An algorithm for the selection of representative Fourier coefficients in smoothing CD spectra

U. Glatter, W. Straßburger, and A. Wollmer

Fachgebiet Struktur und Funktion der Proteine
Abt. Physiologische Chemie, Rheinisch-Westfälische Technische Hochschule Aachen, Schneebergweg 211, D-5100 Aachen

Fourier filtering is widely used in smoothing digital spectroscopic data. The main problem is to separate the Fourier coefficients representing the true signal from those representing noise. This is usually achieved by subjective decision of whether or not the back-transformed spectrum is an appropriate representation of the authentic.
In the algorithm for smoothing CD spectra suggested by C.A. Bush (1), the noise frequencies are identified by a statistical approach. This procedure, though automatic, requires the setting of a parameter according to the experience of the user.
The method presented here was applied to CD data recorded on a Cary 61 spectrometer controlled by a Cromemco microcomputer (2). Measurements of the sample as well as the baseline were taken at equally spaced wavelength intervals to make interpolations unnecessary. The differences between the sample and the baseline spectral data were stored on floppy disks. In order to avoid discontinuities at both ends of the back-transformed spectra data were linearly detrended (3) prior to transformation with the subroutine FFTS (4). The programme provides intermediate storage of the calculated coefficients.

As CD spectra, in particular those of biopolymer backbones, usually consist of relatively few broad bands, less than 32 frequencies should suffice for proper representation. Our cut-off criterion is the minimum number of coefficients assuring that the residuals between the back-transformed and the original spectra lack periodicity. This number was found by means of a procedure analogue to binary search algorithms, starting with 16 frequencies.
The usefulness of our method is demonstrated with gaussian curves superimposed with noise of different standard deviations as well as with genuine CD spectra of proteins.

1) Bush, C.A., (1974)
Anal. Chem. 46, 890.
2) Glatter, U., Straßburger, W., Szameit, H., Wollmer, A., to be published.
3) Hayes, J.W., Glover, D.E., Smith, D.E., (1973), Anal. Chem. 45, 277.
4) Brigham, E.O., (1974), The Fast Fourier Transform Prentice Hall Inc., Englewood Cliffs, New Jersey.