Synergy of Target and Anomaly Detection in Hyperspectral Images

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Hyperspectral Imaging

- Many pixels provide a good sampling for exploratory analysis, detection and classification
  - rapid and non-invasive
- Good for heterogeneous mixtures
  - although quantities to be detected may be low on a volume basis, signal in individual pixels can be dominated by an analyte of interest
  - wet chemistry methods can be hampered by dilution effects

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Typical Algorithms for Hyperspectral

- **Exploratory Analysis and Anomaly detection**
  - finds unusual pixels w/in an image in “any direction”

- **Target detection**
  - finds pixels w/ unusual signal in “specific directions” w/in an image

- **Change detection**
  - finds unusual pixels inter-image
Anomaly Detection

- PCA, others, …
  - Based on exploratory analysis algorithms

**PCA geometry for two variables**

Scores PC 1

Scores on PC 2
Hotelling’s $T^2$


$$T^2 = t\left(\frac{1}{M-1} T^T T\right)^{-1} t^T$$

$$T^2 = \frac{t_1^2}{\lambda_1} + \frac{t_2^2}{\lambda_2} = \tilde{t}_1^2 + \tilde{t}_2^2$$

“whitening”

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Anomaly Detection Example

NIR reflectance image of a cellulosic swipe with ?? on it.

PCA scores 1, 2, 3 (RGB) for -log10, mean-centered data.

a) is an anomaly apparent?
b) where is it?
c) if seen, can the analyte be identified?

Image of Scores on PC 1 (97.73%), PC 2 (1.28%) & PC 3 (0.56%)
T^2 Anomaly Detection

weak anomaly found on PCs 4 to 6

X-block: Swipe_SS_1000_1730.hdr  35208 by 731
Preprocessing: -log10, Mean Center
Num. PCs: 7

<table>
<thead>
<tr>
<th>Principal Component Number</th>
<th>Cov(X)</th>
<th>% Variance Captured This PC</th>
<th>% Variance Captured Total</th>
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Anomaly Detection Summary

- Finds unusual pixels in *any* direction
- Doesn’t tell *what* the anomaly is due to
- Is it possible to utilize what is known about target analyte to choose *a specific* direction?

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Target Detection

- Finds pixels with unusual signal in a **specific direction** within an image
- Provides information on **what** an anomaly is
- **Algorithms:**
  - Generalized least squares (GLS), spectral angle mapper, window target factor analysis

For target detection, it is nice to know how the signal manifests in general...explore the signal.
Target Detection

\[ X = TP^T + E \]

\[ T = XP \]

\[ \hat{c} = X\Sigma^{-1}_c s \left( s^T \Sigma^{-1}_c s \right)^{-1} \]

Image of Scores on PC 1 (97.73%), PC 2 (1.28%), PC 3 (0.56%)

s is the spectrum of RDX

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data set: courtesy OPOTEK, Inc., Carlsbad, CA

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Model System Studied

- ppm levels of melamine in wheat gluten

NIR reflectance hyperspectral image
Powdered Raw Materials

Challenges

- scattering and particle size distributions changes sample-to-sample
- same material from a wide variety of sources

Calibration for typical ILS models difficult

- unlikely to acquire a calibration data set that spans all the sample variation expected to be seen
  - and if you do, the net analyte signal suffers
- unlikely to use one ILS model from a single material for multiple raw materials
Unadulterated Wheat Gluten

Signal from the unadulterated wheat gluten is highly variable and is much stronger than the adulterant.
PCA of Melamine in Wheat Gluten

Eigenvalues for 200 ppm melamine in wheat gluten -log10

Percent Variance Captured by PCA Model

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<th>Principal Component Number</th>
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Target Approach

- 2\textsuperscript{nd} derivative preprocessing
  - eliminates much of the irrelevant clutter signal

- Use library spectrum as the target
  - libraries can be good first approximations
target contributions

visualization saturates the image signal to

\[ c_{\text{lim}} < c < 2c_{\text{lim}} \]

whitening based on all the pixels

\[ c_{\text{lim}} = \left( s^T \sum_{c^+}^{-1} s \right)^{-1/2} \]
Whitened PCA Anomaly Detection

GLS target detection results.

- Define pixels with $c > c_{\text{lim}}$ as $X_s$ and whiten using all other pixels.
- Known target pixels are “signal” and others are “clutter”. We are now supervising the PCA.

$$\Sigma_c^{-\frac{1}{2}} X_s^T X_s \Sigma_c^{-\frac{1}{2}} p = \lambda p$$

$$\Sigma_c = \frac{1}{M_c} X_c^T X_c$$

- If $X_s$ is a single target pixel, $x_s$, the approach reduces to GLS target detection.
- The pixels selected in the image are generally expected to be more relevant as a target than library spectra.
- Whitening based on non-target pixels
Calibrate on Whitened Target Pixels

Pixels identified in target detection are used as “image relevant target signal.”

Off-target pixels are used for whitening (= “clutter signal”)

Image of Scores on PC 1 (94.26%)
Targeted Anomaly Detection

- Target detection based on a library spectrum identified candidate target-rich pixels
- Target-rich pixels replace the library spectrum as target signal, and
- Off-target-rich pixels are clutter and are used to de-weight clutter signal
  - clutter = all signal not of interest / non-target signal
- Whitened PCA is “targeted anomaly detection”
PC 1 ~looks like the GLS target.

1st derivative
center to mean of clutter
autocontrast the scores

Percent Variance Captured by PCA Model

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<td>3</td>
<td>6.70e-01</td>
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Compare GLS & WPCA
Image of Scores on PC 1 (71.80%), PC 2 (3.18%)

1st derivative, SNV center to mean of clutter autocontrast the scores
Conclusions

- Anomaly and Target detection can be used synergistically to find signal of interest
  - signal that may be missed when used independently
- The math behind many methods is similar
  - e.g., GLS and WPCA
  - as shown WPCA can be considered “targeted anomaly detection”
- Differences are in how “signal” and “clutter” are defined
  - Can it be improved further with additional iterations? Automated?