unmixR: Hyperspectral Unmixing in *R*

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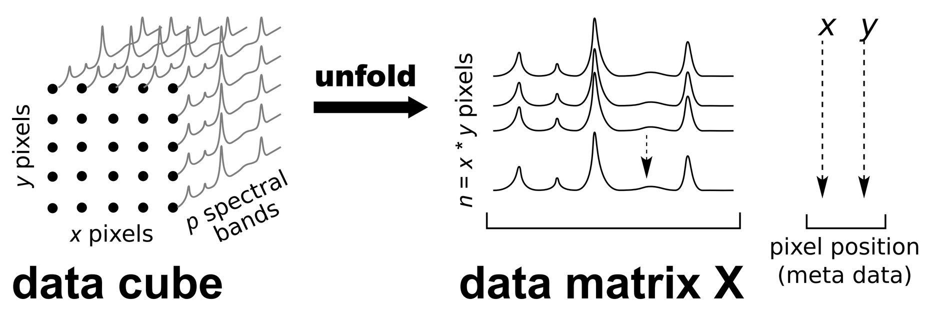
Hyperspectral Imaging

Hyperspectral images are 3D data sets of spectra collected over an x, y grid.



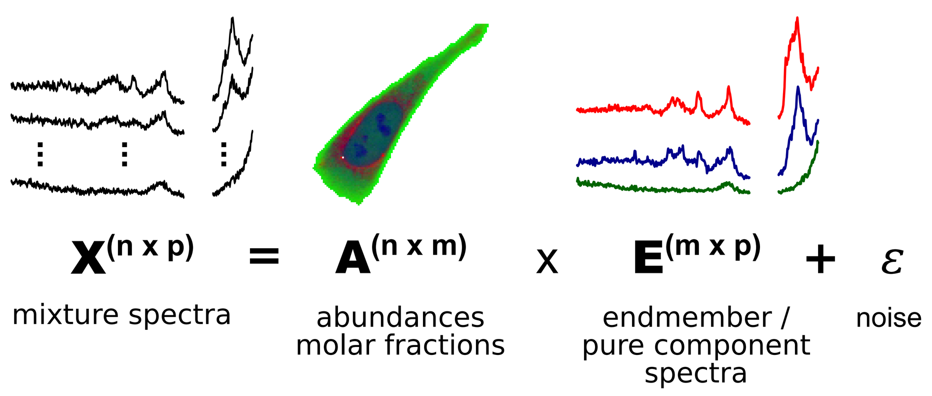
Applications: remote sensing/ airborne or satellite land imaging, biomedical microspectroscopy and art history investigations

Spectra: e.g. visible, near-infrared, mid-infrared, or Raman spectra.

Spectral Unmixing

Identify m pure component spectra in data, then derive respective concentrations.

Bilinear statistical model:



Mixture diagram for m components: $(m-1)$-simplex in $m-1$ dimensions (***A***).

2 components	1-simplex	line
3 components	2-simplex	triangle
4 components	3-simplex	tetrahedron

Vertices are pure component spectra.

Assumptions:

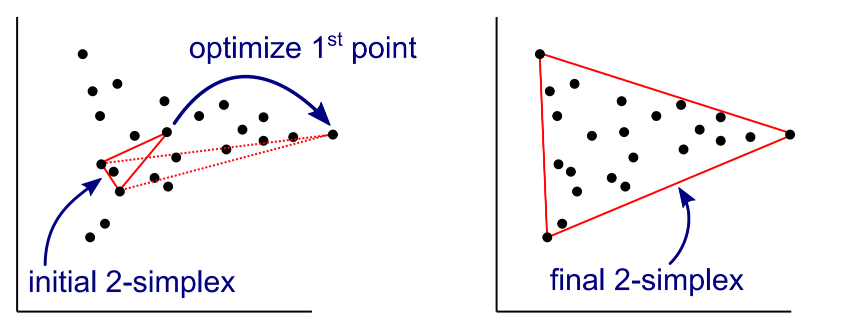
- Data consists of *mixture* spectra
- Spectra of pure components are available somewhere in the data ***X***
- Not too much noise on measurements (possibly after PCA)
- (Other methods relax assumptions 2 and 3)
- Number of pure components m ("chemical rank") provided by user input
- Abundances subject to non-negativity constraint

N-FINDR Algorithm

Heuristic: find m spectra within data set that span $(m-1)$-simplex with *largest volume*

1. Project ***X*** into $(m-1)$-dimensional space (typically by PCA)
2. Initialize simplex with m arbitrary points
3. Iteratively grow simplex:
   For each vertex point in turn:
   exchange by point that maximizes simplex volume (keeping the other $m-1$ points constant)

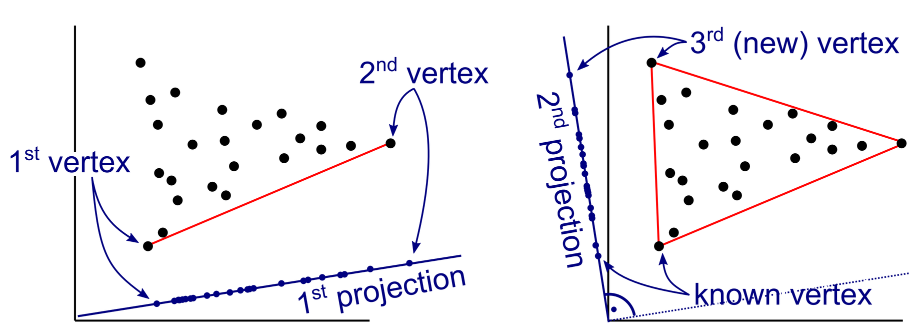
   Iterate/refine until convergence
4. Return corresponding spectra of ***X*** as endmembers
5. `predict` abundances by non-negative least squares [nnls] on found endmembers



VCA Algorithm

Heuristic: projection of points onto arbitrary direction will always have 2 of the m vertices as maximum and minimum.

1. Project ***X*** into $(m-1)$-dimensional space if data is considered too noisy
2. Project ***X*** onto arbitrary direction
3. Find first 2 vertices as min and max
4. Project ***X*** onto arbitrary direction orthogonal to all previously used directions
5. Find next vertex as unknown min or max
6. Repeat 4 and 5 until m vertices are found
7. Return corresponding spectra of ***X*** as endmembers
8. `predict` abundances by non-negative least squares [nnls] on found endmembers



AVIRIS Cuprite Data

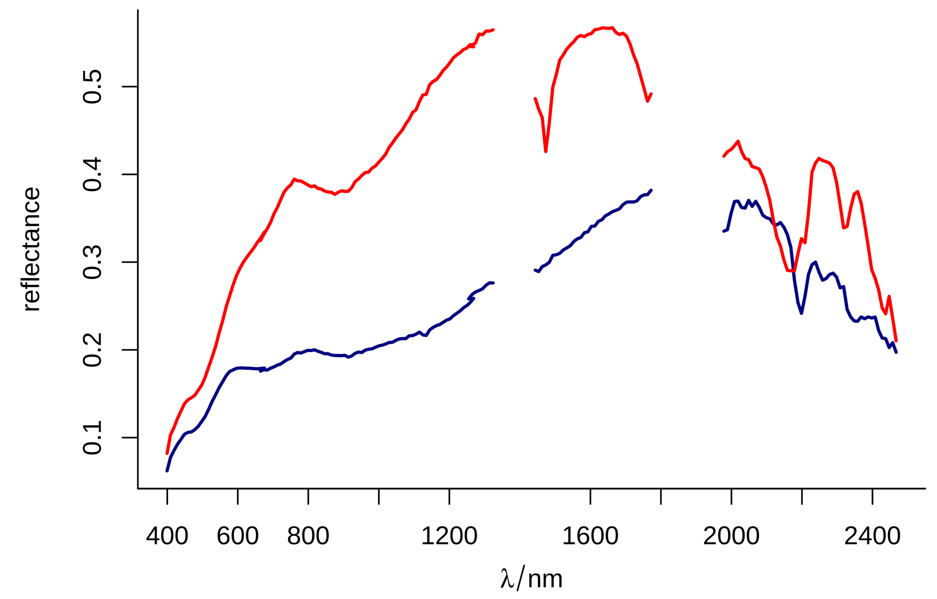
Data Set:

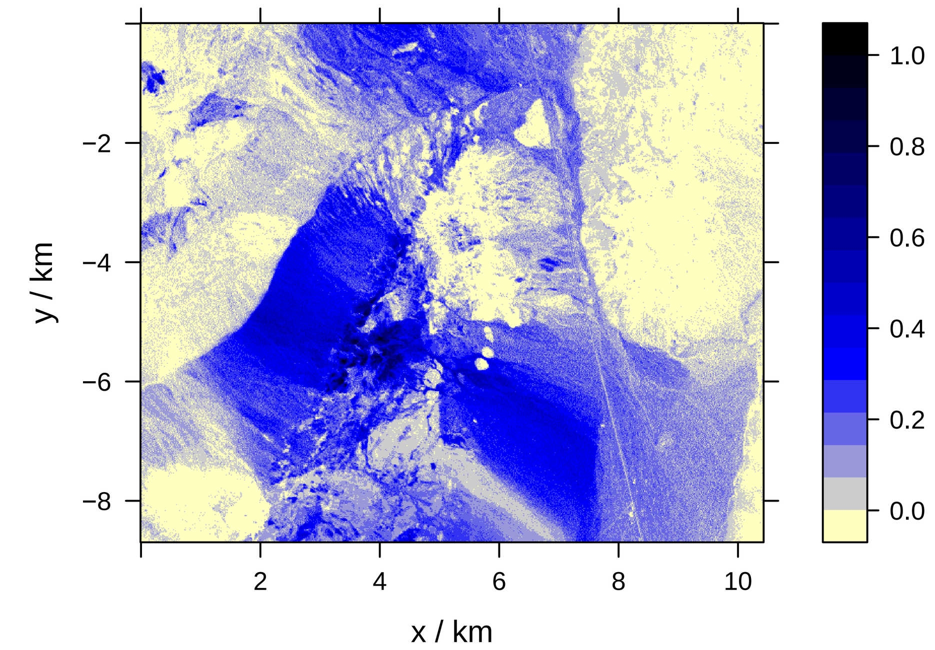
- Acquired by NASA's Airborne Visible/ InfraRed Imaging Spectrometer
- of mining region in the south of Nevada/USA
- 45 × 10 km (300 000 pixel subimage shown)
- 250 - 4 000 nm (224 spectral bands)
- Well-known ground truth

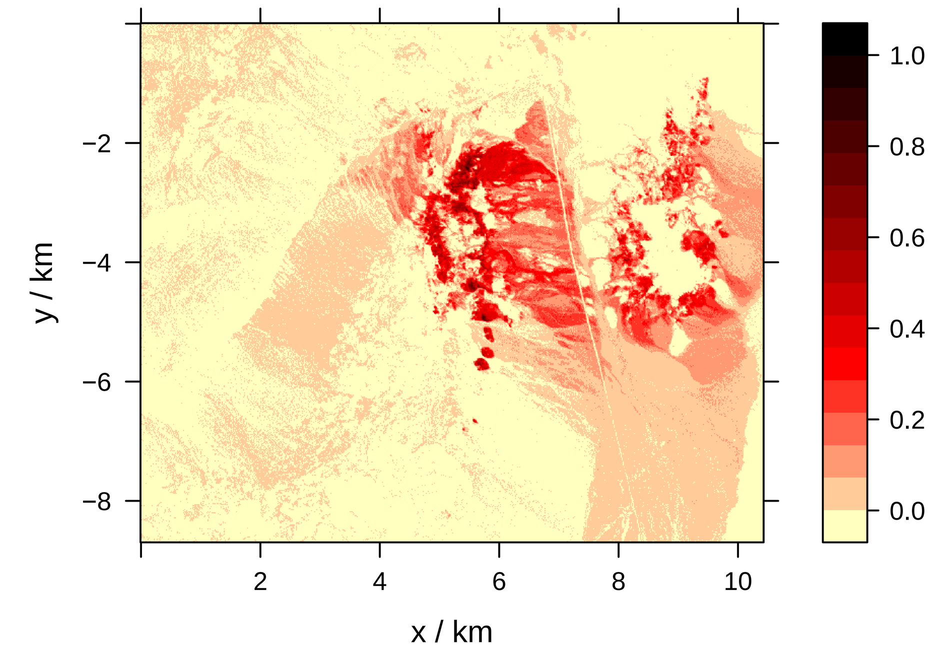
N-FINDR with $m = 19$ endmembers

As example, we show 2 components identified as

- muscovite (mica, $KAl_2(AlSi_3O_{10})(F_OH)_2$), and
- alunite (alumstone, $KAl_3(SO_4)_2(OH)_6$).





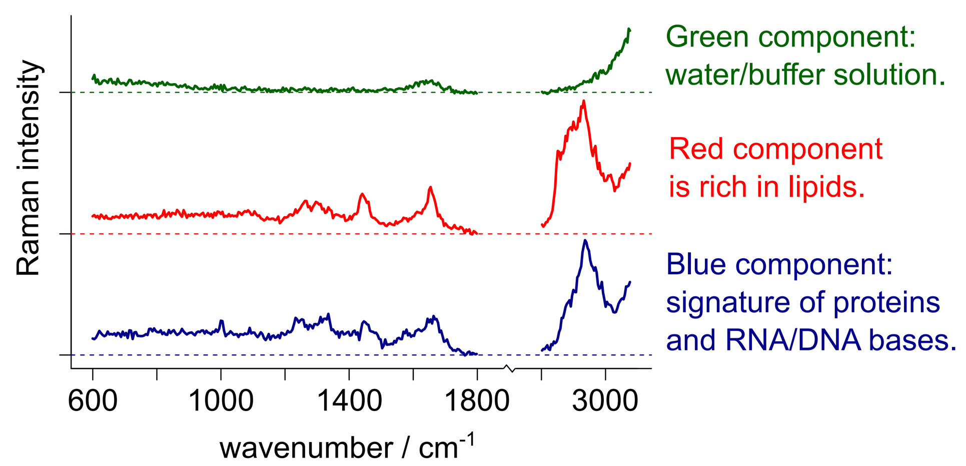


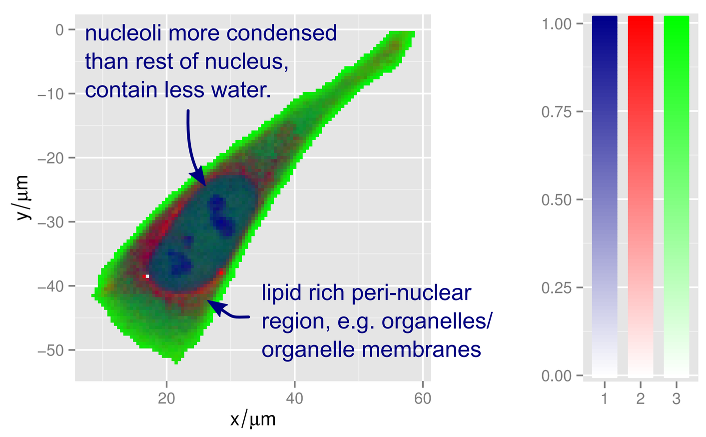
Raman Image of HeLa Cell

Data Set:

- Raman spectra of HeLa cell
- Excitation: 5 mW @ 488 nm, 0.5 s/spectrum
- Spectra: 600 – 1800 + 2800 – 3075 cm^{-1}, 314 bands (after pre-processing)
- Area: 60 × 60 µm, step size 0.5 µm
- For details see reference [HeLa Cell].

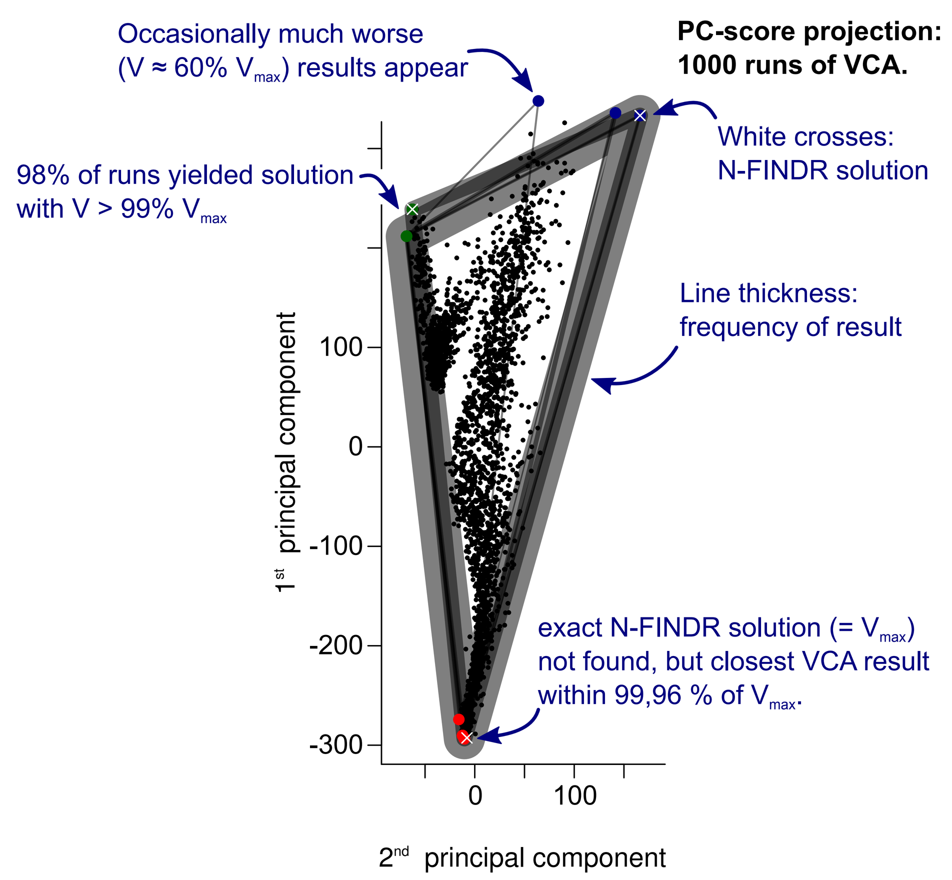
N-FINDR with $m = 3$ endmembers





- Solution is stable: Identical results for 100 runs with random initialization

VCA Results $m = 3$ endmembers



- VCA is expected to be less stable than N-FINDR: no refinement of tentative vertices
- VCA faster than Winter's N-FINDR, but advantage small for improved algorithms.

R package `unmixR`

Conor McManus implemented N-FINDR [Winter, Dowler] and VCA [Nascimento, Lopez] algorithms as R package `unmixR`. He was supervised by Claudia Beleites, Simon Fuller and Bryan Hanson.

Claudia Beleites now maintains the package with help by Bryan Hanson.

The package is available at
`http://github.com/Chathurga/unmixR`

References

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