# Neural Network Tutorial & Application in Nuclear Physics

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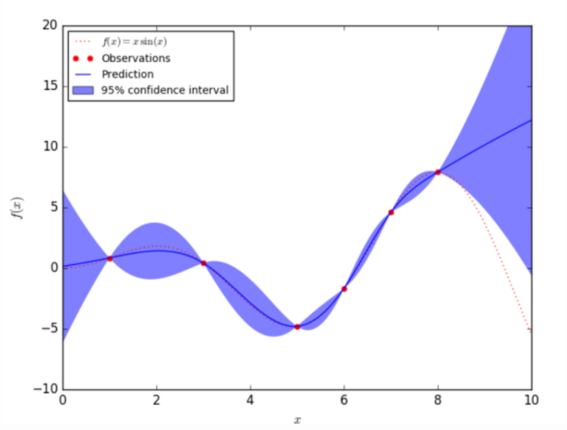
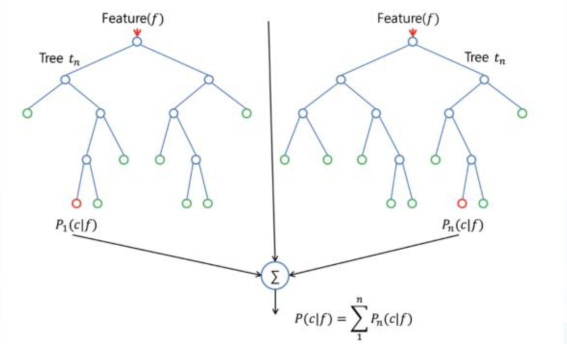
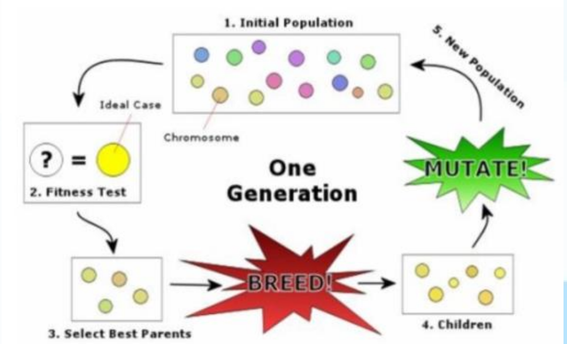
# Machine Learning

- Logistic Regression
- Gaussian Processes
- Neural Network
- Support vector machine
- Random Forest
- Genetic Algorithm

⋮



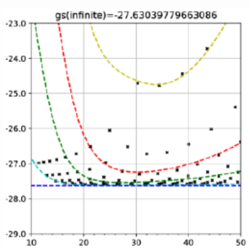



# Machine Learning
# ≈ Establish a function

- Image Reconition
- $f$ (  ) = “Panda”

- Playing Go
- $f$ (  ) = “3-4” (next move)

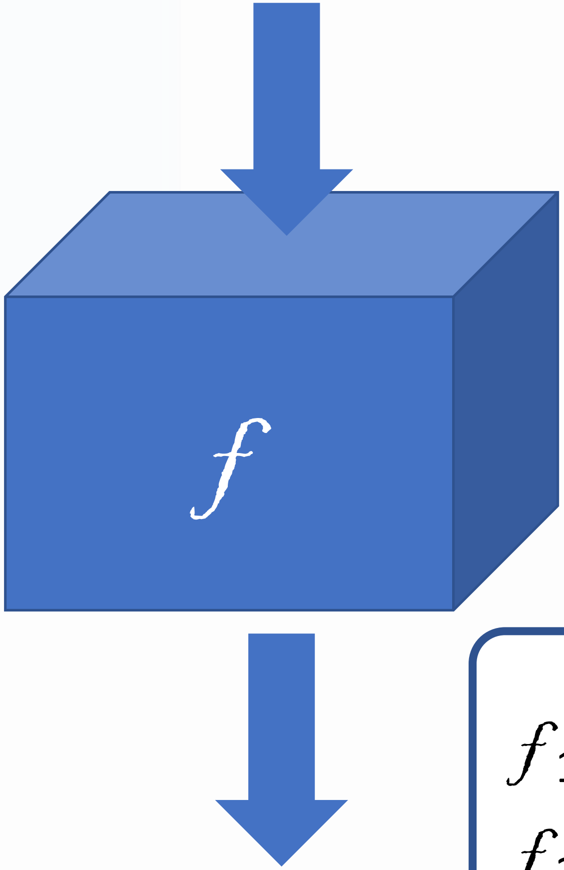
- Extrapolation
- $f$ ( 

) = “g.s. : -27.63 MeV”

# Machine Learning Framework

Image Recognition

$f$ (  ) = "Panda"




- Model :
- Complex function with lots of parameters （black box）

$f_1$ (  ) = "Panda"

$f_1$ (  ) = "Dog"

$f_2$ (  ) = "Panda"

$f_2$ (  ) = "cat"

# Machine Learning
# Supervised Learning

**A set of function**

$f_1$ (  ) = "Panda"

$f_2$ (  ) = "Panda"

⋮

$f_1$ (  ) = "Dog"

$f_2$ (  ) = "cat"

Goodness of the function $f$

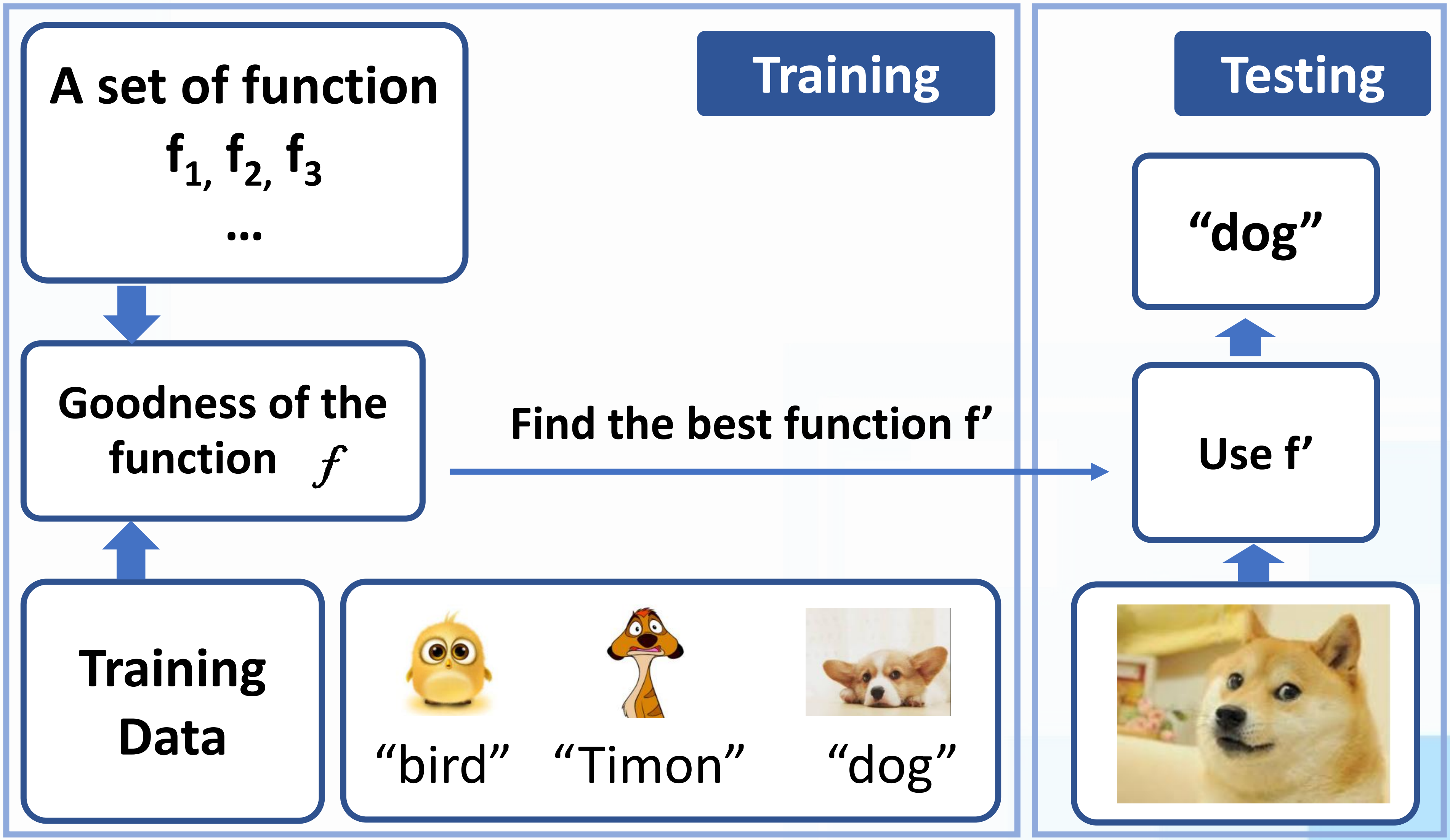
**Training Data**

**Supervised Learning**

Function input:   

Function output: "bird" "Timon" "dog"

# Machine Learning
# Supervised Learning

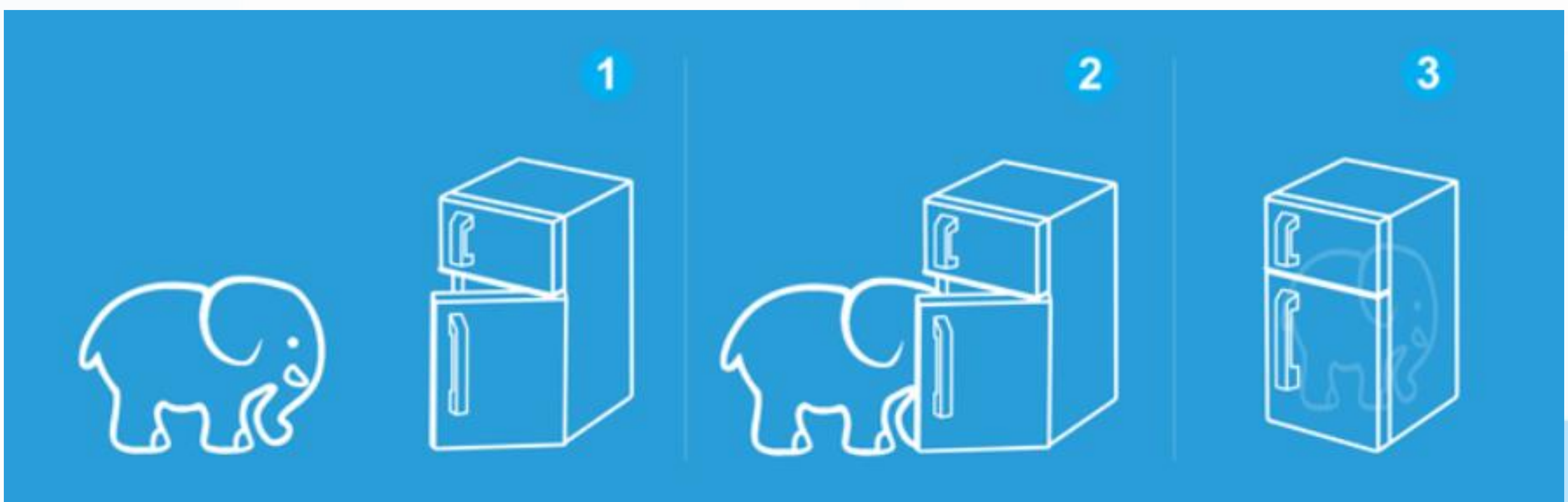


# Three Steps for Machine Learning

**Step 1:**
**Define a set of function**

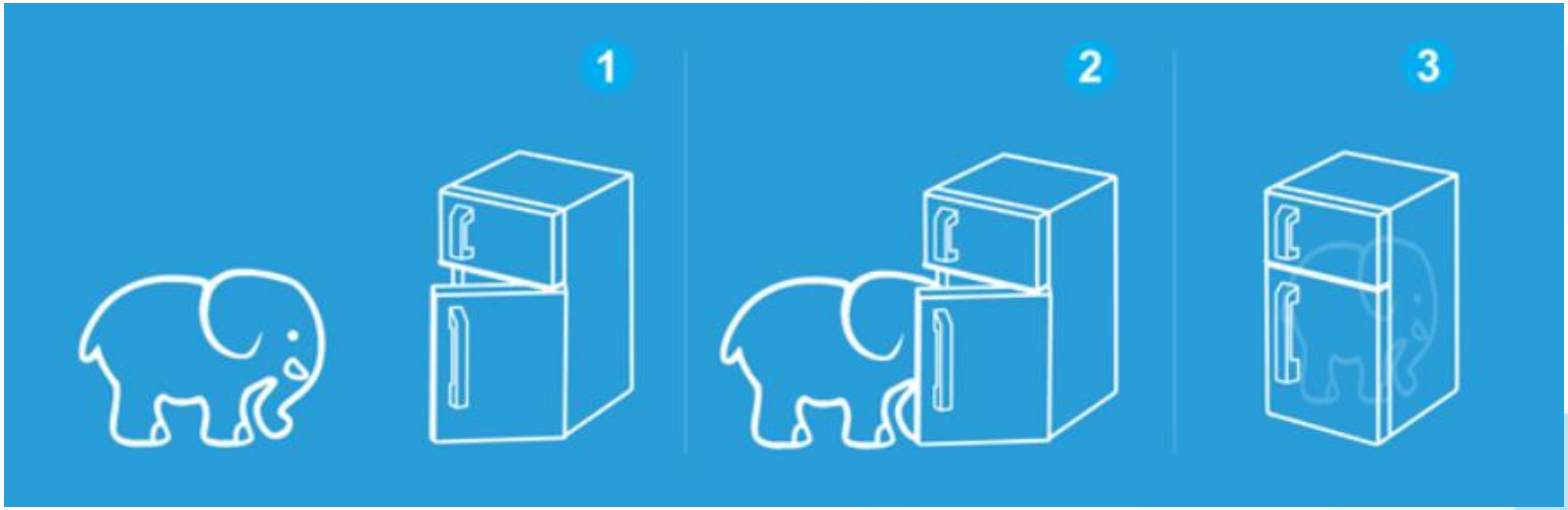
**Step 2:**
**Evaluate the function**

**Step 3:**
**Choose the best function**



# Three Steps for Machine Learning

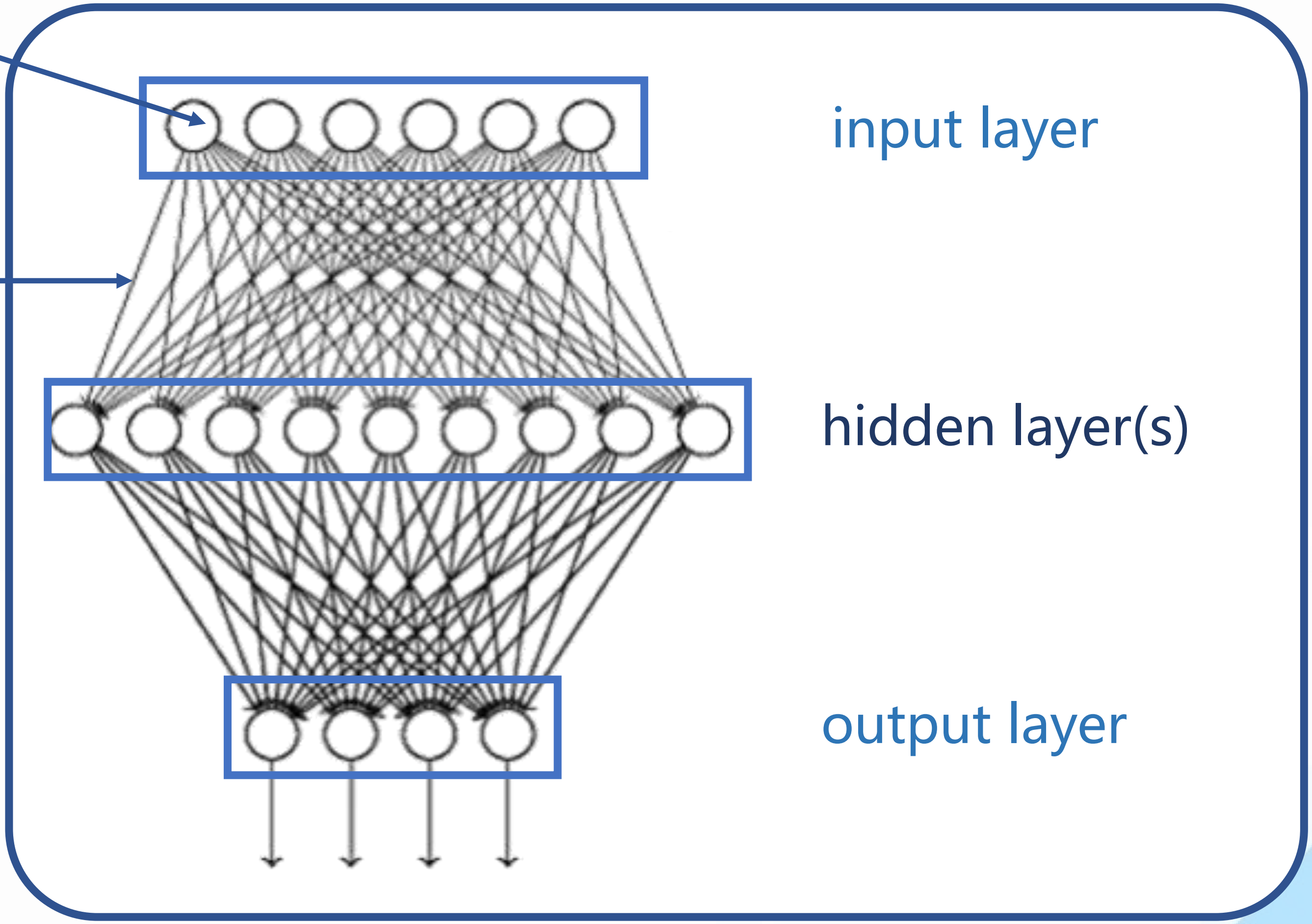
Step 1: Neural Network → Step 2: Evaluate the function → Step 3: Choose the best function



# Neural Network & Machine Learning

neurons

weights

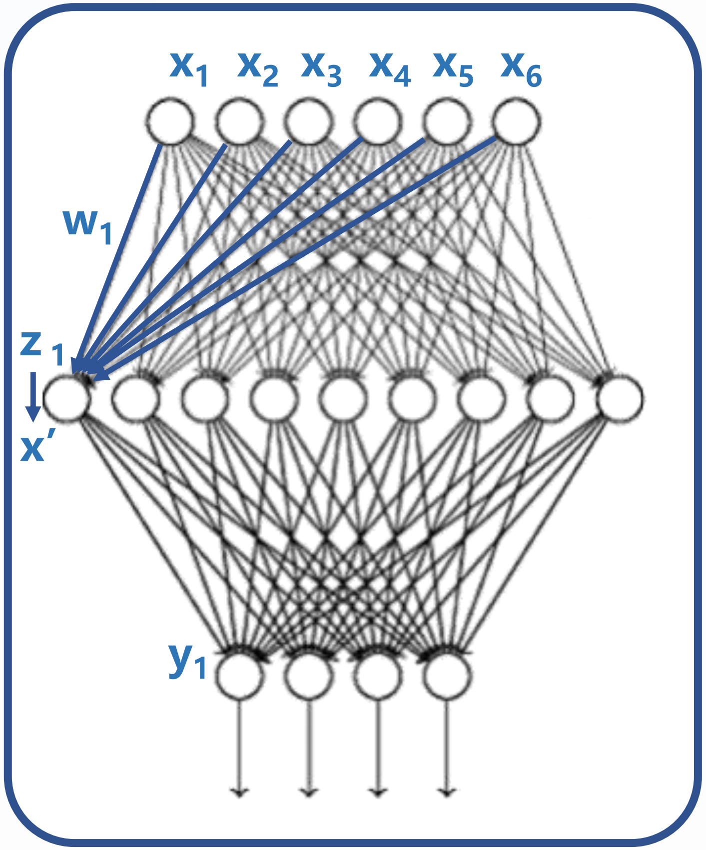



128 X 128 X 3 color = 49152 neurons 0-255 chroma

0 1 0 0 0 ……
“panda”

A sample of feed forward neural network (NN)

# Feedforward Neural Network




$$z_1 = x_1 w_1 + \ldots + x_n w_n + \text{bias}$$

$$\downarrow$$

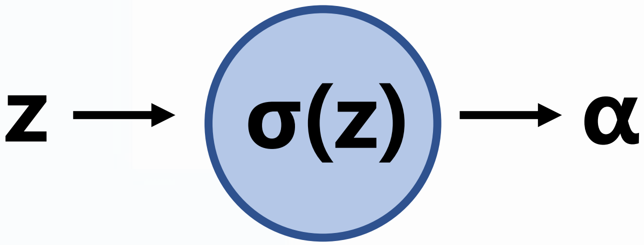
$$z \longrightarrow \sigma(z) \longrightarrow x'$$

**Activation function**

Feedforward:
The value for every neuron only depend on the previous layer.

# Activation function

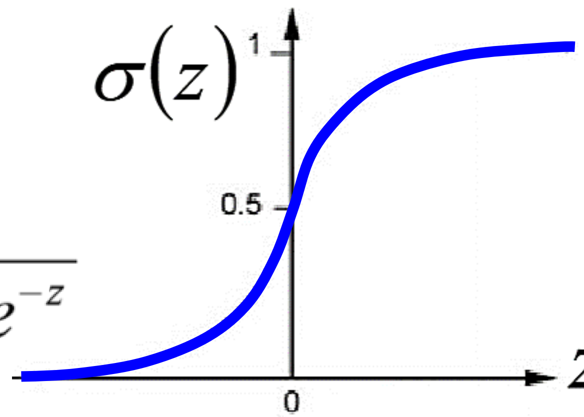
give non-linearity to the NN



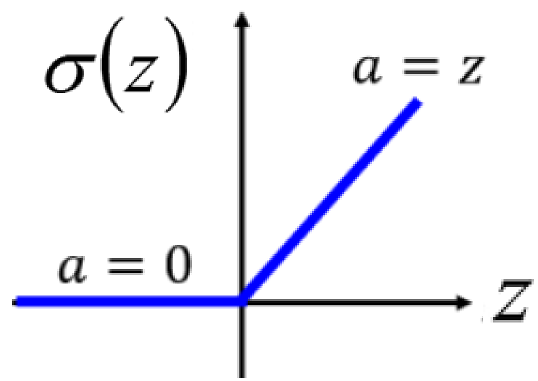

Activation function

**Sigmoid**

$$\sigma(z) = \frac{1}{1+e^{-z}}$$




**ReLU**



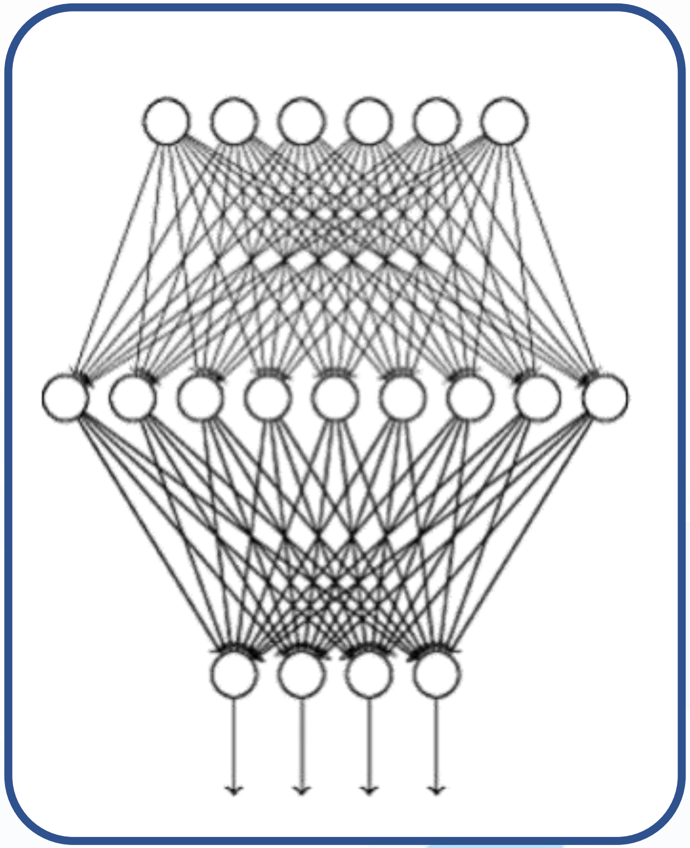
# Neural Network Function

**input layer (X): i neurons**
**one hidden layer: j neurons**
**output layer (Y): k neurons**

$$Z_j = \sum_i X_i W_{ij} + b_j$$

$$X'_j = \sigma\,(Z_j)$$

$$Y_k = \sum_j X'_j W'_{jk} + b'_k$$



# Tensor operation

Training data: p sample

input layer (X): i neurons

one hidden layer: j neurons

output layer (Y): k neurons

$$Z_{(p,j)} = X_{(p,i)} \times W_{(i,j)} + b_{(p,j)}$$

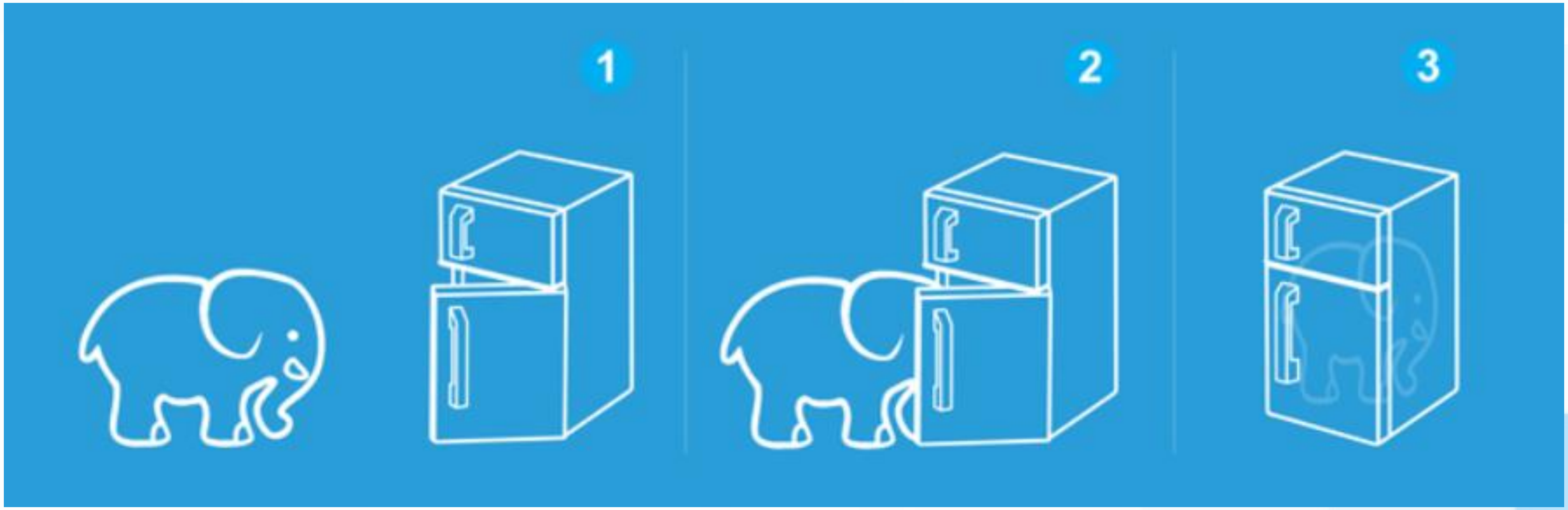
$$\begin{pmatrix} z_{11} & \cdots & z_{1j} \\ \vdots & \ddots & \vdots \\ z_{p1} & \cdots & z_{pj} \end{pmatrix} = \begin{pmatrix} x_{11} & \cdots & x_{1i} \\ \vdots & \ddots & \vdots \\ x_{p1} & \cdots & x_{pi} \end{pmatrix} \times \begin{pmatrix} w_{11} & \cdots & w_{1j} \\ \vdots & \ddots & \vdots \\ w_{i1} & \cdots & w_{ij} \end{pmatrix} + \begin{pmatrix} b_{11} & \cdots & b_{1j} \\ \vdots & \ddots & \vdots \\ b_{p1} & \cdots & b_{pj} \end{pmatrix}$$

$$Y_{(p,k)} = X'_{(p,j)} \times W'_{(j,k)} + b'_{(p,j)}$$

$$\begin{pmatrix} y_{11} & \cdots & y_{1j} \\ \vdots & \ddots & \vdots \\ y_{p1} & \cdots & y_{pj} \end{pmatrix} = \begin{pmatrix} \sigma(z)_{11} & \cdots & \sigma(z)_{1j} \\ \vdots & \ddots & \vdots \\ \sigma(z)_{p1} & \cdots & \sigma(z)_{pj} \end{pmatrix} \times \begin{pmatrix} w'_{11} & \cdots & w'_{1j} \\ \vdots & \ddots & \vdots \\ w'_{i1} & \cdots & w'_{ij} \end{pmatrix} + \begin{pmatrix} b'_{11} & \cdots & b'_{1j} \\ \vdots & \ddots & \vdots \\ b'_{p1} & \cdots & b'_{pj} \end{pmatrix}$$

# Three Steps for Machine Learning

**Step 1:** Neural Network → **Step 2:** Evaluate the function → **Step 3:** Choose the best function



# Evaluate a network

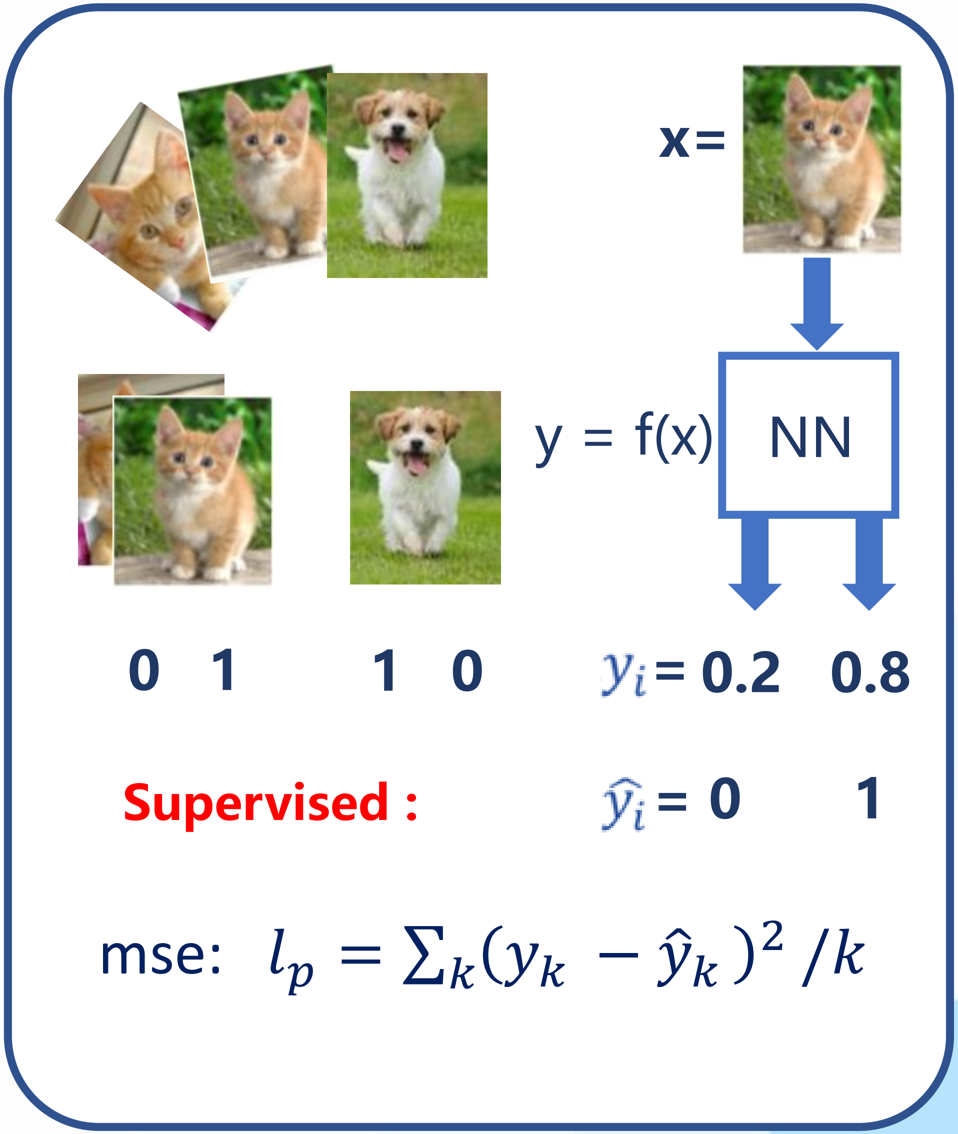
Introduce a loss function to describe the performance of the network
(mse, cross entropy)

Loss:

$$L = \sum_{r=1}^{p} l_p$$

Smaller the better

**Image Recognition**

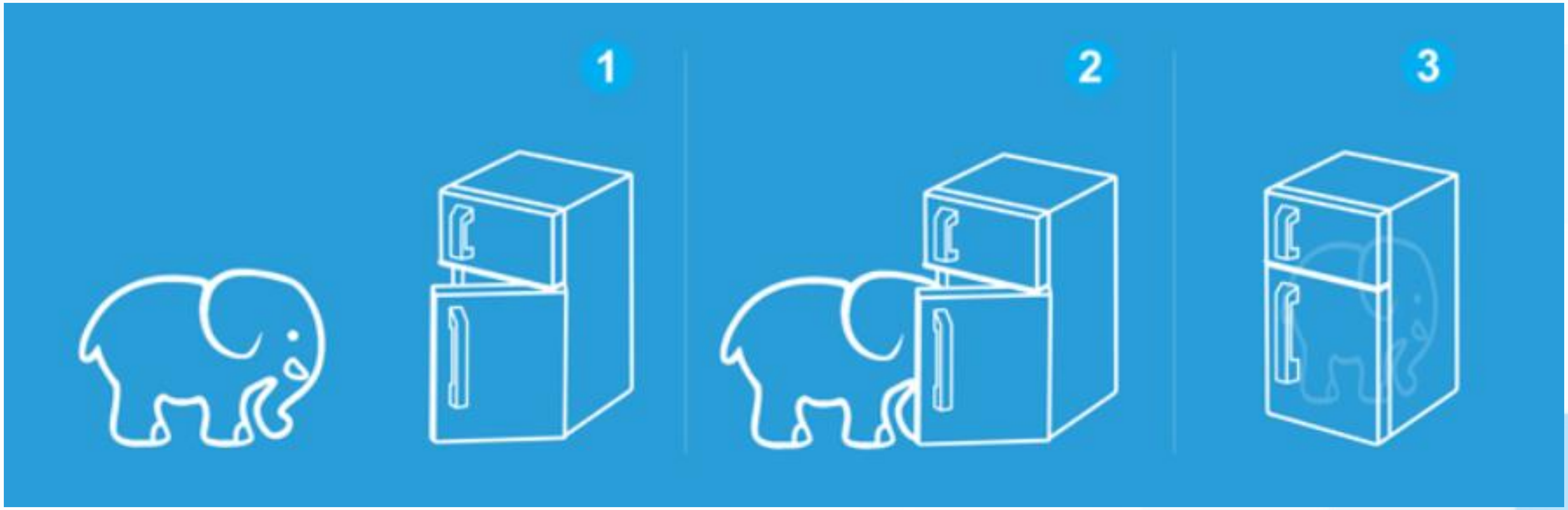


# Three Steps for Machine Learning

**Step 1:**
**Neural Network**

**Step 2:**
**Evaluate the function**

**Step 3:**
**Choose the best function**

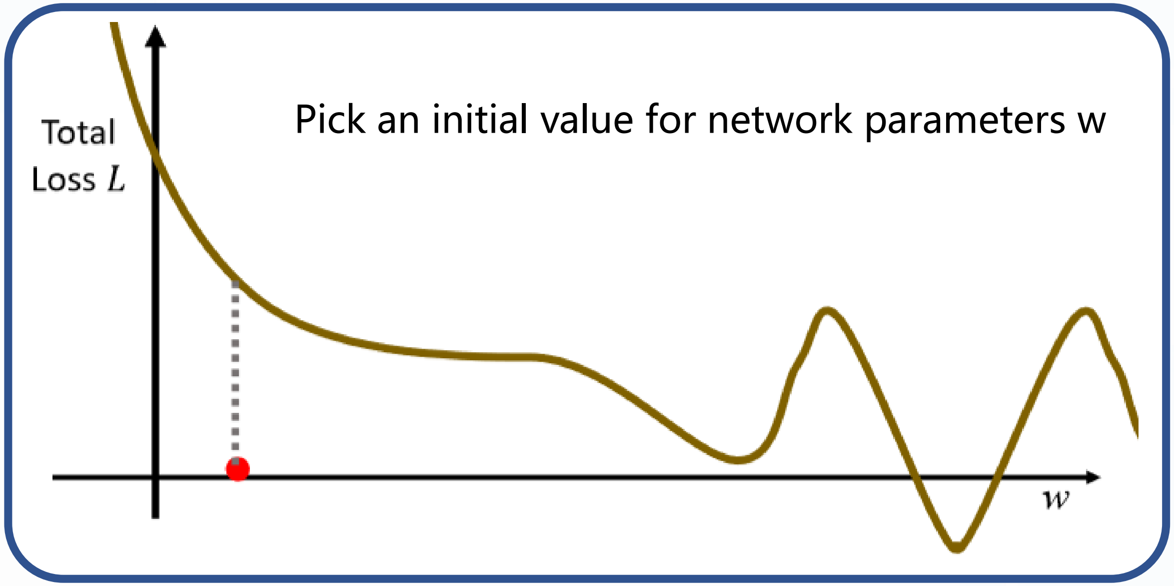


# "Learning" : find the best function

Ultimate goal:

Find the network parameters set that minimize the total loss L

Gradient Descent (even for AlphaGo)




- Compute $\partial L / \partial w$ with training data
- Update the parameters $w \leftarrow w - \eta \partial L / \partial w$
- Repeat until $\partial L / \partial w$ is small enough

This procedure is so call the machine learning.

# Backpropagation

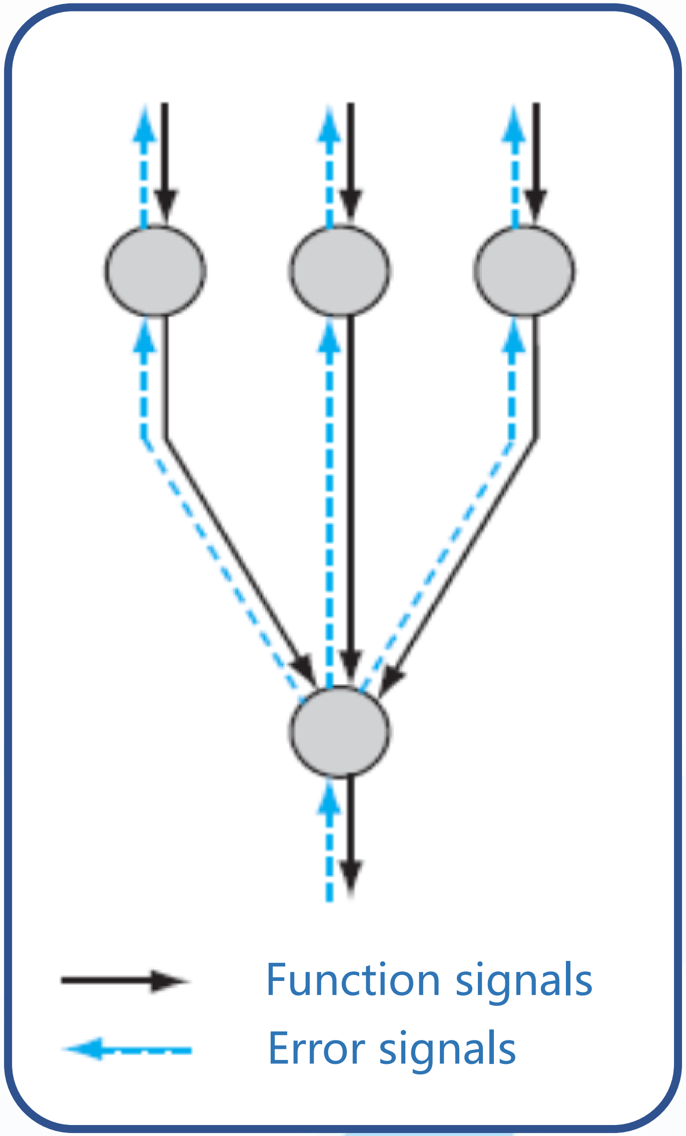
An efficient way to compute $\partial \mathrm{L}/\partial \mathrm{w}$

$$Z_j = \sum_i X_i W_{ij} + b_j$$

$$X'_j = \sigma\,(Z_j)$$

$$Y_k = \sum_j X'_j W'_{jk} + b'_k$$

mse: $l_p = \sum_k (y_k - \hat{y}_k)^2 / k$




Backpropagation (BP)

# Backpropagation

$$Z_j = \sum_i X_i W_{ij} + b_j$$

↓

$$X'_j = \sigma\,(Z_j)$$

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

↓

$$Y_k = \sum_j X'_j W'_{jk} + b'_k$$

↓

mse: $l_p = \sum_k (y_k - \hat{y}_k)^2 / k$

$$\frac{\partial l}{\partial \mathrm{w}} = \frac{\partial l}{\partial z} * \mathrm{x} \qquad \frac{\partial l}{\partial b} = \frac{\partial l}{\partial z}$$

↑

$$\frac{\partial l}{\partial Z} = \frac{\partial l}{\partial x\prime} * \frac{1}{1+e^{-z}} * \left(1 - \frac{1}{1+e^{-z}}\right)$$

↑

$$\frac{\partial l}{\partial \mathrm{w}'} = \frac{\partial l}{\partial y} * \mathrm{x}' \qquad \frac{\partial l}{\partial b'} = \frac{\partial l}{\partial y}$$

↑

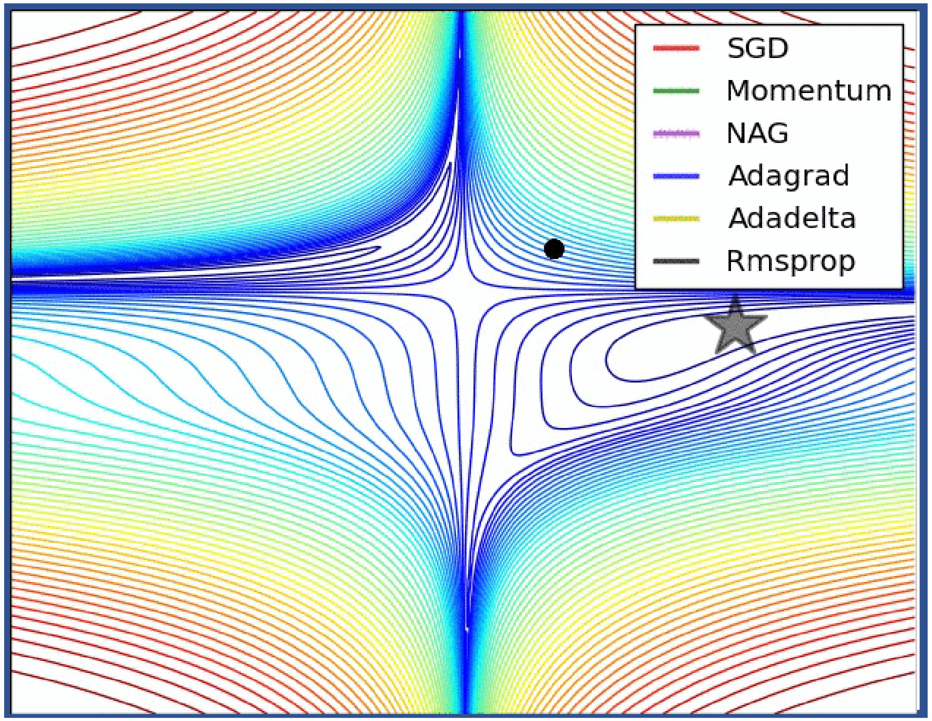
$\frac{\partial l}{\partial y}$ = 2/k * $(y - \hat{y})$

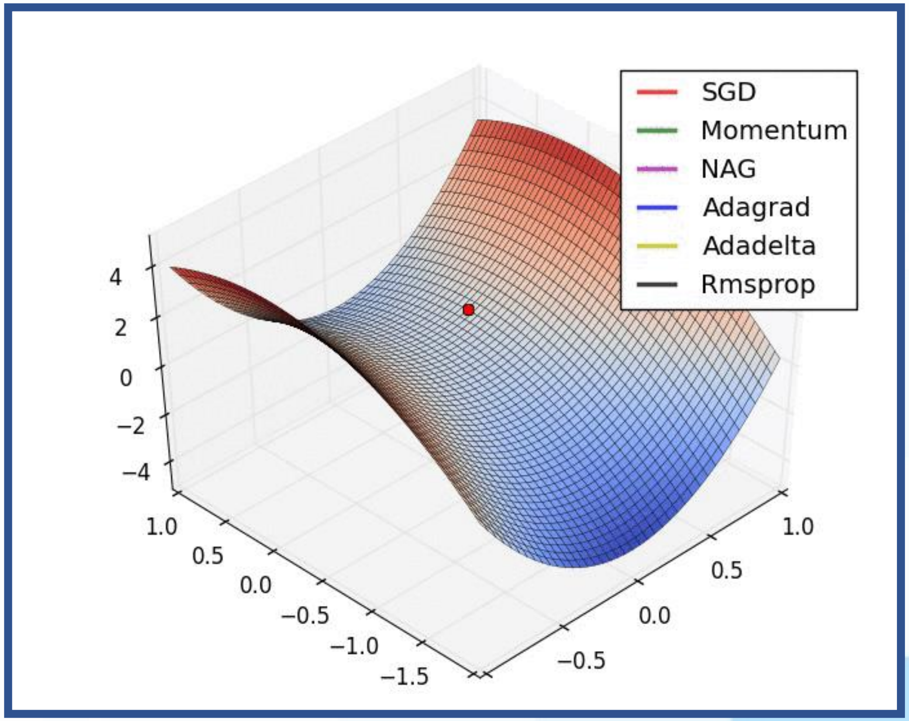
# Optimizer

Gradient Descent :
walking in the desert, blindfold

Cannot see the whole picture

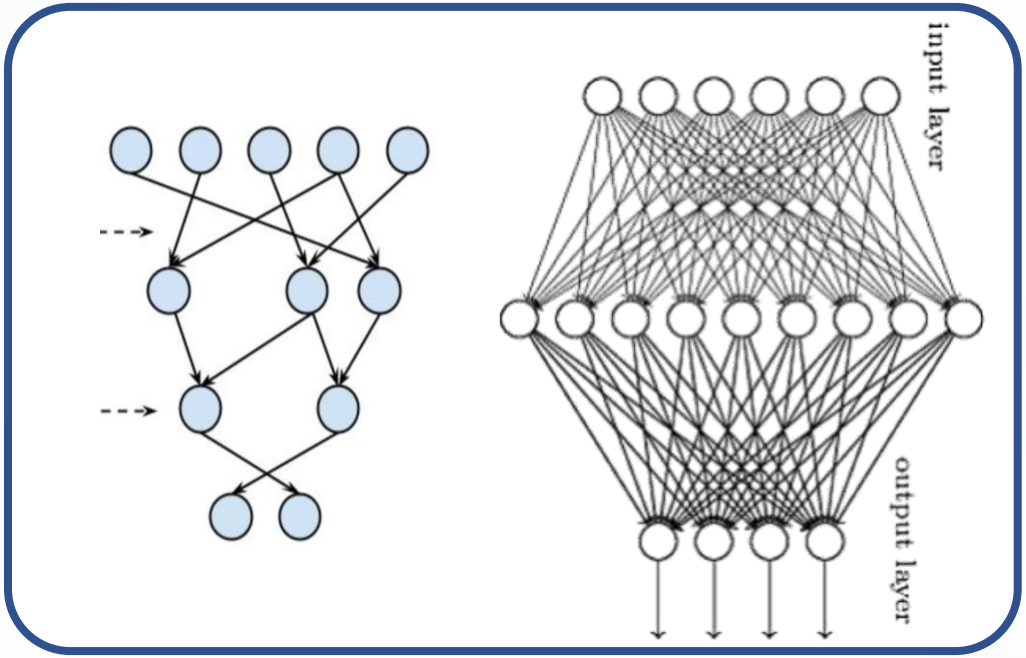
SGD
Momentum
AdaGrad
Adam



# “Deep” learning

Deep just means more hidden layers




“Deep” VS “Wide”

” Deep” is better

But not too deep

# “Deep” learning

Gradient vanishing/exploding problem

n’ hidden layers

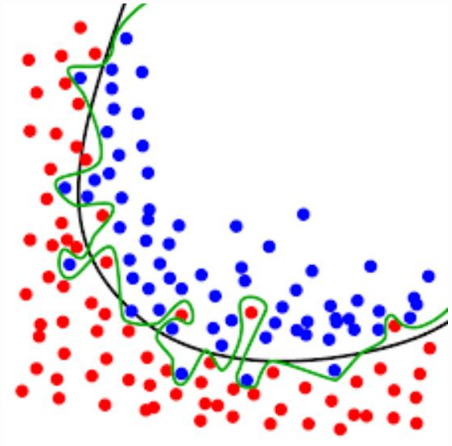
$w_q$ is the weights for “q” th hidden layer

$$\frac{\partial l}{\partial x'} = \frac{\partial l}{\partial y} * \mathrm{w}$$

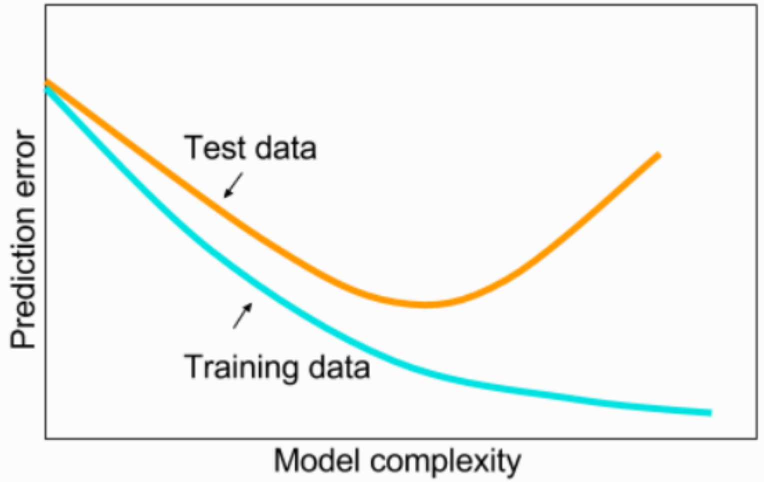
$$\frac{\partial l}{\partial w_q} = \frac{\partial l}{\partial y} * w_n * w_{n-1} * w_{n-2} * \cdots * w_{q+1} * \mathrm{x}$$

# Overfitting

Training data and testing data can be different



**Solution:**
**Get more training data**
**Create more training data**
**Dropout**
**L1/L2 regularization**
**Early Stopping**

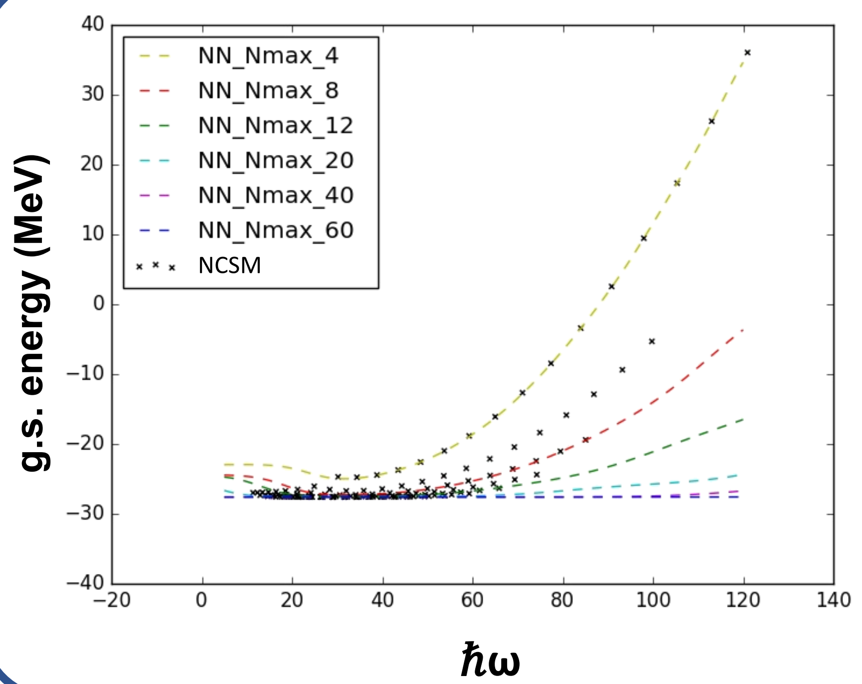


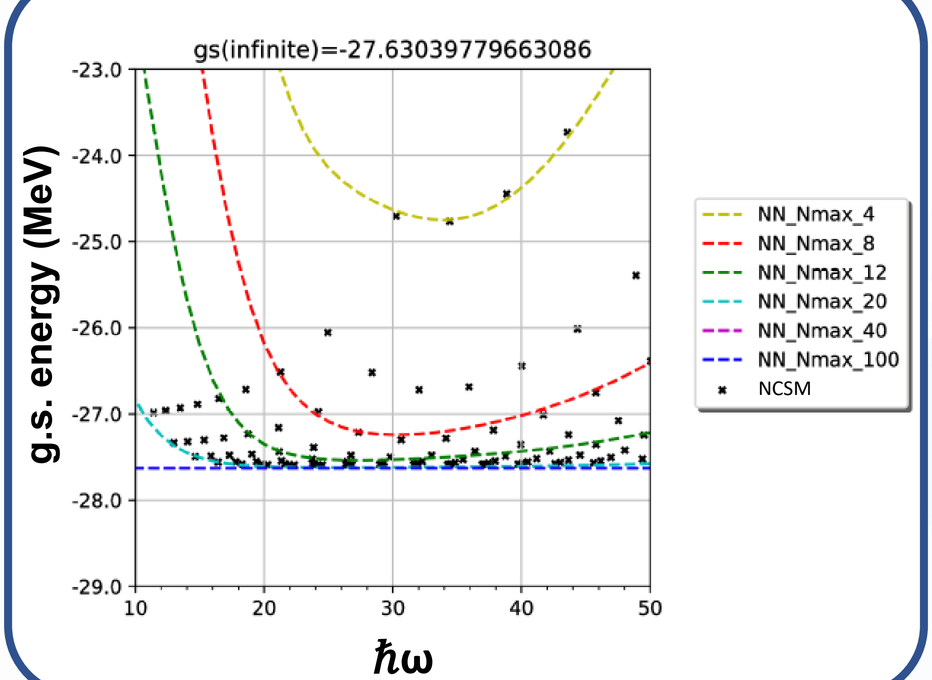
# Friendly tool: Keras


- Python
- $ apt-get install python3-pip
- $ pip3 install keras
- $ pip3 install tensorflow

# Neural network simulation & extrapolation

- NN application in nuclear physics
- $^4$He ground-state energy

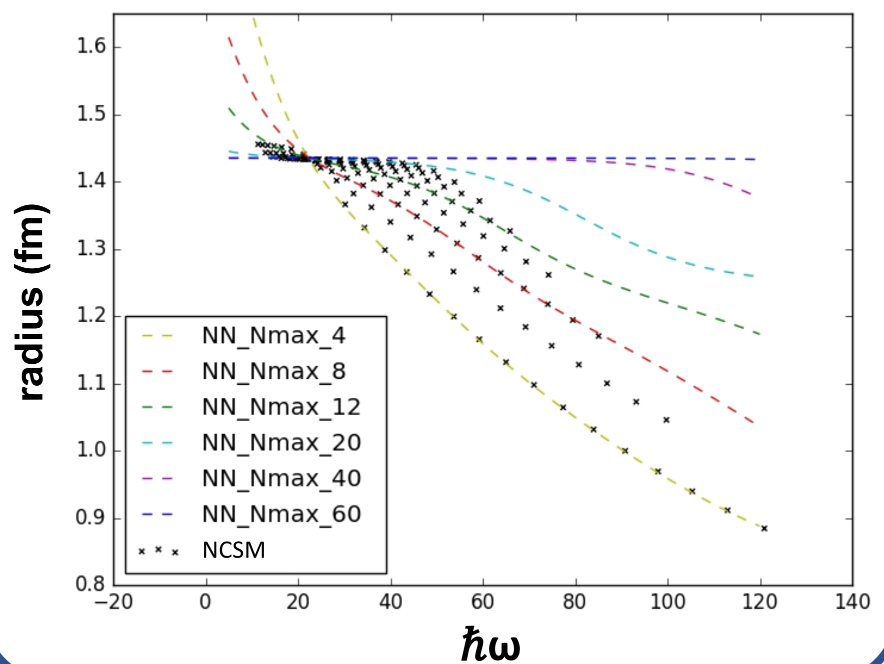


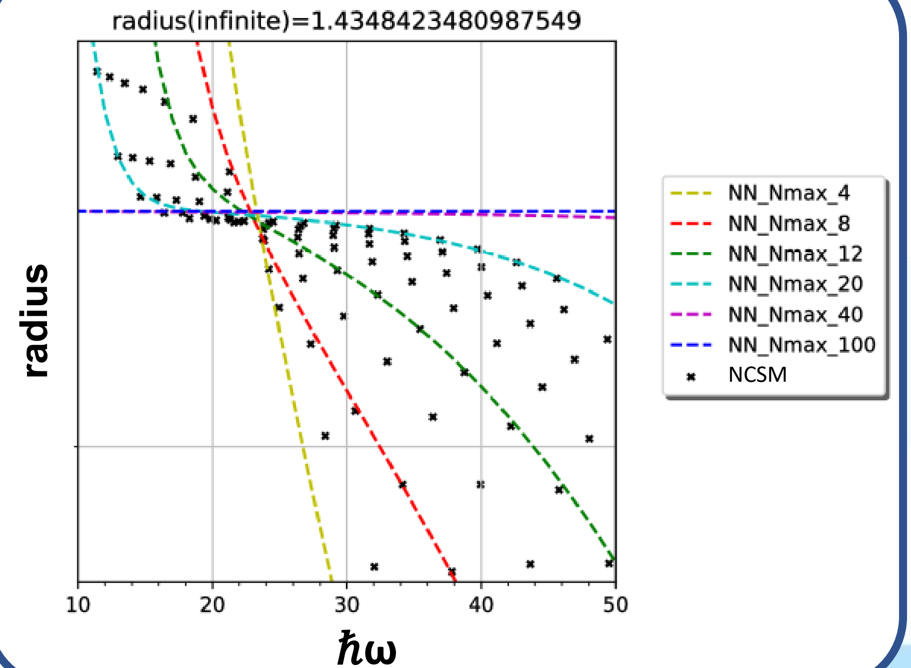




* Negoita G A, Luecke G R, Vary J P, et al. Deep Learning: A Tool for Computational Nuclear Physics[J]. arXiv preprint arXiv:1803.03215, 2018.

# Neural network simulation & extrapolation

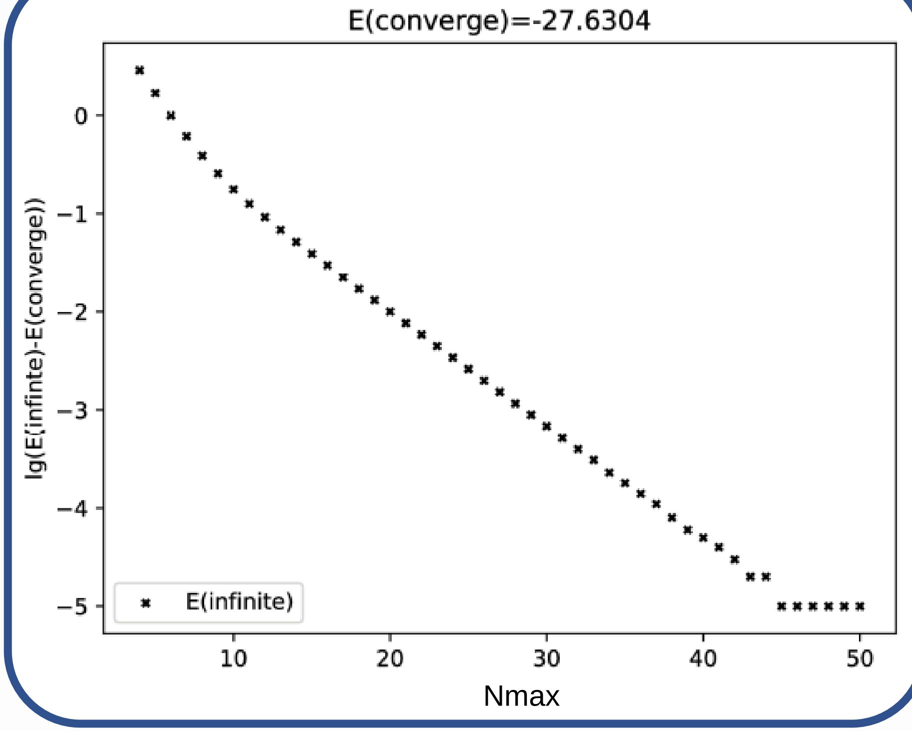
- $^4$He radius

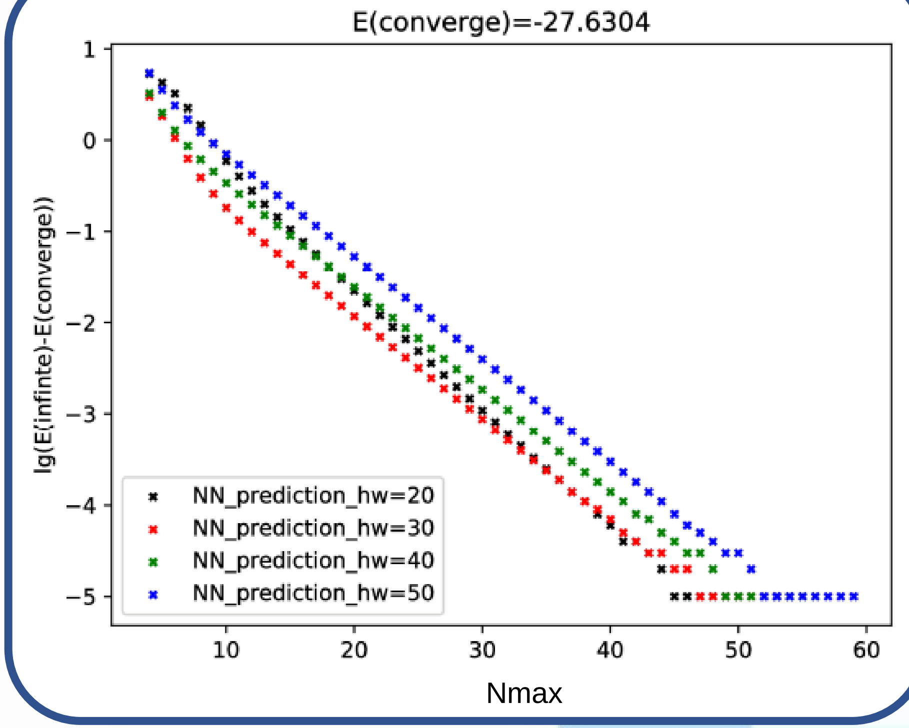


# Neural network simulation & extrapolation

- The minimum g.s energy of each Nmax drops exponentially




* Forssén, C., Carlsson, B. D., Johansson, H. T., Sääf, D., Bansal, A., Hagen, G., & Papenbrock, T. (2018). Large-scale exact diagonalizations reveal low-momentum scales of nuclei. *Physical Review C*, *97*(3), 034328.

# Neural network for Coupled-cluster

$$|\Psi_0\rangle = e^{\hat{T}}|\Phi_0\rangle$$

$$\hat{T} = \sum_i T_i$$

$$\hat{T}_{\text{CCSDT}} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3$$

CCSDT equations:

$$\langle\Phi_i^a|e^{-T}He^{T}|\Phi_0\rangle = 0$$

$$\langle\Phi_{ij}^{ab}|e^{-T}He^{T}|\Phi_0\rangle = 0$$

$$\langle\Phi_{ijk}^{abc}|e^{-T}He^{T}|\Phi_0\rangle = 0$$

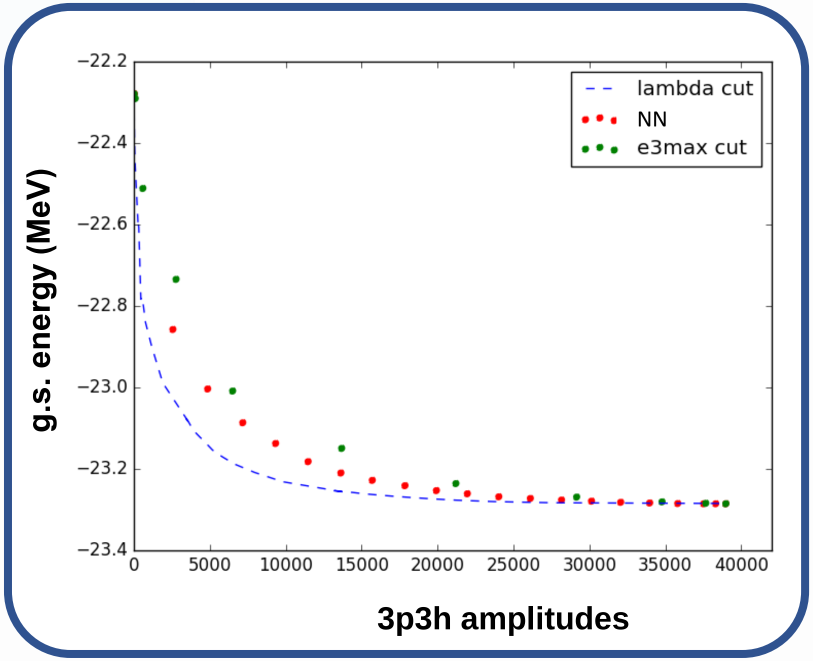
We want to truncate the 3p3h configurations

Introduce NN to select the more important configurations

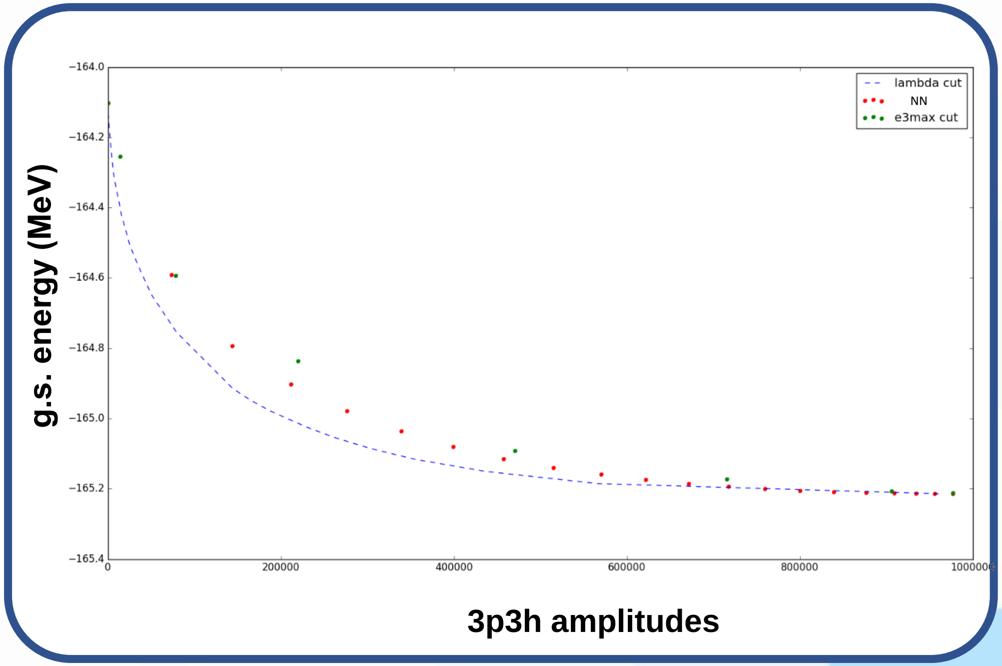
# Neural network for Coupled-cluster

- The input layer include all the quantum numbers of the 3p3h amplitudes ( n l j $j_{tot}$ $t_z$ …).

$^{8}$He

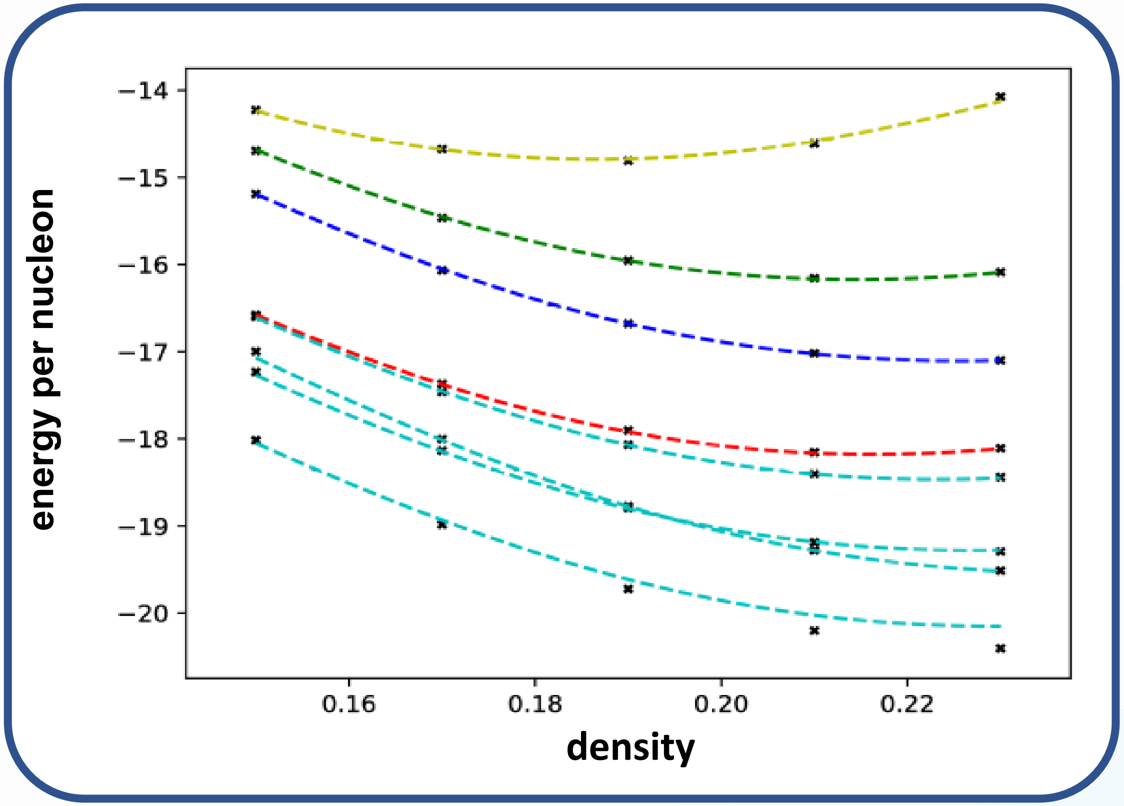



$^{16}$O



# Neural network in nuclear matter

- Train with different combination of cD,cE.



# Neural network
# Uncertainty analysis

- Even with the same input data and network structure, the NN will give different results in mutual independence trainings.

Sources of uncertainty

1. random initialization of neural network parameters

2. different divisions between training data and validation data

3. data shuffle (limit batch size)

Solution

1. ???

2. k-fold cross validation …

3. increase batch size …

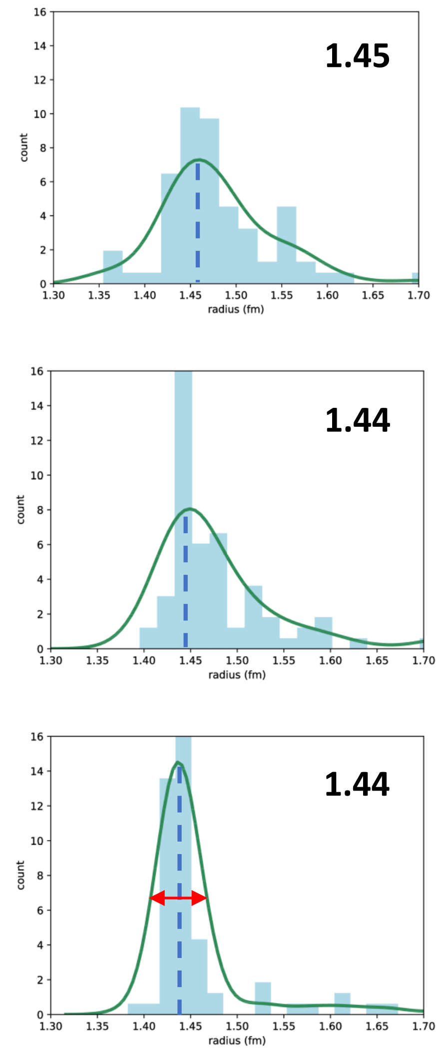
# Ensembles of Neural Networks

- $^4$He radius
- The distribution of NN predict radius is Gaussian.
- Define the full width at half maximum value as the uncertainty for certain NN structure.
- The NN uncertainty reduce with more training data.
- The almost identical value of NN prediction radius indicates that the NN has a good generalization performance.

Nmax 4-12

Nmax 4-16

Nmax 4-20



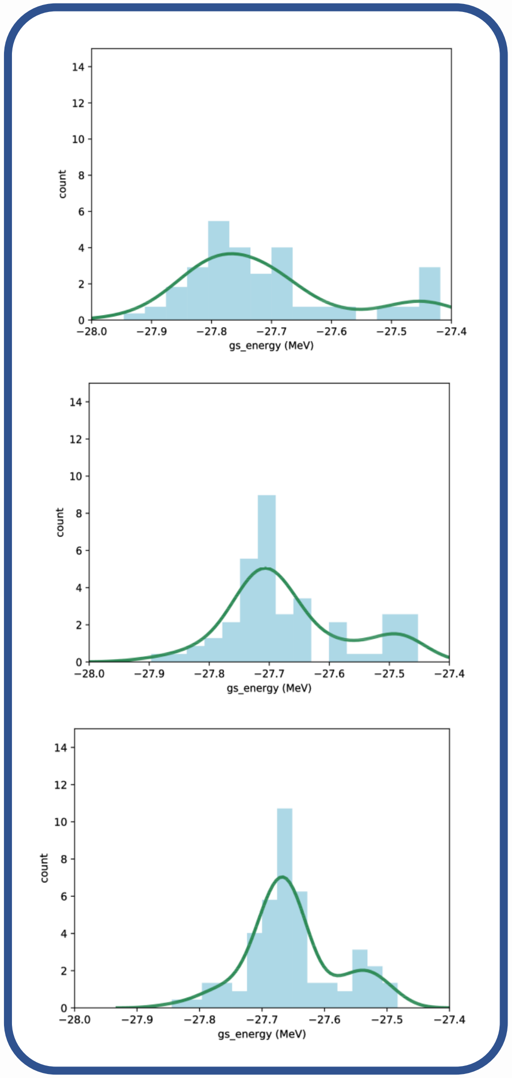
# More complex case:

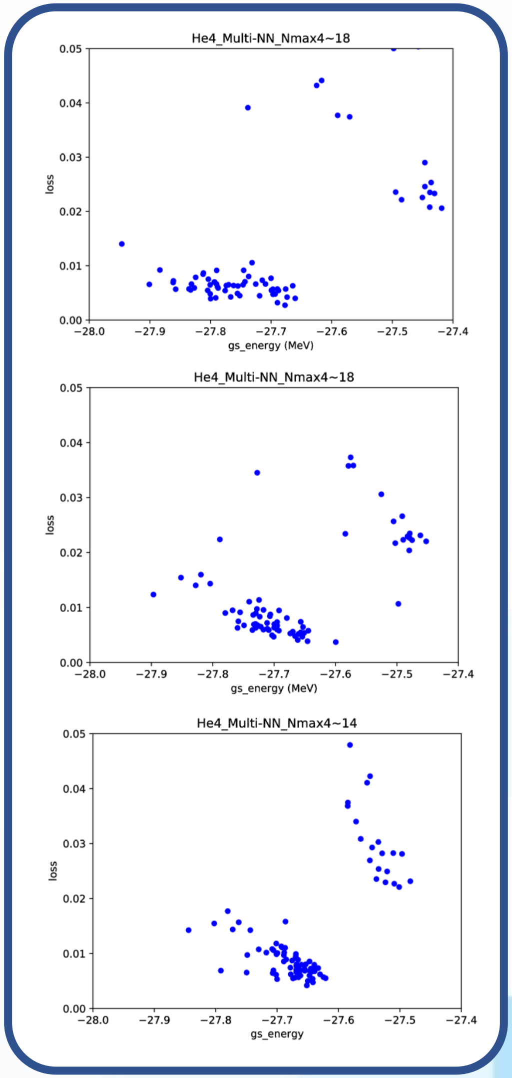
## $^4$He g.s. energy, with two peak

**Nmax 4-10**

**Nmax 4-12**

**Nmax 4-14**



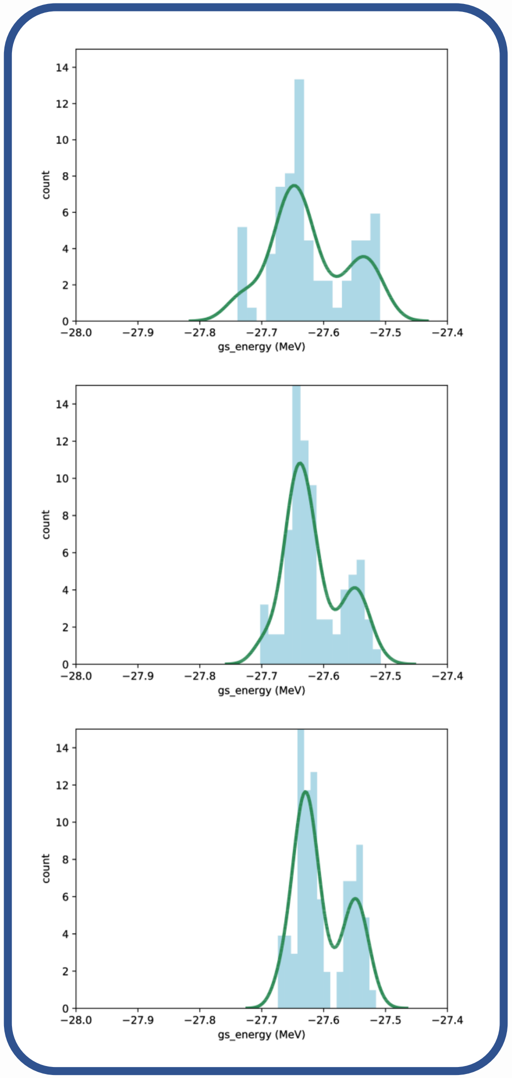



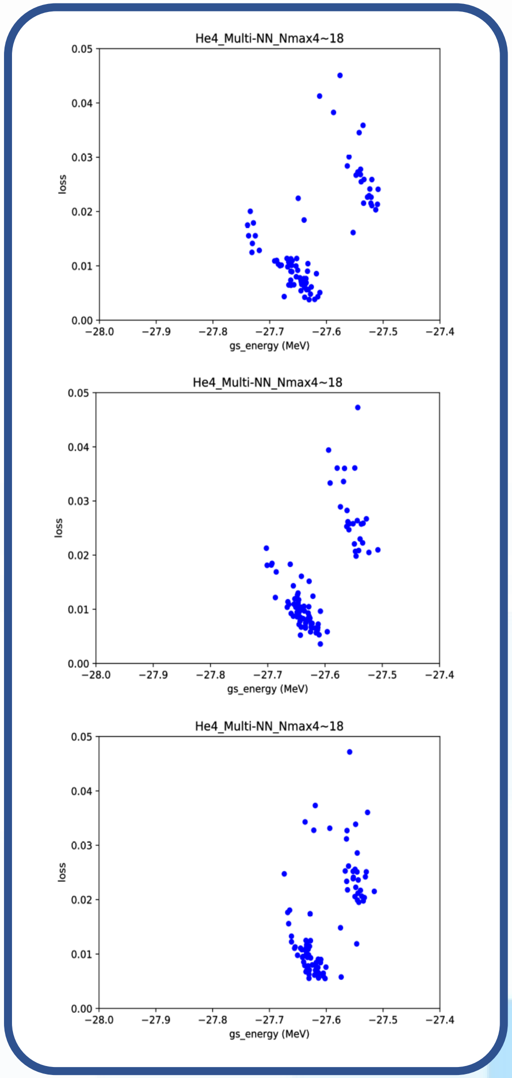
# $^{4}$He g.s. energy, with two peak

Nmax 4-16

Nmax 4-18

Nmax 4-20



We can separate the peaks with features (loss) provided by NN.