Using Lagged Spectral Data in Feedback Control Using Particle Swarm Optimisation

Caleb Rascon * **Barry Lennox** * **Ognjen Marjanovic** *

* *School of Electronic and Electrical Engineering, University of Manchester, UK, M60 1QD*

Abstract: The ability to use spectral data within a control loop is beginning to be considered in many areas, particularly in the Pharmaceutical Industry. However, typical spectral analysis tools, such as Classical Least Squares, are very fragile when handling frequency shifts which may occur in spectral measuring devices as a result of poor calibration or external influences. This paper shows that Particle Swarm Optimisation can be used to offset the effect of shift in measured spectra and improve the performance of any control system which may use this measurement.

Keywords: Spectral Analysis; Shift; Particle Swarm Optimisation; Classical LS Regression

1. INTRODUCTION

The automatic analysis of spectral data has recently seen an increase in interest, particularly in the Pharmaceutical Industry (Yu et al., 2003). In the future, it is anticipated that spectral measurements will be used directly in control systems to regulate product quality. Unfortunately, the consistency of spectral measurements can be affected by the calibration of the instrument and external influences, such as temperature or the presence of an undesired material (Zuppa et al., 2007). In many cases, this results in frequency displacement, or lag, in the spectral measurements, which can have a significant impact on automated analytical tools, which assume that the relationship between frequency and spectral intensity remains constant.

Spectral analysis is typically used to identify the presence or concentration of particular compounds in a mixture. In such applications it is common that the *reference spectra* of the compounds is known a priori (Dyrby et al., 2002). Unfortunately, when frequency shifts exist in spectral measurements it can make the identification of particular compounds difficult. This paper describes an approach which identifies the concentrations of compounds in a mixture by searching for the best linear fit of the reference spectra and comparing them to the measured spectra, taking account of any lags that may be present. Both the magnitude of the lag and the concentration of each spectral component can be identified using Particle Swarm Optimisation (PSO). PSO is a search technique which has been shown to provide a robust and efficient method for identifying the global optima for non-linear cost functions (Kennedy et al., 1995). The benefits of the proposed technique are demonstrated through its application to a simulation of a mixing process.

Section 2 of this paper provides a brief background to PSO; in Section 3, the simulation used to demonstrate the proposed approach is described; in Section 4, the results from a series of experiments are provided; and in Section 5, conclusions and several areas of future work are discussed.

2. BACKGROUND TO PARTICLE SWARM OPTIMISATION

Particle Swarm Optimisation (PSO) is a search algorithm that was introduced in Kennedy et al., 1995. It is based on the inner social behaviour of a flock or a school to find food. To begin, a group of particles (or *swarm*) is randomly placed inside a solution space defined by the given problem, with each variable involved in the problem defining one direction in the solution space. Each particle can 'move' towards different locations in the solution space, with a particular velocity and direction. The location of each particle is graded by a fitness function derived from the problem. Each particle is able to remember the location of the best fitness value it has found and this location is made public to a pre-defined number of neighbours around the particle. During each iteration, the velocities of each particle are modified, through consideration of the location of the best fit found by the particle and the best that has been found by its surrounding neighbours. For one particle, the velocity in one of its directions (x_i) will be modified at each iteration as follows:

$$V_{x_i} \leftarrow V_{x_i} + 2(R(pbest_{x_i} - l_{x_i}) + R(gbest_{x_i} - l_{x_i})) \quad (1)$$

where V_{x_i} is the velocity of the particle in the direction x_i; $pbest_{x_i}$ is the location in direction x_i where the best fit been found by this particular particle; $gbest_{x_i}$ is the location in direction x_i where the best fit that has been found by the surrounding neighbours of the particle; and l_{x_i} is the current position of the particle in direction x_i. R is a stochastic factor which is introduced to avoid having more than one particle in the same location, making the particles 'spread out' in an *area* and not focus on a single point, which improves the chances of finding the true global optima. It is important to note that V_{x_i} and $present_{x_i}$ can be constrained, each having a minimum and

maximum value if necessary. V_{x_i} is modified according to (1) until the best fit found by the whole swarm converges or the maximum number of iterations is exceeded.

The algorithm can be improved by incorporating the concept of a *time-decreasing inertia* (Shi et al., 1998), which forcefully decreases velocities later in the search. This technique helps PSO initially find the area where the global optima is located, and then this area is searched with greater scrutiny for the remainder of the search (when inertia is low), which results in faster and more accurate results (Shi et al., 1998).

PSO has been compared to other stochastic search methods such as Genetic Algorithms (GAs). Kennedy et al. found that PSO did as well or better than GAs in most cases, meaning that it found the same solution in fewer iterations. Considering the relative simplicity of PSO compared to GAs, for example the solution schema does not have to be reduced to a binary form to work efficiently, PSO is an attractive approach for solution searches and was the technique used throughout this work.

3. SIMULATIONS

To test the suitability of using PSO in spectral processing rather than other spectral analysis tools such as Classical Least Squares Regression (CLSR) (see Childers et al., 2002), a mixing process under feedback control was simulated. A schematic of the simulated process is provided in Figure 1. The plant consists of four feed streams (for components 1-4), the flow rate of which can be varied to ensure the concentration of each component in the mixture meets the pre-specified requirements. The output of the plant is a measured spectrum of the mixture. The objective of the control system is to regulate the concentration of each of the four materials in the mixture by manipulating the feed of each component. The concentration of materials in the mixture is not measured directly and must instead be extracted from the spectral measurements. In this study, this is achieved by applying either PSO or CLSR.

Both methods require a set of reference spectra to work with. Four spectral components were artificially created for this purpose, and their basic form is shown in Figure 1 (labelled 'Componet 1-4 Spectrum'). These spectra are also used inside the plant to simulate the measured spectrum of the mixture, where each is multiplied by their corresponding concentration and mixed with the other components and white noise with a signal-to-noise ratio of 70.

The control system was designed to regulate the concentrations of the individuals compounds to specific values in centigrams (cg). These were: 0.5 cg for the first component, 0.6 cg for the second, 0.7 cg for the third, and 0.8 cg for the fourth. The response of the control system when there was no lag on the spectral measurement is shown in Figure 2. This figure shows a 20-second simulated response measured from the outputs of the transfer functions inside the plant. The response in Figure 2 shows that every component has reached its desired concentration. This response was considered in the remainder of this paper as the 'optimal response' of the control system.

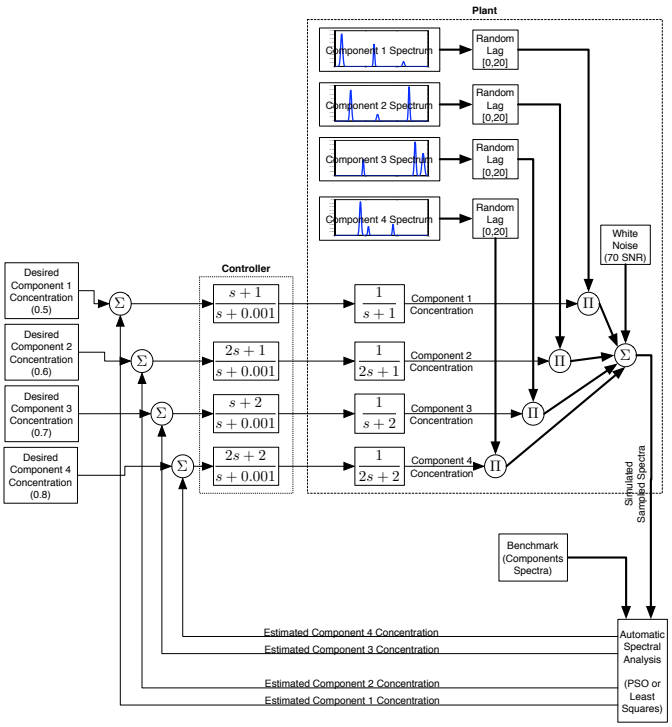

Fig. 1. The whole simulated system.

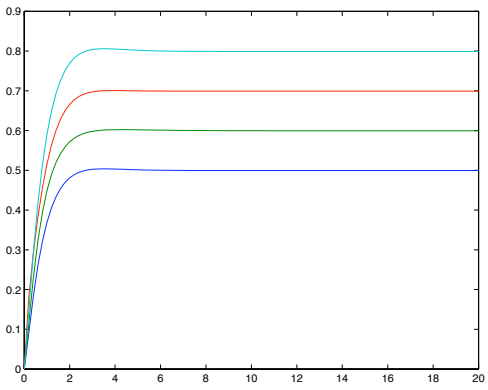

Fig. 2. Control response without using spectral data (i.e. no lag).

In the following section, the effect that frequency shift in the spectral measurements has on the control system is illustrated and the ability of PSO to recover the optimal control performance is investigated.

4. RESULTS

Frequency shift was introduced into the spectral measurements. Following the introduction of the frequency shift, two experiments were conducted. In the first experiment, CLSR was used to resolve the concentrations of each of the components in the mixture directly from the spectral measurement and those concentrations were fed back through the control system. In the second experiment, the concentration of each of the components in the mixture was identified with the aid of PSO, which accounted for the frequency shift in the spectral measurements.

4.1 Classical Least Squares Regression

Classical Least Squares (CLS) is a statistical method which can be used to obtain a set of pure-component spectra from a series of samples. These spectra can then be used to estimate their concentration in other samples using CLS Regression (CLSR), as described in Haaland et al., 1980. The CLSR approach requires knowledge of a reference spectra for each of the components in the mixture. This reference, S, is often available and using the spectra obtained from the mixture, D, the concentrations of each of the components can be identified using the following expression:

$$C = D * S * (S^T * S)^{-1} \tag{2}$$

The concentration obtained using (2) were then fed back through the controller and the resulting concentrations within the mixture are shown in Figure 3. This figure shows that the response of the controller has been severely degraded as a result of the lag, when compared to the response of the control system obtained in Section 3 when there was no lag present.

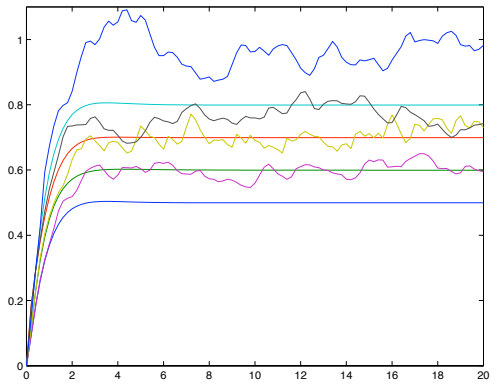

Fig. 3. Control response using lagged data and CLSR as spectral analysis tool.

4.2 Using Particle Swarm Optimization

In this test PSO was used to estimate the concentrations of the components from the spectrum obtained from the mixture. In the PSO, a swarm of 50 particles was created, with each particle considering 5 nearby particles as neighbours. Each particle had 8 directions to 'fly' in, two per component: one direction dealt with the concentration of the component and the other with its spectral lag. To grade the fitness of each particle, each reference spectrum was lagged and multiplied by its corresponding values derived from the location of the particle. The four modified spectra were then linearly mixed, resulting in a 'test spectrum', which was then compared to the spectrum obtained from the plant by calculating the Mean Square Error (MSE) between them. The MSE is a measure of the 'distance' between the ideal value and the acquired value, calculated by the square root of the addition of the squared differences between them at each frequency point. In effect, it is the Euclidian distance between the two spectra, meaning that a value close to zero is desired.

The value of each concentration direction was limited between 0.01 and 1 cg and its velocity between -0.1 and 0.1; every lag direction was limited between -30 and 30 frequency points and its velocity between -3 and 3. These values were obtained empirically and were found to give the best results.

Time-decreasing inertia was also applied, increasingly reducing the velocities from 0% to 60% of their value in the first 300 iterations, and maintaining that value for the remainder of the search. Convergence to a solution was assumed when 120 iterations passed without a change in the identified global optima. The response of the process when the concentrations obtained using the proposed PSO technique were fed back through the control system are displayed in Figure 4.

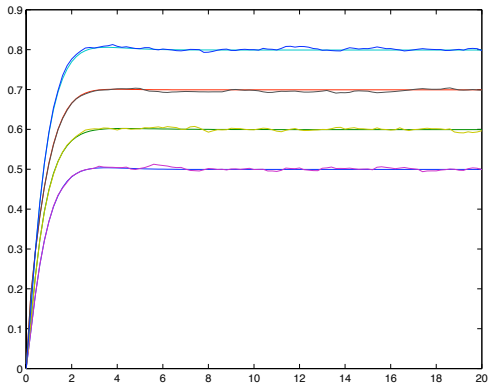

Fig. 4. Control response using lagged data and PSO as spectral analysis tool.

Comparing Figures 3 and 4 shows that the response using the PSO spectral processing technique enables the controller to track much more closely the desired response than was obtained using CLSR. For a more precise comparison, the MSE between each response and the optimal one is provided in the following table and it can be seen that PSO outperforms CLSR significantly.

Mean Square Error using PSO and CLSR				
Component	1	2	3	4
MSE (CLSR)	0.9639	1.0171	0.6966	1.6604
MSE (PSO)	0.0339	0.0319	0.0375	0.0373

5. CONCLUSIONS & DISCUSSION

This paper has shown that using common automatic spectral analysis algorithms, such as Classical Least Squares Regression, may lead to poor control performance if these measurements are used directly in a control system. The reason for this is that frequency shift may be present in the measurements and this can have a significant effect on the controller. CLSR assumes the presence of each spectral component in a constant frequency location, a variation of which results in a deviation of the relationship between frequency and spectral intensity. When this relationship changes and nothing is done to compensate for it, the estimated values of the concentrations of each component will become inaccurate.

Particle Swarm Optimisation was able to consider the possibility that the frequency-intensity relationship could change, and compensated for it by searching for the magnitude of shift affecting each component as well as

their concentration. This lead to accurate estimates of the concentrations, when compared to those produced by CLSR when lag was introduced into the system. Using the concentrations identified using PSO, the performance of the control system was comparable to that achieved when there was no shift present in the spectral measurements.

A limitation with the proposed PSO technique is that each spectrum took approximately 6 minutes to analyse, which is not viable for fast processes. The search parameters of PSO can be re-tuned to speed up the search, but doing so may deteriorate the results it provides. It is left for future work to identify ways to make PSO viable for fast processes.

REFERENCES

L. X. Yu, R. Lionberger, A. Raw, R. D'Costa, H. Wu, and A. Hussain. Applications of process analytical technology to crystallization processes. *Center for Drug Evaluation and Research, Food and Drug Administration*, pages 1–46, August 2003.

M. Zuppa, C. Distante, K. C. Persaud, and P. Siciliano. Recovery of drifting sensor responses by means of dwt analysis. *Sensors & Actuators: B. Chemical*, 120(2):411–416, January 2007.

M. Dyrby, S. Engelsen, and L. Nørgaard. Chemometric quantitation of the active substance (containing c=n) in a pharmaceutical tablet using near-infrared (nir) transmittance and nir ft-raman spectra. *Applied Spectroscopy*, 56(5):579–585, May 2002.

J. Kennedy and R. Eberhart. Particle swarm optimization. *Proceeding of the IEEE International Conference on Neural Networks*, IV:1942–1948, 1995.

Y. Shi and R. C. Eberhart. Parameter selection in particle swarm optimization. *Proceedings of the 7th International Conference on Evolutionary Programming VII*, pages 591–600, 1998.

D. M. Haaland and R. G. Easterling. Improved sensitivity of infrared spectroscopy by the application of least squares methods. *Applied Spectroscopy*, 34(10):539–548, September 1980.

J. W. Childers, W. J. Phillips, E. L. Thompson, D. B. Harris, D. A. Kirchgessner, D. F. Natschke, and M. Clayton. Comparison of an innovative nonlinear algorithm to classical least-squares for analyzing open-path fourier transform infrared spectra collected at a concentrated swine production facility. *Applied Spectroscopy*, 56(3):325–336, March 2002.