

Preface

Graph neural networks (GNNs) are artificial neural networks designed for tasks whose inputs are graphs. Because graphs usually do not have a canonical ordering of their nodes, GNN architectures are commonly designed to be permutation equivariant: reordering the nodes in the input reorders the corresponding node representations in the same way. For graph-level prediction tasks, GNNs typically use a permutation-invariant readout function, whose output is unchanged by the ordering of the nodes. A prominent example is molecular drug design. Molecules can be represented as graphs, with nodes for atoms and edges for atomic bonds, often including known chemical properties as features. Inputs may thus differ in size, due to varying number of atoms and bonds. A graph-level task may be to predict the efficacy of a given molecule for a specific medical application, such as eliminating *E. coli* bacteria.¹

In the present book, ten typical literatures about graph neural networks published on international authoritative journals were selected to introduce the worldwide newest progress, which contains reviews or original researches on graph neural networks. We hope this book can demonstrate advances in graph neural networks as well as give references to the researchers, students and other related people.

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Scientific Research Publishing

September 3rd, 2026

¹ https://en.wikipedia.org/wiki/Graph_neural_network