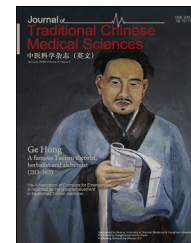


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# Expression model for multiple relationships in the ontology of traditional Chinese medicine knowledge

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## KEYWORDS

Multiple relationships;  
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In traditional Chinese medicine knowledge**Abstract Objective:** To explore multiple relationships in traditional Chinese medicine (TCM) knowledge by comparing binary and multiple relationships during knowledge organization.**Methods:** Characteristics of binary and multiple semantic relationships as well as their associations are described. A method to classify multiple relationships based on the involvement of time is proposed and theoretically validated using examples from the ancient TCM classic *Important Formulas Worth a Thousand Gold Pieces*. The classification includes parallel multiple relationships, restricted multiple relationships, multiple relationships that involve time, and multiple relationships that involve time restriction. Next, construction of multiple semantic relationships for TCM concepts in each classification using Protégé, an ontology editing tool is described.**Results:** Protégé is superior to a binary relationship and less than ideal with multiple relationships during the constitution of concept relationships.**Conclusion:** When applied in TCM, the semantic relationships constructed by Protégé are superior than those constructed by correlation and/or attribute relationships, but less ideal than those constructed by the human cognitive process.© 2016 Beijing University of Chinese Medicine. Production and hosting by Elsevier B.V. This is an open access article under the CC BY-NC-ND license (<http://creativecommons.org/licenses/by-nc-nd/4.0/>).

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## Introduction

Traditional Chinese medicine (TCM) entered the digital era when computer science was introduced into the research of the subject.<sup>1</sup> A large amount of ancient literature on TCM is stored in text. Software is used to present and summarize research results, and predict the evolution of the corresponding disciplines.<sup>2–6</sup> As the expectation of using computers to simulate human thinking has increased, digitization not only means the simple storage of information, but also the storage of information in a way that simulates human thinking. The method for developing software has become object-oriented programming instead of structured programming. Data analysis has been transferred to big data techniques<sup>7,8</sup> from previous statistical and data mining methods.<sup>9–11</sup>

Big data analytics are the main method for researching huge, complicated and associated data, and can be applied to analyzing rules and forecasting related knowledge from data.<sup>12</sup> TCM data belong to intellect-intensive data and have the following features: integrity, hybridity, and relativity. Although the storage content of TCM information is not sufficiently big, Cui et al.<sup>13</sup> believe that TCM data satisfy the requirement of full-scale data,<sup>14</sup> which makes it possible to treat them as big data. Thus, the techniques for investigating big data can be used to process TCM data. Li et al.<sup>15</sup> of the Chinese Academy of Engineering, hold that when analyzing big data, their underlying complex networks, that is, the relational networks that have knowledge structure, need to be analyzed. Thus, the prerequisite for analyzing information for a given field is a proper knowledge model, which can transform information stored in the form of natural language into a form that computers can understand, and make the simulation of human thinking possible.

At present, knowledge models for TCM have been proposed, possessing inquiry, search, and simple inference functions,<sup>16–25</sup> and some models can even exchange information between systems.<sup>26,27</sup> At the same time, the knowledge model for imitating the human brain is still being explored. The object-oriented development method considers the elements of the system as objects in the real world, using terms that are similar to those used in the given field, which makes a computer more similar to the human mind.<sup>28</sup> This is beneficial for analyzing, designing, and programming complex systems. Among these methods, the Unified Modeling Language (UML) is the standard modeling language that dominates the object-oriented field. Ontology is the main development tool for using UML to establish object-oriented models.<sup>29</sup> The semantic models developed by ontology simulate storing information, as the human brain does, which is a proper method for organizing and expressing knowledge, and demonstrates the relational network between pieces of information to a certain degree. The establishment of semantic networks developed by ontology is the precondition for investigating TCM knowledge using big data technologies.

The unified traditional Chinese medical language system (UTCMLS) is the most extensively used semantic network system in the TCM field. UTCMLS was built by the China Academy of Chinese Medical Sciences (CACMS) in 2002 using

ontology.<sup>16</sup> Since then, many research institutions have begun to build semantic networks of TCM.<sup>18,21,30</sup> The building of semantic networks simulates human thinking mainly through constructing relationships between concepts.<sup>31</sup> For some time, this type of method has been limited to the binary relationship construct or has transformed multiple relationships into binary relationships.<sup>32</sup> Semantic relationships in TCM are complicated and multiple relationships in TCM arise almost everywhere. Thus, the discussion and research into multiple relationships in semantic networks is still in its early exploration stage.

Information is the carrier of knowledge and knowledge reacts to information. Computers can store and understand knowledge only through information transformation. The characteristics of TCM information include three aspects. First is the integrality of the meaning. Every piece of information recorded in TCM texts is independent, including basic information on patients, such as age and sex; symptoms; syndrome pattern; and treatment prescriptions. A meaningful knowledge expression conveys a patient's essential state using a complete set of information as presented by the patient. Second is the hybridity in semantics and grammar. The smallest unit in TCM information is the concept. The semantic network construction of a computer is based on conceptual extraction. The concept of TCM information includes a verb, conjunction and preposition at the semantic level, and subject–predicate form, verb–object form and postpositive attributive form at the grammatical level. Third is the complexity of semantics. The same word or word group expresses a different concept and is a different part of speech in different language environments.

The aforementioned characteristics demonstrate that it is very difficult to build semantic networks based on TCM information. Solving the divergence between grammar and semantics is the basis of constructing a semantic network, followed by maintaining the completeness of text information determines the transformation and consistent degree of storing information by the human brain thought analogy.

Through an extensive investigation of ancient TCM works, we found that TCM knowledge is not only a binary relationship, but also a multi-relationship. Based on this understanding, we used the ontology software Protégé to construct a semantic network of the ancient TCM classic, *Important Formulas Worth a Thousand Gold Pieces (Beiji Qianjin Yaofang)*. Our was to develop a multiple relationship expression of TCM information to resolve the completeness of the meaning of TCM. *Important Formulas Worth a Thousand Gold Pieces* is a seminal work in Chinese medicine published in the Tang dynasty in 652. It was written by Sun Simiao, the physician of extraordinary renown in Chinese medical history. The book summarizes pre-Tang medical cases and is believed to have greatly influenced the development of TCM in China. The work lists about 5300 herbal formulas and discusses a wide range of medical topics including gynecology, pediatrics, internal medicine, external medicine, emergency treatment, food therapy and health preservation, acupuncture, among other subjects. We chose this book as our research focus because of its significance the development of TCM and its

extensive records of treatments that are representative of nearly all types of multiple relationships in TCM.

## Binary and multiple relationships

The concepts of binary and multiple relationships originated in mathematics<sup>33</sup> and were later introduced in computer science. In computer ontology, binary and multiple relationships are used to describe the relationship between classes (class is a kind of abstract data; object is the abstraction of objective things; and class is the abstraction of the object<sup>34</sup>). The relationship between class and instance (instance is the construction of the specific object according to the class<sup>34</sup>), and the relationship between instances, which belongs to an expression pattern of subsets are described by binary and multiple relationships. A binary relationship is the relationship between two classes or two instances and often manifests as relationship between two concepts in the knowledge expression. Multiple relationships refer to the relationships among three classes, three instances, multiple classes and multiple instances, and often manifests as relationships among three or more concepts in the knowledge expression. Knowledge is classified as declarative and procedural from the point of view of the advanced cognitive domain. From the perspective of knowledge classification, declarative knowledge represents the property of knowledge that belongs to a binary relationship and procedural knowledge represents a cognitive process that belongs to multiple relationships.<sup>35</sup> For example, in *Important Formulas Worth a Thousand Gold Pieces*, Sun Simiao states “the tongue is the officer of the heart.” This is declarative knowledge and expresses a binary relationship. Sun also states, “when the disease is in the heart, it appears alleviated in the daytime, deteriorate at midnight, and is tranquil in the morning.” Thus, changes in pathology of the heart at different times of the day belongs to procedural knowledge, which expresses multiple relationships among disease, time, and change. Midday, midnight, and morning represent different time periods. Changes in pathology as expressed by “alleviated,” “deteriorated,” and “tranquil” represent changes in pathology.

Currently, the practice TCM ontology construction does not take into account the weight function on, for example, time, selection and limit, in the initial construction of ontology. Thus, this type of semantic network construction is limited only to a binary relationship. Multiple relationships are ignored when constructing ontology knowledge data in TCM or multiple relationship constructions are transformed into binary relationships.

A binary relationship applies to the construction of an objective attribution and incidence relation, which provides a reasonable method for classifying objects and their binary relationship. Multiple relationships within TCM exist everywhere. For example, at the present time, neither the earlier structuring method nor construction method for managing objects can resolve the difficulty in determining varying therapies for a same set of symptoms with different sequence of onset, or determining when to make component modifications according to different sets of symptoms.

Next, we discuss the types of multiple relationships in TCM and their construction based on Protégé.

## Multiple relationships in TCM knowledge

Multiple relationships in TCM knowledge can be divided based on the presence or absence of an involvement of time.

### Multiple relationships that do not involve time

#### Parallel multiple relationships

Parallel multiple relationships are associations among many concepts that belong to parallel relationships in the semantic network. In TCM knowledge, parallel multiple relationships that do not involve time are herbal prescriptions and syndrome patterns. An herbal prescription is typically comprised of several herbs with each herb ascribed a dose (dry weight). Thus, the relationships among all herbs in a prescription can be considered parallel.

#### Restricted multiple relationships

Restricted multiple relationships refer to associations among several concepts that are semantically restricted. In TCM knowledge, restricted multiple relationships that do not involve time are comprised of modifications. For example, in TCM a disease that presents with different symptoms is treated with a different modification based on the fundamental prescription. And, different diseases with the same symptoms are treated with different modifications of a fundamental prescription. Regardless of the situation, the herbs used are limited by both the disease and symptoms. That is, the modification of an herbal prescription is the intersection of the disease and symptoms, such that the relationships among herbs, the disease and symptoms are restricted multiple relationships. For example, in *Important Formulas Worth a Thousand Gold Pieces*, the symptom of “red urine” (concentrated urine) is mentioned twice: when there is red urine with a deficiency syndrome pattern, the herb scutellaria (*Huangqin*, 黄芩) should be added to the prescription Formula for Alcoholic Jaundice (*Jiudanzhe Fang*, 酒疸者方); and when there is a syndrome pattern of abdominal distension and red urine, the prescription should be used without *Huangqin*. Thus, the same symptom but different syndrome patterns require different modifications of the herbal prescription.

### Multiple relationships that involve time

Multiple relationships that involve time concept include timeline and time restriction.

#### Multiple relationships that involve time

These are relationships that emphasize early and late occurrences in a phenomenon. In TCM, these relationships are concerned with the incidence and development of diseases. Symptom occurrence and symptom nature, which include the concepts of early and late, are on a timeline forming the intersection and produces relationships with symptoms or drugs. Concepts on the timeline appear as a relation with two symptom concepts. Again, using an example from *Important Formulas Worth a Thousand Gold Pieces*, for patients with bloody stools, if blood is passed first followed

by stools, the formula Yellow Earth Decoction (*Huangtu Tang*, 黄土汤) should be used; if vice versa, Adzuki Bean Powder (*Chixiaodou San*, 赤小豆散) should be used. Thus, the sequence (timeline) of appearance of the two symptoms of passage of blood and passage of stool, are multiple relationships with the two prescriptions.

#### Multiple relationships that involve time restriction

These are relationships that emphasize the specific time of occurrence of a phenomenon. They contain the multiple relationships of onset, outcome, and treatment. With time restriction of onset and outcome, time is a restricted concept that limits the relationship between disease and outcome. Outcome and the intersection formed by the onset time and disease produce multiple relationships. In TCM, different organs have multiple relationships with disease, time, and disease outcome. For example, in *Important Formulas Worth a Thousand Gold Pieces*, it is said that "Disease in the heart appears alleviated at midday, deteriorated at midnight, and tranquil in the morning"; "Disease in the liver appears alleviated at midday, deteriorated in the afternoon, and tranquil at midnight"; "Disease in the kidney appears alleviated at midnight, deteriorated in the daytime and the four seasons, and tranquil in the afternoon"; and "Disease in the lungs appears alleviated in the afternoon, deteriorated at noon, and tranquil at midnight." In the treatment of disease, the intersection formed by treatment modality, disease, and time produce multiple relationships. A passage in *Important Formulas Worth a Thousand Gold Pieces* describes this concept: "Acupoints for heart disease are *Zhongchong* [PC 9] in the spring, *Laogong* [PC 8] in the summer, *Daling* [PC 7] in the long summer as an adjunct, *Jianshi* [PC 5] in the autumn, and *Quze* [PC 3] in the winter ... ." Thus, a disease that has an onset at different times (in this case, different seasons) is treated differently (in this case, with different acupoints), reflecting that the relationships among disease, acupoints, and time restriction are multiple.

#### Constructions of multiple relationships in TCM in ontology

In information science, ontology is a set of concepts in a domain, including their attributes and relationships.<sup>34</sup> The aforementioned ontologies for a TCM specialty, although aiming to simulate how the human brain develops concept relations, are universally based on a semantic relationship inferior to multiple relationships (though superior to binary relationships). In domain ontology, knowledge storage and multiple relationships are similar to the multi-modal combination in concepts. Our research used the ontology software Protégé to build multiple relationships to define an axiom of concepts and build semantic associations. We primarily used the Superclasses edit box in the axiom function in Protégé to edit multiple relationships (Figs. 1 and 2).

The multiple relationships in this study used "some," "any," and a self-defining semantic relation and semantic type for the purpose of construction. In Protégé, "some" represents optionality and means that there is at least one concept or any concept in the set that has a type of specific relation with another concept or any concept in the set;

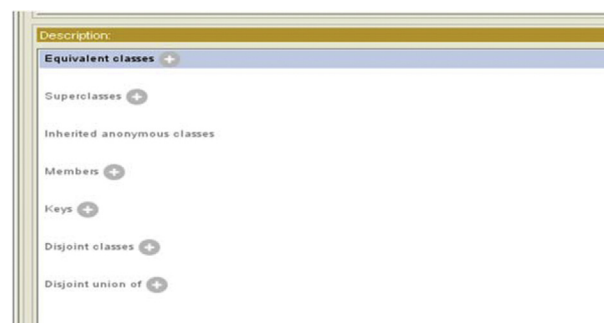


Fig. 1 Axiom text edit in Protégé.

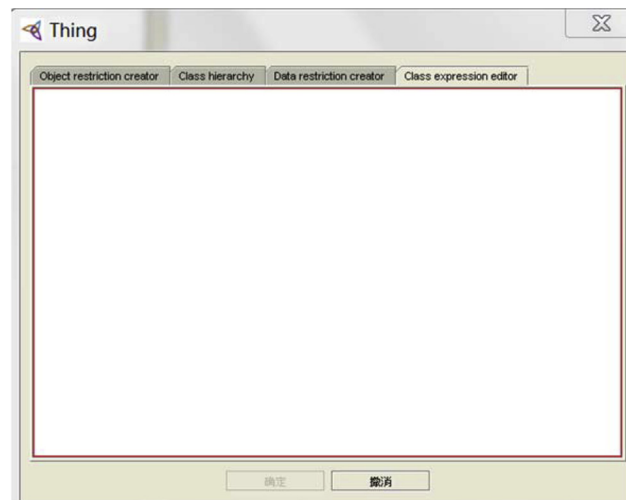


Fig. 2 Superclasses edit text in the axiom function.

and "any" represents uniqueness and means that one concept or any concept in the set has only one type of specific relation with another concept or any concept in the set. The relationships among most concepts belong to "some." The headword should be found first when building the expression model for multiple relationships using Protégé and then constituting a relationship around the headword. The headword is the concept, which is defined by the Protégé axiom editor. It is displayed as a theme in the cognition process, which includes a disease, prescription/drug, and outcome. It can unify other concepts into a central concept under a multiple relationship. For example, in the passage from *Important Formulas Worth a Thousand Gold Pieces* "Angina manifests blue fingers and toes; die in the night if it attacks in the morning and die in the morning if it attacks at night." All the symptom descriptions are centered around the headword "angina," thus "angina" is "the central word."

#### Construction of multiple relationships that do not involve time

##### Construction of parallel multiple relationships

The construction of parallel multiple relationships in the Protégé was accomplished by building associations between the headword and another set, and the concept that demonstrated a parallel relationship, which is also a



multiple relationship between the headword and other parallel concepts. Basic expression model of this kind of multiple relationship is “the headword relationship some (concept A and concept B and concept N).” As an example, a classic prescription described in *Important Formulas Worth a Thousand Gold Pieces* is Four Substance Pill with Tussilago (*Siwu Kuandong Wan*, 四物款冬丸). The text is “*Siwu Kuandong Wan* consists of 21.4 g (1.5 *liang*) *kuan dong*, 21.4 g (1.5 *liang*) *zi yuan*, 7.1 g (0.5 *liang*) *gui xin*, and 3.9 g (6 *zhu*) *fu long gan*.” (*Kuan dong* is the herb tussilago; *zi wan* is aster; *gui xin* is the inner bark of cinnamon; *fu long gan* is soot ash. *Liang* and *zhu* are units of weight.) The prescription contains four medicinals, and their relationships are equal and parallel. The set of parallel relationships formed by the headword “*Siwu Kuandong Wan*” and the four medicinals are “being constituted by...,” (Fig. 3) Note that because of the limitation of the Protégé axiom editor regarding the data property, it is not concerned with the problem of resolving the drug dose (weight).

### Construction of restricted multiple relationships

Restricted multiple relationships are associations between the headword and one or several concepts as constituted by the Protégé axiom editor. The concept being constituted must be limited by other concepts so that it can be related to the headword, which means it is preferable to build multiple relationships of the head-word, concept, and restricted concept. An expression model of this type of multiple relationship is “the head-word relationship some (concept A (relationship some restricted concept B)).” Taking the modification of medicinals based on symptoms as an example, the text is “if the patient is deficient and has yellow urine, *Huangqin* should be added.” The “*Huangqin*” and “yellow urine” have the relationship of treating and being treated, and is based on the syndrome pattern of “deficiency,” without which *Huangqin* would not be used. To summarize, there exist restricted multiple relationships among “*Huangqin*,” “yellow urine,” and “deficiency” (Fig. 4). 4.

### Construction of multiple relationships that involve time

#### Construction of multiple relationships that involve a timeline

The aim of this type of construction is to build a relationship between the headword and a set by establishing early

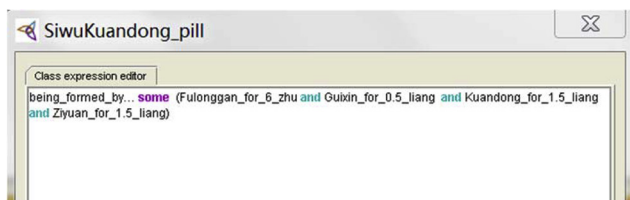


Fig. 3 Construction of parallel multiple relationships using an example of a prescription constitution. *Siwu Kuandong Wan* is the headword; “and” is the parallel connection between each medicinal; “()” is the gathering among the four medicinals; “being formed by ...” is the semantic relation for connecting the relationship between *Siwu Kuandong Wan* and the four medicinals.

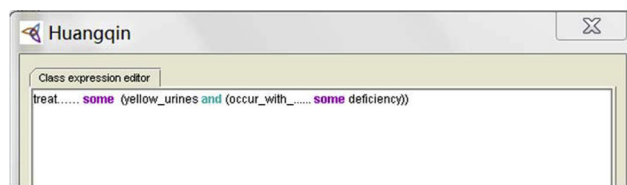


Fig. 4 Construction of restricted multiple relationships modification of medicinals with symptoms. *Huangqin* is the headword. “()” adjuncts “deficiency” and is used to restrict “yellow urine”; “occur with...” is used to connect “yellow urine” and “deficiency” and explains how “yellow urine” occurs; “()” adjuncts “yellow urine” and embodies the gathering of two symptoms; “yellow urine” is the main symptom, “treat...” is the semantic relation that connects the relationships between “*Huangqin*” and “yellow urine.”

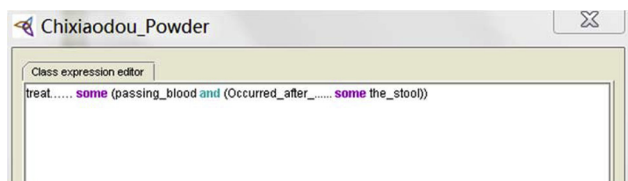
(“happening before”) and late (“occurred after”) times as a semantic relation. This has the semantic relationship of a timeline among concepts in the set, and is a type of special parallel relationship that involves time. The expression model of this type of multiple relationship is “the head-word relationship some (concept A and (happening before ... /occurred after ... some concept B)).” Taking the timeline of symptom onset as an example, the passage from *Important Formulas Worth a Thousand Gold Pieces* is, “for the patient who suffers from blood stools, if blood is passed first followed by stools, Yellow Earth Decoction (*Huangtu Tang*, 黄土汤) should be used; if vice versa, Adzuki Bean Powder (*Chixiaodou San*, 赤小豆散) should be used.” The timeline of “stool” and “blood” determines the constitution relationships with different headwords (Fig. 5).

### Construction of multiple relationships involving time restriction

Construction of multiple relationships involving time restriction mainly takes time as a concept and restricts other concepts through the semantic relation of “happening in ....” This type of relationship belongs to the special expression form of limiting multiple relationships and is used for details on an outcome in the cognitive process. An expression model of this type of multiple relationship is “the head-word relationship some (concept A and (happening in ... some concept B)).” Taking the outcome of disease in TCM as an example and the passage from *Important Formulas Worth a Thousand Gold Pieces*, “Disease in the heart appears alleviated at midday, deteriorated at midnight, and tranquil in the morning.” “Alleviated,” “deteriorated,” and “tranquil” are the results of the disease outcome, and “midday,” “midnight,” and “morning” are the time restrictions of the outcome. A time restriction holds meaning according to TCM theory. Therefore, it is very necessary for a construction of this type of cognitive process (Fig. 6).

## Discussion

At present, the semantic network is a common method applied to imitate the clinical thought process of doctors.



**Fig. 5** Construction of multiple relationships of a sequence of symptoms occurring in a disease. *Chixiaodou* Powder as the headword, states the sequence of “passing blood” and “stools” by building a semantic relation that involves time. “*Chixiaodou San*” has an association with “passing blood” and “stools” by virtue of a time semantic relation with “treat ....”



**Fig. 6** Construction of multiple relationships by taking the outcome of a disease involving time restriction. “Alleviated” is the headword and states the outcome relation of “heart disease” occurs at “midday” by building a semantic relation “happening in...” to restrict the time of “heart disease” occurrence and “result of ....”

The semantic network editor Protégé used in this research is recommended by the World Wide Web Consortium and holds good repute in China. Protégé is superior to a binary relationship and less than ideal with multiple relationships during the constitution of concept relationships. Therefore, when applied in traditional Chinese medicine, the semantic relationships constructed by Protégé are superior than those constructed by correlation and/or attribute relationships, but less ideal than those constructed by the human cognitive process. The present study was aimed at addressing this problem. This research divided multiple relationships during the cognitive process for TCM knowledge into four basic types according to whether there was a time factor. It discussed four basic expression models of multiple relationships using as examples the constitution of herbal prescriptions, symptom combination modification of medicinals, timeline of symptom occurrence, and relation and outcome of treatment, which conforms to the multiple associations that TCM practitioners must think in terms of during the diagnostic and treatment processes of a patient.

Research on building an expressional model of multiple relationships is a supplement to and serves to perfect knowledge model construction in the background of big data. This type of model is a foundation for analyzing the actual associations in traditional Chinese medicine knowledge. Protégé is not customized software for multiple relationships in TCM knowledge. The native language of Protégé is English and the expressional scheme is different than the Chinese language. Moreover, because of the complexity of the semantic expression of TCM knowledge, the model still has certain limitations, such as in querying, graphing, and displaying the existence of headwords. For

these reasons, much research remains to be done in computer/information science and in TCM to develop an autonomous model of multiple relationships in TCM knowledge.

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