CyberMAGICS Workshop: Introduction to Machine Learning

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Machine Learning hands-on: Anikeya Aditya, Nitish Baradwaj, Taufeq Razakh, Liqiu Yang

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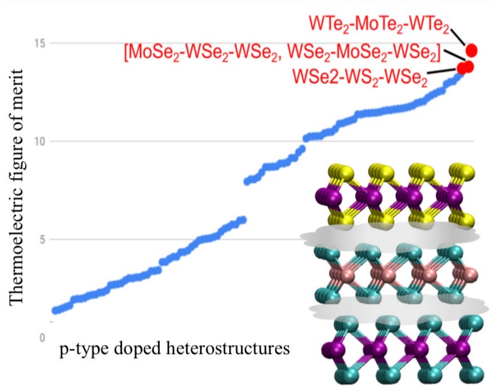
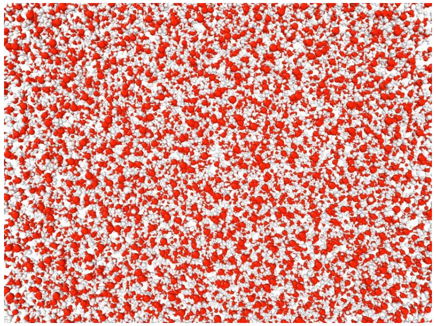
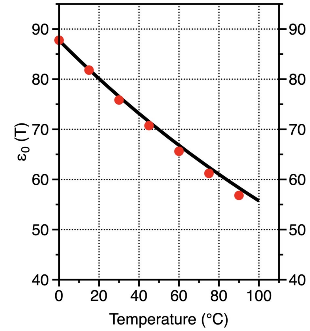
Material Modeling with Machine Learning

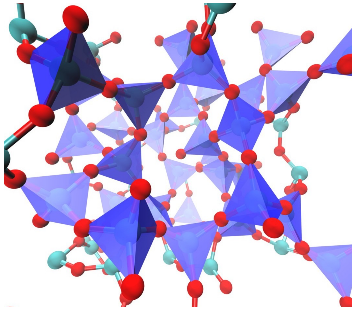
Active learning for accelerated material design

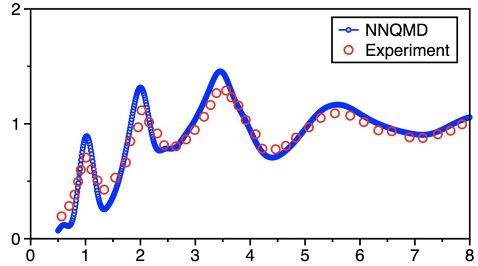


Large-scale and long-time neural network QMD simulations

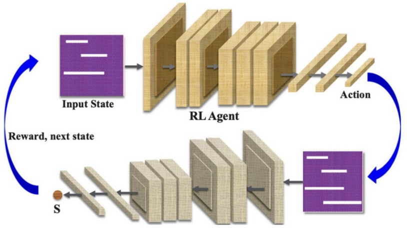


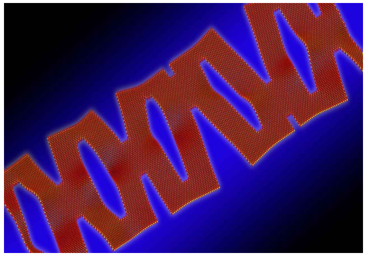


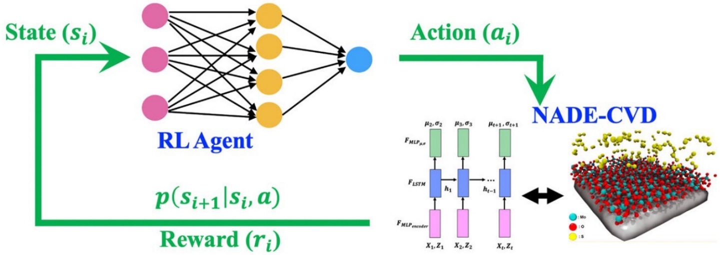




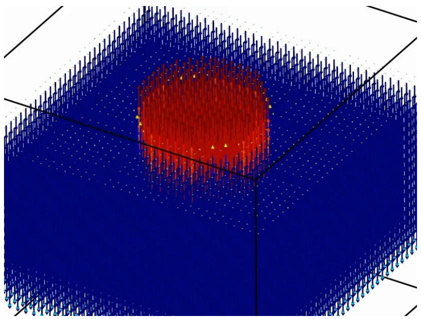
Reinforcement learning for quantum materials synthesis





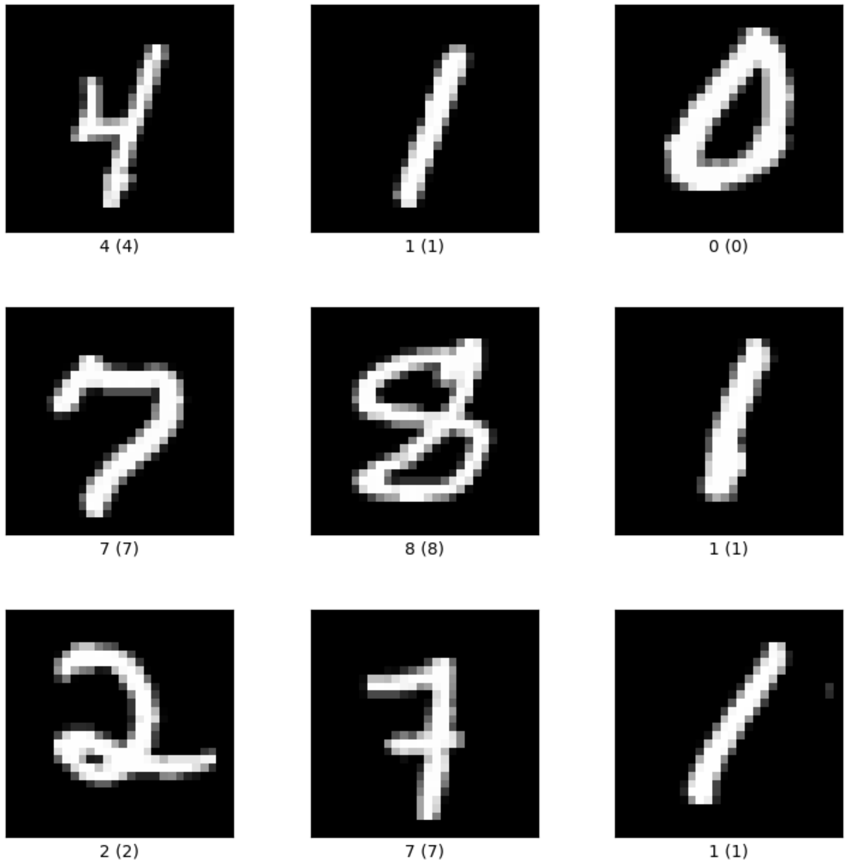


Deep generative model for ferroelectrics



What is Machine Learning?

Image classification using MNIST dataset



What is Machine Learning?

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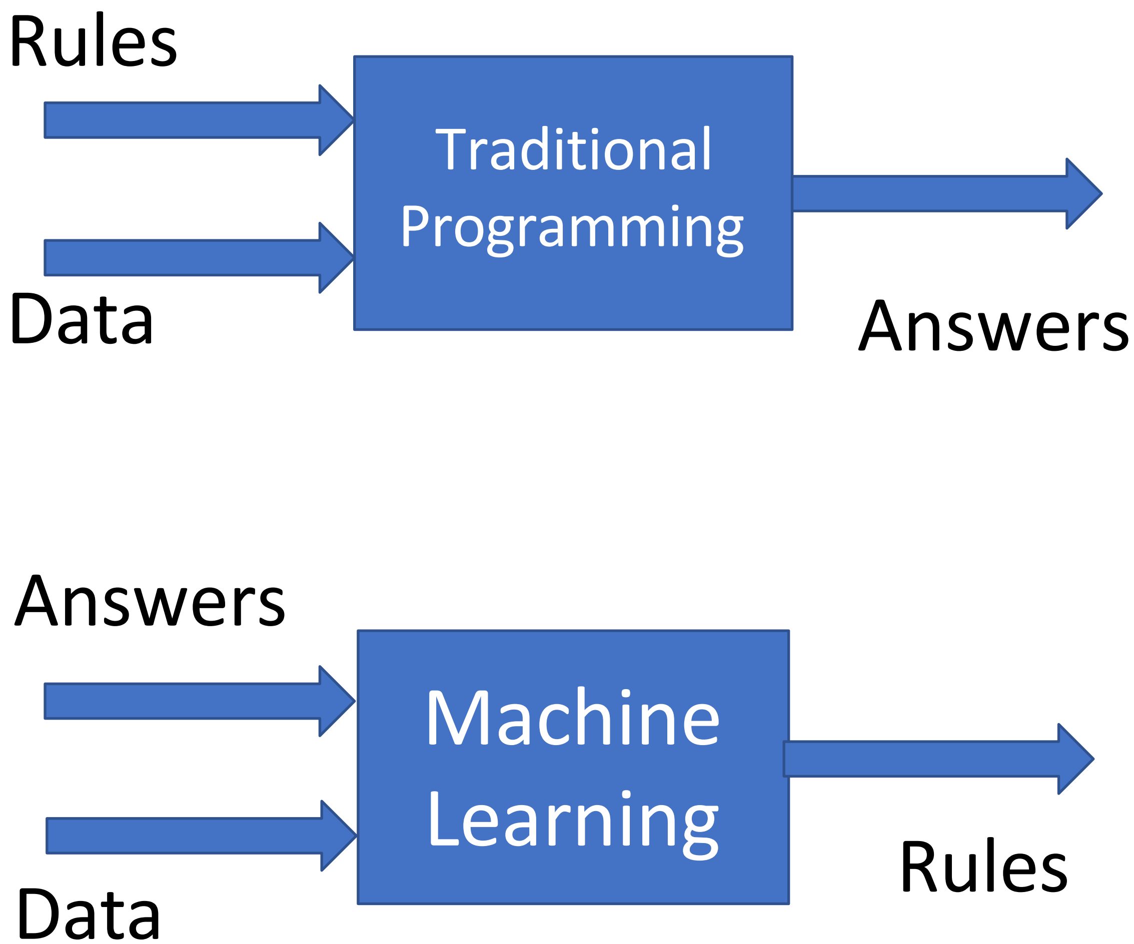
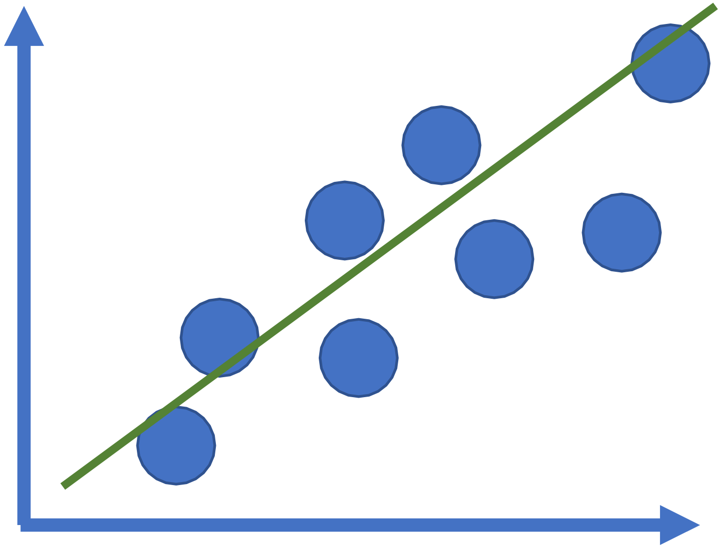


Google I/O 2019

Classification vs Regression

Classification
Predict class label

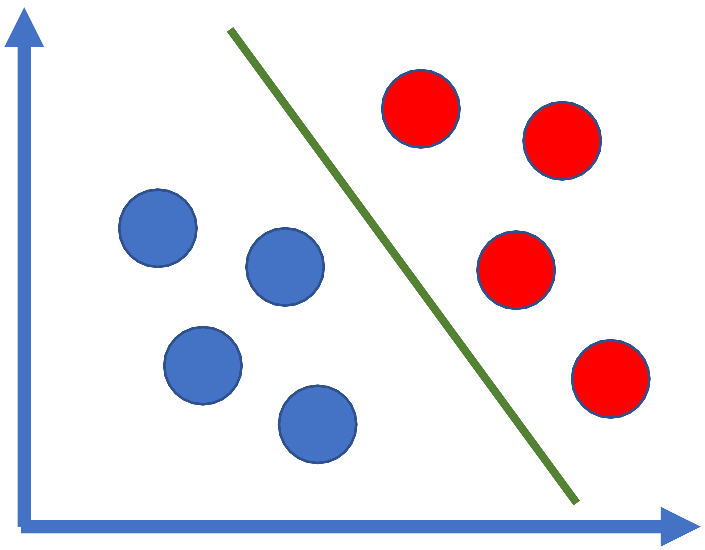
Regression
Predict real value

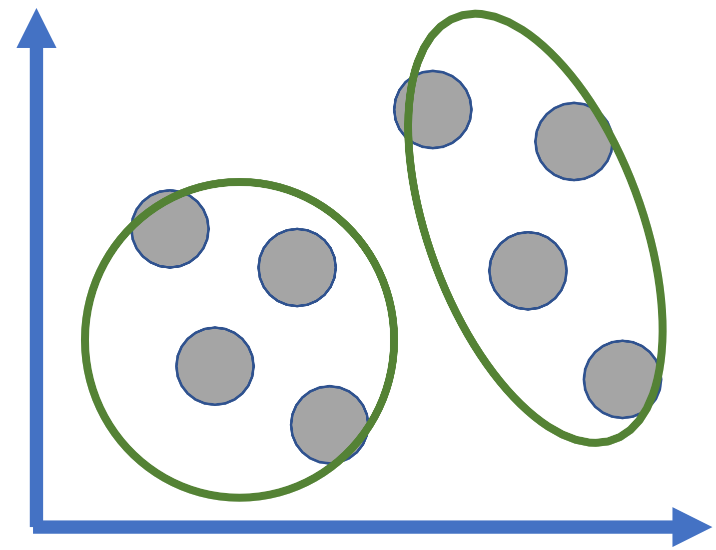


Supervised vs Unsupervised

Supervised:
Data are ”labeled”
classification, regression

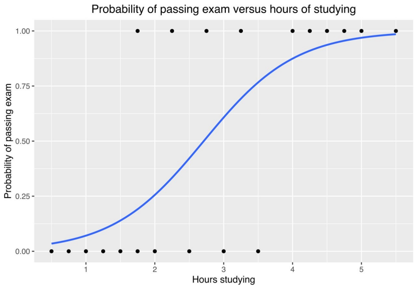
Unsupervised:
Data are “not labeled”
Clustering, dimensionality reduction

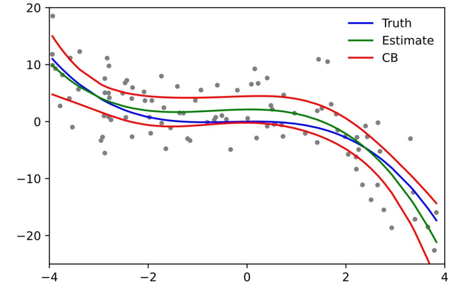


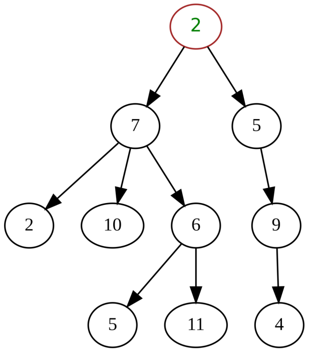


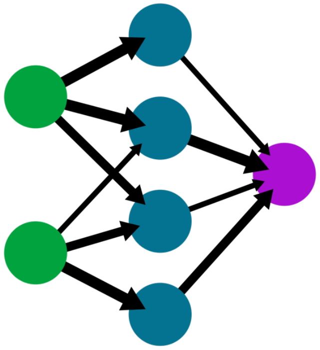
ML Algorithms

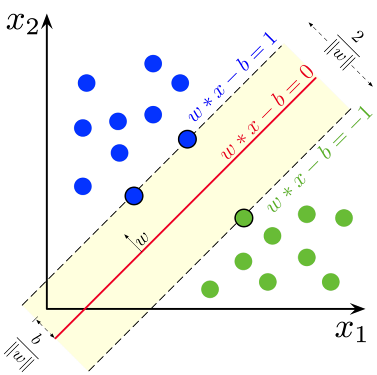
- **Linear/polynomial Regressions**
- **Logistic Regression**
- **K-Nearest Neighbors**
- **Decision Trees**
- **Random Forests**
- **Support Vector Machines**
- **Neural Networks**
- **Bayesian Networks**
- **PCA & t-SNE**

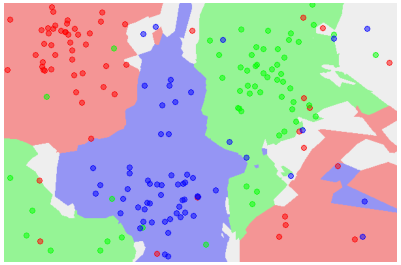








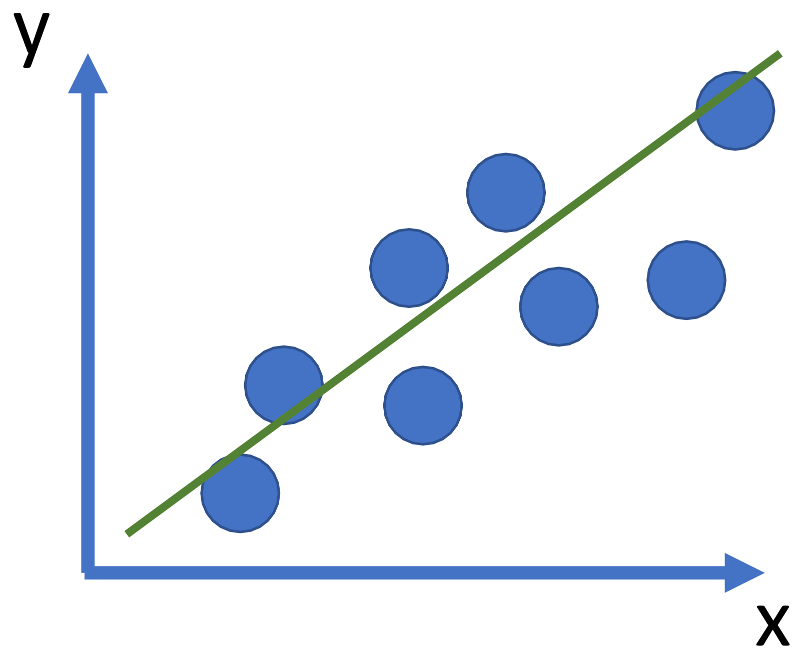




Linear Regression

- **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**

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

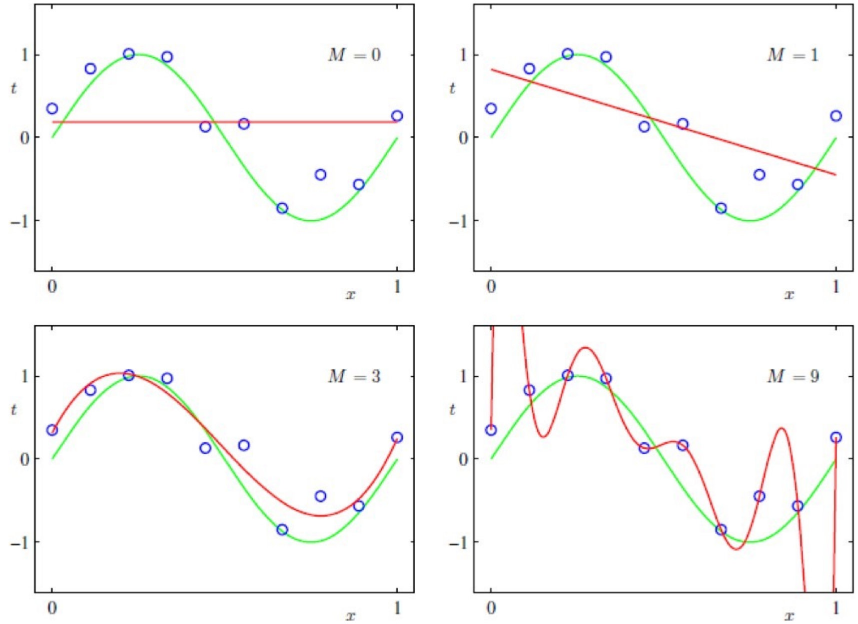


$$L = \frac{1}{N} \Sigma_{i=1}^{N} \left(\widehat{Y}_i - Y_i\right)^2$$

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**

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

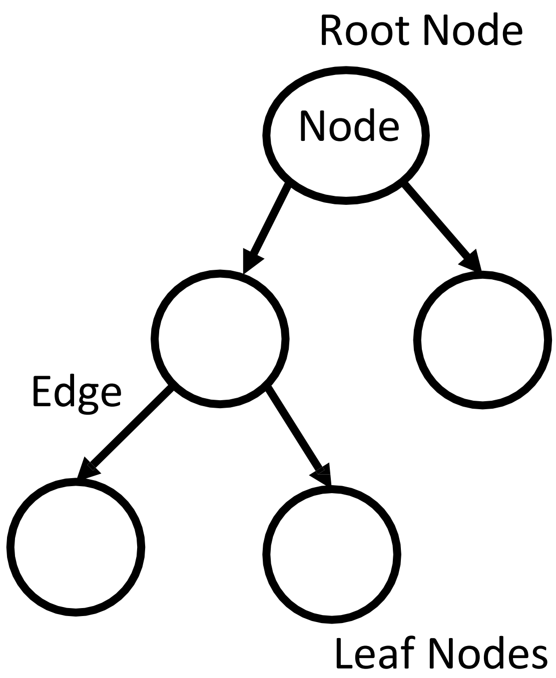


True function
Training data with noise
Model predictions

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

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**

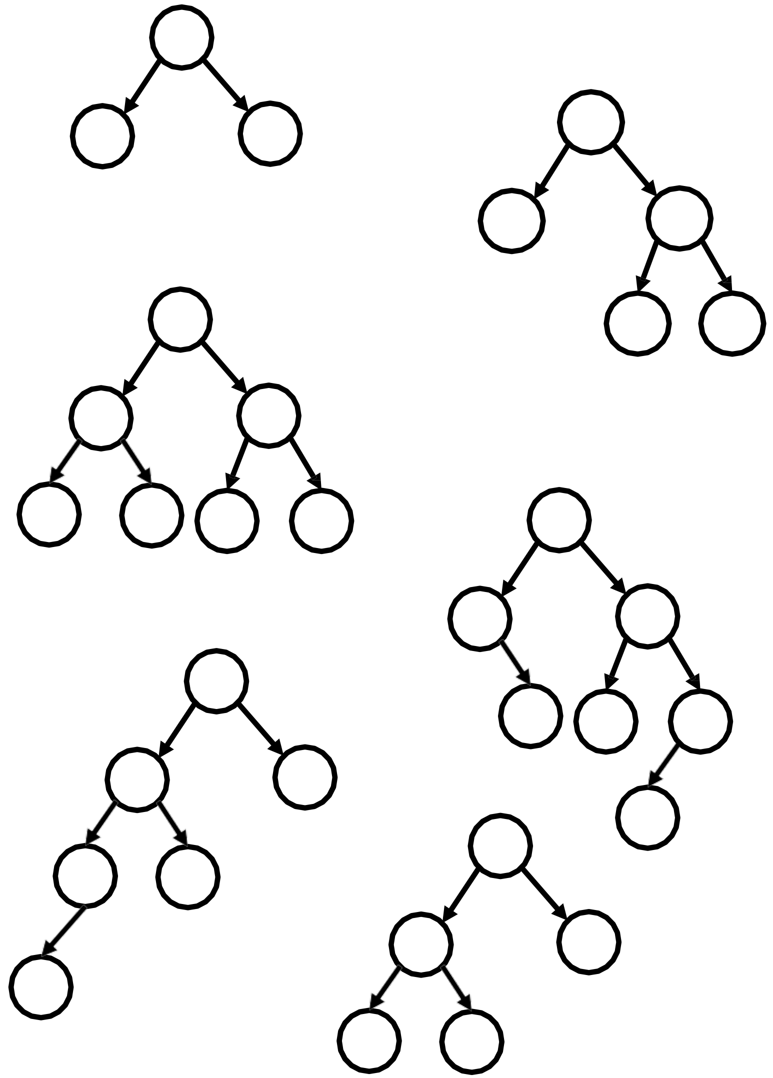


$$I_{Gini} = 1 - \Sigma_j p_j^2$$

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

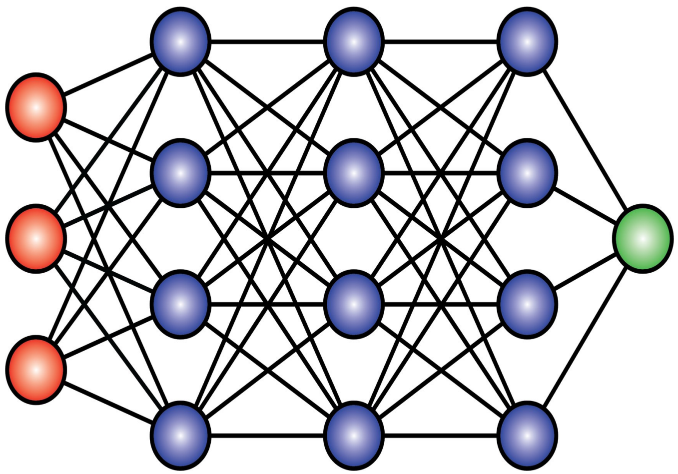
Decision Tree and Random Forest

- 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

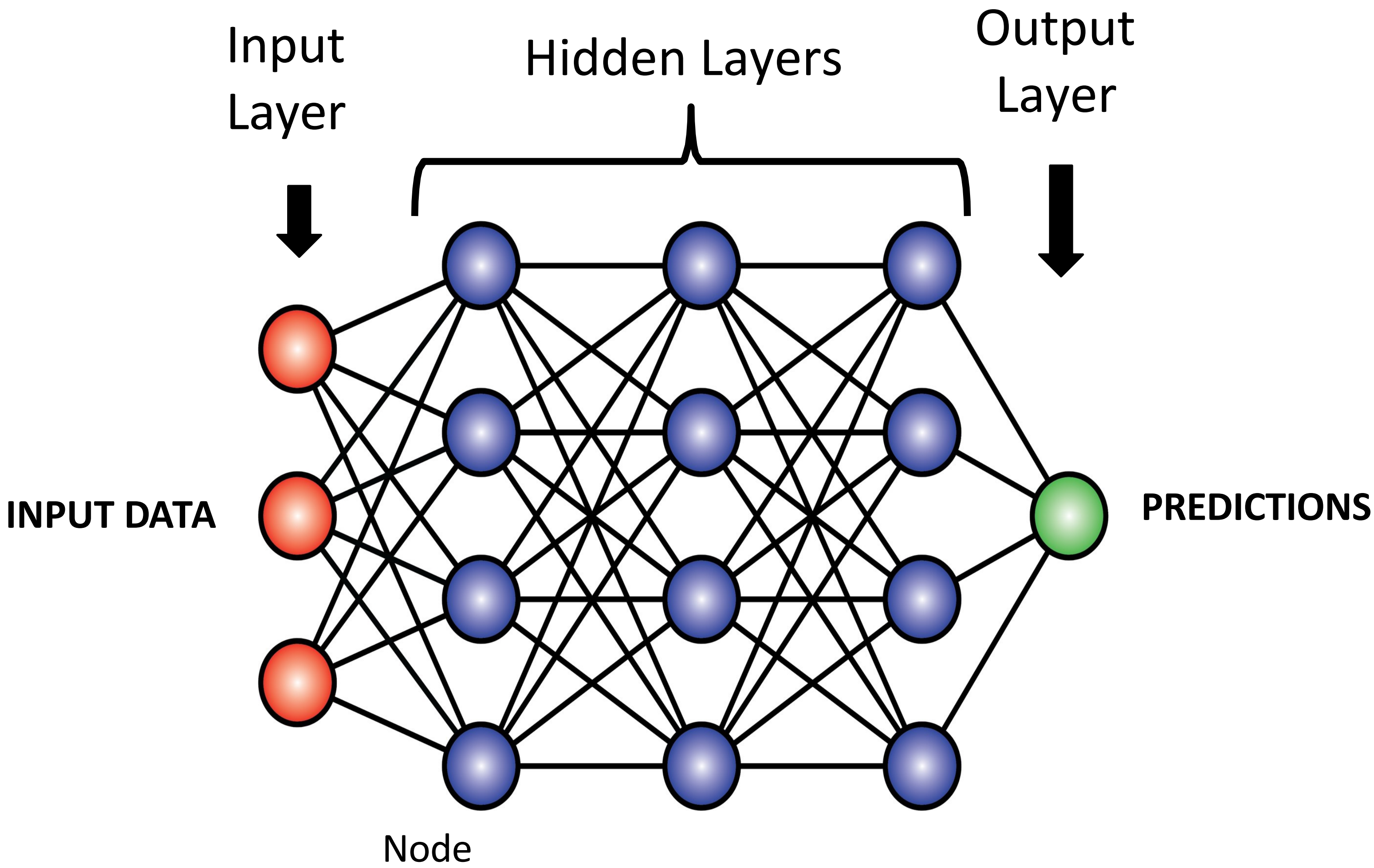


Neural Network

- 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

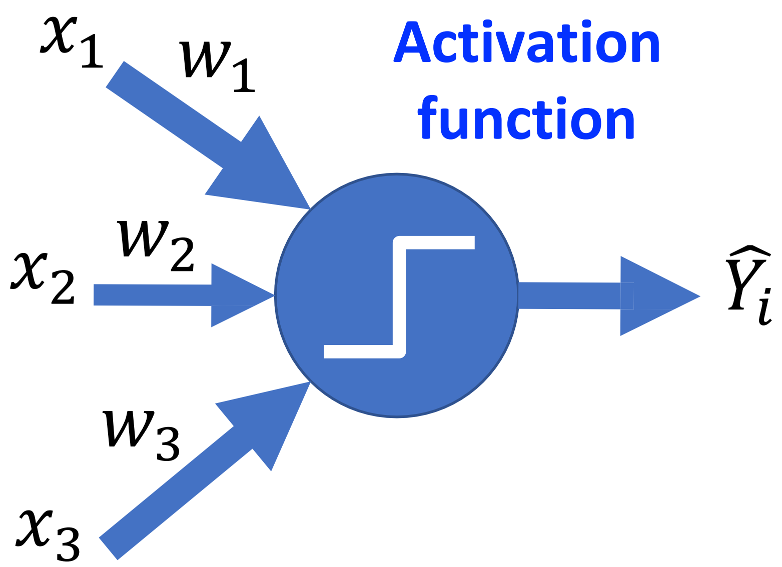


Neural Network



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

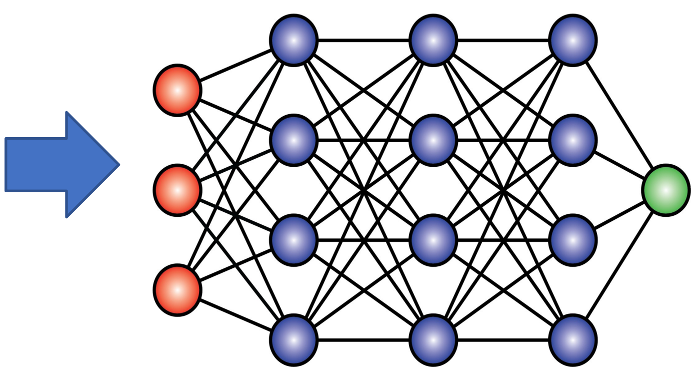


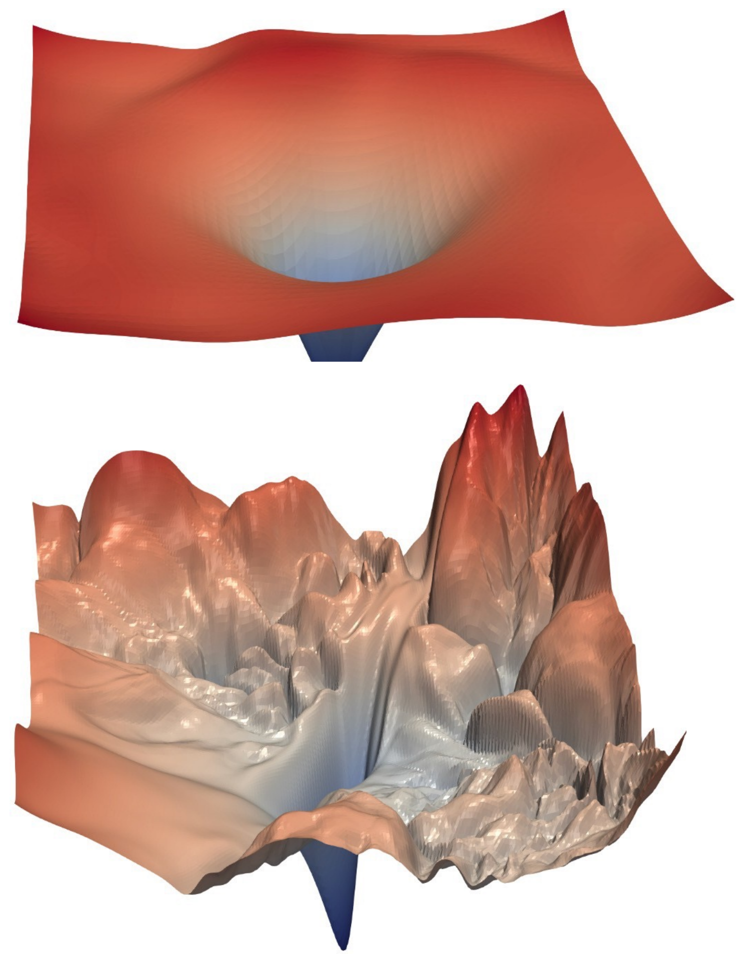
$$L = \frac{1}{N}\Sigma_{i=1}^{N}\left(\widehat{Y}_i - Y_i\right)^2$$

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
  Ian Goodfellow and Yoshua Bengio and Aaron Courville
  https://www.deeplearningbook.org/
  The Elements of Statistical Learning
  Trevor Hastie, Robert Tibshirani, Jerome Friedman
  https://hastie.su.domains/ElemStatLearn/
- **Python Programming**
  Scikit-learn https://scikit-learn.org
  Pytorch https://pytorch.org
  Tensorflow https://www.tensorflow.org