# Ch 10.1: Neural Nets

## Lecture 21 - CMSE 381

Michigan State University
::
Dept of Computational Mathematics, Science & Engineering

Wed, April 10, 2024

# Announcements

**Last time:**

- SVM

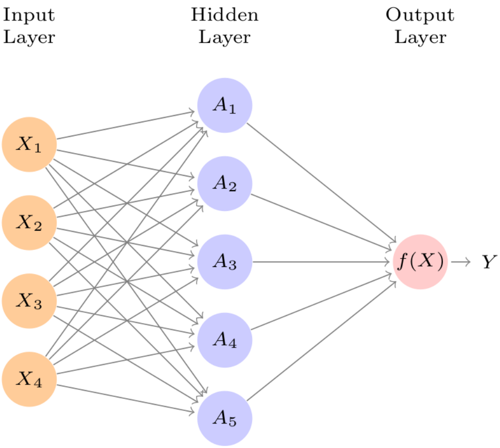
**This lecture:**

- Feed Forward Neural Nets

Section 1

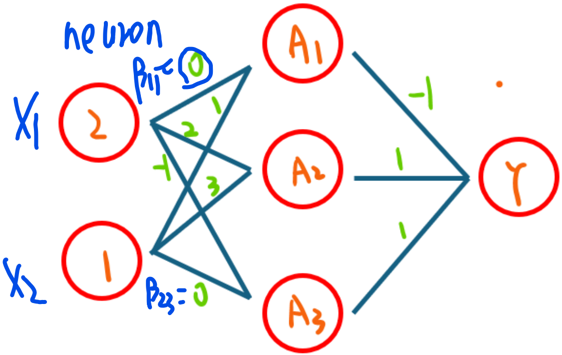
## Neural Nets

# Feed Forward Neural Network




- Input layer is starting data
- Each arrow means taking combo of those values with weights to get next value
- Here there is one hidden layer then the output
- Get to pick how many hidden units $K$, here we have $K = 5$

# Starter: A linear network




*Calculate the prediction for the new data*

$(2, 1)$

$A_1 = 2 \cdot 0 + 1 \cdot 1 = 1$

$A_2 = 2 \cdot 2 + 1 \cdot 3 = 5$

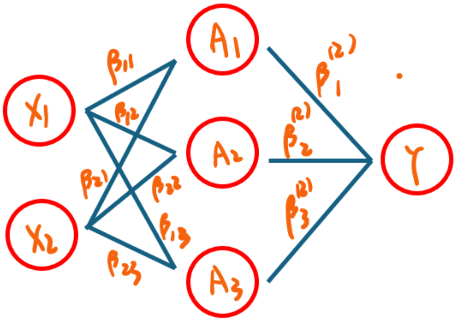
$A_3 = 2 \cdot (-1) + 1 \cdot 0 = -2$

$Y = -1 \cdot A_1 + 1 \cdot A_2 + 1 \cdot A_3 = -1 + 5 - 2 = 2$

predicted $Y$ is 2

$$\beta = \begin{pmatrix} 0 & 2 & -1 \\ 1 & 3 & 0 \end{pmatrix} \qquad \beta^{(2)} = \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}$$

Training data $x^1 = (0,1), y^1 = 1,\ x^2 = (1,1), y^2 = -1.$

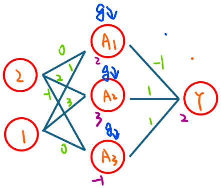



$$\hat{y}_1 = \beta_1^{(2)} A_1 + \beta_2^{(2)} A_2 + \beta_3^{(2)} A_3$$
$$= \beta_1^{(2)} \left( \beta_{11} X_1^1 + \beta_{21} X_2^1 \right) + \beta_2^{(2)} \left( \beta_{12} X_1^1 + \beta_{22} X_2^1 \right)$$
$$+ \beta_3^{(2)} \left( \beta_{31} X_1^1 + \beta_{12} X_2^1 \right)$$
$$= \beta_1^{(2)} \beta_{21} + \beta_2^{(2)} \beta_{22} + \beta_3^{(2)} \beta_{32}$$
$$\hat{y}_2 = \beta_1^{(2)} (\beta_{11} + \beta_{21}) + \beta_2^{(2)} (\beta_{21} + \beta_{22}) + \beta_3^{(2)} (\beta_{31} + \beta_{32})$$
$$\hat{\beta}_{ij}, \hat{\beta}_K^{(2)} = \underset{\beta_{ij}, \beta_K^{(2)}}{\arg\min} (y_1 - \hat{y}_1)^2 + (y_2 - \hat{y}_2)^2 = (1 - \hat{y}_1)^2 + (1 + \hat{y}_2$$
$i = 1, 2,\ j = 1, 2, 3,\ K = 1, 2, 3$

# Adding bias and activation

## Computing $Y$ for $(0, 1)$

$$A_k = g(\beta_{k0} + \sum_{j=1}^{p} \beta_{kj} X_j), \quad y = f(X) = \beta_0^{(2)} + \sum_{k=1}^{K} \beta_k^{(2)} A_k$$




← fully connected neural network

$\begin{cases} \beta_{10} = 2 \\ \beta_{20} = 3 \\ \beta_{30} = -1 \end{cases}$ : bias, $\beta_0^{(2)} = 2$

$g(z) = (z)_+ = \begin{cases} z, & \text{if } z \geq 0 \\ 0, & \text{else} \end{cases}$ ← ReLU function

activation function

# A different example

Find prediction for $(0,1,0)$

- Draw the diagram for a neural net with input data points with $p = 3$ (i.e., $(X_1, X_2, X_3)$) and two units in the hidden layer.
- Using the $\beta$ and $\beta^{(2)}$ matrices, what is the output predicted $Y$ for the point $(2, 0, 1)$?

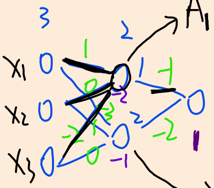
bias

$$\beta = \begin{pmatrix} 1 & 0 & -2 & 2 \\ -3 & 1 & 0 & -1 \end{pmatrix} \qquad \beta^{(2)} = \begin{pmatrix} -1 \\ -2 \\ 1 \end{pmatrix}$$

bias

- Use the activation function

$$g(z) = (z)_+ = \begin{cases} 0 & \text{if } z < 0 \\ z & \text{else.} \end{cases}$$



$$A_1 = g(1\cdot X_1 + 0\cdot X_2 + (-2)X_3 + 2) = g(2) = 2$$

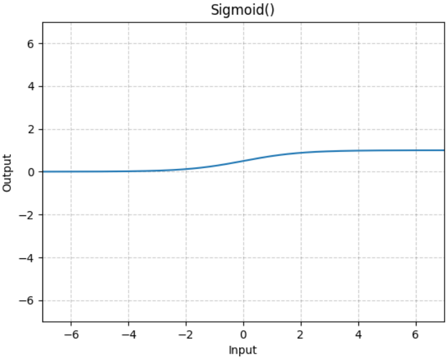
$$A_2 = g(-3X_1 + 1\cdot X_2 + 0\cdot X_3 - 1) = g(1 + (-1)) = g(0) = 0$$

$$y = -1\cdot A_1 + (-2)\cdot A_2 + 1 = -2 + 1 = -1$$

# Choices for activation function

Sigmoid: differentiable

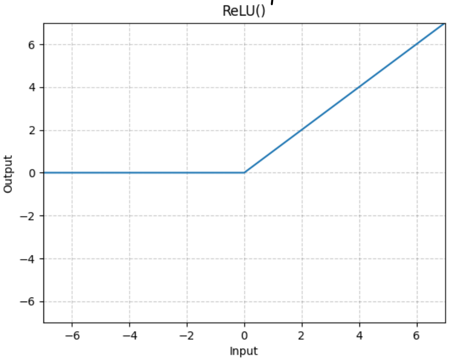
$$g(z) = \frac{e^z}{1 + e^z} = \frac{1}{1 + e^{-z}}$$



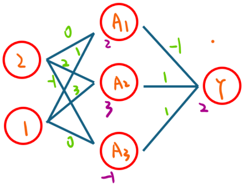

ReLU: Rectified linear unit

$$g(z) = (z)_+ = \begin{cases} 0 & \text{if } z < 0 \\ z & \text{else.} \end{cases}$$

almost everywhere differentiable



# Matrix version: First layer




$\begin{cases}\beta_{10}=2\\ \beta_{20}=3\\ \beta_{30}=-1\end{cases}$ : bias, $\beta_0^{(2)}=2$

$g(z)=(z)_+=\begin{cases} z, & \text{if } z\ge 0\\ 0, & \text{else}\end{cases}$

activation function

$$A_k = g(\beta_{k0} + \sum_{j=1}^{p} \beta_{kj} Xj),$$

$\begin{bmatrix}A_1\\A_2\\A_3\end{bmatrix}$ =

$$A = g(\mathbf{W}\cdot\mathbf{X}) \qquad \mathbf{X}^T = (1\ X_1\ X_2\ \cdots\ X_p)$$

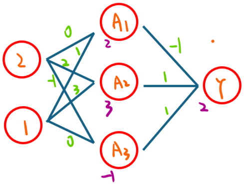
the matrix containing $\beta_{kj}$

*Caclulate out the matrix multiplication using the matrices at left to show that the equations are the same.*

# Matrix version: Output

Testing: new $(\tilde{x}, ?)$

$$\hat{y} = \hat{\beta}^{(2)} g(\hat{w}\cdot\tilde{x})$$




$$f(X) = \beta_0^{(2)} + \sum_{k=1}^{K} \beta_k^{(2)} A_k$$

$$\left\{\begin{array}{l}\beta_{10}=2\\ \beta_{20}=3\\ \beta_{30}=-1\end{array}\right. : \text{bias}, \quad \beta_0^{(2)}=2$$

$$g(z) = (z)_+ = \begin{cases} z, & \text{if } z \ge 0 \\ 0, & \text{else} \end{cases}$$

activation function

$$\left\{\begin{array}{l} Y = \beta^{(2)} \cdot \mathbf{A} \\ A = g(WX) \end{array}\right. \qquad \mathbf{A}^T = (1\ A_1\ A_2\ \cdots\ A_K)$$

previous slide

$$\Rightarrow \hat{Y} = \beta^{(2)} \cdot g(WX)$$

weights (including bias)

Training: Given $(X_i, y_i)$ $i=1,\cdots,n$

$$\hat{\beta}^{(2)}, \hat{w} = \arg\min_{\beta^{(2)}, w} \sum_{i=1}^{n} \left(y_i - \beta^{(2)} \cdot g(WX_i)\right)^2$$

# Now what?

Choose parameters by minimizing RSS, $\sum_{i=1}^{n}(y_i - f(x_i))^2$

**Chosen in advance:**

- Number of layers (more on that next lecture)
- Number of hidden units
- Activation function $g(z)$

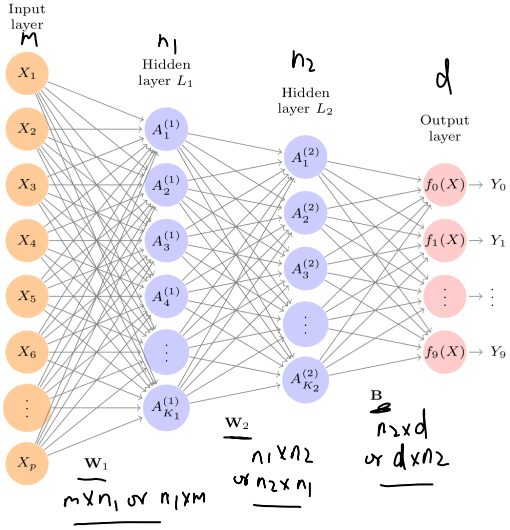
**Found by fitting the data:**

- $\mathbf{W}$
- $\beta^{(2)}$

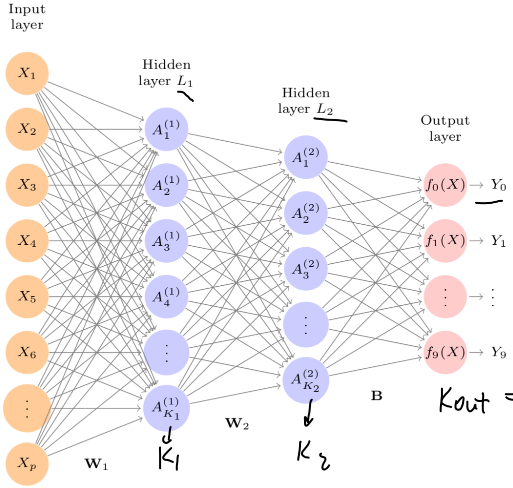
Section 2

# Multilayer Neural Networks

# Multiple layers




- Include more layers
- Can pick number of units per layer
- Each layer is linear combinations of previous




Hidden

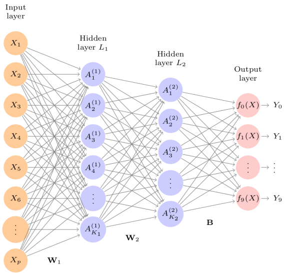
$$
\begin{aligned}
A_k^{(1)} &= \boxed{h_k^{(1)}(X)} \\
&= g(w_{k0}^{(1)} + \textstyle\sum_{j=1}^{p} w_{kj}^{(1)} X_j)
\end{aligned}
$$

$$
\begin{aligned}
A_\ell^{(2)} &= h_\ell^{(2)}(X) \\
&= g(w_{\ell 0}^{(2)} + \textstyle\sum_{k=1}^{K_1} w_{\ell k}^{(2)} A_k^{(1)})
\end{aligned}
$$

$K_{out}$ = number of classes

- Two hidden layers. $L_1$ has 256 units; $L_2$ has 128
- 10 output variables due to class labeling

# More on that architecture

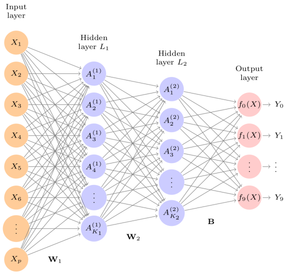



$$
\begin{aligned}
A_k^{(1)} &= h_k^{(1)}(X) \\
&= g(w_{k0}^{(1)} + \textstyle\sum_{j=1}^{p} w_{kj}^{(1)} X_j)
\end{aligned}
$$

$$
\begin{aligned}
A_\ell^{(2)} &= h_\ell^{(2)}(X) \\
&= g(w_{\ell 0}^{(2)} + \textstyle\sum_{k=1}^{K_1} w_{\ell k}^{(2)} A_k^{(1)})
\end{aligned}
$$

- Superscript denotes layer
- $W_1$ denotes entire matrix of weight
- In this setting, size is $785 \times 256 = 200,960$ values
- 785 instead of 784 to involve intercept term (called bias in this literature)

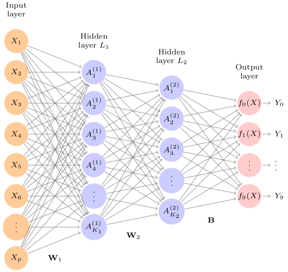
# Matrix version: First layer




$$\begin{aligned} A_k^{(1)} &= h_k^{(1)}(X) \\ &= g(w_{k0}^{(1)} + \textstyle\sum_{j=1}^{p} w_{kj}^{(1)} X_j) \end{aligned}$$

$$A^{(1)} = g(\mathbf{W}^{(1)} \cdot \mathbf{X}) \qquad \mathbf{X}^T = (1 \; X_1 \; X_2 \; \cdots \; X_p)$$

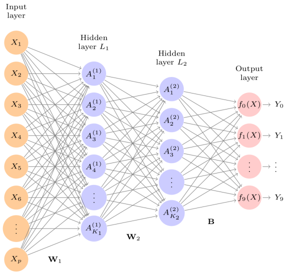
# Matrix version: Second layer




$$
\begin{aligned}
A_\ell^{(2)} &= h_\ell^{(2)}(X) \\
&= g(w_{\ell 0}^{(2)} + \textstyle\sum_{k=1}^{K_1} w_{\ell k}^{(2)} A_k^{(1)})
\end{aligned}
$$

$$
A^{(2)} = g(\mathbf{W}^{(2)} \cdot \mathbf{A}) \qquad (\mathbf{A}^{(1)})^T = (1 \; A_1^{(1)} \; A_2^{(1)} \; \cdots \; A_{K_1}^{(1)})
$$

# Matrix version: Last layer, first step

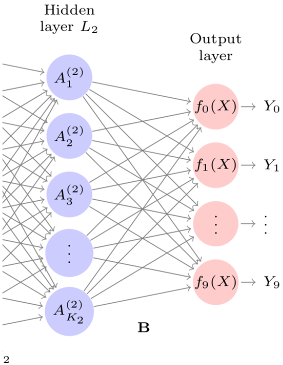



$$\begin{aligned}\underbrace{Z_m}_{} &= \beta_{m0} + \textstyle\sum_{\ell=1}^{K_2} \beta_{m\ell} h_\ell^{(2)}(X) \\ &= \beta_{m0} + \textstyle\sum_{\ell=1}^{K_2} \beta_{m\ell} A_\ell^{(2)},\end{aligned}$$

$$\mathbf{Z} = \beta \cdot \mathbf{A}$$

$\beta$ is $M \times (K_2 + 1)$ matrix $\quad (\mathbf{A}^{(2)})^T = (1\ A_1^{(2)}\ A_2^{(2)}\ \cdots\ A_{K_2}^{(2)})$

# The last column for classification: Softmax




$$f_m(X) = \Pr(Y = m|X) = \frac{e^{Z_m}}{\sum_{\ell=0}^{9} e^{Z_\ell}},$$

- Want this to act like a probability.
- Answer is to use the softmax activation function $f_m(X)$
- Values are non-negative
- Values sum to 1
- Return class with highest probability

# An example

$$Z = \begin{pmatrix} 1 & 3 & -1 & 2 & 5 \end{pmatrix}$$

$$Y_m = \frac{e^{z_m}}{\sum_{j=1}^{K_{out}} e^{z_j}} \qquad m = 1, \cdots K_{out}$$

$m=1$: $\dfrac{e^1}{\Sigma} = Y_1$

$m=2$: $\dfrac{e^3}{\Sigma} = Y_2$

- $\overbrace{e^1 + e^3 + e^{-1} + e^2 + e^5}^{\Sigma} = \underline{178.97}$
- $f =$
  $\begin{pmatrix} 0.01518 & 0.1122 & 0.00205 & 0.04128 & 0.82924 \end{pmatrix}$

$$\vec{Y} = \Big( \underbrace{\frac{e^1}{\Sigma}, \frac{e^3}{\Sigma}, \frac{e^{-1}}{\Sigma}, \cdots \frac{e^5}{\Sigma}}_{\text{probability distribution}} \Big)$$

since $Y_1 + Y_2 + \cdots + Y_5 = 1$

$Y_1$ : probility your sample is in class 1

$\vdots$ . . . . . . . . . . . class k

$Y_K$ : . .

# MNIST

- Goal: Build a model to classify images into their correct digit class
- Each image has $p = 28 \cdot 28 = 784$ pixels
- Each pixel is grayscale value in [0,255]
- Data converted into column order
- Output represented by one-hot vector $Y = (Y_0, Y_1, \cdots, Y_9)$
- 60K training images, 10K test images