Graph Neural Networks - Applications in Bioinformatics

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Graph Neural Networks (GNNs) have emerged as powerful tools for modeling complex, non-Euclidean data structures, making them especially valuable in the life sciences. With the rise of high-throughput technologies, biological data is increasingly represented as graphs—ranging from drug compounds and protein–protein interaction networks to gene regulatory networks. GNNs enable the extraction of meaningful patterns from such data, offering new opportunities in bioinformatics and computational biology. This workshop introduces participants to the foundational principles of GNNs and their applications in life sciences. We will cover the core architecture and mechanisms of GNNs, illustrating how they address three major research challenges: node-level prediction, edge-level prediction, and graph-level prediction. The session will include a case study followed by a hands-on practical segment, where participants will build GNN models for real-world biological data, including steps for graph construction, model training, and evaluation. We will also discuss key considerations such as interpretability challenges, best practices in designing biological graph models, and future directions at the intersection of network biology and machine learning.

References

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