Synergy of Target and Anomaly Detection in Hyperspectral Images

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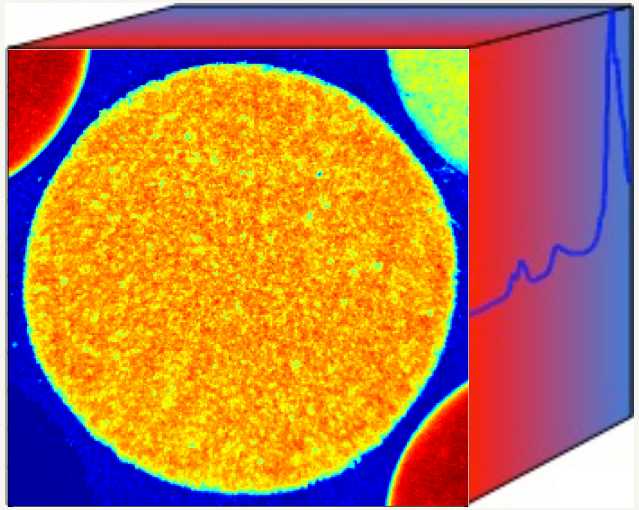
Hyperspectral Imaging



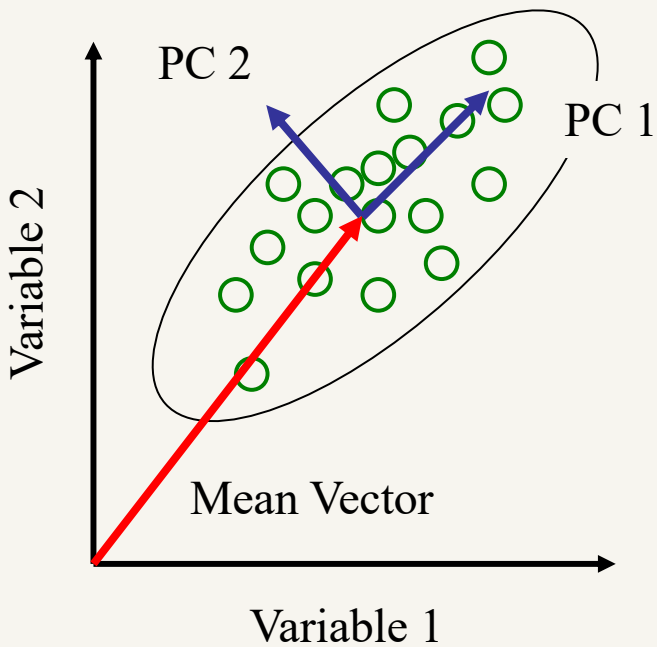
- Many pixels provide a good sampling for exploratory analysis, detection and classification
  - rapid and non-invasive
- Good for heterogeneous mixtures
  - although quantities to be detected may be low on a volume basis, signal in individual pixels can be dominated by an analyte of interest
  - wet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

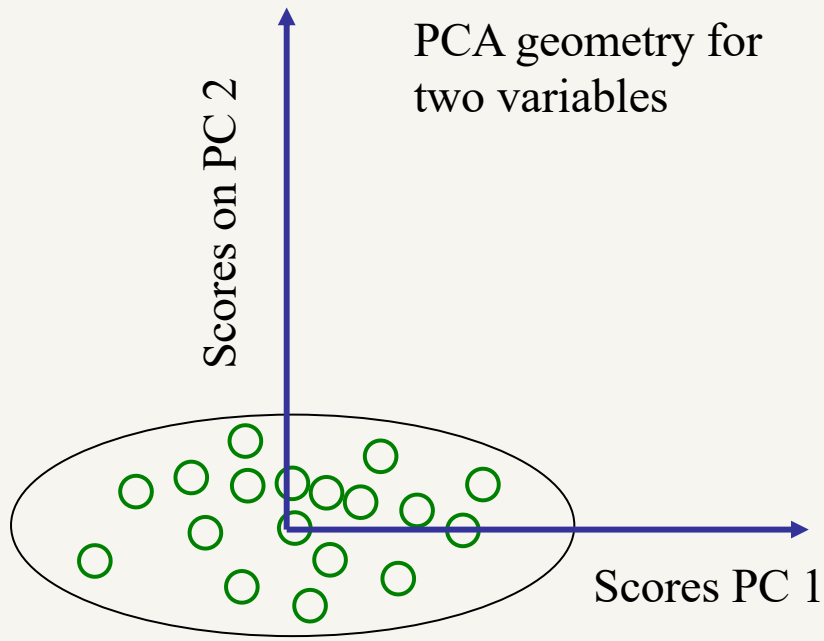
Typical Algorithms for Hyperspectral

- 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





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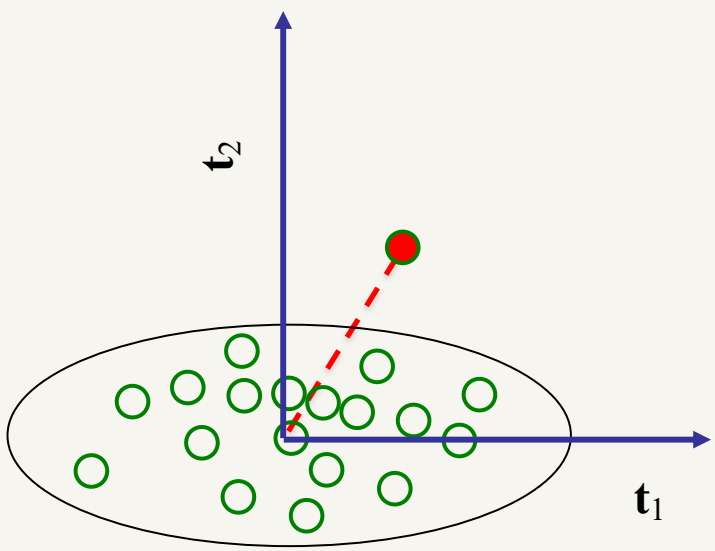
PCA Anomaly Detection

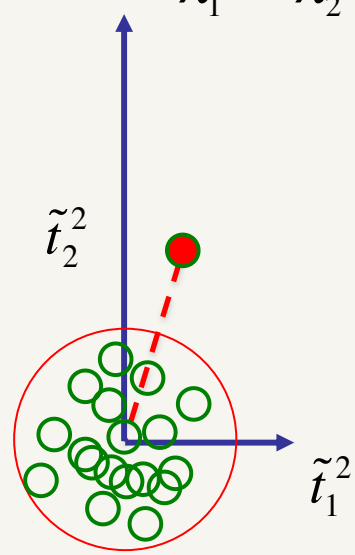
- Hotelling's T^2
  - Hotelling, H, (1931) "The generalization of Student's ratio," *Annals of Mathematical Statistics*," **2**(3), 360-378

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

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

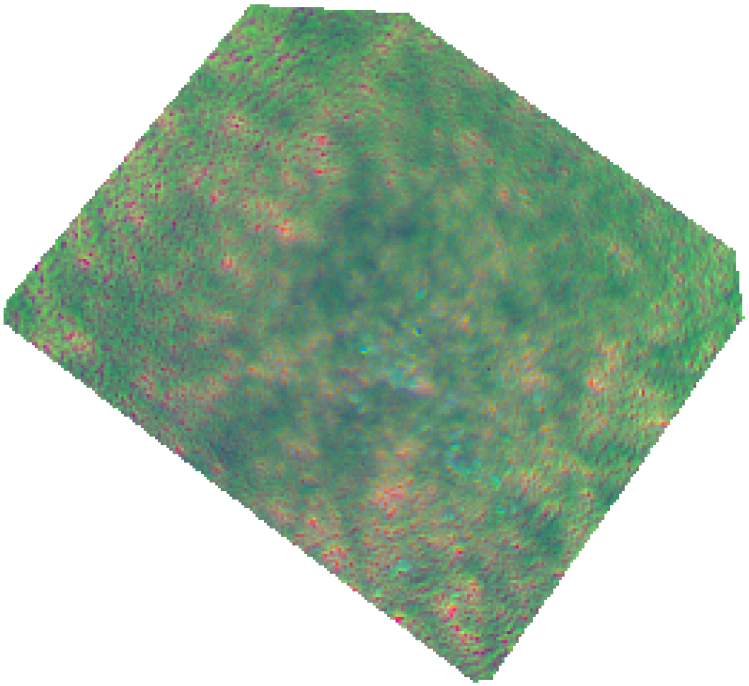
"whitening"





Anomaly Detection Example

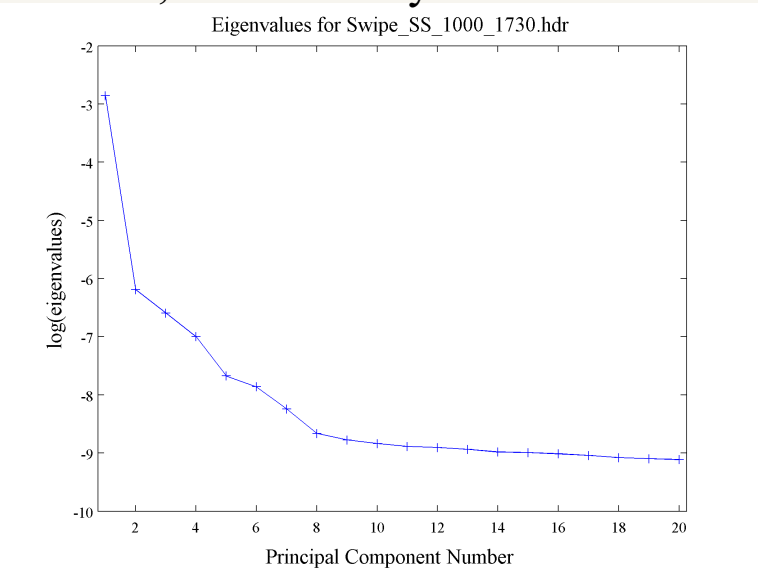
Image of Scores on PC 1 (97.73%), PC 2 (1.28%) & PC 3 (0.56%)



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?



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

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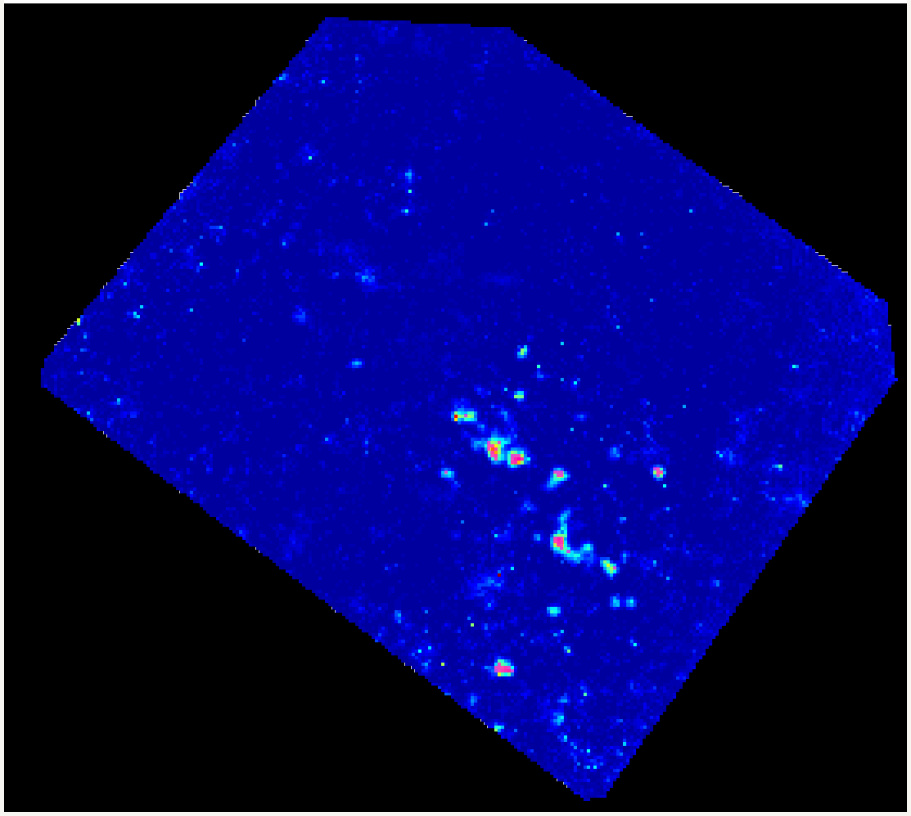
T^2 Anomaly Detection

Image of Hotelling T^2 (99.83%)



weak anomaly found on PCs 4 to 6

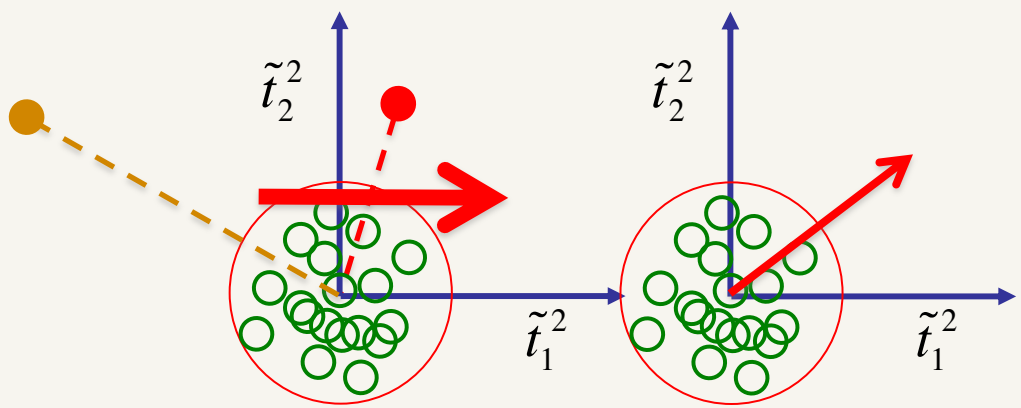
X-block: Swipe_SS_1000_1730.hdr 35208 by 731
Preprocessing: -log10, Mean Center
Num. PCs: 7

Percent Variance Captured by PCA Model

Principal Component Number	Eigenvalue of Cov(X)	% Variance Captured This PC	% Variance Captured Total
1	1.03e+01	97.73	97.73
2	1.35e-01	1.28	99.01
3	5.84e-02	0.56	99.57
4	1.86e-02	0.18	99.75
5	4.28e-03	0.04	99.79
6	3.17e-03	0.03	99.82
7	1.78e-03	0.02	99.83

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?



Target Detection

- Finds pixels w/ unusual signal in a *specific direction* w/in 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

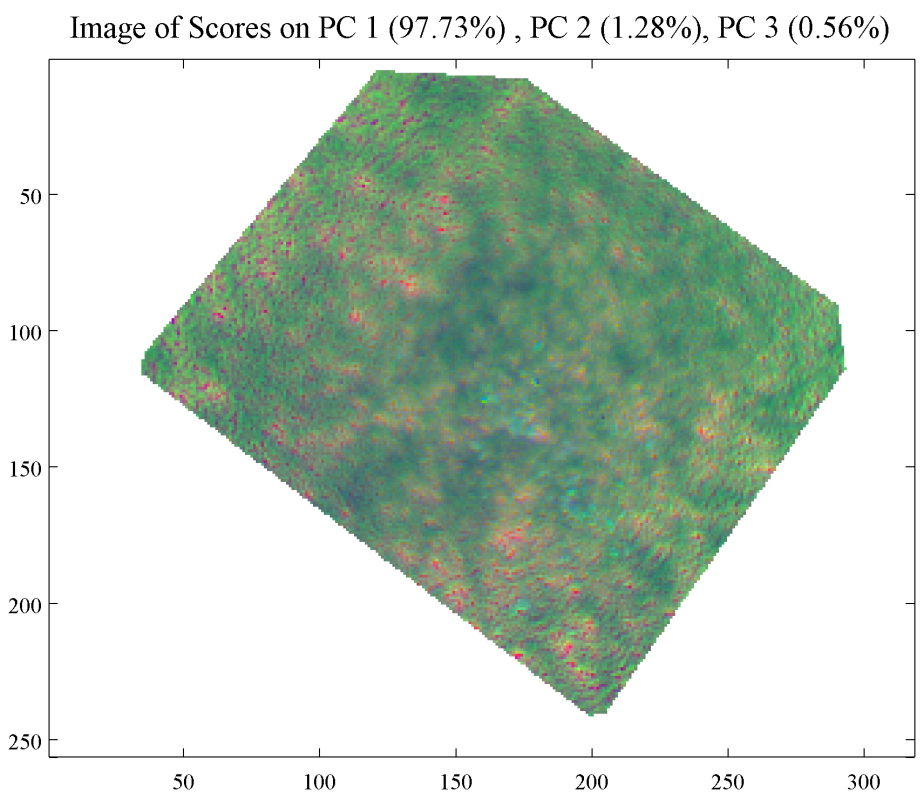
Target Detection

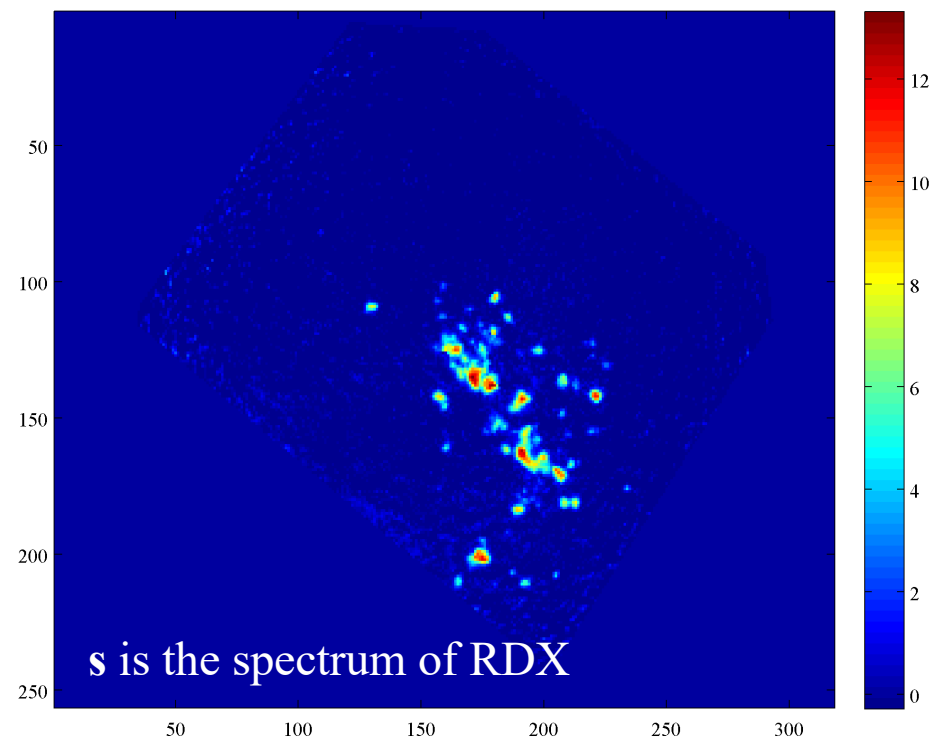
$$\mathbf{X} = \mathbf{T}\mathbf{P}^T + \mathbf{E}$$

$$\mathbf{T} = \mathbf{X}\mathbf{P}$$

$$\mathbf{X} = \mathbf{c}\mathbf{s}^T + \mathbf{E}$$

$$\hat{\mathbf{c}} = \mathbf{X}\boldsymbol{\Sigma}_c^{-1}\mathbf{s}\left(\mathbf{s}^T\boldsymbol{\Sigma}_c^{-1}\mathbf{s}\right)^{-1}$$



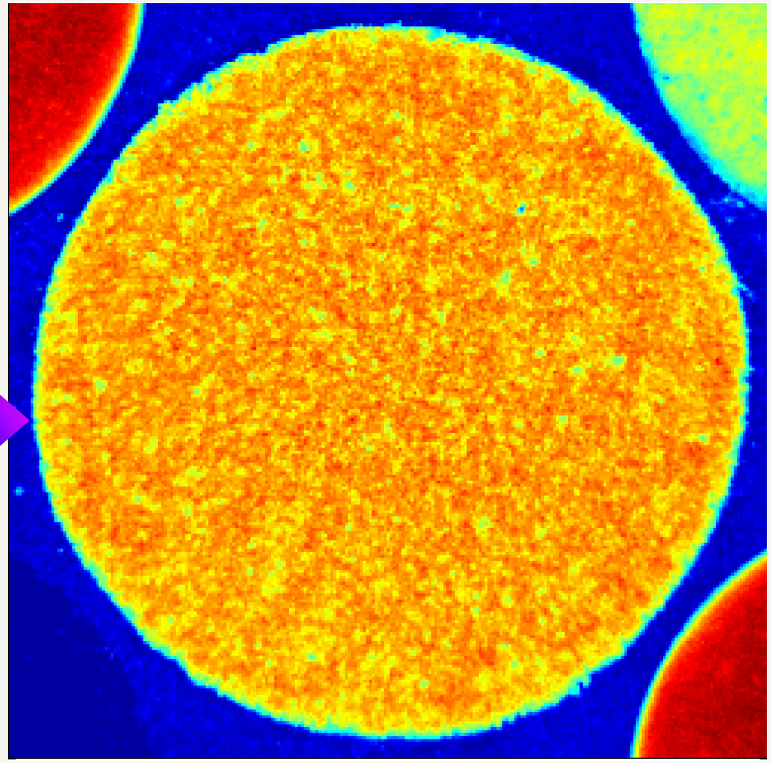


data set: courtesy OPOTEK, Inc., Carlsbad, CA

Model System Studied

- ppm levels of melamine in wheat gluten

NIR reflectance hyperspectral image



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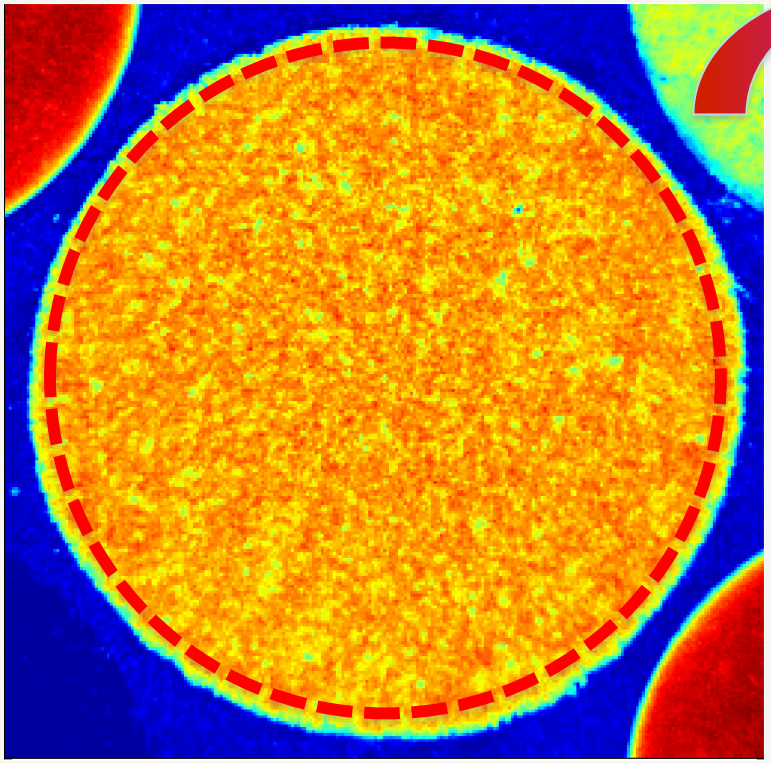
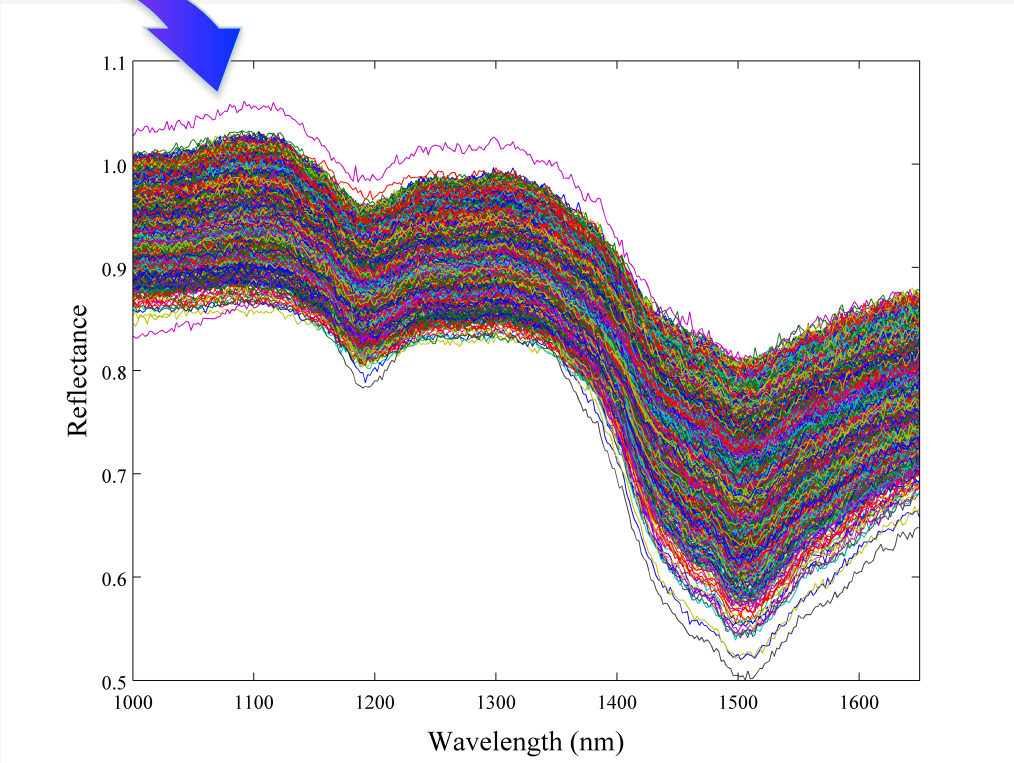
Powdered Raw Materials

- 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.





Unadulterated wheat gluten

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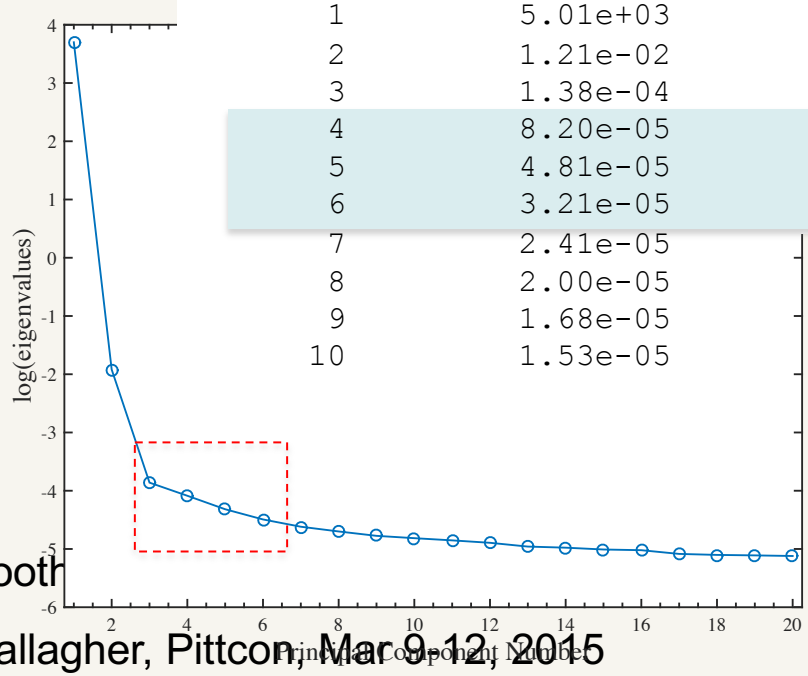
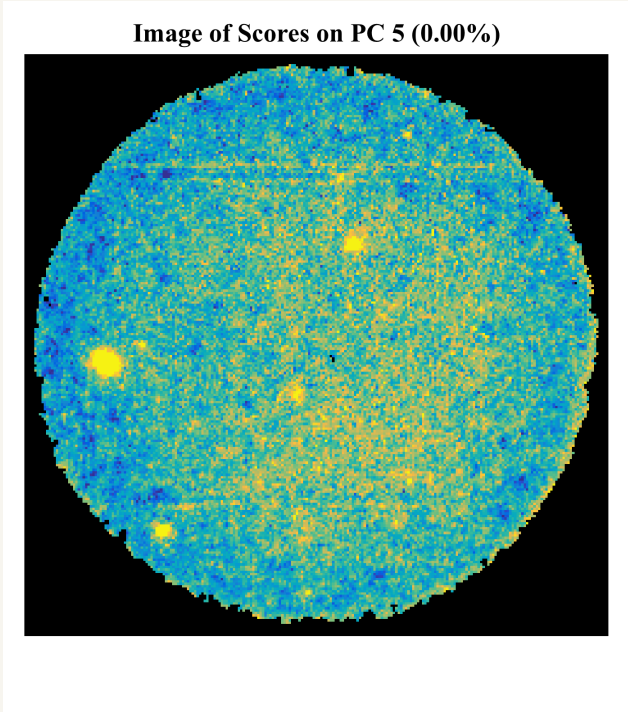
PCA of Melamine in Wheat Gluten

Eigenvalues for 200 ppm melamine in wheat gluten
-log10

Percent Variance Captured by PCA Model

Principal Component Number	Eigenvalue of Cov(X)	% Variance Captured This PC
1	5.01e+03	100.00
2	1.21e-02	0.00
3	1.38e-04	0.00
4	8.20e-05	0.00
5	4.81e-05	0.00
6	3.21e-05	0.00
7	2.41e-05	0.00
8	2.00e-05	0.00
9	1.68e-05	0.00
10	1.53e-05	0.00





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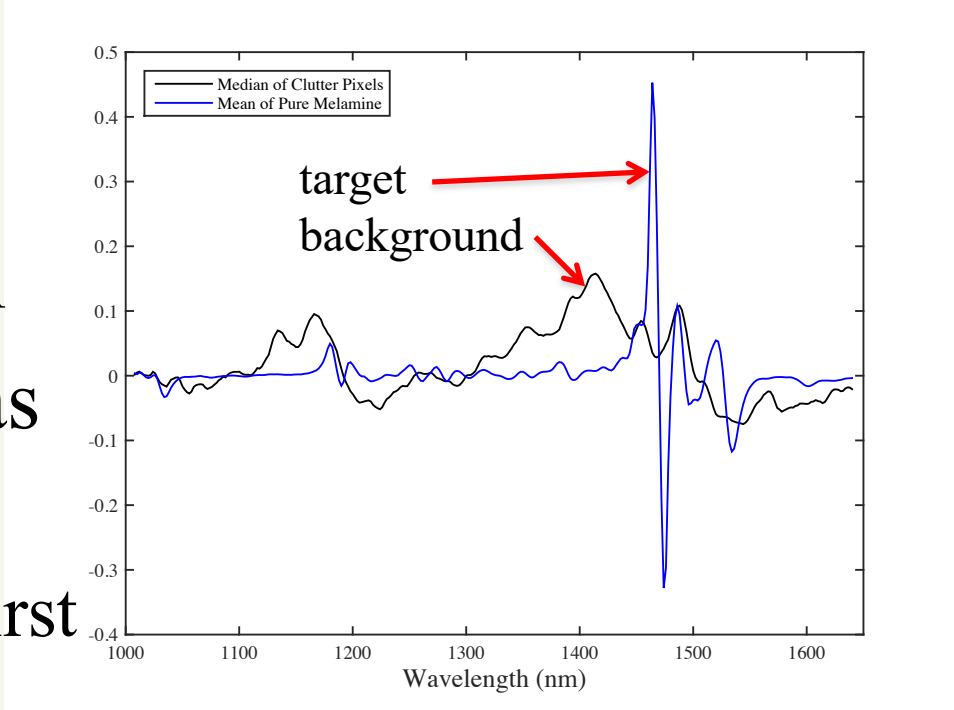
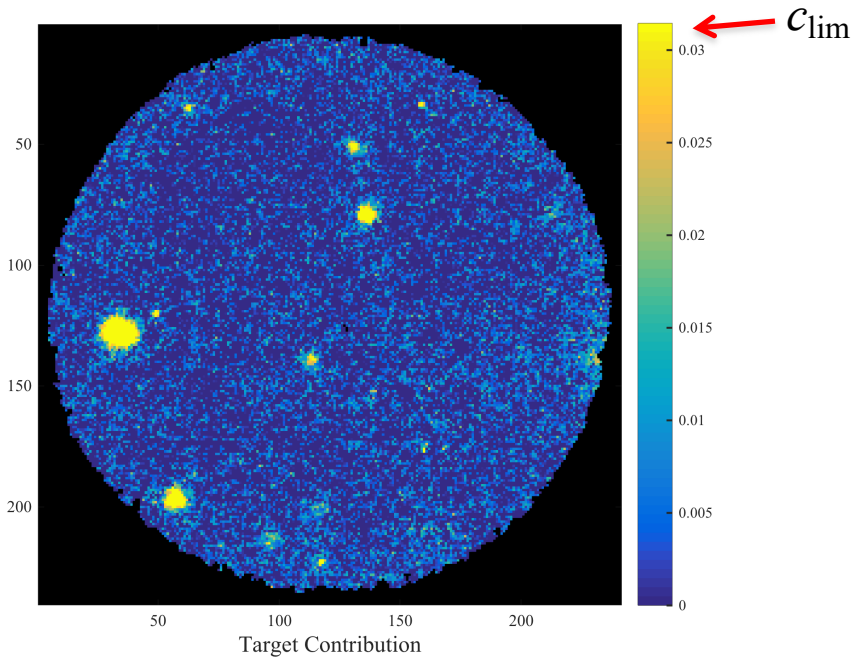
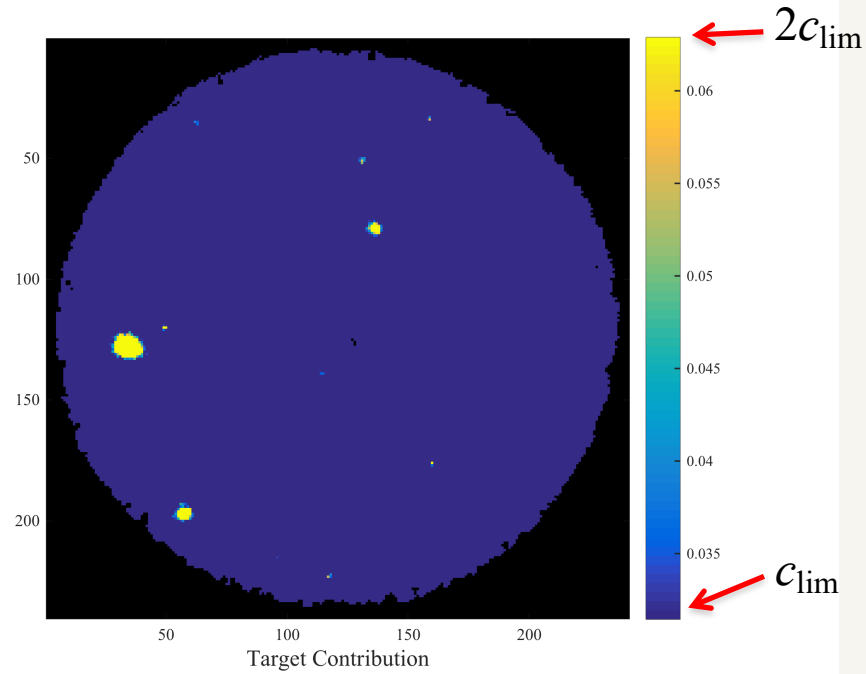
Target Approach

- 2nd derivative preprocessing
  - eliminates much of the irrelevant clutter signal
- Use library spectrum as the target
  - libraries can be good first approximations





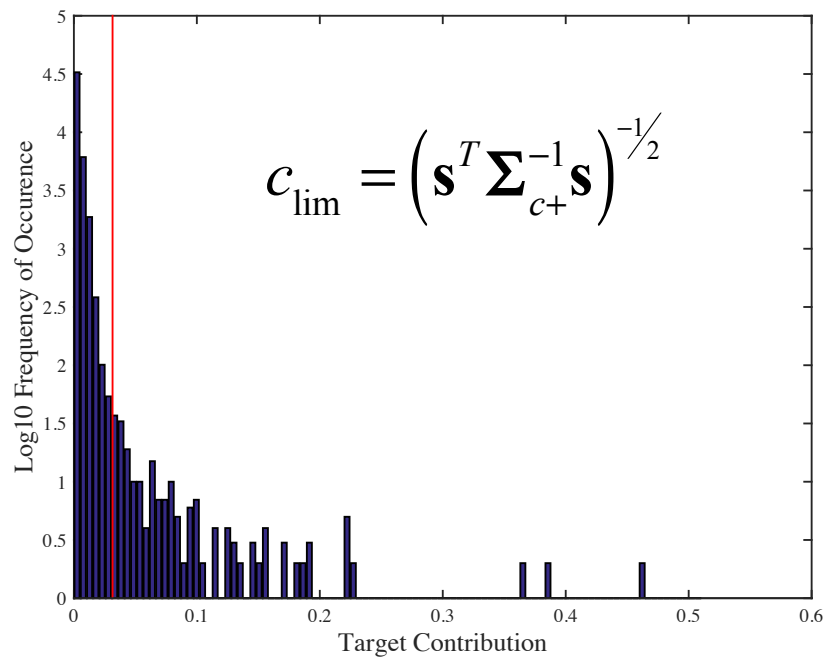


target contributions

visualization saturates the image signal to

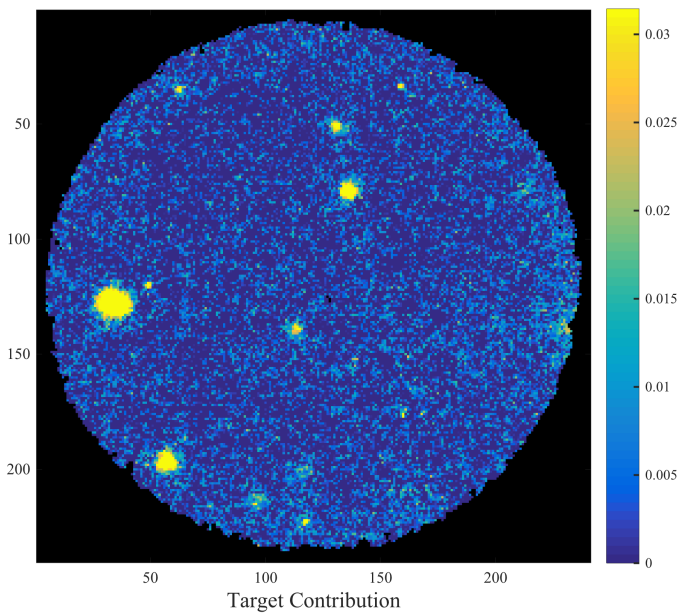
$$c_{\mathrm{lim}} < c < 2c_{\mathrm{lim}}$$

whitening based on all the pixels



Whitened PCA Anomaly Detection

GLS target detection results.



- Define pixels with $c > c_{lim}$ as $\mathbf{X}_s$ and whiten using all other pixels.
- Known target pixels are "signal" and others are "clutter". We are now supervising the PCA.

$$\boldsymbol{\Sigma}_c^{-1/2}\mathbf{X}_s^T\mathbf{X}_s\boldsymbol{\Sigma}_c^{-1/2}\mathbf{p} = \lambda\mathbf{p}$$

$$\boldsymbol{\Sigma}_c = \frac{1}{M_c}\mathbf{X}_c^T\mathbf{X}_c$$

- If $\mathbf{X}_s$ is a single target pixel, $\mathbf{x}_s$, 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

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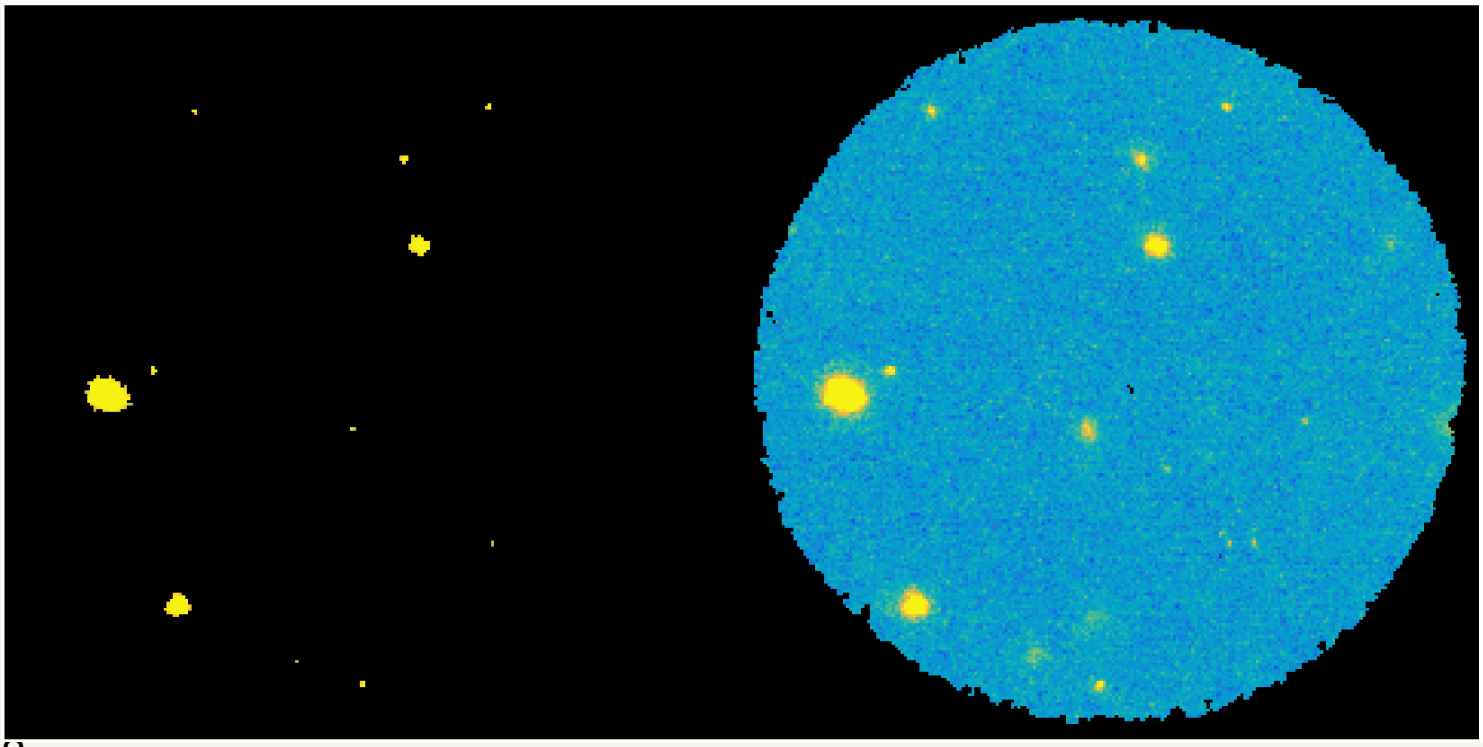
Calibrate on Whitened Target Pixels

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"

Image of Scores on PC 1 (94.26%)

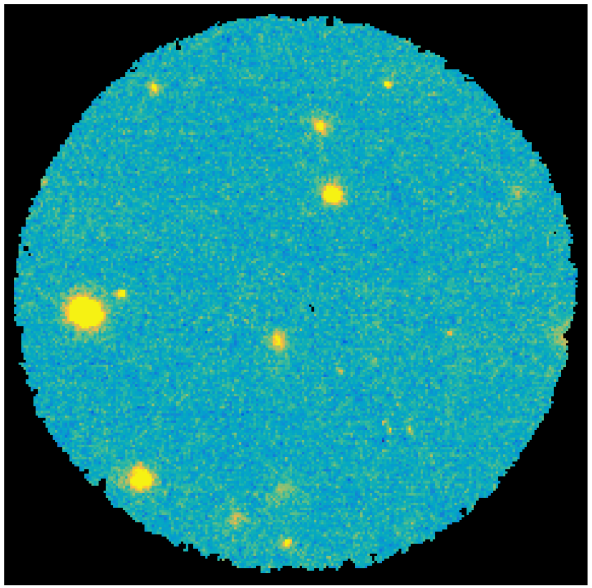
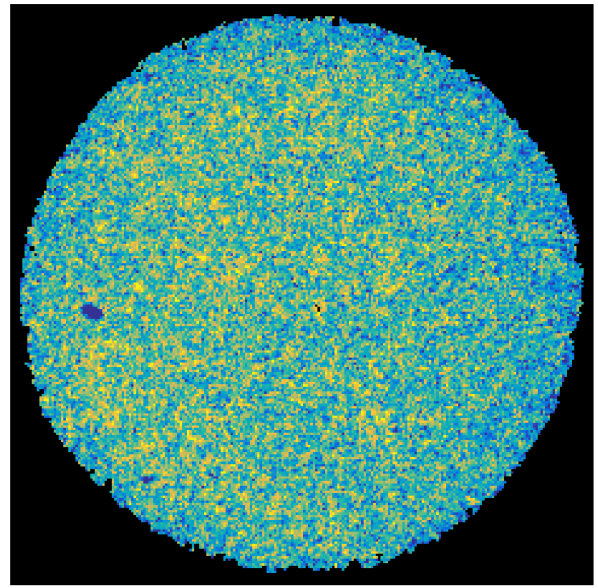
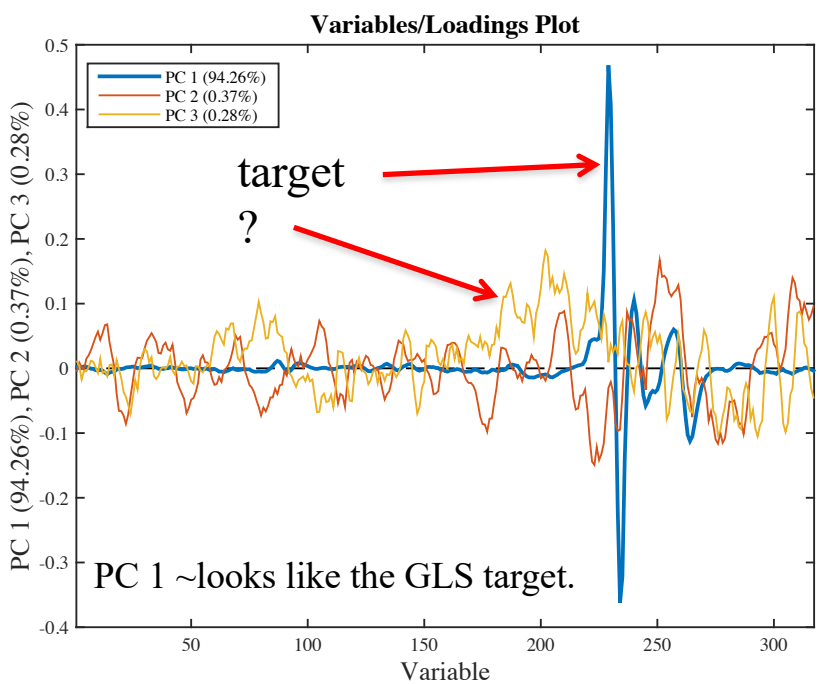


Image of Scores on PC 3 (0.28%)





1st derivative

center to mean of clutter

autocontrast the scores

Percent Variance Captured by PCA Model

Principal Component Number	Eigenvalue of Cov(X)	% Variance Captured This PC
1	2.27e+02	94.26
2	8.93e-01	0.37
3	6.70e-01	0.28

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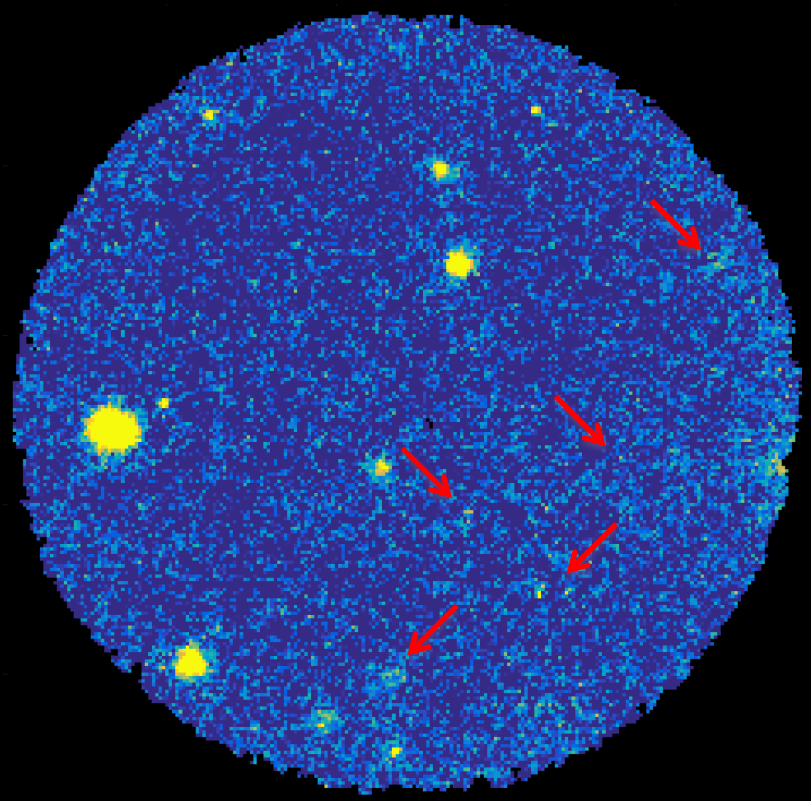
Compare GLS & WPCA



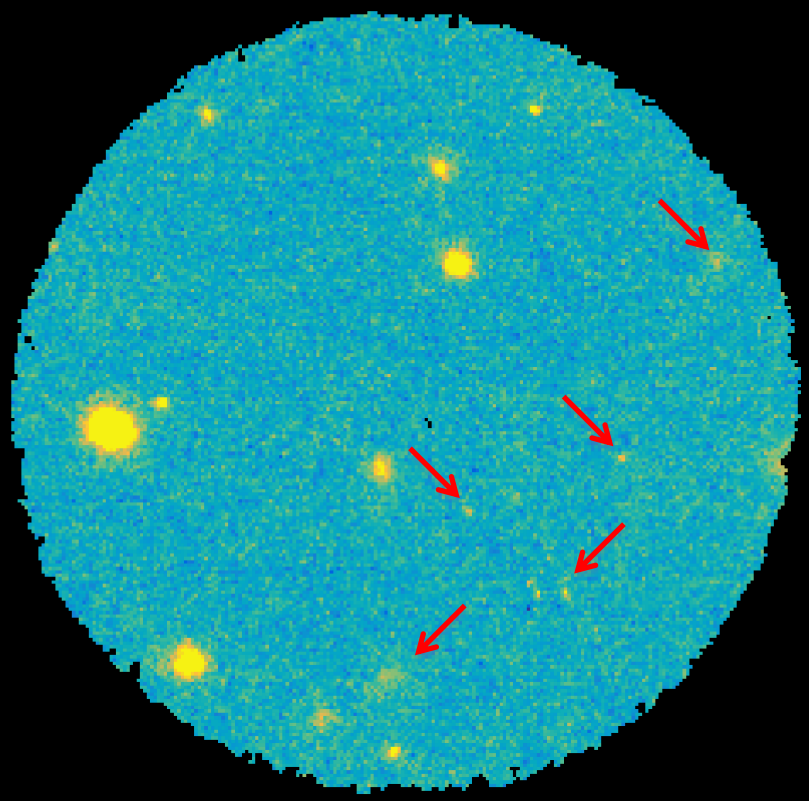


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Image of Scores on PC 1 (71.80%)

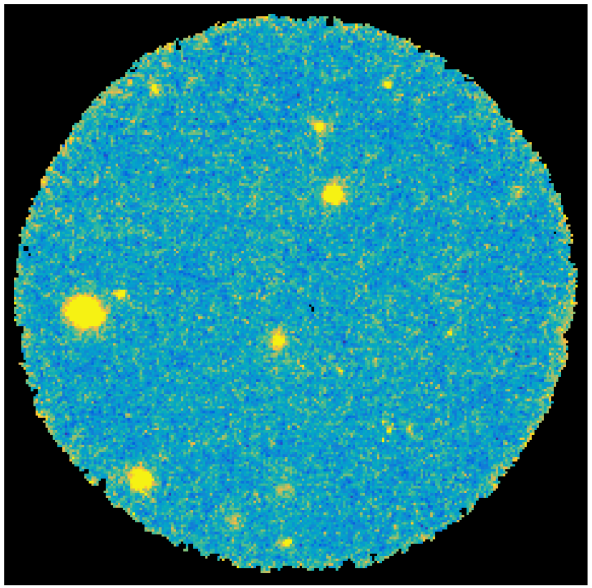


Image of Scores on PC 2 (3.18%)

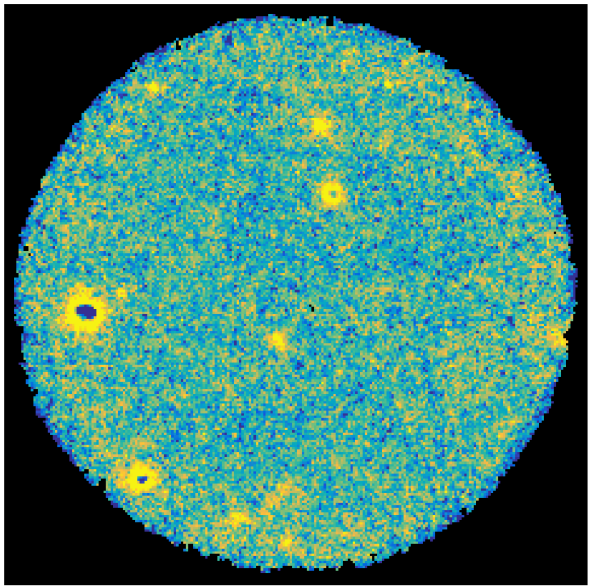
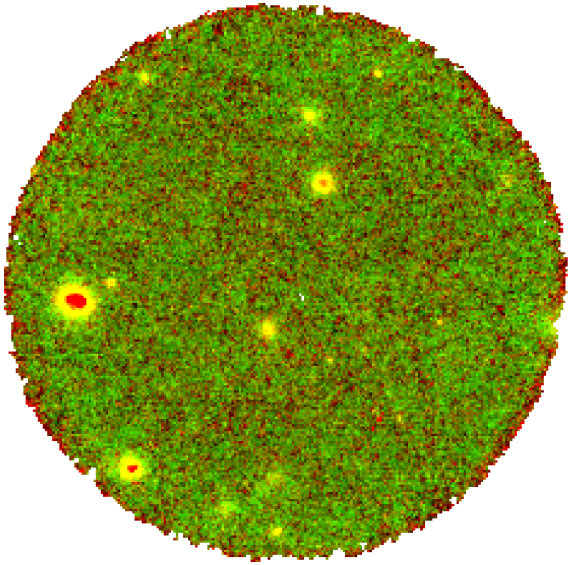
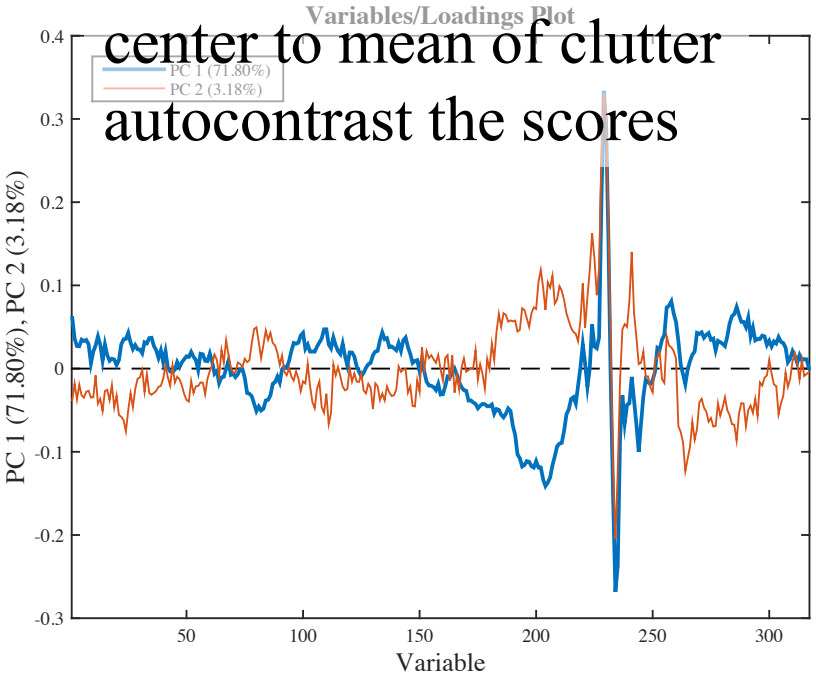


Image of Scores on PC 1 (71.80%) & Scores on PC 2 (3.18%)



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?