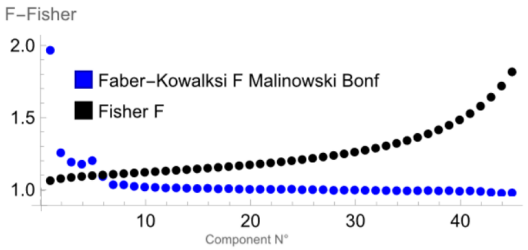
Enhancing Data Understanding: An Integrated Approach using multivariate statistical techniques in Time-resolved Spectroscopy, case of study: Trans-Cl-[Ru(X,X')-dimethyl-2,2'-bipyridine)$(CO)_2Cl_2$].

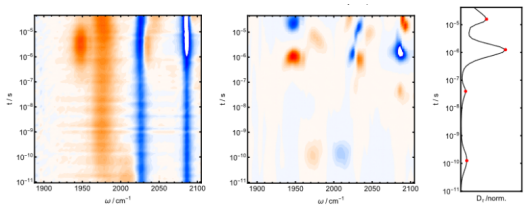
S. Aranda[1], L. Tatarashvili[1], K. Oppelt[1], P. Hamm[1]*

[1]Department of Chemistry, University of Zurich, Zurich, Switzerland

Since the rise of the computing power, the application of mathematical techniques for data analysis has become indispensable across various scientific disciplines. Prior to engaging in exploratory analysis, a comprehensive understanding of the data is important to mitigate the risk of making wrong conclusions or fabricating data, all of which can undermine the acquisition of meaningful insights. The primary objective of this work is to present Singular Value Decomposition (SVD) as a widely adopted and well-established analytical tool, utilized for several decades. The subjectivity involved in discriminating between chemical and mathematical information can be mitigated through the employment of lesser-known mathematical methodologies that facilitate the imposition of statistical boundaries on such data [1].



Additionally, the Shannon's Maximum Entropy Method (MEM), extensively employed in the deconvolution of individual chemical species spectra [2], is used to extract valuable information from the data. Furthermore, we explore the Lifetime Analysis (LTA) technique, an infrequently utilized method grounded in MEM principle to extract information from the kinetics point of view. These methodologies are exemplified through their application to a series of experiments conducted on a Ruthenium bipyridyl complex employing ultrafast time-resolved pump-probe spectroscopy under varying conditions. The significance of this work extends beyond this specific experimental data, as these tools can be effectively applied to other types of multidimensional datasets encompassing diverse domains such as microscopy images, electrochemical spectra, and multidimensional NMR, among others.



[1] Widjaja, Garland, *J Comput Chem,* 2002, 23, 911 - 919
[2] Lorentz-Fonfria, Kandori, *Applied Spectroscopy,* 2016, 60, 407 - 417