Application Note 9

Identification of Incoming Raw Materials: Lemon vs. Lime

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1. Introduction

Customer supplied us with ~7ml of Lemon and Lime flavors. The goal of the experiment was to determine if the Cyranose 320 could distinguish between Lemon and Lime flavors. The customer currently uses a human sensory panel for discrimination, however they are limited in the number of samples per day they can test.

2. Experiment

Sample preparation: 1 ml of each of the Lemon and Lime were placed in 20 ml septum lidded vials. Ten replicates were prepared for each sample. All samples were kept in Lab environment with ambient condition.

Testing Conditions:

Cyranose 320 with a 32-sensor array was used. The instrument was warmed up for 30 minutes before the test. Most of the sensors reached equilibrium (31 out of 32). The method settings are listed in Table I. The training set was obtained by sampling the 20 sealed vials randomly (Refer to Table II).

Data handling:

Data was recorded with digital filter on. The sensor responses were calculated using the minimum of the resistance reading during the baseline purge and the maximum resistance reading during the vapor exposure, which is $(R_{max}-R_{min})/R_{min}$. The 32 sensor responses were auto-scaled and normalized using norm 1. The canonical discriminant analysis (CDA) algorithm was used to build a model and for prediction.

3. Results

The Lemon and Lime flavors clustered into distinct regions in PCA space (Figure 1). The Canonical plot also demonstrates clustering of the two flavors into distinct regions (Figure 2). This indicates a robustness of the training set for prediction in this application. The training process took about 30 minutes and the training set remained robust throughout the 3-day experiment resulting in correct identifications of the Lemon and Lime flavors. The interclass M distance between Lemon and Lime was 15.

4. Conclusion

Analysis with the Cyranose 320 created distinct patterns that allowed samples of Lemon and Lime to be readily identified for at least 3 days.

Table I. Method Settings

C320 Parameters	Time	Pump Speed
Baseline Purge	10 seconds	Low
Sample Draw	30 seconds	Low
Sample Draw 2	0	N/A
Snout removal	0	N/A
1 st Sample Gas Purge	0	N/A
1 st Air Intake Purge	10	High
2 nd Sample Gas Purge	50	High
2 nd Air Intake Purge	0	N/A
Digital Filtering ON		
Substrate Temperature 35°C		
Algorithm	Canonical	
Preprocessing	Autoscaling	
Normalization	Norm 1	

Table II. Random Training order for Lemon vs. Lime

	0
1	1= Lemon,
2	2 = Lime
1	
2	
2	
2	
1	
2	
1	
1	
2	
1	
2	
1	
2	
1	
1	
2	
2	
1	

Figure 1. PCA of Lemon vs. Lime PCA Projection Plot

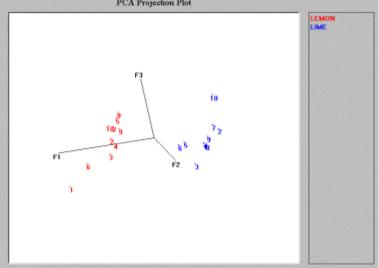


Figure 2. Canonical plot of Lemon vs. Lime Canonical Projection Plot

