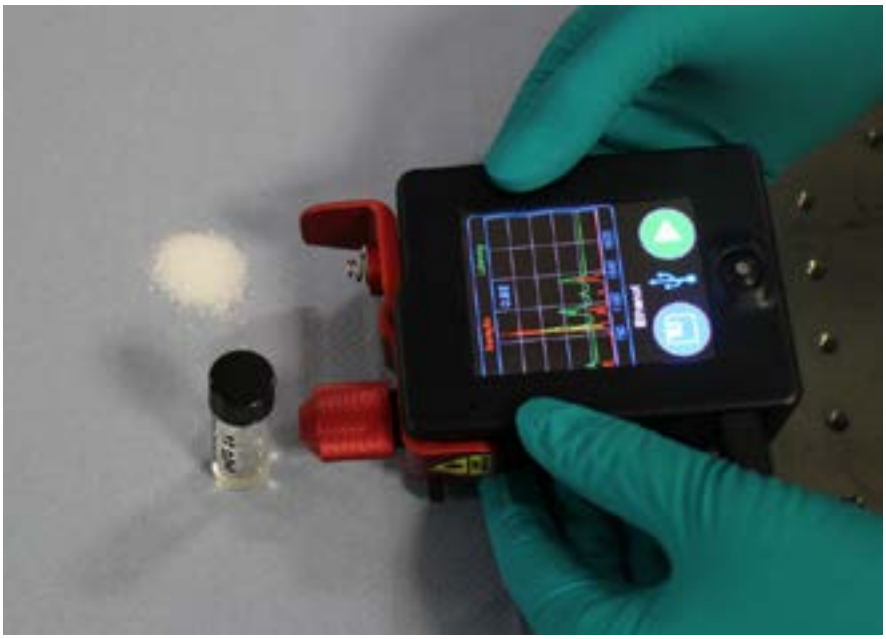
University Defence Research Collaboration in Signal Processing

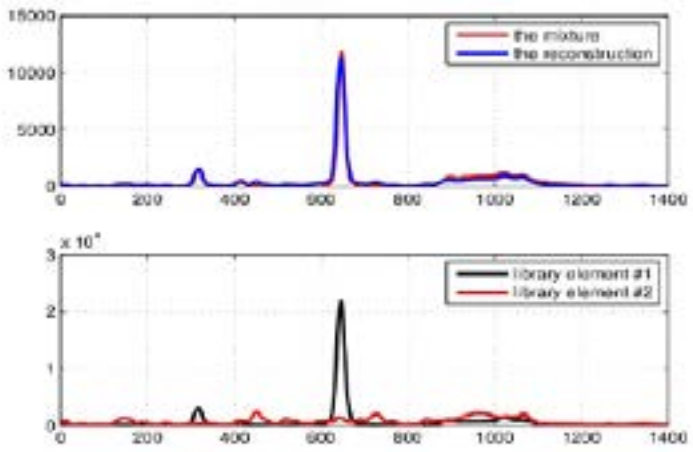
Edinburgh Consortium White Paper

A Sparsity Based Raman Spectral Decomposition

Introduction



Raman spectroscopy is an established and successful method for identifying unknown materials. The technique exposes materials to a narrow band laser beam and measures the scattered light of different energies to provide a unique signature belonging to that chemical. The conventional analysis methods are based on comparing the measured spectrum with a reference spectral library of known chemicals to find the best match. Raman spectroscopy has been used for many applications in Biology, Chemistry and Defence. The success of Raman spectroscopy, has encouraged the European Space Agency (ESA) to plan to send a specially designed Raman spectrometer to Mars in a near future mission. In the defence sector, Raman spectrometers have been demonstrated for identifying unknown toxic and explosive materials.



While it would be a mathematically easy task to identify a single spectrum from the library, the problem is more challenging when the sample is composed of a mixture of different chemicals. In this case, the measured spectrum is a composition of the spectral signatures of the existing components, with different weights, corresponding to the percentages of the presence of materials. If we can overcome the mathematical difficulties, we can decompose the spectrum and even identify the target chemicals, when the sample is substantially contaminated with other unimportant materials.

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Fortunately, the new developments in the sparse component analysis help us to simplify the decomposition problem. Such an analysis is based on the fact that at each instance we typically only have a mixture with a few elements of the library. We then use a sparse approximation technique for the Raman spectral decomposition, when the library of the spectra is given and only a few unknown spectra exist. We have proposed such a technique in [1], in which the algorithm can successfully recover the correct mixtures, even though some components have only a 10% contribution, close to measurement noise level.

The technology of making portable Raman spectrometers has had a significant progress in the last years, such that today we can have hand-held spectrum analysers. This demands a low complexity algorithm to run on the embedded platform, which is normally computation and memory restricted. For such an application, we have developed a fast Raman spectral decomposition technique based on a new fast sparse approximation method [2]. This algorithm has already been evaluated with real mixtures in different measurement scenarios with great success and we are currently porting these algorithms to a hand held device.

The proposed method is very fast and close to real time, i.e. computational time of one second on a normal desktop computer. In future work, other constraints like preferential and structured spectral decomposition, are being explored.

The algorithm has been prepared as a Matlab package, which can handle a given library and an input spectrum. A hardware independent C package has been prepared, to run on a low power real-time platform, after linking with the specific I/O handlers.

References:

[1] "A Sparse Regularized Model for Raman Spectral Analysis", D. Wu, M. Yaghoobi, S. Kelly, M. E. Davies and R. Clewes, Sensor Signal Processing for Defence (SSPD), Edinburgh, September 2014.

[2] "Fast Non-Negative Orthogonal Matching Pursuit", M Yaghoobi, D. Wu, M. Davies, IEEE Signal Processing Letters, September 2015.