Hyperspectral imaging, unmixing and NMF

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What is hyperspectral imaging

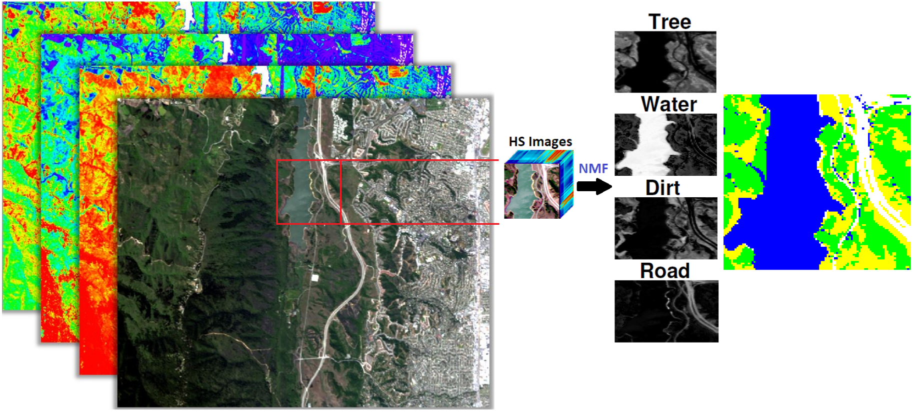
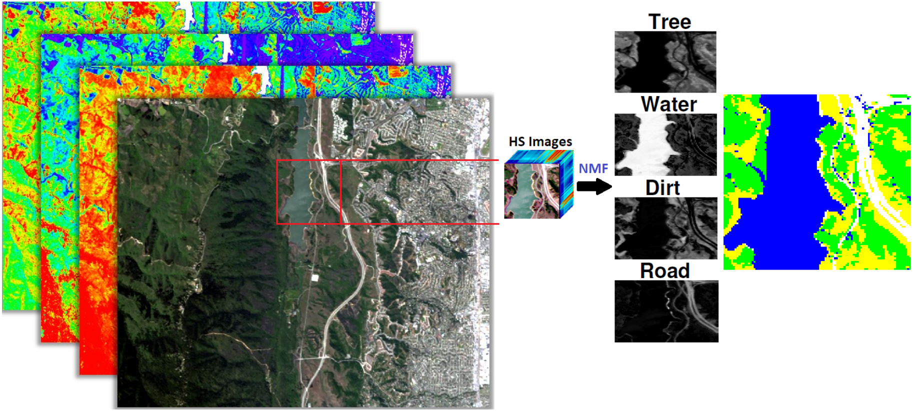


Figure: Left: From HySpeed Computing. Right: From A. & Gillis, 2019

- Ordinary "image" = red green blue.
- Hyperspectral image = in x-ray, infra-red, ultraviolet, etc.
  $\implies$ we have an image cube with the 3rd dimension corresponds to the wavelength dimension.

What is hyperspectral unmixing (HU)



- A scene has a few type of material, called *endmembers*.
- Examples of endmember here: tree, water, dirt, road.
- Task of HU: 1) identify these endmembers, and 2) identify the abundance of each endmemeber in each pixel of the image.

Reflectance (Absorbance) spectrum of material

- Why grass is green: it reflects green light and absorb other light
- This characteristic is described by the reflectance spectrum.
  - x-axis is wavelength / wave number / frequency
  - y-axis is amount of reflection
- Reflectance = normalized amount of reflection, with maximum value 1.
- Absorbance = 1 - reflectance.
- Reflectance or absorbance spectrum are both nonnegative.
- Different material has its own characteristic spectrum.

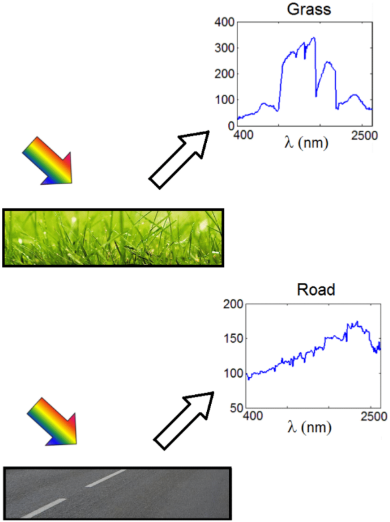
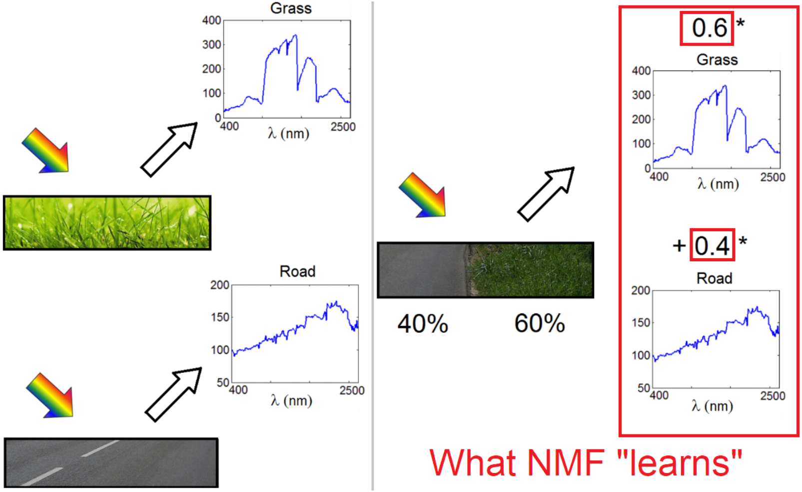


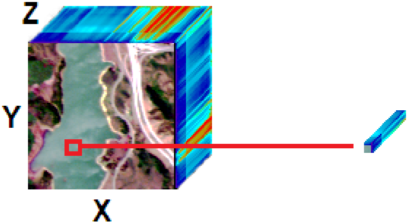
Figure: Figure comes from slide of Nicolas Gillis.

Abundance of the endmember



- For a pixel that consists of 40% grass and 60% road, you expect its spectrum is 40% grass + 60% road.
- The numbers 0.4 and 0.6 here represent the relative abundance of the endmember in that pixel (i.e. they sum to 1).

Hyperspectral pixel



- Recall the data in hyperspectral imaging is a collection of images of the same scene across different wavelengths: the data is a 3rd order tensor of size $X \times Y \times Z$, where X and Y refer to the spatial dimension of the image and Z refers to the wavelength dimension.

- A pixel in the data is a vector $\mathbf{m}$ in $\mathbb{R}^Z_+$ and it represent the spectral behavior across all wavelength at that specific spatial location.

Linear mixing model

- Suppose there are r endmembers in the scene, the spectrum profile of each endmember is represented by a vector $\mathbf{w}_i$, Then a pixel $\mathbf{m}$ can be expressed by the following linear model

$$\mathbf{x} \;\; = \;\; \sum_i \mathbf{w}_i h(i),$$

  where $h(i) \geq 0$ represents the amount of abundance of endmember $\mathbf{w}_i$ presented in the pixel.

- Compact notation: $\mathbf{m} = \mathbf{W}\mathbf{h}$.

- Let $\mathbf{M}$ represents the collections of pixels, then we have $\mathbf{m}_i = \mathbf{W}\mathbf{h}_i$, or equivalently

$$\mathbf{M} = \mathbf{W}\mathbf{H},$$

  where $\mathbf{M}$ is Z-by-XY, $\mathbf{W}$ is Z-by-r, and $\mathbf{H}$ is r-by-XY.

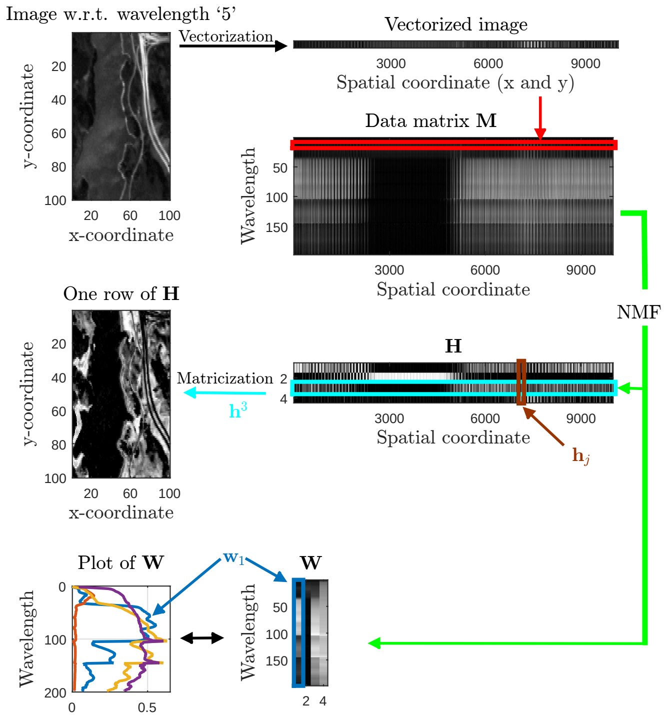


Image w.r.t. wavelength '5'
Vectorization
Vectorized image
3000 6000 9000
Spatial coordinate (x and y)
y-coordinate
20 40 60 80 100
20 60 100
x-coordinate
Data matrix M
Wavelength
50 100 150
3000 6000 9000
Spatial coordinate
NMF
One row of H
H
Matricization
$\mathbf{h}^3$
$\mathbf{h}_j$
2 4
Plot of W
W
$\mathbf{w}_1$
Wavelength
0 100 200
0 0.5
50 100 150
2 4

Hyperspectral unmixing and NMF

- Given a hyperspectral image cube $\mathcal{X}$ (size Y-by-X-by-Z) or a matrix data $\mathbf{M}$ (size Z-by-XY), the goals of Hyperspectral unmixing are
  - Identify the number of endmembers.
    This corresponds to determine the factorization rank r in NMF.
  - Identify the endmembers.
    This corresponds to determine the factor matrix $\mathbf{W}$ in NMF.
  - Identify the abundance of each endmember in all the pixels.
    This corresponds to determine the factor matrix $\mathbf{H}$ in NMF.
- As spectrum and abundance are both nonnegative, so NMF model naturally fits in the application of Hyperspectral unmixing.

NMF

- Given a hyperspectral data matrix $\mathbf{M}$ (size Z-by-XY), assume we know the factorization rank r, then the NMF problem is

$$\min_{\mathbf{W},\mathbf{H}} \frac{1}{2}\|\mathbf{M}-\mathbf{W}\mathbf{H}\|_F^2 \ \text{ s.t. } \ \mathbf{W}\geq 0, \ \mathbf{H}\geq 0.$$

- Considering the fact that columns of $\mathbf{H}$ encode the abundances of endmembers in pixels, then the elements of the column sum to one, and hence we have the additional constraint $\langle \mathbf{h}_j, \mathbf{1}\rangle = 1$ for all j. In compact notation this is $\mathbf{H}^\top\mathbf{1}=\mathbf{1}$, and the NMF problem becomes

$$\min_{\mathbf{W},\mathbf{H}} \frac{1}{2}\|\mathbf{M}-\mathbf{W}\mathbf{H}\|_F^2 \ \text{ s.t. } \ \mathbf{W}\geq 0, \ \mathbf{H}\geq 0, \ \mathbf{H}^\top\mathbf{1}=\mathbf{1}.$$

- This is the basic form of NMF for hyperspectral unmixing problem.

Assumptions on using NMF to solve hyperspectral unmixing problem

- We assumed factorization rank r is known.
  In practice, r is not known and we have to estimate it. This problem is also known as model order selection.

- We assumed all endmembers can be presented by a rank-1 nonnegative matrix in the form of $\mathbf{W}(:,i)\mathbf{H}(i,:)$.
  In practice, this may not be true, and an endmember may need multiple components to represent. Then we can consider the group NMF model: i.e., in stead of using a rank-4 factorization with four rank-1 components to represent four endmembers, we use a rank-r factorization with $r > 4$.

- We assumed the data is relatively clean: the noise in the data is bounded. In practice, data can be corrupted by strong noise or contains outliers. Then we either perform denoising or use robust NMF.

Last page - summary

Discussed

- Brief introduction of hyperspectral imaging.
- How NMF can be used to solve hyperspectral unmixing problem.
- Assumptions made when using NMF to solve hyperspectral unmixing problem.

Not discussed

- Other assumptions in hyperspectral unmixing problem: for example nonlinear mixing effect, spectral variability.
- How to exactly solve the NMF minimization problem.
- Pure-pixel assumption and the minimum volume criterion.

End of document