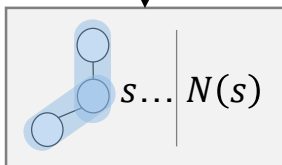
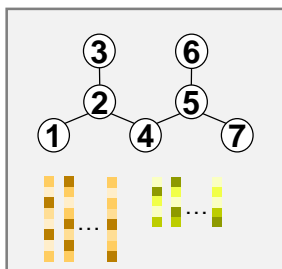
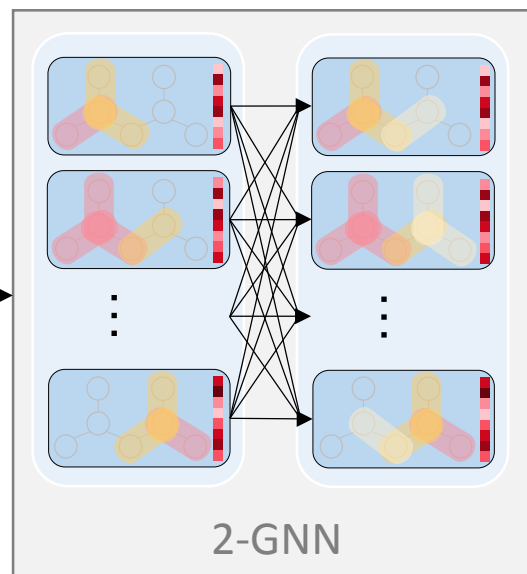
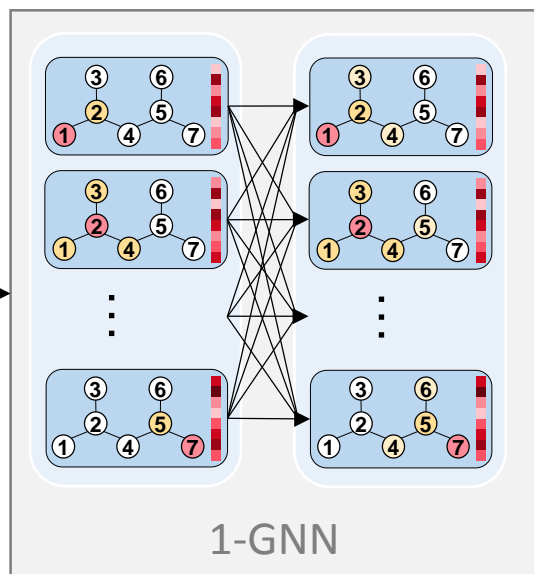


SMILES



Python & RDKit & k-GNN



Python & PyTorch & PyTorch Geometric

Pooling

Pooling

DCN, MON, or RON

DCN

MON

RON