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Setting Up Environment

conda create -n myenv python=3.10

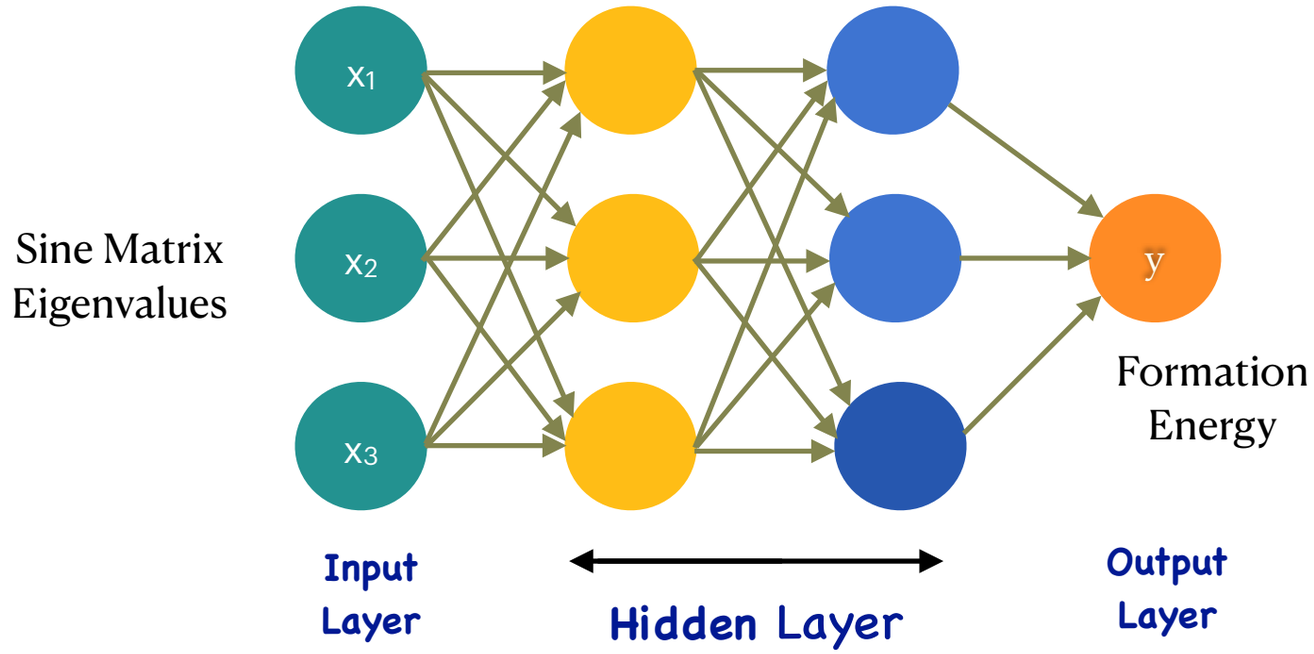
conda activate myenv

pip install torch torchvision torchaudio

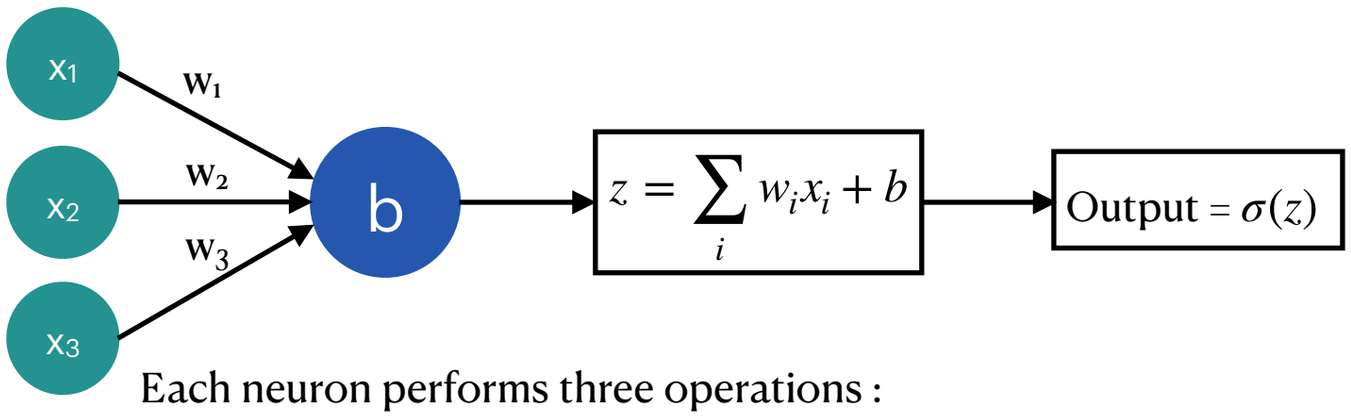
pip install numpy pandas scikit-learn matplotlib tqdm jupyterlab

All these work with python 3.12 also

Goal: Predicting formation energy using Neural Network with sine matrix eigenvalues



The output from one layer is used as input to the next layer. Such network architecture is called "**feedforward neural network**".



Each neuron performs three operations :

- It takes the inputs.
- Then performs the weighted sum of its inputs and adds a bias.
- Finally passes it through some activation function.

Sigmoid : $\sigma(z) = \dfrac{1}{1+e^{-z}}$

ReLU : $\sigma(z) = \max(0,z)$

Training the Model

Training of ANN implies finding the optimal set of weights and biases that will minimise the cost function.

Cost Function

$$C = \frac{1}{2N} \sum_x ||y(x) - a^L(x)||^2$$

actual output predicted output

The sum is over all the training observations x .
L = number of layers in the network.
N = total number of training observations