

1145-AA-1837 **Jeff Knisley*** (knisleyj@etsu.edu) and **Debra Knisley**. *Identifying Biologically Relevant Structures: From Clustering to Manifold Learning.*

Protein tertiary structure determines protein function and is itself determined by the DNA sequence of the gene encoding the protein. However, the relationship between a gene's DNA sequence and the corresponding protein's tertiary structure is imperfectly understood. We can begin to address our understanding of this relationship using spectral clustering, which is a graph partitioning algorithm derived from the Laplacian matrix of a network. The method typically requires only a few of the eigenvectors of the Laplacian, and in fact, a true graph partition only requires a single eigenvector – the Fiedler eigenvector. However, the method can be generalized to use more than a few of the eigenvectors, in which case it is often interpreted as a nonlinear dimensionality reduction technique known as manifold learning. This talk explores the connection between spectral clustering and manifold learning as it can be applied to biological applications, such as for example how clustering can lead to manifold learning when applied to the study of a protein's tertiary structure. (Received September 24, 2018)