A New N-FINDR Algorithm and the unmixR Package for Spectral Unmixing

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In spectral unmixing, a data set $X$ composed of $n$ observed spectra of chemical mixtures with $p$ wavelengths or spectral bands is decomposed to identify pure component spectra. Each spectrum is assumed to be a linear mixture of a limited number $m$ of pure component spectra, in this context also referred to as endmembers. $m$ is also known as chemical rank of the spectra matrix $X$. In matrix notation, this is the bilinear model

$$X^{(n \times p)} = A^{(n \times m)} E^{(m \times p)} + \varepsilon.$$ 

The concentrations or abundances $A$ can be depicted in the mixture diagram of the $m$ components, forming an $(m-1)$ simplex. Also the spectra $X$ lie in an $(m-1)$ simplex. If noise is low and pure component spectra are present in the data, this decomposition can be obtained by finding the corners of the simplex. Two well-known algorithms to achieve this are N-FINDR \cite{1} and Vertex Component Analysis \cite{2}. N-FINDR is a rather slow iterative algorithm. While VCA is much faster, we find that it does not always yield as good decompositions. A number of improved algorithms are known \cite{3, 4}. In addition, we present a new N-FINDR algorithm that uses a fast projection and is particularly suitable for implementation in high-level languages such as R or Matlab where optimized and parallelized BLAS routines can be used but loops are computationally expensive.

unmixR (http://github.com/Chathurga/unmixR) provides different N-FINDR and VCA algorithms as an R package. We demonstrate the correctness of the algorithms by reproducing the results of \cite{5}.

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References


