# unmixR: Hyperspectral Unmixing in *R*

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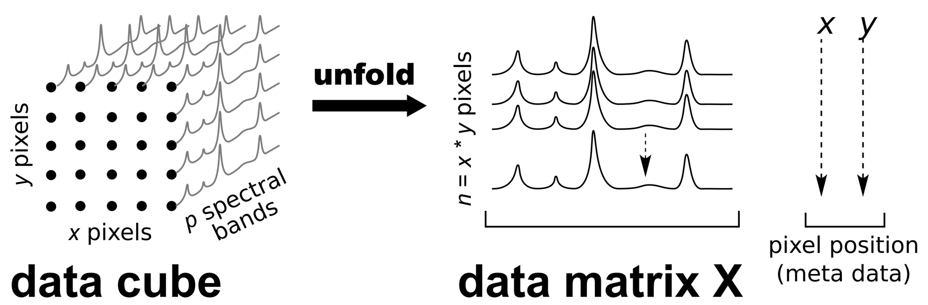
## Hyperspectral Imaging

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



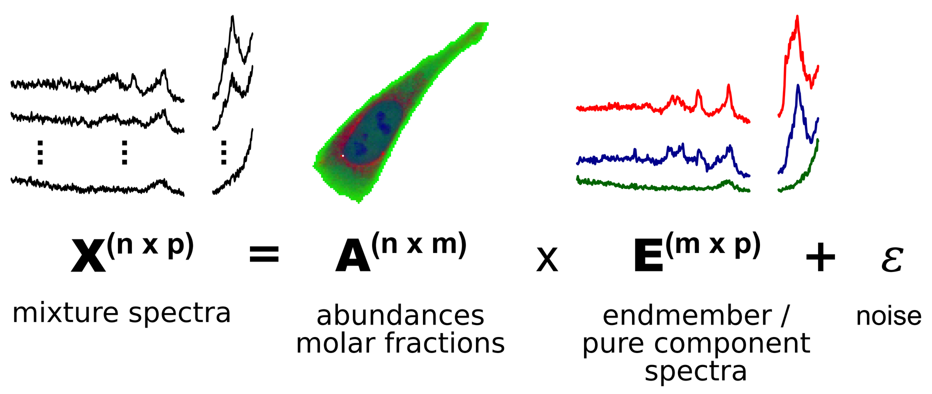

**Applications:** remote sensing/ airborne or satellite land imaging, biomedical microspectroscopy and art history investigations

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

## Spectral Unmixing

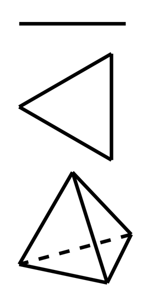
Identify $m$ pure component spectra in data, then derive respective concentrations.

**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:**

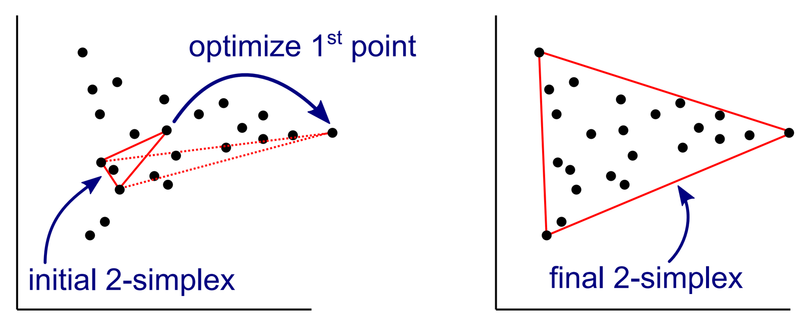
- Data consists of *mixture* spectra
- Spectra of pure components are available somewhere in the data ***X***
- Not too much noise on measurements (possibly after PCA)
- (Other methods relax assumptions 2 and 3)
- Number of pure components $m$ ("chemical rank") provided by user input
- Abundances subject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

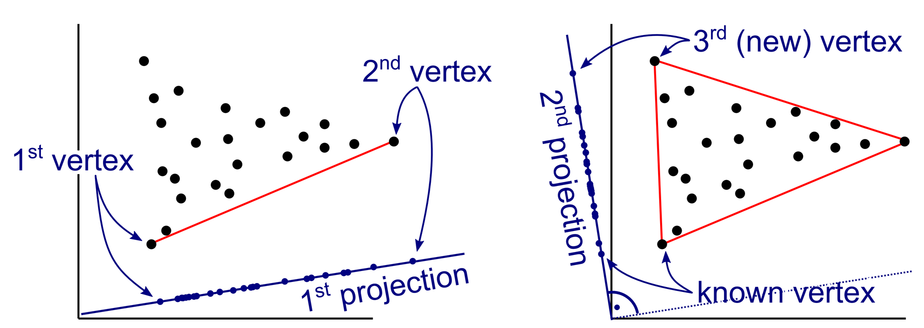
   Iterate/refine until convergence
4. Return corresponding spectra of ***X*** as endmembers
5. `predict` abundances by non-negative least squares [nnls] on found endmembers




## 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

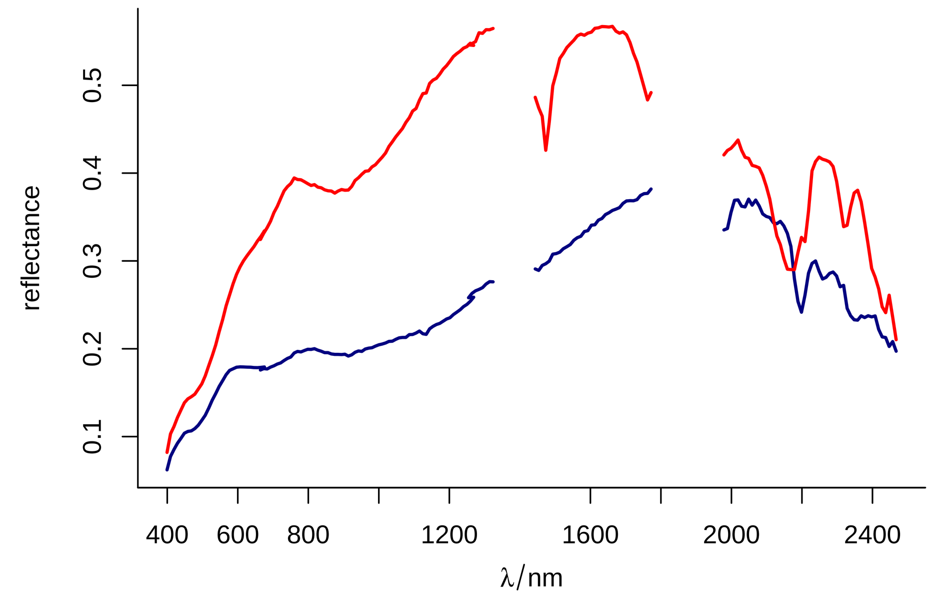
**Data Set:**

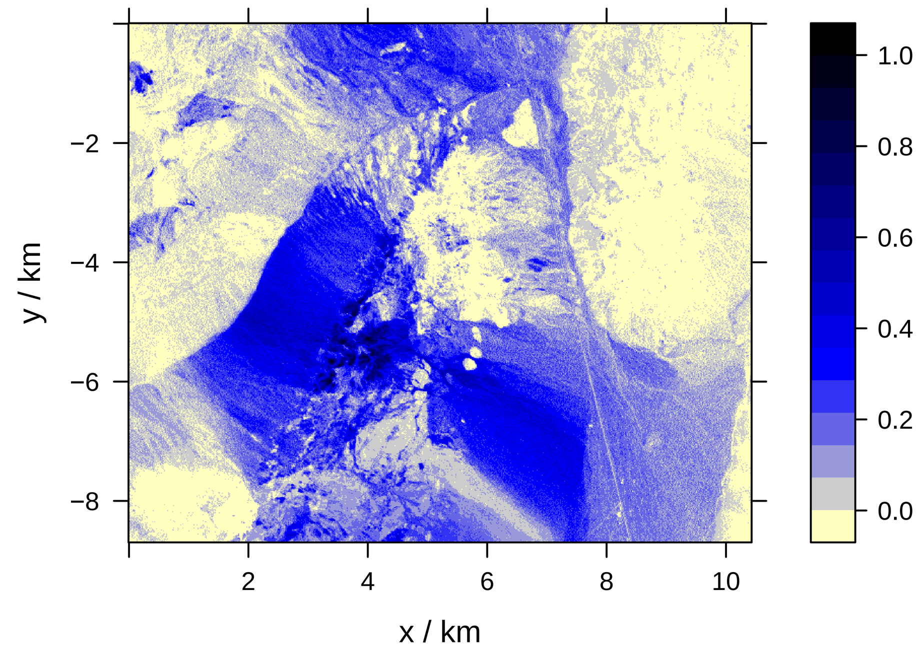
- Acquired by NASA's Airborne Visible/ InfraRed Imaging Spectrometer
- of mining region in the south of Nevada/USA
- 45 × 10 km (300 000 pixel subimage shown)
- 250 - 4 000 nm (224 spectral bands)
- Well-known ground truth

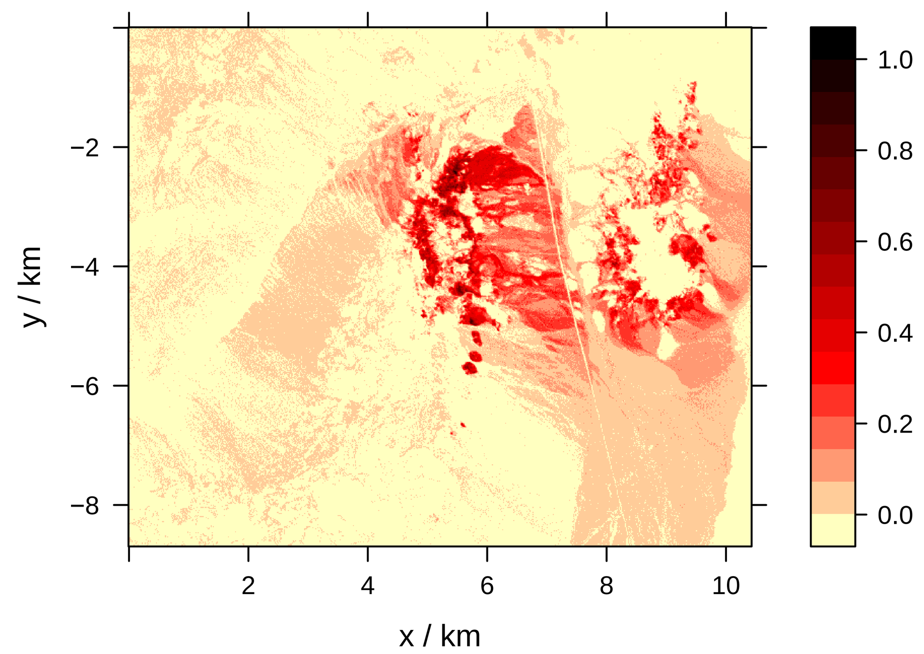
### N-FINDR with $m = 19$ endmembers

As example, we show 2 components identified as

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



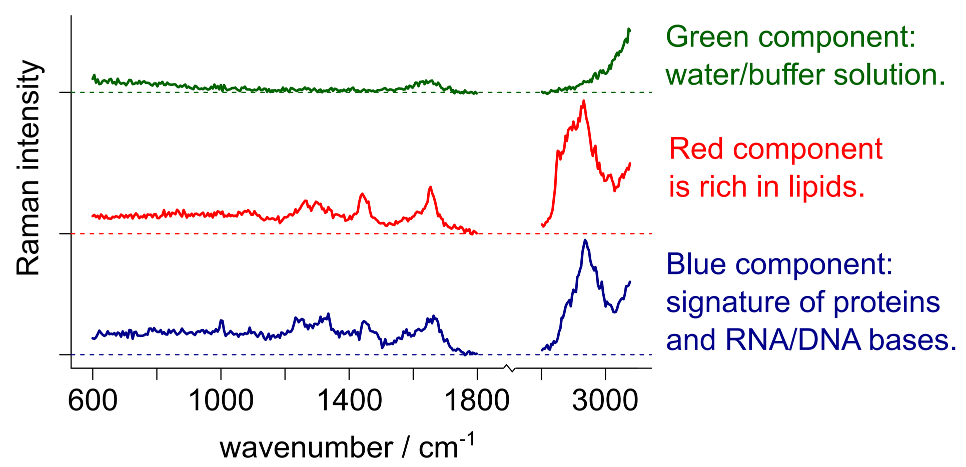



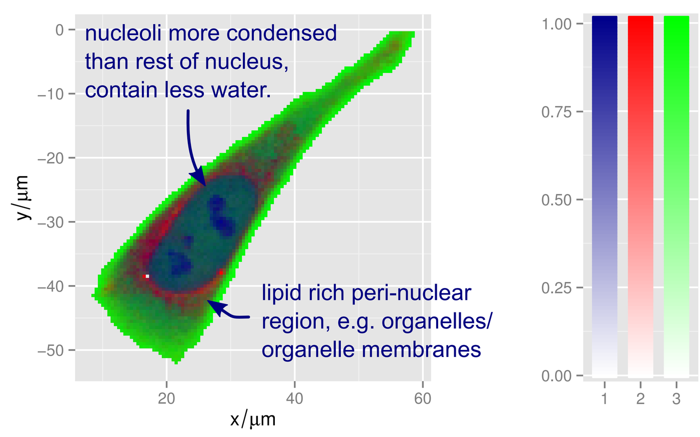

## Raman Image of HeLa Cell

**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].

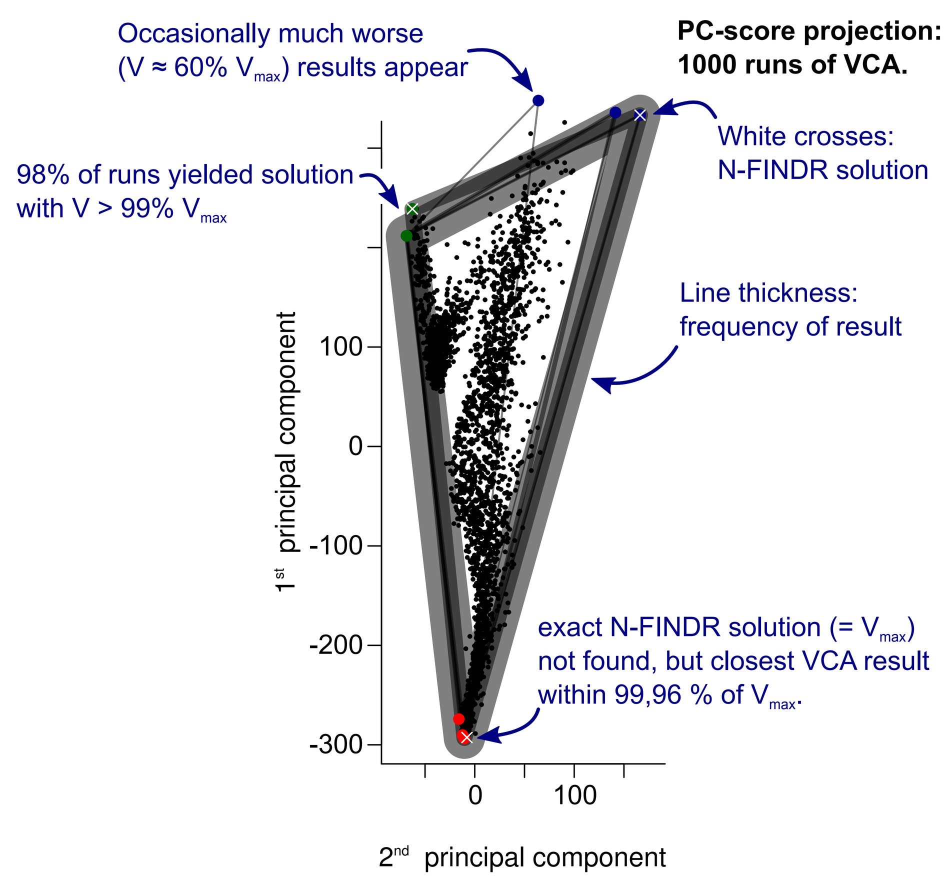
### N-FINDR with $m = 3$ endmembers




- 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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**Dowler** SW *et al.*: Reducing the complexity of the N-FINDR algorithm for hyperspectral image analysis., IEEE Trans Image Process, 22, 2835–2848 (2013). DOI: 10.1109/TIP.2012.2219546

**Nascimento** JMP *et al.*: Vertex Component Analysis: A Fast Algorithm to Unmix Hyperspectral Data, IEEE Trans Geosci. Rem Sens, 43, 898–910 (2005). DOI: 10.1109/TGRS.2005.844293 Iden

**Lopez** S *et al.*: A Low-Computational-Complexity Algorithm for Hyperspectral Endmember Extraction: Modified Vertex Component Analysis, IEEE Geosci Rem Sens Lett, 9, 502-506 (2012). DOI: 10.1109/LGRS.2011.2172771

**Cuprite:** AVIRIS data: `http://aviris.jpl.nasa.gov/data/free_data.html`, spetroscopic and geological information: `http://speclab.cr.usgs.gov/PAPERS/cuprite.clark.93/mineral_map.html`, spetroscopic reference: Clark RN *et al.*: USGS digital spectral library splib06a: U.S. Geological Survey, Digital Data Series 231 (2007).

**HeLa Cell:** Hedegaard M *et al.*: Spectral unmixing and clustering algorithms for assessment of single cells by Raman microscopic imaging, Theor Chem Acc, 130, 1249–1261 (2011). DOI: 10.1007/s00214-011-0957-1

**hyperSpec:** a package to handle hyperspectral data sets in R, Beleites C & Sergo V, Ver. 0.98-20140612 (2014).

**nnls:** The Lawson-Hanson algorithm for non-negative least squares, Mullen KM & van Stokkum IHM, Ver. 1.4 (2012).

**lattice:** Multivariate Data Visualization with R, Sarkar D, Springer (2008). Ver. 0.20-29

**ggplot2:** Elegant Graphics for Data Analysis, Wickham H, Springer (2009). Ver. 1.0.0

## Acknowledgments

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