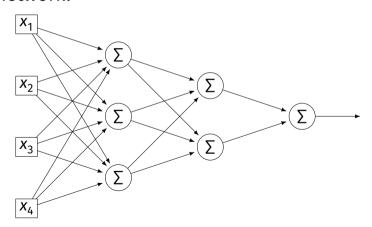
DSC 1408 Representation Learning

Lecture 20 | Part 1

Training Neural Networks

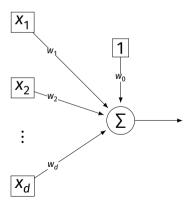
Training

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

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

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

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

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

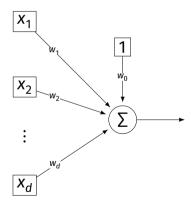
Suppose H is a linear prediction function:

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

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

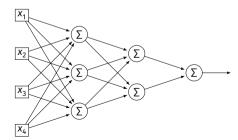
Example: Linear Model

► 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

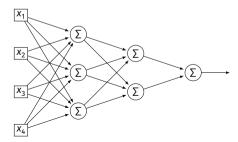
- It is often useful to pack all of the network's weights into a parameter vector, \vec{w} .
- Order is arbitrary:

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

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

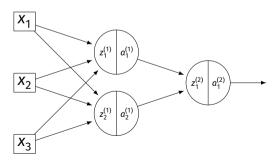
Gradient of Neural Network

- $ightharpoonup \nabla_{\vec{w}} H$ 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} .

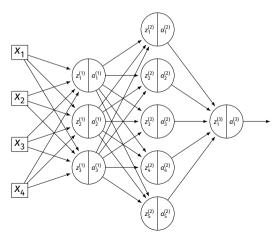


Exercise

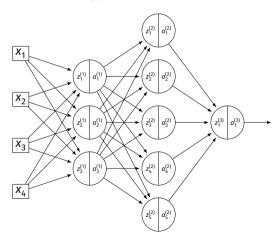
Suppose $W_{11}^{(1)} = -2$, $W_{21}^{(1)} = -5$, $W_{31}^{(1)} = 2$ and $\vec{x} = (3, 2, -2)^T$ and all biases are 0. ReLU activations are used. What is $\partial H/\partial W_{11}^{(1)}(\vec{x}, \vec{w})$?



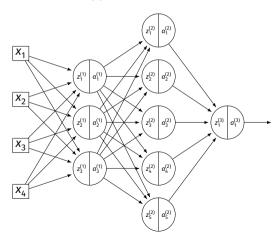
► Consider $\partial H/\partial W_{11}^{(3)}$:



► Consider $\partial H/\partial W_{11}^{(2)}$:



► 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 1408 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

= f'(q(x)) q'(x)

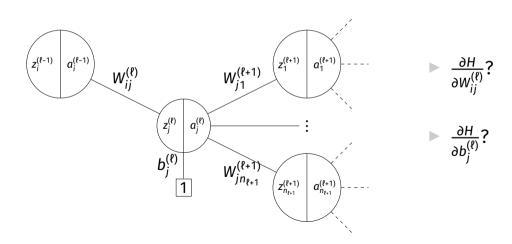
$$\frac{d}{dx}f(g(x)) = \frac{df}{dg}\frac{dg}{dx}$$

Some Notation

► We'll consider an arbitrary node in layer ℓ of a neural network.

- Let *g* be the activation function.
- ho_{ℓ} denotes the number of nodes in layer ℓ .

Arbitrary Node



Claim #1

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

Claim #2

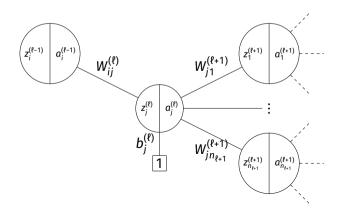
$$\frac{\partial H}{\partial z_i^{(\ell)}} = \frac{\partial H}{\partial a_i^{(\ell)}} g'(z_j^{\ell})$$

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 network¹, we have the following recursive formulas:

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

¹Fully-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, \(\extit{\eta}\); store them.
 - ▶ Use to compute derivatives in layer ℓ 1.
 - ▶ Use to compute derivatives in layer ℓ 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 \{\epsilon\ from last to first:

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

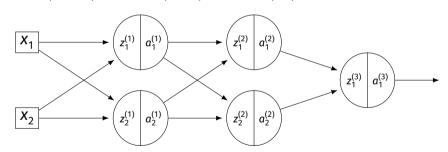
Compute
$$\frac{\partial H}{\partial z_i^{(\ell)}} = \frac{\partial H}{\partial a_i^{(\ell)}} g'(z_j^{\ell})$$

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

Compute
$$\frac{\partial H'}{\partial b_i^{(\ell)}} = \frac{\partial H}{\partial z_i^{(\ell)}}$$

Compute the entries of the gradient given:

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



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

Aside: Derivative of ReLU

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

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

Summary: Backprop

- Backprop is an algorithm for efficiently computing the gradient of a neural network
- It is not an algorithm **you** need to carry out by hand: your NN library can do it for you.