

Research of Digital Based on Network Model in the Fingerprint of Traditional Chinese Medicines (TCM)

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Abstract. In this paper, a network model is used to simulate the fingerprint of TCM, the fingerprint is digitized, it is easy to store and display by simplifying the data processed. Application of digital processing technology and pattern recognition technology sets up the standard fingerprint. According to the standard fingerprint of TCM, Identify the quality and authenticity of the medicines, especially with the lack of medicines. It can realize medicinal materials testing in comprehensive evaluation of internal quality and overall control of the whole matter, according to the fingerprint of TCM. Improve the overall level of the TCM industry and promote the early development of the Chinese medicine industry to the world.

Keywords. Network model; Fingerprint of TCM; Digital pattern recognition

1 The introduction

With the development of the times and the development of medical technology, the research craze of TCM is on the rise. Compared with chemical drugs, Chinese medicine has the advantages of low toxicity side effects and remarkable clinical efficacy, more and more countries and regions have begun to pay attention to the unique diagnosis and treatment methods of Chinese medicine. With the increasing use of Chinese medicine, the quality supervision of TCM has become a popular research direction and the international medical research hotspot[1-2].

Because of the composition of Chinese medicine is complex, quality testing and analysis are difficult. The efficacy of Chinese medicine is restricted, growing environment, territory, collection time, collection site, processing method, storage method, for example[3]. The quality of Chinese medicine must be determined and controlled to ensure the safety and effectiveness of Chinese medicine. By analyzing the ingredients of medicinal materials, it is an effective method to determine the quality of Chinese medicine. The fingerprint of TCM has become an effective means to control the quality of various medicines[4-5].

2 Computer information processing in the fingerprint of TCM

The fingerprint of TCM is an effective method to detect medicine quality. The components of medicinal materials are monitored and evaluated by a variety of disciplines and comprehensive techniques. With the maturity of

various research theories, the integration of various technologies, the importance of applying computer data processing technology to the research of the fingerprint of TCM is gradually noticed[6]. The composition of is complex, the factors affecting the pharmacodynamic effect are more, so the accuracy of artificial fingerprint is open to discussion. It is imperative to combine the fingerprint of TCM with computer data analysis and pattern recognition technology.

With the use of fingerprint in the field of medicine detection and quality control, how to control the pharmacological information of pharmacological substances by fingerprint, Gradually turning into a mathematical method involving a large number of calculations to analyze and process data[7-10]. The common computer processing methods of medicine information data have regression analysis, cluster analysis, artificial neural network, and so on [11-17].

3 Network model and digital expression in the fingerprint of TCM

The fingerprint of TCM is a kind of map that can show the common peaks of certain medicine characteristics. It has the characteristics of overall similarity and individual ambiguity. At present, the application of TCM fingerprint technology is very wide. The digital information processing method urgently needs to be integrated into the fingerprint data processing. In order to explore the deep data relation of fingerprint map and improve the identification method of fingerprint map. At present, the application of signal and digital information processing technology to fingerprint is more and more. Some

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mathematical methods are also gradually applied to the analysis of the fingerprint map. But, some of these methods affect the integrity of the data, complicated, the retention value of chromatographic peak is unstable. These factors add to the difficulty of the analysis of the fingerprint. To resolve these issues, this paper proposes a new method to extract TCM fingerprint based on network diagram theory, the characteristics of fingerprint are simulated by using the graph of network. This kind of research method is clear and easy to understand. The unity of data integrity and fuzziness can be guaranteed.

3.1 Network model in the fingerprint of TCM

With the proliferation of modern analytical instruments, in particular, computer application technology and instrument analysis data fuse together. The data presented in this mode is intelligent and automated. The information on medicinal materials is huge, researchers have been unable to identify the relevant characteristics and internal rules of medicines with their subjective professional experience.

The simple pattern recognition has been unable to obtain the inherent law of data and valuable information. In this paper, the digital expression of medicine data is carried out using the network diagram structure. The data feature selection of pattern recognition field is combined with digital display. This fusion technique is used to analyze the original data set of TCM fingerprint. The information map can reflect the chemical characteristics of the medicine. This kind of digitized reticular structure is used to visually identify and evaluate the quality of medicine. The network model acquisition process of TCM fingerprint is shown below.

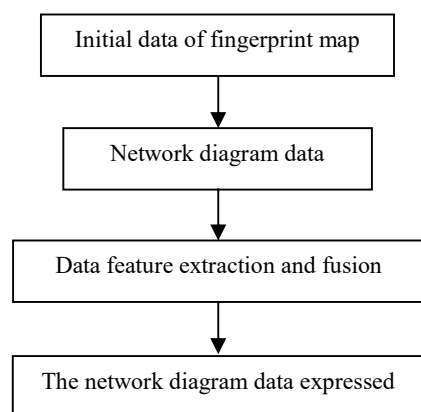


Figure 1. Flow Chart

3.2 Digital expression in the fingerprint of TCM

The data of fingerprint is presented, it is usually based on the integral result or the retention value data as the basis of data statistics. In the processing of data, first, the raw data is analyzed, ignore the external influence of the analysis system. Then a peak of the fingerprint was selected as the reference peak, compare the other peak data to it, based on the relative value obtained compare

the fingerprint patterns.

The basic principle of the digital chromatographic fingerprint is to determine a chromatographic peak as the reference standard in the chromatographic map of all the samples participating in the identification. This determined reference chromatographic peak exists in each sample to be identified. Use it to calculate the relative retention value of each peak. The relative retention value is relatively stable compared with that of the chromatographic peak retention value, the systematic error in the analysis data is eliminated, the drift of the retained value is reduced, in this way, the location of chromatographic peak is ensured. The fingerprint of TCM, which is based on relative retention value, is the digital fingerprint.

Select the peaks that are common to each sample, and the peak time in the residence as the reference peak, the calculation formula of relative retention value is follow, $\alpha = tR_i / tR_s$.

tR_i is the peak time of each group.

tR_s is the peak time of reference peak.

The fingerprint of TCM is transformed into easy-to-display data by means of information, by digitizing the fingerprint map, it makes the quality identification of medicine more convenient and more objective. Digital processing of massive data samples is carried out, fuzzy individual characteristics, it can get a more reliable standard fingerprint. In reality, it is difficult to determine the standard material, but the standard fingerprint map that is determined by technical means is relatively easy. According to the standard fingerprint map, able to identify the quality of medicinal materials.

4 Example analysis

This paper is based on the network diagram representation principle, the species of ginseng was studied by using near-infrared spectroscopy. The fingerprint map was extracted using the network diagram, ensure the integrity and the objectivity of the data. It is an effective research method.

The number of peaks detected when different wave body width is selected from the data of various experimental samples. The data table is as follows. The process flow diagram is as follows.

The peak detection procedure is applied to the peak detection of all sample data. Select the first eight crest characteristics, the characteristic mean of the sample data is used as the characteristic mode of the class. Draw the network diagram of all kinds of samples. The initial data set is composed of all the crest in the spectral curve, when it comes to the fusion of characteristics. The characteristic fusion method is using network diagram, parameter is setting 3 layers, characteristic optimization techniques adopt improved genetic algorithm strategy. The results are as follows.

The results of the experiment can be seen, the method presented in this paper has obtained relatively higher identification accuracy.

Table1. The number of spectral peaks detected of Ginsengs

Crest parameter Data sample	4	8	12	16	20	24	28
Salvia	140	98	43	17	12	10	8
Mountain ginseng	97	78	35	11	8	7	6
Adenophora verticillata	142	112	50	18	8	7	5
Radix pseudostellariae	147	115	44	15	9	6	5

Table 2. The error rate of the recognition experiment

Characteristic presentation method	Linear classifier	Bayes classifier	k nearest neighbor classifier
The original characteristics of standardization(data)	0.1070	0.0925	0.1072
Principal component characteristics of the original data(data+PCA)	0.1362	0.0933	0.1202
The characteristics of the wave crest detected(fengdata4)	0.0402	0.0444	0.0522
Fengdata4+PCA	0.0814	0.0605	0.0496
Presentation in this paper	0.0102	0.0004	0.0035

5 Conclusion

In this paper, the data characteristics of TCM fingerprint are analyzed by using the network graph structure. By building network model, extraction data, digital analysis, calculating relative retention value, determine the standard fingerprint map. It provides a new way of thinking and means for the quality, monitoring and evaluation of medicine.

Acknowledgement

This work was supported by science and technology research project of education department of Heilongjiang Province under grant No. 12531785 and guidance project of the science and technology bureau of Qiqihar, Heilongjiang Province under grant No.GYZD-2017010.

References

1. Xiaohe, Xiao; Luqi, Huang; Xiaojun, Ma. On the new connotation and significance of the modernization of Chinese medicine and traditional Chinese medicine. *China Journal of Chinese Materia Medica*, 28(3):282-286, 2003.
2. Liping, Yang. The thought and exploration of Chinese medicine modernization. *New Journal of Traditional Chinese Medicine*, 36(9):3-4, 2004.
3. Huaizhou, Zhao; Ying, Jia; Shanghua, Zhao, etc. The development of Chinese medicine qi and theory. *China Journal of Chinese Materia Medica*, 30(24):1898-1901, 2005.
4. National pharmacopoeia commission. *Pharmacopoeia of the People's Republic of China* (2005 edition). Beijing: Chemical Industry Press, 2005.
5. Bo, Hong; Wenjing, Li; Shumin, Liu; Jicheng, Liu. HPLC Fingerprinting and Cluster Analysis of Diterpenoids Constituents in *Euphorbia fischerian*. *Natural drug research and development*, 27:617-620, 2015.
6. Xiayan, Wang. The application of modern analytical techniques in the study of traditional Chinese medicine fingerprint. *Chinese Traditional and Herbal Drugs*, 35(7):127-130, 2004.
7. Weiwei, Su; Zhong, Wu; Jian, Quan. Construction of traditional Chinese medicine fingerprint and computer analysis. *Journal of Chinese Medicinal Materials*, 24(4):295-298, 2001.
8. Libo, Yan; Bingren, Xiang. The molecular similarity method is used for the study of the relationship between pharmacological antiphase chromatogram. *Chinese Journal of Chromatography*, 19(5):427-432, 2001.
9. A. Rahman, D.V. Smith, B. Little, A.B. Ingham, P.L. Greenwood, and G.J. Bishop-Hurley, Cattle behaviour classification from collar, halter, and ear tag sensors. *Information Processing in Agriculture* 5(1), 124-133, 2018.
10. N.P. Seeram, and B. Burton-Freeman, The seventh biennial berry health benefits symposium. *Food & Function* 9(1), 20-21, 2018.
11. R. Hu, Y. Zhang, Y. Chen, and G. Lin, Dynamic metabolic profiling in vegetable soybean seed development. *Emirates Journal of Food and Agriculture* 30(2), 90-98, 2018.
12. M. Cruz Campas, A.G. Villalba Villalba, and R. Ramirez Leal, Editorial. *Revista Internacional De Contaminacion Ambiental* 33(SI), I-I, 2017.
13. M. Duan, Z. Liu, D. Yan, W. Peng, and A. Baghban, Application of lssvm algorithm for estimating higher heating value of biomass based on ultimate analysis.

Energy Sources Part a-Recovery Utilization and Environmental Effects 40(6), 709-715, 2018.

Energy Sources Part B-Economics Planning and Policy 13(2), 132-136, 2018.

14. Z. Liu, Economic analysis of energy production from coal/biomass upgrading; Part 1: hydrogen production.

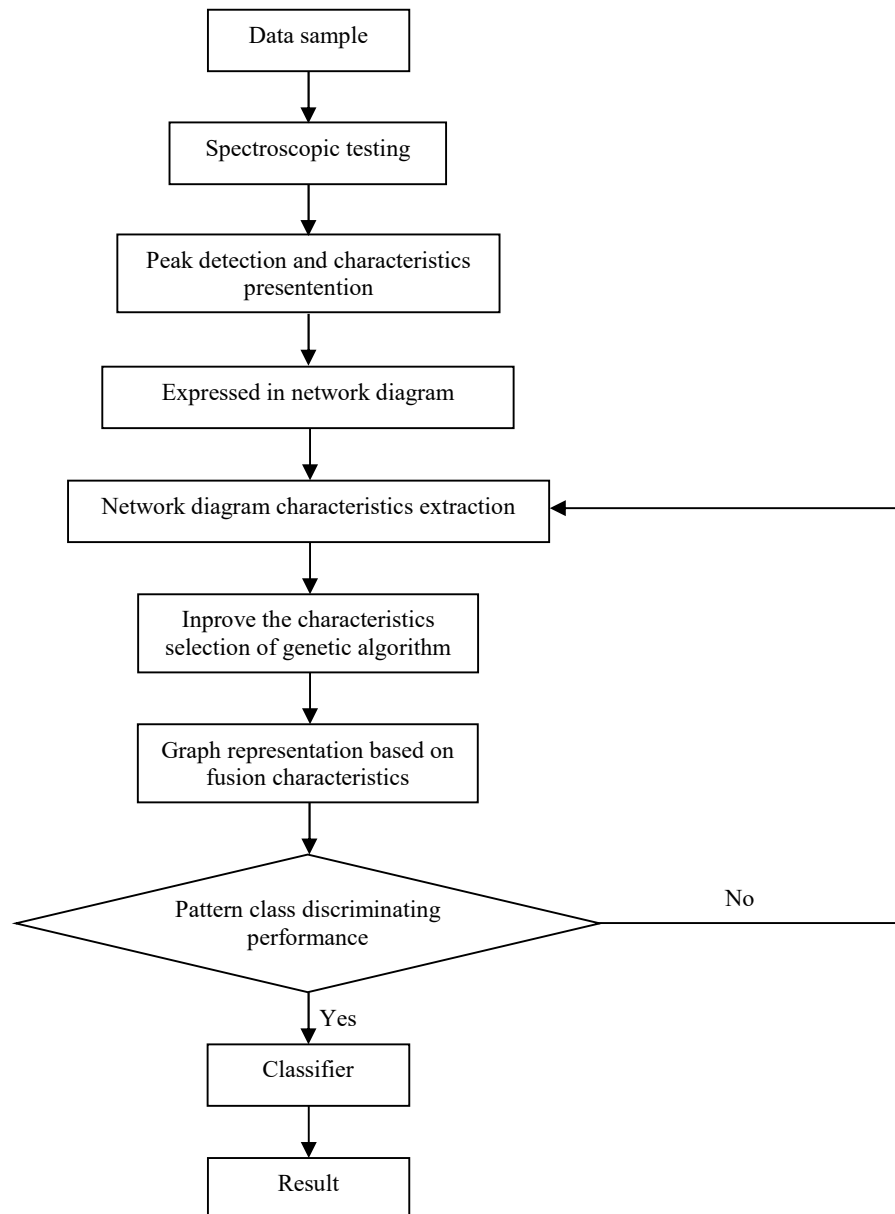


Figure 2. The process flow diagram