MANCHESTER 1824

The University of Manchester

APACT 09

Extraction of Fundamental Components from Distorted Spectral Measurements

Mr. Caleb Rascon
Prof. Barry Lennox
Dr. Ognjen Marjanovic

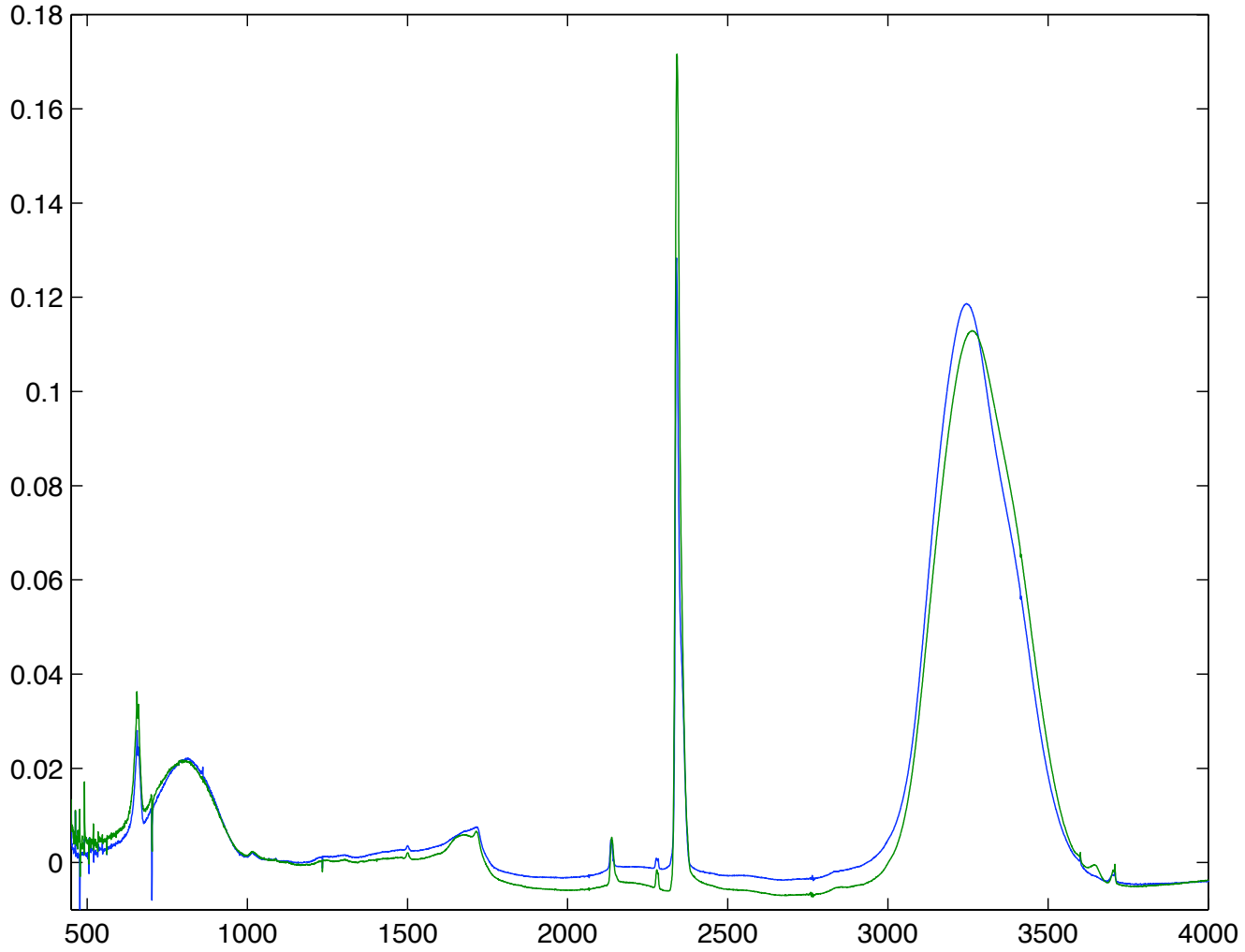
Using Spectral Data in Monitoring

- Crystallisation of active ingredients (Yu et al, 2003)
- Identify material concentrations (Dyrbe et al, 2002)

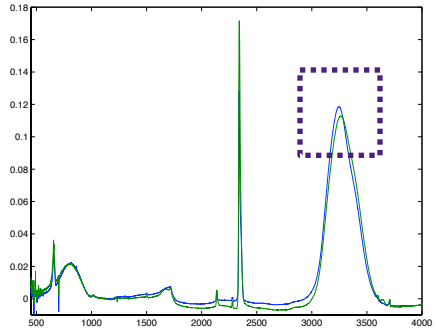
- Component identification
  - Self-Modelling Curve Resolution Methods
    - Alternating Least Squares
    - SIMPLISMA
  - Blind Source Separation
    - Principal and Independent Component Analysis

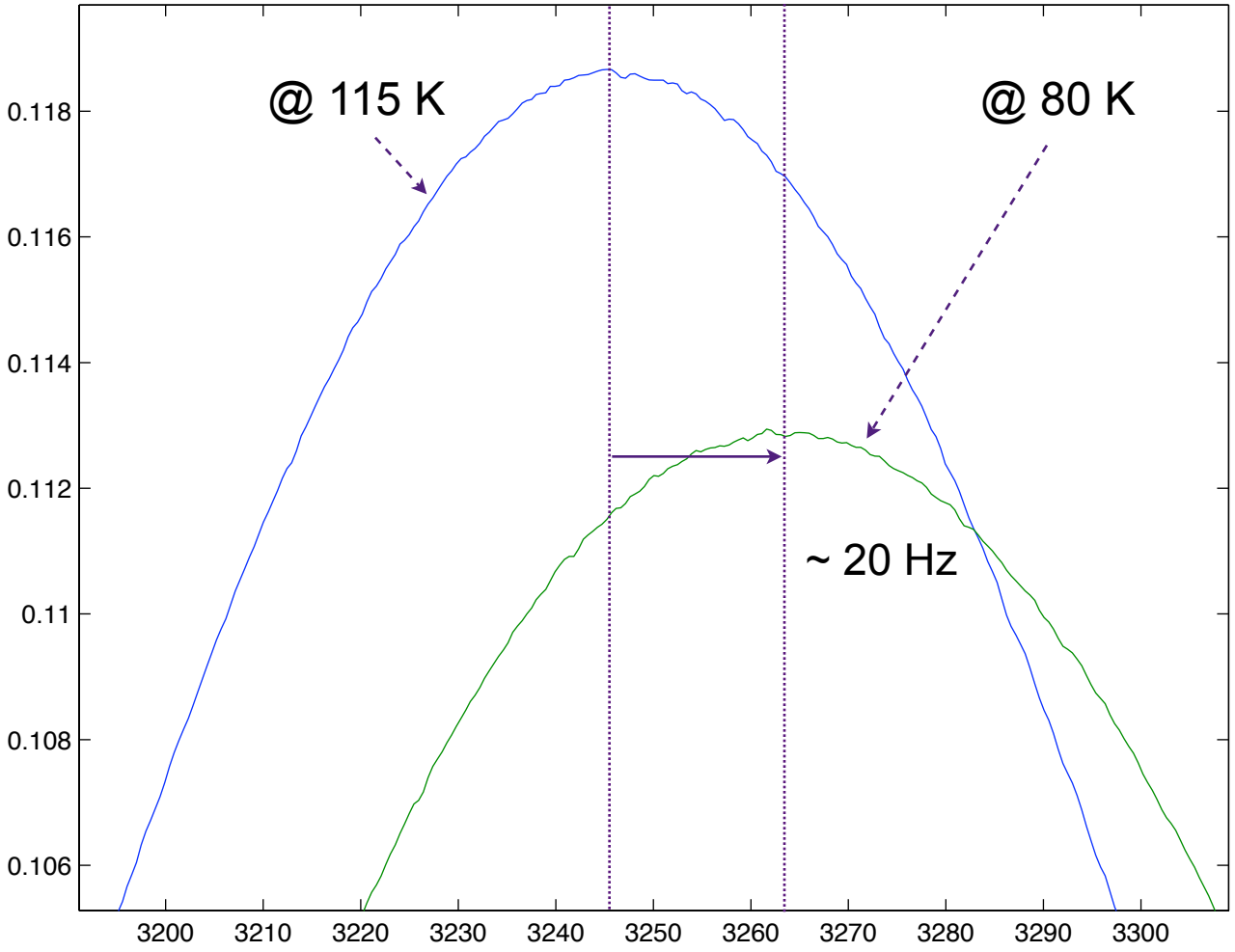
- Viable as observed variables in feedback control
  - Or are they?

Spectral Distortion (Ice Analogs)

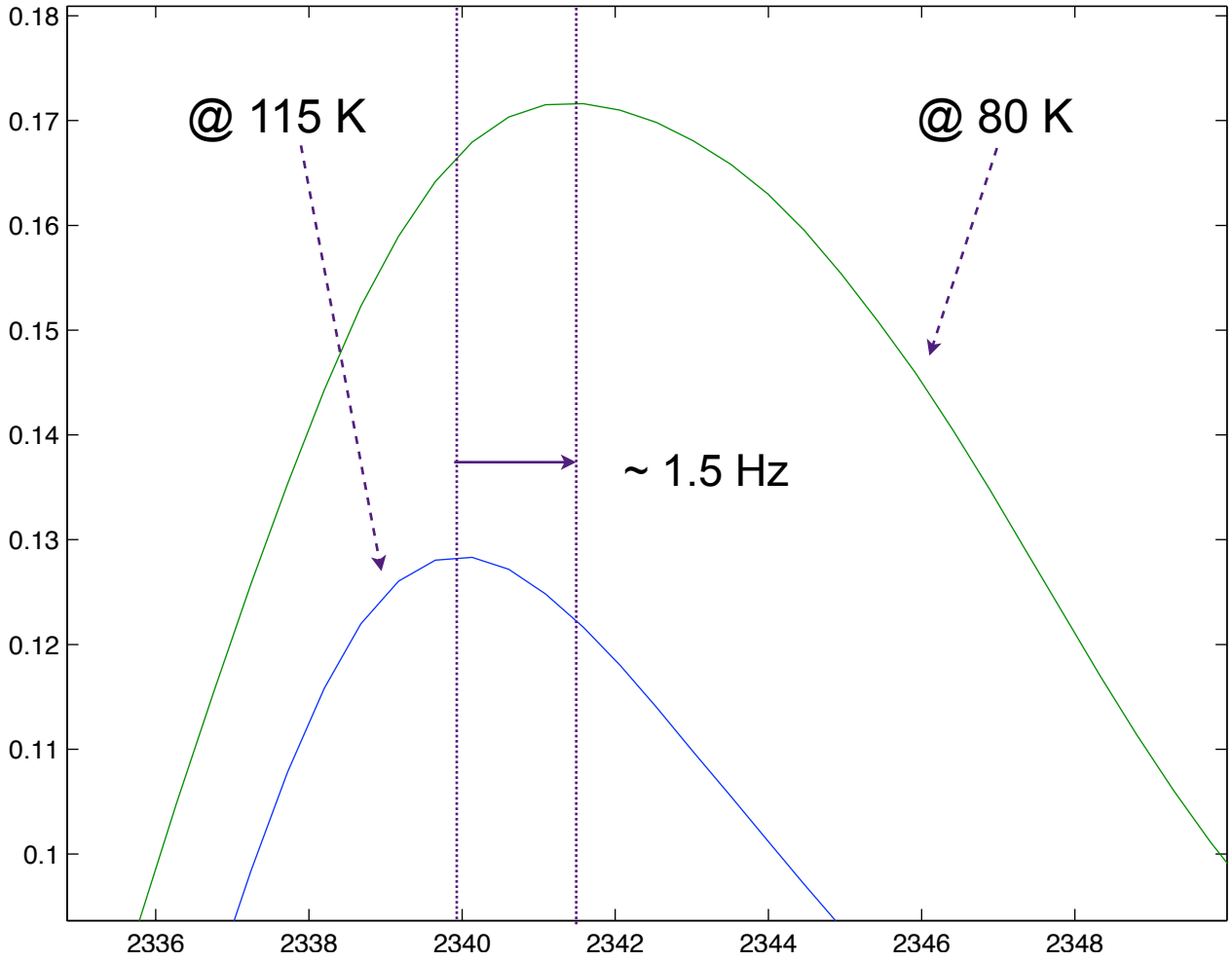


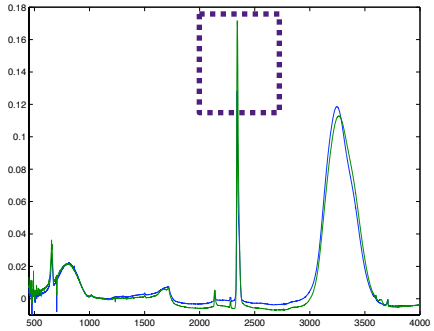
First Component





Second Component





Sources of Spectral Distortion

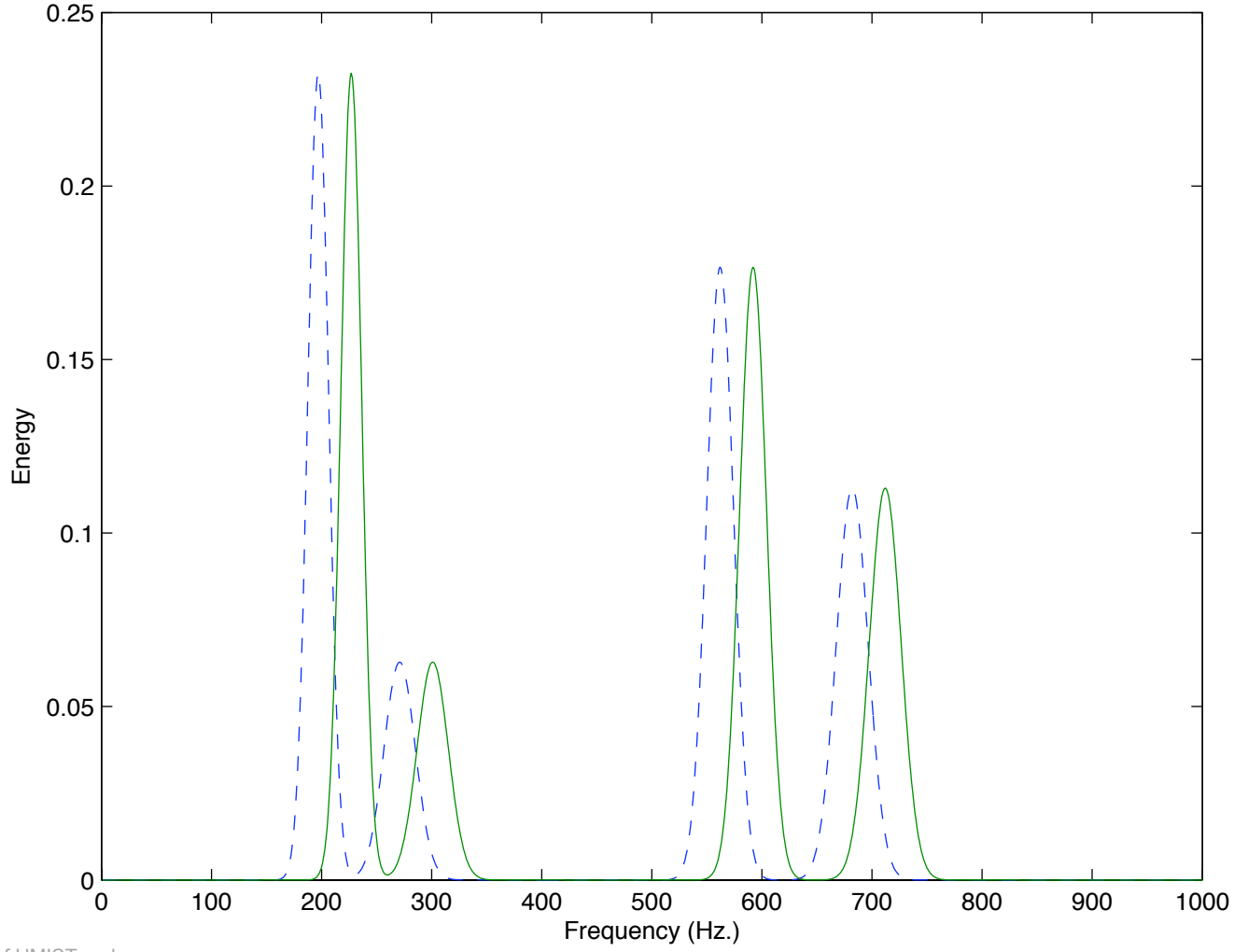
- Temperature changes
- Pressure changes
- Sensor de-calibration
- Foreign components (even external light sources)

- Baggerly et al. (2004) have observed spectral distortion from one instrument to another within the same laboratory.

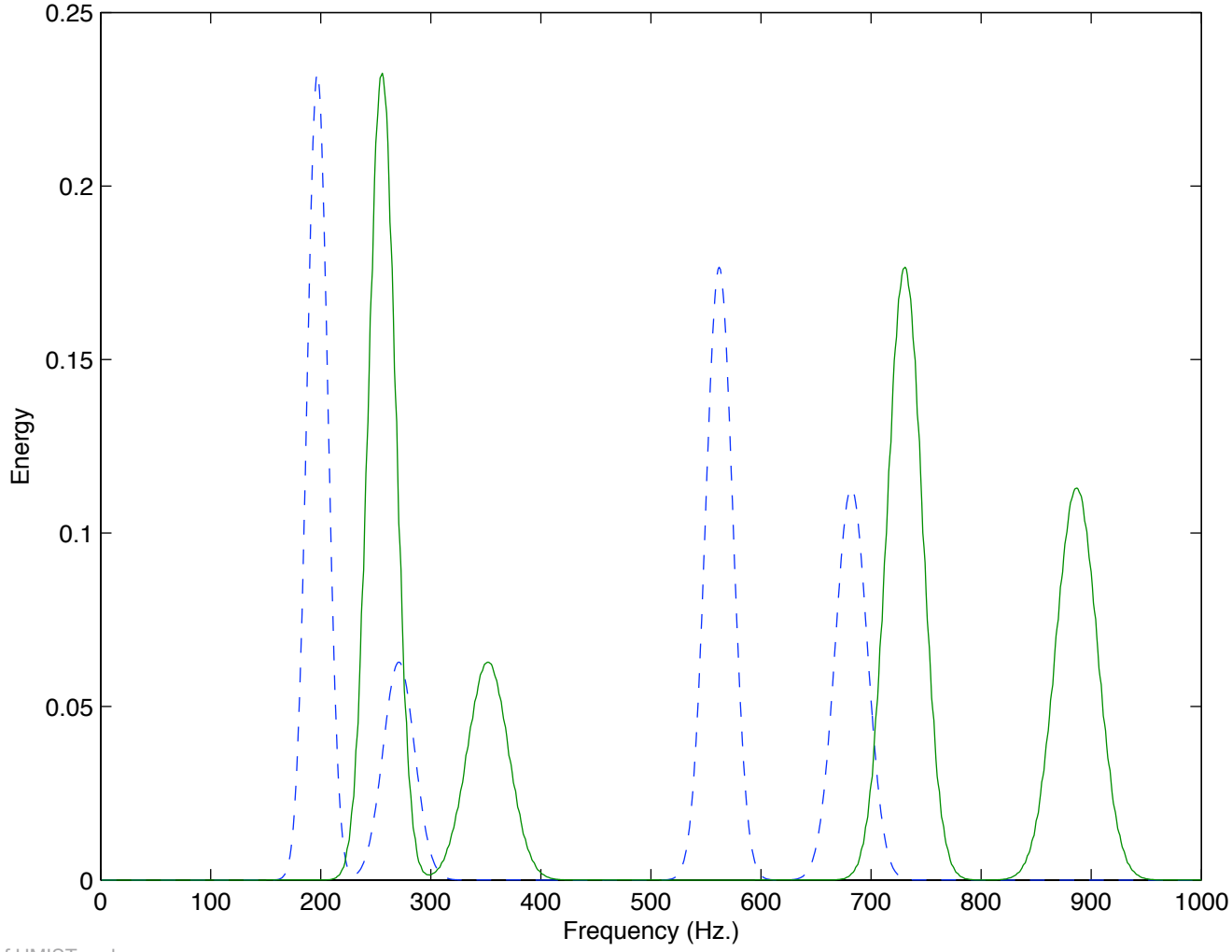
- Most observed:

  -**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.

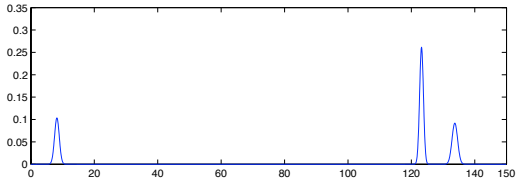
Shift

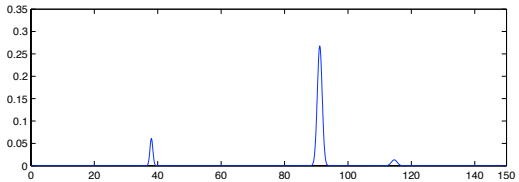

0.25
0.2
0.15
0.1
0.05
0
Energy
0
100
200
300
400
500
600
700
800
900
1000
Frequency (Hz.)

Warp


0.25
0.2
0.15
0.1
0.05
0
Energy
0
100
200
300
400
500
600
700
800
900
1000
Frequency (Hz.)

Effects on Component Identification Methods

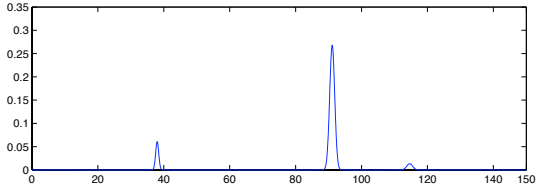


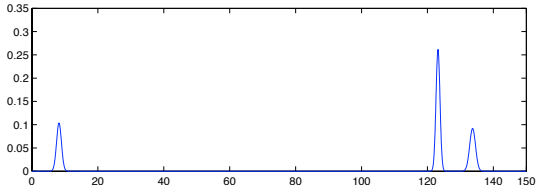


Sources

Data set without shift nor warp

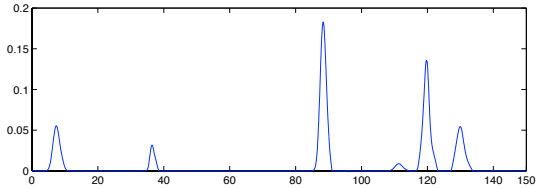
ALS

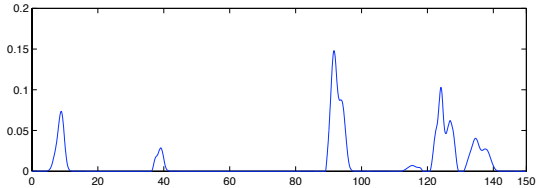




Data set with shifts between [-2 2] Hz and warps between [-5 5] %

ALS

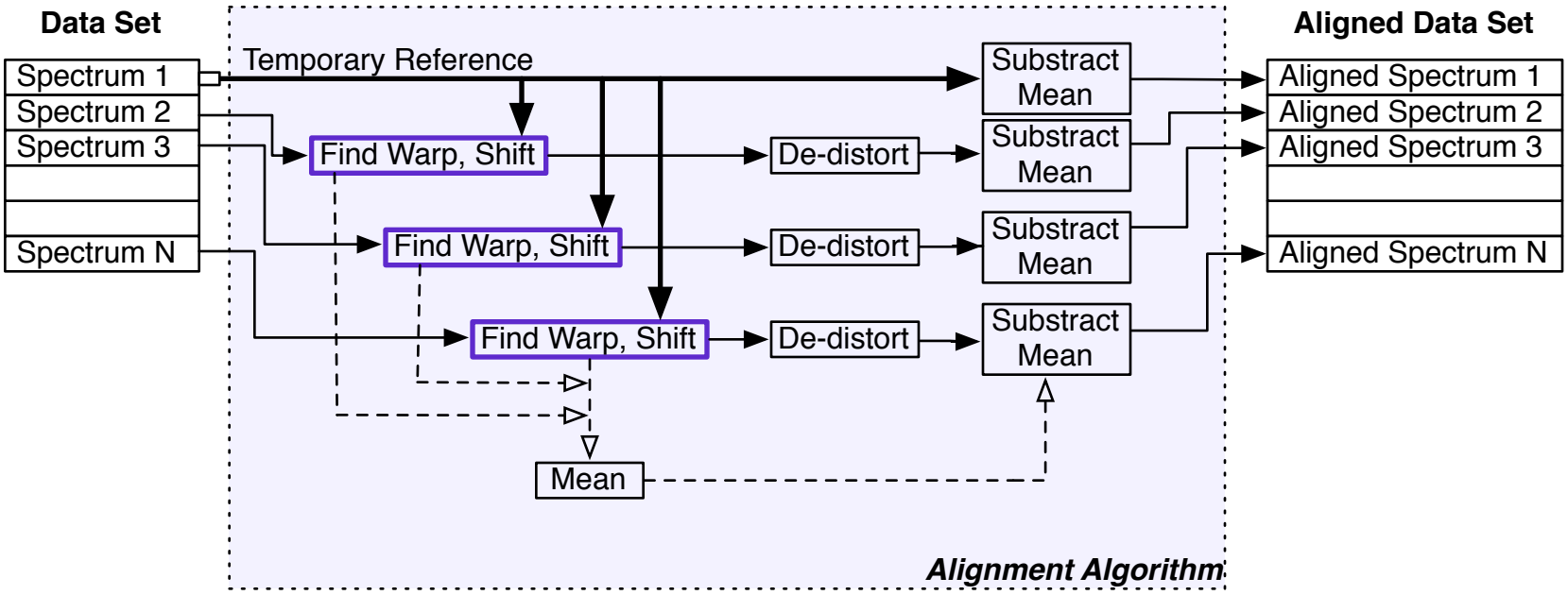




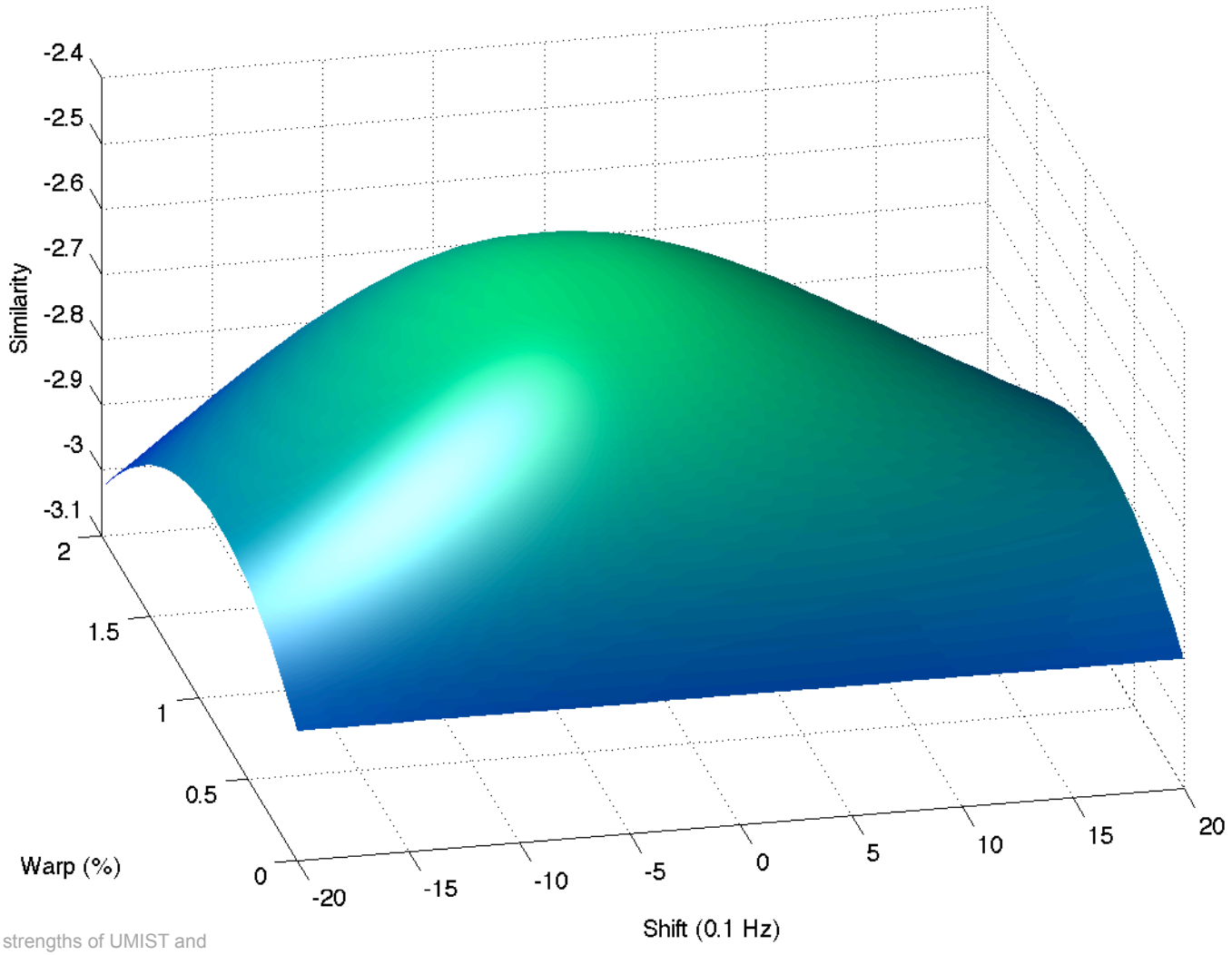
Alignment as an Optimisation Problem

- Components inside a set of spectra need to be aligned to be properly identified.
  - However, the ‘reference’ frequency location is irrelevant in the identification process.
- The spectra can be aligned using any one of the signals as a temporary reference.
- An optimisation algorithm is applied to find the optimal amounts of counter-distortion (de-shift, de-warp, etc.) for each spectrum, to be the most similar to the temporary reference.
- Using information gathered for each aligned spectrum, a mean tendency for each type of distortion is calculated, and assumed as the amount of distortion suffered in the temporary reference.

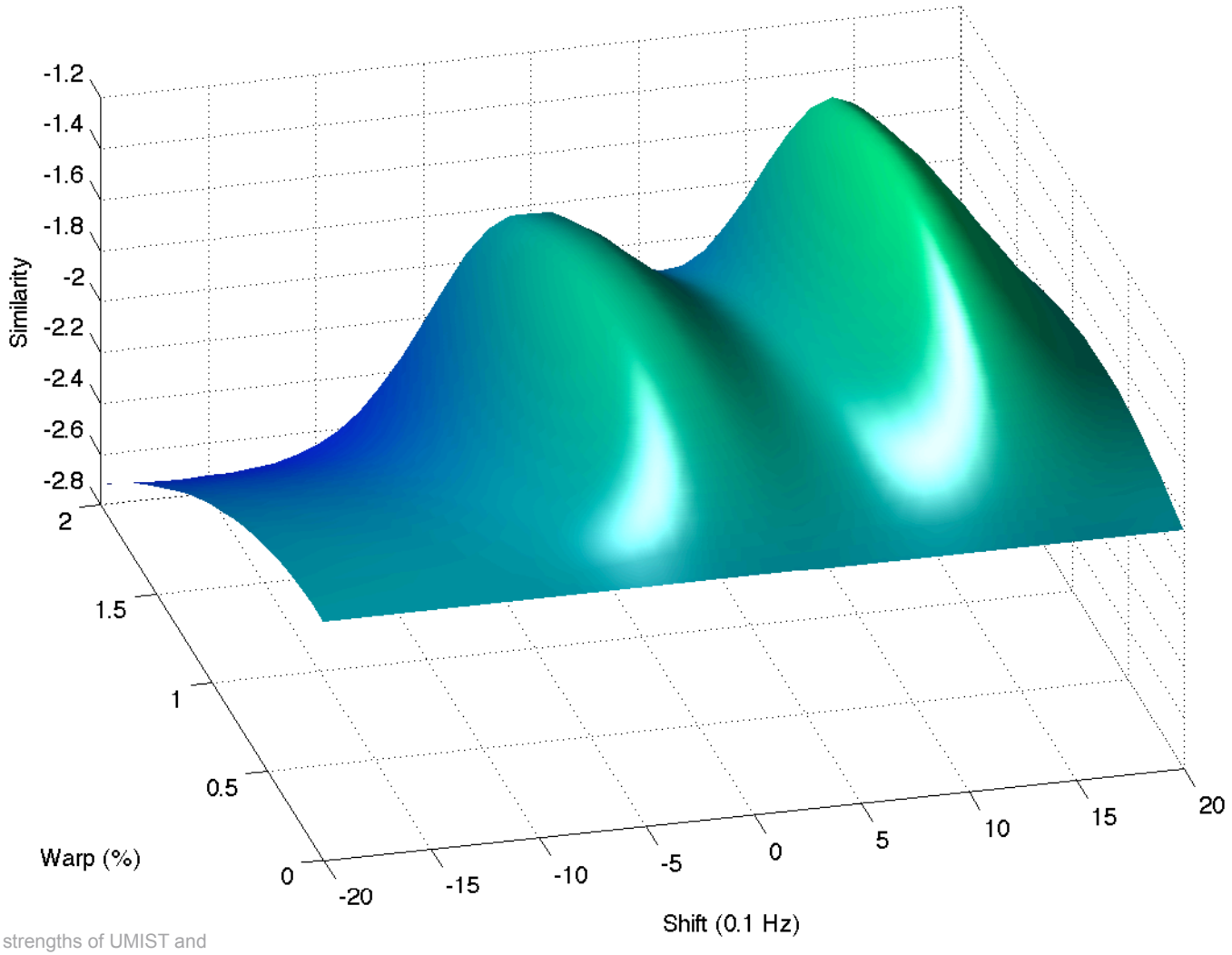
Algorithm Summary



Example of Solution Space Observed



Another Example of Solution Space

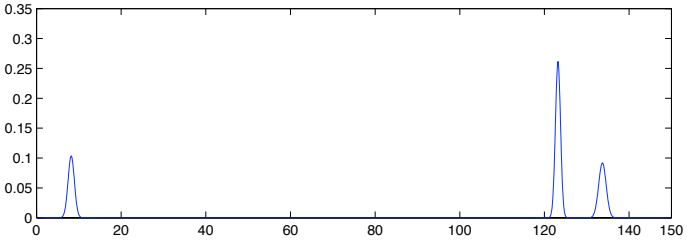


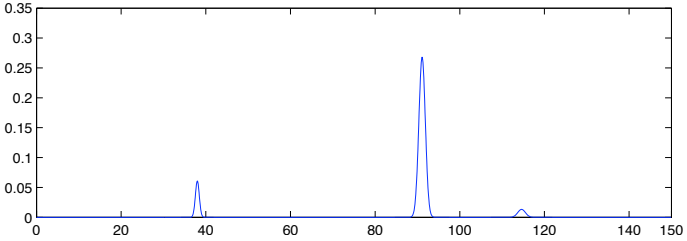
Optimisation Algorithm

- The unpredictable nature of the problem makes it necessary to apply a black-box oriented optimisation algorithm.
- **Particle Swarm Optimisation:**
  - Simulates a flock of bird 'flying' in the solution space.
  - Relatively easy to implement and visualise.
  - Proven to converge under specific tuning parameters (Clerc et al., 2002).
  - As good or better results than Genetic Algorithms (Kennedy et al., 1995).

- Given the definition of the problem, other algorithms can be applied.

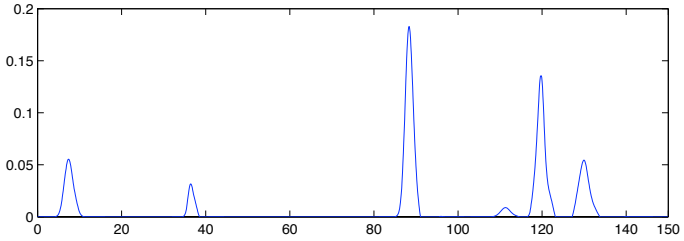
Results of Pre-Aligning before ALS

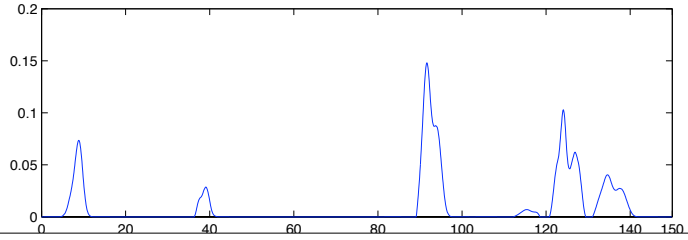




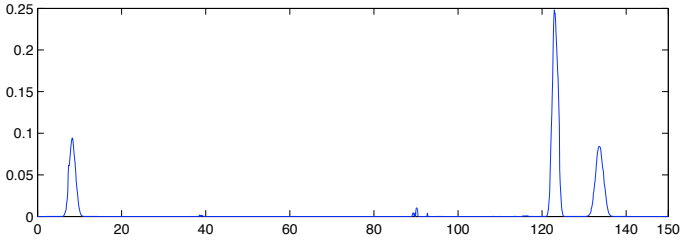
Benchmark Used

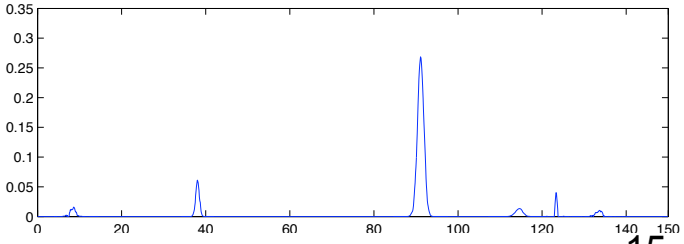
Components obtained *without* Pre-Alignment





Components obtained *with* Pre-Aligned Data





Conclusions & Future Work

- Spectral distortion is an issue of great importance, and sensor de-calibration is currently dealt with in an open-loop manner.
  - The algorithm records every shift encountered, and can automatically indicate if a calibration is necessary.
- The flexibility of this approach is to be noted, as more types of spectral distortion can be considered.

- ALS assumes the number of components is known *a-priori*.
  - Extend spectral distortion robustness towards estimating it.
- Other component identification algorithms, such as ICA, are to be explored.