Targeted Anomaly Detection in Hyperspectral Imaging – Finding Minor Anomalies in a Swamp

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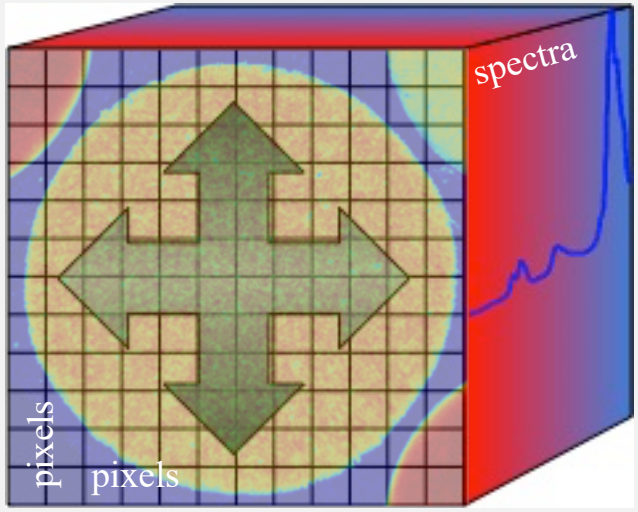
Hyperspectral Imaging



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

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Detection Models

- Compared to the statistical distribution of the data set:
- Anomaly Detection finds unusual signal in any direction
- Target Detection finds signal in a specific direction defined externally
- Targeted Anomaly Detection finds signal in ~specific directions relevant to the image

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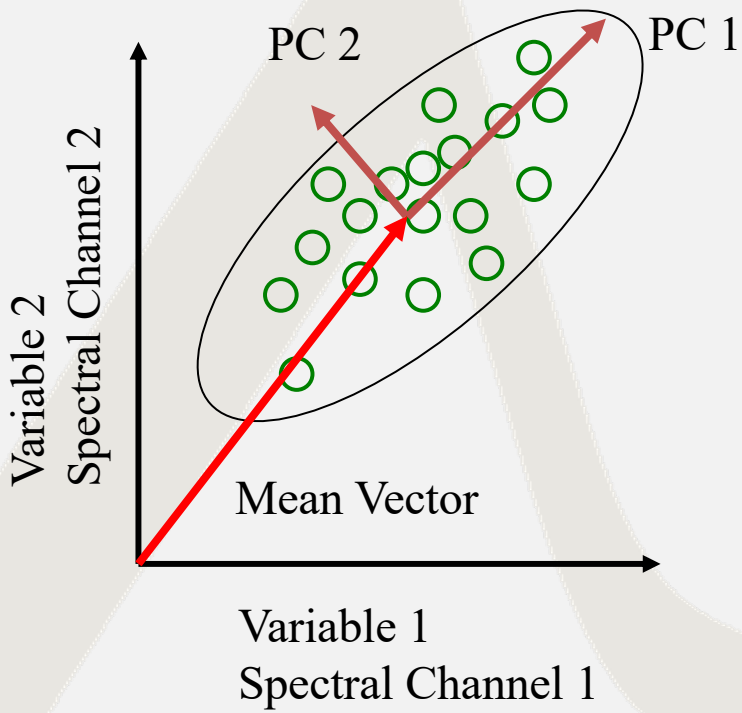
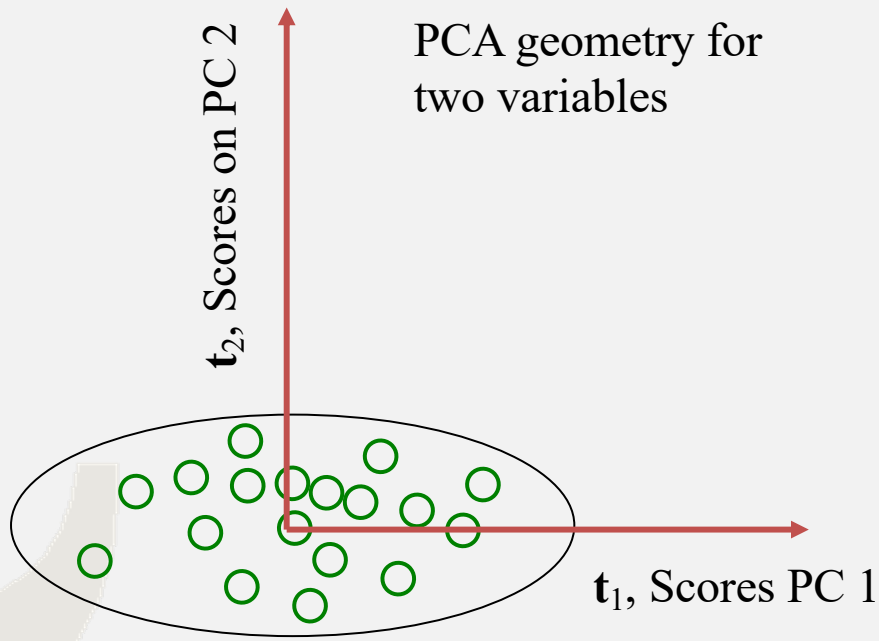
Principal Components Analysis

- PCA, ICA, DistSlct/Purity, …





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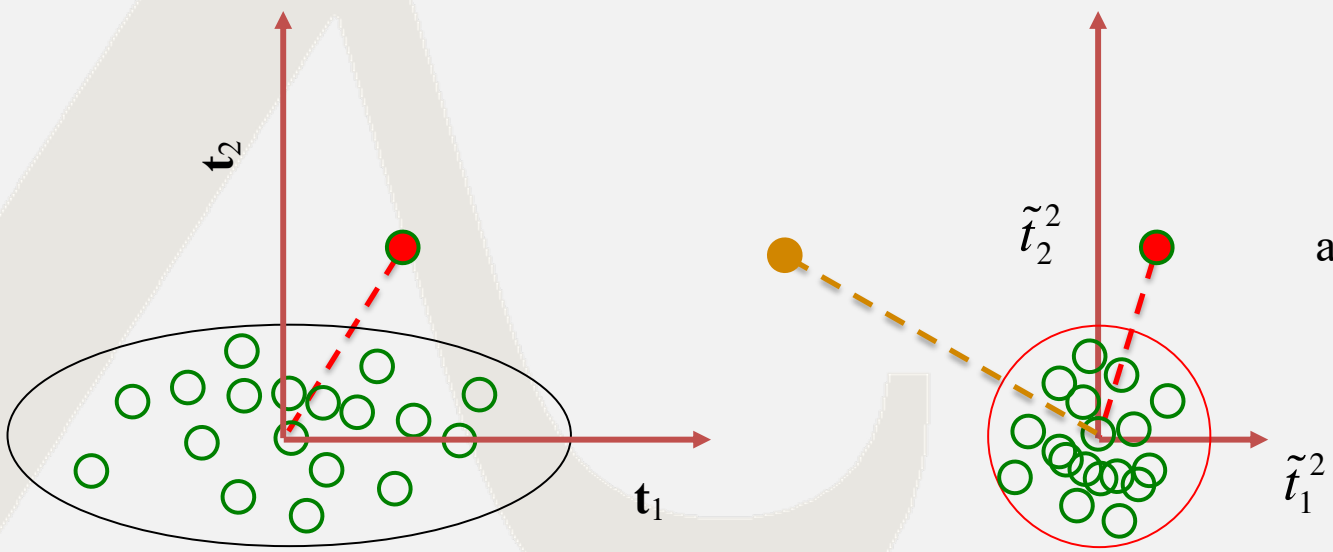
PCA Anomaly Detection w/ T^2

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

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



"whitening"

anomalies are found in any direction

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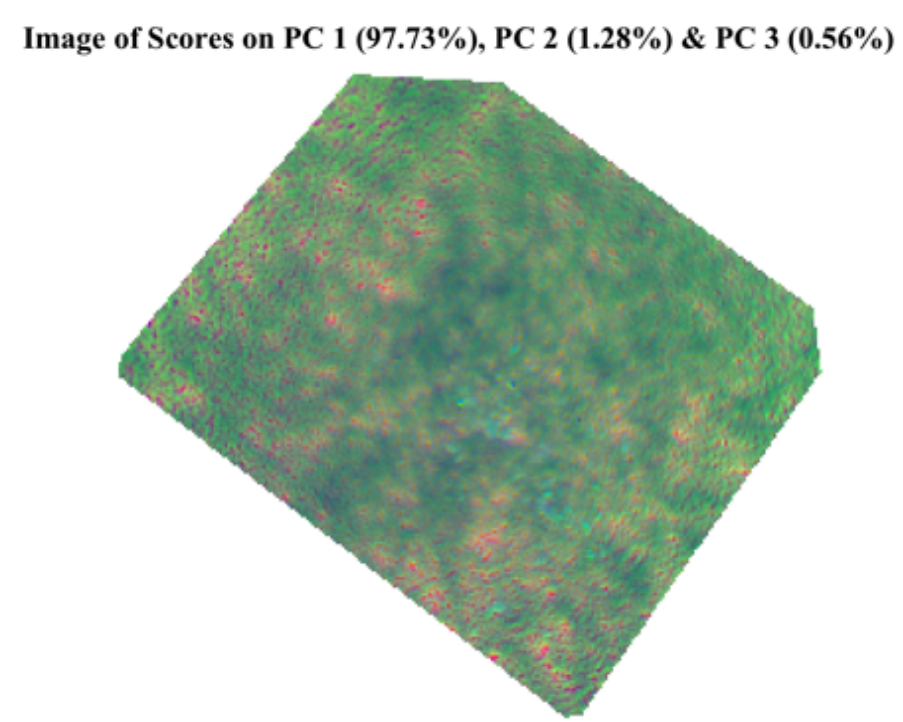
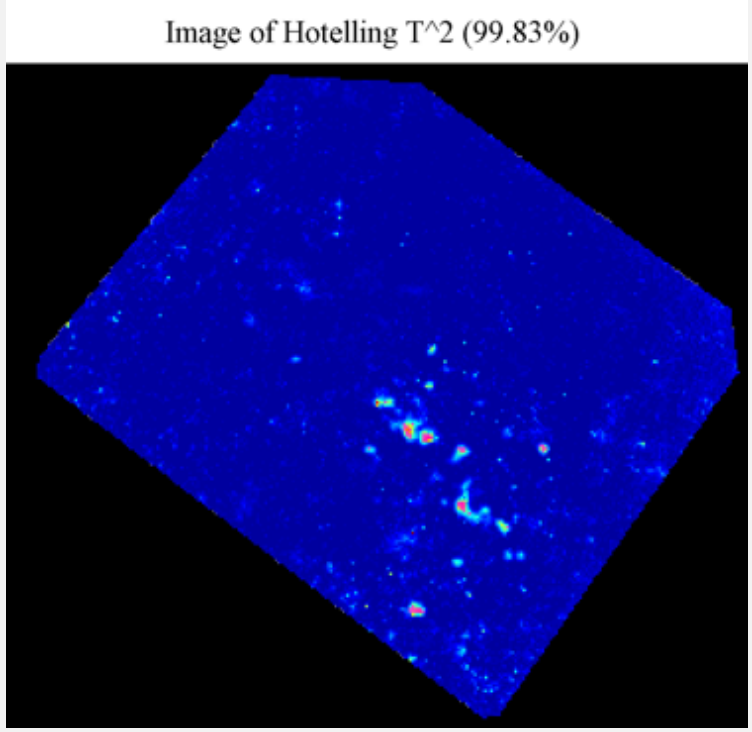
Anomaly Detection Example

NIR reflectance image of a cellulosic swipe.

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

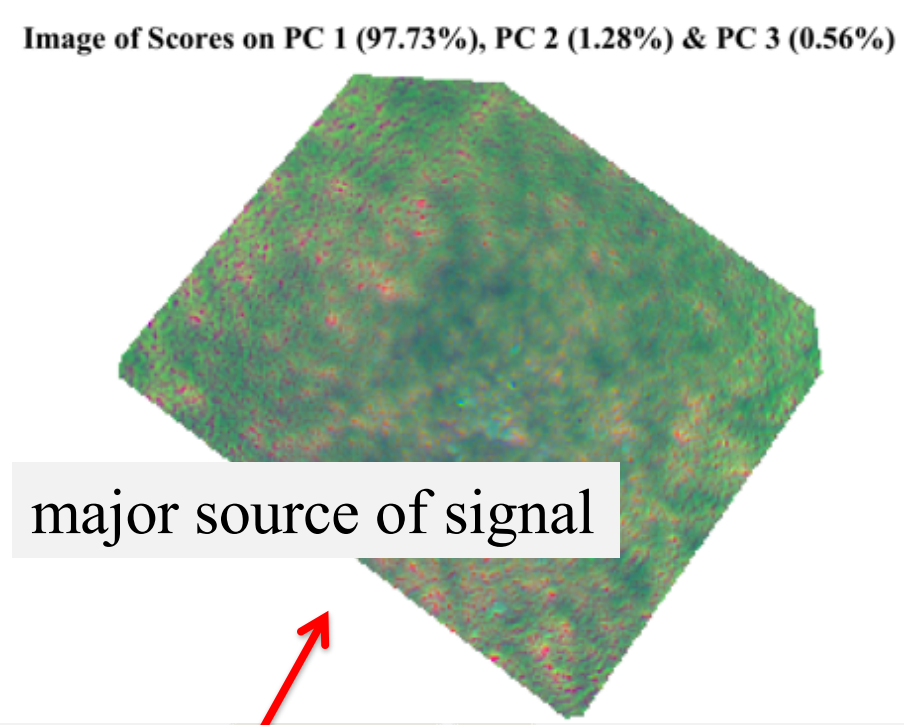
apparent anomaly observed – what is it?



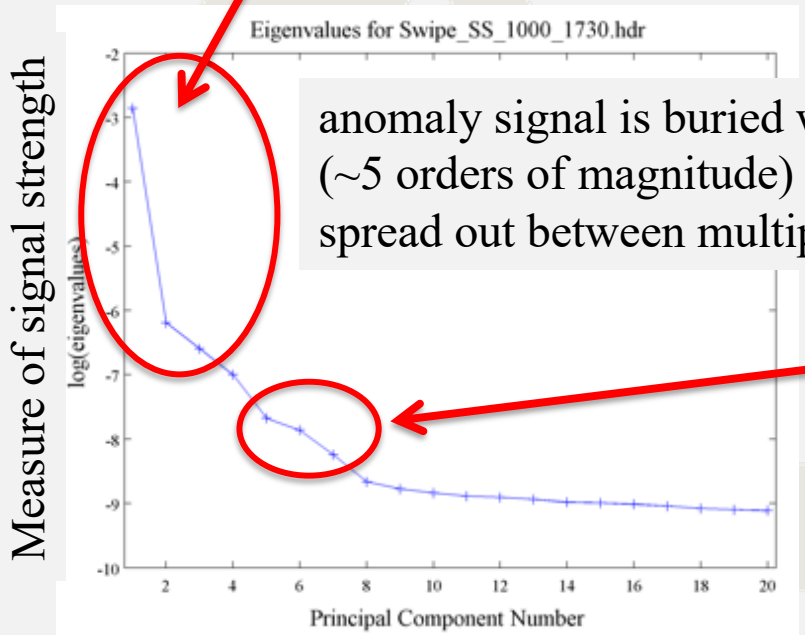


data set: courtesy OPOTEK, Inc., Carlsbad, CA

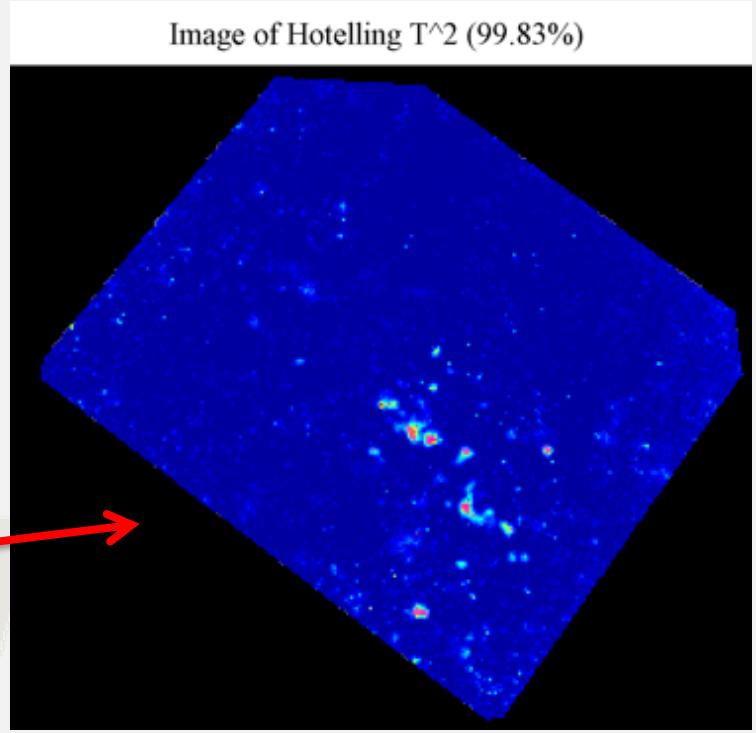
Anomaly Detection Example



apparent anomaly observed – what is it?



anomaly signal is buried waaay (~5 orders of magnitude) and spread out between multiple factors



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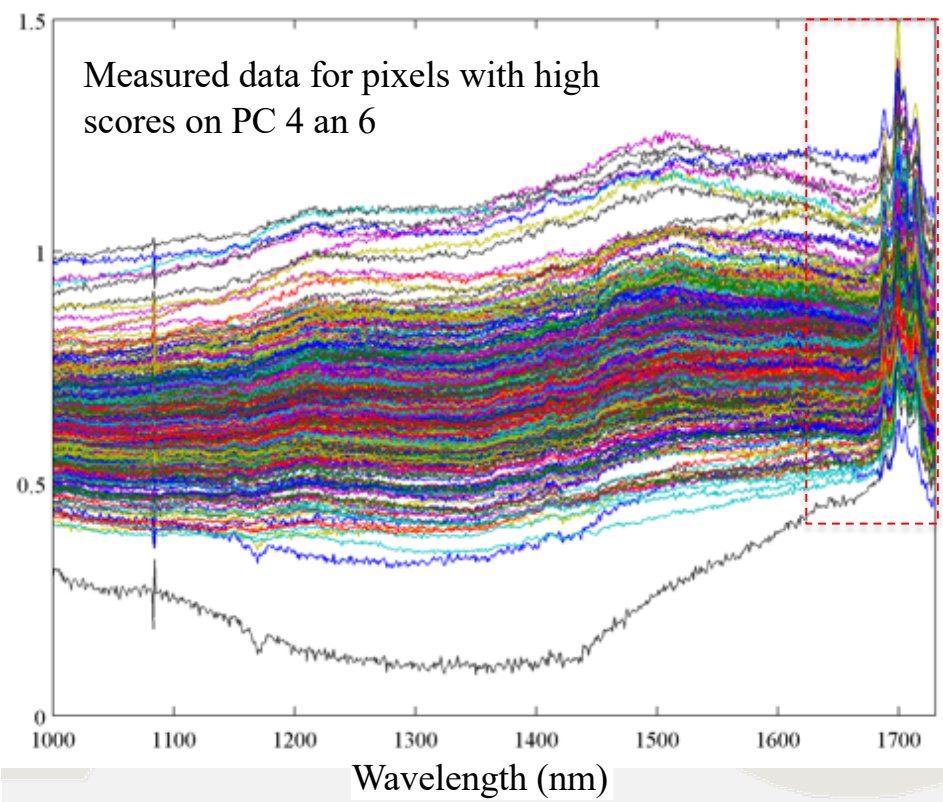
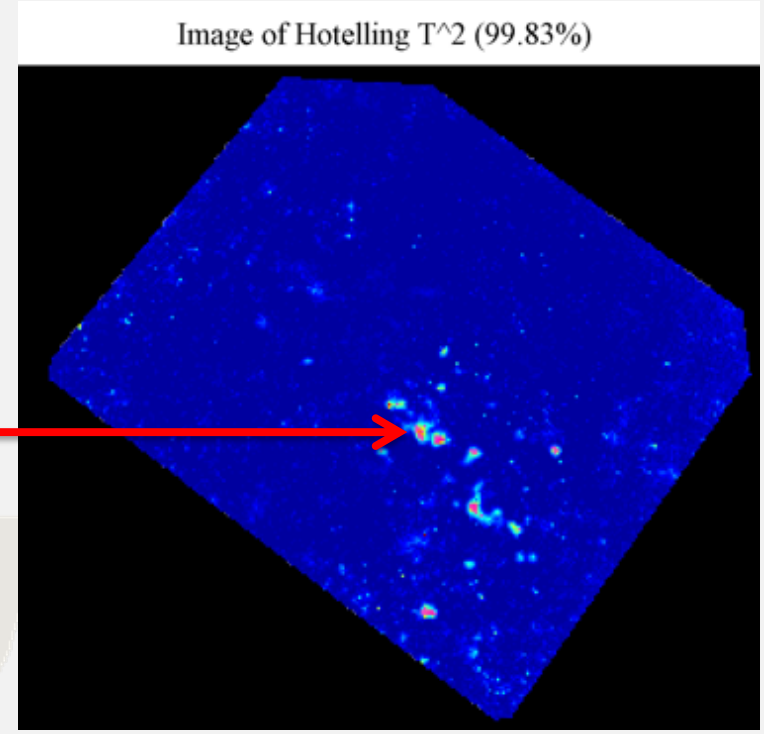
Anomaly Pixels

- Most of the signal is "clutter"

apparent anomaly observed – what is it?





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Anomaly Detection Summary

- Flexible - finds unusual signal
- Minor anomalies may be difficult to detect
  - Could appear like random noise
- Doesn't identify the signal
  - Library search
    - Spectra in library not relevant? Matrix, environment,…
    - Additional processing may be needed for impure signal to remove background

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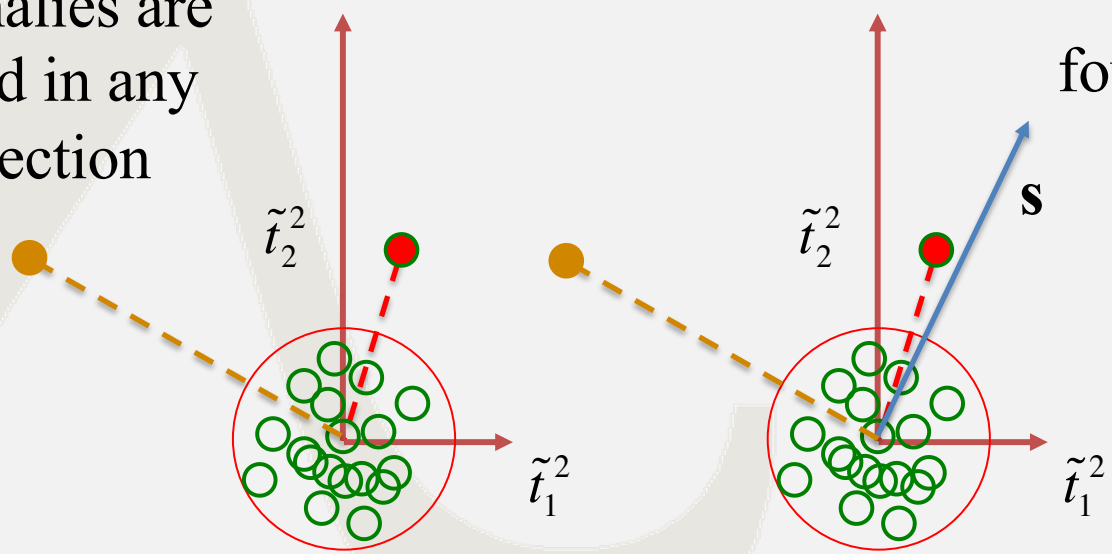
Target Detection

- Aitken Estimator, Generalized Least Squares
  - Alexander C. Aitken, (1935) "On Least Squares and Linear Combinations of Observations", *Proceedings of the Royal Society of Edinburgh*. **55**, 42-48.

anomalies are found in any direction



target signal is found in a specific direction, **s**

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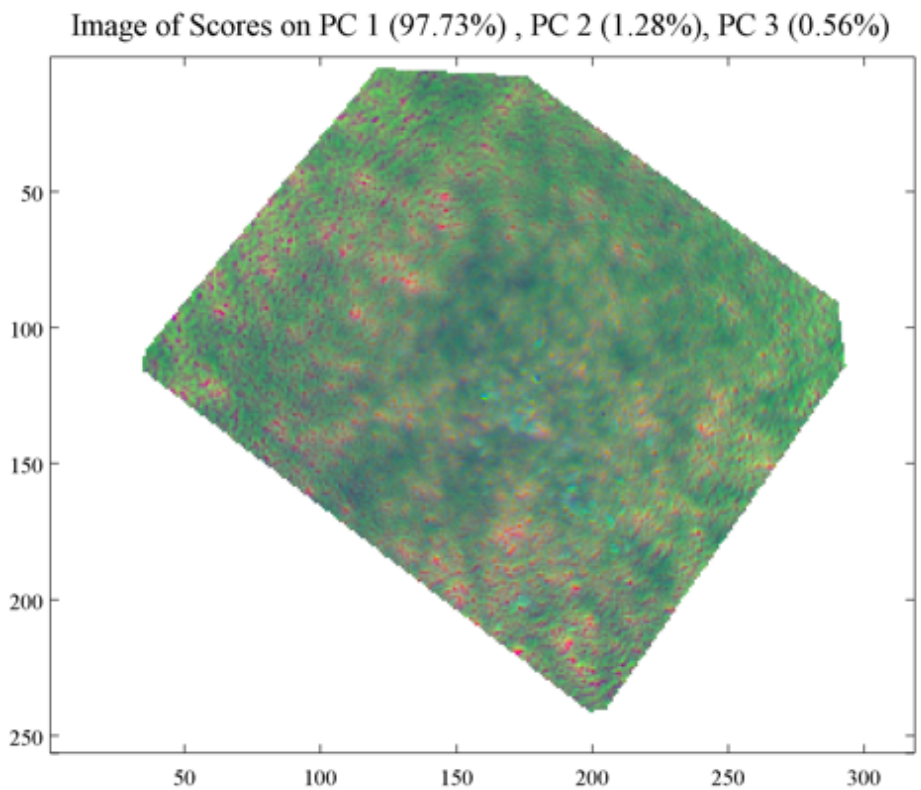
Target Detection Example

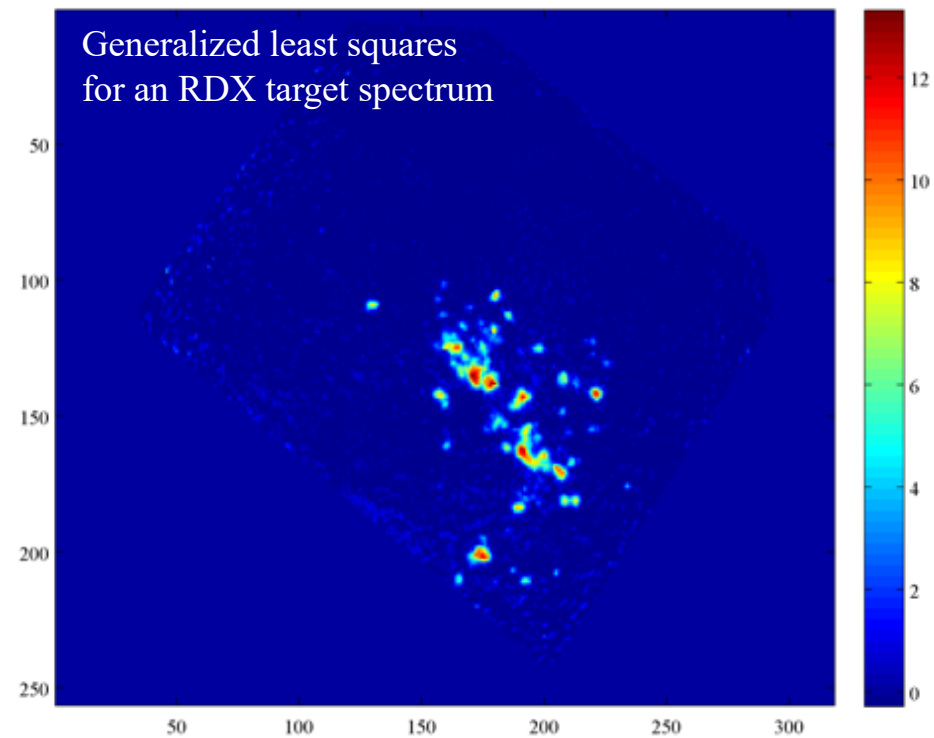
$$\mathbf{X} = \mathbf{T}\mathbf{P}^T + \mathbf{E}$$

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

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

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





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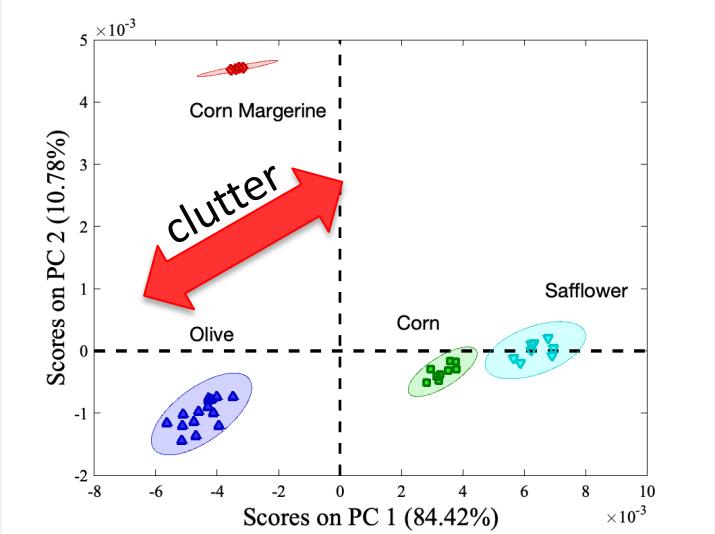
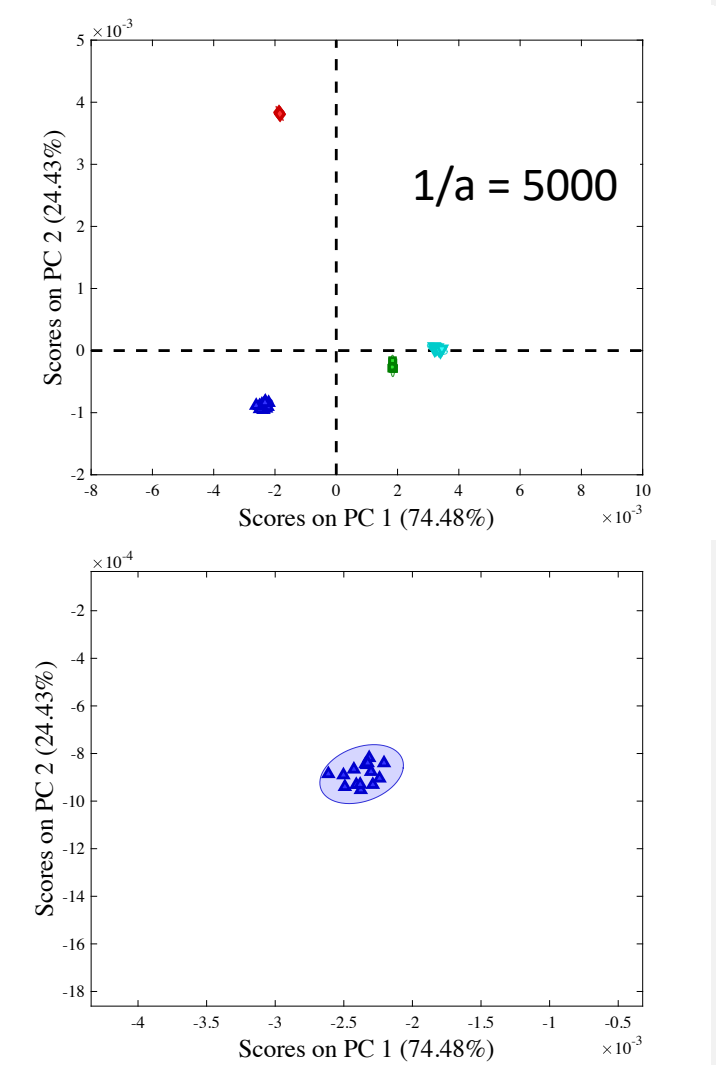
What does "decluttering" do?



generalized least squares weighting is a form of "de-cluttering" that can be used to increase inter- to intra-class variance where 1/a is a measure of how strong the de-weighting is applied.

Paradigm Shift:
Maximize: signal-to-noise → signal-to-clutter
Requires replicates to characterize the intra-class clutter.

GLSW (weighting 1/a)



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Target Detection Example
RDX on a Plate

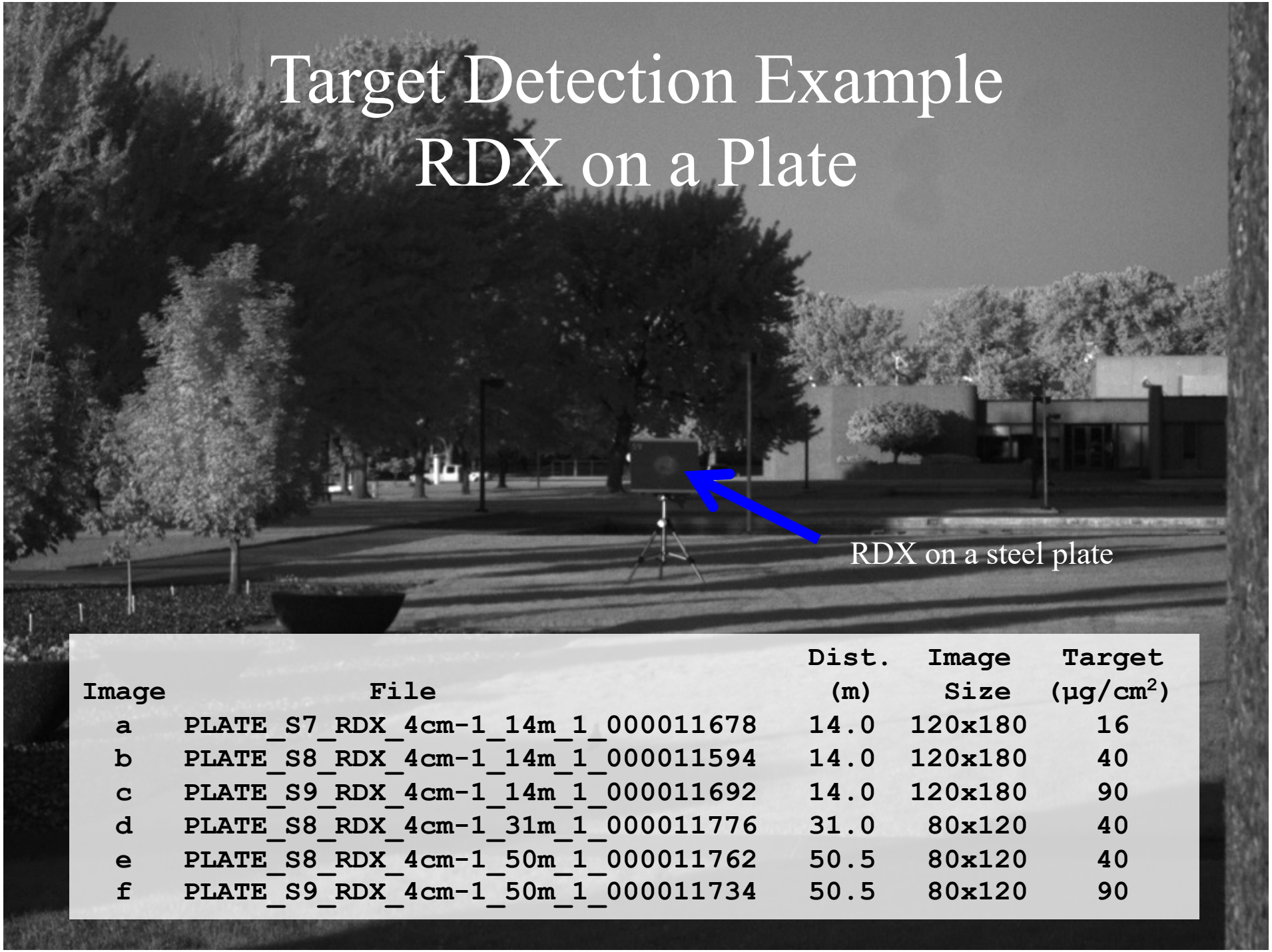
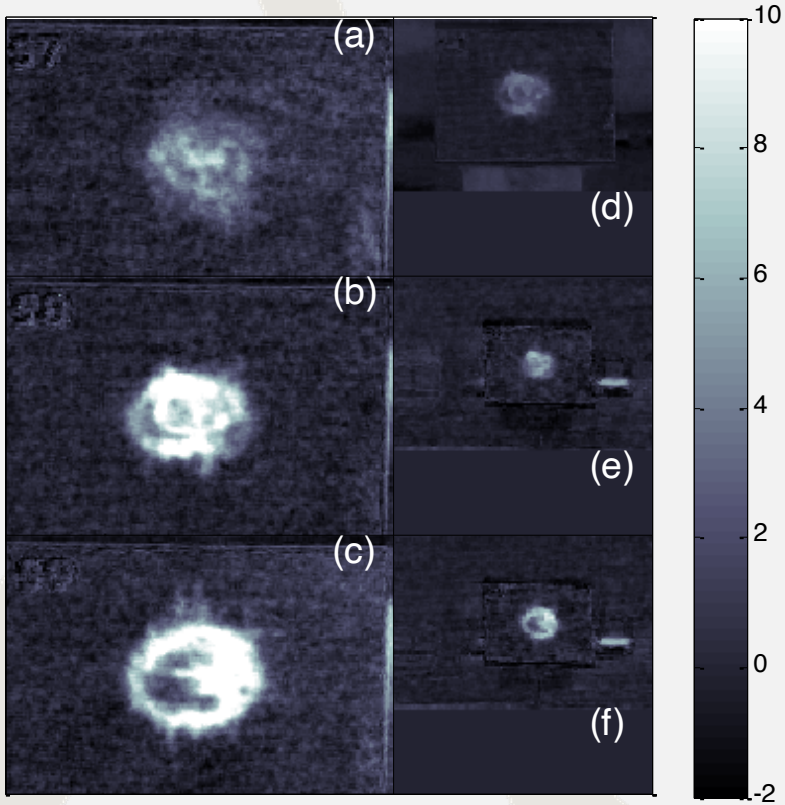


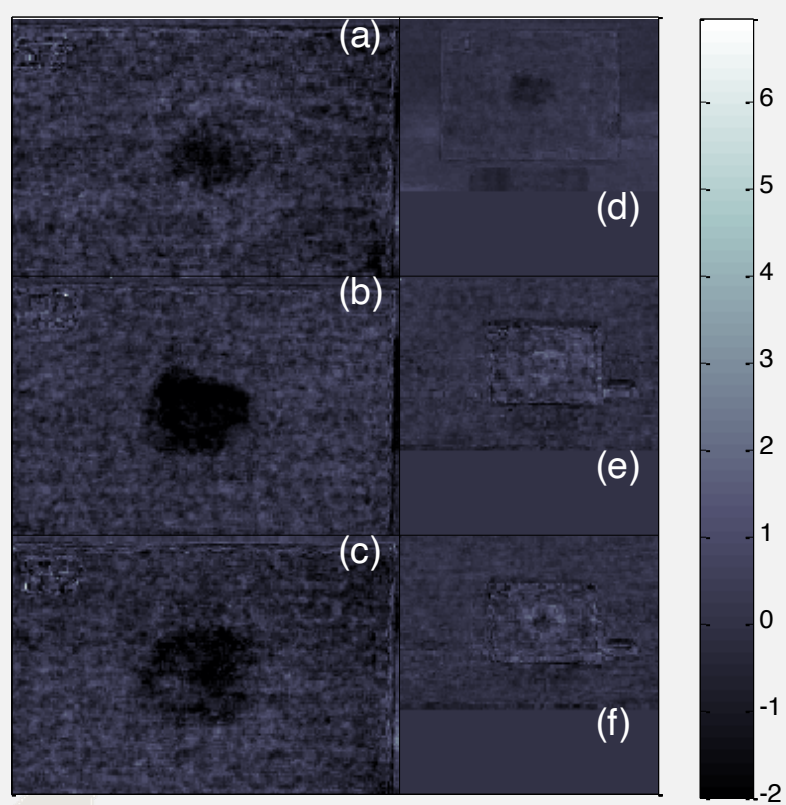
Image	File	Dist. (m)	Image Size	Target (µg/cm^2)
a	PLATE_S7_RDX_4cm-1_14m_1_000011678	14.0	120x180	16
b	PLATE_S8_RDX_4cm-1_14m_1_000011594	14.0	120x180	40
c	PLATE_S9_RDX_4cm-1_14m_1_000011692	14.0	120x180	90
d	PLATE_S8_RDX_4cm-1_31m_1_000011776	31.0	80x120	40
e	PLATE_S8_RDX_4cm-1_50m_1_000011762	50.5	80x120	40
f	PLATE_S9_RDX_4cm-1_50m_1_000011734	50.5	80x120	90

GLS Contributions

RDX



TNT



RDX target is detected at in all images while TNT is not.
False alarms suggested in images d-f but not if residuals are included.
Clutter is based on LH 52 and 48 pixels.

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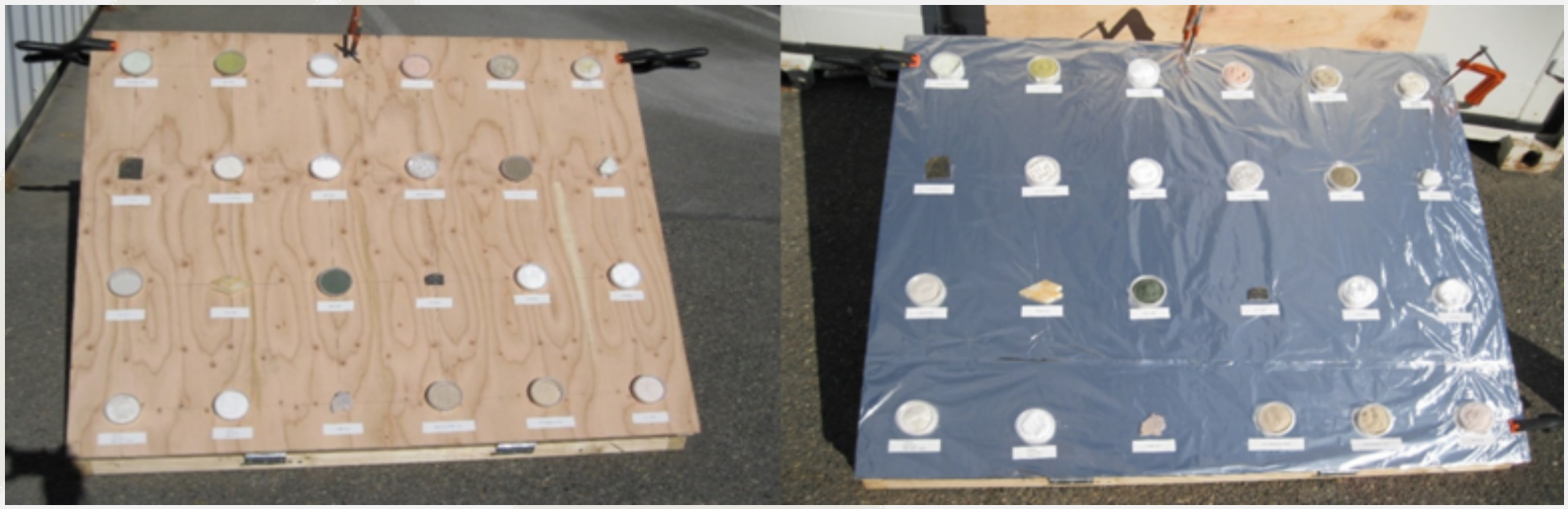
Target Detection Example
Minerals on Plate

- Rock and Minerals (ground in Nalgene cup)
  - Samples: 8 inch columns, 11.3 inch rows
  - Bare plywood and aluminum foil surfaces at 45º at 14 m
  - Rudimentary atmospheric correction



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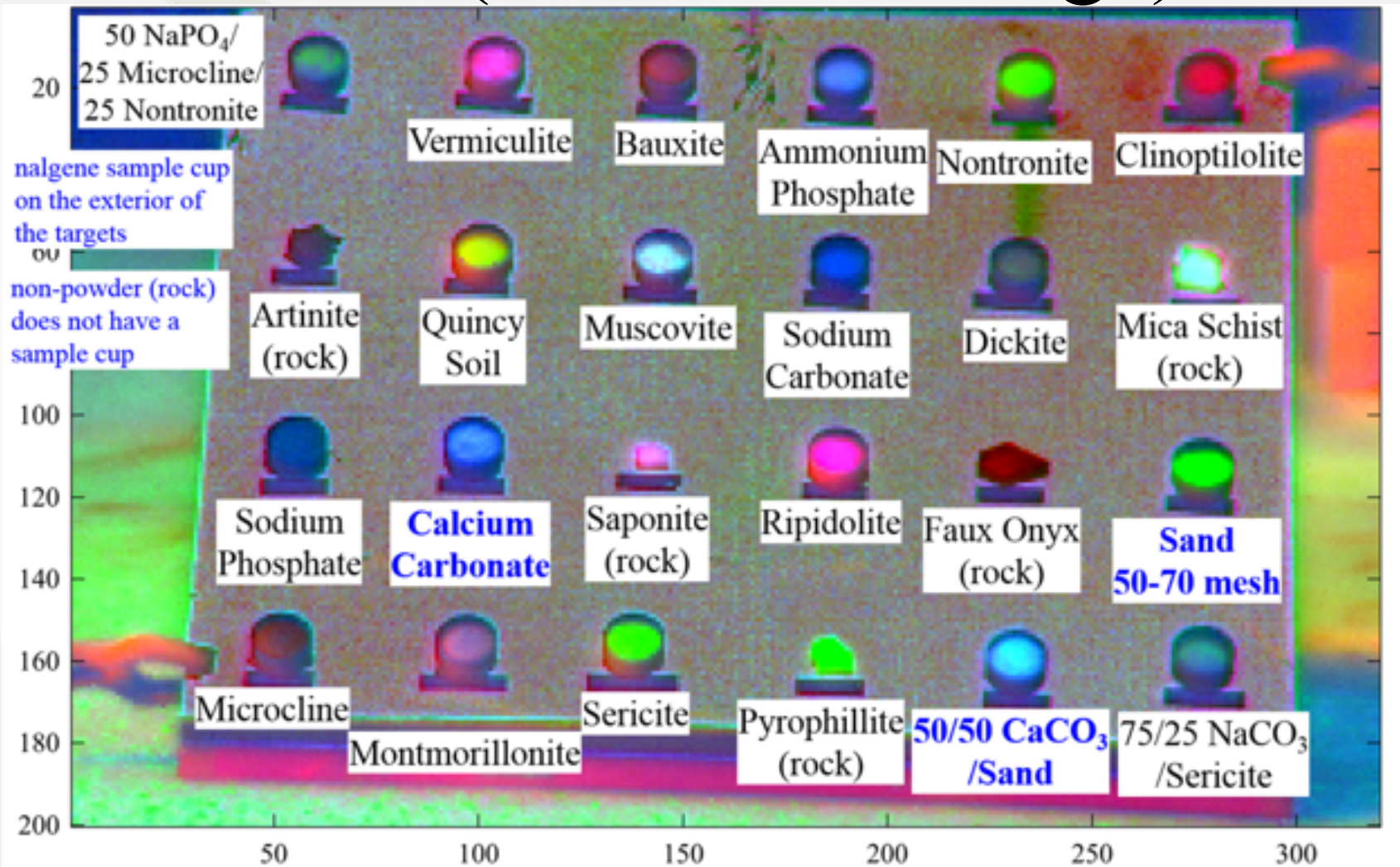
PCA (PC Scores Image)



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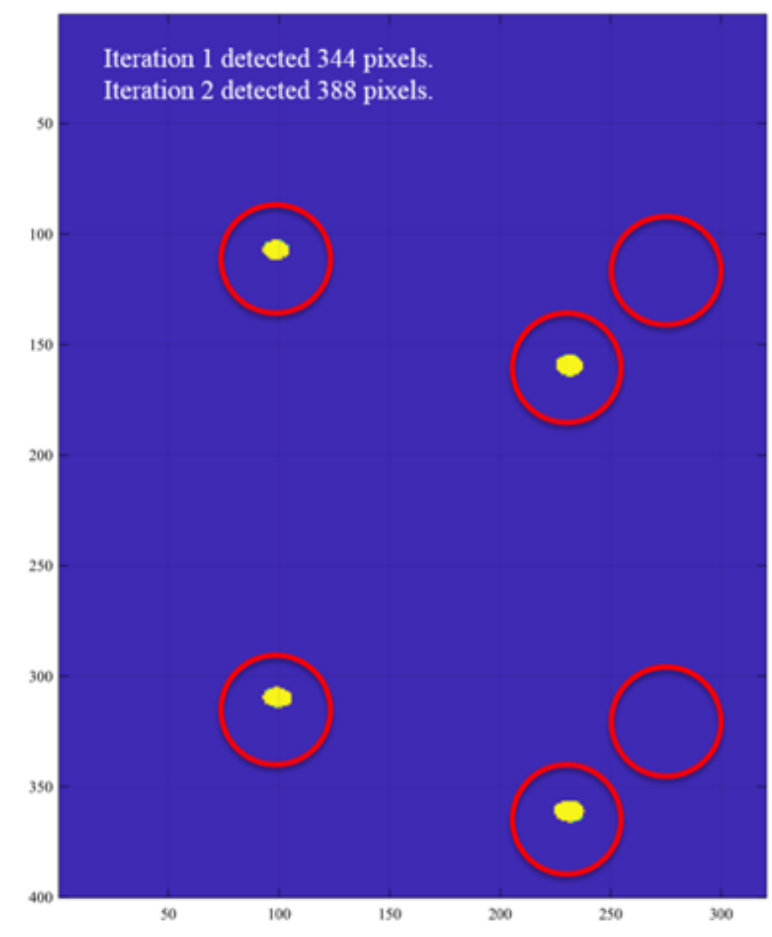
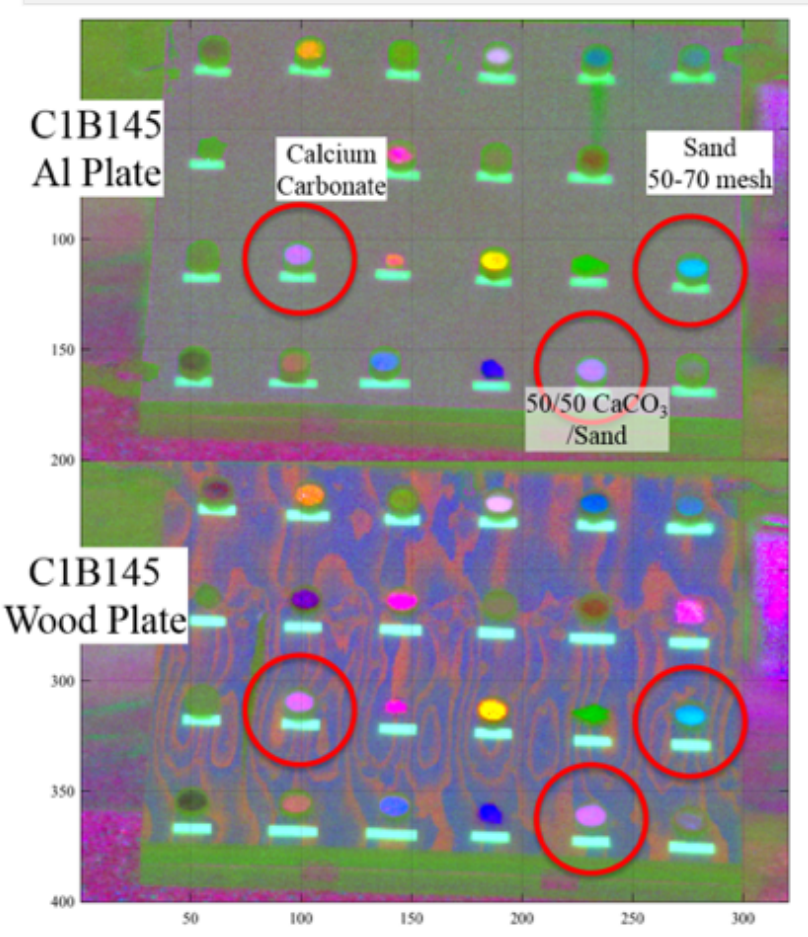
Target Detection for $CaCO_3$

Scores image for visualization





Only $CaCO_3$ is detected (including the 50/50 mixture)!

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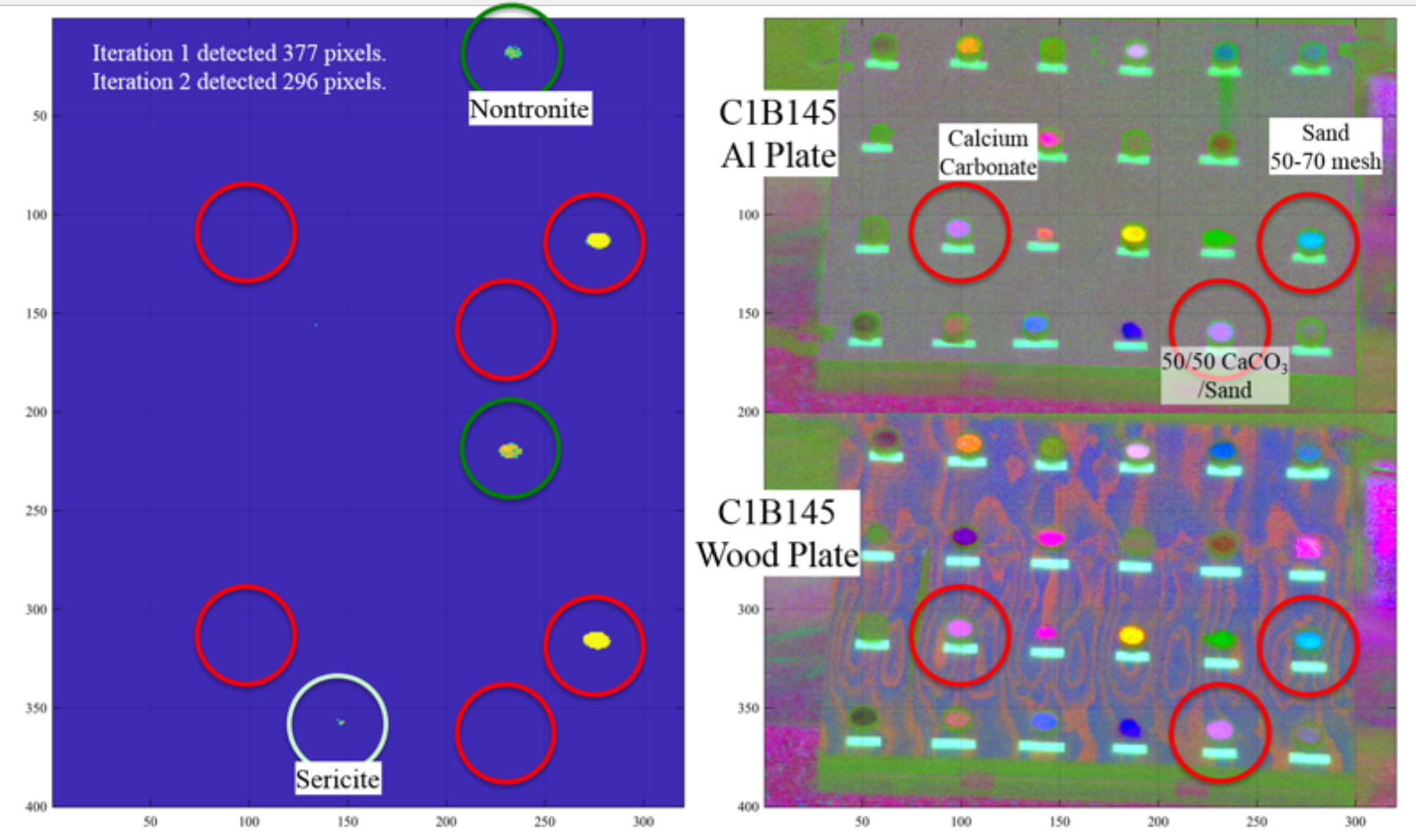
Target Detection for Sand (SiO_2)



Sand is detected (none in the 50/50 mixture with $CaCO_3$).
Nontronite is a false alarm. Sericite has a minor false alarm on the wood plate.

Targeted Anomaly Detection

	detection	classification	quantification
Anomaly Detection	**yes**	no	no
Target Detection	**yes**	**yes**	~yes
Targeted Anomaly Det	**yes**	~yes	~no

- Anomaly Detection
- Target Detection
  - what about multiple targets?
  - is the library target a match for each image?
- Targeted Anomaly Detection
  - use target detection to find possible target pixels
  - the use the detected pixels as target relevant for each image
    - accounts for lighting changes, matrix effects, signal changes and allows for multiple manifestations of a target's signal

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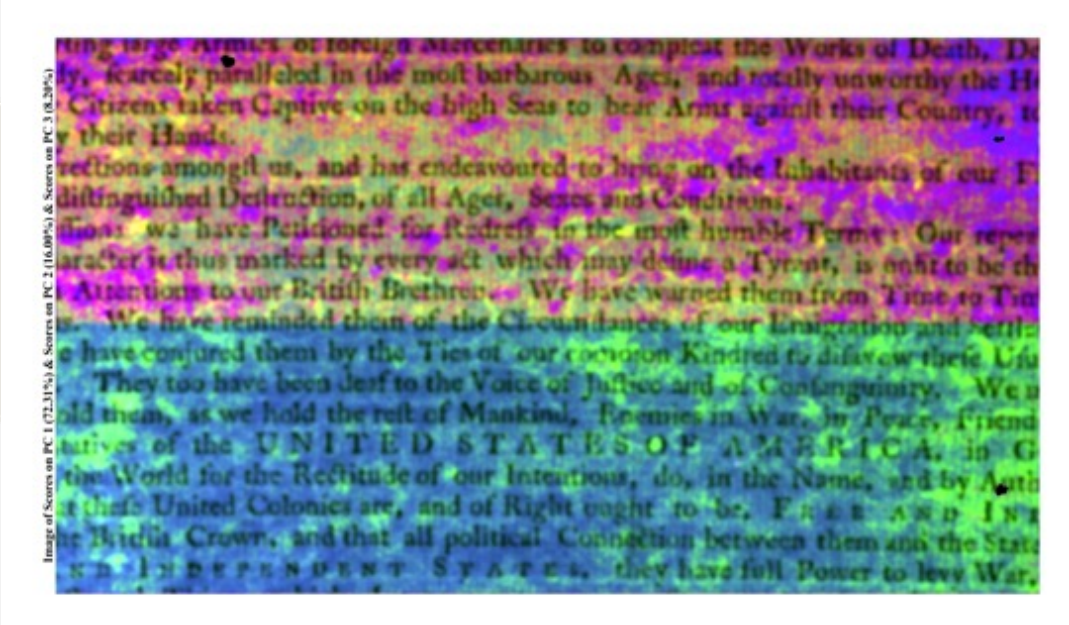
Hidden Watermark

Dunlap Broadside printing of the Declaration of Independence



two major
sources of clutter

Thank you Library of Congress
Meghan Wilson, Preservation Science Specialist
Fenella France, Chief of Preservation Research and Testing Division

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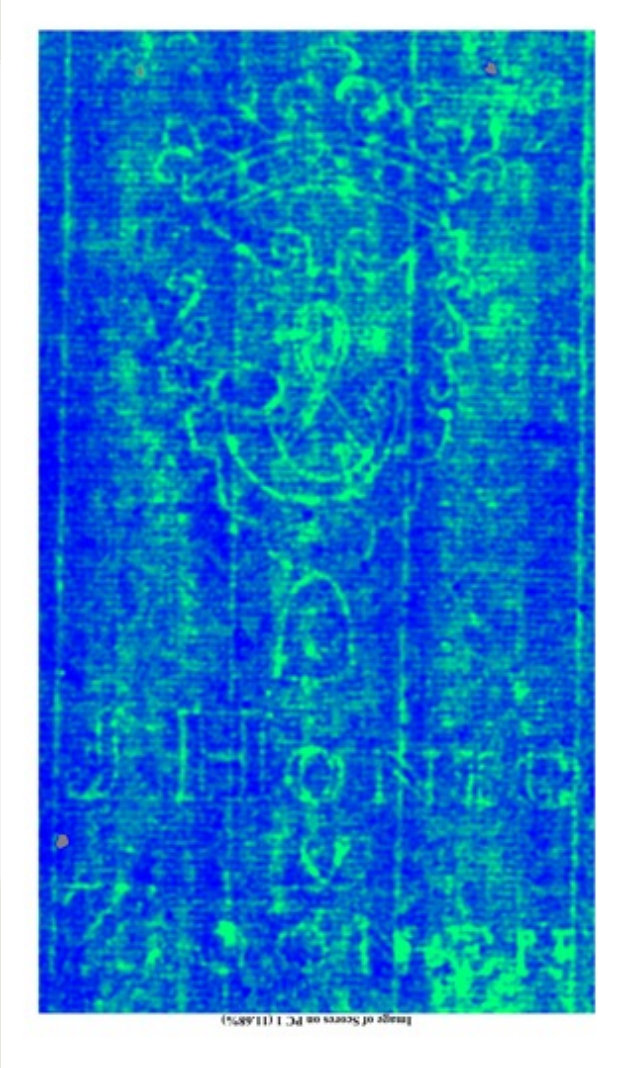
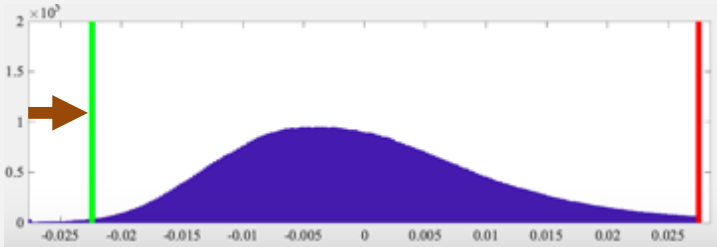
Watermark



colormap winter
enhanced contrast
decluttering (1/**α**=100)
decluttering (1/**α**=10)
decluttering (**α**=1)
decluttering (**α**=0.1)
no decluttering

- GLSW, mean-centering = WPCA
  - 1/**α** larger is stronger de-cluttering
- Scores on PC 1
  - autocontrasted
    - mean-centered & saturated at ±2 std



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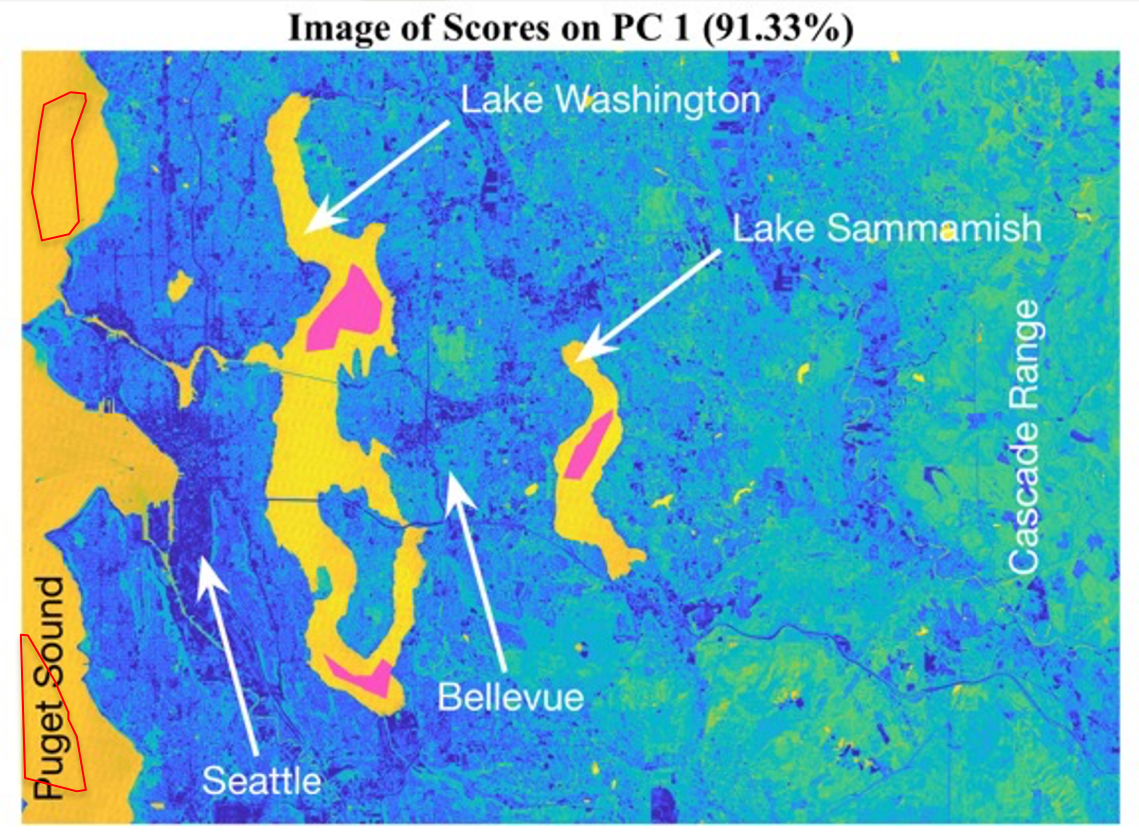
Target Detection Example

Seattle Landsat, USGS/NASA



- Two-target GLS
  - Target: "Lakes" magenta
  - Interference: "Puget Sound"

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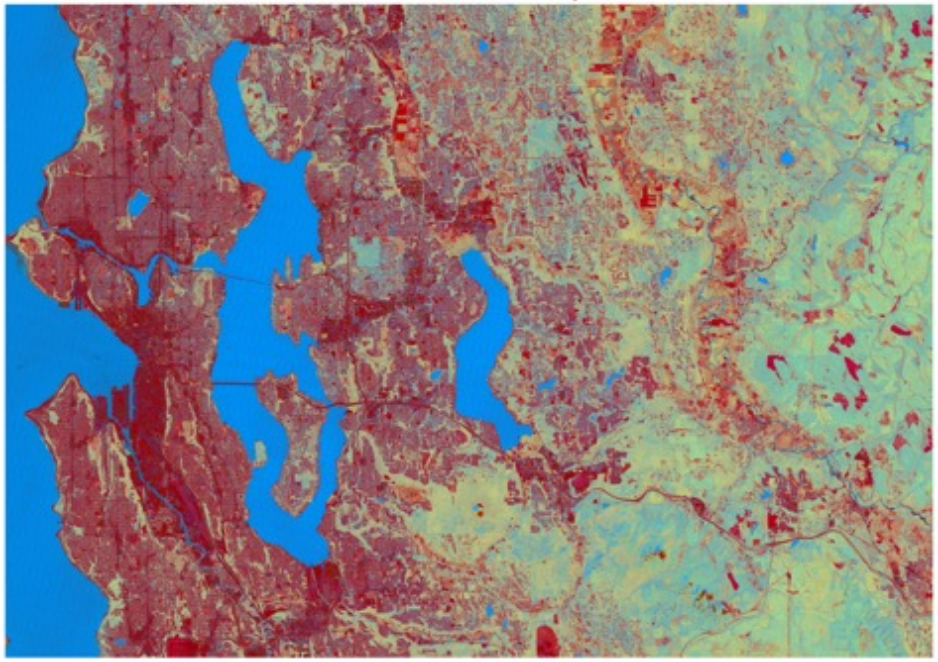
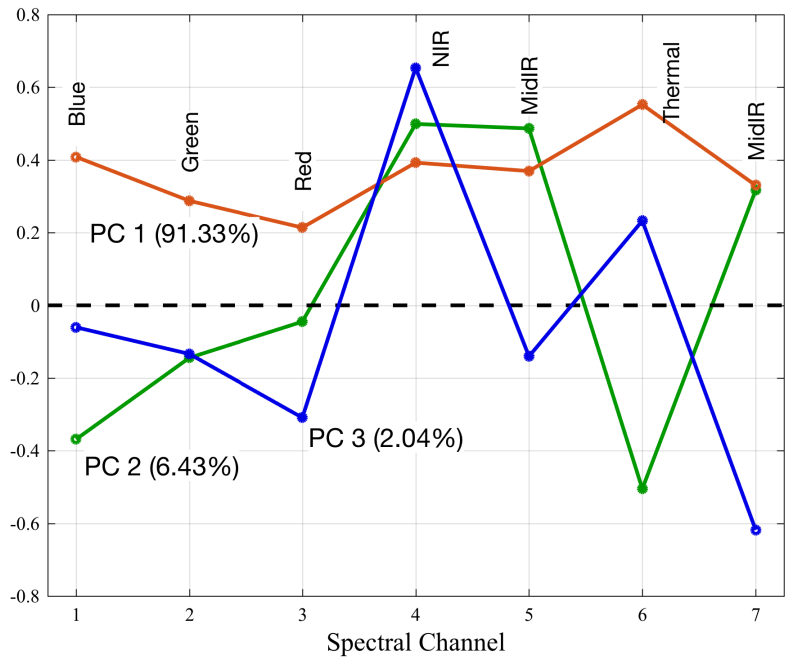
PCA Scores and Loadings

RGB Scores on PC 1,2 & 3





the water signal is minor (it's in PC 3)

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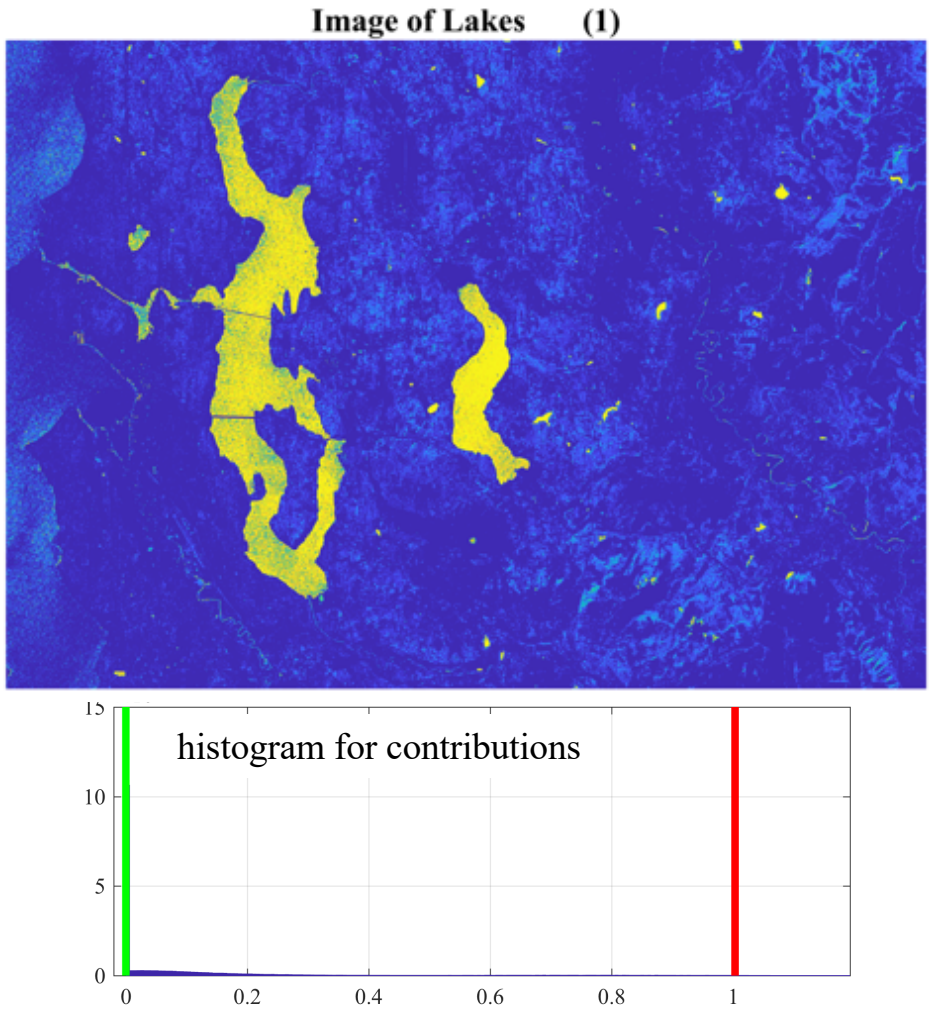
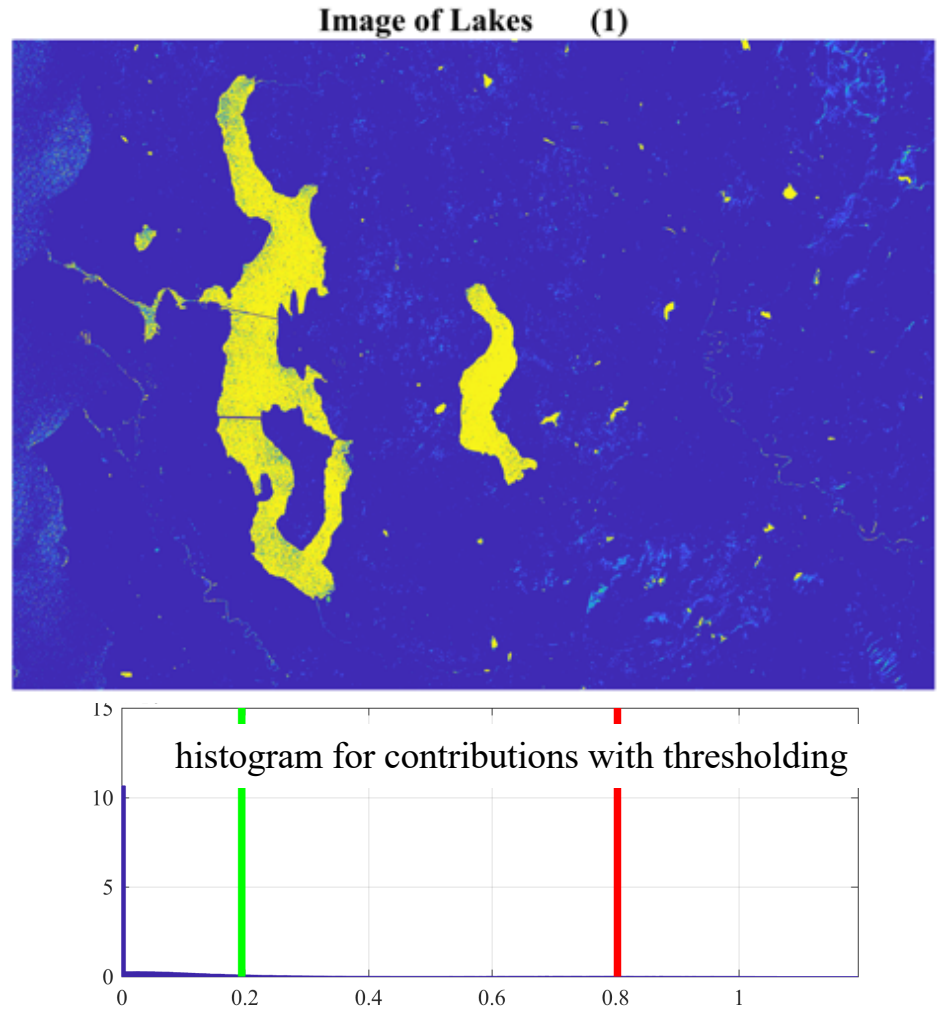
Target Contributions





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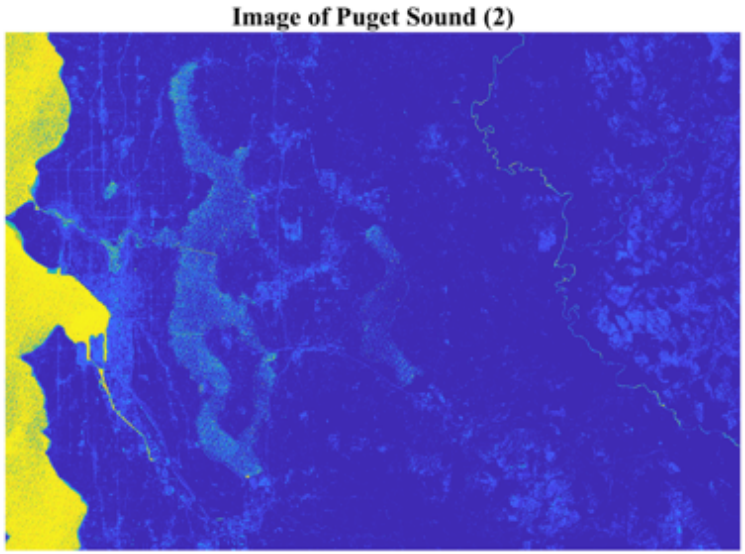
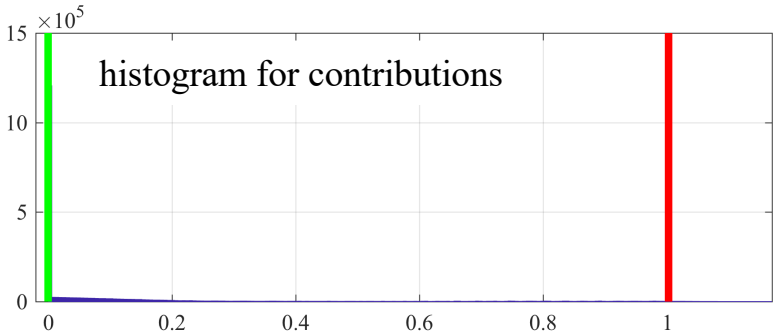
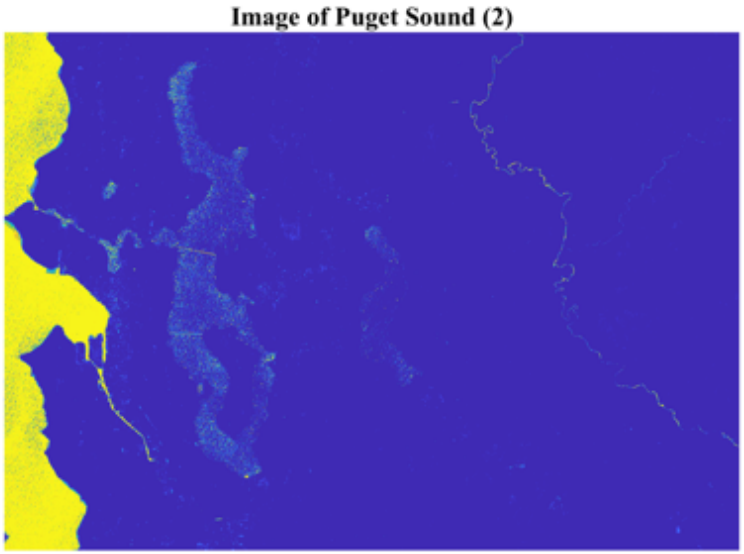
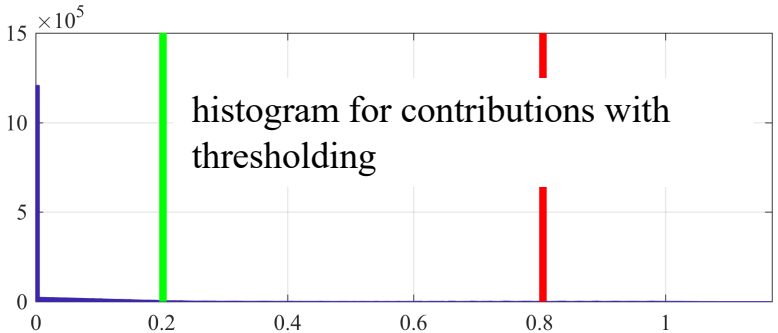
Interference Contributions









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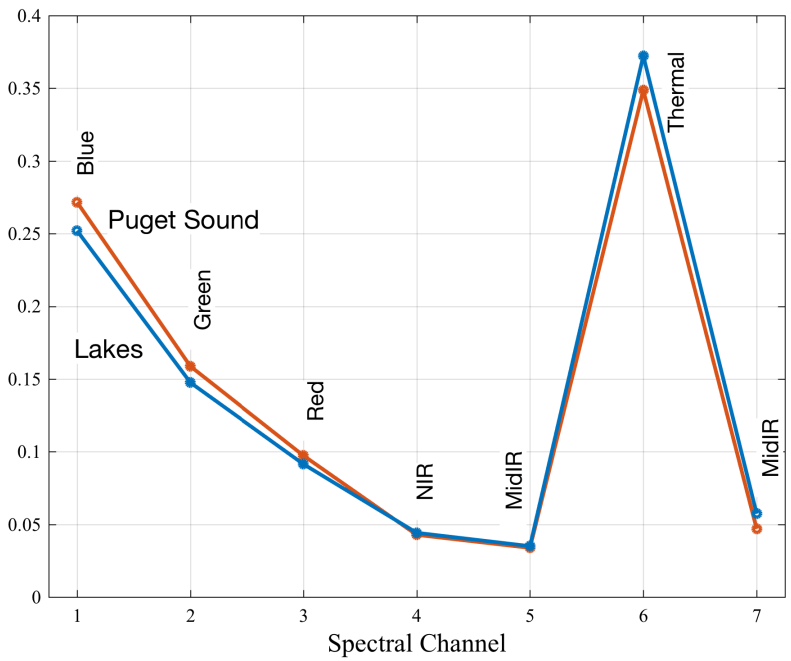
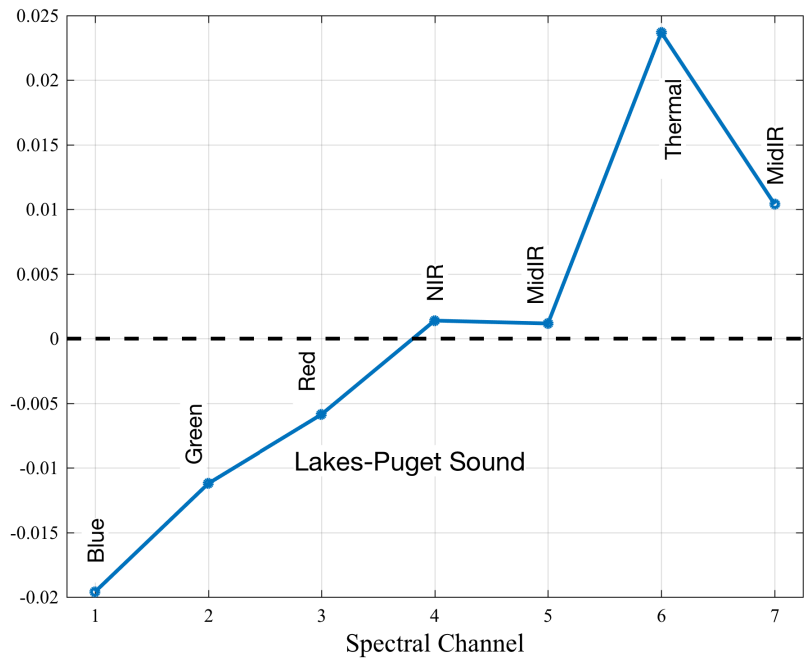
Targets





The target signals are very similar

Lakes appear to have a higher signal on the Thermal channel relative to the Blue channel.

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Conclusions

- The examples differed are in how "signal" and "clutter" are defined depending on the desired signal to enhance and signal to suppress
  - One man's clutter is another's target.
- Anomaly and Target Detection can be used synergistically to find signal of interest
  - signal that may be missed when used independently
  - the result is Targeted Anomaly Detection
  - very flexible approach to targeted image exploration

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https://www.sciencedirect.com/science/article/pii/B9780444639776000110

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