

Partial Least Squares to Identify Functional Dynamics of Proteins

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It has been recently demonstrated on several examples that the (multivariate) partial least squares algorithm can be successfully used to study certain functional mechanisms of proteins. This is achieved by identification of collective modes of internal protein dynamics that maximally correlate to an external order parameter(s) of functional interest. Thereby, the standard partial least squares algorithm need to be adjusted to the specific goals and data types. In this talk we discuss a new multivariate partial least squares algorithm and its statistical properties, as well as performance of (multivariate) partial least squares in presence of serial correlation.

Key Words: collective modes, serial correlated data