

# Smart Sampling and Probing

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*“The eternal mystery of the universe is its comprehensibility...”*  
(by Albert Einstein)

## Abstract

Water quality check and quality control procedures are very common in nowadays environmental studies. Spectroscopic techniques such as UV-vis, fluorescence and NIR have been extensively used for these purpose with several analytical advantages such as, for example, minimal sample volume requirements, fast response time, very low analytical costs and possibility for automatic in-situ monitoring studies [1].

Typical for molecular spectroscopy, this type of spectral information consists in several unresolved broad bands, leading to spectra overlap and conducting to severe selectivity problems.

Several Chemometric methodologies, developed in earlies 90's, such Partial Least Squares (PLS), were essentially devoted to allow for simultaneous calibration and quantification of several analytes in complex matrices based on spectral information.

However, when dealing with real systems, Chemometric techniques faces a basic limitation in terms of deciding the number of independent contributions that are present in a given system under evaluation.

In a recent work [2] we discussed the application of Principal Component Analysis (PCA) and Principal Object Analysis (POA) in unsupervised analysis of complex systems.

In one hand, PCA accesses system information by focusing it attention in terms of the analysis of data variability, and allows to decompose all information into orthogonal contributions.

By opposite, POA is focused in objects, related with system composition in terms of analytical contributions. By this methodology its possible to deconvolute a complex system response in terms of analytes present.

In this work we go a little further in terms of diagnosing underling information in complex systems. By doing this diagnose we are able to perform “smart sampling and probing” - easily and correctly decompose information, predict which variables are not significantly contributing with relevant information and evaluating if the number of collected samples is already suitable for a given analytical purpose.

## References

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