Chapter 5 Deep Learning in Bioinformatics: Principles and Applications

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ABSTRACT

The power of deep learning-based models to process and interpret complex biological data has opened new avenues for research and discovery, offering innovative solutions to longstanding and emerging challenges in bioinformatics. This chapter explores how deep learning is researchers solve some of the most pressing challenges in bioinformatics today. From predicting protein structures to speeding the development of new drugs, these models are at the forefront of bioinformatic research, redefining the boundaries of the. The authors explore applications where deep learning has made significant contributions and the synergy between deep learning techniques and bioinformatics, illustrating how this powerful collaboration is helping to advance medical research, drug discovery, and beyond. The current challenges and limitations of such methods are also covered in this chapter. The goal is to provide insights into the transformative impact of deep learning on bio-

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informatics, underscoring its potential to revolutionize our understanding of life.

1. INTRODUCTION

Bioinformatics employs a variety of tools to achieve its goal of understanding biological processes through computational methods. Among these tools, artificial intelligence (AI) models and techniques, such as machine learning and deep learning, have proven themselves particularly effective in addressing complex problems with poorly understood rules and mechanisms, as illustrated in Figure 1. These AI techniques have enabled significant breakthroughs in bioinformatics challenges such as protein structure prediction, genomic sequence analysis, and drug discovery. By leveraging the power of AI, bioinformatics continues to advance our understanding of biology, providing new insights and accelerating research in molecular biology and genetics.

With the advent of omics, the abundance of data brought answers but also raised new questions and challenges. A great example is high-throughput sequencing, a technology that emerged in the late 20th century that gave us genomics and enabled large-scale endeavors such as the human genome project (International Human Genome Sequencing Consortium, 2001). By reducing the costs and increasing the speed of obtaining genetic sequences of organisms, fields such as phylogenetics (Zhou et al., 2013) have advanced significantly and continue to do so, enabling us to perform more complex analyses and better understand evolution and its dynamics (John et al., 2021). However, this fast-paced increase in available data also brings challenges, such as: (i) How do you interpret all this data? (ii) How do you find patterns in it? Moreover, (iii) how to correlate multiple data layers in multi-omics studies?

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