

0907MLEGLAB group meeting memo

By JingJin

1.

Zhong hao presents a article about using the End-to-end differentiable learning to predict the protein structure. This is a big innovative idea. And this algorithm almost outperform all the existed algorithms. The algorithm is based on a LSTM model. The model takes a sequence of amino acids and PSSMs as input and outputs a 3D structure.

It is comprised of three stages-computation, geometry, and assessment. Firstly, protein sequences are fed one residue at a time to the computational units of a LSTM model, integrating information about its amino acid, PSSM, and from residues upstream and downstream. Then three torsional angles of the residue are predicted. Secondly, the torsional angels are fed to geometric units, which sequentially translate them into Cartesian coordinates to generate the predicted structure. Finally, dRMSD is used to measure deviation from experimental structures. The dRMSD first computes pairwise distances between all atoms in the predicted structure and all atoms in the experimental one(separately), and then computes the root mean square of the distance between these sets of distance.

2.

Ansi Zhang presents a topic in transfer learning in fault diagnosis. The main problem is how to predict the remaining useful life(RUL) of the machine based on data of different sensors. To deal with lacking of data samples in some situation, he proposes a transfer learning algorithm, in which the models can be first trained on different but related dataset and then fine-tuned by the target dataset. Normally this algorithm would improve the performance in situation with small number of samples. But there is an interesting exception that transferring from multi-type operating conditions to single operating conditions deliver a worse result.

Ali: what is the input of the machine?

The input data is 30 *30 dimensional data. For a single input, it contains 30 single-cycle data from every multivariate time series of trajectories and each single-cycle vector comprised of 24 sensors values and 6 other values(including the operating values).

The transfer learning framework is based on LSTM networks. One is for training the large amount of data of the source task, the input is the source data and the output is source RUL. Then the model is further trained with the small amount of the data from the target task, and the output is target RUL.