Training Neural Networks

CMPUT 261: Introduction to Artificial Intelligence

GBC §6.5

Lecture Outline

1. Recap & Logistics
2. Gradient Descent for Neural Networks
3. Automatic Differentiation
4. Back-Propagation

After this lecture, you should be able to:

- trace an execution of forward-mode automatic differentiation
- trace an execution of backward-mode automatic differentiation
- construct a finite numerical algorithm for a given computation
- explain why automatic differentiation is more efficient than the method of finite differences
- explain why automatic differentiation is more efficient than symbolic differentiation
- explain why backward mode automatic differentiation is more efficient for typical deep learning applications

Logisitics

- **Assignment #3** was released last week
  - Due **Thursday, March 23**
  - Submit via eClass
- **Midterm** marks are available on eclass
  - Cc all of the TAs if you have questions about the marking

Recap: Nonlinear Features

$$y = f(\mathbf{x}; \mathbf{w}) = g(\mathbf{w}^T \mathbf{x}) = g\left(\sum_{i=1}^{n} w_i x_i\right)$$

Generalized linear model: **Activation function** g of linear combination of inputs

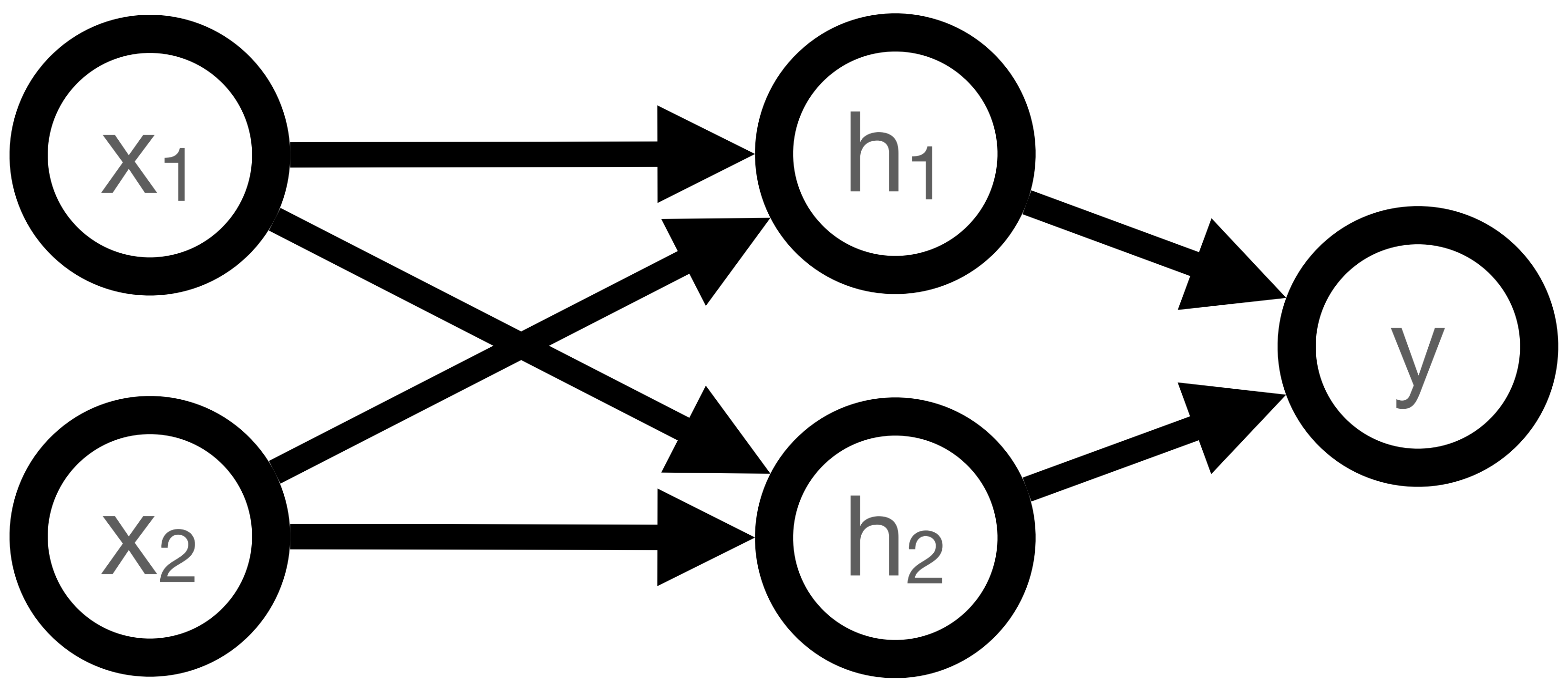
Extension: Learn a generalized linear model on **richer inputs**

1. Define a **feature mapping** $\phi(\mathbf{x})$ that returns **functions** of the original inputs

2. Learn a linear model of the **features** instead of the **inputs**

$$y = f(\mathbf{x}; \mathbf{w}) = g(\mathbf{w}^T \phi(\mathbf{x})) = g\left(\sum_{i=1}^{n} w_i [\phi(\mathbf{x})]_i\right)$$

Recap:
Feedforward Neural Network



$$h_1(\mathbf{x}; \mathbf{w}^{(1)}, b^{(1)}) = g\left(b^{(1)} + \sum_{i=1}^{n} w_i^{(1)} x_i\right)$$

$$y(\mathbf{x}; \mathbf{w}, \mathbf{b}) = g\left(b^{(y)} + \sum_{i=1}^{n} w_i^{(y)} h_i(\mathbf{x}_i; \mathbf{w}^{(i)}, b^{(i)})\right)$$

- A **neural network** is many **units composed** together
- **Feedforward neural network:** Units arranged into **layers**
    - Each layer takes outputs of **previous layer** as its **inputs**

Recap: Chain Rule of Calculus

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$

i.e,

if $z = h(x) = f(g(x))$ and $y = g(x)$

$$h(x) = f(g(x)) \implies h'(x) = f'(g(x))g'(x)$$

If we know formulas for the derivatives of **components** of a function, then we can build up the derivative of their composition mechanically

Chain Rule of Calculus: Multiple Intermediate Arguments

What if $h(x) = f(g_1(x), g_2(x))$?

$$\frac{dh}{dx} = \frac{\partial f}{\partial g_1}\frac{dg_1}{dx} + \frac{\partial f}{\partial g_2}\frac{dg_2}{dx}$$

i.e., $h'(x) = g_1'(x)\left.\frac{\partial f(t_1, t_2)}{\partial t_1}\right|_{\substack{t_1 = g_1(x) \\ t_2 = g_2(x)}} + g_2'(x)\left.\frac{\partial f(t_1, t_2)}{\partial t_2}\right|_{\substack{t_1 = g_1(x) \\ t_2 = g_2(x)}}$

Recap: Training Neural Networks

- Specify a **loss** L and a set of **training examples:**

$$E = (\mathbf{x}^{(1)}, y^{(1)}), \ldots, (\mathbf{x}^{(n)}, y^{(n)})$$

- Training by **gradient descent**:

1. Compute **loss** on training data: $L(\mathbf{W}, \mathbf{b}) = \sum_i \ell\left(\underbrace{f(\mathbf{x}^{(i)}; \mathbf{W}, \mathbf{b})}_{\text{Prediction}}, \underbrace{y^{(i)}}_{\text{Target}}\right)$

Loss function (e.g., squared error)

2. Compute **gradient** of loss: $\nabla L(\mathbf{W}, \mathbf{b})$

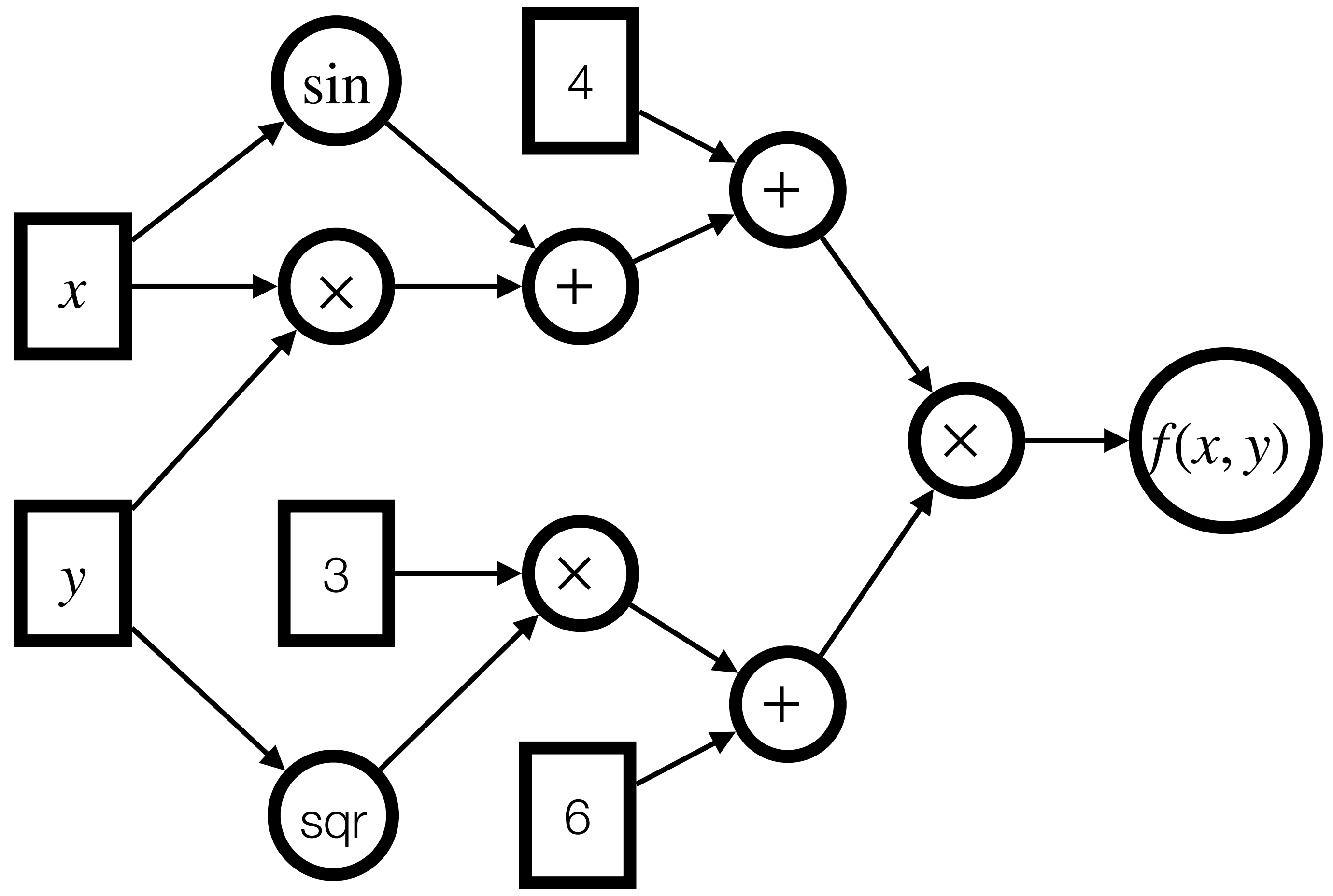
3. **Update parameters** to make loss smaller:

$$\begin{bmatrix} \mathbf{W}^{new} \\ \mathbf{b}^{new} \end{bmatrix} = \begin{bmatrix} \mathbf{W}^{old} \\ \mathbf{b}^{old} \end{bmatrix} - \eta \nabla L(\mathbf{W}^{old}, \mathbf{b}^{old})$$

Three Representations

A function $f(x, y)$ can be represented in multiple ways:

1. As a **formula:**
   $$f(x, y) = (xy + \sin x + 4)(3y^2 + 6)$$
2. As a **computational graph:**



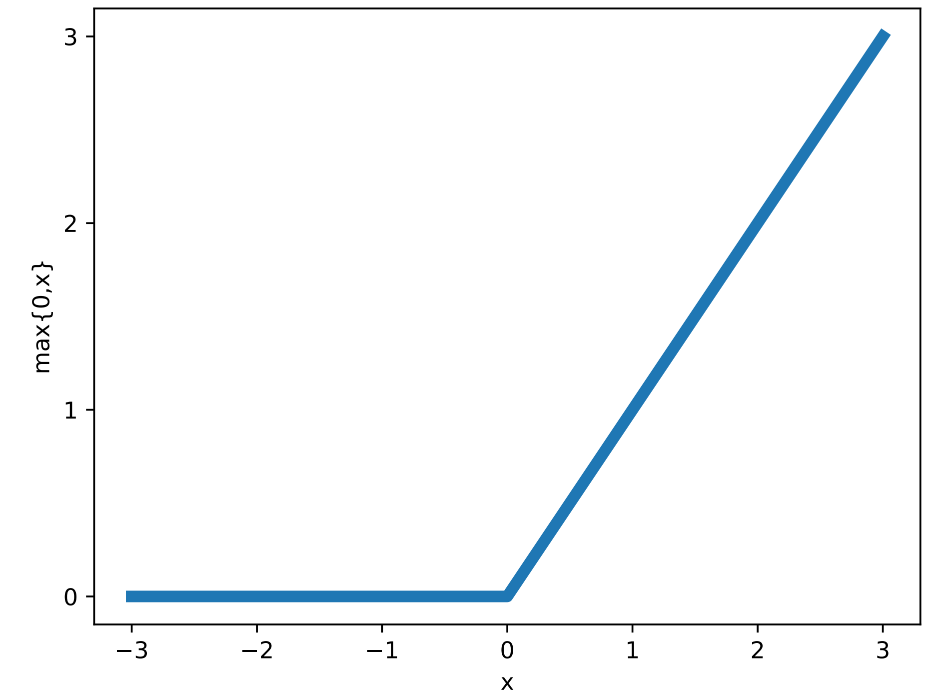
3. As a **finite numerical algorithm**

$$\begin{aligned}
s_1 &= x \\
s_2 &= y \\
s_3 &= s_1 \times s_2 \\
s_4 &= \sin(s_1) \\
s_5 &= s_3 + s_4 \\
s_6 &= s_5 + 4 \\
s_7 &= \mathrm{sqr}(s_2) \\
s_8 &= 3 \times s_7 \\
s_9 &= s_8 + 6 \\
s_{10} &= s_6 \times s_9
\end{aligned}$$

example from [Bücker et al., 2006]

Symbolic Differentiation

$$
\begin{aligned}
z &= f(y) \\
y &= f(x) \\
x &= f(w)
\end{aligned}
\qquad z = f(f(f(w)))
\qquad
\begin{aligned}
\frac{\partial z}{\partial w} &= \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}\frac{\partial x}{\partial w} \\
&= f'(f(f(w)))f'(f(w))f'(w)
\end{aligned}
$$



$$f(w) = \begin{cases} w & \text{if } w > 0 \\ 0 & \text{otherwise.} \end{cases}$$

- We can differentiate a nested **formula** by recursively applying the **chain rule** to derive a **new formula** for the gradient
- **Problem:** This can result in a lot of repeated subexpressions
- **Question:** What happens if the nested function is defined **piecewise**?

Automatic Differentiation: Forward Mode

- The forward mode converts a **finite numerical algorithm** for computing a function into an **augmented** finite numerical algorithm for computing the **function's derivative**

- For each step, a new step is constructed representing the derivative of the corresponding step in the original program:

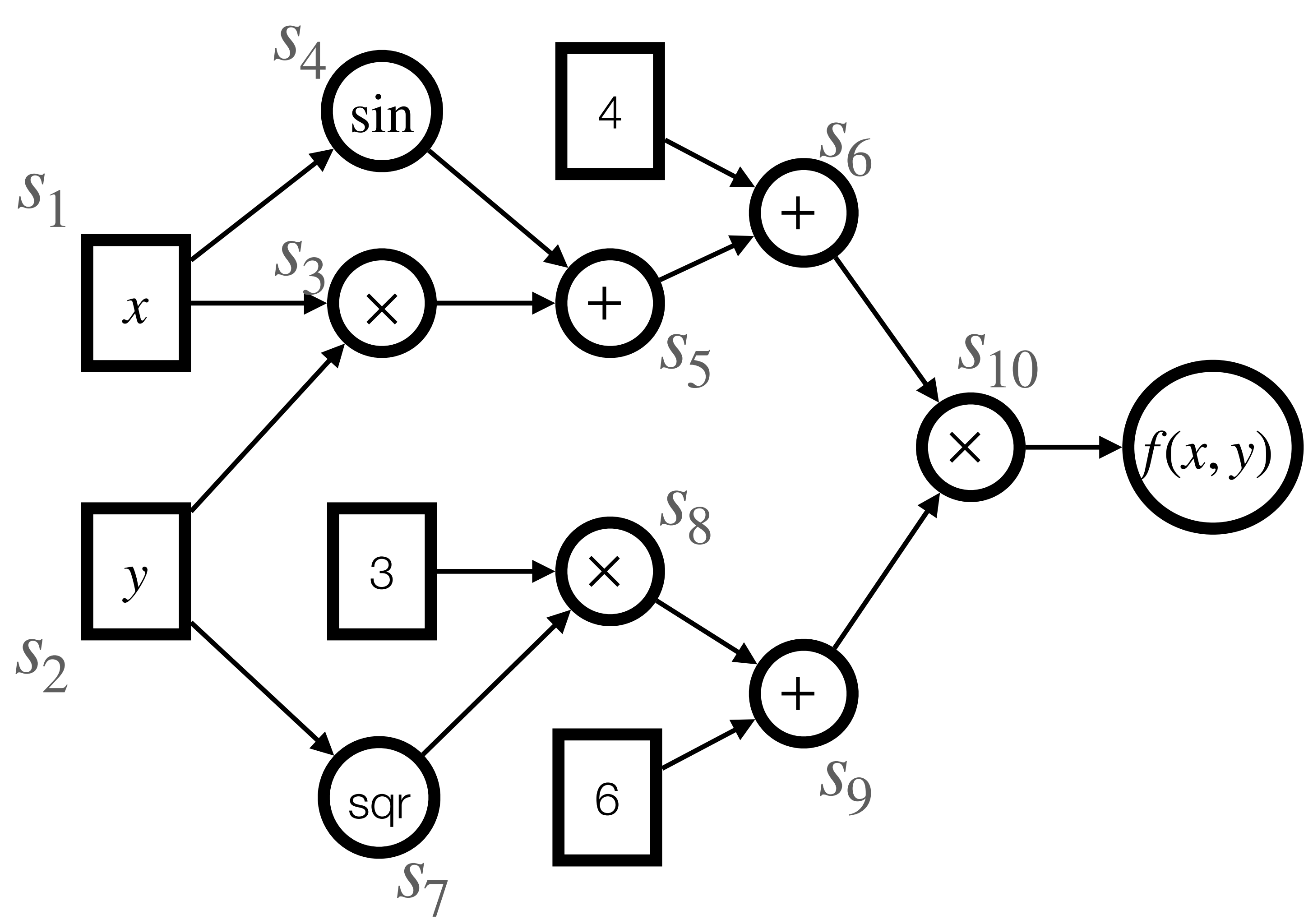
$$
\begin{aligned}
s_1 &= x \\
s_2 &= y \\
s_3 &= s_1 + s_2 \\
s_4 &= s_1 \times s_2 \\
&\vdots
\end{aligned}
\quad \Longrightarrow \quad
\begin{aligned}
s_1' &= 1 \\
s_2' &= 0 \\
s_3' &= s_1' + s_2' \\
s_4' &= s_1 \times s_2' + s_1' \times s_2 \\
&\vdots
\end{aligned}
$$

- To compute the partial derivative $\dfrac{\partial s_n}{\partial s_1}$, set $s_1' = 1$ and $s_2' = 0$ and run augmented algorithm

- This takes roughly twice as long to run as the original algorithm (**why?**)

Forward Mode Example

Let's compute $\left.\frac{\partial f}{\partial y}\right|_{x=2,y=8}$ using forward mode:



$$
\begin{aligned}
s_1 &= x & &= 2 & \quad s_1' &= 0 \\
s_2 &= y & &= 8 & \quad s_2' &= 1 \\
s_3 &= s_1 \times s_2 & &= 16 & \quad s_3' &= s_1 \times s_2' + s_1' \times s_2 = 2 \\
s_4 &= \sin(s_1) & &\approx 0.034 & \quad s_4' &= \cos(s_1) \times s_1' = 0 \\
s_5 &= s_3 + s_4 & &= 16.034 & \quad s_5' &= s_3' + s_4' = 2 \\
s_6 &= s_5 + 4 & &= 20.034 & \quad s_6' &= s_5' = 2 \\
s_7 &= \mathrm{sqr}(s_2) & &= 64 & \quad s_7' &= s_2' \times 2 \times s_2 = 16 \\
s_8 &= 3 \times s_7 & &= 192 & \quad s_8' &= 3 \times s_7' = 48 \\
s_9 &= s_8 + 6 & &= 198 & \quad s_9' &= s_8' = 48 \\
s_{10} &= s_6 \times s_9 & &= 3966.732 & \quad s_{10}' &= s_6 \times s_9' + s_6' \times s_9 = 1357.632
\end{aligned}
$$

Question: What is the problem with this approach for neural networks?

Forward Mode Performance

- To compute the full gradient of a function of m inputs requires computing m partial derivatives
- In forward mode, this requires m forward passes
- For our toy examples, that means running the forward pass twice
- Neural networks can easily have **thousands** of parameters
- We don't want to run the network *thousands of times* for each gradient update!

Automatic Differentiation: Backward Mode

- **Forward mode** sweeps through the graph:
  - For each s_i, computes $s_i' = \dfrac{\partial s_i}{\partial s_1}$ for each s_i
  - The **numerator varies**, and the **denominator is fixed**
- **Backward mode** does the opposite:
  - For each s_i, computes the **local gradient** $\overline{s_i} = \dfrac{\partial s_n}{\partial s_i}$
  - The **numerator is fixed**, and the **denominator varies**
- At the end, we have computed $\overline{x_i} = \dfrac{\partial s_n}{\partial x_i}$ for each input x_i

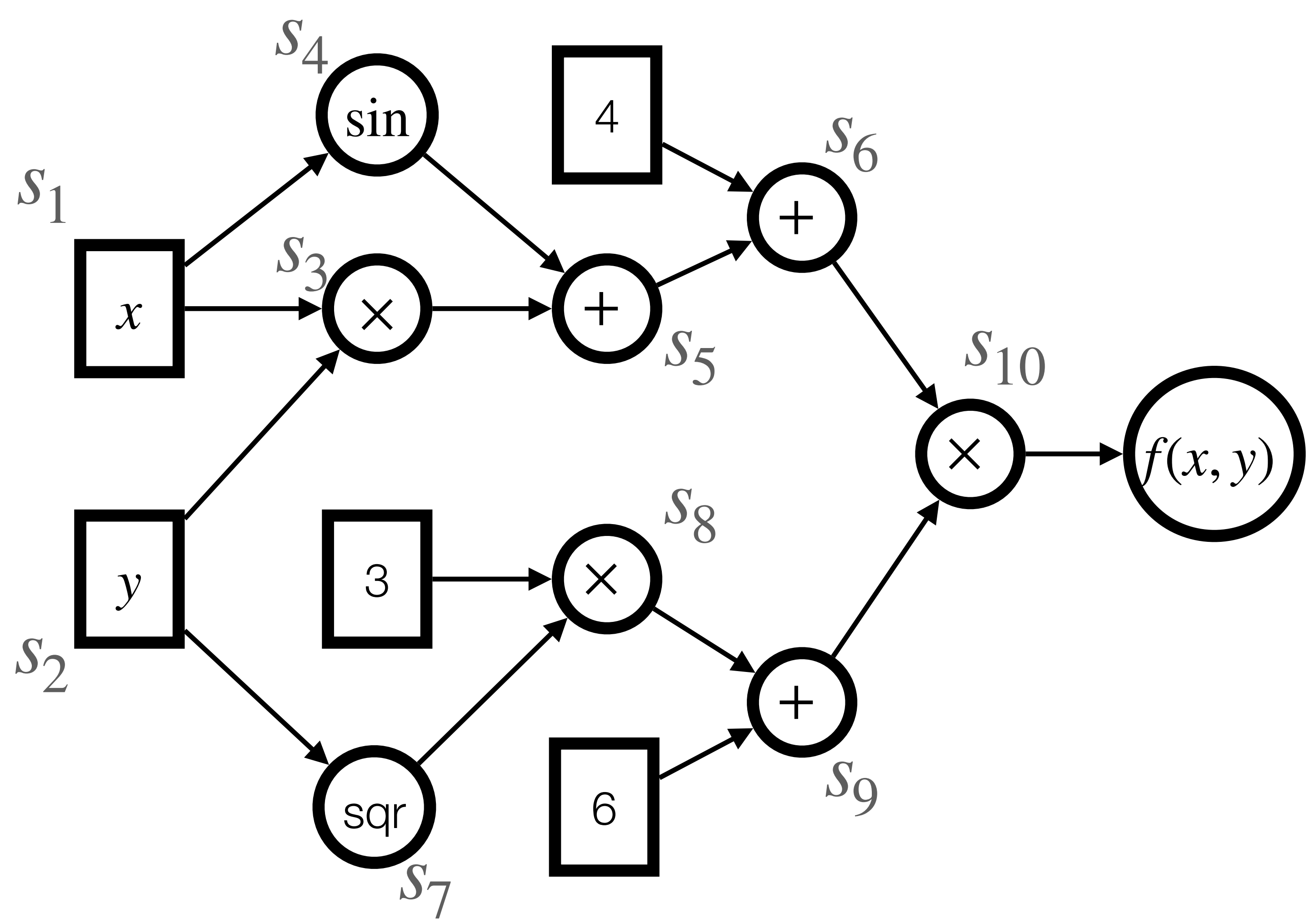
$$\left.\begin{array}{l}\left.\begin{array}{l}s_1 = x\\ s_2 = y\\ s_3 = s_1 \times s_2\end{array}\right\}\dfrac{\partial s_3}{\partial s_1}\\ s_4 = \sin(s_1)\end{array}\right\}\dfrac{\partial s_4}{\partial s_1}$$

$$\begin{array}{l}s_5 = s_3 + s_4\\ s_6 = s_5 + 4\end{array}$$

$$\dfrac{\partial s_{10}}{\partial s_7}\left\{\begin{array}{l}s_7 = \mathrm{sqr}(s_2)\\ \dfrac{\partial s_{10}}{\partial s_8}\left\{\begin{array}{l}s_8 = 3 \times s_7\\ s_9 = s_8 + 6\\ s_{10} = s_6 \times s_9\end{array}\right.\end{array}\right.$$

Automatic Differentiation: Local Derivatives

The augmented algorithm computes local derivatives in **reverse** order:



$$
\begin{aligned}
s_1 &= x \\
s_2 &= y \\
s_3 &= s_1 \times s_2 \\
s_4 &= \sin(s_1) \\
s_5 &= s_3 + s_4 \\
s_6 &= s_5 + 4 \\
s_7 &= \mathrm{sqr}(s_2) \\
s_8 &= 3 \times s_7 \\
s_9 &= s_8 + 6 \\
s_{10} &= s_6 \times s_9
\end{aligned}
$$

$$\overline{s_{10}} = \frac{\partial s_{10}}{\partial s_{10}} = 1$$

$$\overline{s_9} = \frac{\partial s_{10}}{\partial s_9} = \overline{s_{10}} s_6$$

$$\frac{\partial \text{ final output}}{\partial \text{ immediate output}} \quad \frac{\partial \text{ immediate output}}{\partial \text{ self}}$$

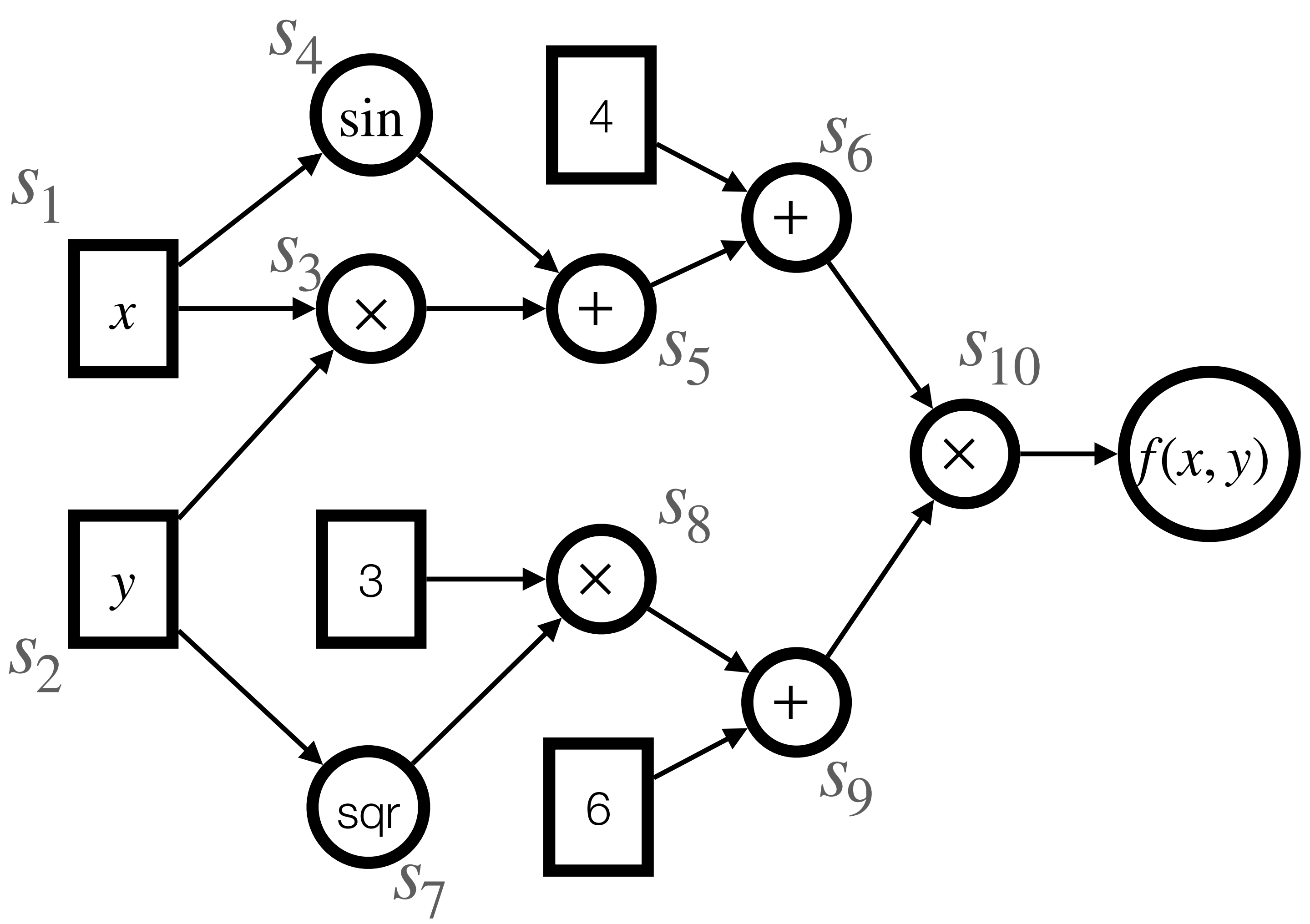
$$\overline{s_8} = \frac{\partial s_{10}}{\partial s_8} = \boxed{\frac{\partial s_{10}}{\partial s_9}}\boxed{\frac{\partial s_9}{\partial s_8}} = \overline{s_9} 1$$

$$\overline{s_7} = \frac{\partial s_{10}}{\partial s_7} = \frac{\partial s_{10}}{\partial s_8} \frac{\partial s_8}{\partial s_7} = \overline{s_8} 3$$

$$\overline{s_6} = \frac{\partial s_{10}}{\partial s_6} = s_9$$

$$\vdots$$

Automatic Differentiation: Local Derivatives (2)



$$
\begin{aligned}
s_1 &= x \\
s_2 &= y \\
s_3 &= s_1 \times s_2 \\
s_4 &= \sin(s_1) \\
s_5 &= s_3 + s_4 \\
s_6 &= s_5 + 4 \\
s_7 &= \mathrm{sqr}(s_2) \\
s_8 &= 3 \times s_7 \\
s_9 &= s_8 + 6 \\
s_{10} &= s_6 \times s_9
\end{aligned}
$$

$$\overline{s_6} = \frac{\partial s_{10}}{\partial s_6} = s_9$$

$$\overline{s_5} = \frac{\partial s_{10}}{\partial s_5} = \frac{\partial s_{10}}{\partial s_6}\frac{\partial s_6}{\partial s_5} = \overline{s_6}1$$

$$\overline{s_4} = \frac{\partial s_{10}}{\partial s_4} = \frac{\partial s_{10}}{\partial s_5}\frac{\partial s_5}{\partial s_4} = \overline{s_5}1$$

$$\overline{s_3} = \frac{\partial s_{10}}{\partial s_3} = \frac{\partial s_{10}}{\partial s_5}\frac{\partial s_5}{\partial s_3} = \overline{s_5}1$$

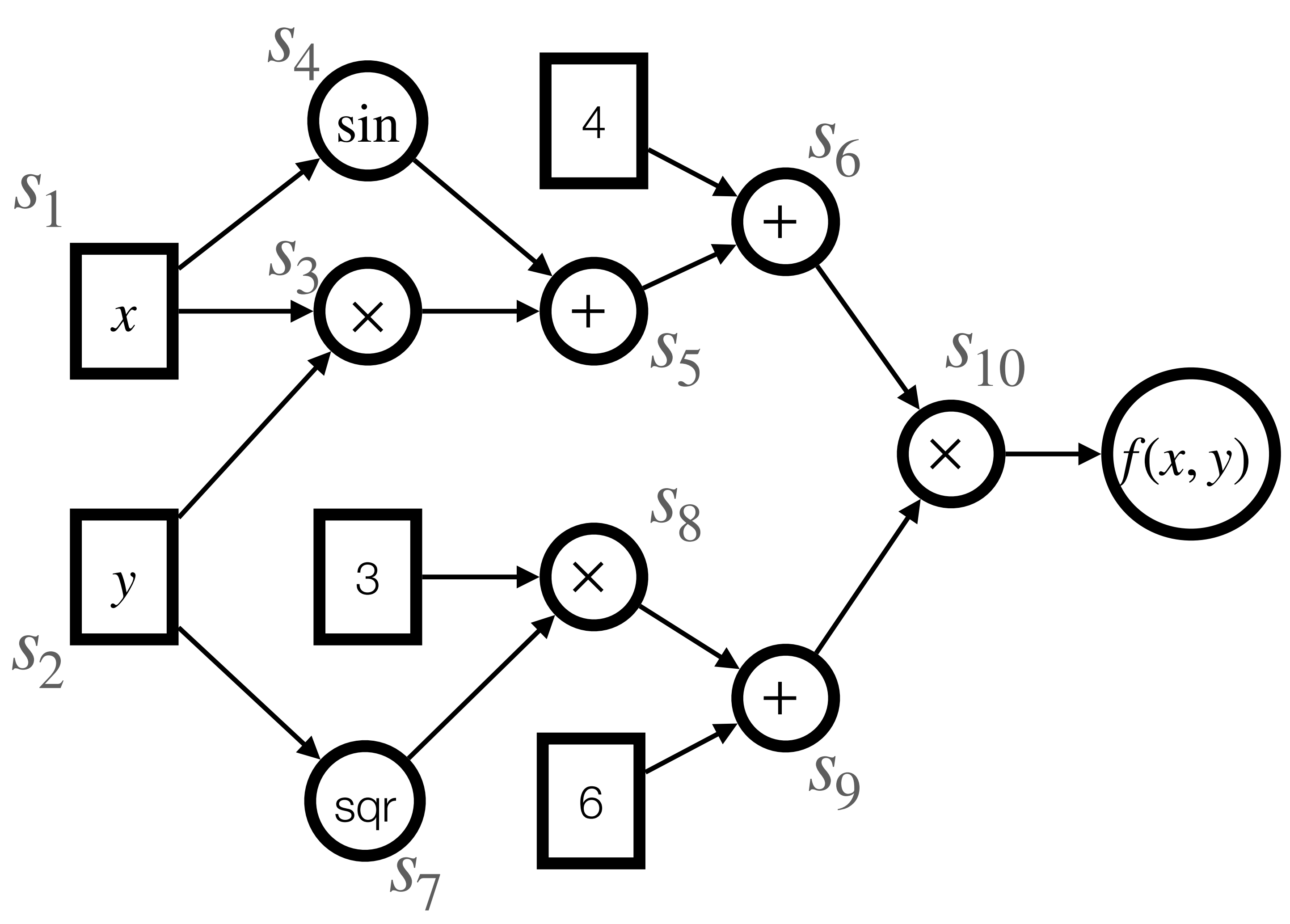
One term for **each** immediate output

$$\overline{s_2} = \frac{\partial s_{10}}{\partial s_2} = \boxed{\frac{\partial s_{10}}{\partial s_3}\frac{\partial s_3}{\partial s_2}} + \boxed{\frac{\partial s_{10}}{\partial s_7}\frac{\partial s_7}{\partial s_2}} = \overline{s_3}s_1 + \overline{s_7}2s_2$$

$$\overline{s_1} = \frac{\partial s_{10}}{\partial s_1} = \frac{\partial s_{10}}{\partial s_3}\frac{\partial s_3}{\partial s_1} + \frac{\partial s_{10}}{\partial s_4}\frac{\partial s_4}{\partial s_1} = \overline{s_3}s_2 + \overline{s_4}\cos s_1$$

Backward Mode Example

Let's compute $\left.\frac{\partial f}{\partial x}\right|_{x=2,y=8}$ and $\left.\frac{\partial f}{\partial y}\right|_{x=2,y=8}$ using backward mode:



$$
\begin{aligned}
s_1 &= x && = 2\\
s_2 &= y && = 8\\
s_3 &= s_1 \times s_2 && = 16\\
s_4 &= \sin(s_1) && \approx 0.034\\
s_5 &= s_3 + s_4 && = 16.034\\
s_6 &= s_5 + 4 && = 20.034\\
s_7 &= \mathrm{sqr}(s_2) && = 64\\
s_8 &= 3 \times s_7 && = 192\\
s_9 &= s_8 + 6 && = 198\\
s_{10} &= s_6 \times s_9 && = 3966.732
\end{aligned}
$$

$$
\begin{aligned}
\overline{s_{10}} &= 1\\
\overline{s_9} &= \overline{s_{10}} s_6 = 20.034\\
\overline{s_8} &= \overline{s_9} 1 = 20.034\\
\overline{s_7} &= \overline{s_8} 3 = 60.102\\
\overline{s_6} &= s_9 = 198\\
\overline{s_6} &= s_9 = 198\\
\overline{s_5} &= \overline{s_6} 1 = 198\\
\overline{s_4} &= \frac{\partial s_{10}}{\partial s_4} = \frac{\partial s_{10}}{\partial s_5}\frac{\partial s_5}{\partial s_4} = \overline{s_5} 1 = 198\\
\overline{s_3} &= \frac{\partial s_{10}}{\partial s_3} = \frac{\partial s_{10}}{\partial s_5}\frac{\partial s_5}{\partial s_3} = \overline{s_5} 1 = 198\\
\overline{s_2} &= \overline{s_3} s_1 + \overline{s_7} 2 s_2 \simeq \boxed{1357.632}\\
\overline{s_1} &= \overline{s_3} s_2 + \overline{s_4} \cos s_1 \simeq \boxed{1781.9}
\end{aligned}
$$

Back-Propagation

$$L(\mathbf{W}, \mathbf{b}) = \sum_i \ell\left(f(\mathbf{x}^{(i)}; \mathbf{W}, \mathbf{b}), y^{(i)}\right)$$

Back-propagation is simply automatic differentiation in **backward mode**, used to compute the gradient $\nabla_{\mathbf{W},\mathbf{b}} L$ of the **loss function** with respect to its **parameters** $\mathbf{W}, \mathbf{b}$:

1. At each layer, compute the **local gradients** of the layer's computations
2. These local gradients will be used as inputs to the **next layer's** local gradient computations
3. At the end, we have a partial derivative for each of the parameters, which we can use to take a **gradient step**

Summary

- The loss function of a **deep feedforward networks** is simply a very nested function of the **parameters** of the model
- **Automatic differentiation** can compute these gradients more efficiently than symbolic differentiation or finite-differences numeric computations
    - Symbolic differentiation is **interleaved** with numeric computation
    - In **forward mode**, m sweeps are required for a function of m parameters
    - In **backward mode**, only a single sweep is required
- **Back-propagation** is simply automatic differentiation **applied to neural networks** in backward mode