●	●	●	●														●
o4	●	●	●	●	●				●	●									
o16	●	●			●														●
o8	●	●	●	●	●												●		
o19	●		●	●	●							●							●
o1	●	●	●	●	●			●		●									
o2	●	●	●	●	●			●		●									

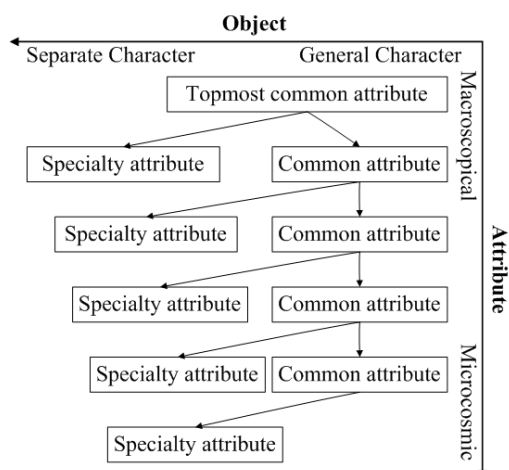
Fig.2 The formal context of the Cassia twig decoction and its derivatives

Index for objects (decoctions) : {o1:Cassia twig-Ephedra 1:1 Integrated Decoction, o2:Cassia twig-Ephedra 2:1 Integrated Decoction, o3:Cassia twig Decoction plus Mangnolia officinalis Bitter apricot seed, o4:Cassia twig-Spleen effusing 2:1 Integrated Decoction, o5: Cassia twig Decoction plus Monkshood, o6:Cassia twig Decoction plus Rheum officinale, o7:Cassia twig Decoction plus Pueraria, o8: Small Jianzhong Decoction, o9:Cassia twig Decoction plus Peony Fresh giner Ginseng, o10: Cassia twig Decoction, o11:Cassia twig Decoction plus Peony, o12: Cassia twig Decoction plus Cassia twig, o13: Cassia twig Decoction minus Peony plus Monkshood, o14:Cassia twig Decoction minus Peony plus Antifebrile dichroa branchlet and leaf Fossil fragments Concha ostreae, o15:Cassia twig Decoction minus Peony, o16: Poria cocos Cassia twig Liquorice and Chinese-date Decoction, o17:Cassia twig Liquorice Fossil fragments and Concha ostreae Decoction, o18:Cassia twig and Liquorice Decoction, o19:Cassia twig Decoction minus Cassia twig plus Poria cocos White atractylodes }.

Index for attributes (herbs) : a1:Liquorice, a2: Cassia twig, a3: Fresh giner, a4: Peony, a5:Chinese-date, a6: Monkshood, a7: Mangnolia officinalis, a8: Bitter apricot seed, a9: Gypsum, a10: Ephedra, a11: Rheum officinale, a12: White atractylodes, a13: Antifebrile dichroa branchlet and leaf, a14: Concha ostreae, a15: Pueraria, a16: Fossil fragments, a17: Gum yee, a18: Ginseng, a19: Poria cocos }.

#### CALCULATION OF THE PARTIAL-ORDER ATTRIBUTE DIAGRAM

According to the FCA theory, by programming in the environment of VSTO 2010, we can calculate the data in Fig.2 to generate the partial-order attribute diagram. Fig.3 is a conceptual view of general partial-order attribute diagram. The Hierarchical structure can be used to find common and special attributes. In this paper, the authors introduced it to find concepts and knowledge in TCP. Detail refers to the section of results and discussion.

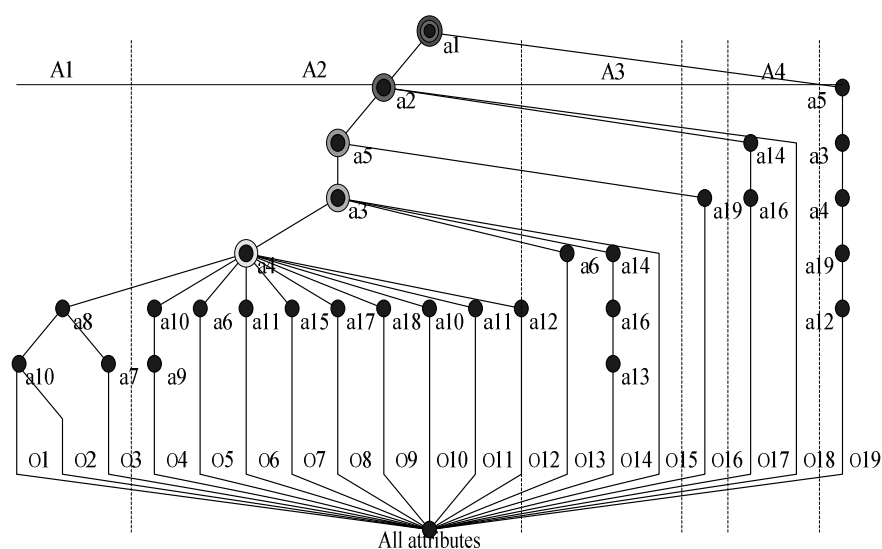
**Fig.3 The conceptual view of the partial-order attribute diagram**

## RESULTS AND DISCUSSION

The partial-order attribute diagram of the Cassia twig decoction and its derivatives calculated from Fig.2 is shown as Fig.4. where clusters (derivative decoctions): A1 cluster: the compound recipe of Cassia twig and Ephedra Decoction, A2 cluster: Cassia twig Decoction plus Peony, A3 cluster: Cassia twig Decoction plus Fresh giner, A4 cluster: Cassia twig Decoction plus Fossil fragments and Concha ostreae and Poria cocos.

It is known that the Cassia twig Decoction is composed of the five attribute elements a1-a5, o1-o15 derived from this through adding one or two herbs or replaced one based on it, thus the five attribute are the habit combination medication prescription to use of Cassia twig Decoction. Fig.4 indicates that the addition and subtraction relationships between Cassia twig Decoction and each other formulations of decoctions. This visualized result has important significance.

In Fig.4, branches of o6 and o11 are exactly the same, but in fact they are different in the amount of peony, this can be verified by other authoritative discourses. The different efficacies because of different doses. Cassia twig is the main ingredients of the Cassia twig Decoction, its main function is to relieve muscle surface fever and pain feeling of a patient with the syndrome of cold and sweat; however the main medicine in Cassia twig Decoction plus Peony is Peony, aimed at effect of treating Taiyin disease in empirical, dredging the main and collateral channels of spleen and stopping abdominal pain.

**Fig.4 The partial-order attribute diagram of the Cassia twig decoction and its derivative**

**THE COMMON ATTRIBUTE——THE HIGH FREQUENCY MEDICATION**

The partial-order attribute diagram is constructed layer by layer based on the inclusion relationship among attributes, so the high frequency properties must be located in the higher layer. Although research object of this paper is studying on the Cassia twig decoction, Cassia twig did not figure in the first layer, attribute element which situated on the first layer is the "Liquorice", because there is a prescription o19 does not have the "Cassia twig" attribute. The fact that each prescription here contains "Liquorice" reflects that Liquorice is the highest frequency medication in the most common attribute in this group of TCP due to its medical function of reconciling.

Secondly, attribute element which situated on the second layer is the "Cassia twig" and "Chinese-date", is in accordance with the premise that "Cassia twig" as keywords in the text mining of these nineteen decoctions.

**THE DERIVATIVE ATTRIBUTES**

In clinic, a decoction maybe has different efficacies due to adding one or more ingredient herbs. Such as a1 and a2 in Fig.4, branches contain the objects in a2 are all belong to a1, meet the associated definition of the derivative attribute. On the other hand, it demonstrated the rule that a1 and a2 as the combination used in Cassia twig Decoction frequently.

From the Cluster Perspective, there are four paired drugs in Cassia Twig Decoction generally, they are Cassia Twig—Peony, Cassia Twig—Liquorice, Peony—Liquorice, and Fresh ginger — Liquorice, as shown in Fig.4, the four paired herbs are on positive correlation, can work in with each other. Cassia Twig—Peony, cassia twig match with Peony is "opposite and complementary", through the opposing functions both of them, cassia twig dredging the main and collateral channels of spleen, peony clear heat and cool blood, two-way adjustment, thereby restoring the body to healthy and balanced state. From the perspective of dialectical treatment of TCM, combined with fresh ginger and ginseng is scientifically reasonable. Decoction combined with fresh ginger and Monkshood accords with the four inverse methods in TCM.

**THE UNIQUE ATTRIBUTE (UNIQUE KEYWORD)**

If a property is included only in one branch, then the attribute is the unique attribute. This means a very high value for text mining research. In Fig.4, because o4 and o10 also have the a10 attribute, and in addition to o3, other objects do not contain the a7 attribute, so a7 is the unique attributes, while a10 is not. The o3 is composed of the Cassia twig decoction plus Bitter apricot seed is bitter and warm, has the function of ventilating the lung and resolving phlegm, relieving cough and asthma. Therefore, this prescription has the function of expelling wind. It is still known as a famous cough remedy decoction.

Analysis above indicates that we can do much more refined text mining research following the branches of the partial-order attribute diagram. Hierarchical structure of the partial-order attribute diagram can be used as a visualized approach in studying on the formulations of decoctions in TCM.

**CONCLUSION**

Based on the FCA theory, this paper presented a partial-order attribute diagram method for studying on the formulations of decoctions in TCM. As an example, the author selects the context of Cassia twig decoction and its derivatives which was chosen from Zhongjing Zhang's "Treatise on Febrile Diseases", a historical masterpiece in TCM. Through the related concepts of "properties" in the formal context, the author analyzed some typical findings respectively. Regularities found in the context are all consistent with the theory of traditional Chinese medicine. These findings verified the feasibility and scientific significance of this research method.

Generally speaking, the hierarchical structure of the partial-order attribute diagram can be used as a visualized approach in studying on the discovery of knowledge and regularities in the use of herbs in TCM as well as other domains such as modern pharmaceutical industries.

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