CS230

Towards More Accurate Herbal Medicine Classification with Electronic Nose under Sensor Drift (Feature Engineering and Data Drift Mitigation)

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Abstract

Anti-drift is important in sensor-related areas. In this research, we use several combinations of feature extraction methods and neural networks to classify herbal medicine. To solve the problem of sensor drift, DRCA, a subspace projection method, is used to find a subspace in which data collected by different sensors have similar distributions. Experiments show the effectiveness of DRCA with different feature extraction method and neural networks.

1 Introduction

Alternative herbal medicines are valuable in medical research and therapies. Previous research demonstrated that supervised learning based on data collected by electronic nose can effectively classify herbal medicines. However, the labor-intensive manual labeling and sensor drift negatively impact the efficiency and effectiveness of this method. In this study, we try to use deep learning to classify traditional Chinese herbal medicine and mitigate sensor drift by feature engineering and DRCA(domain regularized component analysis). Our inputs are electronic nose signals with feature extraction. The input is basically time-series data. Our outputs are the categories of the given samples.

2 Related work

To solve the problem of herbal medicine classification, Zhan, Xianghao, et al.[2] classified 12 categories of herbal medicines by SVM and LDA and introduced conformal predictions based on 1NN (1-Nearest Neighbor) and 3NN (3-Nearest Neighbor). Liu, Li, et al[3] investigated the effectiveness of multiple feature engineering approaches on classifying herbal medicine origins. PCA was used in this research to reduce time expenditure required for classification, however the accuracy would decrease. The research built a herbal medicine library and inspired us to use other methods to get a better classification.

Liu, Li, et al. [4] provided a systematic analysis on 5 data augmentation strategies for boosting the alternative herbal medicine classification model generalizability. The future work might include the 5 methods to train models better.

Several researches were done to solve the problem of sensor drift. Zhang et al.[5] used DRCA for anti-drift and found the method effective compared to state-of-art methods. Zhang, Lei, and David Zhang[6] proposes a unified framework called domain adaptation extreme learning machine (DAELM) for drift compensation as well as gas recognition in E-nose systems. Martinelli, Eugenio, et al.[7] introduced a modified version of an Artificial Immune System algorithm for chemical sensor

CS230: Deep Learning, Autumn 2021, Stanford University, CA.

drift mitigation. These researches show us multiple ways to solve the sensor drift problem, and due to the described well behavior of DRCA we decided to use DRCA as a method to improve models' behavior.

3 Dataset and Features

The dataset is collected from the State Key Laboratory of Industrial Control Technology in Zhejiang University, using an electronic nose system that contains 16 TGS(Taguchi Gas Sensors) type metal oxide semi-conductive(MOS) sensors bought from Figaro Engineering Inc[1]. Dataset is further divided into source dataset and target dataset by the sensor used for data collection. The source dataset is used for model training and the target dataset is used for measuring the transferability of models. The source dataset contains 160 samples for 3 categories each and the target dataset contains 50 samples for 3 categories each. The raw data is time-series data in the shape of (1,16,31800). For down-sampling feature extraction, we resample the primitive data with 100 Hz sample rate on each 16 sensors. For aggregation feature extraction, 8 features are extracted from each sensor: the maximum voltage, the integral value of voltage, the maximum and minimum value of 3 types of exponential moving average(EMA) of the derivative of voltage[2]. The source dataset is divided into the training set, valid set, and test set according to the ratio of 70:15:15 since the total number of samples is limited. The whole target dataset is used as a target set.

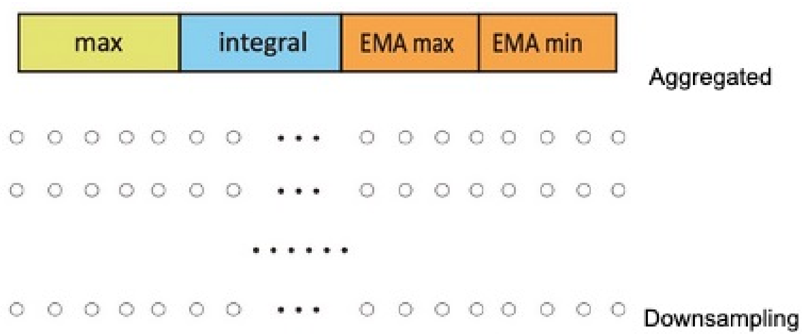

Figure 1: Feature Extraction[3]

4 Methods

4.1 Models

We use different combinations of feature extraction methods and neural networks to classify herbal medicine and compare their transferability. Aggregated and down-sampling are tested as feature extraction methods. Neural networks are common neural networks, 1D-CNN(1D-convolutional neural network) and LSTM(long short-term memory).

The combinations we have tested are: aggregated feature extraction and common neural network; aggregated feature extraction and 1D-CNN; down- sampling and 1D-CNN; down-sampling and LSTM. In a common neural network, there are 1 input layer, 3 hidden layers and 1 output layer. The number of nodes in hidden layers are 64, 32 and 16 respectively.The learning rate is 0.0005. Dropout is used as regularization and the keep-probability is 0.7. In the CNN model, the learning rate is set as 0.0001. The model has 3 convolutional layers and 3 max pooling layers. Each convolutional layer is followed by a max pooling layer. The number of filters are 32, 64, and 64 respectively. The sizes of convolutional kernels are 2, 2 and 3 respectively. No paddling is used and strides are always 1. A fully connected layer is used as the last layer to form a 3-class prediction output. Dropout is used as regularization and the keep-probability is 0.5. In the LSTM model, the learning rate is set as 0.0001. The dimension of the hidden layer is 128. The number of recurrent layers is 3. The model is bidirectional. Dropout is used as regularization and the keep-probability is 0.5.

4.2 DRCA

Assume source dataset $X_S \in R^{D\times N_S}$, and target dataset $X_T \in R^{D\times N_T}$. The principle of DRCA is to find a projection P that projects source and target dataset to a subspace that minimized the mean distribution discrepancy(MDD) between them.

$$X'_S = P^T X_S \tag{1}$$

$$X'_T = P^T X_T \tag{2}$$

$$\min ||\mu_S - \mu_T||_2^2 = \min ||\frac{1}{N_S}\sum_{i=1}^{N_S} X_S^{i\,\prime} - \frac{1}{N_T}\sum_{j=1}^{N_T} X_T^{j\,\prime}||_2^2 \tag{3}$$

The procedure of computing optimal P^* is described below:

1. Choose hyperparameters λ and d.
2. Calculate the centroid of source data and target data.

$$\mu = \frac{1}{N}\sum_{i=1}^{N} X^i \tag{4}$$

3. Compute matrix A as :

$$A = ((\mu_S - \mu_T)(\mu_S - \mu_T)^T)^{-1}(X_S X_S^T + \lambda X_T X_T^T) \tag{5}$$

4. Perform the eigenvalue decomposition of A by $AP = \rho P$. Choose the eigen-vectors of the first d largest eigenvalue to get the optimal projection $P^* = [P_1, P_2, ...Pd]$

5 Experiments/Results/Discussion

We trained the models with original datasets and DRCA augmented datasets, respectively, and compared their performance on the test set and target set.

5.1 Experiment on Original Dataset

As shown in table 1, all models achieve desirable accuracy and F1 score on the test set. For aggregated features, the common neural network(Accuracy 91.67%) works slightly better than 1D-CNN(Accuracy 87.50%). On the other hand, 1D-CNN and LSTM perform almost the same on down-sampling features. However, all models perform poorly on the target set. The highest accuracy is only 46.67% obtained by the common neural network. Rest of the models only achieved 34 35% accuracy.

The results show that all combinations of features and models can classify herbal medicine well when using the same electronic nose for data collection. At the same time, sensor drift indeed greatly affects the performance of the model. Models trained with dataset collected by specific electronic noses cannot be applied to dataset collected by other electronic noses.

Table 1 Performance of the models trained on the original dataset

Feature	Model	Test Accuracy	Test F1 score	Target Accuracy	Target F1 Score
Aggregated	NN	91.67%	92.02%	46.67%	38.84%
Aggregated	1D-CNN	87.50%	87.91%	35.33%	25.71%
Down-sampling	1D-CNN	94.44%	94.48%	34.00%	18.06%
Down-sampling	LSTM	94.44%	94.26%	34.67%	22.86%

5.2 Experiment on DRCA Augmented Dataset

After DRCA transformation, the accuracy and F1 score of the models on the test decreased by 8 18% and 8 20%, respectively. The LSTM model with down-sampling features outperforms other models and its drop in accuracy after DRCA is the lowest. For the target set, though most models remain the same as before(Accuracy 32 35%, F1 Score 20 23%), the performance of the common neural network significantly improves after DRCA transformation(Accuray from 46.67% to 65.35%, F1 Score from 38.84% to 65.17%). The confusion matrix and ROC curve(Figure 2, 3) show that the common neural network can better classify class 0 and 2 at target set with the help of DRCA.

The results indicate that DRCA transformation generally slightly decreases the performance of the models and different models are affected by different levels. Common neural networks with aggregated features benefit from DRCA transformation in mitigating sensor drift. It performs similarly in test set and target set.

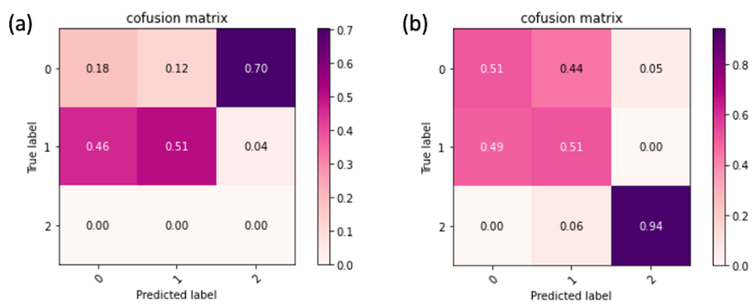

Figure 2: Confusion matrix of common neural network with aggregated features at target set
(a) Original Dataset; (b) DRCA augmented Dataset

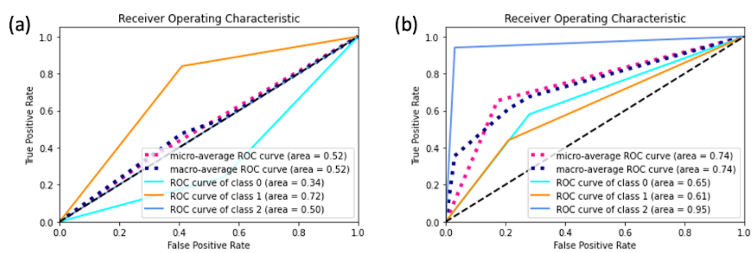

Figure 3: ROC curve of common neural network with aggregated features at target set
(a) Original Dataset; (b) DRCA augmented Dataset

Table 2 Performance of the models trained on the DRCA augmented dataset

Feature	Model	Test Accuracy	Test F1 score	Target Accuracy	Target F1 Score
Aggregated	NN	73.61%	71.47%	65.35%	65.17%
Aggregated	1D-CNN	79.17%	79.30%	35.33%	20.73%
Down-sampling	1D-CNN	77.78%	76.72%	32.00%	23.28%
Down-sampling	LSTM	86.11%	85.12%	35.33%	20.69%

5.3 DRCA Analysis

In our experiments, the accuracy of the models decreases by 8 18% after DRCA transformation. DRCA transformation tries to mitigate sensor drift by minimizing the mean distribution discrepancy(MDD) between source and target dataset. Since it projects the original features to a lower dimension subspace for minimizing MDD, the loss of information is inevitable which leads to the overall decrease in model performance. Hence, there is a trade off between transferability and model accuracy.

The experiment result shows that common neural networks with aggregated features work best in the target set. There are two possible reasons. a) Aggregated features are more suitable for DRCA compared to down-sampling features. Aggregated features represent the numerical range of collected time-series data. As DRCA minimizes MDD, the discrepancy in numerical range caused by sensor drift can be reduced or eliminated. However, for down-sample features, while DRCA minimizes MDD of different features in each time step, it also breaks the continuity of time-series data as shown in Figure 4. Although 1D-CNN and LSTM can learn to fit messy time-series data, the transferability of the models is impaired. b) The convoluted layer of 1-D CNN has a lower ability to extract features from input compared to the fully connected layers of a common neural network. As shown in table 2, the common neural network has better transferability than 1D-CNN even without DRCA.

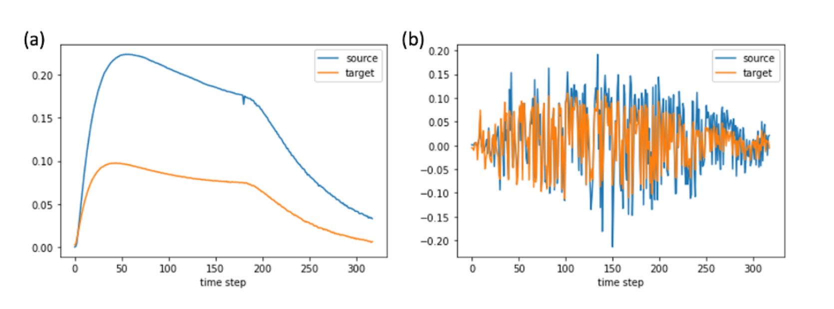

Figure 4: Down-sampling feature of test and target set
(a) Original Dataset; (b) DRCA augmented Dataset

6 Conclusion/Future Work

Four combinations of feature extraction and neural network are tested in this research. DRCA is used to solve the problem of sensor drift. After combining with DRCA, common neural networks and aggregated features achieved significant improvement in transferability. But other combinations of features and models didn't exhibit meaningful improvement. In conclusion, DRCA helps to mitigate sensor drift and improve model transferability in herbal medicine classification, but its effectiveness is highly dependent on feature extraction and model architectures. Experiments must be conducted to analyze the effectiveness of DRCA before application.

Our future work includes data augmentation to get more data for training our models. Testing other combinations of feature extraction methods and neural networks and finding one with the best transferability are required in our next work. Feature extraction methods to be investigated include long-line and Fast Fourier transformation.

7 Contributions

Zikun Cui contributed to the construction and revision of models. Jialuo Yuan contributed to the revision of models and tuning of hyperparameters. Both of them took part in writing this paper and making the presentation video. Li Liu and Xianghao Zhan offered the code of the DRCA method from their previous research and feature extraction of raw data.

References

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