ML methods for materials discovery

1. Classical Machine Learning

1a. Supervised Learning

Regression
- e.g., linear regression, SVM
- predict quantitative materials properties
(e.g., bandgap, hardness, thermal conductivity)

Classification
- e.g., decision tree, random forests
- predict categorical outcomes
(e.g., crystal structure type, phase stability)

1b. Unsupervised Learning
- e.g., PCA, t-SNE
- clustering, Dimension Reduction
- materials categorization, discovery new phases

2. Deep Learning

2a. Feedforward Neural Networks (FNN)
- most basic deep learning architecture
- predict material properties from descriptors

2b. Convolutional Neural Networks (CNN)
- designed to process image data
- microscopy & diffraction image analysis

2c. Graph Neural Networks (GNN)
- molecules/Crystal structures as graphs
(nodes = atoms, edges = bonds)

2d. Generative Models
- e.g., GANs, VAEs
- propose new compounds or structures

Reinforcement Learning
- optimize sequential decision-making tasks
- reaction pathways optimization

Baysian Optimization
- probablistic model guiding next experiment
- minimize the number of trials

Active learning
- model-driven selection of informative experiments
- maximizing information gain

Natural Language Processing
- text mining & literature analysis
- automatic extraction of data from articles