Extraction of Fundamental Components from Distorted Spectral Measurements

Spectral Data in Monitoring

Spectral data is of great interest to be used in quality monitoring, as it holds a great amount of information that potentially could be used in feedback control.

Essential information in quality monitoring, such as material signatures and concentrations, can be estimated from a sampled spectrum using algorithms similar to Alternating Least Squares or Independent Component Analysis.

Spectral Distortion

A big obstacle in using spectral data is its energy-to-location inconsistency that results from external influences and/or sensor de-calibration. Two frequently observed distortion were studied:

-**Shift**, aka *Frequency Displacement*, reported to be caused by changes in pressure, temperature, or a foreign component.
-**Warp**, aka *Frequency "Stretching"* or *"Shrinking"*, reported also to be caused by a change in temperature.

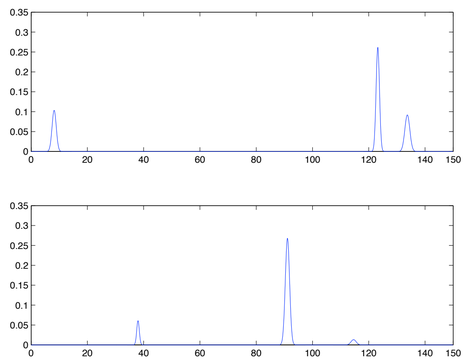
Optimisation Approach

To compensate for the distortion experienced in the data, a sample is defined as a temporary reference of which every other spectrum is aligned to. The alignment procedure aims to find the optimal combination of anti-warp and anti-shift values, with which the spectrum is the most similar to the temporary reference.

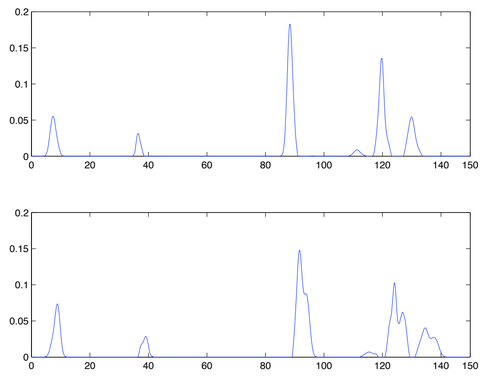
The mean of the values are removed from the all the spectra, to eliminate at most possible all bias experienced from the temporary reference.

Results of Pre-Aligning

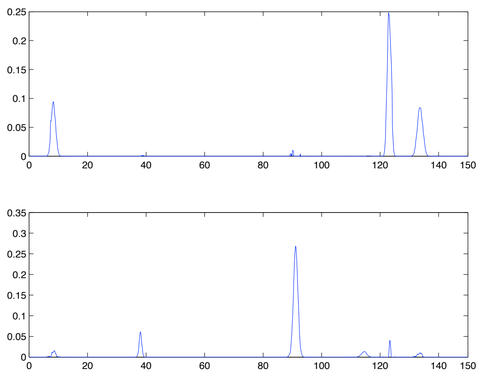
Alternating Least Squares was applied to a data set that experienced severe shifts and warps.



Components of underlying components



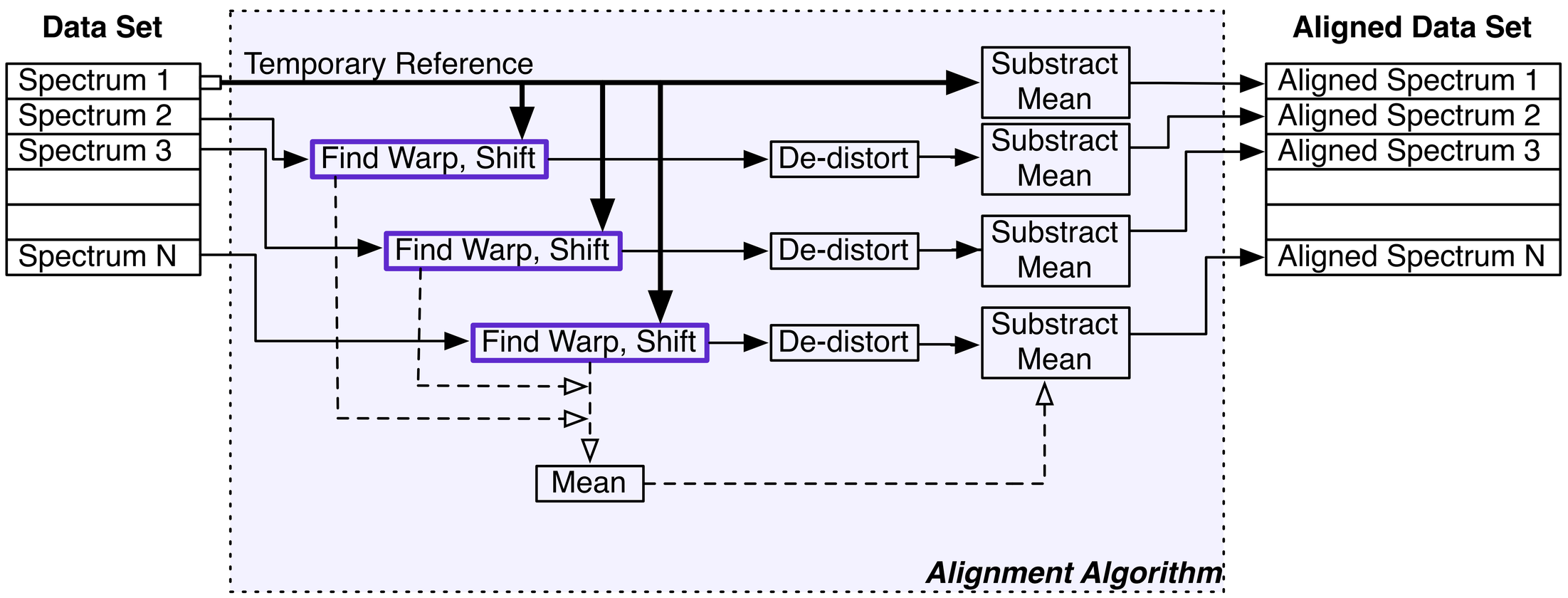
Estimated components from original data set



Estimated components from aligned data set

Conclusion

Sensorial displacement is frequently observed in practical situations, where underlying components of data are of interest to be obtained. Pre-aligning can successfully counter the distortions that plague sampled spectra in the industry. Because of the varied nature of the spectral distortions observed, an optimisation approach is preferred as it is able to consider many types of distortion.



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