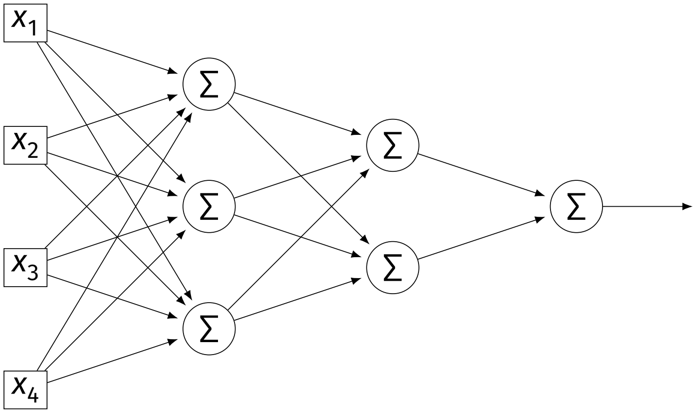
DSC 140B
Representation Learning

Lecture 20 | Part 1

Training Neural Networks

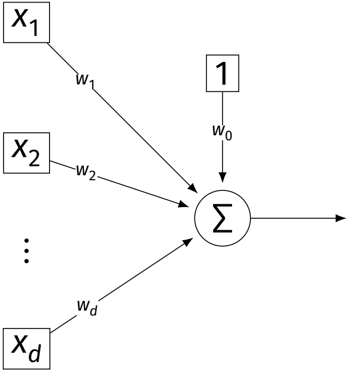
Training

- How do we learn the weights of a (deep) neural network?



Remember...

- How did we learn the weights in linear least squares regression?



Empirical Risk Minimization

0. Collect a training set, $\{(\vec{x}^{(i)}, y_i)\}$

1. Pick the form of the prediction function, H.

2. Pick a loss function.

3. Minimize the empirical risk w.r.t. that loss.

Remember: Linear Least Squares

0. Pick the form of the prediction function, H.
   - E.g., linear: $H(\vec{x}; \vec{w}) = w_0 + w_1 x_1 + \ldots + w_d x_d = \text{Aug}(\vec{x}) \cdot \vec{w}$
1. Pick a loss function.
   - E.g., the square loss.
2. Minimize the empirical risk w.r.t. that loss:

$$R_{\text{sq}}(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} (H(\vec{x}^{(i)}) - y_i)^2 = \frac{1}{n} \sum_{i=1}^{n} (\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i)^2$$

Minimizing Risk

- To minimize risk, we often use **vector calculus**.
  - Either set $\nabla_{\vec{w}} R(\vec{w}) = 0$ and solve...
  - Or use gradient descent: walk in opposite direction of $\nabla_{\vec{w}} R(\vec{w})$.

- Recall, $\nabla_{\vec{w}} R(\vec{w}) = (\partial R / \partial w_0, \partial R / \partial w_1, \ldots, \partial R / \partial w_d)^T$

In General

- Let ℓ be the loss function, let $H(\vec{x}; \vec{w})$ be the prediction function.

- The empirical risk:

$$R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

- Using the chain rule:

$$\nabla_{\vec{w}} R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \frac{\partial \ell}{\partial H} \nabla_{\vec{w}} H(\vec{x}^{(i)}; \vec{w})$$

Gradient of H

- To minimize risk, we want to compute $\nabla_{\vec{w}} R$.
- To compute $\nabla_{\vec{w}} R$, we want to compute $\nabla_{\vec{w}} H$.
- This will depend on the form of H.

Example: Linear Model

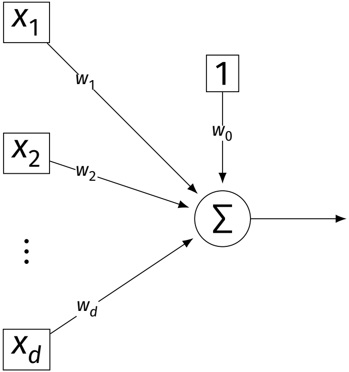
- Suppose H is a linear prediction function:

$$H(\vec{x}; \vec{w}) = w_0 + w_1 x_1 + \ldots + w_d x_d$$

- What is $\nabla_{\vec{w}} H$ with respect to $\vec{w}$?

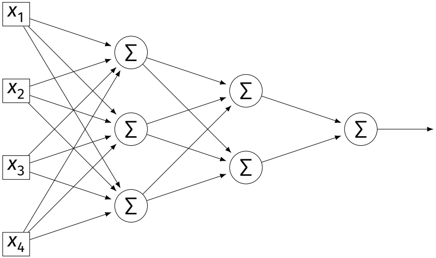
Example: Linear Model

- Consider $\partial H / \partial w_1$:



Example: Neural Networks

- Suppose H is a neural network (with nonlinear activations).
- What is ∇H?
  - It's more complicated...



Parameter Vectors

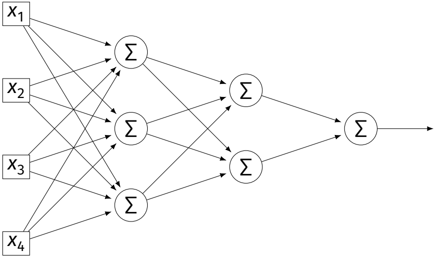
- It is often useful to pack all of the network's weights into a **parameter vector**, $\vec{w}$.
- Order is arbitrary:

$$\vec{w} = (W_{11}^{(1)}, W_{12}^{(1)}, \ldots, b_1^{(1)}, b_2^{(1)}, W_{11}^{(2)}, W_{12}^{(2)}, \ldots, b_1^{(2)}, b_2^{(2)}, \ldots)^T$$

- The network is a function $H(\vec{x}; \vec{w})$.
- Goal of learning: find the "best" $\vec{w}$.

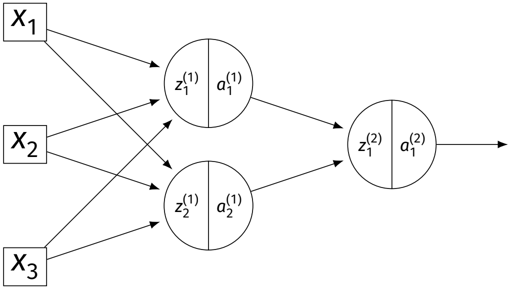
Gradient of Neural Network

- $\nabla_{\vec{w}} H$ is a vector-valued function.
- Plugging a data point, $\vec{x}$, and a parameter vector, $\vec{w}$, into $\nabla_{\vec{w}} H$ "evaluates the gradient", results in a vector, same size as $\vec{w}$.



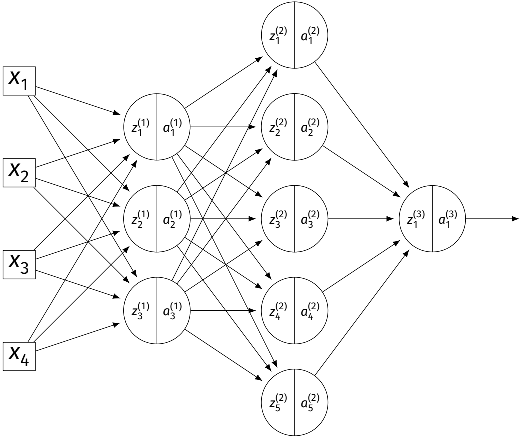
Exercise

Suppose $W_{11}^{(1)} = -2, W_{21}^{(1)} = -5, W_{31}^{(1)} = 2$ and $\vec{x} = (3, 2, -2)^T$ and all biases are 0. ReLU activations are used. What is $\partial H / \partial W_{11}^{(1)}(\vec{x}, \vec{w})$?



Example

- Consider $\partial H / \partial W_{11}^{(1)}$:



A Better Way

- Computing the gradient is straightforward...
- But can involve a lot of repeated work.
- **Backpropagation** is an algorithm for efficiently computing the gradient of a neural network.

DSC 140B

Representation Learning

Lecture 20 | Part 2

Backpropagation

Gradient of a Network

- We want to compute the gradient $\nabla_{\vec{w}} H$.
  - That is, $\partial H / \partial W_{ij}^{(\ell)}$ and $\partial H / \partial b_i^{(\ell)}$ for all valid i, j, ℓ.
- A network is a composition of functions.
- We'll make good use of the **chain rule**.

Recall: The Chain Rule

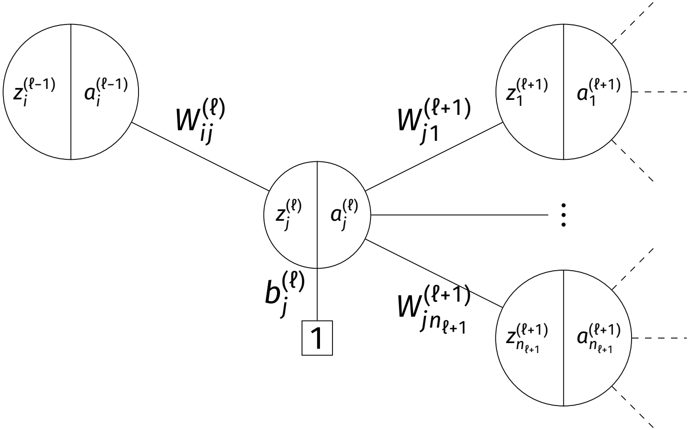
$$\frac{d}{dx} f(g(x)) = \frac{df}{dg}\frac{dg}{dx}$$

$$= f'(g(x))\, g'(x)$$

Some Notation

- We'll consider an arbitrary node in layer ℓ of a neural network.
- Let g be the activation function.
- n_ℓ denotes the number of nodes in layer ℓ.

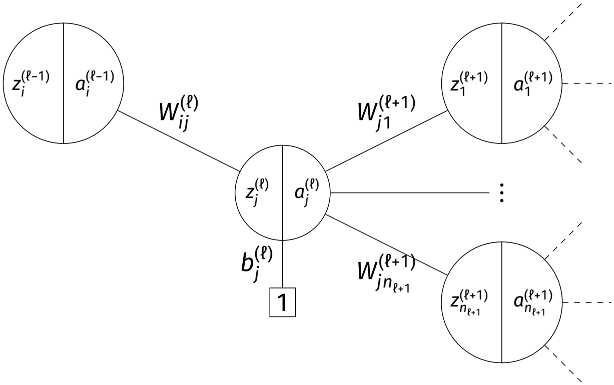
Arbitrary Node



- $\dfrac{\partial H}{\partial W_{ij}^{(\ell)}}$?
- $\dfrac{\partial H}{\partial b_j^{(\ell)}}$?

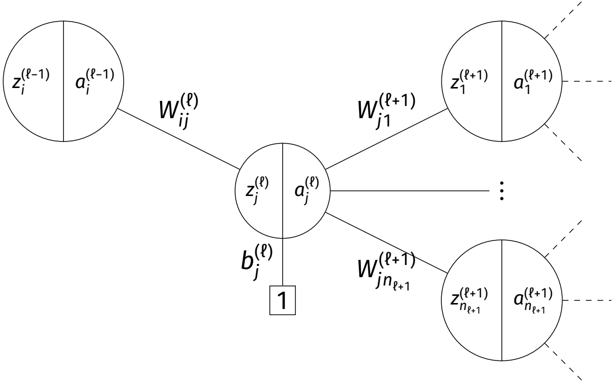
Claim #1

$$\frac{\partial H}{\partial W_{ij}^{(\ell)}} = \frac{\partial H}{\partial z_j^{(\ell)}} a_i^{(\ell-1)}$$



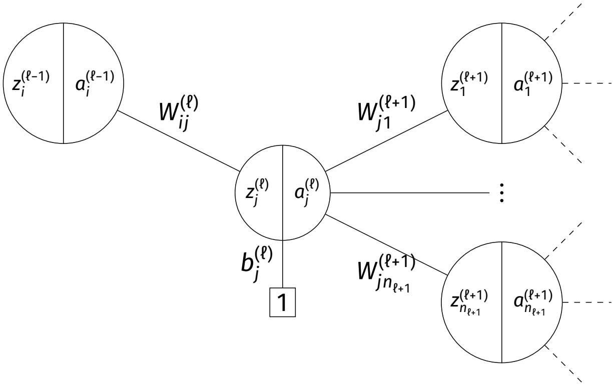
Claim #2

$$\frac{\partial H}{\partial z_j^{(\ell)}} = \frac{\partial H}{\partial a_j^{(\ell)}} g'(z_j^{\ell})$$



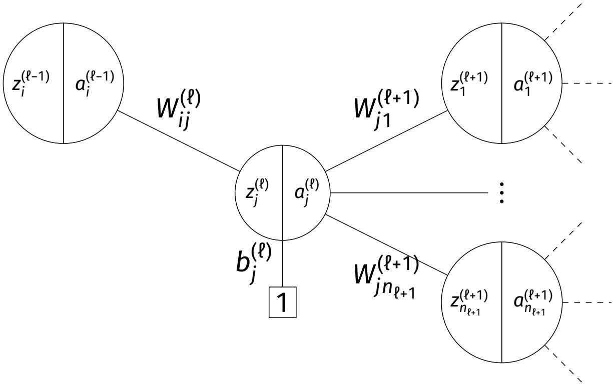
Claim #3

$$\frac{\partial H}{\partial a_j^{(\ell)}} = \sum_{k=1}^{n_{\ell+1}} \frac{\partial H}{\partial z_k^{(\ell+1)}} W_{jk}^{(\ell+1)}$$



Exercise

What is $\partial H / \partial b_j^{(\ell)}$?



General Formulas

- For any node in any neural network[1], we have the following recursive formulas:
  - $\frac{\partial H}{\partial a_j^{(\ell)}} = \sum_{k=1}^{n_{\ell+1}} \frac{\partial H}{\partial z_k^{(\ell+1)}} W_{jk}^{(\ell+1)}$
  - $\frac{\partial H}{\partial z_j^{(\ell)}} = \frac{\partial H}{\partial a_j^{(\ell)}} g'(z_j^{\ell})$
  - $\frac{\partial H}{\partial W_{ij}^{(\ell)}} = \frac{\partial H}{\partial z_j^{(\ell)}} a_i^{(\ell-1)}$
  - $\frac{\partial H}{\partial b_j^{(\ell)}} = \frac{\partial H}{\partial z_j^{(\ell)}}$

[1]Fully-connected, feedforward network

Main Idea

The derivatives in layer ℓ depend on derivatives in layer $\ell + 1$.

Backpropagation

- **Idea:** compute the derivatives in last layers, first.
- That is:
  - Compute derivatives in last layer, ℓ; store them.
  - Use to compute derivatives in layer $\ell - 1$.
  - Use to compute derivatives in layer $\ell - 2$.
  - ...

Backpropagation

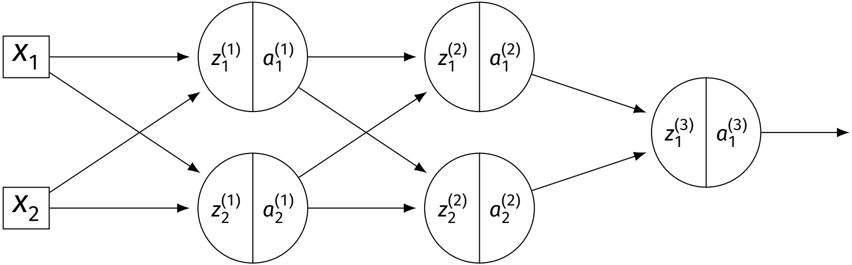
Given an input $\vec{x}$ and a current parameter vector $\vec{w}$:

1. Evaluate the network to compute $z_i^{(\ell)}$ and $a_i^{(\ell)}$ for all nodes.
2. For each layer ℓ from last to first:
   - Compute $\frac{\partial H}{\partial a_j^{(\ell)}} = \sum_{k=1}^{n_{\ell+1}} \frac{\partial H}{\partial z_k^{(\ell+1)}} W_{jk}^{(\ell+1)}$
   - Compute $\frac{\partial H}{\partial z_j^{(\ell)}} = \frac{\partial H}{\partial a_j^{(\ell)}} g'(z_j^{\ell})$
   - Compute $\frac{\partial H}{\partial W_{ij}^{(\ell)}} = \frac{\partial H}{\partial z_j^{(\ell)}} a_i^{(\ell-1)}$
   - Compute $\frac{\partial H}{\partial b_j^{(\ell)}} = \frac{\partial H}{\partial z_j^{(\ell)}}$

Example

Compute the entries of the gradient given:

$$W^{(1)} = \begin{pmatrix} 2 & -3 \\ 2 & 1 \end{pmatrix} \quad W^{(2)} = \begin{pmatrix} 2 & 1 \\ 0 & 1 \end{pmatrix} \quad W^{(3)} = \begin{pmatrix} 3 \\ -2 \end{pmatrix} \quad \vec{x} = (2, 1)^T \quad g(z) = \text{ReLU}$$



$$\frac{\partial H}{\partial a_j^{(\ell)}} = \sum_{k=1}^{n_{\ell+1}} \frac{\partial H}{\partial z_k^{(\ell+1)}} W_{jk}^{(\ell+1)} \qquad \frac{\partial H}{\partial z_j^{(\ell)}} = \frac{\partial H}{\partial a_j^{(\ell)}} g'(z_j^{\ell}) \qquad \frac{\partial H}{\partial W_{ij}^{(\ell)}} = \frac{\partial H}{\partial z_j^{(\ell)}} a_i^{(\ell-1)}$$

Aside: Derivative of ReLU

$$g(z) = \max\{0, z\}$$

$$g'(z) = \begin{cases} 0, & z < 0 \\ 1, & z > 0 \end{cases}$$