

Data Processing in Circular Dichroism Spectroscopy

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Abstract:

Circular Dichroism (CD) spectroscopy is a method for the biophysical characterisation of protein molecules. It is able to tell the user the percentage composition of secondary structure components that are present in the protein molecule. The advantages of this technique are that concentrations can be very low and the protein does not need to exist in any particular special form in order for the process to be undertaken, in contrast to other techniques.

A number of methods of characterisation and comparison of CD spectroscopy of proteins have been developed in the past. I have been investigating ways to extend such methods of comparison of protein CD spectra with each other by the development of a comparison metric. In addition to this work, I have also been using machine learning methods (namely Support Vector Machines and some Gaussian processes) to try to improve the accuracy of prediction of the amount of secondary structure elements in the protein under investigation. Our group has developed a carefully calibrated dataset using synchrotron radiation CD spectroscopy which has extended the quality and wavelength range of training data used in this method. Using this data, I aim to improve upon methods of characterisation that currently exist.