Exponentials: beautiful functions, useful chemometrics

A. Gomez[1,2], O. Devos[1], R. Vitale[1], A. de Juan[2], C. Ruckebusch[1]
[1]*Dynamics, Nanoscopy and Chemometrics (Dynachem)*, LASIRE, CNRS, U Lille
[2]*Chemometrics group*, U BARCELONA
Cyril.ruckebusch@univ-lille.fr

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1 Introduction

Exponential functions have very interesting properties which are widely used in all fields of science. Very well-known examples of the utility of exponential functions are the modelling of the growth of biological organisms, decays of radionuclides, first-order chemical reactions or intensity decays of the emission of luminescent materials. In signal processing, the use of exponential functions is ubiquitous as for discrete Fourier transformation. In this presentation, some applications of the mathematical properties of exponential functions in chemometric analysis are discussed.

2 Methods

The main mathematical feature of the exponential function is that a constant change in the independent variable *x* gives the same proportional change in the dependent variable *y*, for all values *x*, i.e. the exponential function equals its own derivative. For a decaying exponential signal, this translates into the property in Eq. 1.

$$\left(e^{\frac{-t}{\tau}}\right)' = -\frac{1}{\tau}\left(e^{\frac{-t}{\tau}}\right) \qquad (1).$$

The exponential function also satisfies other interesting features, such as the translation property in Eq. 2. By applying lags of different durations to an exponential decay, the pre-exponential amplitude factor varies while the characteristic time remains constant.

$$e^{\frac{-(t-t_0)}{\tau}} = e^{\frac{-t}{\tau}} e^{\frac{t_0}{\tau}} = \alpha e^{\frac{-t}{\tau}} \qquad (2).$$

The linear relationship in Eq. 2 has actually been exploited in chemometrics to produce and analyze three-way data arrays from two-way matrices of multi-exponential signals. Direct exponential curve resolution analysis (DECRA) [1] was introduced in 1997 to resolve series of NMR mixture spectra in which the contribution of the components varies with a decaying exponential. This procedure was later called *Slicing* [2] and combined to parallel factor analysis (PARAFAC). Recently, the approach has also been extended to multivariate curve resolution - alternating least squares (MCR-ALS) to allow unmixing signals that are combinations of exponential and non-exponential component profiles [3].

Another interesting property is related to the convolution of exponential signals *f(t)* with a kernel function *g(t)*, as in Eq. 3.

Consider $f(t) = Ae^{\frac{-t}{\tau}}$

and $g(t)$ a kernel function with $t = 0$ outside of $[0, m]$

it can be shown that:

$$y(t) = f(t) * g(t) = \int_{-\infty}^{+\infty} f(t-\delta)g(\delta)\,d\delta = \lambda f(t)\ for\ t \geq m \qquad (3).$$

Equation 3 means that the characteristic time τ of the resulting exponential signal *y(t)* is unchanged, and only the preexponential factor is being affected. For multiexponential signals, Eq. 3 translates into the fact that the relative contribution of each individual component to the total signal changes. Thus, by applying a set of kernels to a two-way matrix, somehow *Kernelizing* the data [4], trilinear data sets can be generated and, as for the abovementioned *Slicing* approach, subsequent trilinear data decomposition can be performed.

Additionally, advantage can be also be taken from the property in Eq. (1) to extract and handle instrument response function for "autodeconvolution" of mono-exponential signals, or tail fitting of multi-exponential signals [4].

3 Results and discussion

We will discuss the results obtained applying the data *Tensorization* approaches mentioned above for analyzing time-lapsed and time-resolved fluorescence microscopy images of biological samples. Emphasis will be on the versatility of hybrid bilinear-trilinear MCR-ALS data decomposition models. For the sake of illustration, we provide in the Figure below the results of a fluorescence microscopy photobleaching/recovery live-cell experiment generating a four-way slicing data set and analyzing patches of the data with three-component models.

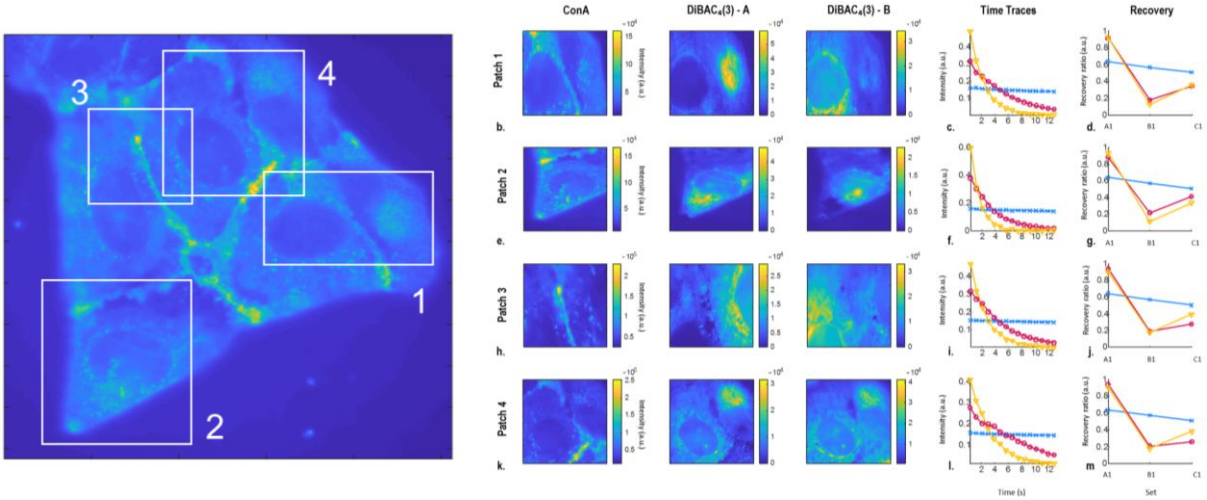

Figure: Multilinear slicing for exponential unmixing of time-lapse photobleaching/recovery fluorescence images [5].

4 References

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