

Deep Learning Approach for Classifying Contamination Levels with Limited Samples

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Abstract

The detection of the contaminants in daily food and drinking water is crucial for global public health. For heavy metals detection of Mercury (Hg) and Arsenic (As), our group has proposed a novel paper-based and microfluidic device integrated with a mobile phone and an image analysis pipeline to capture and analyze the sensor images on-site. Still, the detection of lower contamination levels remains challenging due to the small number of available data samples and large intra-class variance of our application. To overcome this challenge, we explore traditional data augmentation and GAN-based augmentation techniques for synthesizing realistic colorimetric images; and we propose a CNN classifier for five-contamination-levels classification. Our proposed system is trained and evaluated on a limited dataset of 126 phone captured images of five contamination levels. Our system yields 88.1% classification accuracy and 91.92% precision, demonstrating the feasibility of this approach. We believe that this approach of training deep learning models on limited detection images datasets presents a clear path toward phone-based contamination-levels detection.

Introduction

To address the threats of heavy metals As and Hg to food safety, our group has proposed a novel paper-based, microfluidic biosensor. Fig. 1 shows the proposed detection mechanism of our biosensors and the test interpretation. Two kinds of the aptamer-functionalized particles specific to Hg^{2+} and As^{3+} are preloaded on each of the upper, and lower two circular pads, respectively. Test samples are dropped in the inlet of the biosensors. The biosensor shows colorimetric responses in the presence of the target after the test solution interacts with the corresponding particles deposited on the testing areas [1].

To detect and measure heavy metal contaminants in food or liquids, we propose two image analysis methods to obtain a higher prediction accuracy with our developed paper-based devices in our previous work. (1) We convert images of the colorimetric response captured with a mobile phone camera to grayscale images, and then we use ΔE from a white background as our baseline method to correlate the optical properties with the different concentrations of the target, and optimally quantize these responses into five groups to evaluate the prediction accuracy [2], [3]. The prediction accuracy is shown in Table 1. The ΔE from the global background method shows an average prediction performance of

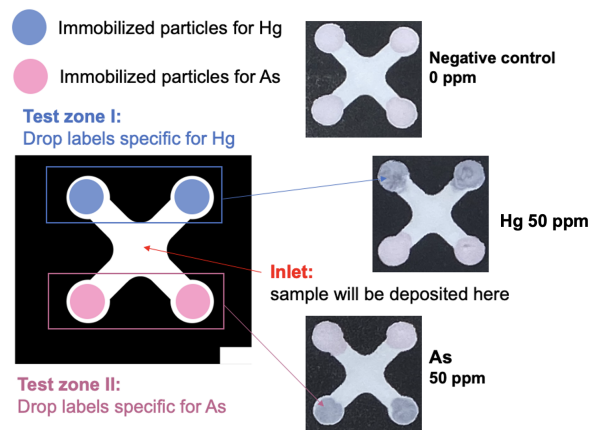


Figure 1. Detection mechanism of our biosensors and test interpretation. (To illustrate the different particles specific for Hg and As, the particles specific for Hg are labeled blue in the figure; but the actual particles are colored light pink.)

60%. Its effectiveness is restricted by the limited dataset and the insufficient utilization of the spatial information contained in the sensor pad images.

Table 1: Performance of the method based on ΔE from the global background.

Class	C 1	C 2	C 3	C 4	C 5
Accuracy	91%	60%	43%	20%	86%

(2) To further improve the accuracy, we consider the use of the spectral reflectance of the sensor pad, then develop two different machine learning approaches: k-nearest-neighbor with sequential forward feature selection to determine the best set of features, and random forest with principal component analysis for feature reduction for classifying the level of contamination by As^{3+} into one of five categories. The accuracy of these two models is compared by implementing them with the same training and test datasets. It turns out that the RF model with PCA feature selection performs well in terms of accuracy compared to the k-NN classifier. Table 2 shows the prediction accuracy of the RF model with PCA features. The classification performance yields 86.6%

average accuracy which is higher than the baseline model. The challenging part of the spectral imaging model is that the spectral data must be obtained using an expensive and professional optical component, like a spectroradiometer [4].

Table 2: Performance of the RF model with PCA features.

Class	C 1	C 2	C 3	C 4	C 5
Accuracy	82%	80%	71%	100%	100%

Nowadays, convolutional neural networks (CNN) have gained tremendous popularity in computer vision, especially in the image classification domain for better performance than popular image processing methods [5], [6]. Deep learning algorithms yield high classification accuracy by using large, annotated datasets of images. Therefore, to develop accurate image classifiers for the contamination-levels classification task, we need a large dataset of images of colorimetric responses. However, obtaining large-scale datasets of detection images of contamination levels is challenging because of limited test samples.

One approach to overcome this challenge is to use data augmentation, a standard procedure to obtain good performance by deploying rotation, flip, translation, and scaling techniques. Another emerging deep learning generative model inspired by game theory to synthesize images is the Generative Adversarial Network (GAN) [7]. The GAN model consists of a generator to create fake images and a discriminator to distinguish between the real and fake images. These two parts are trained in an adversarial process. Different variations of the classic GAN models have been proposed. As a representative example, pix2pix is a GAN model addressing image-to-image translation problems [8]. Recent medical and biological imaging applications have shown that the GAN framework can successfully generate images and obtain reasonable performance [9], [10], [11]. Therefore, it is appropriate to apply a GAN model to generate synthetic images for training purposes.

We aim to solve the classification problem posed by a small scale of data samples and large intra-class variance. In this paper, we propose an approach to generate high-quality colorimetric responses from our detection images captured by a phone camera and apply a CNN based on EfficientNet-B0 [12] for the contamination-levels multi-classification. The proposed method is evaluated on five contamination levels, and is compared with our previous work. We hope that the proposed methods can be a strong candidate for phone-based contamination-levels detection. Because the user need only take an image of the test response using their phone camera and feed the captured image into the proposed model, the model can automatically classify the test sample's contamination level.

The rest of the paper is organized as follows. In Section 2, we present the dataset, explore two methods for generating realistic synthetic images, and evaluate the classification results achieved by the proposed CNN classifier. Section 3 reports the experimental results for classifying contamination levels. In Section 4, the conclusions are given.

Methodology

The main challenges of our project are the small scale of available data samples and the large intra-class variance. To over-

come these challenges, we first use traditional data augmentation techniques to enlarge the training dataset of the colorimetric signals (AUG data), then train the proposed CNN model with these training sets, and test with the real test dataset. Finally, we synthesize realistic images using pix2pix (GAN data), and observe the classification accuracy after adding the GAN data to the AUG training set.

Dataset description

In this study, the colorimetric responses of 5 contamination levels (As^{3+}) are used as the experimental data. Our optical system first acquires the colorimetric signals of the biosensors. The optical system mainly consists of a photo studio booth (Amzdeal, purchased from Amazon.com) for providing the controlled D65 illumination environment, a mobile phone camera (iPhone 11 Pro Max, CA, USA), and a fixture to hold the mobile phone. Next, we extract the regions of interest and obtain the corresponding segmentation masks, as illustrated in Fig. 2. Through the above-mentioned steps, our dataset consists of 126 phone captured images: 35 in Class 1 (0, 1, 2 ppm), 32 in Class 2 (4, 5 ppm), 22 in Class 3 (10 ppm), 15 in Class 4 (20, 30 ppm), and 22 in Class 5 (50 ppm). All the ROIs are resized to a uniform dimension of 200×200 pixels. Finally, we divide the original dataset into a training set, a validation set, and a test set according to the ratio 5: 2: 3, as shown in Table 3.

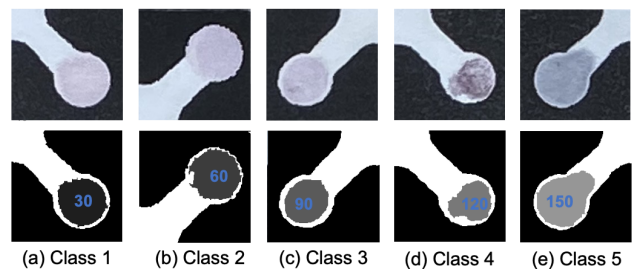


Figure 2. Dataset examples of 5 contamination levels: the ROI images of the colorimetric signal and the corresponding segmentation masks (The numbers in blue are the grayscale values. To distinguish different classes, we use different grayscale values to label different classes' response areas).

Table 3: Overview of the small-scale dataset showing the division, respectively, into training, validation, and test sets.

Class	Training set	Validation set	Test set	Total
Class 1	17	7	11	35
Class 2	16	6	10	32
Class 3	11	4	7	22
Class 4	7	3	5	15
Class 5	11	4	7	22

Traditional data augmentation

Deep learning algorithms yield high classification accuracy by using large, annotated datasets of images to train a network. This can cause a danger of overfitting when a deep network deals with a limited numbers of training images. One standard method to address this problem uses traditional data augmentation meth-

ods. Classic data augmentation techniques include scaling, cropping, flipping, rotation, translation, and other deformations. The color of the image is important to our application, and we aim to train a classifier to predict the unknown test image's contaminant level based on its colorimetric signal. Therefore, we choose the rotation, flipping, and shifting data augmentation methods, and avoid color deformation.

Generative adversarial network

Another promising tool to generate synthetic images is the Generative Adversarial Net (GAN). The GAN model consists of a discriminator D to discriminate between the real and fake images, and a generator G generating fake images to fool the discriminator. These two parts are trained in an adversarial process. Recent studies have shown that the GAN framework can successfully generate images and obtain good performance [13]. Inspired by [10], we explore pix2pix, a variant of conditional GANs for learning the translation from the binary segmentation images to the colorimetric signal images. The loss function is shown in (1).

$$G^* = \arg \min_G \max_D L_{cGAN}(G, D) + \lambda L_{L1}(G) \quad (1)$$

Here the generator G tries to minimize this loss function, whereas the discriminator D tries to maximize it, λ is the hyperparameter that balances the $L1$ loss term, which is used to obtain sharp images. One of the limitations of pix2pix is that it requires paired images to train the network. For our application, the input paired images to train the network are the ROI images of the colorimetric signal and the corresponding segmentation masks, as illustrated in Fig. 2. Then, we only feed the segmentation masks to the trained pix2pix network to generate realistic colorimetric signals.

Proposed CNN architecture

EfficientNet models are based on uniformly scaling the network width, depth, and resolution to yield higher test accuracy and better efficiency with a smaller number of parameters than previous ConvNets, like ResNet-50, and Inception-v2 [14], [15]. EfficientNet consists of a series of models from B0 to B7, and the number of parameters varies from 5×10^6 to 66×10^6 [12]. Considering that we focus on a phone-based contamination detection application, we use EfficientNet-B0 with the least number of parameters for transfer learning and to extract features of the generated detection images. To perform the five-contamination-levels classification task, we add a sequence of two fully connected layers with batch normalization, RELU activation functions, and a dropout layer. Finally, the classification layer contains five output units for 5-class classification based on using the softmax activation function. To test the performance of our proposed CNN classifier, we use accuracy, precision, and F-1 score as the evaluation metrics.

Experiments and results

To solve the multi-class classification problem posed by the small scale of our dataset and its large intra-class variance, we explore two kinds of data augmentation techniques, and compare their effectiveness for classifying the five contamination levels. The experiments are set up as follows:

(1) We enlarge our training dataset (AUG training data) by using traditional data augmentation, then calculate the test accu-

rary of our proposed CNN model trained with the different numbers of the AUG data.

(2) To compare the classification effects between the traditional data augmentation method and pix2pix, we use the AUG training dataset that yields the highest test accuracy to train pix2pix. Then we input the specific segmentation masks to pix2pix to generate the corresponding realistic colorimetric signal images.

Traditional data augmentation evaluation

According to the proposed approach, we first apply rotation, flipping, and shifting to produce a large number of images for the training and validation datasets. Here, $N_{rotation} = 70$, $N_{flip} = 2$, and $N_{trans} = 24$. Inspired by [16], we randomly sample the augmented images to additively form the different training dataset groups $D_{train1} \subset D_{train2} \subset \dots \subset D_{train8}$ such that D_{train1} only consists of the original training dataset, each class of D_{train2} includes 1,000 samples, ..., and each class of D_{train8} includes 7,000 images. Then, we randomly select 1,000 images per class for the validation dataset.

We train the proposed CNN classifier separately for each set of the training groups and evaluate the test results on the same original test dataset. The accuracy results for five contamination levels with the increasing training datasets are illustrated in Fig. 3. It shows that the classification results improve from 61.9% with no AUG data to 88.1% (D_{train4} , the optimal AUG data group). We also notice that after D_{train4} , the classification results drop down slightly and continue to fluctuate around 80%. Table 4 presents the confusion matrix for the optimal AUG training data group D_{train4} . The classification performance using only classic data augmentation (D_{train4}) yields 91.92% average precision, 86.6% average recall, and 86.7% average F-1 score.

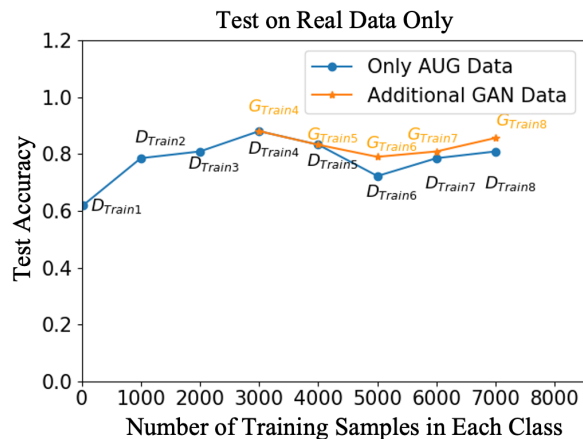


Figure 3. Classification results for the five-classes test data as a function of the training set size.

Pix2pix data augmentation evaluation

Researchers have reported that the augmented images produced by the traditional data augmentation approach are highly correlated; and GANs are a promising approach to generate a large, diversified dataset of images for training purposes [10], [16]. So, we use the optimal AUG data group D_{train4} to train pix2pix and input the segmentation masks of the well-trained

Table 4: Confusion matrix for the CNN model trained with the D_{train4} group.

Ground Truth	Predicted Class					Precision	Recall
	C1	C2	C3	C4	C5		
C1	11	0	0	0	0	84.6%	100%
C2	1	9	0	0	0	75%	90%
C3	1	3	3	0	0	100 %	42.9%
C4	0	0	0	5	0	100%	100%
C5	0	0	0	0	7	100%	100%

pix2pix to generate a realistic colorimetric images dataset. Here, we also additively form the synthetic training group datasets (GAN data) $D_{train4} \subset G_{train5} \subset G_{train6} \subset G_{train7} \subset G_{train8}$. To avoid the influence of the edges in the training group on the classification, the segmentation masks of G_{train5} and D_{train5} are the same, and this requirement applies to the rest of the training groups, i.e. G_{train6} and D_{train6} are the same, and so on.

Fig. 4 shows the synthesized high-quality colorimetric images of five-classes with the well-trained pix2pix. Fig. 3 shows

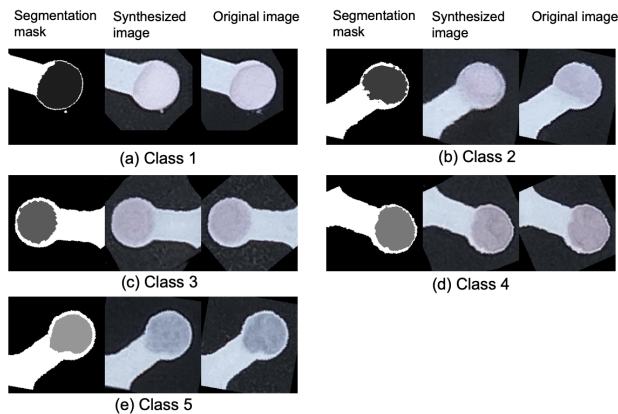


Figure 4. Synthesized examples of five-classes with pix2pix. For each class, the figures from left to right are a segmentation mask, a synthesized image generated by a well-trained pix2pix, and the colorimetric signal's original image.

the test accuracy of the GAN-based synthetic augmentation experiments. Even though the highest classification result is still obtained with D_{train4} , adding the synthetic training data does improve the accuracy for the training sets G_{train6} , G_{train7} , and G_{train8} , compared with the same training set number in the AUG training group. It also reduces the fluctuation in accuracy.

Conclusion

In this paper, we focus on solving the multi-class classification problem posed by a small scale dataset and large intra-class variance. We propose a CNN classifier and explore two kinds of data augmentation techniques to compare their effectiveness for a classification task. Moreover, we conclude that this proposed approach demonstrates promising results for a contamination-levels classification task with limited data.

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