Hyperspectral Image Analysis for Visualizing Grain Compounds

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Outline

1. Introduction
    - What are these hyperspectral images?
    - The linear and convex geometry model.
    - Wheat and maize kernel data.
2. Image Acquisition & Processing
    - The hyperspectral camera.
    - Pre-processing pipeline.
3. The Unmixing Model
    - Decomposing wheat and maize kernels.
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Hyperspectral image analysis

Introduction

- Classic image analysis is usually conducted on photographes having up to 3 RGB colors, sufficient for visualization.
- *Hyperspectral images* includes multiple color bands, typically > 50 bands and thus offers a more detailed analysis.

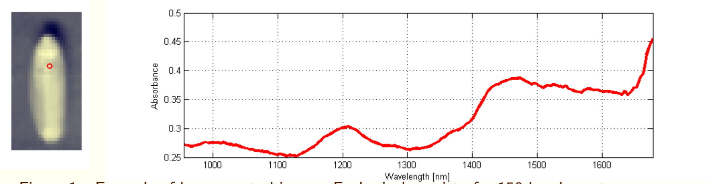

Figure 1 : Example of hyperspectral image. Each pixel consist of a 150 band spectra.

- Light reflection from sample contains information of material.
- The observed spectra is dominated by a linear mix of pure components.
- The objective is to decompose the image to into these pure spectral signatures.

Linear Modeling

The mixing of the constituents can be approximated linearly as

$$\mathbf{X} = \mathbf{WH} + \epsilon, \tag{1}$$

where **W** are the spectral signatures, **H** denote the fractional abundances (concentrations) and ϵ is the residual white Gaussian noise.

Constraints

- Non-Negativity, intensities can not be negative :

$$x_{i,j} \geq 0 \qquad \wedge \qquad w_{i,j} \geq 0 \qquad \wedge \qquad h_{i,j} \geq 0 \tag{2}$$

- Additivity, concentrations must sum to one : $\sum_i h_{i,j} = 1$

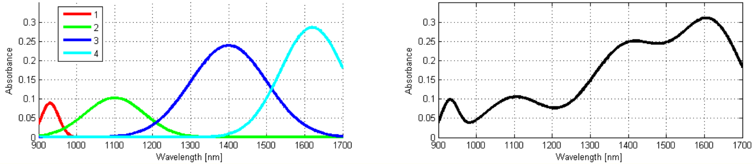

Figure 2 : Linear mixing of spectral signature into observed pixel spectra.

Convex Geometry Model

- These constraints lead to the following geometry for the 2 component case.

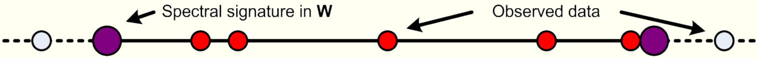

Figure 3 : Simple mixing with only 2 vertices.

- Purple vertices are the basis vertices denoted *endmembers*.
- Red points inside designate valid observed samples.
- Gray points outside are invalid due to noise (constraints violated).

For multiple endmembers the structure becomes an N-simplex.

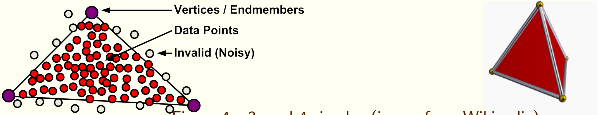

Figure 4 : 3- and 4-simplex (image from Wikipedia).

Objective is to locate the vertices as the basis spectral signatures based only on the observed data (unsupervised learning).

Grain Kernel Datasets

Expected identifiable components in grain kernels:

- Starch in endosperm (maize has both horny and floury starch).
- Protein in a matrix structure with starch and in aleurone layer.
- Oil in the germ.
- Background pixels.

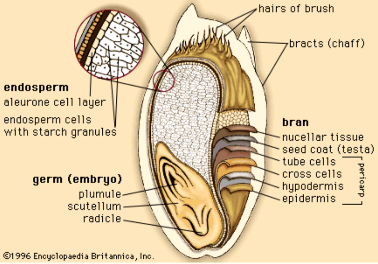

Figure 5 : Wheat kernel anatomy.

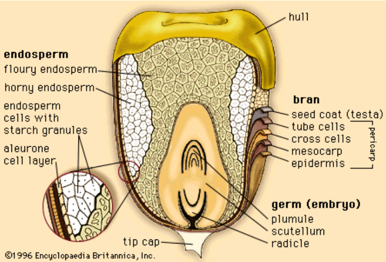

Figure 6 : Maize kernel anatomy with both horny and floury starch.

Image Acquisition

- Hyperspectral line-scan NIR camera sensitive from $900 - 1700$nm in 165 bands.
- Two datasets: 14 Wheat kernels and 8 Maize kernels (front and backside).
- Data format of each image is a $320 \times 150 \times 165$ tensor.
- Unfortunately no ground truth reference set, e.g. single kernel protein levels.

Figure 7 : Hyperspectral camera setup.

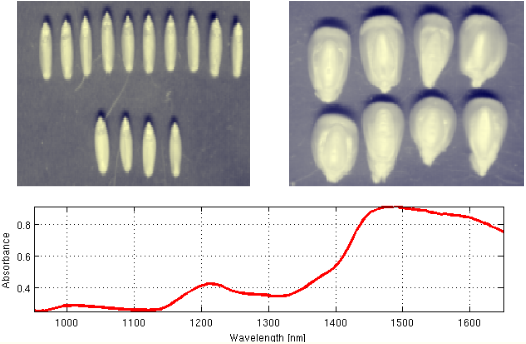

Figure 8 : Grain kernel datasets.

Data Processing Pipeline

Prior to decomposing the hyperspectral data a series of pre-processing steps are taken.

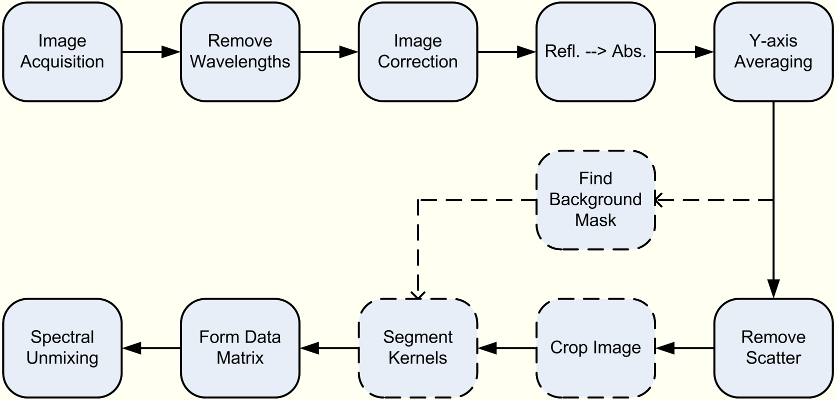

Figure 9 : Pre-processing pipeline.

Initial Pre-Processing

- Remove spectral range: Poor response at 900-950nm & 1650-1700nm (165 $\rightarrow$ 145 bands).
- Image correction: White reference and dark current image compensation.
- Line y-axis averaging: $2 \times$ Oversampling.
- Convert to Absorbance.

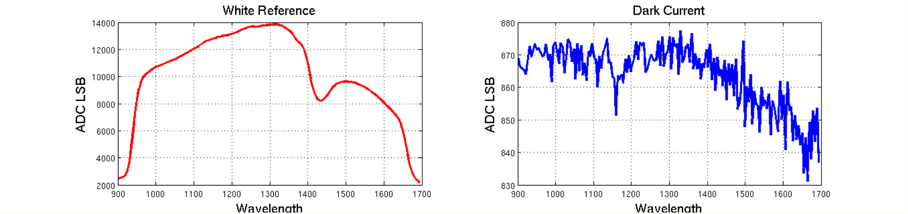

Figure 10 : White reference and dark current spectra.

- White light source to show poor SNR at spectral edges.
- Spectral dip at 1430nm is due to light guide fiber characteristics.

Scatter effects

- Main contribution to scatter effect appear due to surface structures of grains.
- Different types of scatter removal approaches: MSC, SNV, Detrending (Cubic Splines, SG-Smoothing etc.), Derivatives etc.
- NIR spectra are very smooth and thus complex detrending can prove fatal as important spectral information is suppressed.

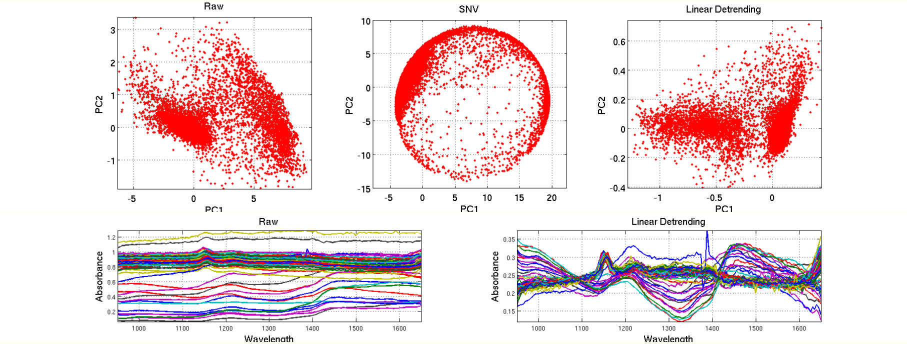

Figure 11 : Comparison of different antiscatter approaches.

Wheat Kernel Segmentation

- Each kernel is cropped into small $26 \times 44 \times 145$ images.
- Background pixels (black cardboard) are identified by a simple threshold applied to the 1st PC image.

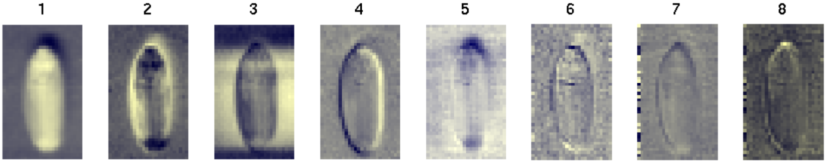

Figure 12 : Principal component images.

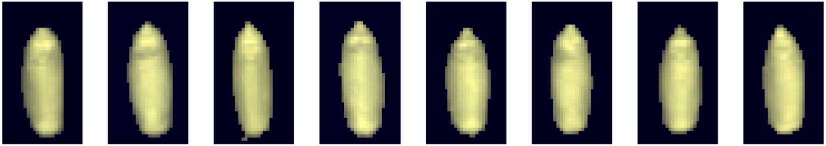

Figure 13 : Segmented wheat kernel images.

The Unmixing Model

- Linear NMF model $\mathbf{X} = \mathbf{WH} + \epsilon$ subject to the constraints (2).
- Augmented volume regularization with cost function

$$E = \frac{1}{2}||\mathbf{X} - \mathbf{WH}||^2 + \lambda J_W(\mathbf{W}) \tag{3}$$

- Regularization term $J_W(\mathbf{W})$ encourages tight volume of simplex around the observed data points.

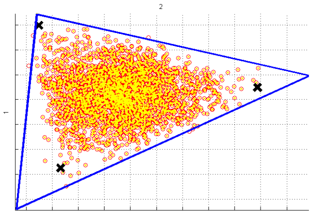

Figure 14 : No regularization

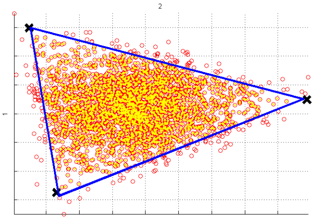

Figure 15 : Optimal regularization.

- Model parameter λ can be tuned to suppress inherit noise.

Wheat Kernel Dataset

- Constituents successfully identified: *Starch*, *Oil* and *Background*.

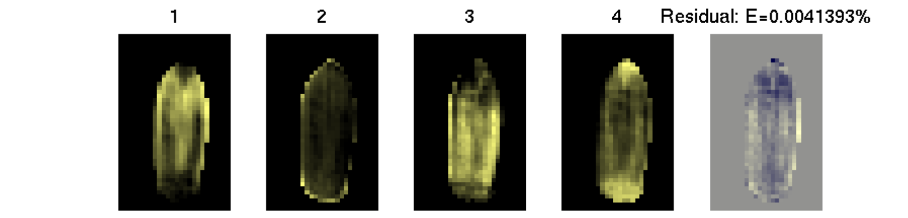

Figure 16 : Image components i wheat kernel dataset.

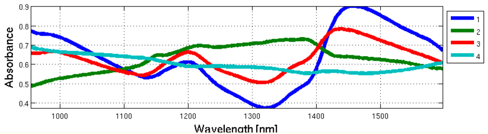

Figure 17 : Pure spectral signatures.

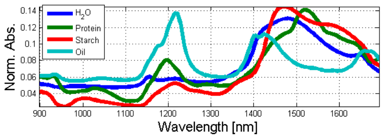

Figure 18 : Reference spectral signatures.

- Limitations: High correlation between constituents, mixing profile of compounds (simplex not filled) and penetration depth (difficult to asses).

Maize Kernel Dataset

- Constituents successfully identified: *Starch (Horny & Floury)*, *Oil*, *Background* and *Shadows*.

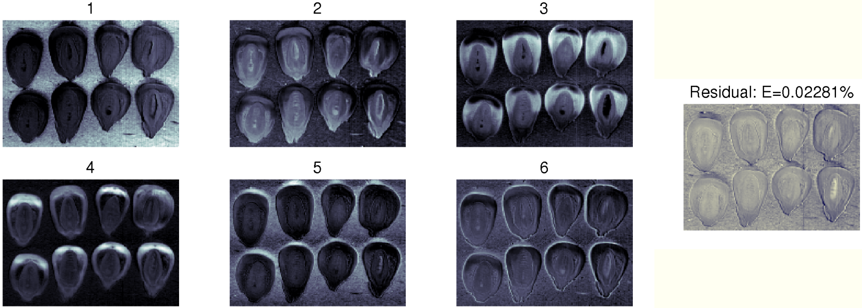

Figure 19 : Image components in maize kernel dataset.

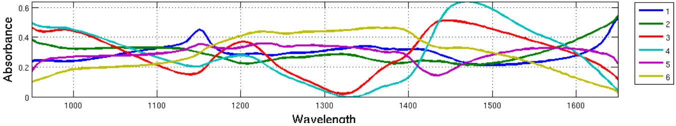

Figure 20 : Image component and spectral signatures.

Advanced Models

Bayesian NMF with volume prior

- Bayesian framework leads to probability distributions providing confidence of endmember estimate.

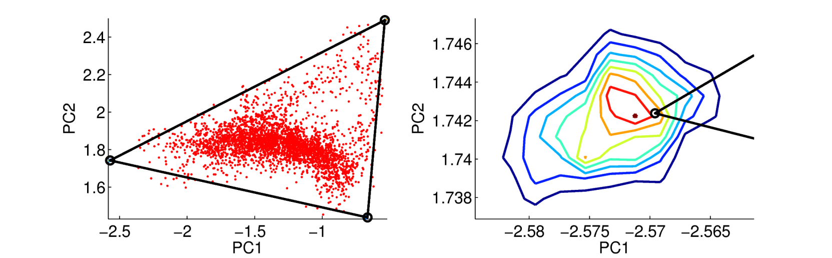

Figure 21 : Bayesian volume NMF applied on wheat kernel dataset.

- Achieve variance estimation not acquired by regular NMF.

Summary

Conclusions

- Hyperspectral images can be decomposed efficiently using NMF algorithms with *volume* regularizations.
- Pre-processing of data is important to achieve reasonable decomposition.
- Structure of dataset can set limitations, such as component correlation and mixing profile.

Near future work

- Incorporate spatial information, e.g. smoothing.