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Deep learning for prediction and analysis of protein structures

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Abstract

The three-dimensional (3D) structure of a protein is related to its function and is important for life science applications such as drug discovery. However, experimentally determining three-dimensional protein structures is costly and time-consuming. Thus, many computational methods for predicting protein 3D structures from amino acid sequences have been developed. These days, deep learning, which utilizes an artificial neural network with huge number of the hidden layers, has been applied to the field. Before, the improvement by deep learning in this field was not impressive because researchers just replaced classical machine learning algorithms to deep neural network. However, these days, several specific neural network architectures that can directly deal with 3D coordinates of atoms belong to a protein were developed. Such neural network architectures, including 3D convolutional neural network, graph neural network, have enabled the end-to-end learning and achieved significant improvements. Particularly, AlphaFold2 developed by DeepMind achieved almost perfect protein structure prediction in CASP14 that was an international benchmark of protein structure prediction held in 2020 [1]. In this talk, I introduce recent progress of this field by introducing our recent researches related to protein structure prediction [2][[3][4]. Additionally, I will discuss the practicality of AlphaFold2's predicted structures and the limitation of current technology.

1. Jumper, J., Evans, R., Pritzel, A., Green, T., Figurnov, M., Ronneberger, O., ... & Hassabis, D. (2021). Highly accurate protein structure prediction with AlphaFold. Nature, 596(7873), 583-589.
2. Sato, R., & Ishida, T. (2019). Protein model accuracy estimation based on local structure quality assessment using 3D convolutional neural network. PloS one, 14(9), e0221347.
3. Makigaki, S., & Ishida, T. (2020). Sequence alignment using machine learning for accurate template-based protein structure prediction. Bioinformatics, 36(1), 104-111.
4. Takei, Y., & Ishida, T. (2021). P3CMQA: Single-Model Quality Assessment Using 3DCNN with
5. Profile-Based Features. Bioengineering, 8(3), 40.