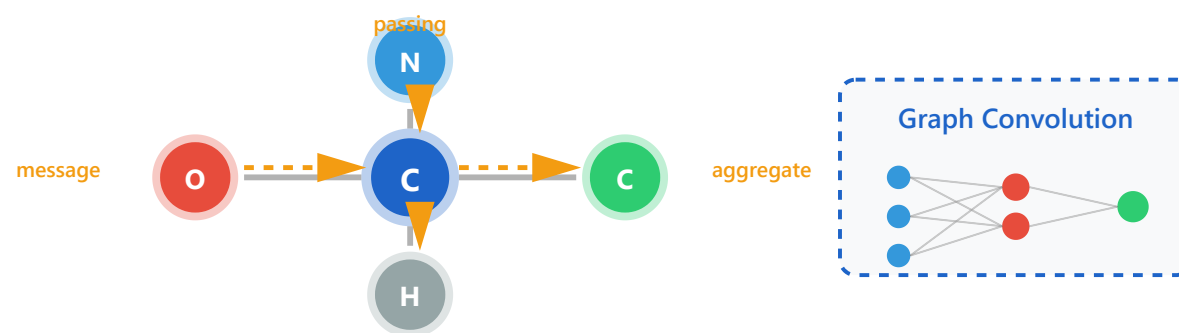


Graph Neural Networks



● Atoms (Nodes) — Bonds (Edges) — Message Flow

Molecular graphs

Atoms as nodes, bonds as edges

Message passing

Information flow between atoms

Graph convolutions

Feature aggregation operations

Attention mechanisms

Weighted information aggregation

Pooling strategies

Graph-level representations