Analyze IQ® Lab Application Notes

1: Identifying Acetonitrile in Mixtures

Comparing **SIMCA** (implemented in Unscrambler V8.0) with two **Analyze IQ Lab** techniques. Using 74 samples: 53 with Acetonitrile and 21 without Acetonitrile. Computing average error from 5 runs of 10-fold cross-validation.

Acetonitrile Classification	% Error
Unscrambler: SIMCA	8.65±2.23
Analyze IQ: Weighted Spectral Linear Kernel	2.16±1.54
Analyze IQ: Spectral Attribute Voting	1.08±1.13

## 2: Chlorinated Solvents; Acetaminophen with Excipients

Comparing the standard technique of **Principal Component Regression** with **Analyze IQ Lab**'s kernel-based techniques for classification of a target in a mixture.

Dataset 1: Acetaminophen in various concentrations, mixed with common narcotic excipients; 217 samples in total. **Dataset 2:** Mixtures of chlorinated and non-chlorinated solvents; 230 samples in total. Results from 10 x 10-fold cross-validation.

Dataset 1: Acetaminophen + Excipients	PCR Classification	Analyze IQ WS Lin Kernel	Analyze IQ WS RBF Kernel
% Error in Identifying Acetaminophen	4.47 %	1.93 %	0.41 %
Dataset 2: Chlorinated Solvents			
% Error in Identifying 1-1-1 Trichloroethane	18.73 %	2.43 %	2.39 %
% Error in Identifying Dichloromethane	7.87 %	0.96 %	0.87 %
% Error in Identifying Chloroform	13.49 %	0.91 %	0.87 %

3: Visualization of Clusters

Comparing the Principal Components found using standard **Principal Component Analysis** and using Analyze IQ's Weighted Spectral Linear Kernel. Analysis based on a dataset of mixtures with Acetaminophen (blue) and without Acetaminophen (red).

Standard PCA   **Weighted Spectral Linear Kernel**
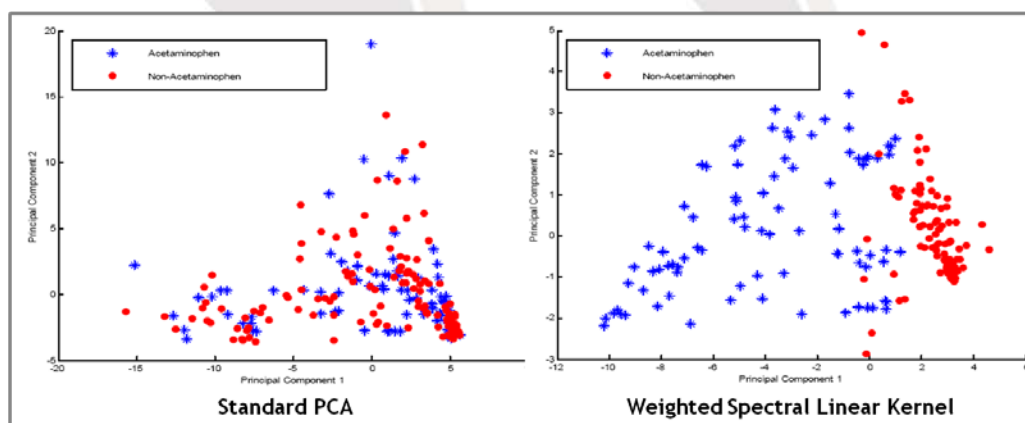
In both cases, we plot PC1 vs PC2. The PCs computed with Analyze IQ's Weighted Spectral Linear Kernel clearly separate the samples, whereas standard PCA does not.