Towards a fully automated exploration of chemical space
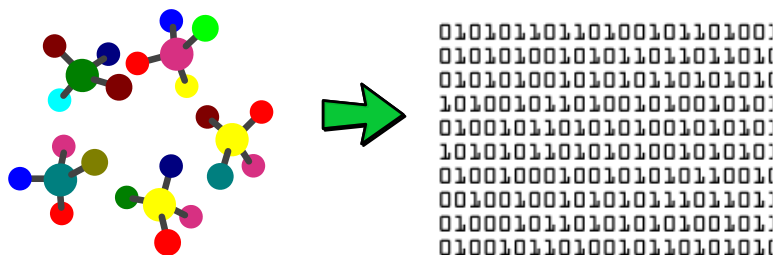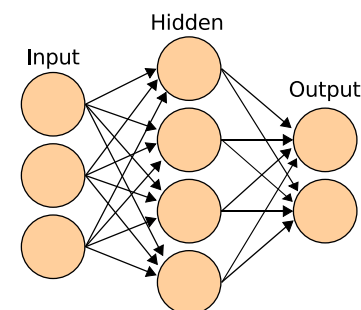
Molecule generation

Feature representations
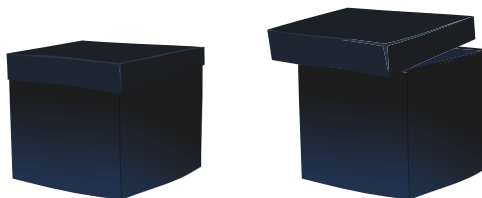

Models

Search in discrete spaces

Multi-objective optimization

Scheduling of tasks to resources