

1035-62-1859

Taylor R Pressler* (taylor.pressler@gmail.com), 93 College St. Apt. 3, South Hadley, MA 01075, and **Sean M Decatur** (sdecatur@mtholyoke.edu), 50 College St, South Hadley, MA 01075. *Singular Value Decomposition and Its Applications to Fourier Transform Infrared Spectroscopy Studies of Amyloid Protein Dynamics.*

Singular Value Decomposition (SVD) is a type of component analysis that can be used to decompose a real $m \times n$ matrix and where $m \geq n$. SVD can be very useful when analyzing large sets of spectroscopic data collected as a function of time. Fourier Transform Infrared Spectroscopy (FTIR) is used to study the conformational changes of proteins. This technique is widely used in biophysical chemistry research on the misfolding of proteins associated with Alzheimer's Disease. A time series of FTIR spectra is regarded as a matrix, in which each row corresponds to a frequency at a fixed time. A useful way to analyze the data is to decompose the matrix into a sum of terms by SVD. The individual terms in this decomposition then hold a real physical significance. This allows a purely mathematical operation to isolate physical effects as different terms. For example, a protein change can be comprised of both fast and slow processes and in a typical application these are separated by SVD. Other contributions to the spectra such as buffer and water vapor, which would have to be subtracted out through data processing, are also isolated into individual terms. This can help eliminate artifacts which arise from data processing and preserve data integrity. (Received September 20, 2007)