unmixR: Hyperspectral Unmixing in *R*

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Hyperspectral images are 3D data sets collected over an x, y grid, where the pixel at each x, y is composed of a spectrum. In hyperspectral unmixing, such a data set $\mathbf{X}$ composed of n observed spectra with p wavelengths or spectral bands is decomposed to identify the pure component spectra. Such data sets are found in airborne land imaging studies, biomedical and art history investigations as well as time series (kinetics) of chemical reactions. The spectra are typically visible, infrared, near-infrared, Raman spectra or mass spectrometric data sets.

Each spectrum is assumed to be a linear mixture of a limited number m of pure component spectra, the so-called endmembers. m is also referred to as chemical rank of the spectra matrix $\mathbf{X}$. Endmembers are suitable for direct interpretation in the domain of the study (e.g. Raman spectra of cancerous tissue, reflectance spectra of minerals) and the goal is to identify them. The spectra matrix $\mathbf{X}^{(n \times p)}$ can be thought of as a sum:

$$\mathbf{X}_{np} = \sum_m \mathbf{A}_{nm}\mathbf{E}_{mp} + \varepsilon \qquad \text{or in matrix notation:} \qquad \mathbf{X}^{(n \times p)} = \mathbf{A}^{(n \times m)}\mathbf{E}^{(m \times p)} + \varepsilon \tag{1}$$

Where n is the number of spectra and m is the number of endmembers. Thus, $\mathbf{E}_{mp}$ is the m^{th} endmember spectrum composed of p bands, and the abundances A_{nm} give the contribution of the m^{th} endmember to the n^{th} sample spectrum. ε is (Gaussian) noise. The abundances $\mathbf{A}$ can be depicted in a mixture diagram of the m components which forms a $(m-1)$-simplex. Thus the spectra $\mathbf{X}$ lie in a $(m-1)$-simplex. If pure component spectra of all m components are available in the data and the noise level is low, the decomposition given above can be obtained by finding the corners of the $(m-1)$-simplex in $\mathbf{X}$.

N-FINDR achieves this by first projecting the data into $(m-1)$-dimensional space, usually by PCA. Starting from a set of m (randomly chosen) potential endmembers, an iterative procedure to maximize the volume of the simplex is used: $m-1$ endmembers are kept fixed and the simplex volume is maximized by varying the remaining point. This is in turn done with each corner of the simplex until a stable solution is reached.

Vertex component analysis (VCA), in contrast, projects the spectra onto an orthogonal set of m axes and chooses the extreme points as endmembers.

Physically, both $\mathbf{E}$ and $\mathbf{A}$ are subject to non-negativity constraints as $\mathbf{E}$ takes the role of pure component spectra and $\mathbf{A}$ correspond to concentrations or molar fractions. If $\mathbf{A}$ is formulated as molar fraction, the rows of $\mathbf{A}$ must sum to 1. Thus, once the endmember spectra are found, $\mathbf{A}$ is obtained by a non-negative least squares fit of the remaining spectra.

unmixR (`http://github.com/Chathurga/unmixR`) provides different N-FINDR and VCA algorithms as an *R* package. The Google Summer of Code 2013 supported Conor McManus to implement the algorithms, supervised by Claudia Beleites, Simon Fuller and Bryan Hanson. Claudia Beleites now maintains the package. Claudia Beleites thanks the BMBF for funding via the project "RamanCTC" (13N12685).