Multilayer Perceptrons (MLP)

Rowel Atienza
rowel@eee.upd.edu.ph
University of the Philippines

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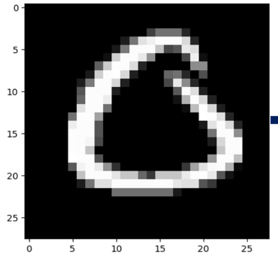
Problem Definition (Supervised Learning)

Given a dataset $\mathcal{D} = (\boldsymbol{x}, \boldsymbol{y})$, find a function $f: \boldsymbol{x} \in \mathbb{R}^N \rightarrow \boldsymbol{y} \in \mathbb{R}^M$



$$f(\cdot)$$

$$\boldsymbol{y} = 0 \in \mathbb{R}^1$$

$$\boldsymbol{x} \in \mathbb{R}^{28 \times 28 \times 1}$$

What is $f(\cdot)$?

$f(\cdot)$ is generally a non-linear function that maps an input distribution $\boldsymbol{x} \sim p(\boldsymbol{x})$ to an output distribution $\boldsymbol{y} = p(\boldsymbol{y}|\boldsymbol{x})$:

$$\boldsymbol{y} = f(\boldsymbol{x}) = p(\boldsymbol{y}|\boldsymbol{x})$$

$f(\cdot)$ is an estimator of density $p(\boldsymbol{y}|\boldsymbol{x})$

General Function Approximator

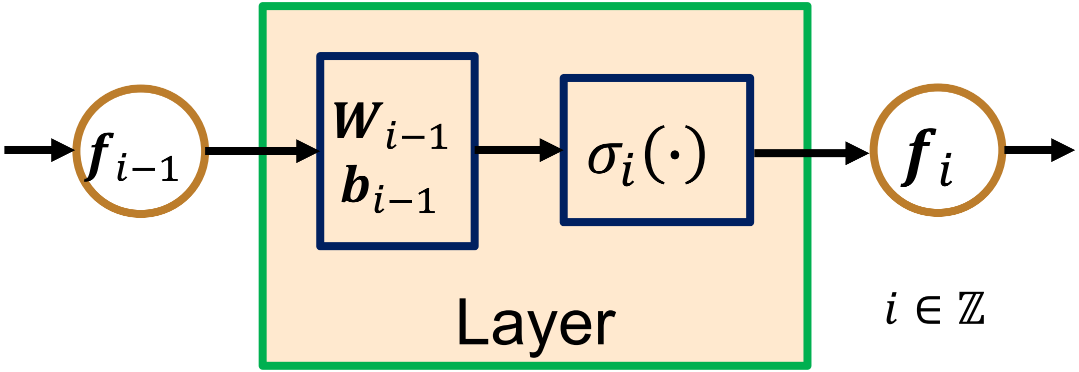
Theorem: Any function $f(\cdot)$ can be approximated by a composition of several smaller functions f_i:

$$\boldsymbol{y} = f(\boldsymbol{x}) \approx f_n \circ f_{n-1} \circ f_{n-2} \circ \cdots \circ f_1 (\boldsymbol{x})$$

$\ni f_0 = \boldsymbol{x}, n \in \mathbb{Z}$

f_i: Dense Layer (`tf.keras`) or Fully-Connected Layer (PyTorch)

$$\boldsymbol{f}_i(\boldsymbol{f}_{i-1};\ \boldsymbol{\theta}_{i-1}) = \sigma_i(\boldsymbol{W}_{i-1}\boldsymbol{f}_{i-1} + \boldsymbol{b}_{i-1})$$



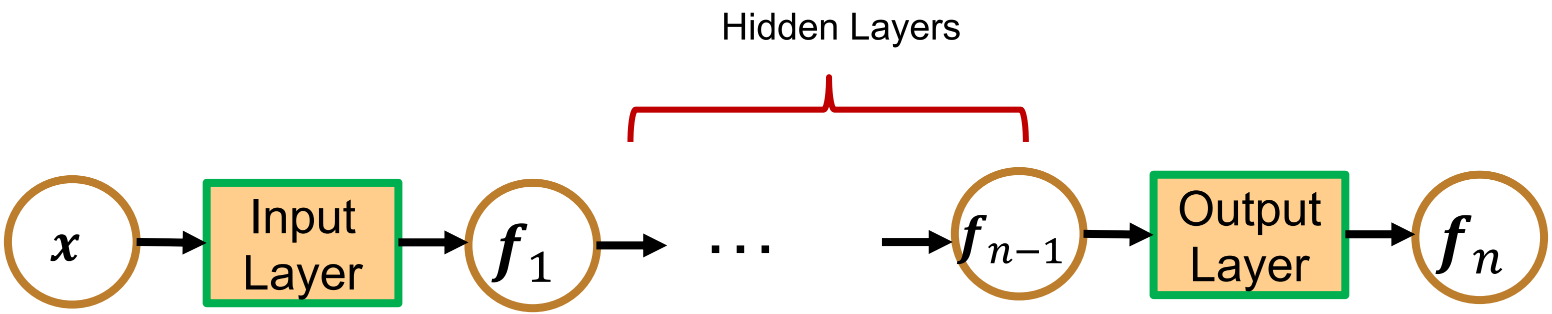
$i \in \mathbb{Z}$

Weights: $\boldsymbol{W} = \{\boldsymbol{W}_0, \boldsymbol{W}_1, \dots, \boldsymbol{W}_{n-1}\}$ Biases: $\boldsymbol{b} = \{\boldsymbol{b}_0, \boldsymbol{b}_1, \dots, \boldsymbol{b}_{n-1}\}$

Weights, Biases := Parameters: $\boldsymbol{\theta} = \{\boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_{n-1}\}$ $\boldsymbol{\theta}_{i-1} = \{\boldsymbol{W}_{i-1}, \boldsymbol{b}_{i-1}\}$

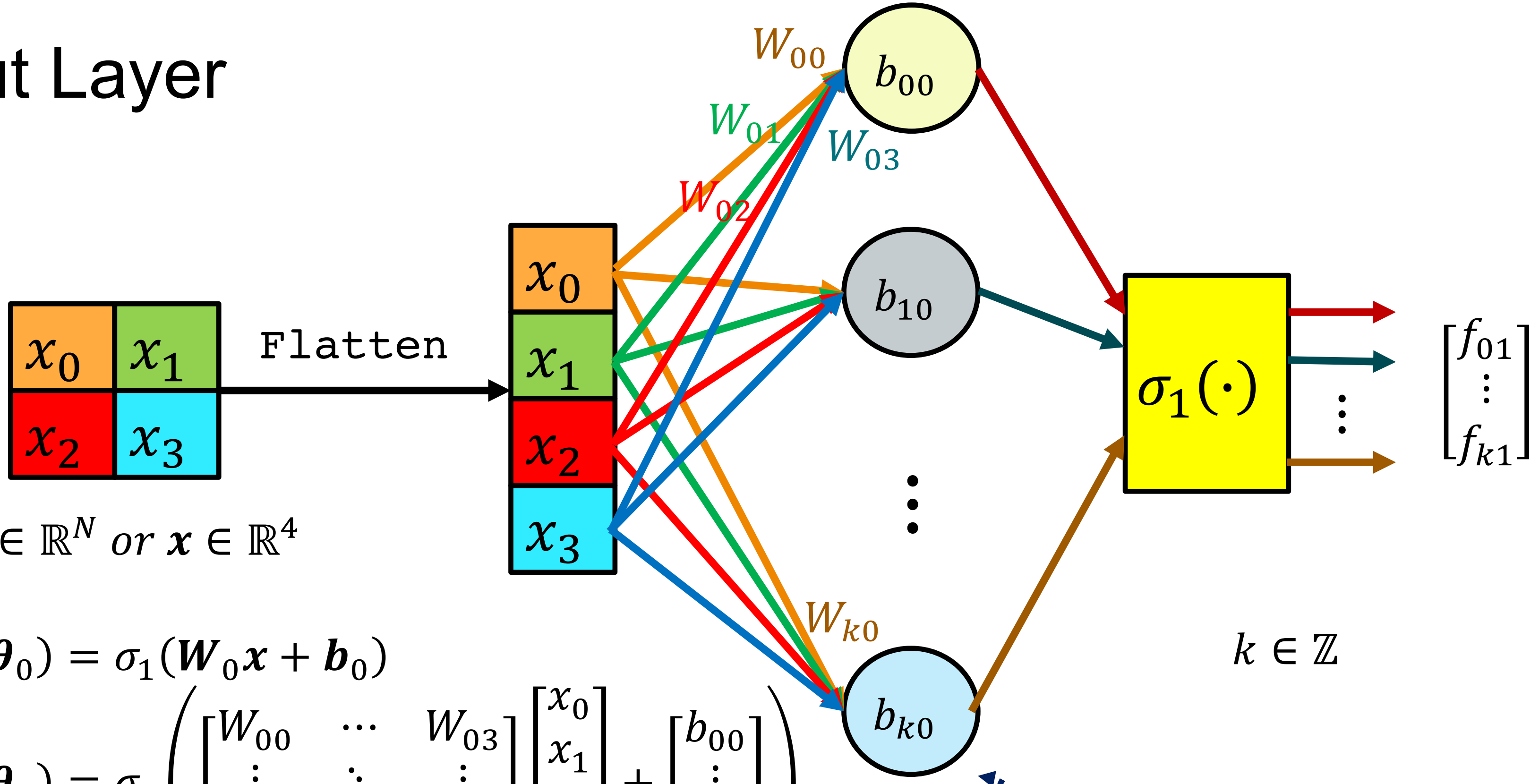
Activation function: $\sigma(\cdot)$

MLP: Function Approximator Implementation



$$\boldsymbol{y} = f(\boldsymbol{x}) \approx f_n \circ f_{n-1} \circ f_{n-2} \circ \cdots \circ f_1(\boldsymbol{x})$$
$$\ni f_0 = \boldsymbol{x},\, n \in \mathbb{Z}$$

Input Layer



$\boldsymbol{x} \in \mathbb{R}^N$ *or* $\boldsymbol{x} \in \mathbb{R}^4$

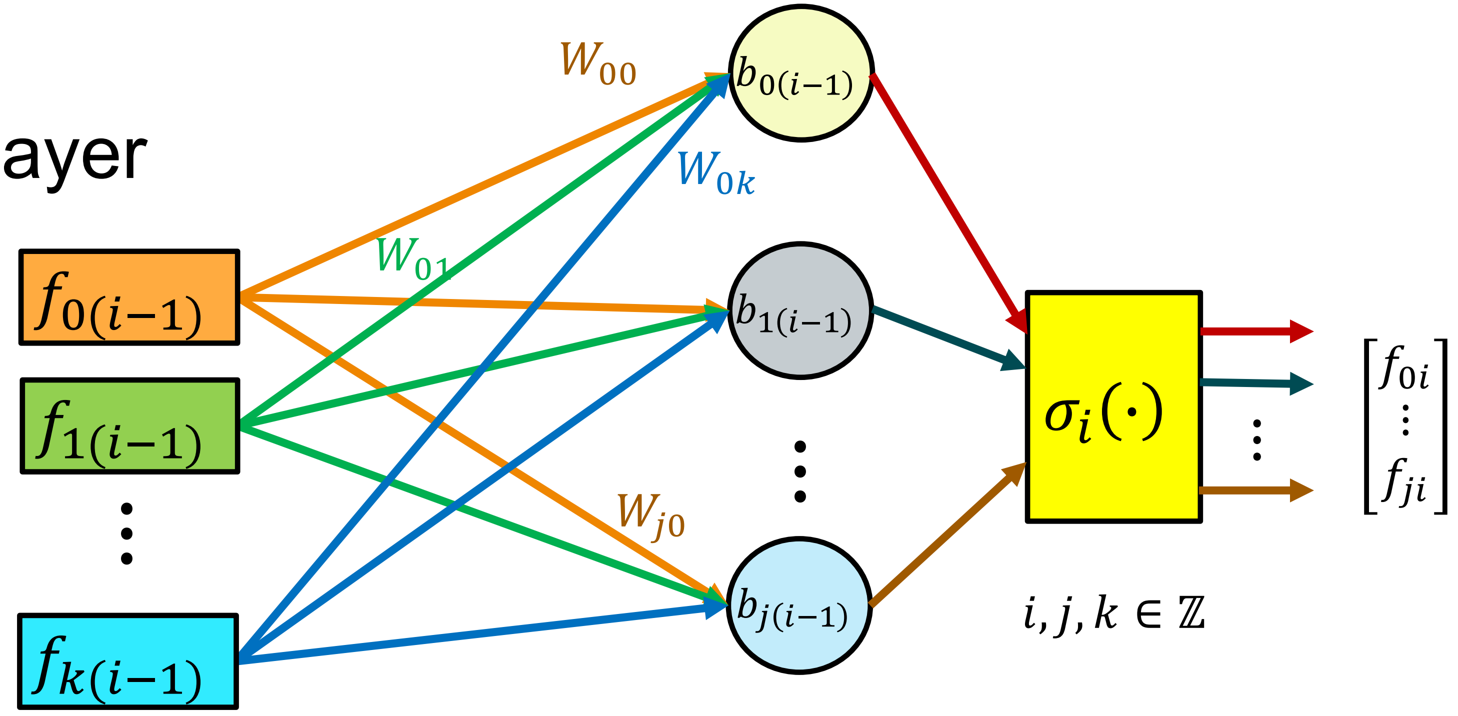
$k \in \mathbb{Z}$

$$\boldsymbol{f}_1(\boldsymbol{x};\ \boldsymbol{\theta}_0) = \sigma_1(\boldsymbol{W}_0\boldsymbol{x} + \boldsymbol{b}_0)$$

$$\boldsymbol{f}_1(\boldsymbol{x};\ \boldsymbol{\theta}_0) = \sigma_1\left(\begin{bmatrix} W_{00} & \cdots & W_{03} \\ \vdots & \ddots & \vdots \\ W_{k0} & \cdots & W_{k3} \end{bmatrix}\begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_{00} \\ \vdots \\ b_{k0} \end{bmatrix}\right)$$

Perceptron Unit

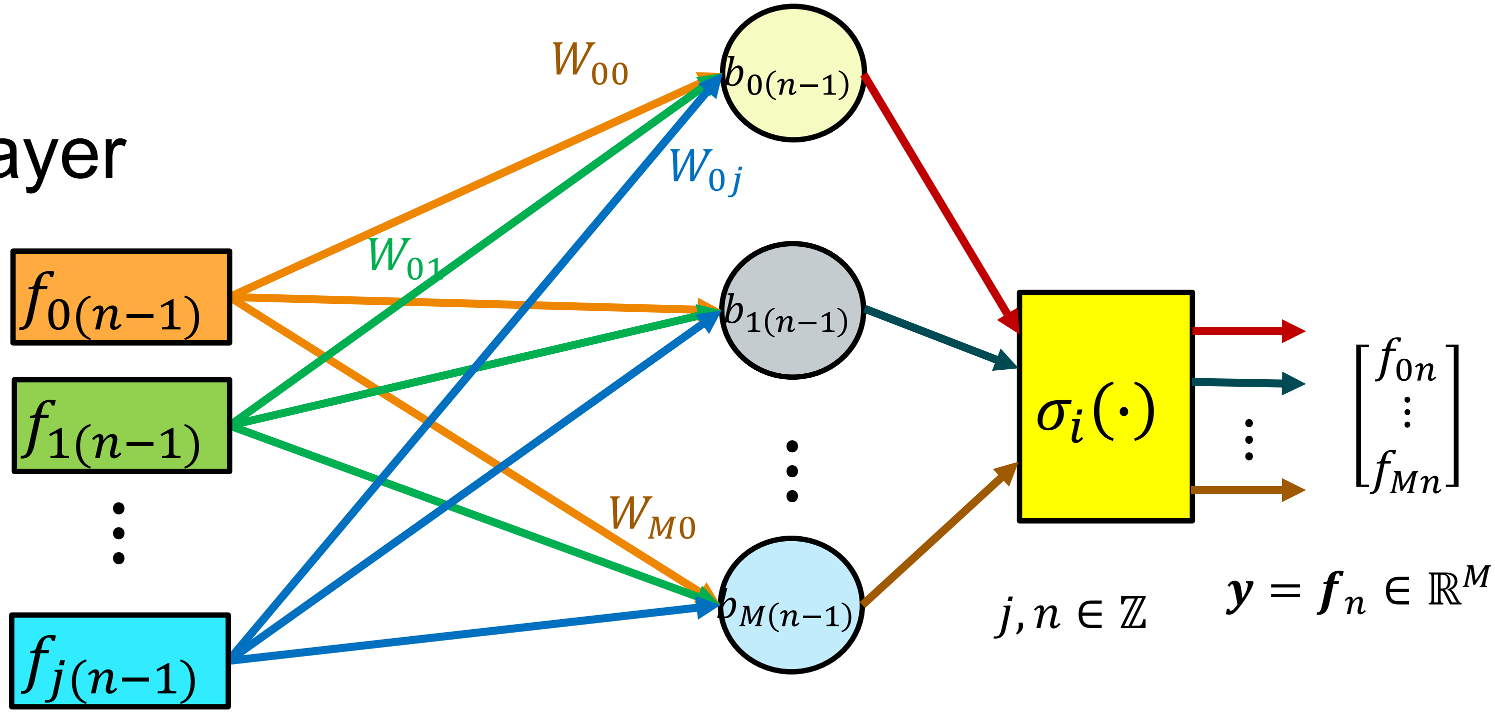
Hidden Layer



$i, j, k \in \mathbb{Z}$

$$\boldsymbol{f}_i(\boldsymbol{f}_{i-1};\ \boldsymbol{\theta}_{i-1}) = \sigma_i\left(\begin{bmatrix} W_{00} & \cdots & W_{0k} \\ \vdots & \ddots & \vdots \\ W_{j0} & \cdots & W_{jk} \end{bmatrix}\begin{bmatrix} f_{0(i-1)} \\ f_{1(i-1)} \\ \vdots \\ f_{k(i-1)} \end{bmatrix} + \begin{bmatrix} b_{0(i-1)} \\ \vdots \\ b_{j(i-1)} \end{bmatrix}\right)$$

Output Layer



$$\boldsymbol{f}_n(\boldsymbol{f}_{n-1};\, \boldsymbol{\theta}_{n-1}) = \sigma_n\left(\begin{bmatrix} W_{00} & \cdots & W_{0j} \\ \vdots & \ddots & \vdots \\ W_{M0} & \cdots & W_{Mj} \end{bmatrix}\begin{bmatrix} f_{0(n-1)} \\ f_{1(n-1)} \\ \vdots \\ f_{j(n-1)} \end{bmatrix} + \begin{bmatrix} b_{0(n-1)} \\ \vdots \\ b_{M(n-1)} \end{bmatrix}\right)$$

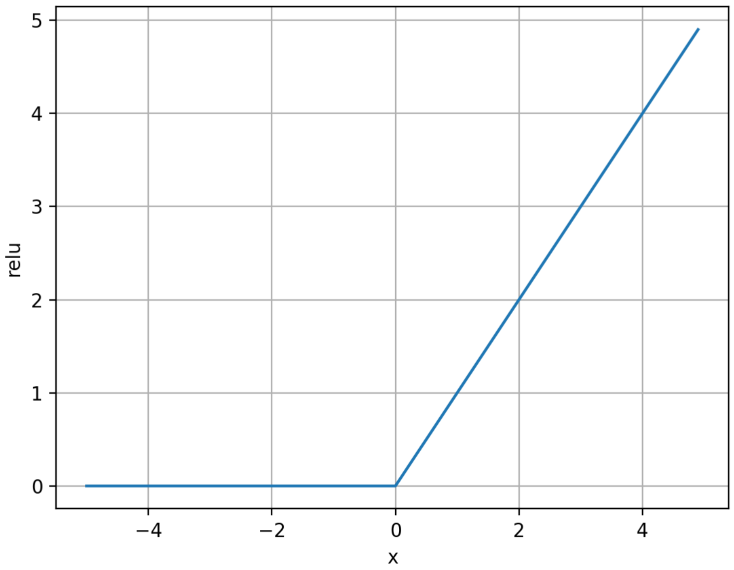
Activation Function: $\sigma_i(\cdot)$

Identity or Linear:

$$\sigma(x) = x$$

Rectified Linear Unit:

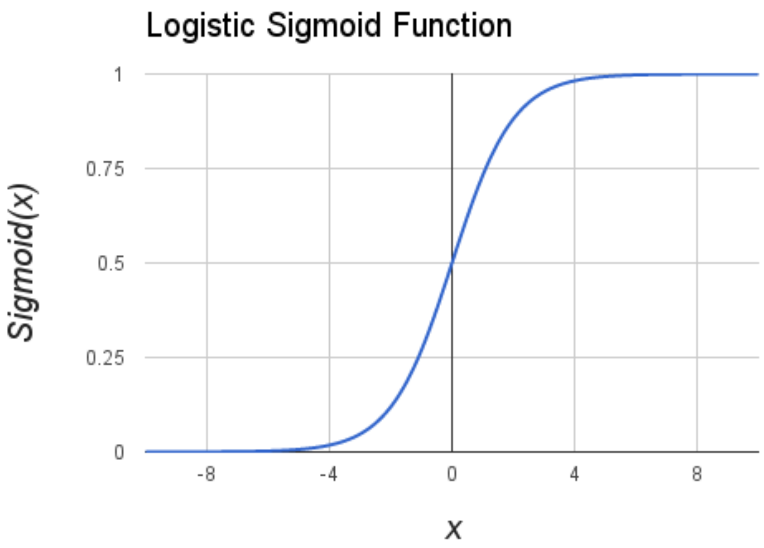
$$\sigma(x) = ReLU(x) = \begin{cases} 0, & x < 0 \\ x, & x \geq 0 \end{cases}$$



Activation Function: $\sigma_i(\cdot)$

Sigmoid:

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



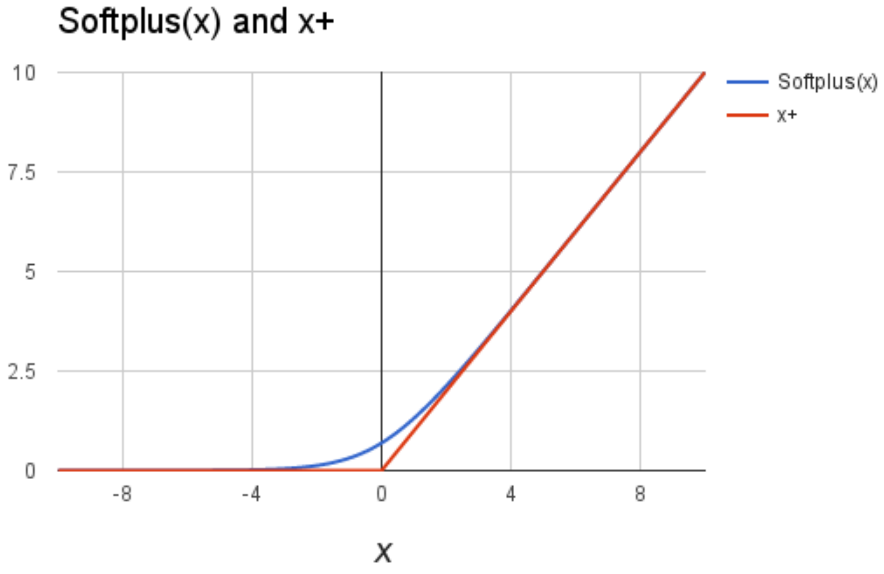
Activation Function: $\sigma_i(\cdot)$

Hyperbolic tangent:

$$\sigma(x) = \tanh x$$

Softplus:

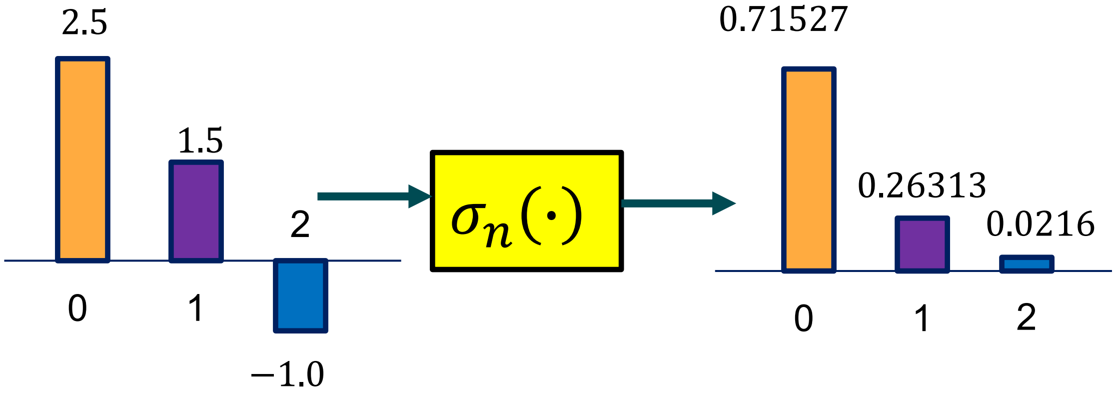
$$\sigma(x) = \ln(1 + e^x)$$



Activation Function: $\sigma_i(\cdot)$

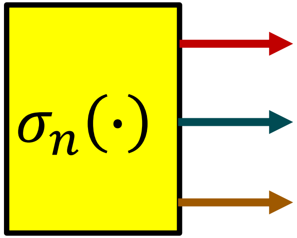
Softmax:

$$\sigma(x_i) = \frac{e^{x_i}}{\sum_{k=0}^{C} e^{x_k}}$$



Probabilities
Sum is 1.0

$$\begin{bmatrix} 2.5 \\ 1.5 \\ -1.0 \end{bmatrix}$$



$$\sigma_n\left(\begin{bmatrix} f_{0n} \\ f_{1n} \\ f_{3n} \end{bmatrix}\right) = softmax\left(\begin{bmatrix} 2.5 \\ 1.5 \\ -1.0 \end{bmatrix}\right) = \begin{bmatrix} 0.71527 \\ 0.26313 \\ 0.02160 \end{bmatrix}$$

Which activation to use?

Input and Hidden Layers

Linear – recommended

ReLU – recommended

Softplus – complex, avoid!!!

Output Layer

Linear – Un-normalized Linear Regression

Sigmoid – Bernoulli Distribution, Normalized Linear Regression

Softmax – Logistic Regression

How to learn $f(\cdot)$ from data?

Recall: Norms, Metrics, Distances from ML

Objective is to reduce the distance of the *prediction* $\boldsymbol{y} = f(\boldsymbol{x})$ from the ground truth *label* $\tilde{\boldsymbol{y}}$

This distance, norm, or metric is oftentimes called a ***Loss Function*** or an ***Objective Function***

Loss Function	**Equation**
Mean Squared Error (MSE)	$\frac{1}{categories} \sum_{i=1}^{categories} \left(y_i^{label} - y_i^{prediction}\right)^2$
Mean Absolute Error (MAE)	$\frac{1}{categories} \sum_{i=1}^{categories} \left\lvert y_i^{label} - y_i^{prediction}\right\rvert$
Categorical Cross Entropy (CE)	$-\sum_{i=1}^{categories} y_i^{label} \log y_i^{prediction}$
Binary Cross Entropy (BCE)	$-y_1^{label} \log y_1^{prediction} - \left(1 - y_1^{label}\right) \log\left(1 - y_1^{prediction}\right)$

Optimization

Given the dataset $\mathcal{D} = (\boldsymbol{x}, \boldsymbol{y}) = (\widetilde{\boldsymbol{x}}, \widetilde{\boldsymbol{y}}) = \{(\widetilde{\boldsymbol{x}}_{train}, \widetilde{\boldsymbol{y}}_{train}), (\widetilde{\boldsymbol{x}}_{test}, \widetilde{\boldsymbol{y}}_{test})\} = \{\mathcal{D}_{train}, \mathcal{D}_{test}\}$, we minimize the loss function on $\mathcal{D}_{train}$ and we measure the performance on $\mathcal{D}_{test}$

Optimization Algorithm: **Stochastic Gradient Descent (SGD)**

Variants of SGD: Adam, RMSprop

SGD Optimization Recipe

Initialize all weights by random values

Biases by zero or small positive values

Better initializers: Glorot, Uniform, Normal, LeCun, He

Preprocessing of Data

Input

Normalize such that $x_i \in [0., 1.]$

Adjust such that inputs has zero mean and unit variance

Output

In logistic regression, convert all labels to one-vectors

Example: In MNIST, digit 8 label is $\tilde{y} = [0,0,0,0,0,0,0,1,0,0]^T$

In linear regression, normalize outputs such that such that $y_i \in [0., 1.]$ or such that $y_i \in [-1., 1.]$

Hyper-parameters

Tunable network parameters

Depth or value of n in f_n

Width values of k and j in the input and hidden layers

Tunable training parameters

Learning rate

Learning rate scheduler

Batch size, Epochs

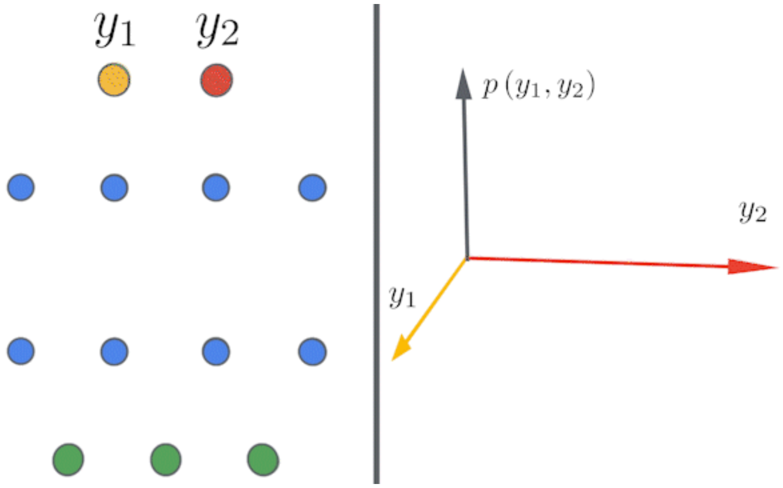
Optimization algorithm

In Summary

MLP is an implementation of the general function approximator

MLP is made of layers as building blocks

Design choices such as hyper-parameters, activation functions, etc



Left: A schematic showing how deep neural networks induce simple input / output maps as they become infinitely wide. Right: As the width of a neural network increases , we see that the distribution of outputs over different random instantiations of the network becomes Gaussian.

https://ai.googleblog.com/2020/03/fast-and-easy-infinitely-wide-networks.html