


Chapter 66

Structural and Functional Data Processing in Bio- Computing and Deep Learning

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ABSTRACT

The goal of new biocomputing research is to comprehend bio molecules' structures and functions via the lens of biofuturistic technologies. The amount of data generated every day is tremendous, and data bases are growing exponentially. A majority of computational researchers have been using machine learning for the analysis of bio-informatics data sets. This chapter explores the relationship between deep learning algorithms and the fundamental biological concepts of protein structure, phenotypes and genotype, proteins and protein levels, and the similarities and differences between popular deep learning models. This chapter offers a useful outlook for further research into its theory, algorithms, and applications in computational biology and bioinformatics. Understanding the structural aspects of cellular contact networks helps to comprehend the interdependencies, causal chains, and fundamental functional capabilities that exist across the entire network.

INTRODUCTION

The massive amounts of biological data from genomics, proteomics, metabolomics, transcriptomics, drug development, and other fields need to be supported by mathematical and computational models. Biological challenges like alignment of gene sequence, gene discovery, assembly of gene, prediction of protein structure, gene expression analysis, protein-protein connections, and the modelling of evolution have all been solved using computational biology. By studying the order of biological molecules like DNA and proteins, functional and morphological information, computational tools and software for the evaluation of bioinformatics sought to solve biological puzzles (Chou et al., 2004).

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In microbiology, understanding the structural aspects of cellular contact networks helps us to comprehend the interdependencies, causal chains, and fundamental functional capabilities that exist across the entire network (Klamt et al., 2006). Advances in molecular biology and imaging techniques such as X-ray, electron microscopy and Nuclear Magnetic Resonance (NMR) have led to a revolution in structural biology. Thus permit us to see the complex three-dimensional shapes of protein structures and their functions such as interaction with other proteins and ligands. The growing technological advancements in imaging techniques are visualizing the exact structure of individual-atom in 2-Dimension and 3-Dimension, protein molecules, other body organ structures and blood flow in veins (functional MR Image) (Sljoka et al., 2022).

The computational models explain the various biological processes that are carried out by specific nucleic acid, result in a specific phenotype changes in gene series or protein expression or localization result in a specific disease, and how modifications to cell organisation affect cell behaviour. It is also known as “bioinformatics” the bioinformatics data sets are holding the information. In order to create models for various types of experimental data, such as concentrations, sequences, images, molecules, cells, tissues, and organs, etc., computational biology employs techniques from a broad range of mathematical and computational fields, including complexity theory, algorithms, machine learning, robotics, etc.

COMPUTATIONAL METHODS

Computing scientists must be able to identify computational methods and techniques that can be used to address problems that may arise in unfamiliar fields. The necessary biological concepts will be used to describe the problems. The typical stages of computational processing include data pre-processing, model selection, model validation, hyper parameter adjustment, and performance evaluation. Recent works employs machine learning for all the works. The remaining chapter describes the machine learning models and recent research works employed machine learning for structural and functional analysis.

Artificial Neural Network (ANN)

ANN is the imitation of human brain and a network made up of computational concepts. It includes several layers with ascends of neurons. The neurons are connected with other neurons in the same layer and with neurons in different layers. Three kinds of layers such as input layer, hidden layer and output layer compiled as common. Each neuron performs computation on the input data with additionally added weight value. Usually, two stages of processes carried out in ANN that are known as training stage and testing stage. The weight value of a connection determination is the primary work in the training stage. The weighted sum of all inputs is passed to the activation function. The activation function plays a role as threshold detection that finalize the node to fire or not. There are distinctive activation functions available. They are,

- Logistic sigmoid function
- Hyperbolic tangent function
- Softmax function
- Rectified Linear Unit (ReLU) function
- Parametric ReLU function

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