CyberMAGICS Workshop: Introduction to Machine Learning

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Machine Learning hands-on: Tian Sang, Ruru Ma, Ken-ichi Nomura

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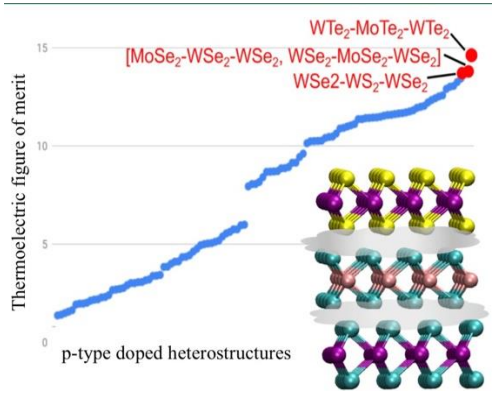
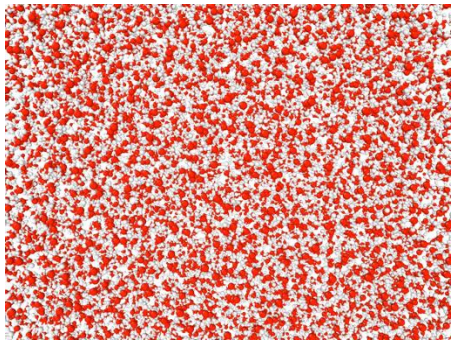
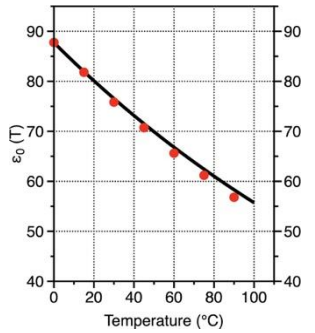
Material Modeling with Machine Learning

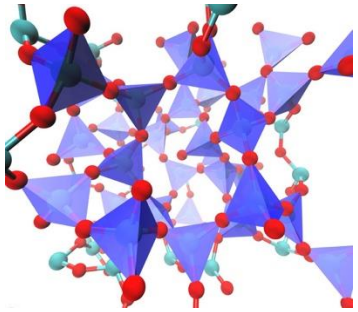
Active learning for accelerated material design

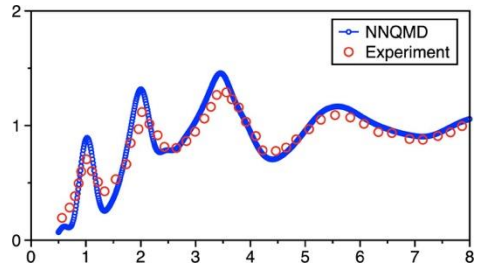


Large-scale and long-time neural network QMD simulations

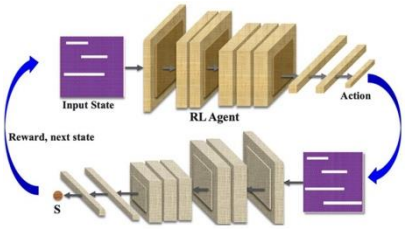


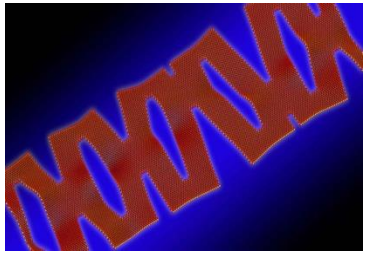


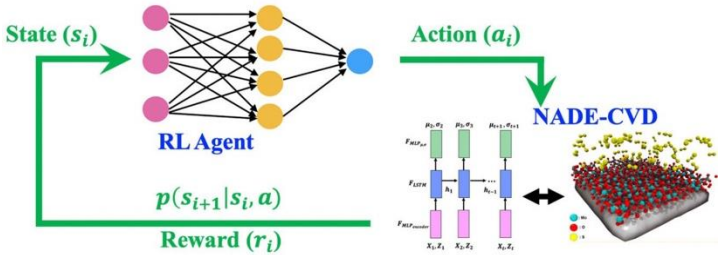




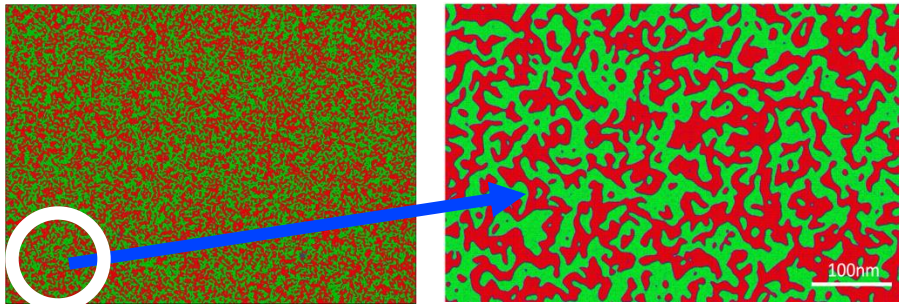
Reinforcement learning for quantum materials synthesis







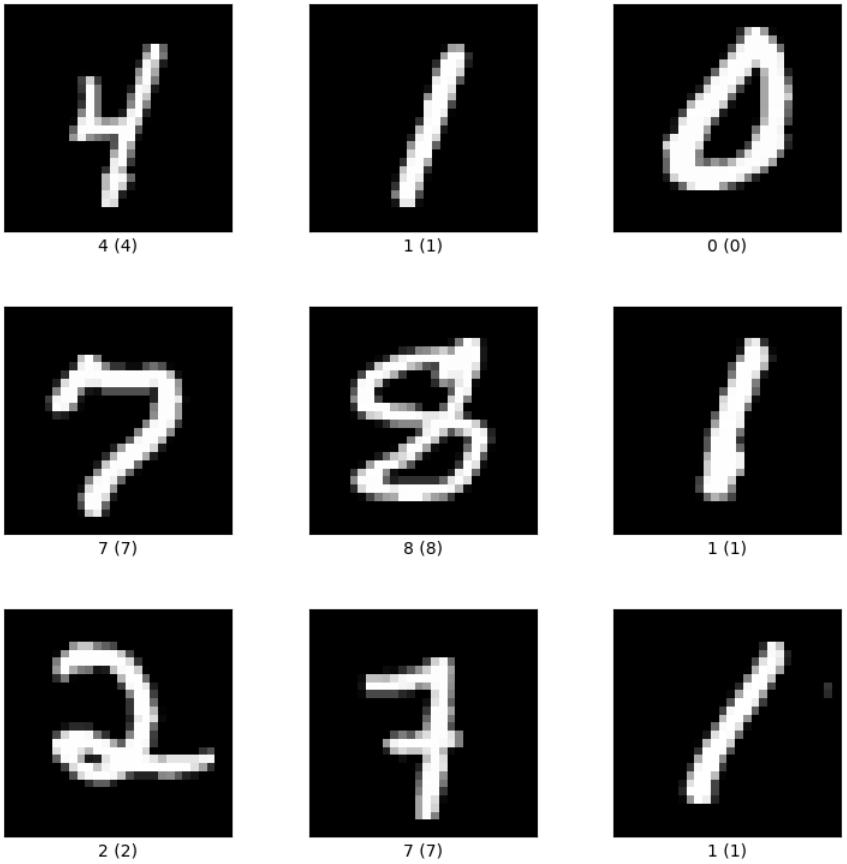
Laser-induced topological pattern formation



$3.8\ \mu m$

What is Machine Learning?

Image classification using MNIST dataset



What is Machine Learning?

What is Machine Learning?

Google I/O 2019

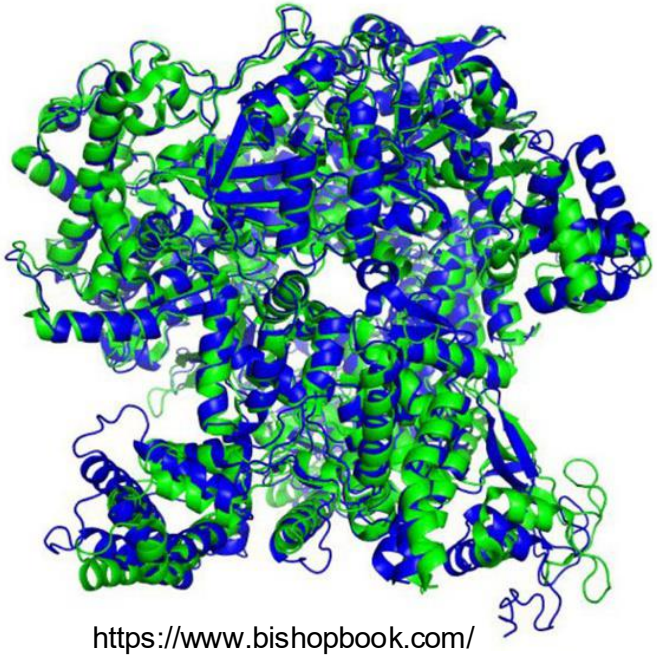
Other Machine Learning Applications

- **Protein Fold – AlphaFold**
  - Amino acid sequence predication and 3D structure analysis

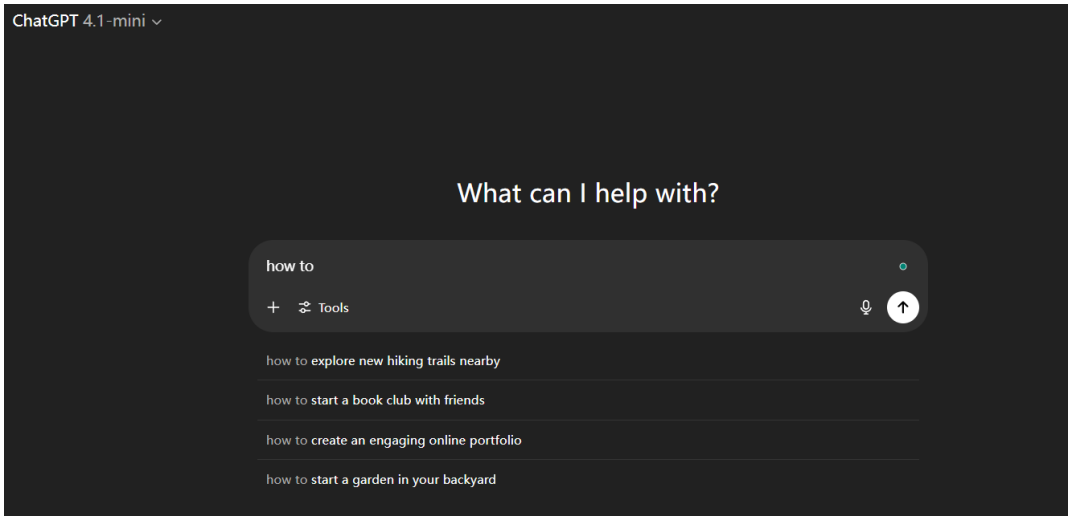
- **Natural Language Processing**
  - Large language models like OpenAI's GPT

- **Computer Vision**
  - Facial Recognition
  - Self-driving Cars

- **Financial Modeling and so on…**



https://www.bishopbook.com/



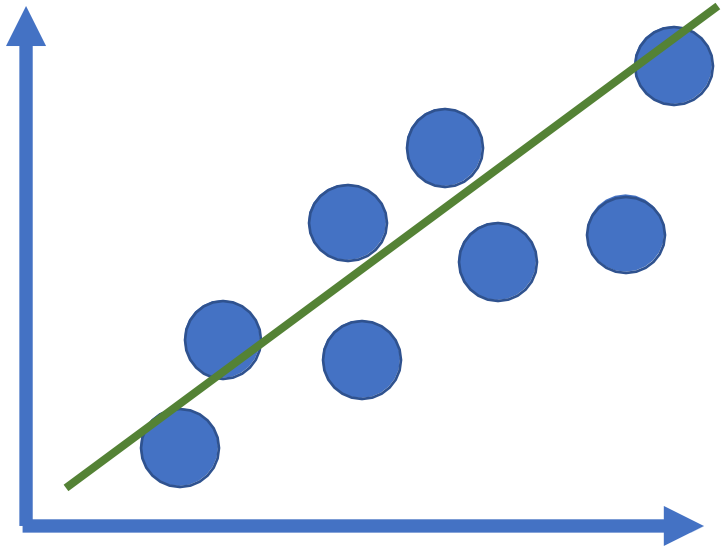
Classification vs Regression

Classification

Predict class label

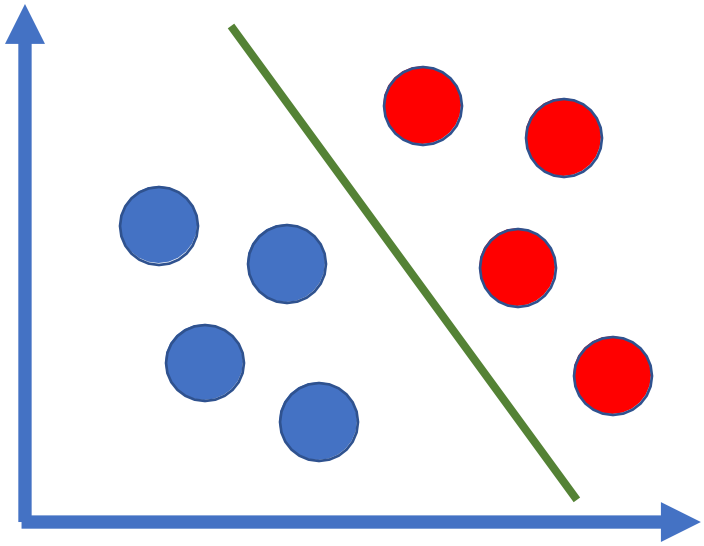
Regression

Predict real value

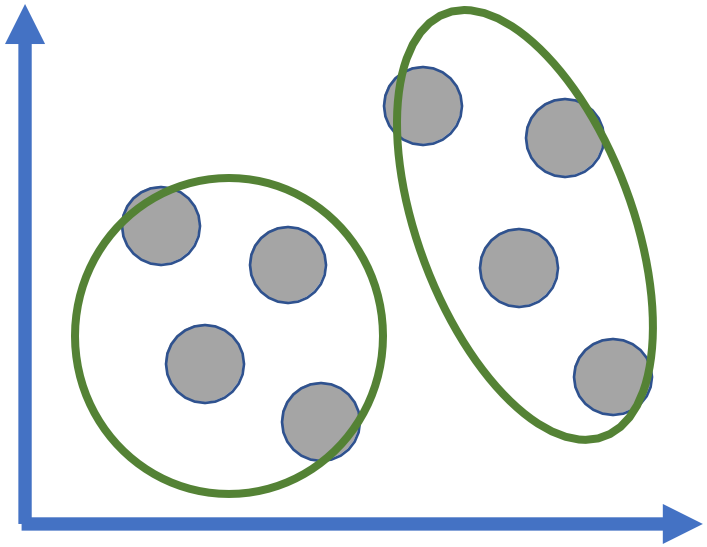


Supervised vs Unsupervised

Supervised:
Data are "labeled"
classification, regression

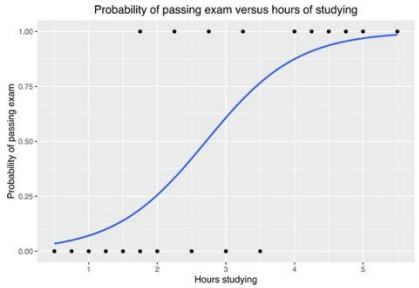


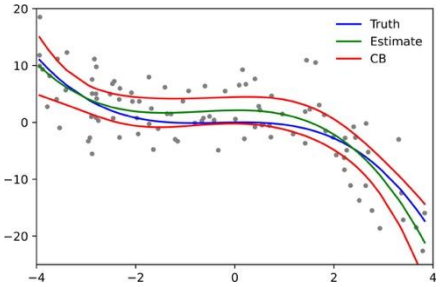
Unsupervised:
Data are "not labeled"
Clustering, dimensionality reduction

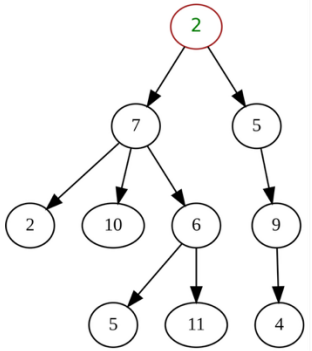


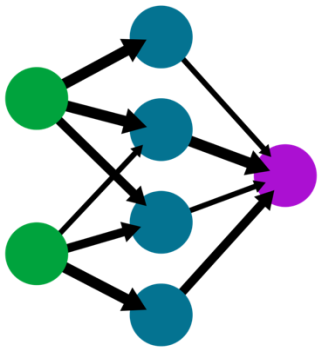
ML Algorithms

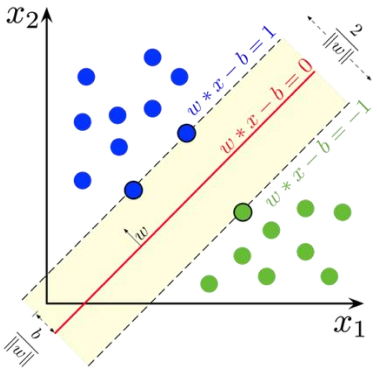
- Linear/polynomial Regressions
- Logistic Regression
- K-Nearest Neighbors
- Decision Trees
- Random Forests
- Support Vector Machines
- Neural Networks
- Bayesian Networks
- PCA & t-SNE

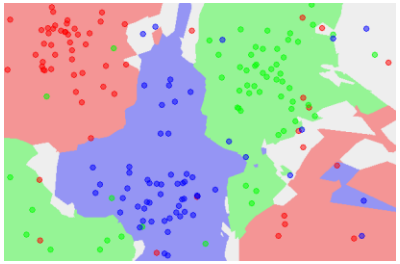








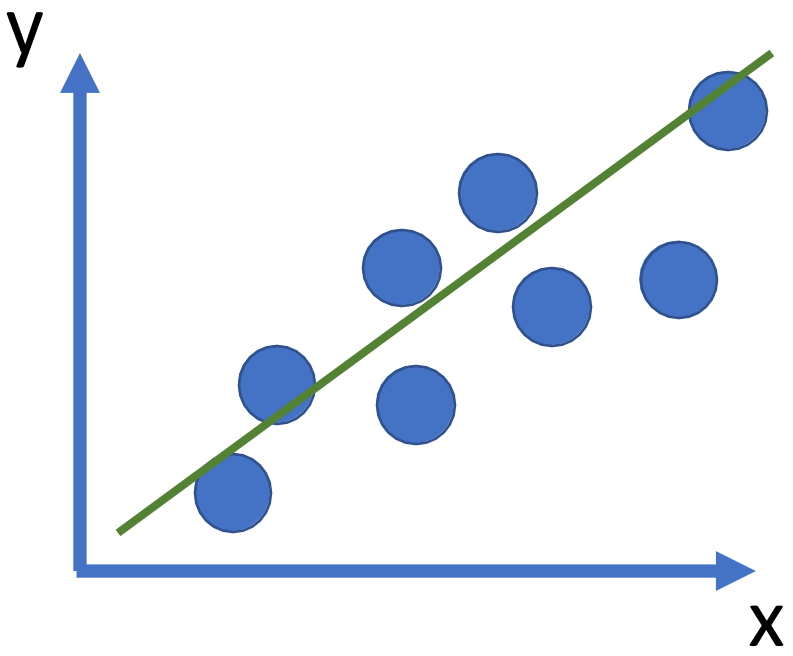




Linear Regression

- **Assumes a linear relationship between the input variable(s) and the output variable (y)**
- **Can be univariate, multivariate, polynomial, logarithmic, …**
- **Coefficients (b_i) are obtained by minimizing the sum of the difference between all data and line**

$$\hat{y} = \beta_0 + \beta_1 x_1 + \cdots + \beta_n x_n = \boldsymbol{x}_i^T \boldsymbol{\beta}$$

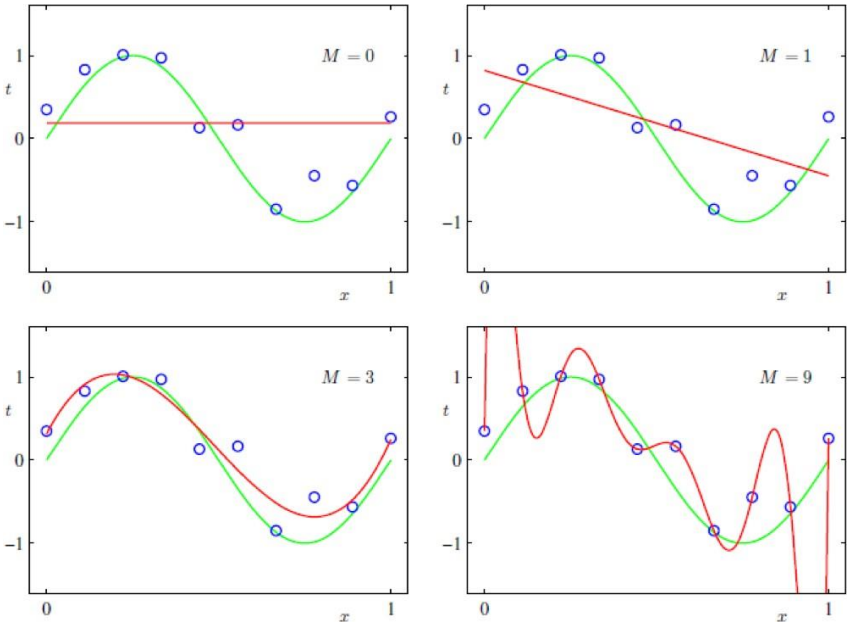


$$L = \frac{1}{N} \Sigma_{i=1}^{N} \left(\hat{Y}_i - Y_i \right)^2$$

Overfitting and Regularization

- A good ML model should accurately predict existing training data as well as "unseen" (out-of-sample) data
- A model with many parameters tends to pick up noise in data and poorly perform on unseen data, i.e. overfitting
- Regularizations, such as Ridge and LASSO

$$\hat{y} = \beta_0 + \beta_1 x_1 + \cdots + \beta_n x_n = \boldsymbol{x}_i^T \boldsymbol{\beta}$$

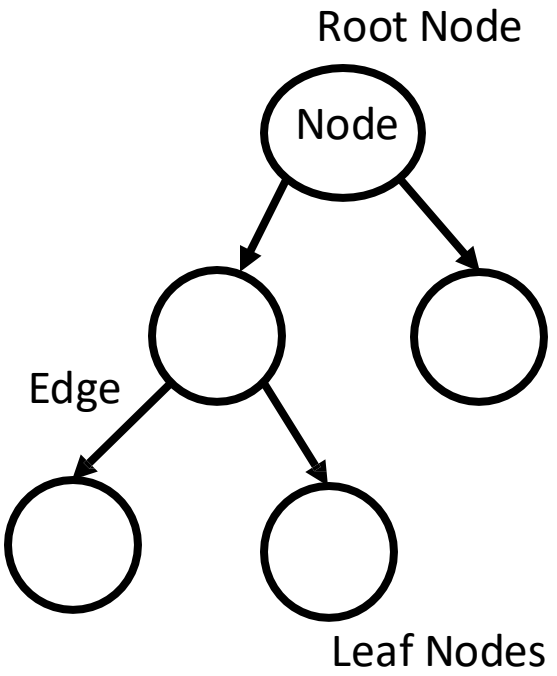


True function
Training data with noise
Model predictions

$$\min_{\beta,\beta_0} \left\{ \frac{1}{N} \|y - X\beta\|^n \right\} \; with \; \|\beta\| \leq t \; or \; \|\beta\|^2 \leq t$$

Decision Tree and Random Forest

- Used for classification or regression
- Starting from root node, "ask a question and select an answer" until a leaf node is reached
- Tree construction based on information theory
  - Gini index/entropy for classification
  - Variance/RMSE for regression
- Easy to construct and interpret, but also overfit

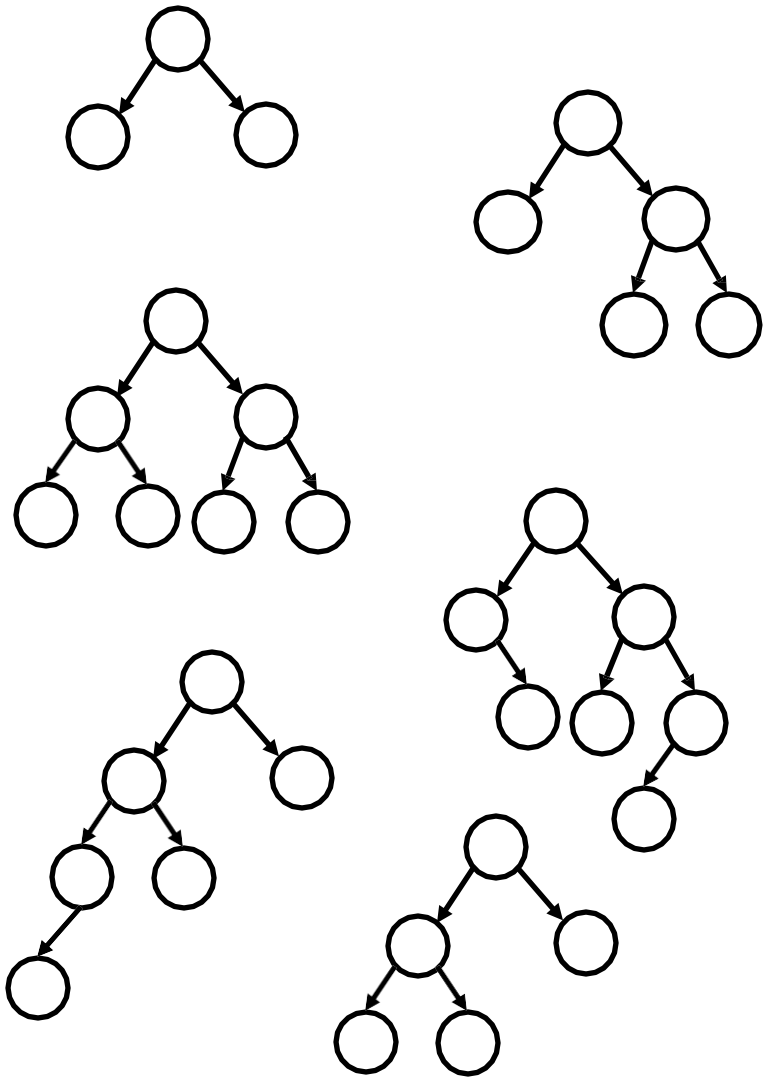


$$I_{Gini} = 1 - \Sigma_j p_j^2$$

$$I_{entropy} = -\Sigma_j p_j \log(p_j)$$

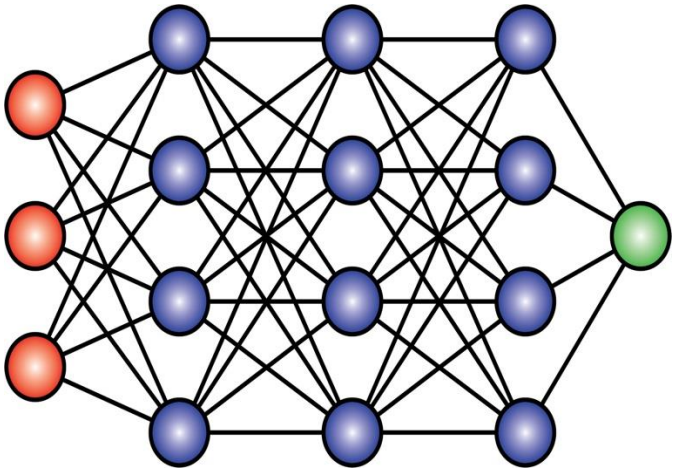
Decision Tree and Random Forest

- Ensemble of decision trees
- Aggregate predictions from each tree as the model prediction
- Good prediction accuracy, generalizability, robust to overfitting
- Less interpretability to single decision tree

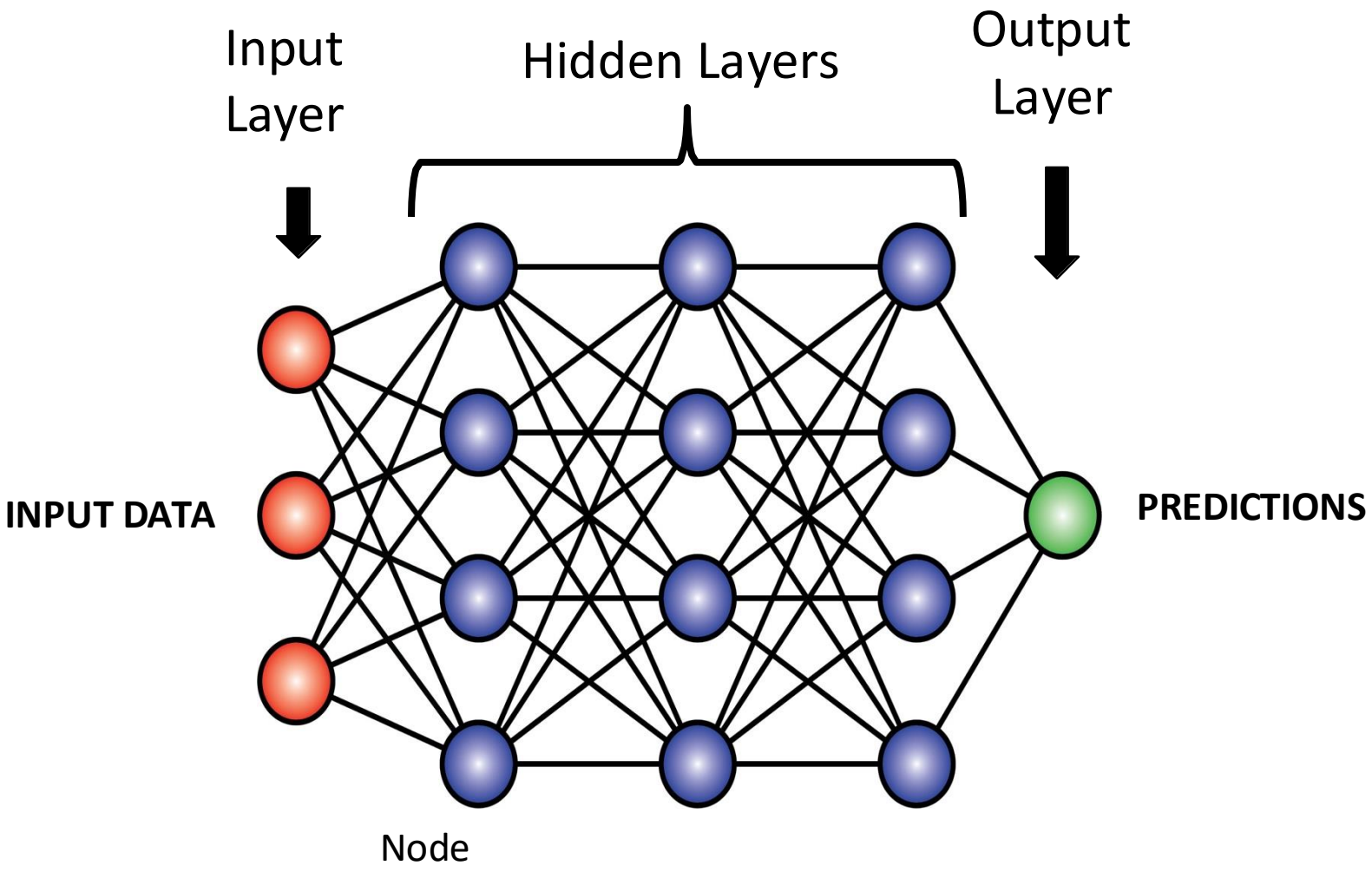


Neural Network

- Inspired by biological brain
- A universal function approximator
- A key component in other deep learning algorithms
- Hyperparameters
  - Number of nodes
  - Degree of connectivity of nodes
  - Number of layers in network

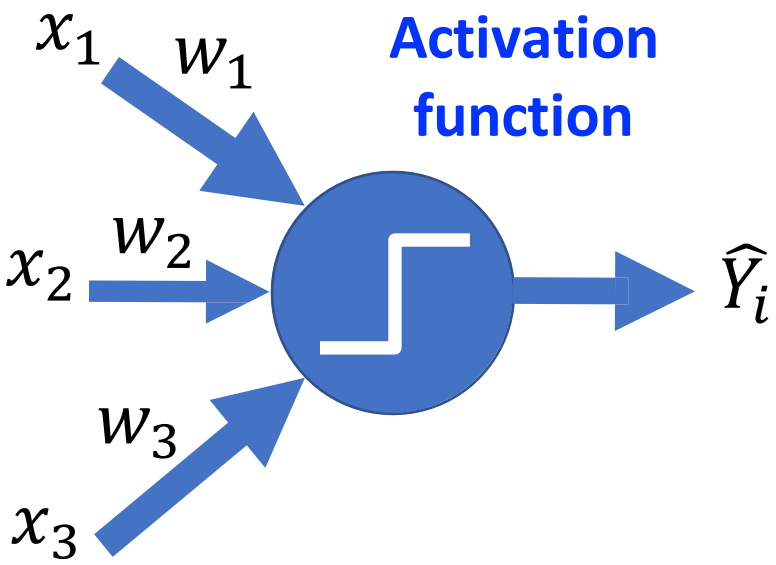


Neural Network



Neural Network

- On each node, outputs (x) from previous layer are aggerated with weights (w)
- A non-linear activation function transforms the aggregated inputs and pass it to next layer
- Compute Loss function (difference between model prediction and given true value) after the output layer

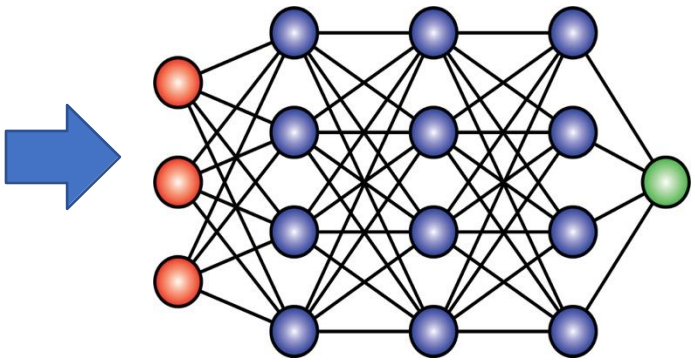


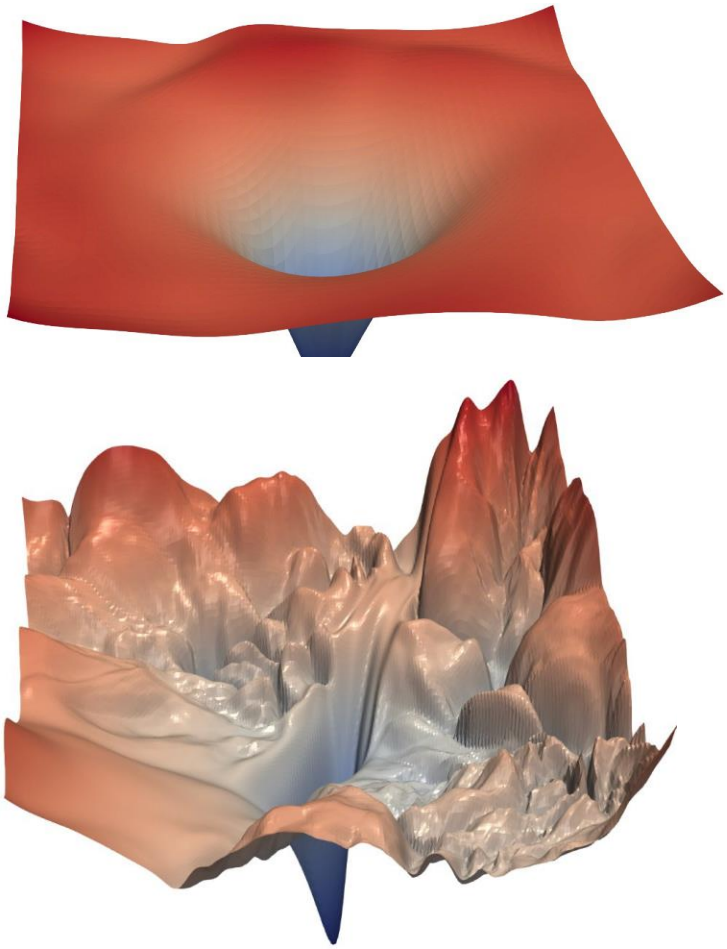
$$L = \frac{1}{N}\Sigma_{i=1}^{N}\left(\widehat{Y}_i - Y_i\right)^2$$

Neural Network Training

- **Network parameters are "trained" by minimizing loss function**
- **Stochastic gradient decent is commonly used**

$$\Delta w = -\partial L / \partial w$$





Loss function landscape

H. Li et al., *"Visualizing the Loss Landscape of Neural Nets,"* arXiv:1712.09913v3

Moving Forward

- **Linear algebra, Statistics & Probability, Python**
- **Online courses**
  https://www.coursera.org/browse/data-science/machine-learning
- **Textbooks**
  Deep Learning Foundations and Concepts:
  https://www.bishopbook.com
  Deep Learning: https://www.deeplearningbook.org/
  The Elements of Statistical Learning:
  https://hastie.su.domains/ElemStatLearn/
- **Python Programming**
  Scikit-learn https://scikit-learn.org
  Pytorch https://pytorch.org
  Tensorflow https://www.tensorflow.org