Using Lagged Spectral Data in Feedback Control Using Particle Swarm Optimisation

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Using Spectral Data in Monitoring

- Pharmaceutical Industry
  - Crystallisation of active ingredients (Yu et. al., 2003)
  - Confirm sample temperature
  - Identify material concentrations

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

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Difficulties of Using Spectral Measurements

- Known for inconsistency due to:
  - Instrument de-calibration
  - External and/or sample temperature
  - Presence of undesired material

- Results in frequency displacement (aka, shift, lag)

- Disastrous if using reference spectra for analysis

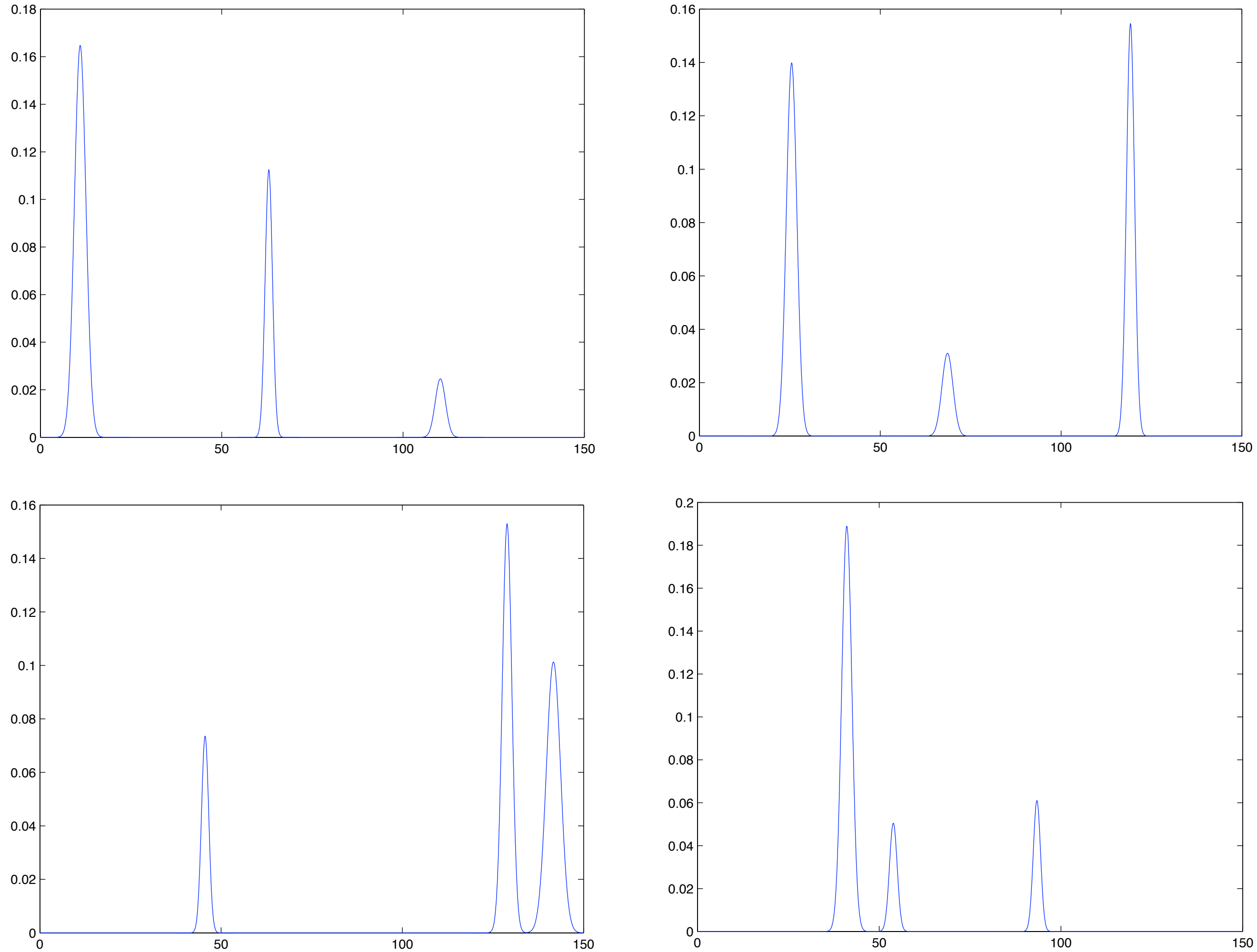
Classical Least Square Regression

$$C = DS(S^T S)^{-1}$$

- D: a spectral measurement
- S: set of reference spectra
- C: set of concentrations

- S and C need to be aligned

Example: Components



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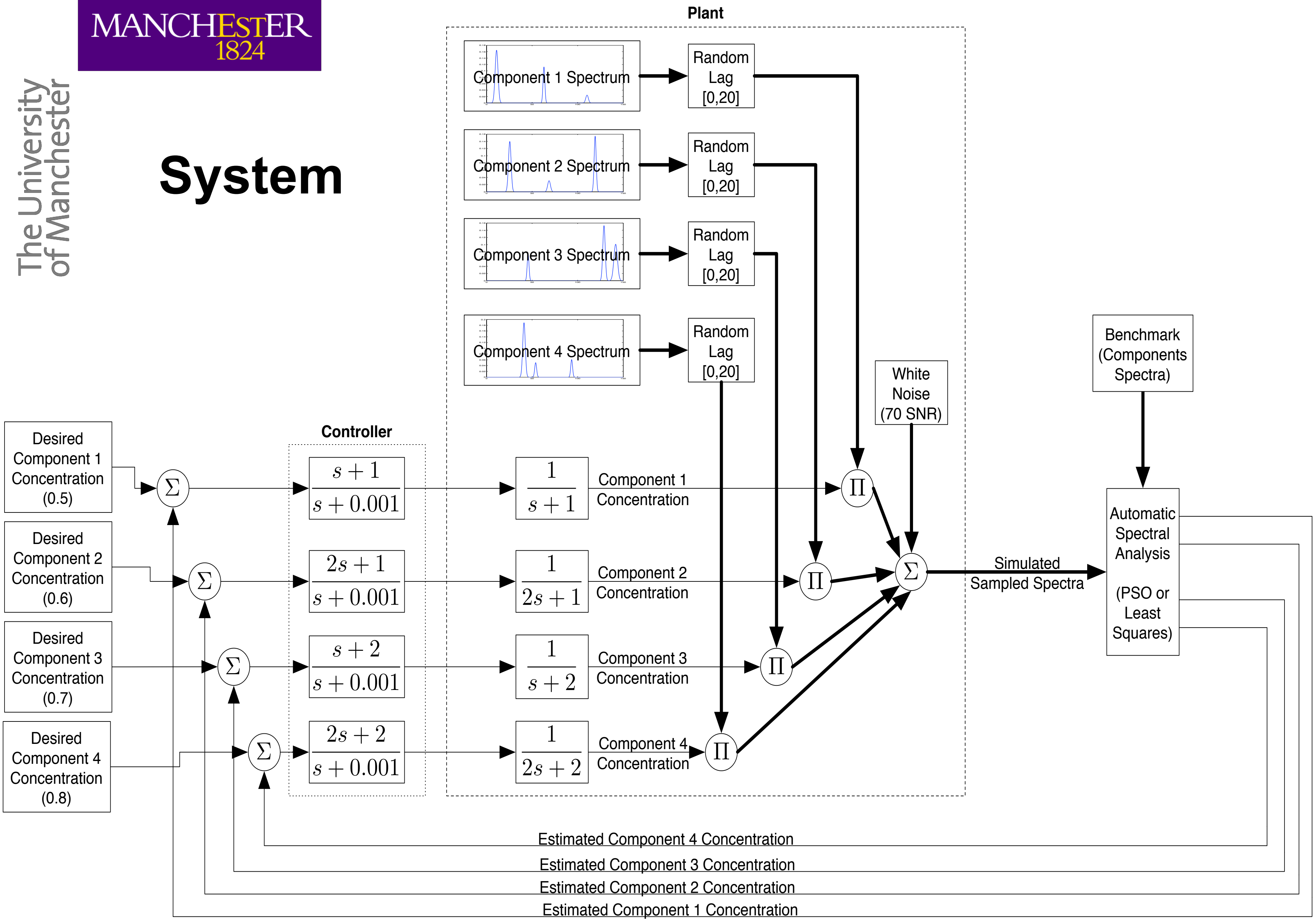
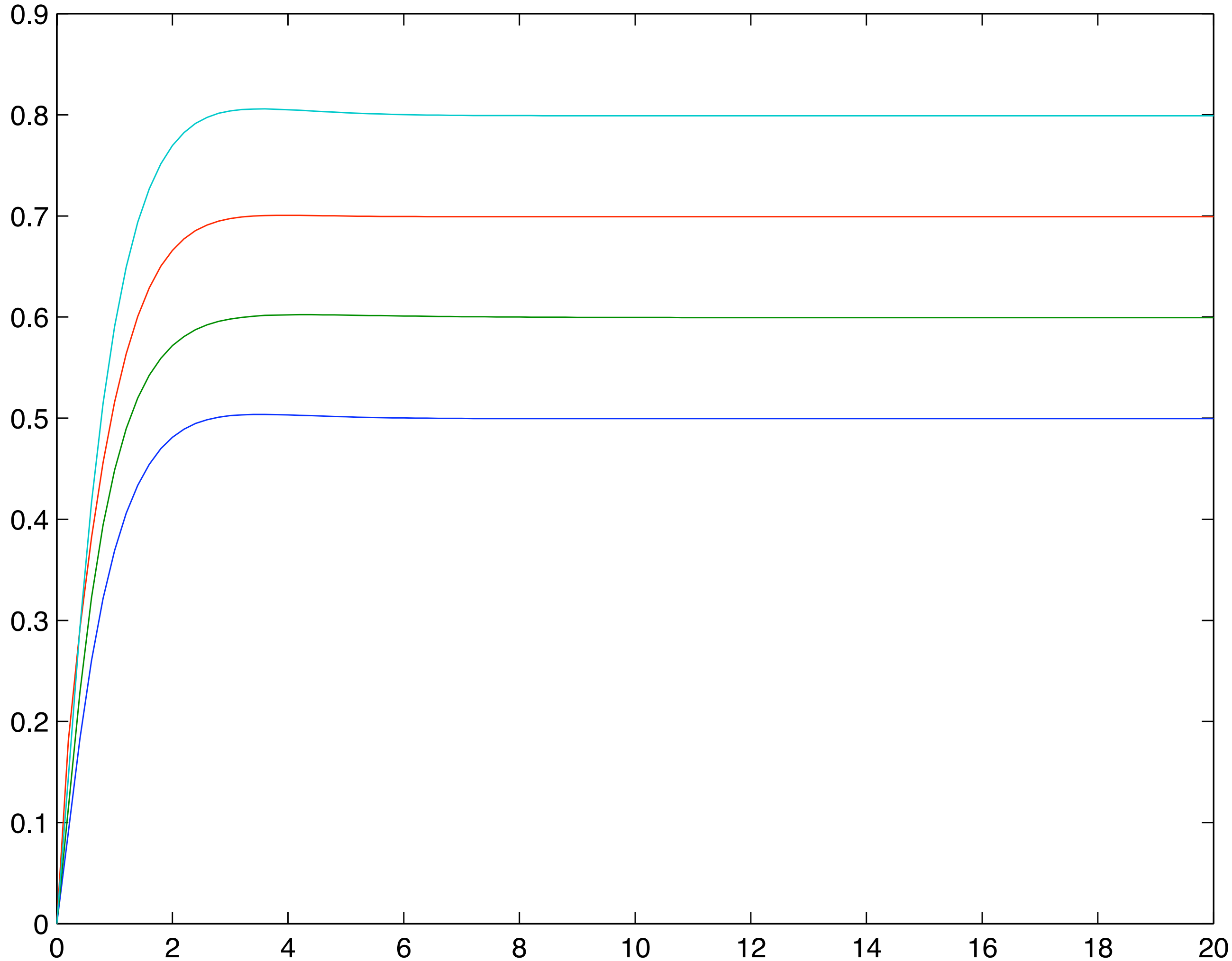
System



Response using CLSR wo. Applying Lag



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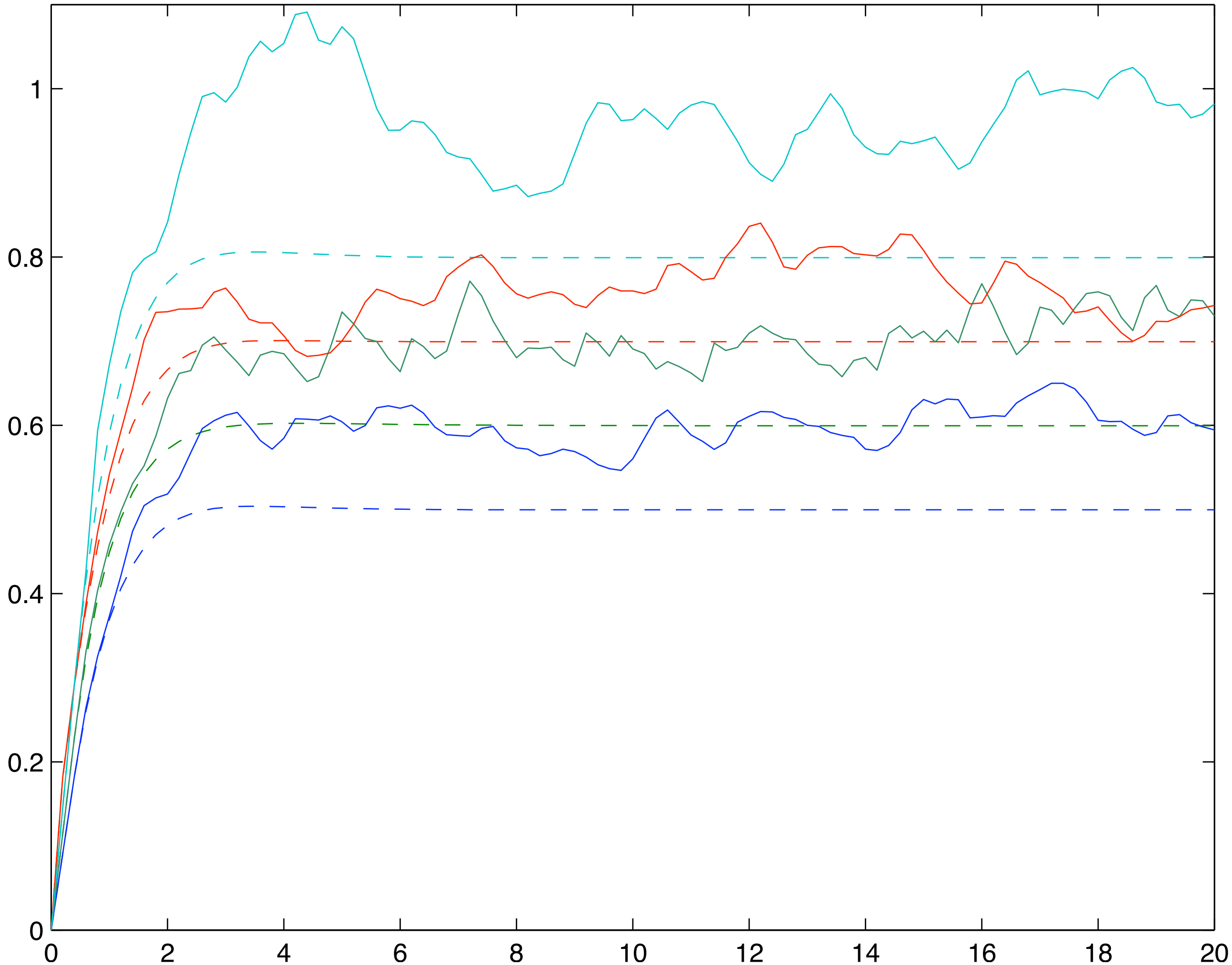
Response using CLSR Applying Lag



Approach as a Search Problem

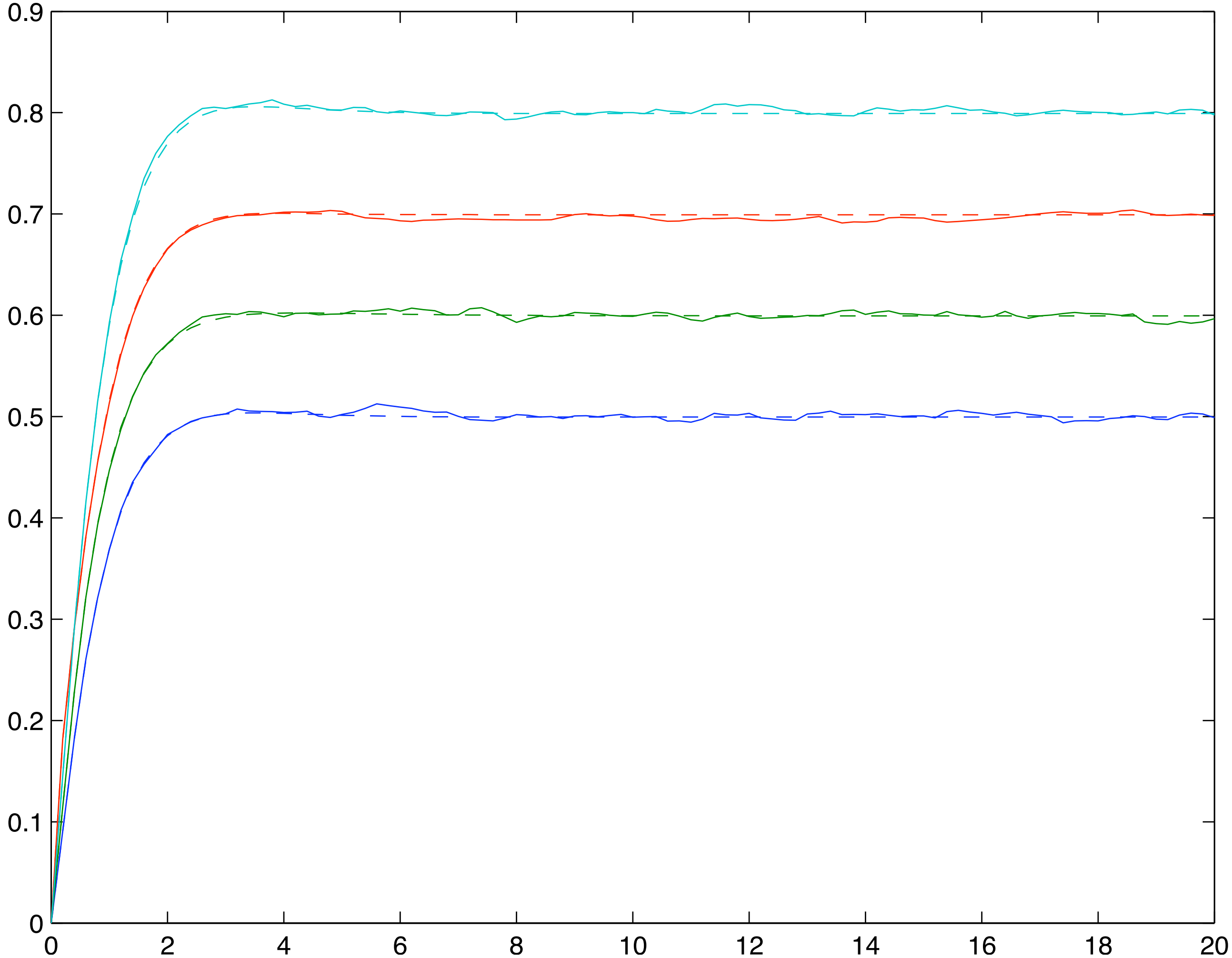
- Find combination of reference spectra that best fits sample
- For each reference spectrum, look for:
  - Magnitudes → concentrations
  - Shift suffered
  - [Others can be added…]

- Use Euclidian distance to grade the combination

Particle Swarm Optimisation

- Created by Kennedy in 1995
- Simulates a flock of birds ‘flying’ in the solution space
- Proven to do as well or better than Genetic Algorithms (Kennedy et. al., 1995)
- Easier to implement and visualise
- Can incorporate the concept of inertia to speed up search

Response using PSO Applying Lag



Comparison

Mean Square Error of responses using CLSR and PSO

Component	*1*	*2*	*3*	*4*
MSE w. **CLSR**	0.9639	1.0171	0.6966	1.6604
MSE w. **PSO**	0.0339	0.0319	0.0375	0.0373

The baseline of comparison is the response obtained when no lag was applied.

Conclusions & Future Work

- Classical spectral analysis methods are frail towards lag
- As a search problem, lag can be factored in
  - Other disturbances too
- Useful in monitoring:
  - Inform the need for sensor calibration
  - Alternative temperature measurements

- Search per sample: ~ 6 min
  - Future work: shortening time of completion