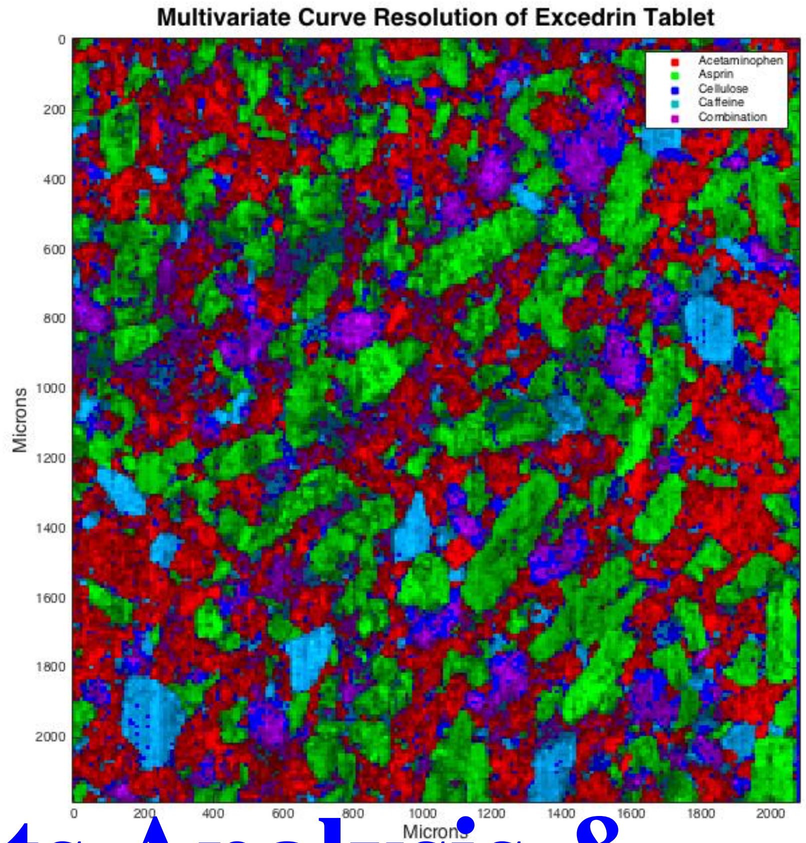


# Introduction to Principal Components Analysis & Related Methods on Multivariate/Hyperspectral Images

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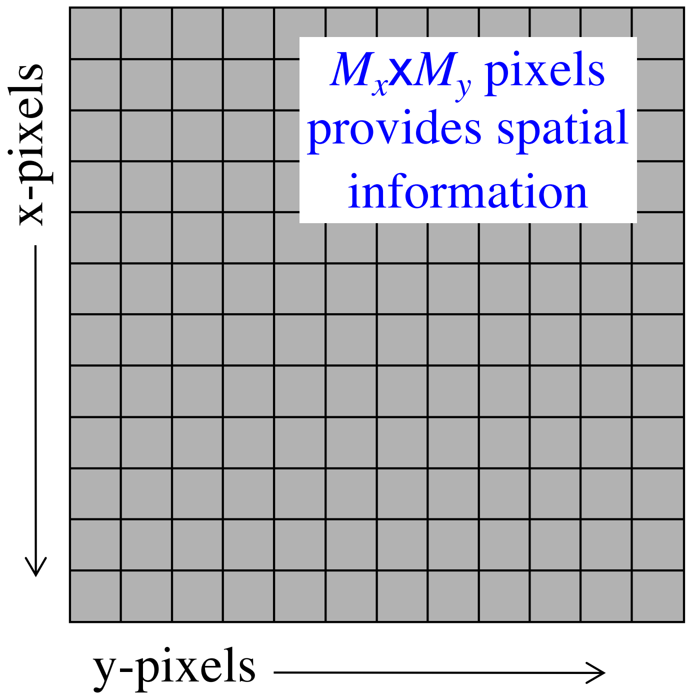
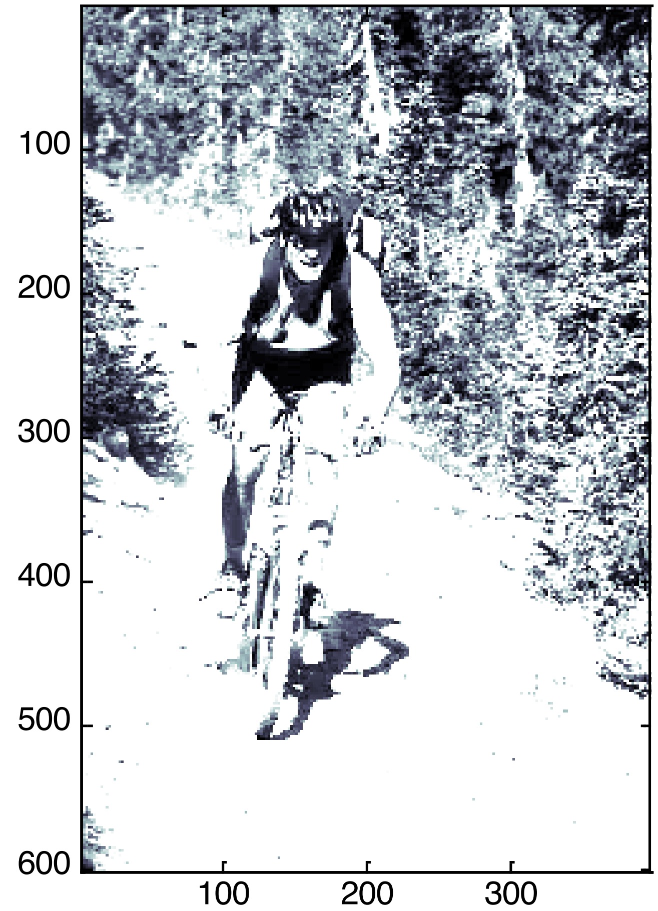
# *Outline*

- Intro to 3-way arrays and simple visualizations
- Principal Components Analysis (PCA)
- Multivariate Curve Resolution (MCR)
- Independent Components Analysis (ICA)
- Other methods: MAF, MDF, GLS, EPO
- Cluster Analysis (time permitting)
- Conclusions

# Univariate Image

- Grey scale
  - each pixel is an number defining an intensity level e.g.,
    - integer (0 to 255) unsigned 8-bit
    - integer (0 to 4095)
    - double (floating point)

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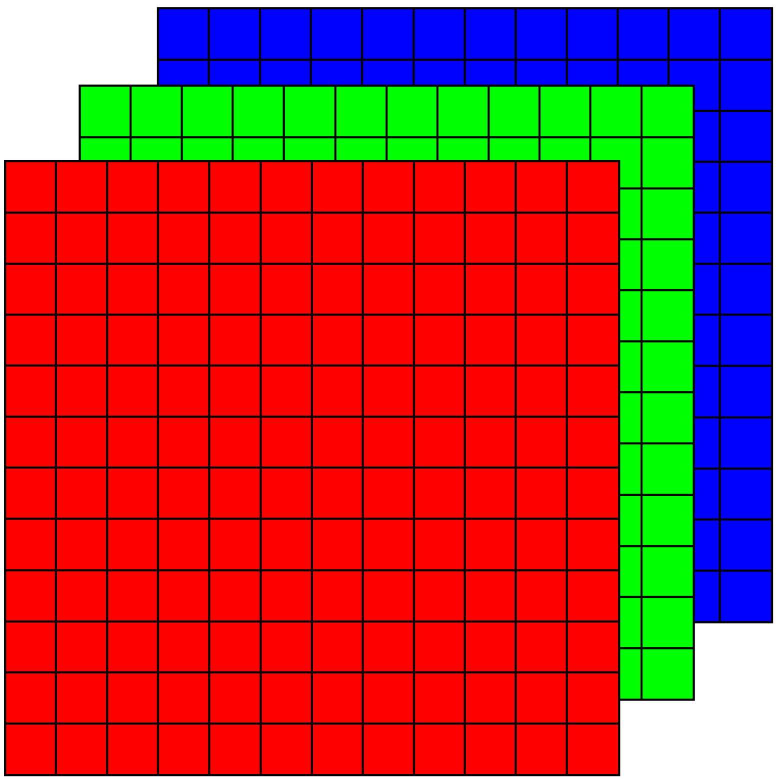
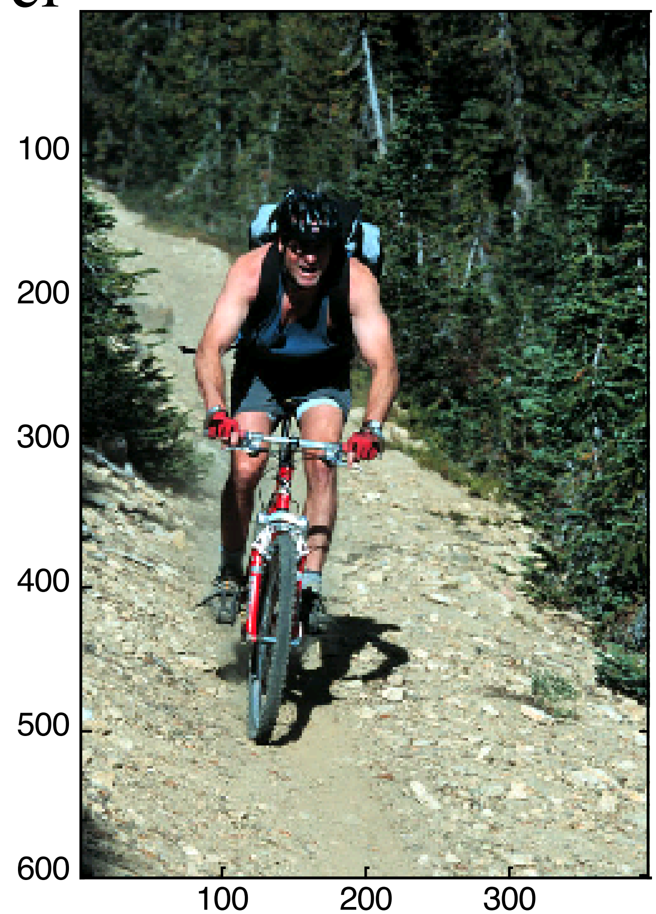
# Multivariate Image
## (3 Variables)

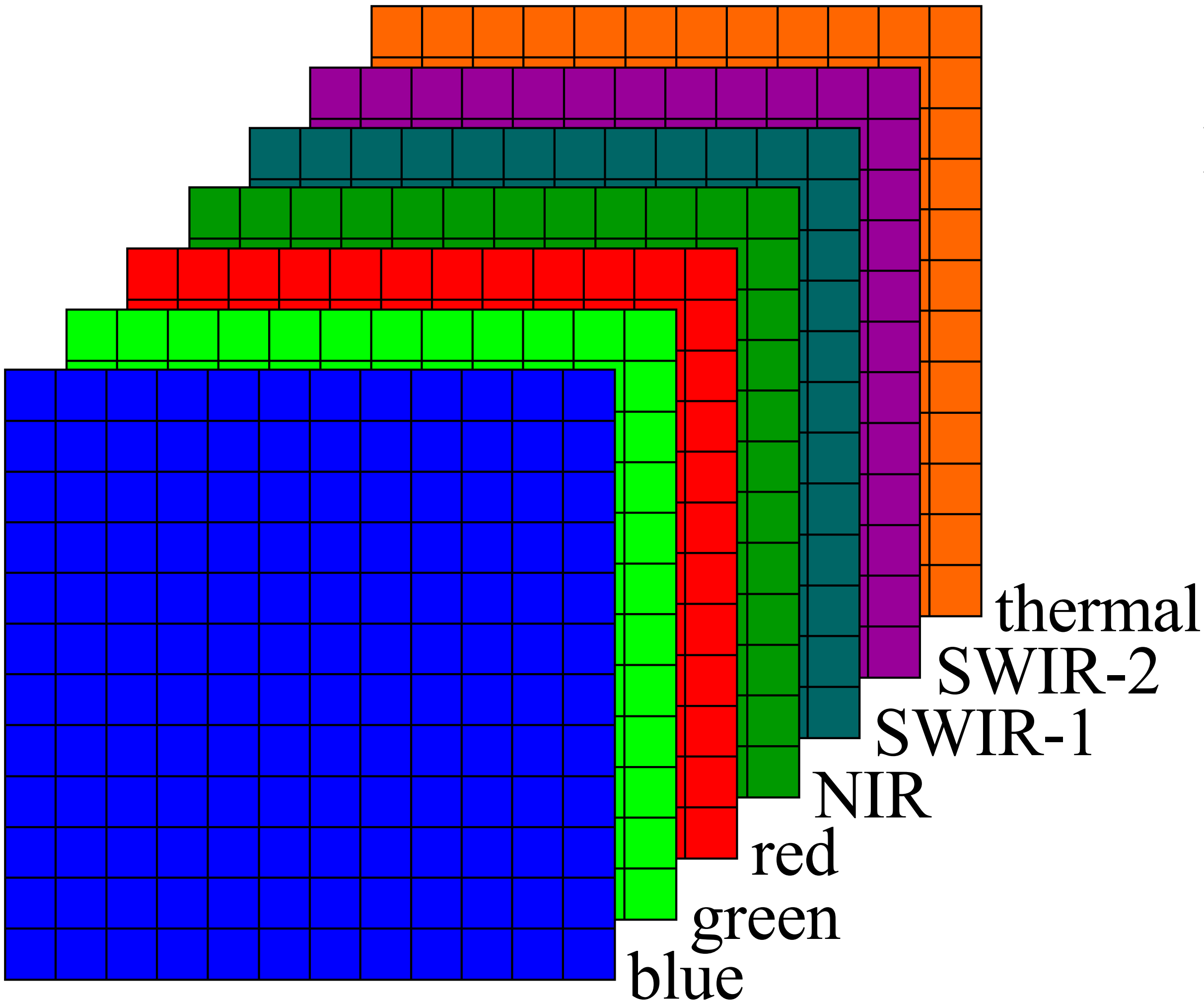
- Red/Green/Blue (RGB) (e.g. JPEG)
  - each layer defines color intensity level
  - much more information-rich





# Multivariate Image
## (4-10 Variables)

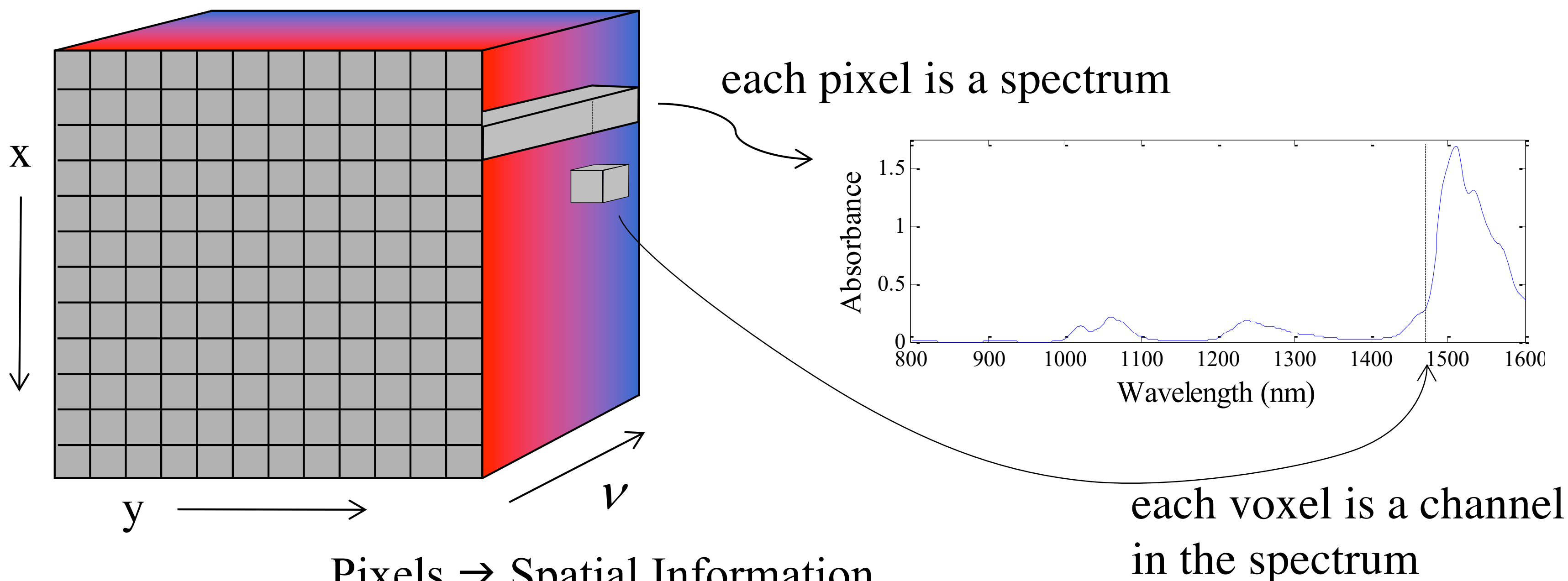
- Measure at several wavelengths (e.g., Landsat)




How should we display a seven variable image?

# Hyperspectral Image
## (>10 Variables)

- Spectrum at each pixel
  - could be 100-1000s of variables
  - often floating point double 10-100s Mbytes




Pixels → Spatial Information

Spectral → Chemical Information

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# Image Analysis

- Many methods have been developed to examine the spatial structure w/in an image
  - the methods recognize spatial patterns within an image
    - based on the light / dark contrast and continuity of regions
- MIA has been traditionally applied to the spectral dimension first followed by spatial analysis
  - some methods that examine both are appearing



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# Multivariate Images

- Data array of *dimension three* (or more)
  - where the first two dimensions are *spatial* and
  - the last dimension(s) is a function of another variable (e.g, spectroscopy).
- Chemical system(s) of interest include
  - microscopic, medical, machine vision, process monitoring crystallization, stand-off and remote sensing, …
  - vapors, liquids, solids (or combination)
  - visible, infra-red, Raman, mass spectroscopy, …

# Displaying a Multivariate Image

- Can choose any 3 variables (wavelengths) and display any image in RGB
- Doesn't choosing ignore potential information in the remaining variables?
- How could information be extracted from the multivariate image?
- Factor-based techniques—Principal Components Analysis
  - data reduction/compression
  - bring relevant information to surface
  - enhance S/N

Image of blue & NIR & thermal

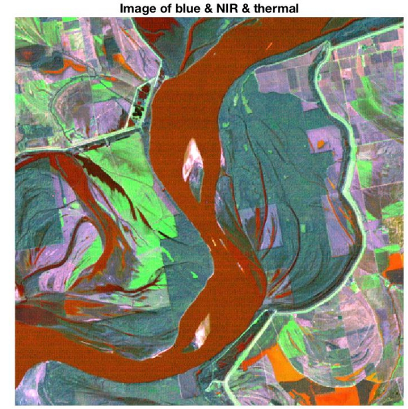
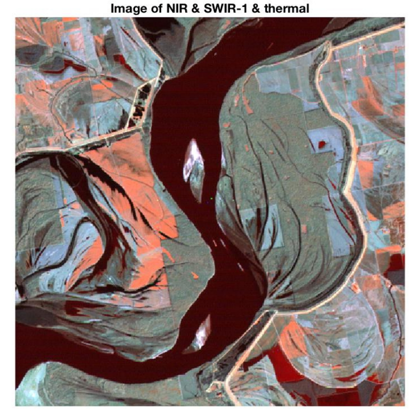


Image of NIR & SWIR-1 & thermal



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# Image Principal Components Analysis

- Math
- Matricizing
- PCA: scores, scores images, loadings
  - unusual samples Q and $T^2$
  - score-score plots, density plots
  - linking scores and image plane(s)

# PCA Math

- For a data matrix **X** with $M$ samples and $N$ variables (generally assumed to be mean centered and properly scaled), the PCA decomposition is

$$\mathbf{X} = \mathbf{t}_1\mathbf{p}_1^T + \mathbf{t}_2\mathbf{p}_2^T + \ldots + \mathbf{t}_K\mathbf{p}_K^T + \ldots + \mathbf{t}_R\mathbf{p}_R^T$$

  Where $R \leq \min\{M,N\}$, and the $\boldsymbol{t}_k\boldsymbol{p}_k^T$ pairs are ordered by the amount of variance captured.

- Generally, the model is truncated to $K$ PCs, leaving some small amount of variance in a residual matrix **E**:

$$\mathbf{X} = \mathbf{t}_1\mathbf{p}_1^T + \mathbf{t}_2\mathbf{p}_2^T + \ldots + \mathbf{t}_K\mathbf{p}_K^T + \mathbf{E} = \mathbf{TP}^T + \mathbf{E}$$

- where **T** is $M$x$K$ and **P** is $N$x$K$.

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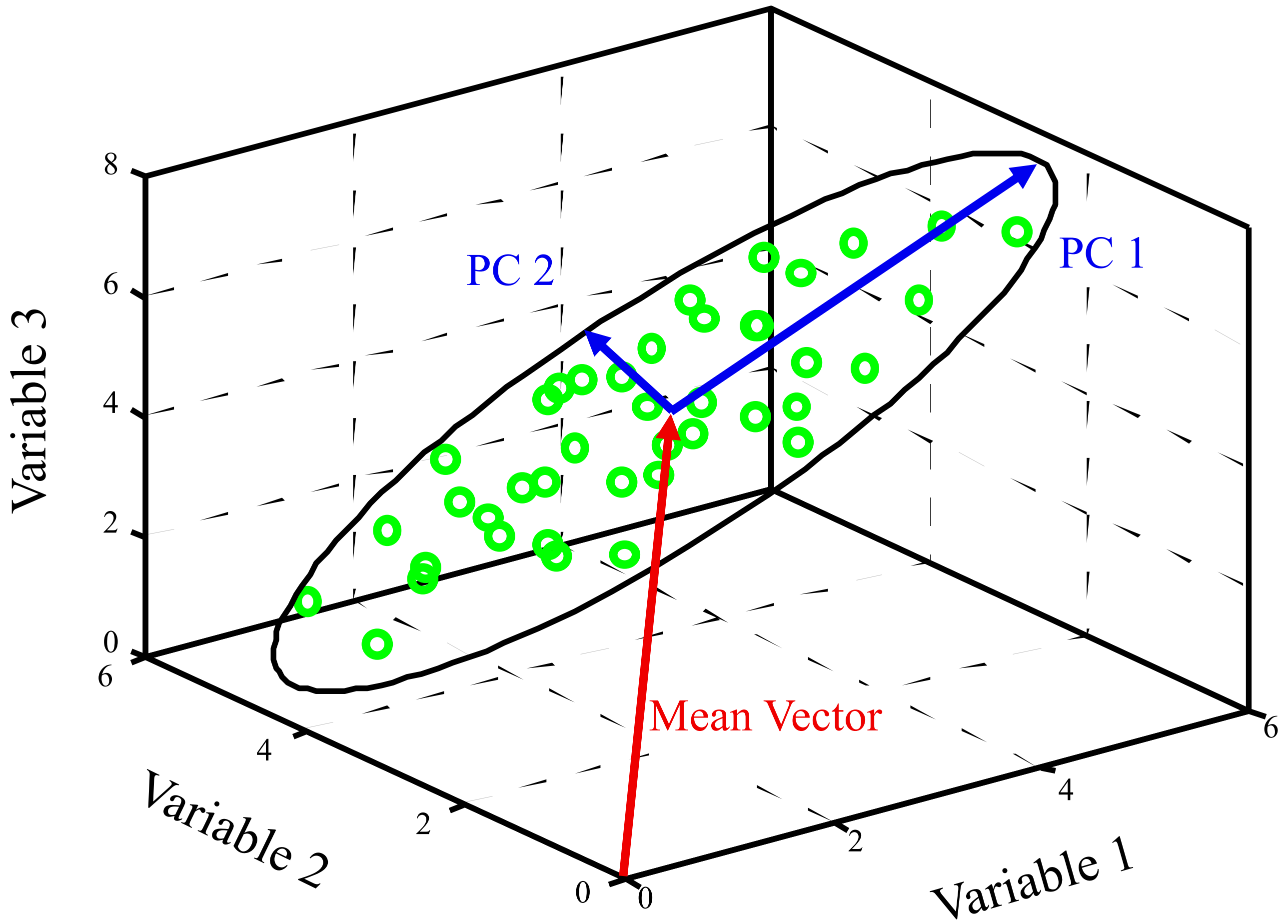
# Properties of PCA

$$\mathbf{X} = \mathbf{t}_1\mathbf{p}_1^{\mathrm{T}} + \mathbf{t}_2\mathbf{p}_2^{\mathrm{T}} + .. + \mathbf{t}_K\mathbf{p}_K^{\mathrm{T}} + \mathbf{E}$$

- $\mathbf{t}_k$,$\mathbf{p}_k$ ordered by amount of *variance captured*
  - $\lambda_k$ are the eigenvalues of $\mathbf{X}^{\mathrm{T}}\mathbf{X} \rightarrow \mathbf{X}^{\mathrm{T}}\mathbf{X}\mathbf{p}_k = \lambda_k\mathbf{p}_k$
  - $\lambda_k$ are $\propto$ variance captured
- $\mathbf{t}_k$ (*scores*) form an orthogonal set $\mathbf{T}_K$ ($M$x$K$)
  - describe relationship between *samples* → *pixels* ($M = M_xM_y$)
- $\mathbf{p}_k$ (*loadings*) form an orthonormal set $\mathbf{P}_K$ ($N$x$K$)
  - describe relationship between *variables*

# PCA Graphically

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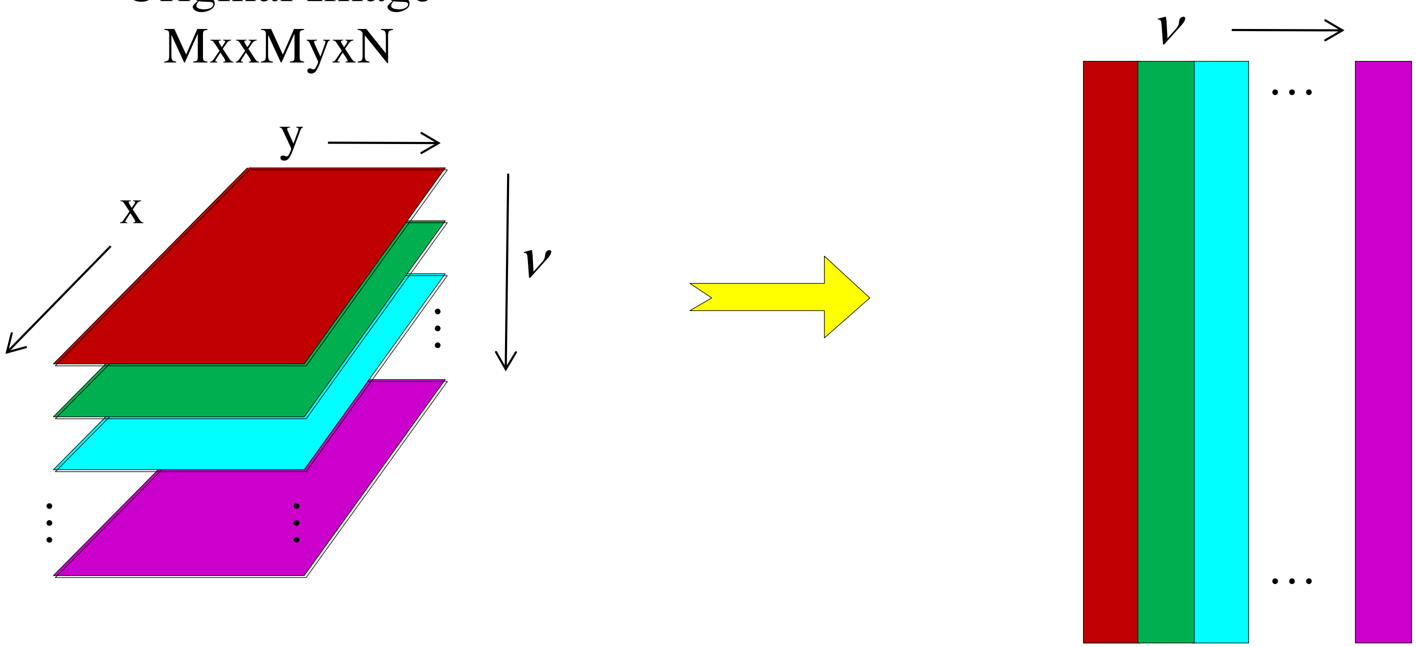
# *Matricizing (a.k.a. Unfolding)*

- PCA works on X (MxN) but the image is MxxMyxN
  - reshape by matricizing such that each pixel is a row in a new MxMyxN matrix

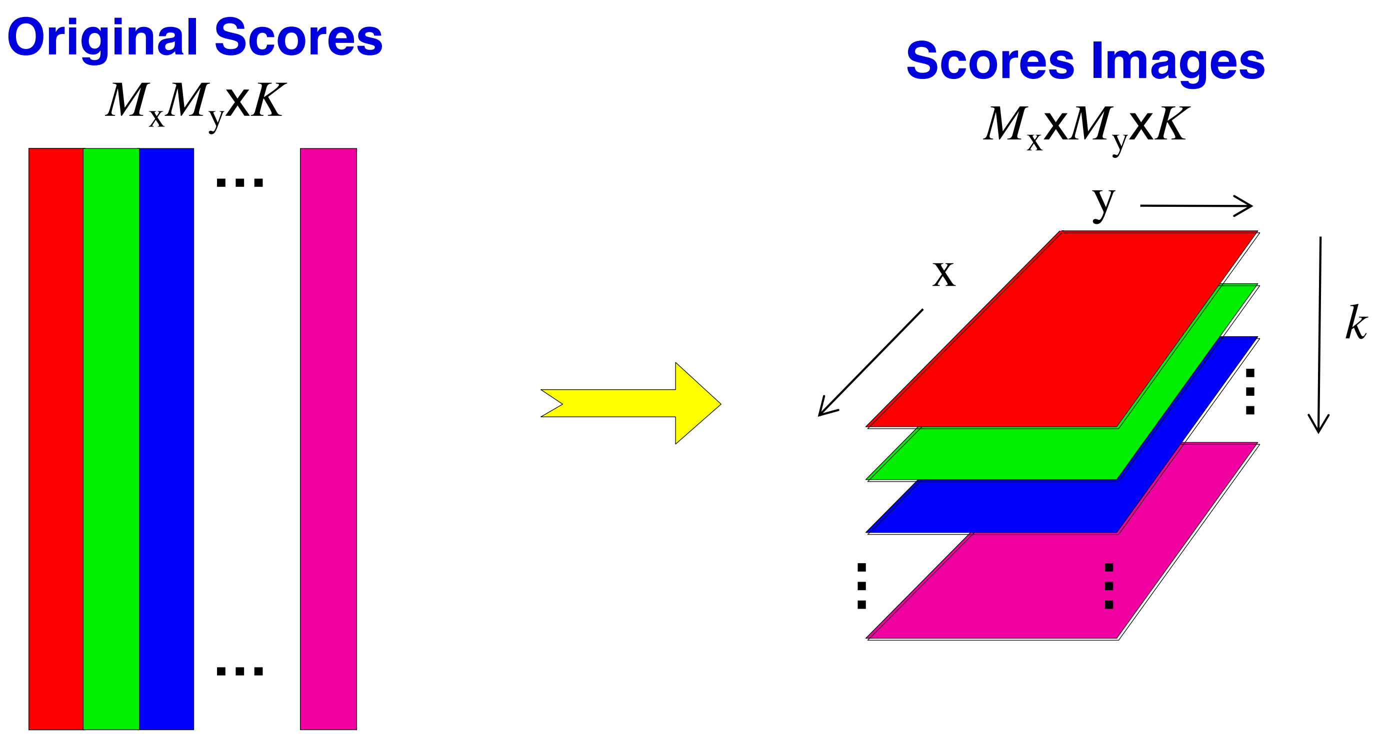
Original Image
MxxMyxN

Matricized Image
MxMyxN



# Reshape Scores To Images

- PCA gives scores **T** ($M$x$K$) which is reshaped to scores images ($M_x$x$M_y$x$K$)
  - each score vector is a $M_x$x$M_y$ scores image

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# Plots / Images for PCA

- scores and loadings plots are interpreted in pairs
  - plot $\mathbf{t}_k$ vs sample number
    - find relationship between *samples* → *pixels*
    - each $M_x M_y$x1 score vector is reshaped to a $M_x$x$M_y$ matrix that can be visualized as a "*scores image*" showing spatial relationships between pixels
  - $\mathbf{p}_k$ vs variable number
    - relationship between *variables* responsible for observations in samples
- it is useful to plot $\mathbf{t}_{k+1}$ vs. $\mathbf{t}_k$ and $\mathbf{p}_{k+1}$ vs. $\mathbf{p}_k$
  - examine image and score / score plots

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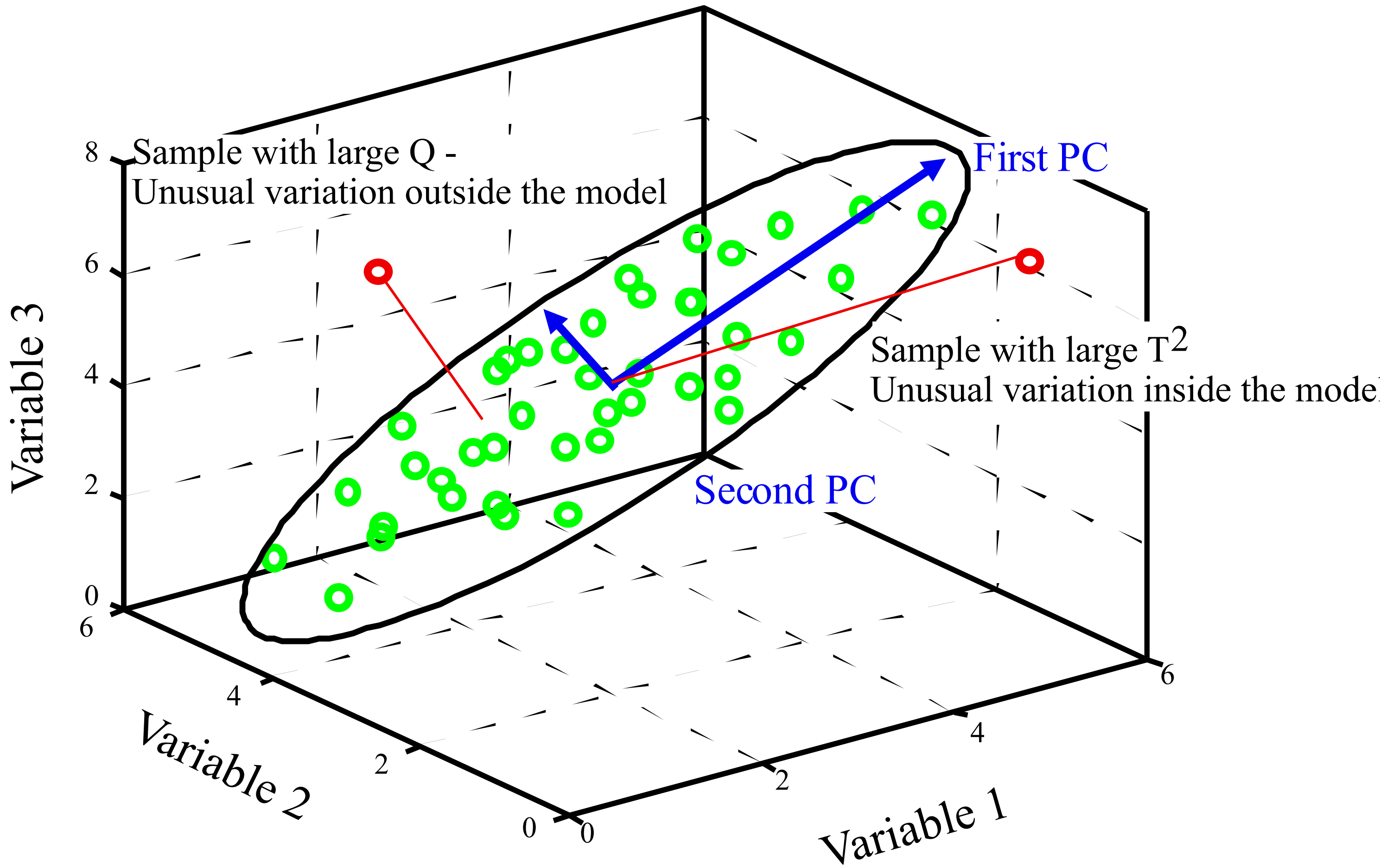
# Geometry of Q and $T^2$



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# PCA Statistics

- Limits can be set for
  - Q residual: lack of fit statistic
    - for a row of $\mathbf{E}$, $\mathbf{e}_m$, and a row of $\mathbf{X}$, $\mathbf{x}_m$, $m = 1, \ldots, M$

$$\mathrm{Q}_m = \mathbf{e}_m \mathbf{e}_m^T = \mathbf{x}_m (\mathbf{I}-\mathbf{P}_K \mathbf{P}_K^T) \mathbf{x}_m^T$$

  - Hotelling's $T^2$ statistic
    - for a row of $\mathbf{T}_K$, $\mathbf{t}_m$, and $K \times K$ diagonal matrix $\lambda$

$$\mathrm{T}_m^2 = \mathbf{t}_m \lambda^{-1} \mathbf{t}_m^T = \mathbf{x}_m \mathbf{P}_K \lambda^{-1} \mathbf{P}_K^T \mathbf{x}_m^T$$

  - and also for individual columns:
    - scores, $\mathbf{t}_{mk}$
    - residuals $\mathbf{e}_{mk}$

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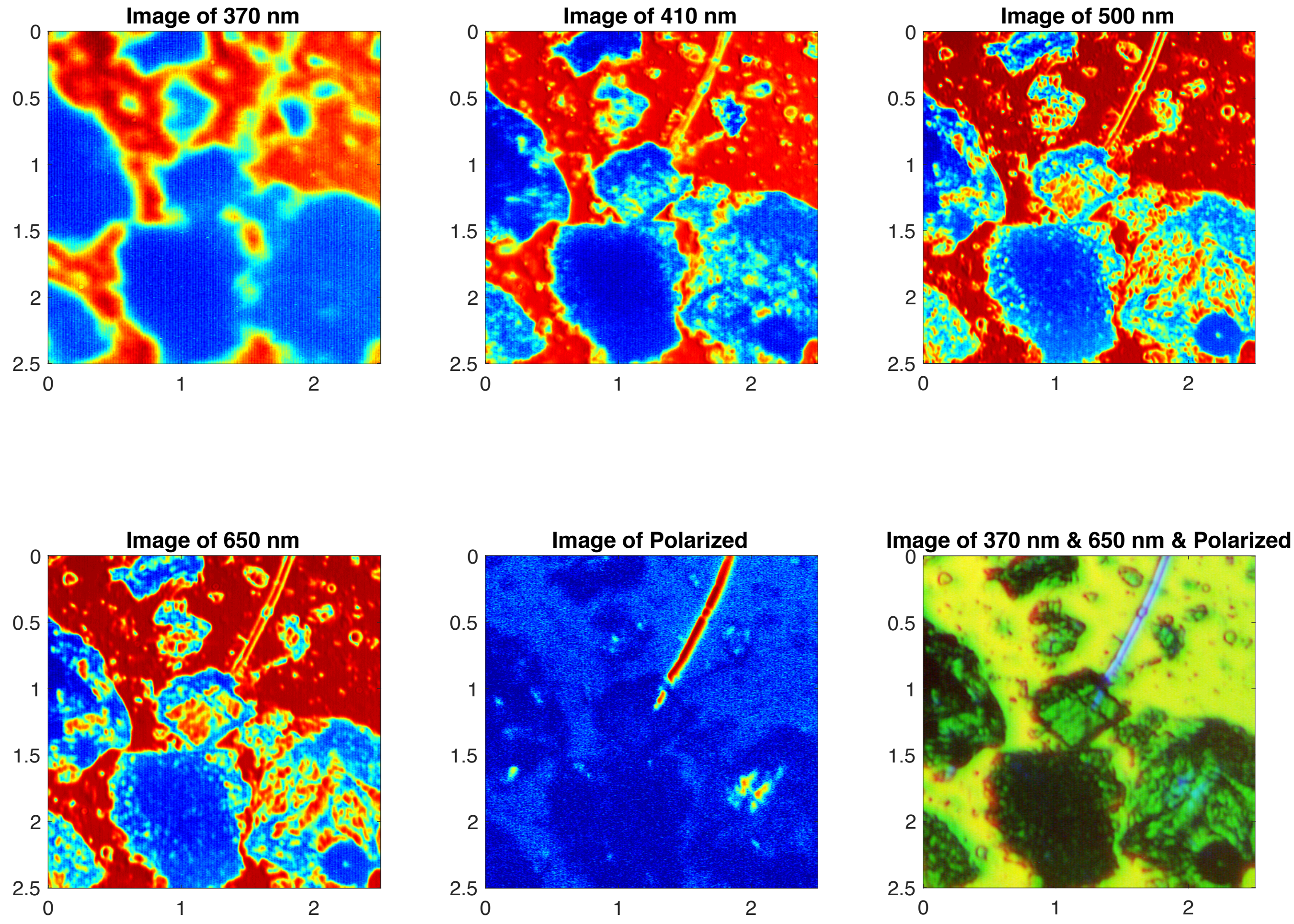
# Example: Bread

- Image of Swedish knäckebröd at 4 different wavelengths (370, 410, 500 & 650nm) plus visible light with a polarizing filter
- Image is 500 by 500 by 5
- Thanks to Paul Geladi for the data!

# Slices of the Bread

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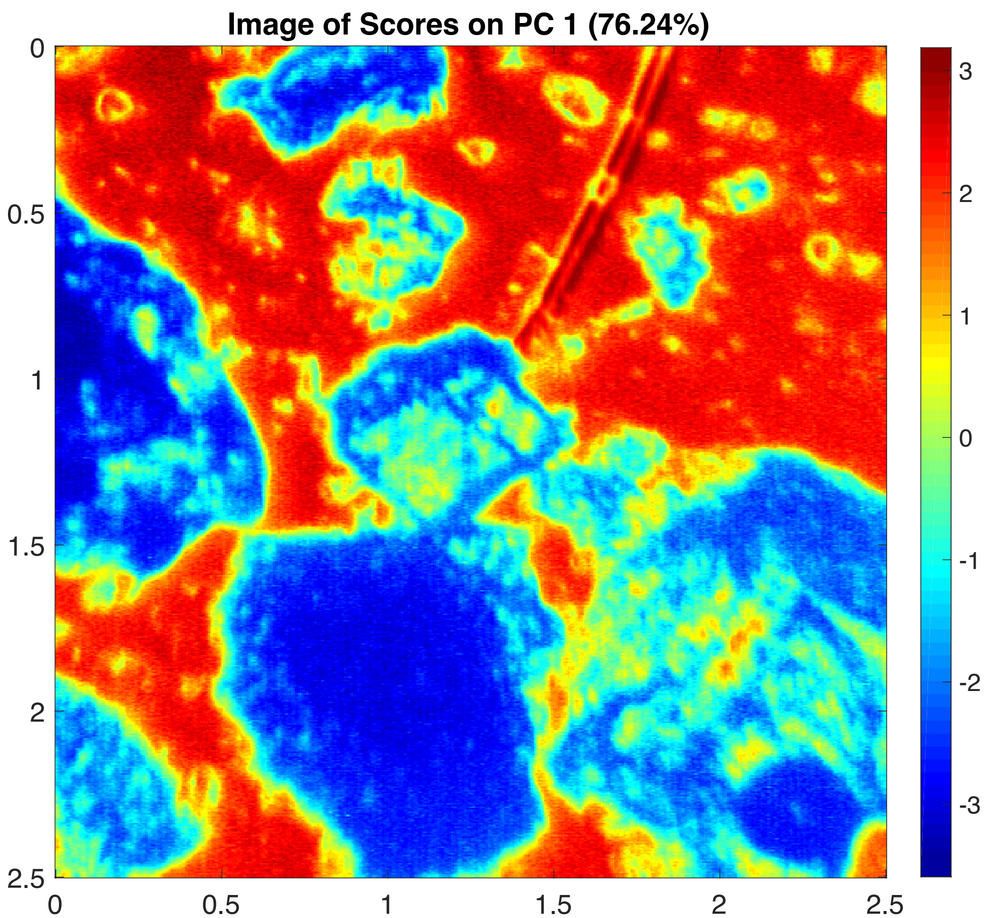
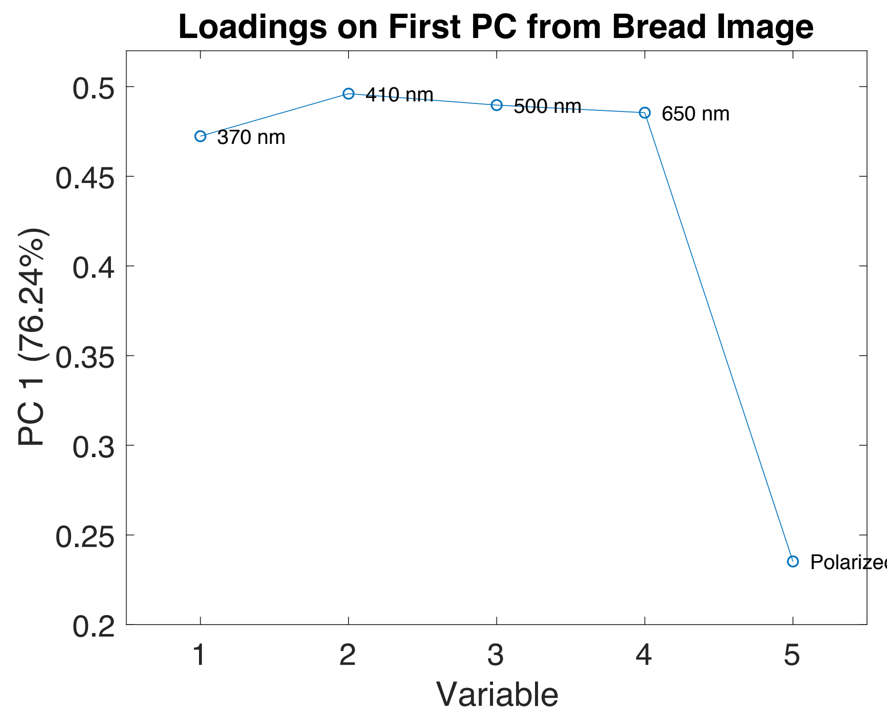
# Variance Captured Table

Percent Variance Captured by PCA Model

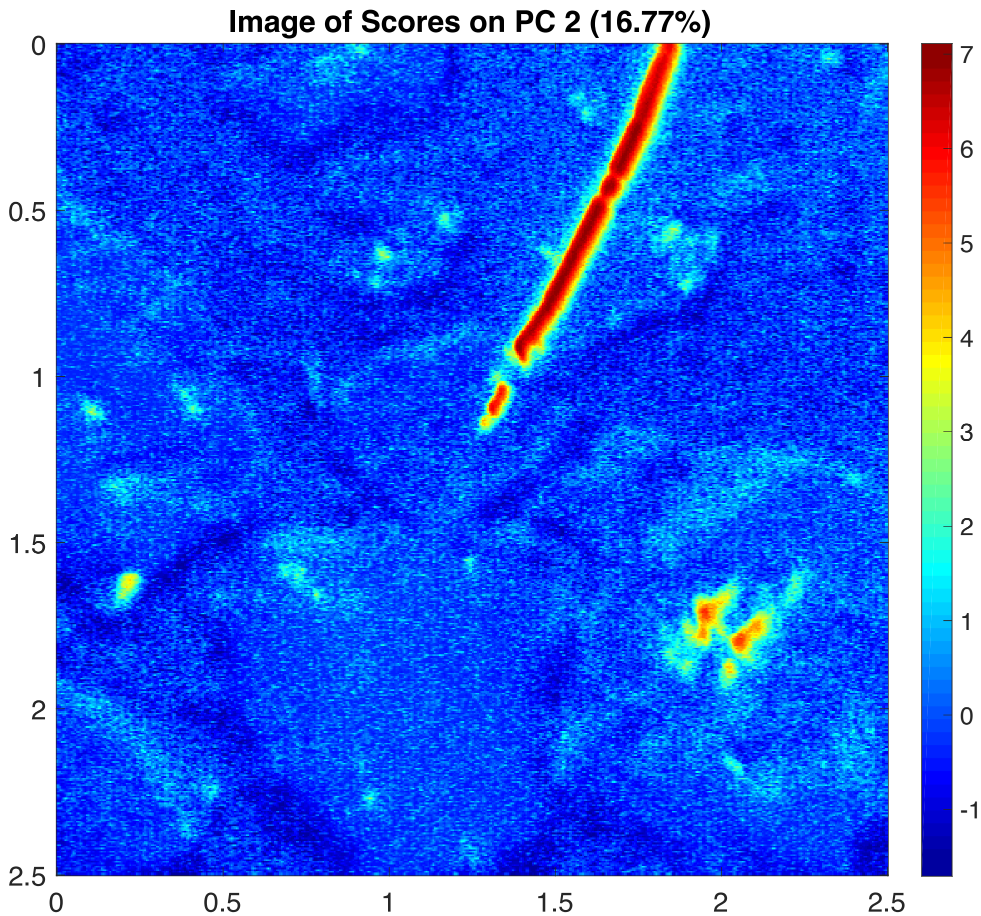
| Principal Component Number | Eigenvalue of Cov(X) | % Variance Captured This PC | % Variance Captured Total |
|---|---|---|---|
| 1 | 3.81e+00 | 76.24 | 76.24 |
| 2 | 8.38e-01 | 16.77 | 93.00 |
| 3 | 2.25e-01 | 4.51 | 97.51 |
| 4 | 7.98e-02 | 1.60 | 99.11 |
| 5 | 4.46e-02 | 0.89 | 100.00 |

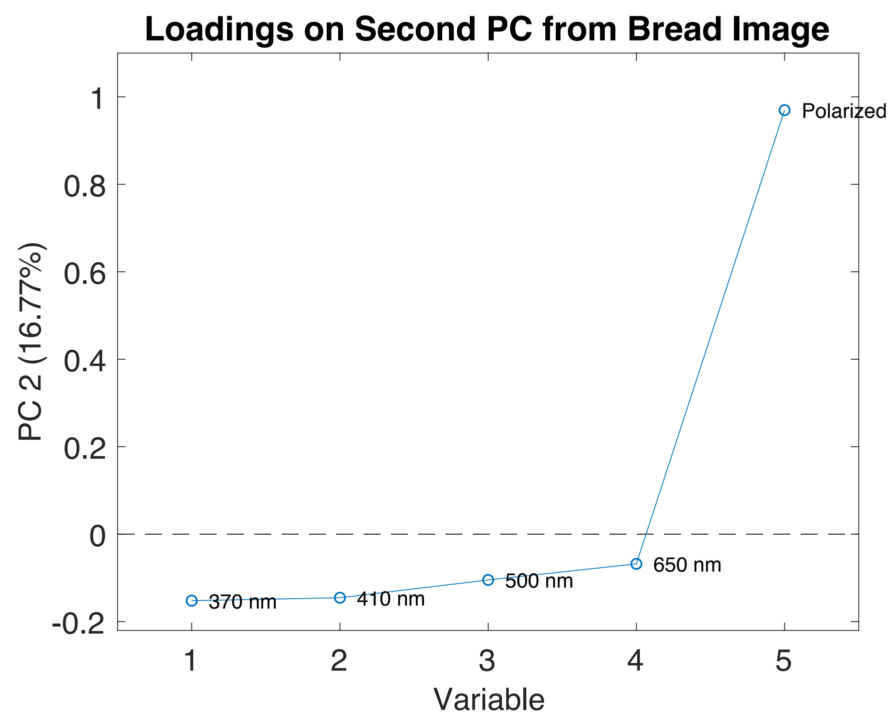
# First PC Scores & Loadings



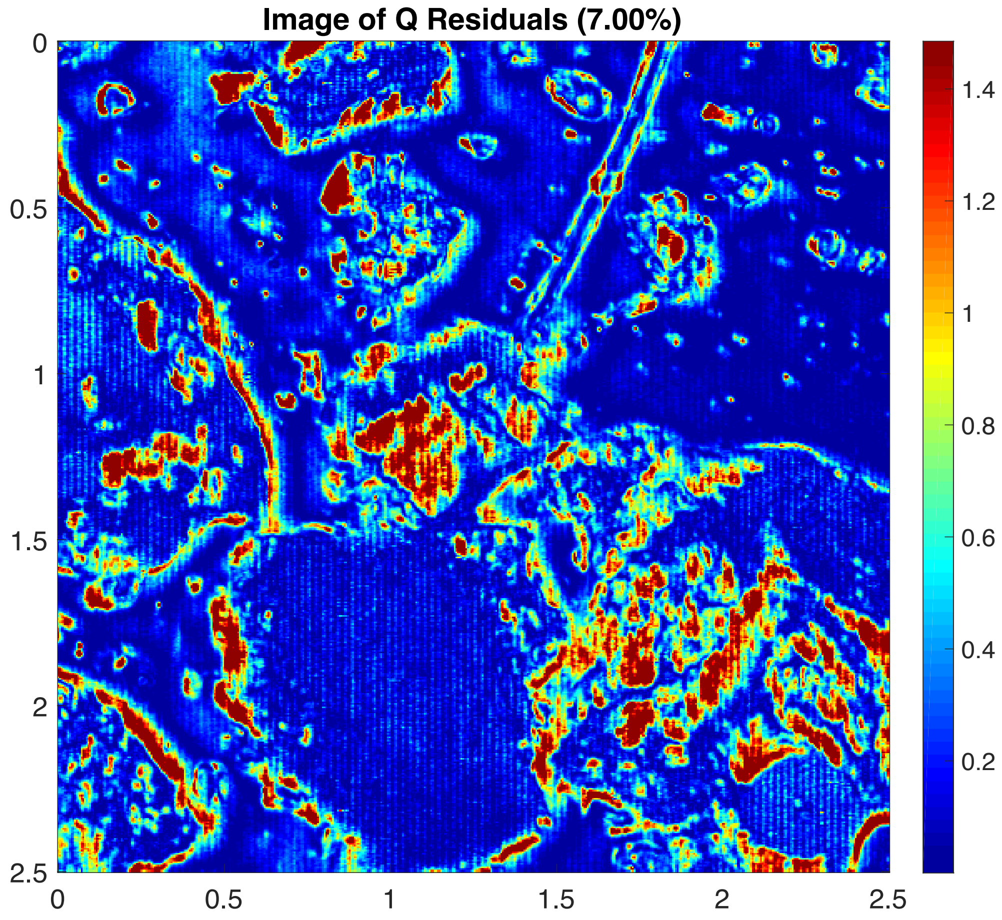



# Second PC Scores & Loadings



# Residual Image

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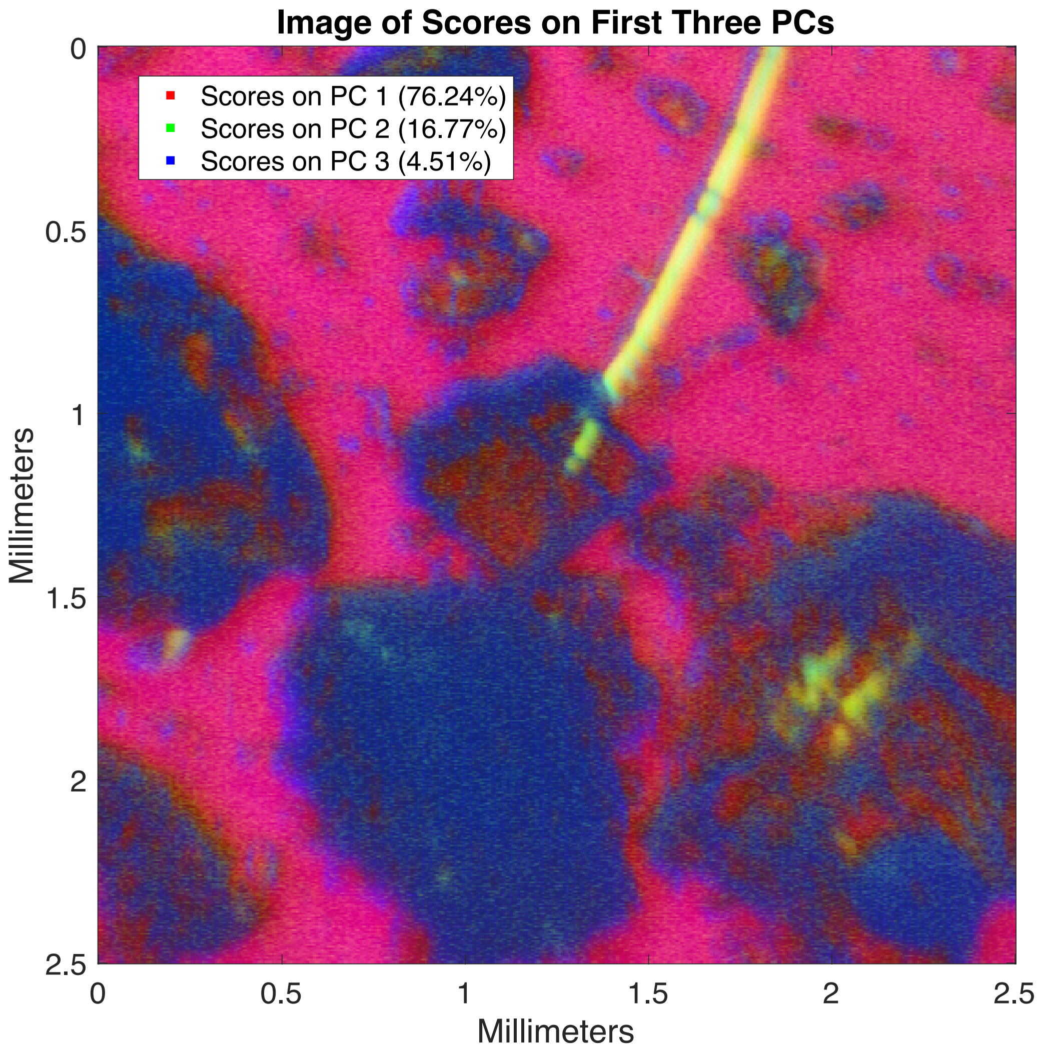
# Creating False Color Images

- Color images are made up of three layers: red, green, blue
- Scores on the PCs can be used to define the intensity of each of the three layers
- Easy to do PC1 = red, PC2 = green, PC3 = blue

# False Color Image



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# Bivariate Scores Plots

- Plot the scores for each pixel from one PC against the scores from another PC
- Problem: lots of points on the plot!
  - For this example: 500*500 = 250,000 points
  - Would look like single blob if plotted as one color
- Solution: score density plots
  - Calculate number of pixels with identical scores
  - Color code score plot according to number of pixels at each point
  - Can be useful to use log scale



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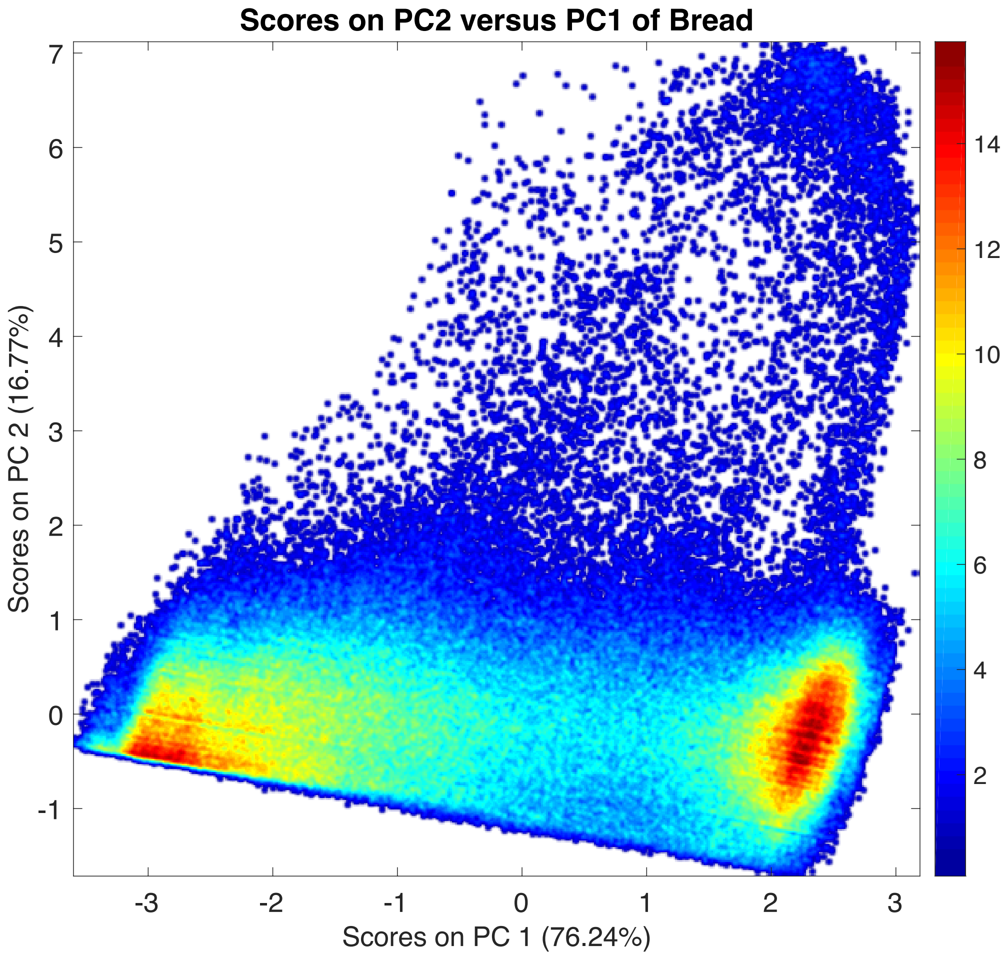
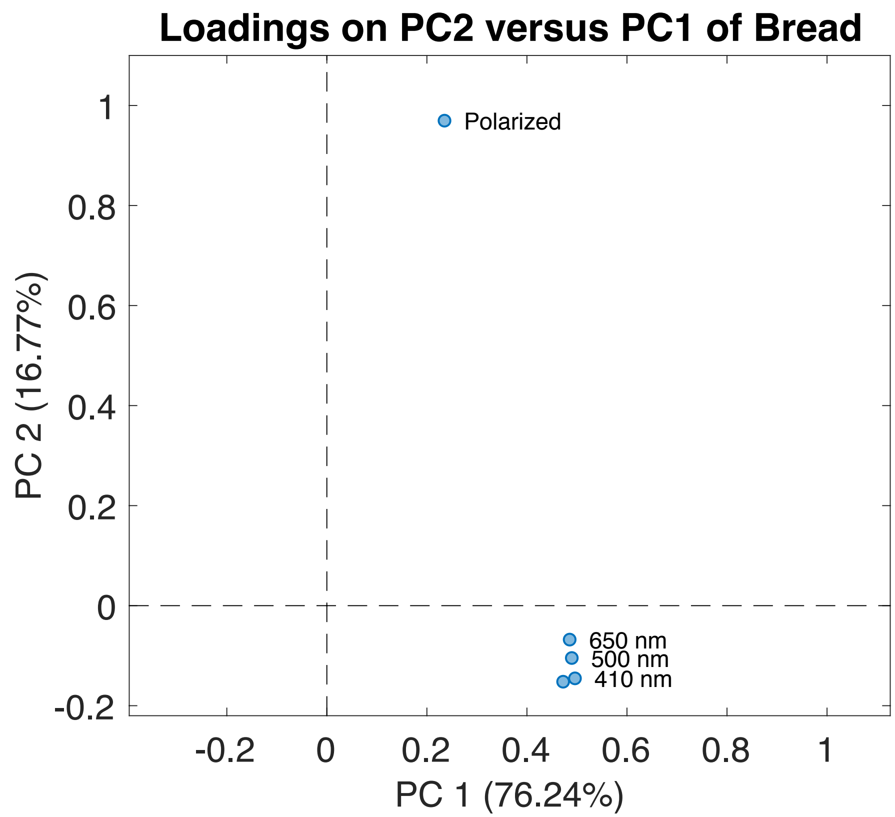
# Scores and Loadings



# Interpreting Scores and Loadings Plots

- Interpretation of scores and loading exactly the same as in conventional PCA
  - Look for clusters of pixels in scores plots
  - Use loadings to determine which original variables are responsible for differences in the scores
- Problem: what do scores clusters correspond to in the image plane?
- Solution: Linking

# Linking Scores and Image Plane Plots

- Interpretation of image PCA models is easier when features in scores plots and the image plane are linked
- Pixels associated with scores in user defined polygons are highlighted in all plots
- Areas in image plane can also be linked to scores plots



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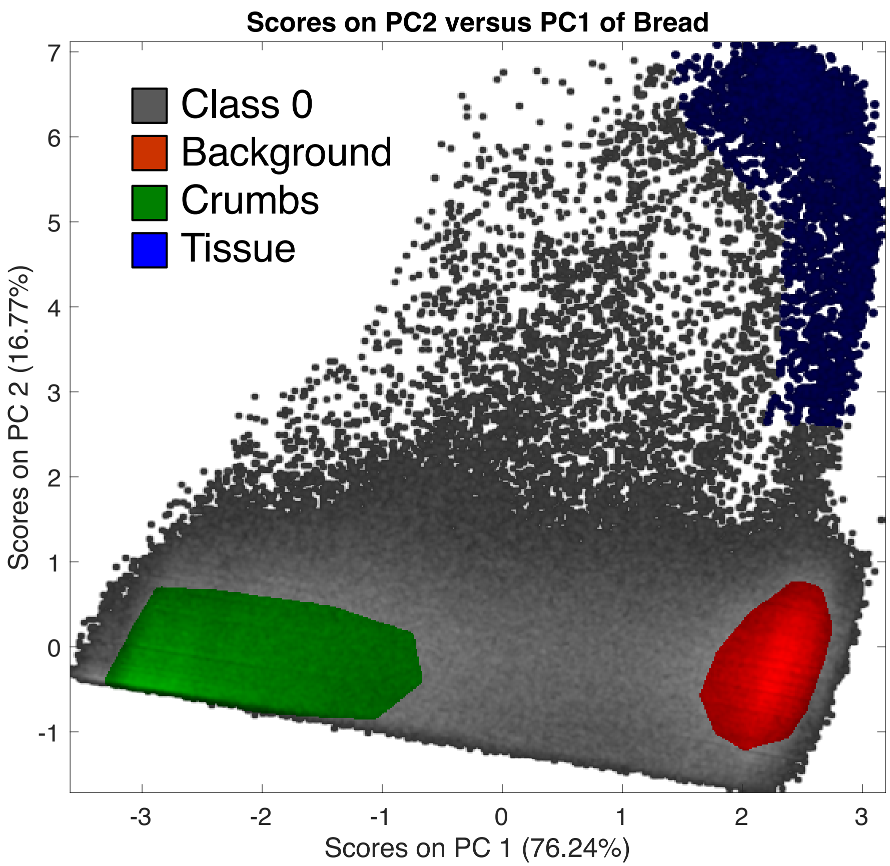
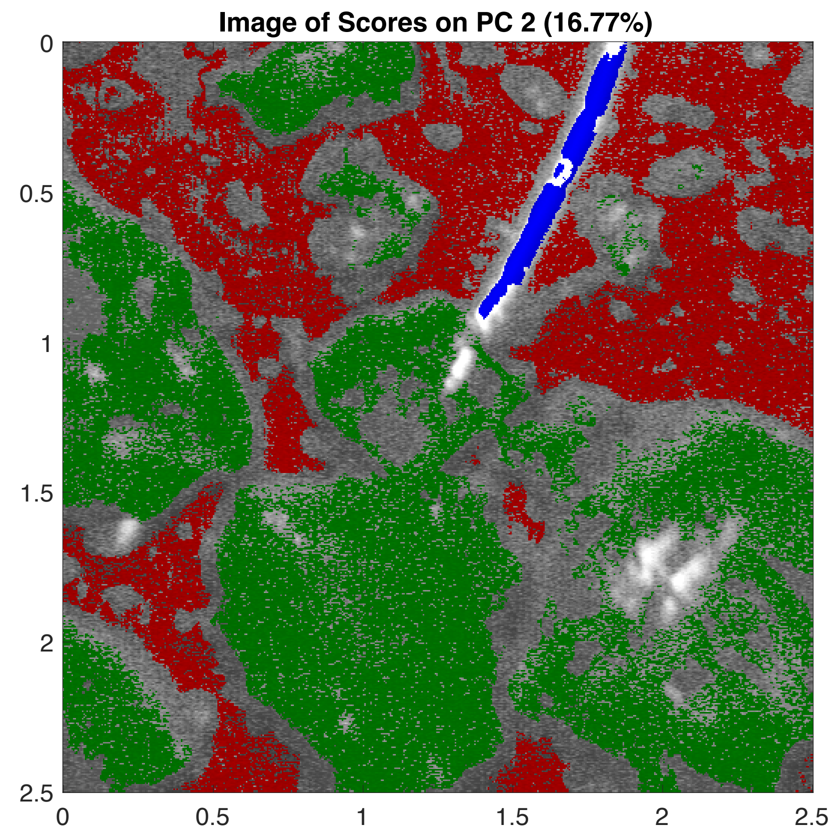
# Linked Scores Plots

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# Multivariate Curve Resolution

- With a minimum of *a priori* information, decompose a data matrix or image into chemically meaningful factors
    - “pure analyte” spectra (in contrast to loadings and weights)
    - “pure analyte” concentrations (in contrast to scores)
- Easy to interpret
    - can be used for process monitoring, QC, …



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# Classical Least Squares

- Classical Least Squares (CLS)
  - commonly used with spectra

$$\mathbf{X} = \mathbf{C}\mathbf{S}^{\mathrm{T}} + \mathbf{E}$$

- Useful for estimating **C** when *all* $K$ analyte spectra are known
  - $\mathbf{X}_{M\mathrm{x}N}$ are measured spectra
    - **X** can be an "unfolded" image where $M$ is the total number of pixels and $N$ is the number of channels
  - $\mathbf{C}_{M\mathrm{x}K}$ are concentrations
  - $\mathbf{S}_{N\mathrm{x}K}$ are pure analyte spectra

# *Alternating Least Squares (ALS)*

- What if we don't know **S** or **C**?
- Given *initial guess* $\mathbf{S}_0$ (or $\mathbf{C}_0$)...

$$\mathbf{C}_i = \mathbf{X}\mathbf{S}_{i-1}(\mathbf{S}_{i-1}^{\mathrm{T}}\mathbf{S}_{i-1})^{-1}$$

$$\mathbf{S}_i = (\mathbf{C}_i^{\mathrm{T}}\mathbf{C}_i)^{-1}\mathbf{C}_i^{\mathrm{T}}\,\mathbf{X}$$

- Iterate until convergence
  - Usually non-negatively constrained ($\mathbf{C}>0$ and $\mathbf{S}>0$)
  - and each $\mathbf{s}_k^T\mathbf{s}_k=1$ (i.e., unit length **S** vectors)
- Most popular method for multivariate curve resolution (MCR)

a.k.a. self-modeling curve resolution, self-modeling mixture analysis, end-member extraction



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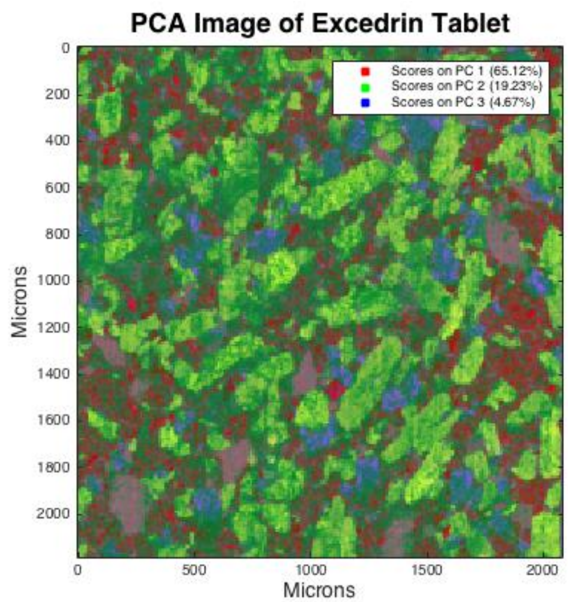
# Example: MCR on Excedrin

- Excedrin is a mixture of aspirin, acetaminophen, caffeine and microcrystalline cellulose
- Tablet imaged with tunable laser from 800 to 1800 $cm^{-1}$ over ~2mm
- Thanks to Agilent for data!





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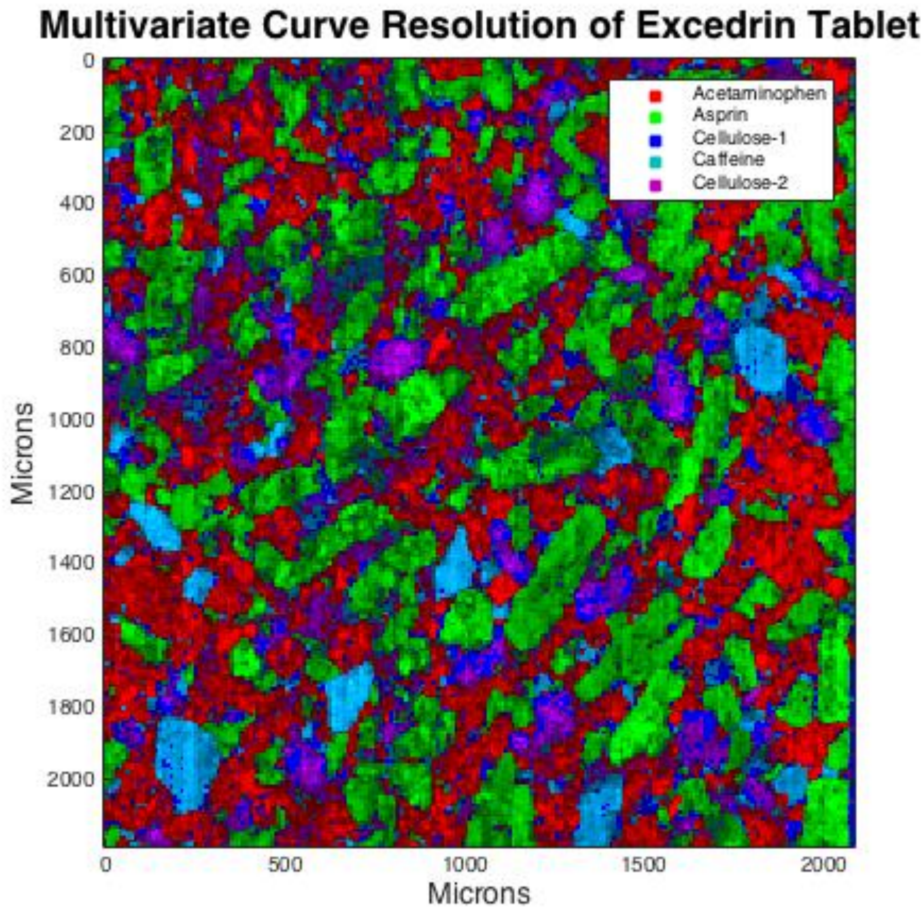
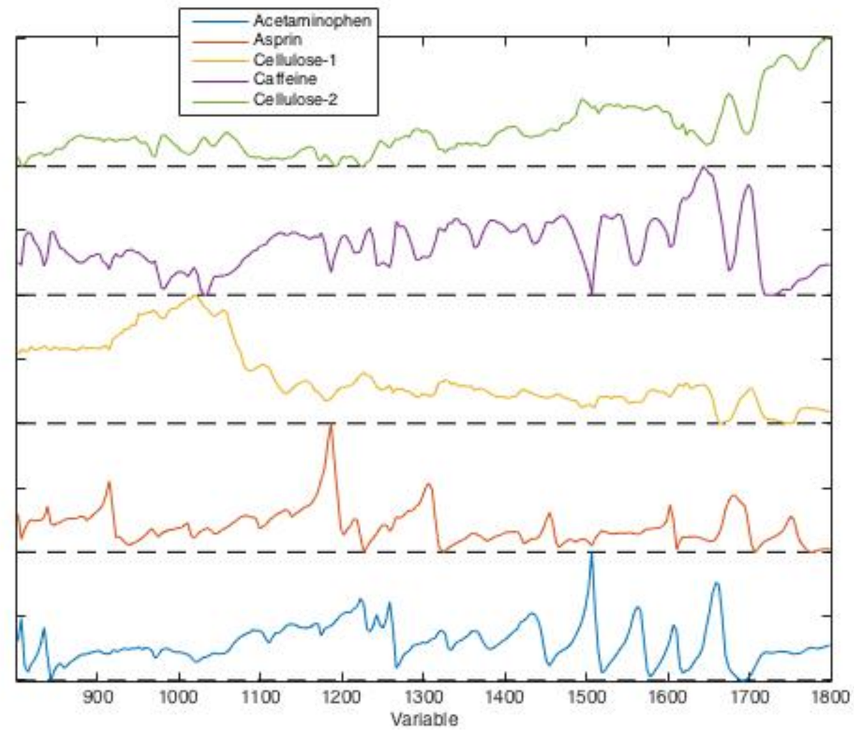
# MCR on Excedrin Results



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# *Further possibilites*

- Export score images to particle analysis
  - Determine particle size distributions of ingredients
  - Check formulation for composition
- Convert MCR model to CLS model
  - Extract loadings from MCR model
  - Load as CLS model
  - Assign component names
  - Use on new images



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# Independent Components Analysis

- Factor based method similar to PCA
- Central limit theorm says that sums of distributions tend towards Gaussian regardless of parent distributions
- ICA factors are computed to be as non-Gaussian as possible by maximizing the excess Kurtosis of the scores

$$k_{excess} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})^4}{\frac{1}{n}\left(\sum_{i=1}^{n}(x_i - \bar{x})^2\right)^2} - 3$$

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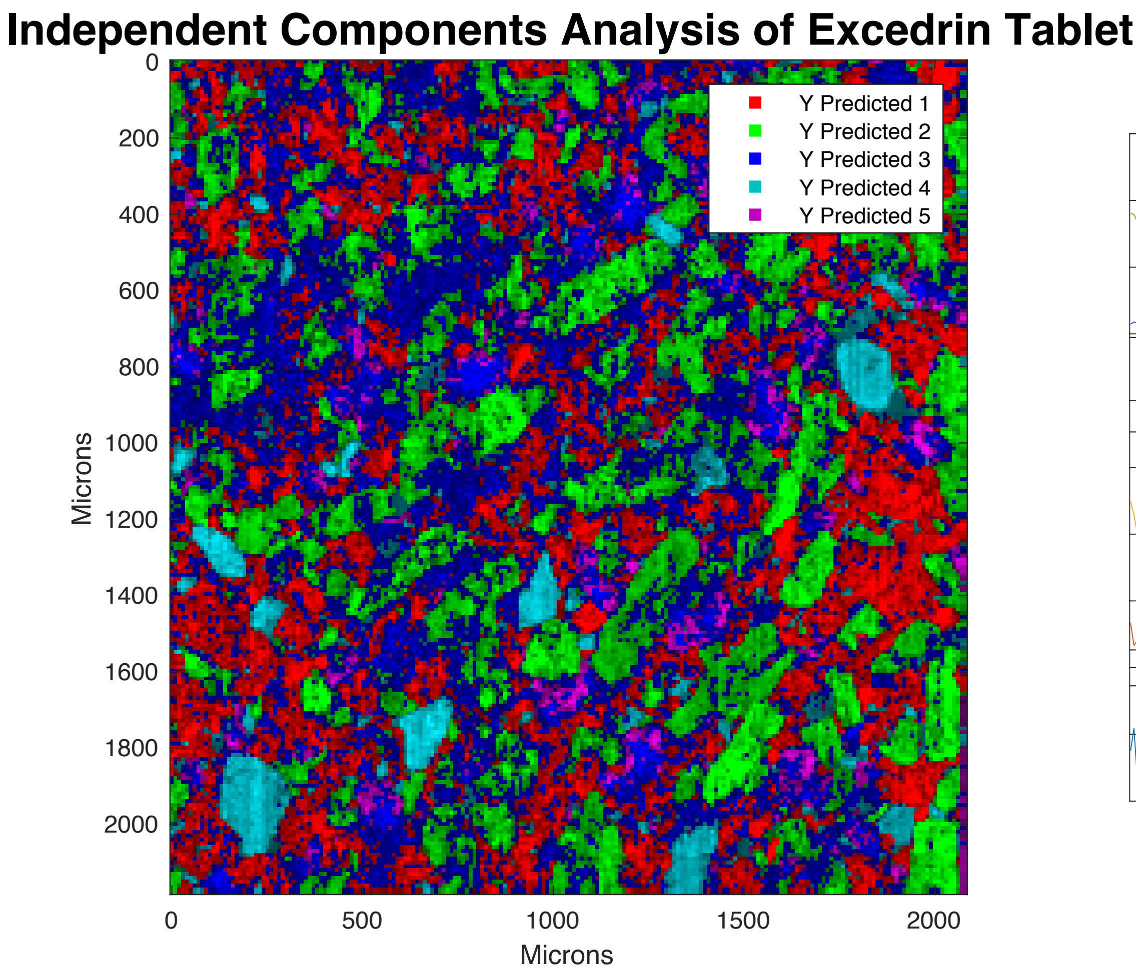
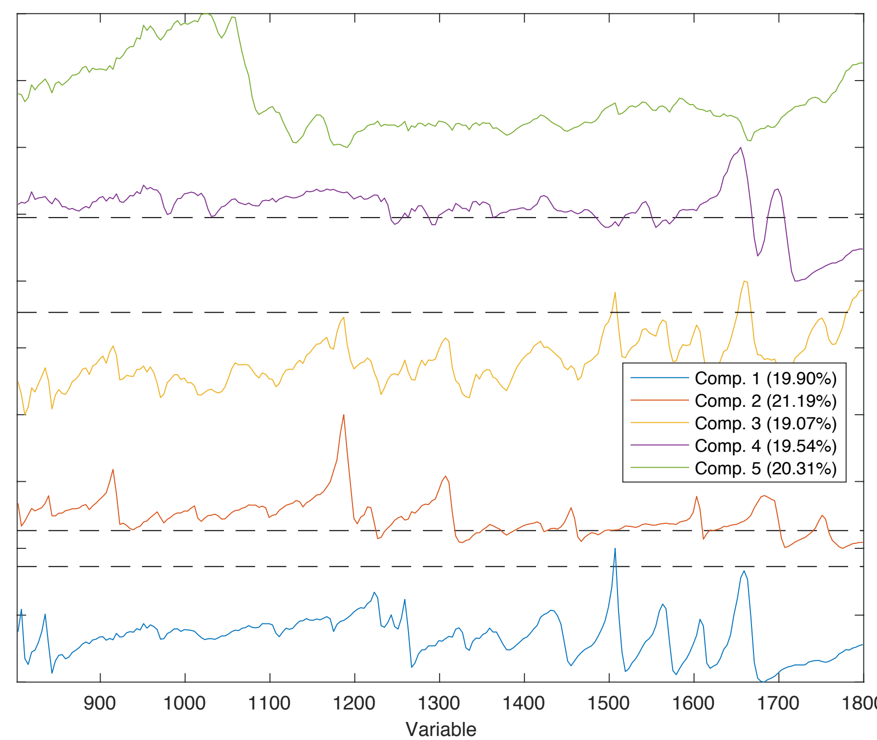
# ICA on Excedrin Results

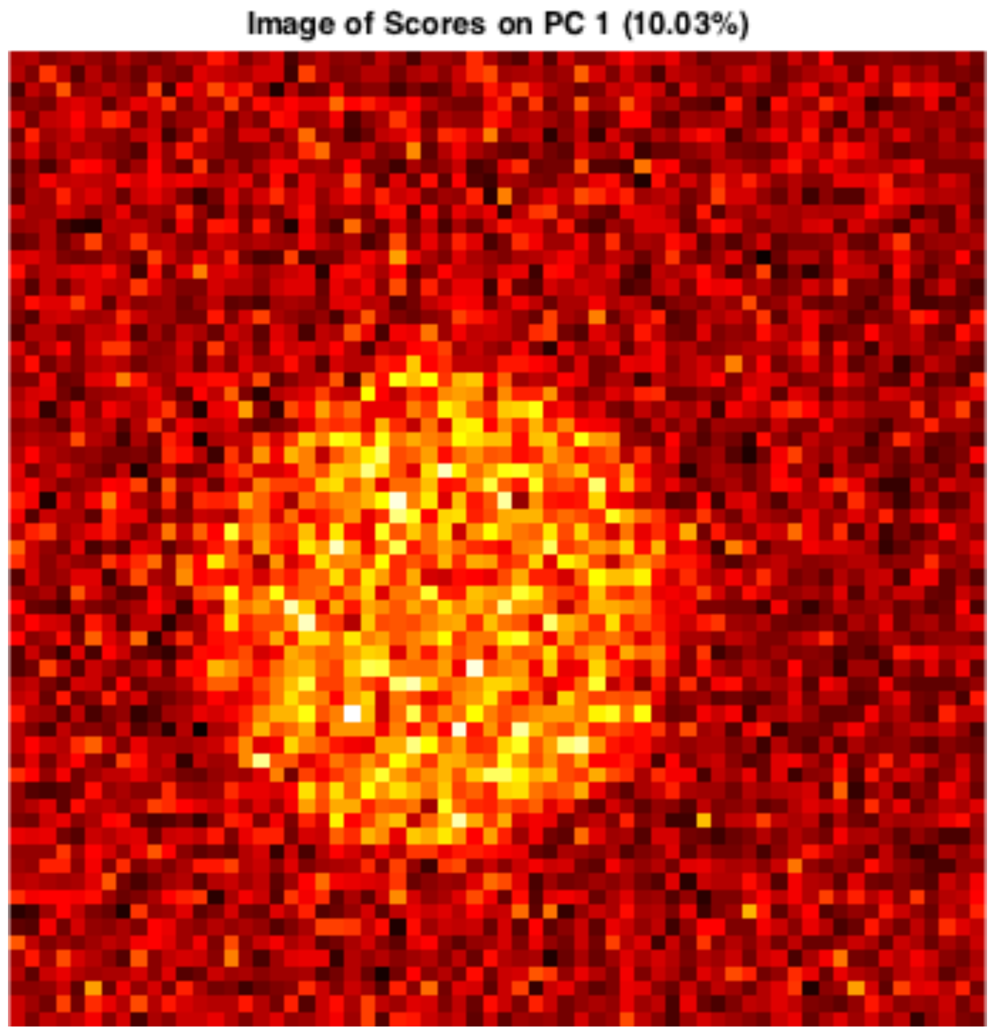


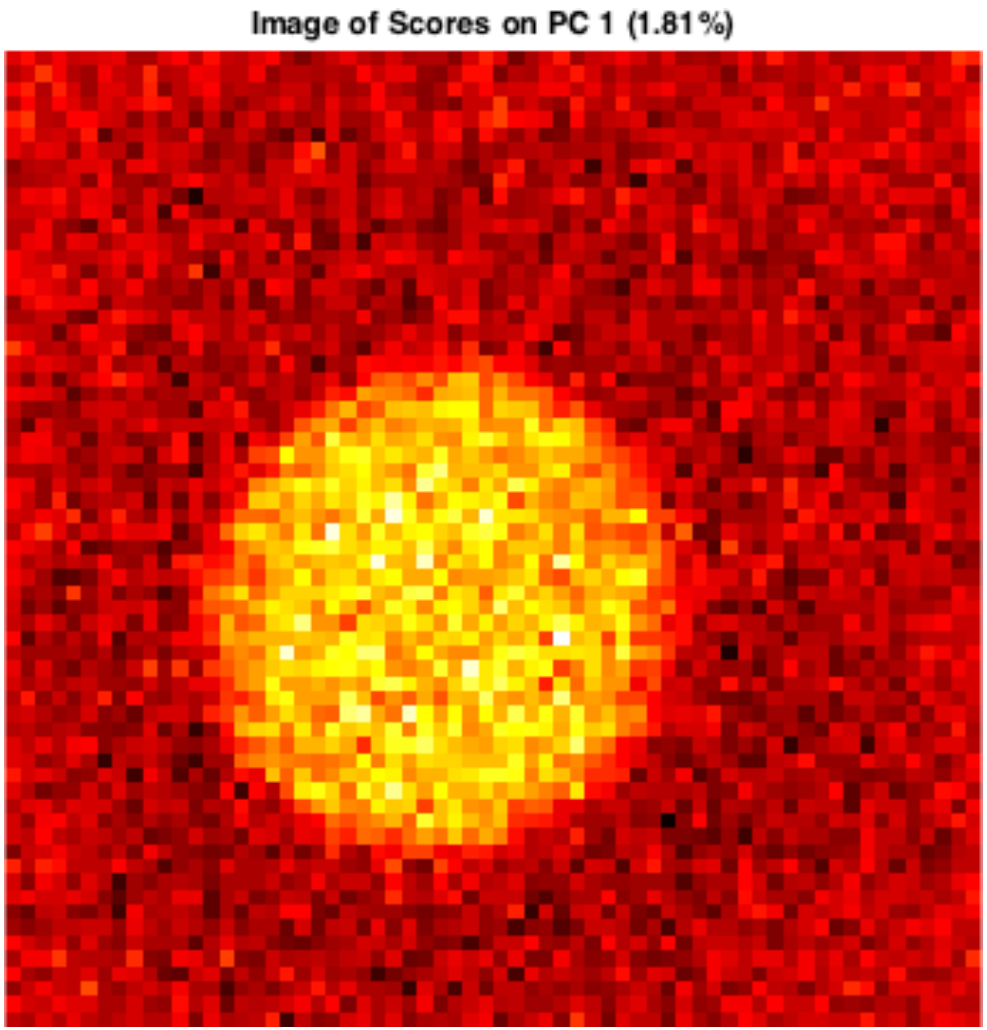
# Other Ways of Focusing on Variance of Interest

- Maximum Autocorrelation Factors (MAF) – find variance with spatial correlation
- Maximum Difference Factors (MDF) – find variance with spatial transitions (edge detection)
- Generalized Least Squares Weighting (GLS) – ignore variance from specified regions
- External Parameter Orthogonalization (EPO) – same idea as GLS

# MAF on SIMS Image of PVA




PCA




MAF

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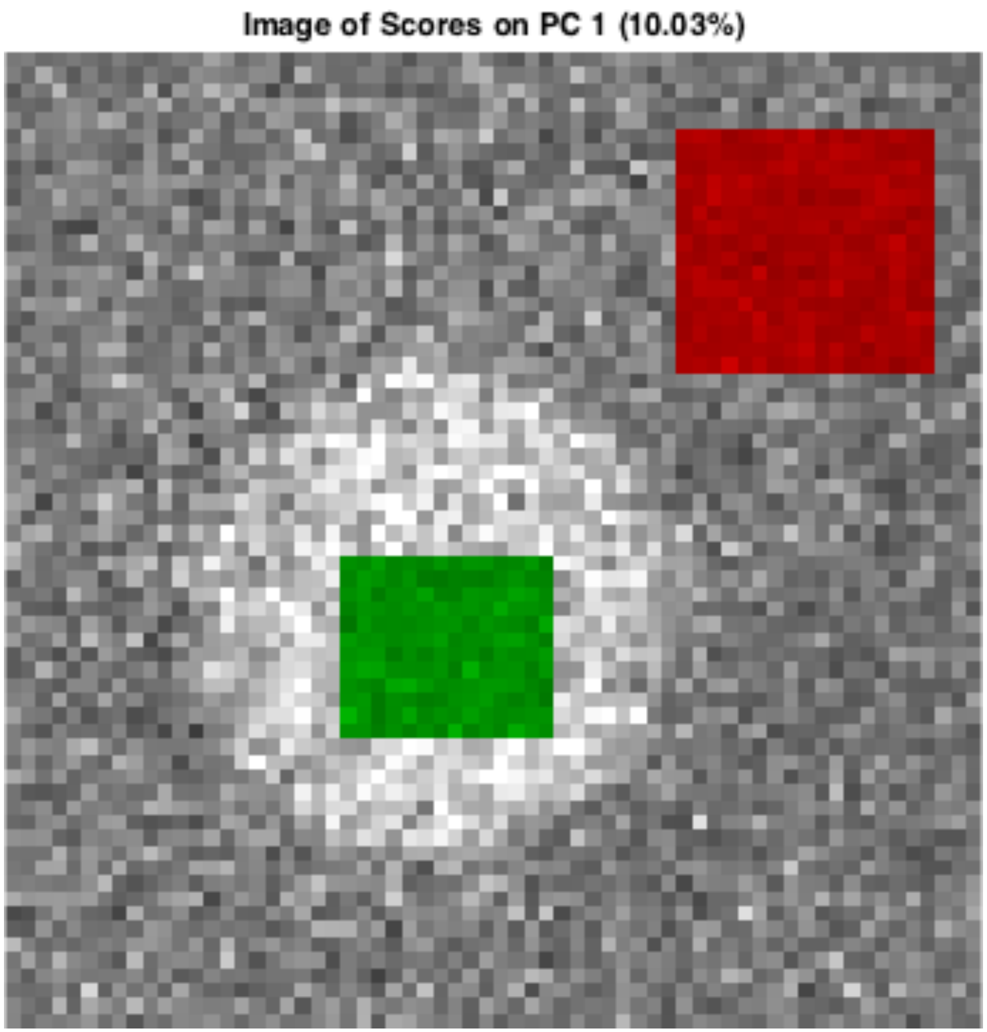
# Clutter Filters

- Define areas where only variance is due to noise or other unwanted variation
- Develop filter to minimize this variance
  - Generalized Least Squares (GLS) Weighting
    - Inverse square root of clutter covariance
  - External Parameter Orthogonalization (EPO)
    - Project out first PCs of clutter covariance

# Define Clutter Areas




Only variation in marked areas is due to “noise”

Center each area to its own mean, then combine areas

Develop GLS weighting from combined areas

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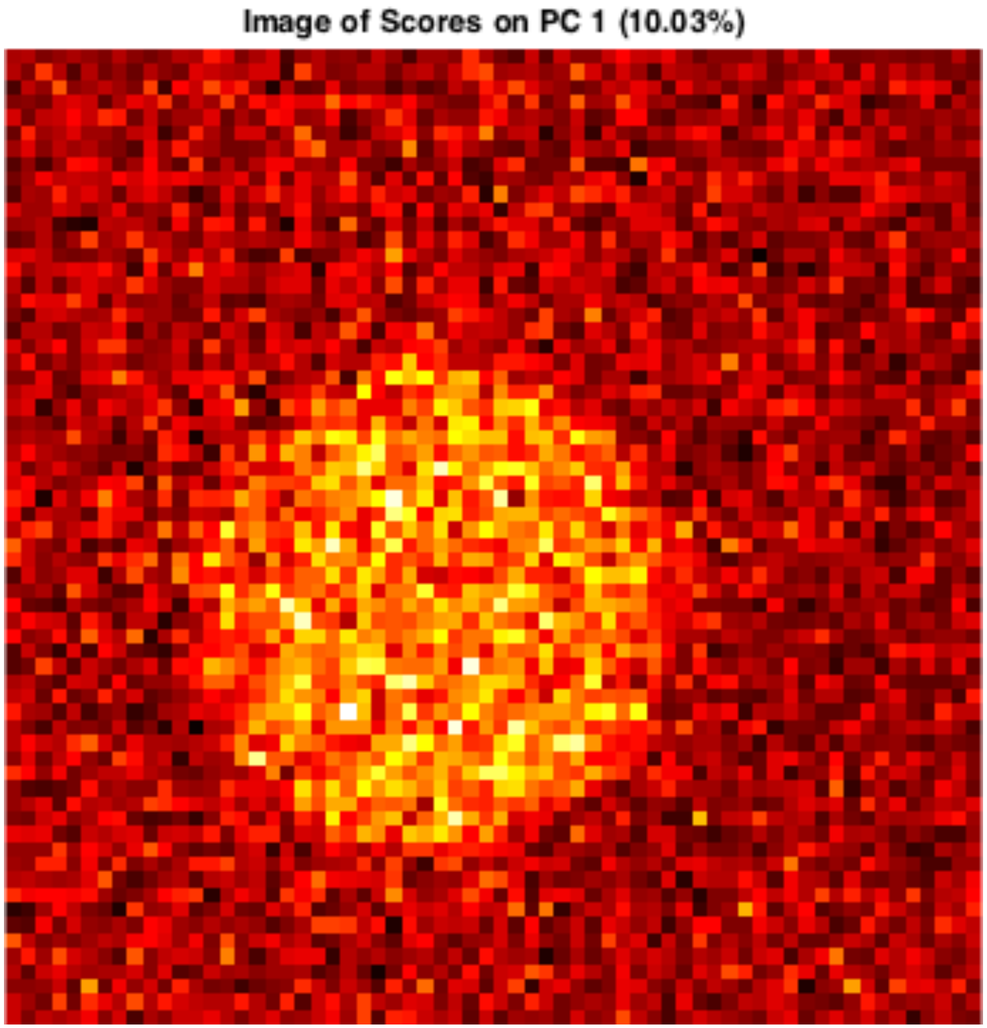
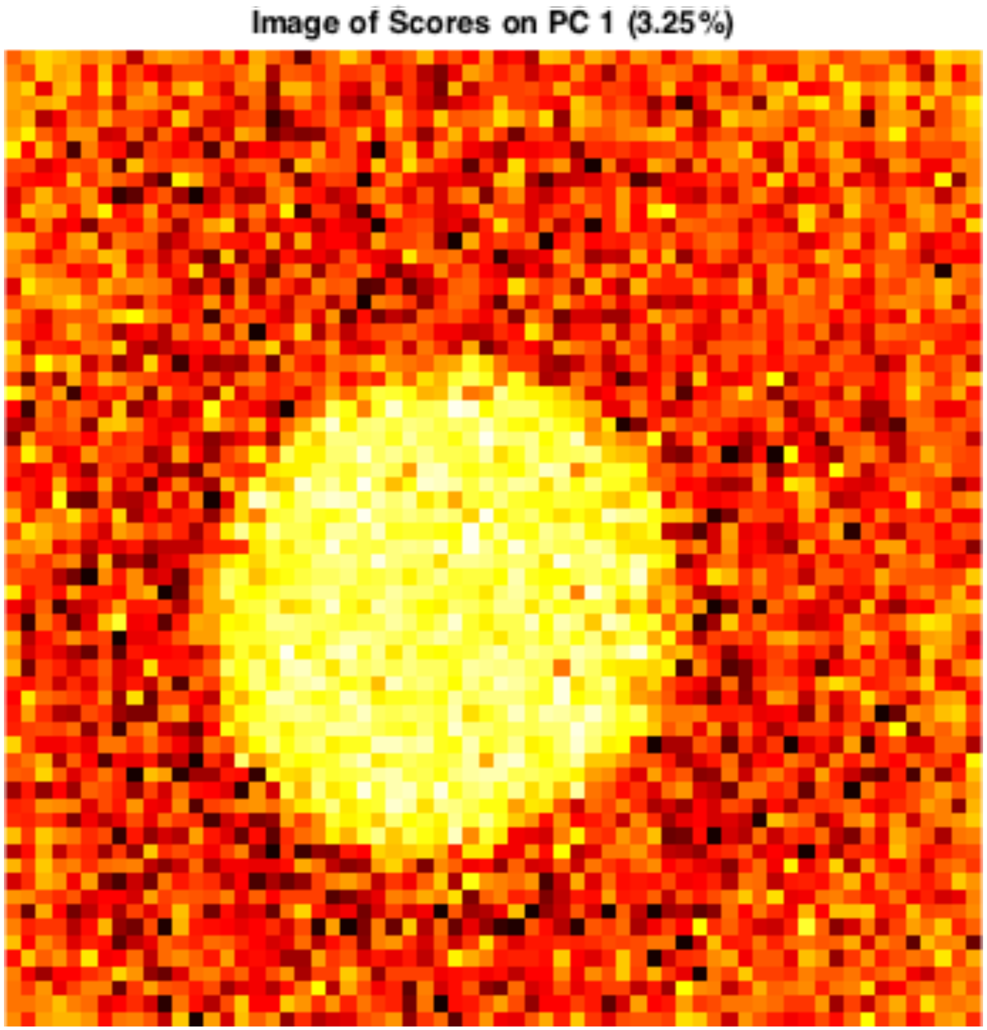
# GLS Filtered PVA




PCA




PCA with GLS

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# Cluster Analysis

- **Clustering:** Identification of natural groupings (classes) of samples without using prior knowledge of their identity – unsupervised classification
- **Agglomerative Clustering:** Start with each object as it's own cluster, then ***combine*** these into larger clusters
- **Partitional Clustering:** Start with all objects in one cluster, then ***separate*** them into smaller clusters
  - Better for image data



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# K-Means Partitional Clustering

- Choose *K* samples as cluster "targets"
  - random selection of samples
  - "pure samples": choose samples on outside of data (furthest from all other samples)
- Classify all samples into one of those *K* clusters.
- Calculate mean of each cluster's samples
- Repeat classification and cluster means until no samples are re-classed after mean recalculation.
- Much faster, but dependent on initial guess of samples and number of clusters *K*.


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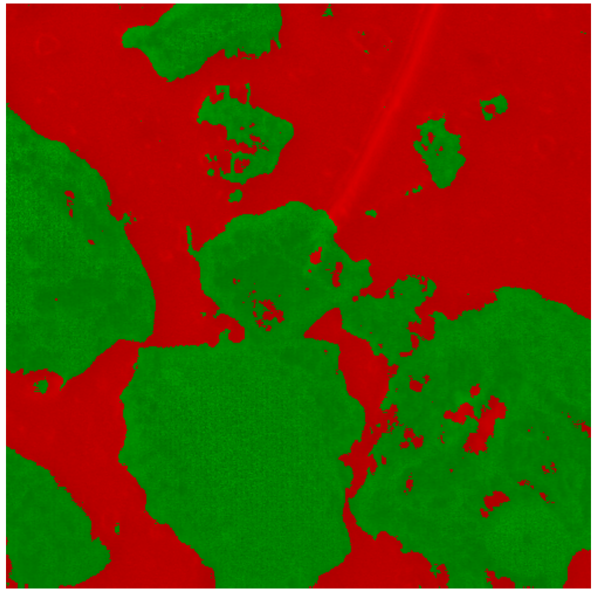
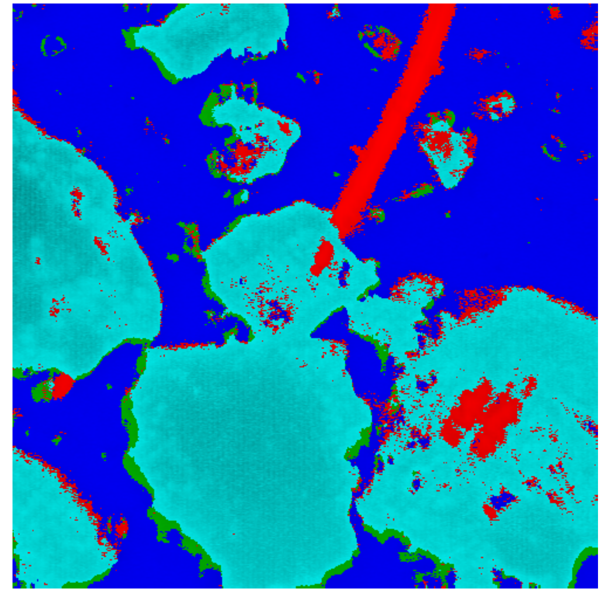
# Cluster Results

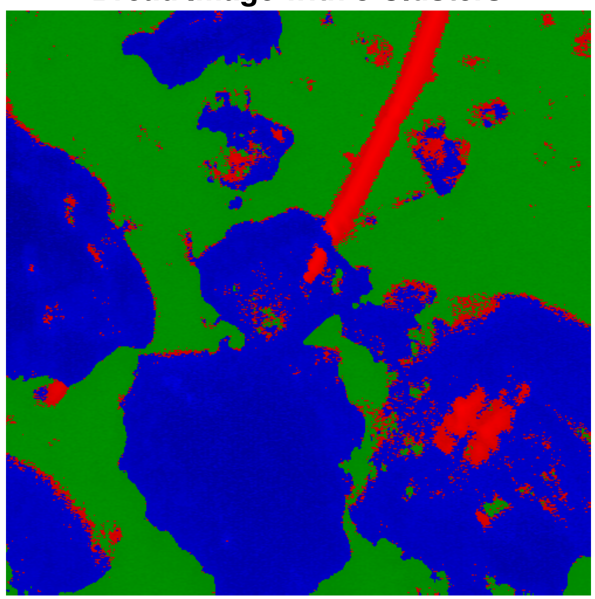
Bread Image with 2 Clusters



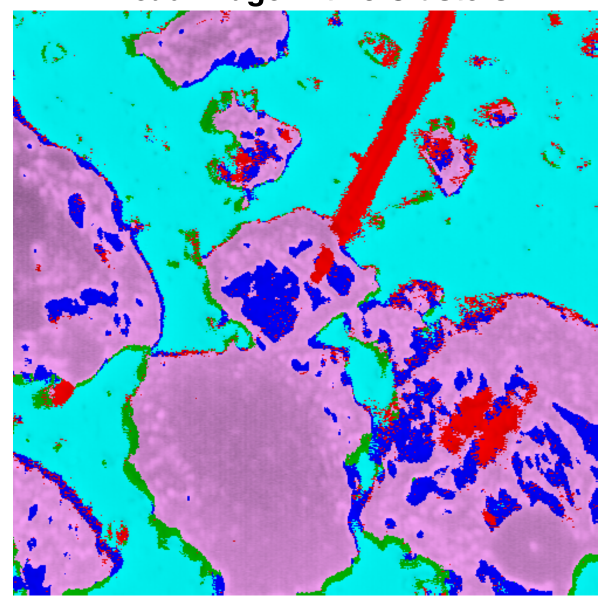
Bread Image with 4 Clusters



Bread Image with 3 Clusters



Bread Image with 5 Clusters



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# Conclusions

- PCA and related techniques focus on structure in the spectral (as opposed to spatial) dimension
- Condenses information from many variables, improves signal to noise
- MCR and ICA attempt to get chemically meaningful factors
- Anything that can be done with 2-way data tables can also be done with multivariate/hyperspectral images