Neural Network Learning basics

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https://github.com/roboticcam/machine-learning-notes

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Check the **regression** notes on:

- revise on **sigmoid** and **tanh** function
- revise on **logistic** and **softmax** regression
- Then we talk about neural networks and multilayer perceptron

Feedforward Neural Network in a nutshell

We begin Feedforward Neural networks, in a nutshell, comprised of the following steps:

- Feedforward

$$f(\mathbf{x}) = f_L(\dots f_2(f_1(\mathbf{x}; \boldsymbol{\theta}_1); \boldsymbol{\theta}_2)\dots), \boldsymbol{\theta}_L)$$

- The objective is to minimize the overall cost:

$$L(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, f(\mathbf{x}_i; \boldsymbol{\theta}))$$

- To put it in a gradient descent framework, i.e.,

$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^t - \eta_t \frac{\partial f}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}^t)$$

Something about $\frac{\partial f}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}^t)$

We know all about it already from high school mathematics:

- **Product rule**:

$$\frac{\partial f}{\partial \boldsymbol{\theta}}\left(f(\boldsymbol{\theta})\, g(\boldsymbol{\theta})\right) = f(\boldsymbol{\theta})\, \frac{\partial}{\partial \boldsymbol{\theta}} g(\boldsymbol{\theta}) + \frac{\partial}{\partial \boldsymbol{\theta}} f(\boldsymbol{\theta})\, g(\boldsymbol{\theta})$$

- **Derivative of sums**:

$$\frac{\partial f}{\partial \boldsymbol{\theta}}\left(f(\boldsymbol{\theta}) + g(\boldsymbol{\theta})\right) = \frac{\partial}{\partial \boldsymbol{\theta}} f(\boldsymbol{\theta}) + \frac{\partial}{\partial \boldsymbol{\theta}} g(\boldsymbol{\theta})$$

- **Chain rule**

$$\begin{aligned}\frac{\partial f}{\partial \boldsymbol{\theta}_l} &= \frac{\partial}{\partial \boldsymbol{\theta}_l} f_L(\dots f_2(f_1(\mathbf{x}; \boldsymbol{\theta}_1); \boldsymbol{\theta}_2)\dots), \boldsymbol{\theta}_L) \\ &= \frac{\partial f_L}{\partial f_{L-1}^\top} \frac{\partial f_{L-1}}{\partial f_{L-2}^\top} \cdots \frac{\partial f_{l+2}}{\partial f_l^\top} \frac{\partial f_l}{\partial \boldsymbol{\theta}_l^\top}\end{aligned}$$

Multivariable Chain Rule

We know all about it already from high school mathematics:

- **Product rule**:

$$\frac{\partial f}{\partial \boldsymbol{\theta}}\left(f\left(\boldsymbol{\theta}\right) g\left(\boldsymbol{\theta}\right)\right) = f\left(\boldsymbol{\theta}\right) \frac{\partial}{\partial \boldsymbol{\theta}} g\left(\boldsymbol{\theta}\right) + \frac{\partial}{\partial \boldsymbol{\theta}} f\left(\boldsymbol{\theta}\right) g\left(\boldsymbol{\theta}\right)$$

- **Derivative of sums**:

$$\frac{\partial f}{\partial \boldsymbol{\theta}}\left(f\left(\boldsymbol{\theta}\right) + g\left(\boldsymbol{\theta}\right)\right) = \frac{\partial}{\partial \boldsymbol{\theta}} f\left(\boldsymbol{\theta}\right) + \frac{\partial}{\partial \boldsymbol{\theta}} g\left(\boldsymbol{\theta}\right)$$

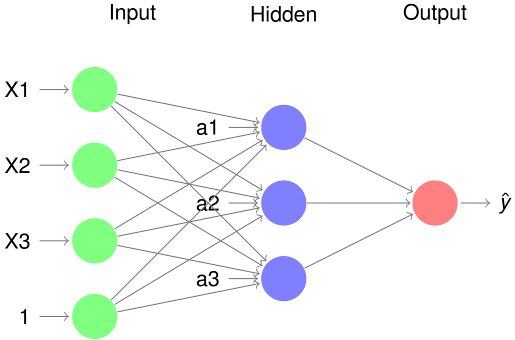
- **Chain rule**

$$\begin{aligned}\frac{\partial f}{\partial \boldsymbol{\theta}_l} &= \frac{\partial}{\partial \boldsymbol{\theta}_l} f_L(\ldots f_2(f_1(\mathbf{x}; \boldsymbol{\theta}_1); \boldsymbol{\theta}_2) \ldots), \boldsymbol{\theta}_L) \\ &= \frac{\partial f_L}{\partial f_{L-1}^\top} \frac{\partial f_{L-1}}{\partial f_{L-2}^\top} \cdots \frac{\partial f_{l+2}}{\partial f_l^\top} \frac{\partial f_l}{\partial \boldsymbol{\theta}_l^\top}\end{aligned}$$

Look at Neural network systematically: Feed Forward (1)

$$\hat{y} = U^\top f(Wx + b)$$
$$= U^\top \underbrace{f(\underbrace{Wx + b}_{z})}_{a} = U^\top a$$

let $\hat{y}$ be a **scalar** score instead of a **softmax** this time.



$$\hat{y} = U^\top f\left(\begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}\right)$$

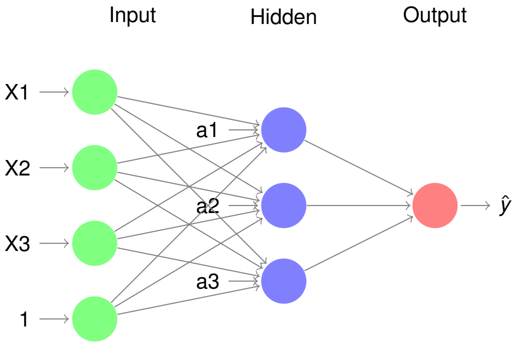
$$z_1 = W_{1,:}^\top X + b_1 = \sum_i W_{1,i} X_i + b_1$$

$$z_2 = W_{2,:}^\top X + b_2 = \sum_i W_{2,i} X_i + b_2$$

$$z_3 = W_{3,:}^\top X + b_3 = \sum_i W_{3,i} X_i + b_3$$

Therefore:

$$W_{(\text{index of } a, \text{index of } X)}$$



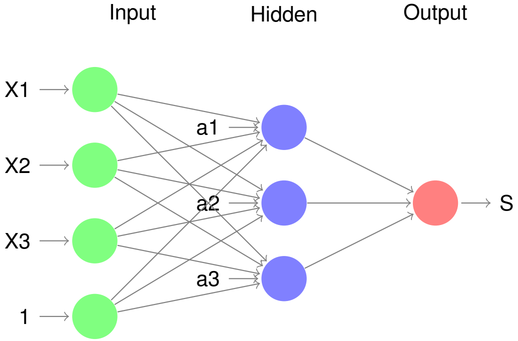
$$\hat{y} = U^\top f\left(\begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \right)$$

Neural network: Backpropagation

$$\hat{y} = U^\top f(Wx + b)$$
$$= U^\top \underbrace{f(\underbrace{Wx + b}_{z})}_{a} = U^\top a$$

Careful of their dimensions:

$$\frac{\partial \hat{y}}{\partial W} = \underbrace{\frac{\partial \hat{y}}{\partial a}\frac{\partial a}{\partial z}}_{\text{column vector}} \times \underbrace{\frac{\partial z}{\partial W}}_{\text{row vector}}$$
$$= \underbrace{(U \odot f'(z))}_{\text{column vector}} \times \underbrace{x}_{\text{row vector}}$$



$$\hat{y} = U^\top f\left(\begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix}\begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}\right)$$

$$\hat{y} = \underbrace{U^\top \underbrace{f(Wx + b)}_{z}}_{a} = U^\top a$$

If dimensionality of derivative of W is too hard to see, then we perform derivative one element $W_{I,j}$ at the time:

$$W_{(\text{index of } a, \text{index of } X)}$$

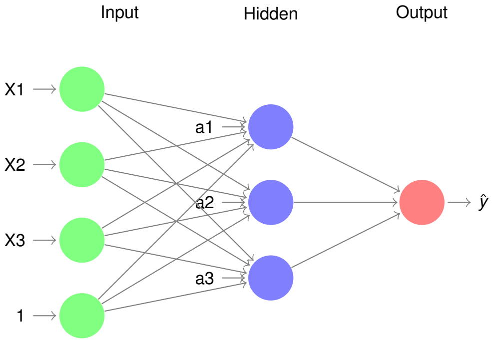
If we were to compute $\frac{\partial S}{W_{i,j}}$:

$$\frac{\partial \hat{y}}{\partial W} = \frac{\partial \hat{y}}{\partial a}\frac{\partial a}{\partial z}\frac{\partial z}{\partial W}$$

$$\Longrightarrow \frac{\partial \hat{y}}{\partial W_{i,j}} = \frac{\partial \hat{y}}{\partial a_i}\frac{\partial a_i}{\partial z_i}\frac{\partial z_i}{\partial W_{i,j}}$$

$$= \underbrace{U_i f'(z_i)}_{\delta_i} X_j$$

$$= \underbrace{U_i f'(W_{i,:}^\top X + b_i)}_{\delta_i} X_j$$



$$\hat{y} = U^\top f\left(\begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix}\begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}\right)$$

important to remember:

$$z_i = W_{i,:}^\top X + b_i = (WX + b)_i$$

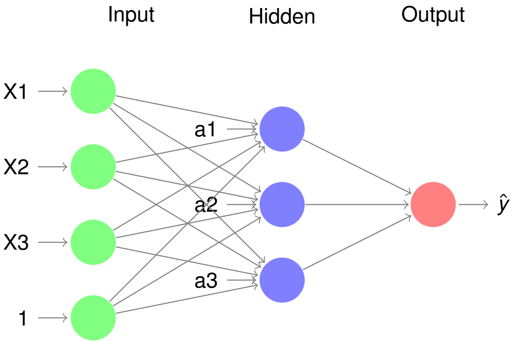
Backpropagation for W

If we were to compute $\frac{\partial \hat{y}}{W_{i,j}}$:

$$\frac{\partial \hat{y}}{\partial W_{i,j}} = \underbrace{U_i f'(W_{i,:}^{\top} X + b_i)}_{\delta_i} X_j$$

$$\delta = \begin{bmatrix} U_1 f'(W_{1,:}^{\top} X + b_1) \\ U_2 f'(W_{2,:}^{\top} X + b_2) \\ U_3 f'(W_{3,:}^{\top} X + b_3) \end{bmatrix}$$
$$= U \odot f'(WX + B)$$

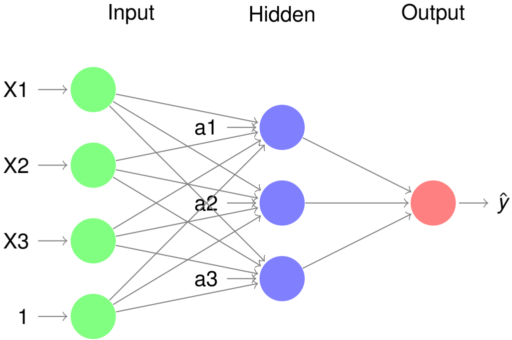
$$\frac{\partial \hat{y}}{\partial W} = \begin{bmatrix} \delta_1 X_1 & \delta_1 X_2 & \delta_1 X_3 \\ \delta_2 X_1 & \delta_2 X_2 & \delta_2 X_3 \\ \delta_3 X_1 & \delta_3 X_2 & \delta_3 X_3 \end{bmatrix}$$
$$= \delta X^{\top}$$



$$\hat{y} = U^{\top} f\left(\begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \right)$$

$$
\delta = \begin{bmatrix} U_1 f'(W_{1,:}^\top X + b_1) \\ U_2 f'(W_{2,:}^\top X + b_2) \\ U_3 f'(W_{3,:}^\top X + b_3) \end{bmatrix} = U \odot f'(WX + B)
$$

$$
\frac{\partial \hat{y}}{\partial W} = \begin{bmatrix} \delta_1 X_1 & \delta_1 X_2 & \delta_1 X_3 \\ \delta_2 X_1 & \delta_2 X_2 & \delta_2 X_3 \\ \delta_3 X_1 & \delta_3 X_2 & \delta_3 X_3 \end{bmatrix} = \delta X^\top
$$



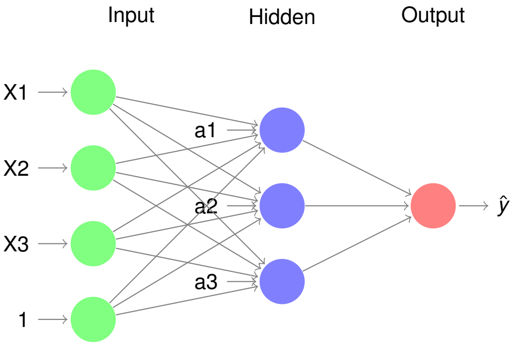
- δ is the error signal, i.e., $\frac{\partial \hat{y}}{\partial z}$
- δ involves the derivatives of all the activation function $\{a_i = f(z_i)\}$

$$
\hat{y} = U^\top f\left(\begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \right)
$$

Backpropagation for b

$$\frac{\partial \hat{y}}{\partial b_i} = \underbrace{U_i f'(W_{i,:}^\top X + b_i)}_{\delta_i} 1$$

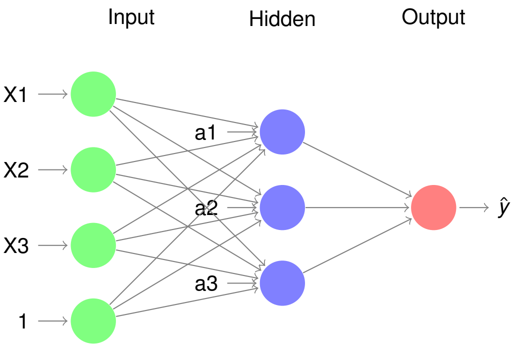
$$= \delta_i$$



$$\hat{y} = U^\top f\left(\begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix}\begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}\right)$$

Note each x_j is contributed by all $\{a_i\}$

$$
\begin{aligned}
\frac{\partial \hat{y}}{\partial x_j} &= \sum_{i=1}^{3} \frac{\partial \hat{y}}{\partial a_i} \frac{\partial a_i}{\partial x_j} \\
&= \sum_{i=1}^{3} \frac{\partial U^\top a}{\partial a_i} \frac{\partial a_i}{\partial x_j} \\
&= \sum_{i=1}^{3} U_i \frac{\partial f(W_{i,:}x + b)}{\partial x_j} \\
&= \sum_{i=1}^{3} \underbrace{U_i f'(W_{i,:}x + b)}_{\delta_i} \frac{\partial W_{i,:}x}{\partial x_j} \\
&= \sum_{i=1}^{3} \delta_i W_{i,j} = \delta^\top W_{:,j}
\end{aligned}
$$



$$
\hat{y} = U^\top f\left(\begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \right)
$$

Backpropagation for two layers with respect to $W^{(2)}$

$$a^{(0)} = x \quad \text{(input)}$$

$$z^{(1)} = W^{(1)} a^{(0)} + b^{(1)} \quad \text{(linear)}$$
$$a^{(1)} = f\left(z^{(1)}\right) \quad \text{(non-linear)}$$

$$z^{(2)} = W^{(2)} a^{(1)} + b^{(2)} \quad \text{(linear)}$$
$$a^{(2)} = f\left(z^{(2)}\right) \quad \text{(non-linear)}$$

$$\hat{y} = U^\top a^{(2)} \quad \text{(output)}$$

$$\hat{y} = U^\top f\left(W^{(2)} f\left(W^{(1)} x + b^{(1)}\right) + b^{(2)}\right)$$

$$\frac{\partial \hat{y}}{\partial W_{i,j}} = \underbrace{U_i f'(z_i)}_{\delta_i} X_j \qquad \text{(one layer case)}$$

$$\Longrightarrow \frac{\partial \hat{y}}{\partial W^{(2)}_{i,j}} = \underbrace{U_i f'(z_i^{(2)})}_{\delta_i^{(2)}} a_j^{(2)}$$

$$\Longrightarrow \frac{\partial \hat{y}}{\partial W^{(2)}} = \delta^{(2)} a^{(2)\top} \qquad \text{where } \delta^{(2)} = U \odot f'(z^{(2)})$$

Backpropagation for two layers with respect to $W^{(1)}$

$$
\begin{aligned}
a^{(0)} &= x && \text{(input)}\\
z^{(1)} &= W^{(1)} a^{(0)} + b^{(1)} && \text{(linear)}\\
a^{(1)} &= f\left(z^{(1)}\right) && \text{(non-linear)}\\
z^{(2)} &= W^{(2)} a^{(1)} + b^{(2)} && \text{(linear)}\\
a^{(2)} &= f\left(z^{(2)}\right) && \text{(non-linear)}\\
\hat{y} &= U^{\top} a^{(2)} && \text{(output)}
\end{aligned}
$$

$$
\begin{aligned}
\hat{y} &= U^{\top} f\left(W^{(2)} f\left(W^{(1)} x + b^{(1)}\right) + b^{(2)}\right)\\
&= U^{\top} f\Bigg(\underbrace{W^{(2)} f\Big(\underbrace{W^{(1)} x + b^{(1)}}_{z^{(1)}}\Big) + b^{(2)}}_{z^{(2)}}\Bigg)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \hat{y}}{\partial W^{(1)}} &= \underbrace{U f'\left(W^{(2)} f\left(W^{(1)} x + b^{(1)}\right) + b^{(2)}\right)}_{\frac{\partial \hat{y}}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial z^{(2)}}} \underbrace{W^{(2)}}_{\frac{\partial z^{(2)}}{\partial a^{(1)}}} \underbrace{f'\left(W^{(1)} X + b^{(1)}\right)}_{\frac{\partial a^{(1)}}{\partial z^{(1)}}} \underbrace{X}_{\frac{\partial z^{(1)}}{\partial W^{(1)}}}\\
&= \underbrace{\underbrace{\frac{\partial \hat{y}}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial z^{(2)}}}_{\delta^{(2)}} \frac{\partial z^{(2)}}{\partial a^{(1)}} \frac{\partial a^{(1)}}{\partial z^{(1)}}}_{\delta^{(1)}} \frac{\partial z^{(1)}}{\partial W^{(1)}}\\
&= \underbrace{\delta^{(2)} W^{(2)} f'(z^{(2)})}_{\delta^{(1)}} X
\end{aligned}
$$

Putting them in the “correct” form of the matrix operations and generalise:

$$
\begin{aligned}
&= \underbrace{\left({W^{(2)}}^\top \delta^{(2)}\right) \odot f'(z^{(2)})}_{\delta^{(1)}} X^\top \\
&\implies \delta^{(1)} = \left({W^{(2)}}^\top \delta^{(2)}\right) \odot f'(z^{(2)}) \\
&\implies \delta^{(l)} = \left({W^{(l)}}^\top \delta^{(l+1)}\right) \odot f'(z^{(l)})
\end{aligned}
$$

Backpropagation in action!

$$a^{(0)} = x \quad \text{(input)}$$

$$z^{(1)} = W^{(1)} a^{(0)} + b^{(1)} \quad \text{(linear)}$$
$$a^{(1)} = f\left(z^{(1)}\right) \quad \text{(non-linear)}$$

$$z^{(2)} = W^{(2)} a^{(1)} + b^{(2)} \quad \text{(linear)}$$
$$a^{(2)} = f\left(z^{(2)}\right) \quad \text{(non-linear)}$$

$$\hat{y} = U^{\top} a^{(2)} \quad \text{(output)}$$

To generalise this:

$$\delta^{(l)} = \left(W^{(l)\top} \delta^{(l+1)}\right) \odot f'(z^{(l)})$$

- step 1: compute δ of the last layer L:

$$\delta^{(L)} = U \odot \underbrace{f'(z^{(L)})}_{\text{from feed-forward}}$$

- step 2: Generate the whole sequence of $\{\delta^{(l)}\}_1^L$

$$\delta^{(l)} = \left(W^{(l)\top} \delta^{(l+1)}\right) \odot f'(z^{(l)})$$

- step 3: compute gradients at each layers $\left\{ \frac{\partial s}{\partial W^{(l)}} \right\}_1^{(L-1)}$:

$$\frac{\partial \hat{y}}{\partial W^{(l)}} = \delta^{(l+1)} a^{(l)\top}$$

Note that $\frac{\partial \hat{y}}{\partial W^{(l)}}$ can be obtained as soon as $\delta^{(l+1)}$ becomes available.