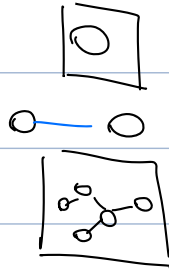


# <1-2> Applications of Graph ML

## • Tasks

- Node classification
- Link prediction
- Graph classification
- Clustering
- Graph generation
- Graph evolution



ex:

knowledge graph completion  
Molecule property prediction

## • Examples

### Node level

#### • Protein Folding

a.a. sequence  $\xrightarrow{\text{predict}}$  protein 3D structure

> Alpha Fold

Protein  $\xrightarrow{\text{as}}$  spatial graph

① Node : a.a.

② Edge : a.a. — a.a.  
proximity

### (link level)

### Edge level

#### • Recommender System

①

2 types of Node

user



item



predict

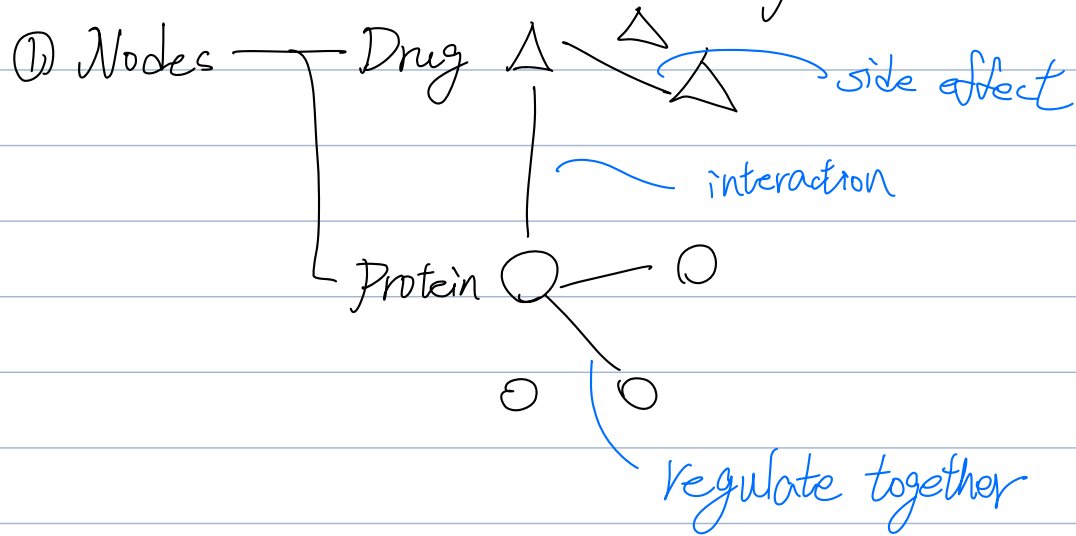
buy

② Edge:

User-item  
interaction

## • Drug Side Effect

patient take mutiple drugs  $\Rightarrow$  Task: Given a Pair of drugs  
predict adverse side effects.



subgraph level

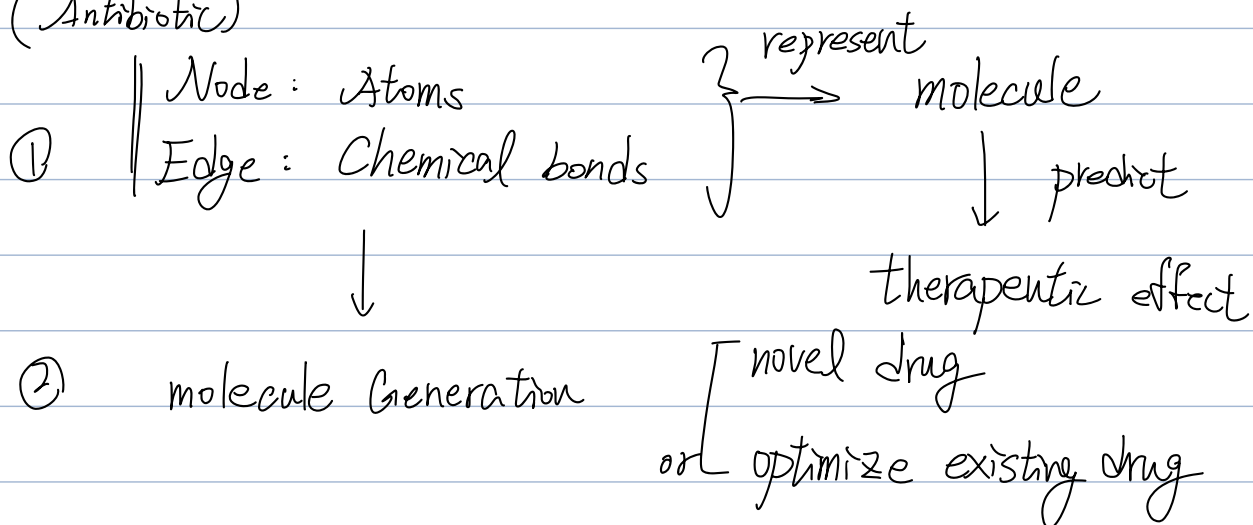
## • Traffic Prediction

Node : Road segments

Edge : Connectivity between road segments

Graph level

## • Drug Discovery (Antibiotic)



# • Physics Simulation

Node : Particle

Edge : Interactions between particles

Graph  $\rightarrow$  Graph

