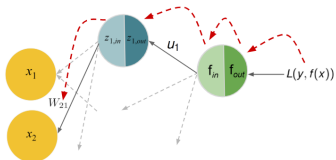


# Deep Learning

## Chain Rule and Computational Graphs



Learning goals

- 
- 
-

# CHAIN RULE OF CALCULUS

- The chain rule can be used to compute derivatives of the composition of two or more functions.
- Let  $\mathbf{x} \in \mathbb{R}^m$ ,  $\mathbf{y} \in \mathbb{R}^n$ ,  
 $g : \mathbb{R}^m \rightarrow \mathbb{R}^n$  and  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ .
- If  $\mathbf{y} = g(\mathbf{x})$  and  $z = f(\mathbf{y})$ , the chain rule yields:

$$\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j} \cdot \frac{\partial y_j}{\partial x_i}$$

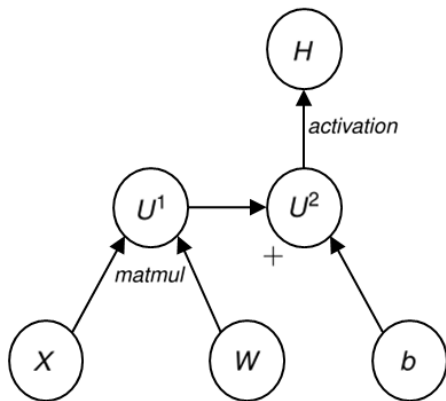
or, in vector notation:

$$\nabla_{\mathbf{x}} z = \left( \frac{\partial \mathbf{y}}{\partial \mathbf{x}} \right)^\top \nabla_{\mathbf{y}} z,$$

where  $\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$  is the  $(n \times m)$  Jacobian matrix of  $g$ .

# COMPUTATIONAL GRAPHS

- Computational graphs are a very helpful language to understand and visualize the chain rule.
- Each node describes a variable.
- Operations are functions applied to one or more variables.



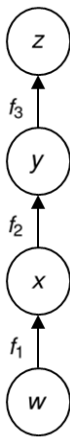
source : Goodfellow et al. (2016)

**Figure:** The computational graph for the expression  $H = \sigma(XW + B)$  with activation function  $\sigma(\cdot)$ .

# CHAIN RULE OF CALCULUS: EXAMPLE 1

- Suppose we have the following computational graph.
- To compute the derivative of  $\frac{\partial z}{\partial w}$  we need to recursively apply the chain rule. That is:

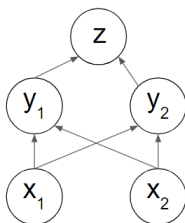
$$\begin{aligned}\frac{\partial z}{\partial w} &= \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x} \cdot \frac{\partial x}{\partial w} \\ &= f'_3(y) \cdot f'_2(x) \cdot f'_1(w) \\ &= f'_3(f_2(f_1(w))) \cdot f'_2(f_1(w)) \cdot f'_1(w)\end{aligned}$$



source : Goodfellow et al. (2016)

**Figure:** A computational graph, such that  $x = f_1(w)$ ,  $y = f_2(x)$  and  $z = f_3(y)$ .

# CHAIN RULE OF CALCULUS: EXAMPLE 2



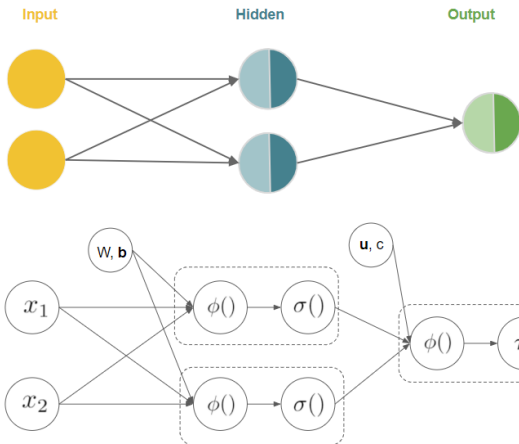
To compute  $\nabla_{\mathbf{x}} z$ , we apply the chain rule

- $\frac{\partial z}{\partial x_1} = \sum_j \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_1} = \frac{\partial z}{\partial y_1} \frac{\partial y_1}{\partial x_1} + \frac{\partial z}{\partial y_2} \frac{\partial y_2}{\partial x_1}$
- $\frac{\partial z}{\partial x_2} = \sum_j \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_2} = \frac{\partial z}{\partial y_1} \frac{\partial y_1}{\partial x_2} + \frac{\partial z}{\partial y_2} \frac{\partial y_2}{\partial x_2}$

Therefore, the gradient of  $z$  w.r.t  $\mathbf{x}$  is

$$\bullet \nabla_{\mathbf{x}} z = \begin{bmatrix} \frac{\partial z}{\partial x_1} \\ \frac{\partial z}{\partial x_2} \end{bmatrix} = \underbrace{\begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} \end{bmatrix}}_{\left(\frac{\partial \mathbf{y}}{\partial \mathbf{x}}\right)^\top} \underbrace{\begin{bmatrix} \frac{\partial z}{\partial y_1} \\ \frac{\partial z}{\partial y_2} \end{bmatrix}}_{\nabla_{\mathbf{y}} z} = \left(\frac{\partial \mathbf{y}}{\partial \mathbf{x}}\right)^\top \nabla_{\mathbf{y}} z$$

# COMPUTATIONAL GRAPH: NEURAL NET



**Figure:** A neural network can be seen as a computational graph.  $\phi$  is the weighted sum and  $\sigma$  and  $\tau$  are the activations.

Note: In contrast to the top figure, the arrows in the computational graph below merely indicate **dependence**, not weights.

# REFERENCES



Ian Goodfellow, Yoshua Bengio and Aaron Courville (2016)

Deep Learning

*<http://www.deeplearningbook.org/>*