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Protein functional motifs: A random matrix approach

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Random matrix theory (RMT), which was formulated 50 years ago, has a wide application in modeling and understanding the diverse areas of research including nuclear physics, disordered systems, information theory, string theory, statistical physics, biological sciences, finance, social systems. In the current work, we use the tools from the random matrix theory to understand the structural and functional organization of a protein family. The method is based on the the random matrix theory which uses various amino acid physiochemical properties along with the multiple sequence alignment data to detect the functional and structural sites and motifs within a protein family. The method is successfully applied to various protein families including the beta-lactamase, serine protease, HSP70, G-proten, HTH1 family etc. In this method a protein sequence is represented as a multi-dimensional time series, which makes it possible to compare the evolutionary distance between the protein sequences based on the physiochemical properties. This gives an easy, fast and informative way to compare different protein sequences using the physiochemical properties. The entropic measures shows that during the evolutionary history of the protein family, it is the certain physiochemical properties that are conserved rather than the type of amino acids. For each physiochemical property, the correlation matrix between positions is calculated, while using an ensemble of Wishart matrices from the random matrix theory for the noise estimation and information filtering. The spectral properties of correlation matrices are calculated and compared with the analytical results for the Wishart matrices. It is shown that the distribution of the eigenvalues outside the random matrix bound deviates significantly from the eigenvalues distribution for Wishart matrices. These eigenvalues and corresponding eigenvectors contains significant information and can determine the structure and functional motifs within the protein family. For proteins, it is found that the eigenvector corresponding to the small eigenvalues are more informative as compared to the large eigenvalues. These small eigenvectors can group positions into sectors with well defined structural and functional role.

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