

Classifying herbal medicine origins by temporal and spectral data mining of electronic nose

1st Li Liu

*Institute of Cyber-system and Control
Zhejiang University
Hangzhou, China
email: liliu@zju.edu.cn*

1st Xianghao Zhan

*Department of Bioengineering
Stanford University
Stanford, USA
email: xzhan96@stanford.edu*

3rd Ziheng Duan

*Institute of Cyber-system and Control
Zhejiang University
Hangzhou, China
email: duanziheng@zju.edu.cn*

4th Yi Wu

*Institute of Intelligent Agricultural Equipment
Zhejiang University
Hangzhou, China
3190100214@zju.edu.cn*

5th Rumeng Wu

*Institute of Cyber-system and Control
Zhejiang University
Hangzhou, China
email: 3150102424@zju.edu.cn*

6th Xiaoqing Guan

*Institute of Cyber-system and Control
Zhejiang University
Hangzhou, China
email: 3150103730@zju.edu.cn*

7th Zhan Wang

*Institute of Cyber-system and Control
Zhejiang University
Hangzhou, China
email: 11732003@zju.edu.cn*

8th You Wang*

*Institute of Cyber-system and Control
Zhejiang University
Hangzhou, China
email: king_wy@zju.edu.cn*

9th Guang Li

*Institute of Cyber-system and Control
Zhejiang University
Hangzhou, China
email: guangli@zju.edu.cn*

Abstract—The origins of herbal medicines are important for their treatment effect, which could be potentially distinguished by electronic nose system. As the odor fingerprint of herbal medicines from different origins can be tiny, the discrimination of origins can be much harder than that of different categories. Better feature extraction methods are significant for this task to be more accurately done, but there lacks systematic studies on different feature extraction methods. In this study, we classified different origins of three categories of herbal medicines with different feature extraction methods: manual feature extraction, mathematical transformation, deep learning algorithms. With 50 repetitive experiments with bootstrapping, we compared the effectiveness of the extractions with a two-layer neural network w/o dimensionality reduction methods (principal component analysis, linear discriminant analysis) as the three base classifiers. Compared with the conventional aggregated features, the Fast Fourier Transform method and our novel approach (longitudinal-information-in-a-line) showed a significant accuracy improvement ($p < 0.05$) on all 3 base classifiers and all three herbal medicine categories. Two of the deep learning algorithm we applied also showed partially significant improvement: one-dimensional convolution neural network (1D-CNN) and a novel graph pooling based framework - multivariate time pooling (MTPool).

Index Terms—electronic nose; feature engineering; herbal medicine origins

I. INTRODUCTION

Different alternative herbal medicines have distinct pharmaceutical values, because of not only different categories but also different geographical origins [1]. Therefore, the medicines from different geographical locations have a high variance in price, leaving space for frauds. For better

treatment, it is necessary to distinguish the categories and geographical origins. However, the similarities in appearances and odors make it difficult for experts to discriminate herbal medicines of the same category but from different origins. An accurate and cheap analytic method capturing the subtle differences is in need.

Electronic nose (e-nose), has been proved to be effective and affordable in pattern recognition based on volatile organic compounds (VOCs). It has been successfully applied in lung cancer detection [2], dendrobiums identification [3], and herbal medicine category classification [4], [5].

Although the previous research showed prototypical success in classifying herbal medicine origins [6], there is much room for improvement. First, features extracted from e-nose signals significantly influences the classification performance. However, most previous publications in herbal medicine classification did not systematically compare the feature extraction methods. As there is no universal features for e-nose agreed by researchers, several studies adopted the aggregated features and deemed them as a standard pipeline [6], [7]. The aggregated features involved the steady-state and transient information [8] of the signals, which was mainly based on subjective domain-expert experience but only partially exploited the signal information without mining temporal and spectral details. E.g., Zhan et al. revealed the overabundance and low predictive power of some aggregated features [6]. Therefore, more universally applicable feature engineering methods worth further investigation. Second, in the previous publication [6], leave-one-out cross validation

was used. The test data were used both in hyperparameter tuning and model evaluation. This might lead to overestimated accuracy. Furthermore, the previous study [6] did not verify the model robustness or test the statistical significance with repeated experiments.

In this study, we improved our previous study on herbal medicine origin classification by systematically comparing different feature engineering methods with parallel experiments, to explore effective feature extraction methods with temporal and spectral information for higher classification accuracy. With a stricter model development and evaluation design, we also tested the statistical significance, which addressed the limitations in previous studies.

II. MATERIALS AND METHODS

A. Data and feature extraction

We used three categories of alternative herbal medicines: Radix Angelicae, Angelica Sinensis and Radix Puerariaem. Each included 160 samples from 4 different origins [6] collected with an e-nose system [2], [3], [6], [7] with 16 semi-conductive sensors from Dec. 2017 to Jan. 2018, with details shown in Tabel I and the previous publication [4], [6]:

TABLE I
THREE CATEGORIES OF HERBAL MEDICINE FROM DIFFERENT ORIGINS

Categories	Origin 1	Origin 2	Origin 3	Origin 4
Radix Angelicae	Anhui	Sichuan	Hubei	Zhejiang
Angelica Sinensis	Shaanxi	Gansu	Hubei	Sichuan
Radix Puerariae	Sichuan	Hubei	Anhui	Hunan

1) *Manual extraction methods*: The manual extraction methods are shown in Fig. 1 and Table. II. The primitive signal contained the 16-sensor responses in 318 seconds with a sampling rate of 100Hz, with baseline removed. In Fig. 1 A, each bar denotes a temporal response of one sensor. As the signals were not changing rapidly, we used the down-sampling method with a sampling rate of 1Hz to reduce dimensionality. The aggregated method extracted 5 features from each sensor, including: the maximum voltage, the integral value, and the median of the temporal data series, the maximum and minimum value of the exponential moving average (EMA) of the derivative of voltage, with $\alpha = 1/SR$, $SR = 100$. The details of aggregated features were shown in the previous publication [4], [6]. The longitudinal-information-in-a-line (long-line) method was a variant version of the aggregated method proposed by us, with the aggregated features from 6 separate windows instead of the entire time range. In Fig. 1 B, each cell (e.g. max) denotes an array of the results extracted from 16 sensors. In fig.1 C, each sub-cell (e.g. the sub-cell in max) denotes an array with results from 16 sensors.

2) *Mathematical transformation*: To extract spectral features, we applied two time-frequency transformations: Fast Fourier transform (FFT) and scalogram analysis. FFT extracts

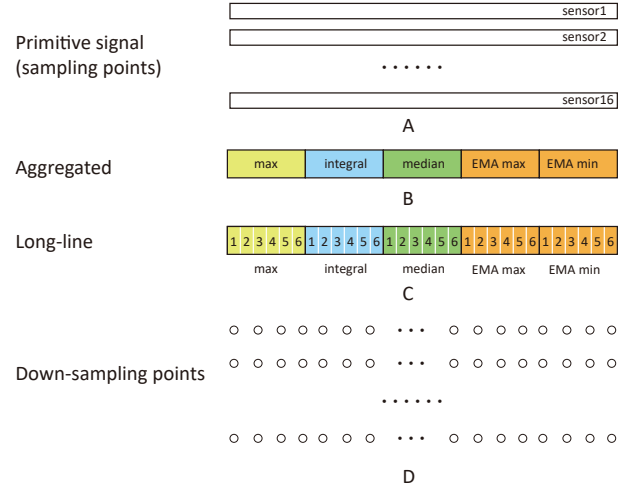


Fig. 1. The manual feature extraction process

spectral densities of a signal, which decomposes the original sequence into several components with different frequencies [9]. Scalogram uses continuous wavelet transform filter bank (in MATLAB) to decompose signals and display the time frequency information with the graph form [10]. In this study, the sampling signals in Fig.1 A was used as the transformation input. We took the absolute value of FFT results. Because the main frequency components gathered in 0-0.5HZ, we used 10 frequency windows with a length of 0.05Hz to extract the information. The maximum, mean and median values in each window were collected as the features. The scalogram method requires image recognition method to extract numeral features from the scalograms, and we adopted pre-trained neural network - VGG16 [11]. To extract the coarse information of scalograms, such as the edges and lines, we chose VGG's fully connected layer 7 as the output before further processing.

3) *Deep learning algorithms*: To explore the data-driven feature extraction method, we employed three deep learning algorithms: recurrent neural network with long short-term memory (LSTM), one dimensional convolution neural network (1D-CNN), a newly proposed graph pooling based framework (MTPool) specific for multi-sensor data pattern recognition. Those algorithms can learn parameters to extract features from the primitive signals in a data-driven manner. Considering the size of our dataset, computational cost and to avoid overfitting, we chose the down-sampling points in Fig.1 D as the input. LSTM is a recurrent neural network (RNN) suited for time series data, and it is featured with connection gates to utilize the information in previous state [12]. We designed an LSTM layer followed by a linear layer for further information processing, which was further connected with the output layer. 1D-CNN is a special deep neural network which uses a convolution kernel to generate the information in a graph, and the kernel only moves in time rather than across sensors [13]. After the convolution operation, three fully connected layers were employed to give the output. MTPool is a novel graph pooling based framework [14], which uses pairwise dependencies of multivariate time series to refine the nodes

TABLE II
THE FEATURE EXTRACTION METHODS AND MACHINE LEARNING ALGORITHMS

Feature extraction types	Method	Dimensionality reduction method	Classifier
Manual Extraction	Aggregated	PCA, LDA	DNN
	long-line	PCA, LDA	DNN
Signal Sampling	Sampling points	PCA, LDA	DNN
	down-sampling points	PCA, LDA	DNN
Time-frequency Transformation	Fast Fourier transformation	PCA, LDA	DNN
	Scalogram	PCA, LDA	VGG+DNN
Deep Learning		LSTM	
		1D-CNN	
		MTPool	

[15]. It uses an 'encoder-decoder' mechanism to determine adaptive clustering centroids and improve robustness.

B. Prediction and evaluation protocol

To avoid overestimating accuracy, we adopted hold-out test instead of the 'leave-one-out' validation in previous study[Feature engineering]: the test set for model evaluation was independent of the training and hyperparameter tuning process. For each category in Table I, we randomly selected 120 samples for the training set, leaving the rest 40 for testing.

For manual extraction and mathematical transformation, we firstly applied them on the entire dataset, and then split it into training set and test set. In this study, we chose DNN as the basic classifier as it does not require strict model assumptions. To condense the extracted feature, we employed 2 dimensionality reduction methods: principal component analysis (PCA), linear discriminant analysis (LDA), and combine them with the base classifier DNN to form the following three base classifiers: original DNN, PCA-DNN, LDA-DNN. To tune the hyperparameters, we used 5-fold cross validation method within the training set. The hyperparameters included the length of width of the fixed spectral window in FFT, the reduced dimensionality in PCA and LDA, the image processing network (VGG or Inception) and its output layer, the number of hidden layers and number of hidden units of DNN, and the number of fully connected layers and the hidden units of 1D-CNN. To statistically evaluate the features, we repeated 50 times parallel experiments with bootstrapping 120 samples, and then we recorded the prediction accuracy of the test set. With fifty results, we performed Wilcoxon signed-rank tests to test statistical significance.

For deep learning methods, we split the dataset into 80/40/40 for train/validation/test sets. The validation set was used for hyperparameter tuning process, which included the convolution kernel size and the network structure in 1D-CNN, the hidden unit dimensionality, number of units in the linear layer after the recurrent layer, learning rate and training epochs in LSTM, the number of centroid heads and pooling layers in MTPool. With the hyperparameters tuned, we retrained the deep learning models using training set in the same bootstrapping pipeline, and tested its prediction accuracy performance on test set.

We took the feature extraction method used in previous studies (aggregated features) as the baseline [4], [6], and applied Wilcoxon signed-rank tests to test the statistical significance.

III. RESULTS

The accuracies of different feature extraction methods in the herbal medicine origin classification are shown in Fig. IV. For Radix Angelicae, except for the scalogram with VGG network, all the other feature extraction methods outperformed baseline on three classifiers($p < 0.05$). The highest median classification accuracy was 0.775 reached by LSTM. For Angelica Sinensis, the long-line, down-sampling and FFT methods outperformed the baseline on three classifiers($p < 0.05$). Besides, 1D-CNN outperformed the baseline (median accuracy: 0.625). For Radix Puerariae, long-line and FFT methods performed better than baseline on classifiers. The best performance was from sampling points with LDA-DNN as the classifier (median accuracy: 0.725).

IV. DISCUSSION

Compared with the conventional aggregated features, the long-line and FFT feature extraction methods generally improved the classification accuracy with three classifiers on all three categories of herbal medicines. Two feature extraction methods always performed better than baseline when using same classifiers: down-sampling points with DNN and LDA-DNN, sampling points methods with LDA-DNN. For the deep learning methods, 1D-CNN and MTPool showed a general improvement on three categories tasks, which also manifested the power of deep learning. Compared with deep learning, the manual feature extraction methods(such as long-line, FFT) still show more effectiveness on our dataset. This is probably due to the small number of our samples, which may lead to the overfitting in the complicated deep learning models.

We provide users willing to classify herbal medicine origins with e-nose with the following suggestions: with undetermined classifiers, for higher robustness, long-line, and FFT are preferred than the conventional aggregated method; To pursue a faster feature extraction and classification process, down-sampling points and sampling points with LDA-DNN are recommended.

This study showed more convenient and efficient feature extraction methods than the aggregated features. However, in the experiments, the advantages of those methods might slightly vary when adopted on different categories of herbal medicines. This was probably due to the limitation of our small-scale dataset, and the further validation will be done

on larger datasets with more categories of herbal medicines originated from different regions.

Besides the comprehensive analysis and comparison of feature extraction methods in this dataset, we published this dataset with the feature engineering methods we used (aggregated features, long-line, down-sampling points, sampling points, FFT) on Github (<https://github.com/xzhan96-stf/Herbal-medicine-origin-e-nose>) for researchers to develop better algorithms, which can be compared with the results in this study as the benchmark.

ACKNOWLEDGMENT

The work is supported by the Natural Science Foundation of China (Grant No. 61773342) and the Science Fund for Creative Research Groups of NSFC (Grant No.61621002).

REFERENCES

- [1] N. Li, Y. Wang, and K. Xu, "Fast discrimination of traditional chinese medicine according to geographical origins with fir spectroscopy and advanced pattern recognition techniques," *Optics Express*, vol. 14, no. 17, pp. 7630–7635, 2006.
- [2] X. Zhan, Z. Wang, M. Yang, Z. Luo, Y. Wang, and G. Li, "An electronic nose-based assistive diagnostic prototype for lung cancer detection with conformal prediction," *Measurement*, vol. 158, p. 107588, 2020.
- [3] Y. Wang, J. Diao, Z. Wang, X. Zhan, B. Zhang, N. Li, and G. Li, "An optimized deep convolutional neural network for dendrobium classification based on electronic nose," *Sensors and Actuators A: Physical*, vol. 307, p. 111874, 2020.
- [4] X. Zhan, X. Guan, R. Wu, Z. Wang, Y. Wang, and G. Li, "Discrimination between alternative herbal medicines from different categories with the electronic nose," *Sensors*, vol. 18, no. 9, p. 2936, 2018.
- [5] X. Zhan, X. Guan, R. Wu, Z. Wang, Y. Wang, Z. Luo, and G. Li, "Online conformal prediction for classifying different types of herbal medicines with electronic nose," 2018.
- [6] X. Zhan, X. Guan, R. Wu, Z. Wang, Y. Wang, and G. Li, "Feature engineering in discrimination of herbal medicines from different geographical origins with electronic nose," in *2019 IEEE 7th International Conference on Bioinformatics and Computational Biology (ICBCB)*. IEEE, 2019, pp. 56–62.
- [7] Z. Wang, X. Sun, J. Miao, Y. Wang, Z. Luo, and G. Li, "Conformal prediction based on k-nearest neighbors for discrimination of ginsengs by a home-made electronic nose," *Sensors*, vol. 17, no. 8, p. 1869, 2017.
- [8] A. Vergara, S. Vembu, T. Ayhan, M. A. Ryan, M. L. Homer, and R. Huerta, "Chemical gas sensor drift compensation using classifier ensembles," *Sensors and Actuators B: Chemical*, vol. 166, pp. 320–329, 2012.
- [9] E. O. Brigham, *The fast Fourier transform and its applications*. Prentice-Hall, Inc., 1988.
- [10] J. M. Lilly and S. C. Olhede, "Generalized morse wavelets as a super-family of analytic wavelets," *IEEE Transactions on Signal Processing*, vol. 60, no. 11, pp. 6036–6041, 2012.
- [11] Z. Ren, K. Qian, Z. Zhang, V. Pandit, A. Baird, and B. Schuller, "Deep scalogram representations for acoustic scene classification," *IEEE/CAA Journal of Automatica Sinica*, vol. 5, no. 3, pp. 662–669, 2018.
- [12] S. Hochreiter and J. Schmidhuber, "Long short-term memory," *Neural computation*, vol. 9, no. 8, pp. 1735–1780, 1997.
- [13] S. Albawi, T. A. Mohammed, and S. Al-Zawi, "Understanding of a convolutional neural network," in *2017 International Conference on Engineering and Technology (ICET)*. Ieee, 2017, pp. 1–6.
- [14] H. Xu, Z. Duan, Y. Bai, Y. Huang, A. Ren, Q. Yu, Q. Zhang, Y. Wang, X. Wang, Y. Sun *et al.*, "Multivariate time series classification with hierarchical variational graph pooling," *arXiv preprint arXiv:2010.05649*, 2020.
- [15] H. Xu, Y. Huang, Z. Duan, J. Feng, and P. Song, "Multivariate time series forecasting based on causal inference with transfer entropy and graph neural network," *arXiv preprint arXiv:2005.01185*, 2020.

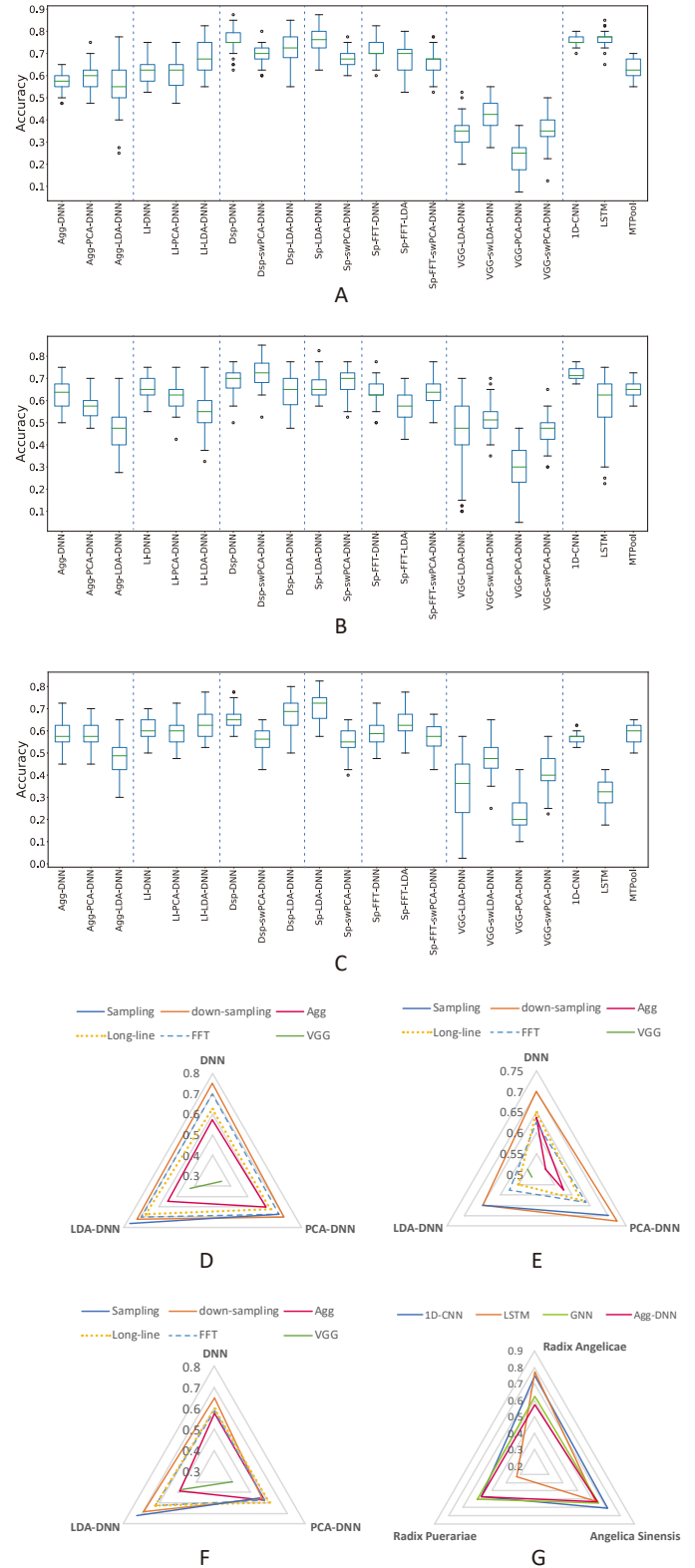


Fig. 2. The classification accuracy of different feature extraction methods on classifying herbal medicine origins for three categories(A: Radix Angelicae, B: Angelica Sinensis, C: Radix Puerariae), and the comparison of their corresponding median values (shown in D,E,F with the same category order). Specially, the results of deep learning algorithms are shown in G. Abbreviation: Agg: aggregated; L1:long-line; Dsp:down-sampling points; Sp: sampling points; Sw: sensor-wise