The Phasor Approach to Multivariate Curve Resolution

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1 Introduction

In multivariate curve resolution, the identification of the number of components and of the purest information underlying the data at hand remains a real challenge in practice [1]. Existing approaches proposed for this purpose, such as principal components analysis (PCA)-based algorithms (e.g. pixel purity index [2], vertex component analysis [3]) or simple-to-use interactive self-modelling mixture analysis (SIMPLISMA), require some parameters to be chosen which overall turns into user- dependent results.

A phasor is a two-dimensional polar plot representing the values of the sine-cosine transforms of a signal provided by the Fast Fourier transformation (FFT). Originally, the phasor analysis was proposed as a way to visualize the angular difference of two sinusoidal waveforms in electronics [4]. It was later adapted to analyze time-resolved fluorescence data [5].

Here, we propose to use the phasor approach to visualize the information measured for each sample of a spectral dataset as a point in the bidimensional phasor plot [5]. The phasor transform has nice features that can be exploited for a more robust and automatic multivariate curve resolution: it is fast, it can be performed independently on each signal (it does not need to process the whole data), and most importantly, it is a linear transformation. It means that the phasor of a mixed signal is a linear combination of multiple individual phasors, which represent the individual species. Under proper normalization, pure(st) spectra of a mixture are thus to be found at the vertices of a convex geometry in a two-dimensional phasor plot, whatever the number of components in the spectral mixture.

2 Material and methods

We consider for illustration a “mixture” data set underlain by four “pure” components (see Figure 1a). The corresponding scores in a normalized principal component subspace are plotted. It is clear that the convex geometry of the four-component data cannot be captured in a bi-dimensional scores plot (see Figure 1b).

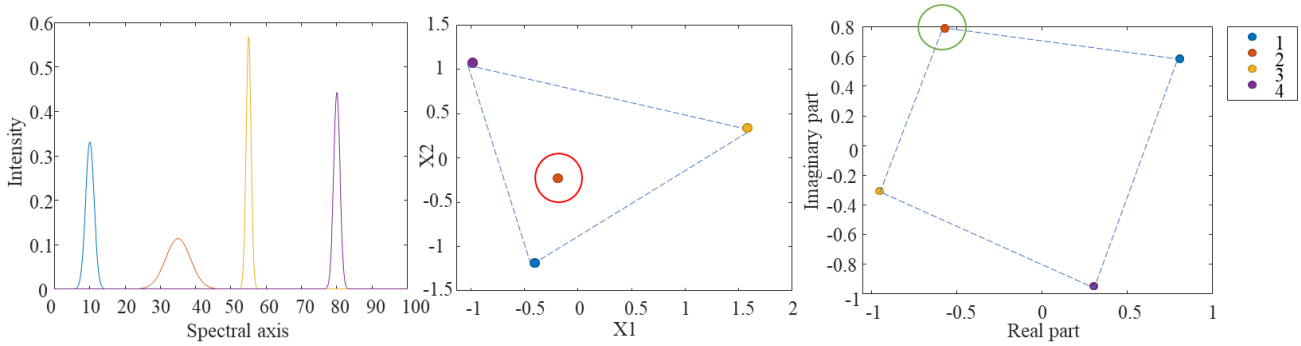

Figure 1 – (a) Four-component data (b) scores in a normalized PCA subspace and (c) in the Fourier subspace.

By contrast, a phasor representation of the same data results in a four-vertices geometry, from which pure spectra can be identified by a geometrical approach (see Fig 1c). This result is generalizable to a larger number of components and any spectral shape.

3 Results and discussion

Results obtained on a seven-component Raman hyperspectral data will be discussed. (see Figure 2). All corresponding pure pixels can be found on the convex envelope of the data set in the bi-dimensional phasor plot. As a first result, it is interesting to note that the convexity is verified in phasor subspace because the purest spectra will be each time on the outer point of the data cloud obtained in the complex space (green circles on Figure 2).

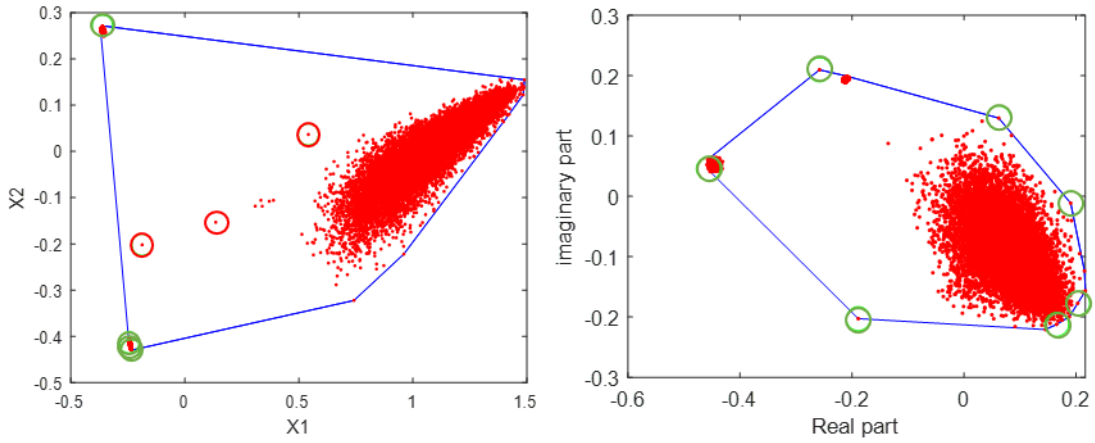

Figure 2: Comparison of the results of spectral identification for the two subspaces (PCA subspace at the right, phasor at the left). The green circles are the purest spectra. It can be seen that seven species can be found in the Fourier space against 4 on PCA subspace.

4 Conclusion

This work suggests that the identification of the purest information encoded in a spectral mixture dataset can be performed more easily and more reliably by computing a phasor transform of the original measurements than by means of PCA. We will discuss this aspect in the framework of MCR-ALS [6-7].

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5 References

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