



PyBioMed

--PyBioMed Protein features



**COMPUTATIONAL BIOLOGY &
DRUG DESIGN GROUP**
CENTRAL SOUTH UNIV., CHINA

There three different methods of calculating interaction descriptors of chemical-chemical interaction, protein-protein interaction and DNA-DNA interaction. Next, we will show how to construct an interaction feature by the protein-protein interaction example.

Protein-protein interaction descriptors

Let $\mathbf{F}_a = \{\mathbf{F}_a(i), i = 1, 2, \dots, p\}$ and $\mathbf{F}_b = \{\mathbf{F}_b(i), i = 1, 2, \dots, p\}$ are the two descriptor vectors for interaction protein A and protein B, respectively. There are three methods to construct the interaction descriptor vector \mathbf{F} for A and B:

(1) Two vectors \mathbf{F}_{ab} and \mathbf{F}_{ba} with dimension of $2p$ are constructed: $\mathbf{F}_{ab} = (\mathbf{F}_a, \mathbf{F}_b)$ for interaction between protein A and protein B and $\mathbf{F}_{ba} = (\mathbf{F}_b, \mathbf{F}_a)$ for interaction between protein B and protein A.

(2) One vector \mathbf{F} with dimension of $2p$ is constructed: $\mathbf{F} = \{\mathbf{F}_a(i) + \mathbf{F}_b(i), \mathbf{F}_a(i) \times \mathbf{F}_b(i), i = 1, 2, \dots, p\}$.

(3) One vector \mathbf{F} with dimension of p^2 is constructed by the tensor product: $\mathbf{F} = \{\mathbf{F}(k) = \mathbf{F}_a(i) \times \mathbf{F}_b(j), i = 1, 2, \dots, p, j = 1, 2, \dots, p, k = (i-1) \times p + j\}$.

There two different methods of calculating interaction descriptors of calculating chemical-protein interaction, protein-DNA interaction, chemical-DNA interaction. Next, we will show how to construct an interaction feature by the chemical-protein interaction example.

Chemical-protein interaction descriptors

There are two methods for construction of descriptor vector \mathbf{F} for chemical-protein interaction from the protein descriptor vector $\mathbf{F}_t(\mathbf{F}_t(i), i = 1, 2, \dots, p_t)$ and chemical descriptor vector $\mathbf{F}_d(\mathbf{F}_d(i), i = 1, 2, \dots, p_d)$:

(1) One vector \mathbf{V} with dimension of $p_t + p_d$ are constructed: $\mathbf{F} = (\mathbf{F}_t, \mathbf{F}_d)$ for interaction between protein T and ligand D.

(2) One vector \mathbf{V} with dimension of $p_t \times p_d$ is constructed by the tensor product: $\mathbf{F} = \{\mathbf{F}(k) = \mathbf{F}_t(i) \times \mathbf{F}_d(j), i = 1, 2, \dots, p_t, j = 1, 2, \dots, p_d, k = (i-1) \times p_t + j\}$.