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Calculation of weights for protein connectivity network

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The Protein Connectivity Network (PCN) is constructed from sequence fragments of a unique size (typically 15-25 amino-acids), with edges connecting similar fragments displaying sufficiently small hamming distance. The PCN can be used for hidden protein homology detection, sequence alignment, evolutionary studies and for many other tasks. Introduction of the weighted PCN (WPCN) should significantly increase the efficiency of the method. It makes possible considering such parameters as level of similarity, similarity of context, positions of matches, sequence complexity and so on. The weight can reflect probability of two protein fragments (corresponding to neighboring nodes in the PCN) to be similar or alternatively, they can reflect level of similarity of the fragments. In our current study we are concerning only to structural similarity calculated by root mean square deviation (RMSD) function, but generally any other type of similarity (functional, for example) can be considered. The task of the weights calculation is reduced to finding a function based on a training dataset, which obtains two protein sequence fragments and providing a value (weight of the edge). These weights are used for calculation of connectivity through the network between any pair of the remote nodes. Currently, we use flow and electrical models for calculation of this connectivity, which is the main parameter for the hidden homology prediction. The prediction accuracy of the WPCN is the main parameter for quality estimation of the constructed function of weights.

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