

Supplementary file: Asymmetric-based framework for efficient balanced learning of protein–protein interaction

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1 Benchmark datasets

Table S1: The details of benchmark datasets

	SHS27K	SHS148K	SYS30K	SYS60K
sequence number	1,690	5,189	2,685	3,549
interaction number	12,517	44,488	30,074	60,357
average degree	14.81	17.15	22.62	34.01
average sequence length	571	597	558	541
maximum sequence length	5,171	5,636	4,910	4,901
minimum sequence length	51	45	51	50

2 Details of features for the GCN and DNN that used as baseline

Six features are used as input for Graph Convolutional Networks (GCN) and Deep Neural Networks (DNN). The details of each feature are as follows:

Conjoint triad: The conjoint triad feature combines k -mer and amino acid type. The k -mer denotes substrings of length k within a biological sequence, commonly used in proteomic and genomic data analysis. In the computation of conjoint triads, amino acids are divided into seven classes. With k set to 3, each 3-mer is considered a unit, and all 3-mers are classified based on the classes of their amino acids. Therefore, each protein sequence is represented by $7^3 = 343$ entries.

Amino acid composition (AAC): AAC calculates the fraction of each amino acid within a protein sequence. Each protein is represented as a vector with 20 entries, where each entry indicates the occurrence of one amino acid within the sequence, normalized by the sequence length.

Pseudo-amino acid composition (PAAC): A combination of conventional AAC and discrete sequence correlation factors, for sequence $S = [a_1, a_2, \dots, a_L]$, the λ -order correlation factor is defined as:

$$\theta_\lambda = \frac{1}{L-\lambda} \sum_{i=1}^{L-\lambda} O(a_i, a_{i+\lambda})$$
$$O(a_i, a_j) = \frac{1}{3} [(H_1(R_j) - H_1(R_i))^2 + (H_2(R_j) - H_2(R_i))^2 + (M(R_j) - M(R_i))^2]$$
(1)

$H_1(a)$, $H_2(a)$ and $M(a)$ denotes the hydrophobicity, hydrophilicity and side-chain mass of a . The sequence is represented as a vector with length $20 + \lambda$:

$$v_i = \begin{cases} \frac{f_i}{\sum_{j=1}^{20} f_j + \omega \sum_{k=1}^{\lambda} \theta_k}, & i \leq 20 \\ \frac{\omega \theta_{i-20}}{\sum_{j=1}^{20} f_j + \omega \sum_{k=1}^{\lambda} \theta_k}, & i > 20 \end{cases} \quad (2)$$

$i \in 1, 2, \dots, (20 + \lambda)$

f_i denotes the frequency of i th amino acid in sequence. It is clear that λ should be smaller than L , in practice, Chou et al. set λ as 30, we follow the same strategy in this work.

CTDT: The transition descriptor in CTD (Composition, Transition and Distribution). For 13 physicochemical properties of amino acids, the amino acids are divided into three functional groups by each property, and transition (T) is the frequency of dipeptides. Finally, a vector with length 39 is computed by the original sequence.

ProVec1D: A feature derived from ProtVec, in which each 3-mer in protein sequence is mapped to a vector with length 100, ProVec1D sums the 100 components as single numeric value.

Global position information: the sum of position information of each amino acid in protein divided by sequence length, where the position information denotes the relative position of amino acid in corresponding sequence.