## Automatic Differentiation

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Some slides are taken from "Alice's Adventures in a Differentiable Wonderland" by Simone Scardapane.

# Why not numerical differentiation?

 We could directly apply the definition of gradients to obtain a suitable numerical approximation of the gradient.

$$\partial_{x_i} f(\mathbf{x}) = \frac{\partial y}{\partial x_i} = \lim_{h \to 0} \frac{f(\mathbf{x} + h\mathbf{e}_i) - f(\mathbf{x})}{h},$$

However, each scalar value to be differentiated requires 2
function calls in a naive implementation, making this
approach unfeasible except for numerical checks over the
implementation.

# Why not symbolic differentiation?

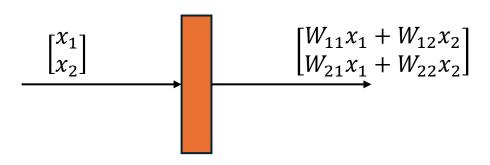
- We can ask a symbolic engine to pre-compute the full, symbolic equation of the derivative. This is called symbolic differentiation.
- Finding an optimal implementation for the Jacobian which avoids any unnecessary computation is an NP-complete task (optimal Jacobian accumulation).

```
import sympy as sp
x, a, b = sp.symbols('x a b')
y = a*sp.sin(x) + b*x*sp.sin(x)
sp.diff(y, x) # [Out]: acos(x)+bxcos(x)+bsin(x)
```

**Box C.6.1:** *Symbolic differentiation in Python using SymPy.* 

f(x, w) adalah sebuah fungsi "fully-connected layer" dengan input vektor ~ (c) dan output vektor ~ (c); dan mempunyai parameter  $W \sim (c, c)$ .

#### Contoh, untuk c = 2:



$$f(\mathbf{x}, \mathbf{W}) = \mathbf{W}\mathbf{x} = \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

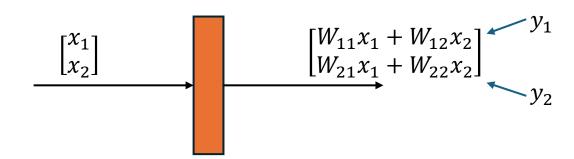
Saat proses optimization untuk mencari  $\mathbf{W}$ , biasanya kita membutuhkan perhitungan dua buah kuantitas:

Input Jacobian :  $\partial_x f(x, W)$ 

Weight Jacobian :  $\partial_W f(x, W)$ 

f(x, w) adalah sebuah fungsi "fully-connected layer" dengan **input vektor** ~ (c) dan output vektor ~ (c); dan mempunyai parameter W ~ (c, c).

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Untuk contoh di atas:

#### Input Jacobian $\sim$ (2, 2):

$$\partial_{\boldsymbol{x}} f(\boldsymbol{x}, \boldsymbol{W}) = \boldsymbol{W} = \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix}$$

Weight Jacobian ~ (2, 2\*2): 
$$\partial_{W} f(x, W) = \begin{bmatrix} \frac{\partial y_{1}}{\partial W_{11}} & \frac{\partial y_{1}}{\partial W_{12}} & \frac{\partial y_{1}}{\partial W_{21}} & \frac{\partial y_{1}}{\partial W_{22}} \\ \frac{\partial y_{2}}{\partial W_{11}} & \frac{\partial y_{2}}{\partial W_{12}} & \frac{\partial y_{2}}{\partial W_{21}} & \frac{\partial y_{2}}{\partial W_{22}} \end{bmatrix}$$

$$\partial_{\boldsymbol{W}} f(\boldsymbol{x}, \boldsymbol{W}) = \begin{bmatrix} x_1 & x_2 & 0 & 0 \\ 0 & 0 & x_1 & x_2 \end{bmatrix}$$

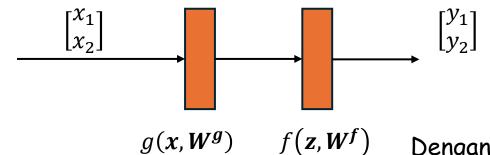
Setelah Anda mengetahui cara menghitung input jacobian dan weight jacobian dari sebuah fungsi fully-connected layer berparameter, sekarang kita mencoba jika terdapat 2 buah layer.

 $W^f$  bukan berarti W pangkat f; tetapi parameter W pada fungsi f. Fungsi f dan g punya parameter yang berbeda.

Sekarang, seandainya ada 2 layer:

$$f(\mathbf{z}, \mathbf{W}^f) = \mathbf{W}^f \mathbf{z} = \begin{bmatrix} W_{11}^f & W_{12}^f \\ W_{21}^f & W_{22}^f \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$$

$$g(\mathbf{x}, \mathbf{W}^g) = \mathbf{W}^g \mathbf{x} = \begin{bmatrix} W_{11}^g & W_{12}^g \\ W_{21}^g & W_{22}^g \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$



Dengan kata lain, ini adalah komposisi fungsi:

$$y = f(g(x, W^g), W^f)$$

Biasanya, kita ingin menghitung  $\partial y/\partial W^g$  dan  $\partial y/\partial W^f$ .

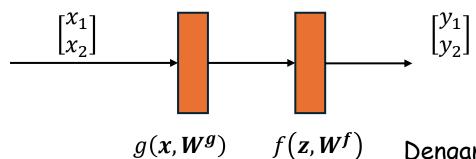
Bagaimana caranya?

 $W^f$  bukan berarti W pangkat f; tetapi parameter W pada fungsi f. Fungsi f dan g punya parameter yang berbeda.

Sekarang, seandainya ada 2 layer:

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Dengan kata lain, ini adalah komposisi fungsi:

$$y = f(g(x, W^g), W^f)$$

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$$\frac{\partial \mathbf{y}}{\partial \mathbf{W}^{\mathbf{g}}} = \frac{\partial f}{\partial \mathbf{W}^{\mathbf{g}}} = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial \mathbf{W}^{\mathbf{g}}}$$

Input Jacobian f:  $\partial_x f(., W^f)$ 

Weight Jacobian g:  $\partial_{W^g} g(., W^g)$ 

$$\frac{\partial \mathbf{y}}{\partial \mathbf{W}^f} = \frac{\partial f}{\partial \mathbf{W}^f}$$

Weight Jacobian  $\mathbf{f}$ :  $\partial_{\mathbf{W}^f} f(., \mathbf{W}^f)$ 

$$f(\mathbf{z}, \mathbf{W}^f) = \mathbf{W}^f \mathbf{z} = \begin{bmatrix} 1 & 2 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$$

$$g(\mathbf{x}, \mathbf{W}^g) = \mathbf{W}^g \mathbf{x} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$\begin{array}{c|cccc}
 & & & & & & \\
\hline
 & & & & & \\
g(\mathbf{x}, \mathbf{W}^g) & & f(\mathbf{z}, \mathbf{W}^f)
\end{array}$$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{W}^{\mathbf{g}}} = \frac{\partial f}{\partial \mathbf{W}^{\mathbf{g}}} = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial \mathbf{W}^{\mathbf{g}}}$$

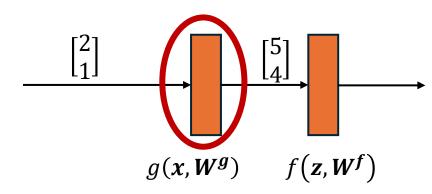
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$$g(\mathbf{x}, \mathbf{W}^g) = \mathbf{W}^g \mathbf{x} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 5 \\ 4 \end{bmatrix}$$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{W}^g} = \frac{\partial f}{\partial \mathbf{W}^g} = \frac{\partial f}{\partial g} \left[ \frac{\partial g}{\partial \mathbf{W}^g} \right]$$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{W}^f} = \frac{\partial f}{\partial \mathbf{W}^f}$$



$$\partial_{\mathbf{W}^g} g(\mathbf{z}, \mathbf{W}^g) = \begin{bmatrix} x_1 & x_2 & 0 & 0 \\ 0 & 0 & x_1 & x_2 \end{bmatrix}$$

$$\partial_{\boldsymbol{W}^{\boldsymbol{g}}} g(\boldsymbol{z}, \boldsymbol{W}^{\boldsymbol{g}}) = \begin{bmatrix} 2 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1 \end{bmatrix}$$

Buat sebuah matrix  $\widehat{W}^g$  yang diinisialisasi dengan Weight Jacobian g:

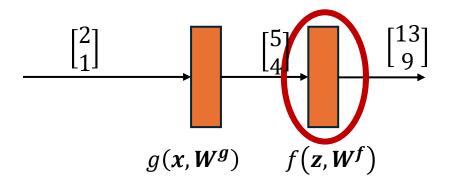
$$\widehat{W^g} \leftarrow \begin{bmatrix} 2 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1 \end{bmatrix}$$

$$f(\mathbf{z}, \mathbf{W}^f) = \mathbf{W}^f \mathbf{z} = \begin{bmatrix} 1 & 2 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 5 \\ 4 \end{bmatrix} = \begin{bmatrix} 13 \\ 9 \end{bmatrix}$$

$$g(\mathbf{x}, \mathbf{W}^g) = \mathbf{W}^g \mathbf{x} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 5 \\ 4 \end{bmatrix}$$

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$$\frac{\partial \mathbf{y}}{\partial \mathbf{W}^f} = \frac{\partial f}{\partial \mathbf{W}^f}$$



$$\partial_{\mathbf{z}} f(\mathbf{z}, \mathbf{W}^f) = \begin{bmatrix} W_{11}^f & W_{12}^f \\ W_{21}^f & W_{22}^f \end{bmatrix}$$

$$\partial_{\mathbf{z}} f(\mathbf{z}, \mathbf{W}^f) = \begin{bmatrix} 1 & 2 \\ 1 & 1 \end{bmatrix}$$

$$\partial_{\mathbf{W}^f} f(\mathbf{z}, \mathbf{W}^f) = \begin{bmatrix} z_1 & z_2 & 0 & 0 \\ 0 & 0 & z_1 & z_2 \end{bmatrix}$$

$$\partial_{\mathbf{W}^f} f(\mathbf{z}, \mathbf{W}^f) = \begin{bmatrix} 5 & 4 & 0 & 0 \\ 0 & 0 & 5 & 4 \end{bmatrix}$$

Update matrix  $\widehat{W}^g$  dikali dengan Input Jacobian  $\mathbf{f}$ .

$$\widehat{W^g} \leftarrow \partial_{\mathbf{z}} f(\mathbf{z}, W^f) \times \widehat{W^g}$$

$$\widehat{W}^g \leftarrow \begin{bmatrix} 1 & 2 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 4 & 2 \\ 2 & 1 & 2 & 1 \end{bmatrix}$$

Buat sebuah matrix  $\widehat{W^f}$  yang diinisialisasi dengan Weight Jacobian f:

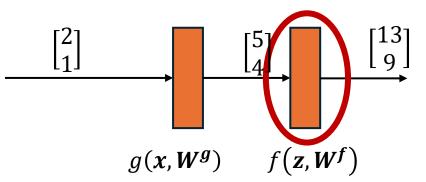
$$\widehat{W^f} \leftarrow \begin{bmatrix} 5 & 4 & 0 & 0 \\ 0 & 0 & 5 & 4 \end{bmatrix}$$

$$f(\mathbf{z}, \mathbf{W}^f) = \mathbf{W}^f \mathbf{z} = \begin{bmatrix} 1 & 2 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 5 \\ 4 \end{bmatrix} = \begin{bmatrix} 13 \\ 9 \end{bmatrix}$$

$$g(\mathbf{x}, \mathbf{W}^g) = \mathbf{W}^g \mathbf{x} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 5 \\ 4 \end{bmatrix}$$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{W}^g} = \frac{\partial f}{\partial \mathbf{W}^g} = \underbrace{\frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial \mathbf{W}^g}}_{\mathbf{g}} = \widehat{W}^g$$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{W}^f} = \left( \frac{\partial f}{\partial \mathbf{W}^f} \right) = \widehat{W}^f$$



$$\frac{\partial y_1}{\partial W_{12}^g} \qquad \qquad \frac{\partial y_2}{\partial W_{22}^g}$$

$$\widehat{W}^g = \begin{bmatrix} 2 & 1 & 4/2 \\ 2 & 1 & 2 & 1 \end{bmatrix}$$

$$\widehat{W^f} = \begin{bmatrix} 5 & 4 & 0 & 0 \\ 0 & 0 & 5 & 4 \end{bmatrix}$$

Sekarang, kita perumum semuanya, dan bungkus dalam sebuah konsep yang Bernama "Automatic Differentiation"

#### Automatic Differentiation: Problem Statement

Consider a sequence of I primitive calls:

$$h_1 = f_1(x, W_1)$$

$$h_2 = f_2(h_1, W_2)$$

$$\vdots$$

$$h_l = f_l(h_{l-1}, W_l)$$

This is called an evaluation trace of the program. Roughly, the first l-1 operations can represent several layers of a differentiable model, operation l can be a per-input loss (e.g., cross-entropy).

Hence, the output of our program is always a scalar, since we require it for numerical optimization.

#### Automatic Differentiation: Problem Statement

**Definition D.6.1 (Automatic differentiation)** Given a program  $F(\mathbf{x})$  composed of a sequence of differentiable primitives, **automatic differentiation** (AD) refers to the task of simultaneously and efficiently computing all weight Jacobians of the program given knowledge of the computational graph and all individuals input and weight Jacobians:

$$AD(F(\mathbf{x})) = \left\{ \partial_{\mathbf{w}_i} y \right\}_{i=1}^l$$

There are two major classes of AD algorithms, called forward-mode and backward-mode, corresponding to a different ordering in the composition of the individual operations.

We will also see that the backward-mode (called back-propagation in the neural networks' literature) is significantly more efficient in our context.

$$\boldsymbol{h_1} = f_1(\boldsymbol{x}, \boldsymbol{W_1})$$

$$\boldsymbol{h_2} = f_2(\boldsymbol{h_1}, \boldsymbol{W_2})$$

:

$$\boldsymbol{h_l} = f_l(\boldsymbol{h_{l-1}}, \boldsymbol{W_l})$$

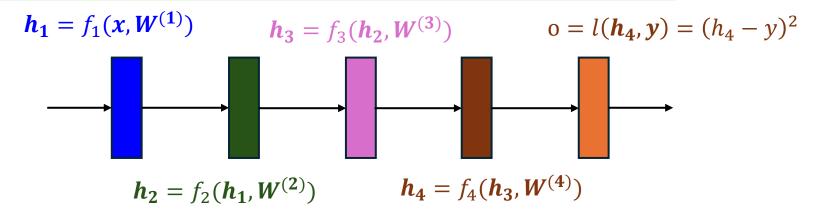
The idea is that every time we apply a primitive function, we initialize its corresponding weight Jacobian (called **tangent** in this context)  $\widehat{W}_i$ , while simultaneously updating all previous tangent matrices.

#### What we want to compute:

$$\frac{\partial h_{l}}{\partial W_{1}} = \frac{\partial h_{l}}{\partial h_{l-1}} \cdot \frac{\partial h_{l-1}}{\partial h_{l-2}} \dots \cdot \frac{\partial h_{2}}{\partial h_{1}} \cdot \frac{\partial h_{1}}{\partial W_{1}}$$

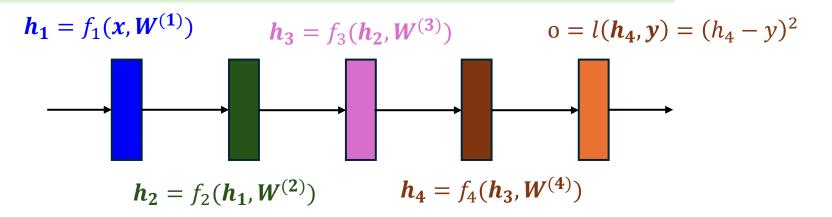
$$\frac{\partial h_{l}}{\partial W_{2}} = \frac{\partial h_{l}}{\partial h_{l-1}} \cdot \frac{\partial h_{l-1}}{\partial h_{l-2}} \dots \frac{\partial h_{2}}{\partial W_{2}}$$

Input jacobian of  $f_i$   $\widehat{W}_j \leftarrow \left[\frac{\partial h_i}{\partial h_{i-1}}\right] \widehat{W}_j \quad \forall j < i$   $\widehat{W}_i \leftarrow \frac{\partial h_i}{\partial W_i}$  Weight jacobian of  $f_i$ 



Misal, Input adalah vektor ~ (2).

Misal, 3 layer pertama adalah fully-connected models dengan output ~ (2); layer ke-4 adalah fully connected model dengan output scalar; dan layer terakhir adalah fungsi loss, yaitu squared loss, yang mengembalikan scalar.



$$f_{1}(x, \mathbf{W}^{(1)}) = \mathbf{W}^{(1)}x = \begin{bmatrix} W_{11}^{(1)} & W_{12}^{(1)} \\ W_{21}^{(1)} & W_{22}^{(1)} \end{bmatrix} \begin{bmatrix} x_{1} \\ x_{2} \end{bmatrix}$$

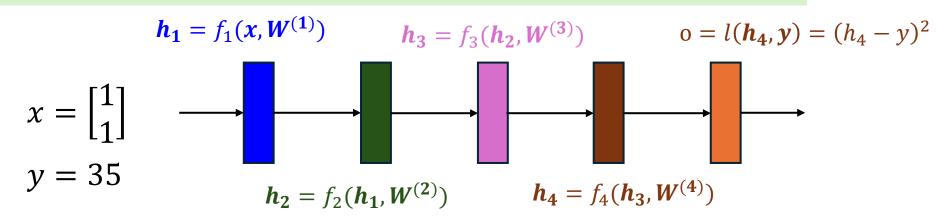
$$f_{2}(\mathbf{h}_{1}, \mathbf{W}^{(2)}) = \mathbf{W}^{(2)}\mathbf{h}_{1} = \begin{bmatrix} W_{11}^{(2)} & W_{12}^{(2)} \\ W_{21}^{(2)} & W_{22}^{(2)} \end{bmatrix} \begin{bmatrix} h_{11} \\ h_{12} \end{bmatrix}$$

$$f_{3}(\mathbf{h}_{2}, \mathbf{W}^{(3)}) = \mathbf{W}^{(3)}\mathbf{h}_{2} = \begin{bmatrix} W_{11}^{(3)} & W_{12}^{(3)} \\ W_{21}^{(3)} & W_{22}^{(3)} \end{bmatrix} \begin{bmatrix} h_{21} \\ h_{22} \end{bmatrix}$$

$$f_4(\mathbf{h}_3, \mathbf{W}^{(4)}) = \mathbf{W}^{(4)}\mathbf{h}_3 = \begin{bmatrix} W_{11}^{(4)} & W_{12}^{(4)} \end{bmatrix} \begin{bmatrix} h_{31} \\ h_{32} \end{bmatrix}$$

$$l(h_4, \mathbf{y}) = (h_4 - \mathbf{y})^2$$

## Total ada 14 parameter!



$$f_1(x, W^{(1)}) = W^{(1)}x = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

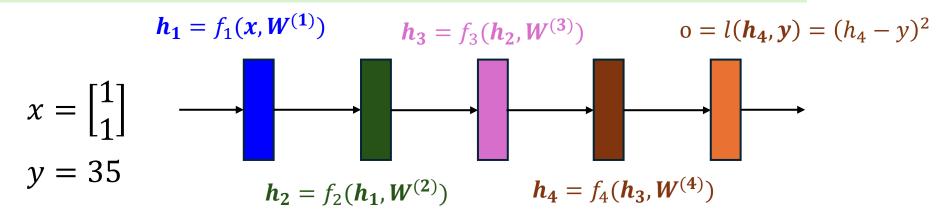
$$f_2(\mathbf{h_1}, \mathbf{W}^{(2)}) = \mathbf{W}^{(2)}\mathbf{h_1} = \begin{bmatrix} 1 & 2 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} h_{11} \\ h_{12} \end{bmatrix}$$

$$f_3(\mathbf{h_2}, \mathbf{W}^{(3)}) = \mathbf{W}^{(3)}\mathbf{h_2} = \begin{bmatrix} 1 & 1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} h_{21} \\ h_{22} \end{bmatrix}$$

$$f_4(h_3, W^{(4)}) = W^{(4)}h_3 = \begin{bmatrix} 2 & 1 \end{bmatrix} \begin{bmatrix} h_{31} \\ h_{32} \end{bmatrix}$$

$$l(h_4, \mathbf{y}) = (h_4 - y)^2$$

Misal, kita mulai dari inisialisasi parameter tertentu (random); dan untuk input x & y tertentu.



$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial W^{(1)}}$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial W^{(2)}}$$

$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial W^{(3)}}$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial W^{(4)}}$$

Input dan output loss function sudah scalar. Turunannya juga scalar:

$$\frac{\partial \boldsymbol{l}}{\partial \boldsymbol{h_4}} = 2(h_4 - y) = 2(h_4 - 2)$$

$$\frac{\partial \boldsymbol{l}}{\partial \boldsymbol{h_4}} = 2(h_4 - 2)$$

$$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$y = 35$$

$$h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$$

$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \underbrace{\frac{\partial h_1}{\partial W^{(1)}}}$$

$$\widehat{W_1} \leftarrow \frac{\partial h_1}{\partial W^{(1)}}$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial W^{(2)}}$$

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$$\widehat{\boldsymbol{W}_1} \leftarrow \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial W^{(2)}}$$

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$$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$y = 35$$

$$h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix} \quad h_2 = \begin{bmatrix} 6 \\ 4 \end{bmatrix}$$

$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial W^{(1)}}$$

$$\frac{\partial l}{\partial l} \quad \partial l \quad \partial h_4 \quad \partial h_3 \quad \partial h_2$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \underbrace{\frac{\partial h_2}{\partial W^{(2)}}}$$

$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial W^{(3)}}$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial W^{(4)}}$$

$$\widehat{W}_1 \leftarrow \frac{\partial h_2}{\partial h_1} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}$$

$$\widehat{W}_2 \leftarrow \frac{\partial h_2}{\partial W^{(2)}}$$

$$\frac{\partial \boldsymbol{l}}{\partial \boldsymbol{h_4}} = 2(h_4 - 2)$$

$$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$y = 35$$

$$h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix} \quad h_2 = \begin{bmatrix} 6 \\ 4 \end{bmatrix}$$

$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial W^{(1)}}$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \left( \frac{\partial h_2}{\partial W^{(2)}} \right)$$

$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial W^{(3)}}$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial W^{(4)}}$$

$$\widehat{\boldsymbol{W}_1} \leftarrow \begin{bmatrix} 1 & 2 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}$$

$$\widehat{\boldsymbol{W}_2} \leftarrow \begin{bmatrix} 2 & 2 & 0 & 0 \\ 0 & 0 & 2 & 2 \end{bmatrix}$$

$$\frac{\partial \boldsymbol{l}}{\partial \boldsymbol{h_4}} = 2(h_4 - 2)$$

$$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

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$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial W^{(3)}}$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial W^{(4)}}$$

$$\widehat{\boldsymbol{W}_1} \leftarrow \begin{bmatrix} 1 & 1 & 2 & 2 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

$$\widehat{\boldsymbol{W}_2} \leftarrow \begin{bmatrix} 2 & 2 & 0 & 0 \\ 0 & 0 & 2 & 2 \end{bmatrix}$$

$$\frac{\partial \boldsymbol{l}}{\partial \boldsymbol{h_4}} = 2(h_4 - 2)$$

$$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$y = 35$$

$$h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix} \quad h_2 = \begin{bmatrix} 6 \\ 4 \end{bmatrix} \quad h_3 = \begin{bmatrix} 10 \\ 16 \end{bmatrix}$$

$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_2}{\partial h_2} \cdot \frac{\partial h_1}{\partial W^{(1)}}$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial W^{(2)}}$$

$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial W^{(3)}}$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial W^{(3)}}$$

$$\widehat{W}_{1} \leftarrow \frac{\partial h_{3}}{\partial h_{2}} \begin{bmatrix} 1 & 1 & 2 & 2 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

$$\widehat{W}_{2} \leftarrow \frac{\partial h_{3}}{\partial h_{2}} \begin{bmatrix} 2 & 2 & 0 & 0 \\ 0 & 0 & 2 & 2 \end{bmatrix}$$

$$\widehat{W}_{3} \leftarrow \frac{\partial h_{3}}{\partial W^{(3)}}$$

$$\frac{\partial \boldsymbol{l}}{\partial \boldsymbol{h_4}} = 2(h_4 - 2)$$

$$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$y = 35$$

$$h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix} \quad h_2 = \begin{bmatrix} 6 \\ 4 \end{bmatrix} \quad h_3 = \begin{bmatrix} 10 \\ 16 \end{bmatrix}$$

$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \left[ \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial W^{(1)}} \right]$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \left[ \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial W^{(2)}} \right]$$

$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \frac{\partial h_3}{\partial W^{(3)}}$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial W^{(4)}}$$

$$\widehat{\boldsymbol{W}_1} \leftarrow \begin{bmatrix} 1 & 1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 2 & 2 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

$$\widehat{\boldsymbol{W}_2} \leftarrow \begin{bmatrix} 1 & 1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 2 & 2 & 0 & 0 \\ 0 & 0 & 2 & 2 \end{bmatrix}$$

$$\widehat{\boldsymbol{W}_3} \leftarrow \begin{bmatrix} 6 & 4 & 0 & 0 \\ 0 & 0 & 6 & 4 \end{bmatrix}$$

$$\frac{\partial \boldsymbol{l}}{\partial \boldsymbol{h_4}} = 2(h_4 - 2)$$

$$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$y = 35$$

$$h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix} \quad h_2 = \begin{bmatrix} 6 \\ 4 \end{bmatrix} \quad h_3 = \begin{bmatrix} 10 \\ 16 \end{bmatrix}$$

$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial W^{(1)}}$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \left[ \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial W^{(2)}} \right]$$

$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \frac{\partial h_3}{\partial W^{(3)}}$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial W^{(4)}}$$

$$\widehat{W}_1 \leftarrow \begin{bmatrix} 2 & 2 & 3 & 3 \\ 3 & 3 & 5 & 5 \end{bmatrix}$$

$$\widehat{\boldsymbol{W}_2} \leftarrow \begin{bmatrix} 2 & 2 & 2 & 2 \\ 4 & 4 & 2 & 2 \end{bmatrix}$$

$$\widehat{\boldsymbol{W}_3} \leftarrow \begin{bmatrix} 6 & 4 & 0 & 0 \\ 0 & 0 & 6 & 4 \end{bmatrix}$$

$$\frac{\partial \boldsymbol{l}}{\partial \boldsymbol{h_4}} = 2(h_4 - 2)$$

$$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$y = 35$$

$$h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix} \quad h_2 = \begin{bmatrix} 6 \\ 4 \end{bmatrix} \quad h_3 = \begin{bmatrix} 10 \\ 16 \end{bmatrix} \quad h_4 = 36$$

$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \left[ \frac{\partial h_4}{\partial h_3}, \frac{\partial h_3}{\partial h_2}, \frac{\partial h_2}{\partial h_1}, \frac{\partial h_1}{\partial W^{(1)}} \right]$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \left[ \frac{\partial h_4}{\partial h_3}, \frac{\partial h_3}{\partial h_2}, \frac{\partial h_2}{\partial W^{(2)}} \right]$$

$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \left[ \frac{\partial h_4}{\partial h_3}, \frac{\partial h_3}{\partial W^{(3)}} \right]$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \left[ \frac{\partial h_4}{\partial h_3}, \frac{\partial h_3}{\partial W^{(3)}} \right]$$

$$\widehat{W}_{1} \leftarrow \frac{\partial h_{4}}{\partial h_{3}} \begin{bmatrix} 2 & 2 & 3 & 3 \\ 3 & 3 & 5 & 5 \end{bmatrix}$$

$$\widehat{W}_{2} \leftarrow \frac{\partial h_{4}}{\partial h_{3}} \begin{bmatrix} 2 & 2 & 2 & 2 \\ 4 & 4 & 2 & 2 \end{bmatrix}$$

$$\widehat{W}_{3} \leftarrow \frac{\partial h_{4}}{\partial h_{3}} \begin{bmatrix} 6 & 4 & 0 & 0 \\ 0 & 0 & 6 & 4 \end{bmatrix}$$

$$\widehat{W}_{4} \leftarrow \frac{\partial h_{4}}{\partial W^{(4)}}$$

$$\frac{\partial \boldsymbol{l}}{\partial \boldsymbol{h_4}} = 2(h_4 - 2)$$

$$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$y = 35$$

$$h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix} \quad h_2 = \begin{bmatrix} 6 \\ 4 \end{bmatrix} \quad h_3 = \begin{bmatrix} 10 \\ 16 \end{bmatrix} \quad h_4 = 36$$

$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \begin{bmatrix} \frac{\partial h_4}{\partial h_3} & \frac{\partial h_3}{\partial h_2} & \frac{\partial h_2}{\partial h_1} & \frac{\partial h_1}{\partial W^{(1)}} \end{bmatrix}$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \left[ \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial W^{(2)}} \right]$$

$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial W^{(3)}}$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \frac{\partial h_4}{\partial W^{(4)}}$$

$$\widehat{W}_1 \leftarrow \begin{bmatrix} 2 & 1 \end{bmatrix} \begin{bmatrix} 2 & 2 & 3 & 3 \\ 3 & 3 & 5 & 5 \end{bmatrix}$$

$$\widehat{\boldsymbol{W}_2} \leftarrow \begin{bmatrix} 2 & 1 \end{bmatrix} \begin{bmatrix} 2 & 2 & 2 & 2 \\ 4 & 4 & 2 & 2 \end{bmatrix}$$

$$\widehat{\boldsymbol{W}_3} \leftarrow \begin{bmatrix} 2 & 1 \end{bmatrix} \begin{bmatrix} 6 & 4 & 0 & 0 \\ 0 & 0 & 6 & 4 \end{bmatrix}$$

$$\widehat{W}_4 \leftarrow [10 \quad 16]$$

$$\frac{\partial \boldsymbol{l}}{\partial \boldsymbol{h_4}} = 2(h_4 - 2)$$

$$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$y = 35$$

$$h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix} \quad h_2 = \begin{bmatrix} 6 \\ 4 \end{bmatrix} \quad h_3 = \begin{bmatrix} 10 \\ 16 \end{bmatrix} \quad h_4 = 36$$

$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \begin{bmatrix} \frac{\partial h_4}{\partial h_3} & \frac{\partial h_3}{\partial h_2} & \frac{\partial h_2}{\partial h_1} & \frac{\partial h_1}{\partial W^{(1)}} \end{bmatrix}$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \left[ \frac{\partial h_4}{\partial h_3}, \frac{\partial h_3}{\partial h_2}, \frac{\partial h_2}{\partial W^{(2)}} \right]$$

$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \left[ \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial W^{(3)}} \right]$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \frac{\partial h_4}{\partial W^{(4)}}$$

$$\widehat{\boldsymbol{W}_1} \leftarrow [7 \quad 7 \quad 11 \quad 11]$$

$$\widehat{W_2} \leftarrow [8 \ 8 \ 6 \ 6]$$

$$\widehat{W}_3 \leftarrow [12 \quad 8 \quad 6 \quad 4]$$

$$\widehat{W_4} \leftarrow [10 \quad 16]$$

$$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$y = 35$$

$$h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix} \quad h_2 = \begin{bmatrix} 6 \\ 4 \end{bmatrix} \quad h_3 = \begin{bmatrix} 10 \\ 16 \end{bmatrix} \quad h_4 = 36 \quad o = 1$$

$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial W^{(1)}}$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial W^{(2)}}$$

$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial W^{(3)}}$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_4} \cdot \frac{\partial h_3}{\partial W^{(4)}}$$

$$\widehat{W}_1 \leftarrow [476 \ 476 \ 748 \ 748]$$

$$\widehat{\mathbf{W}_2} \leftarrow [544 \quad 544 \quad 408 \quad 408]$$

$$\widehat{W}_3 \leftarrow [816 \quad 544 \quad 408 \quad 272]$$

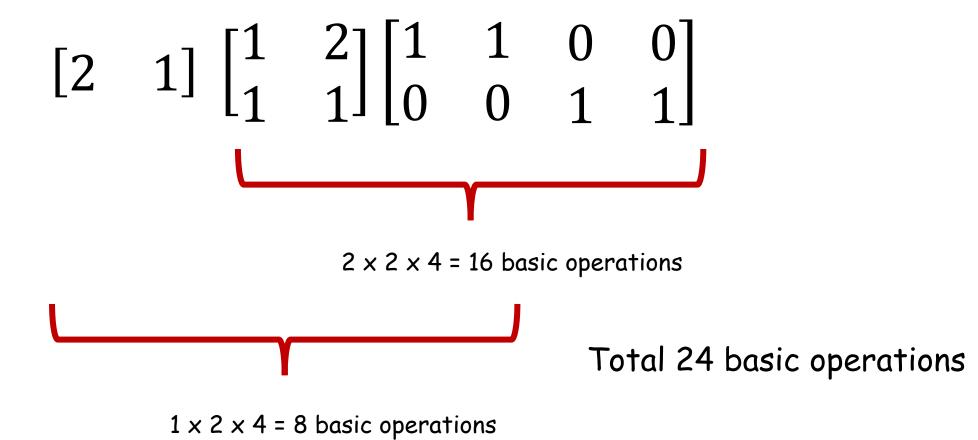
$$\widehat{W}_{4} \leftarrow [680 \ 1088]$$

$$\frac{\partial \boldsymbol{l}}{\partial \boldsymbol{h_4}} = 2(h_4 - 2) = 68$$

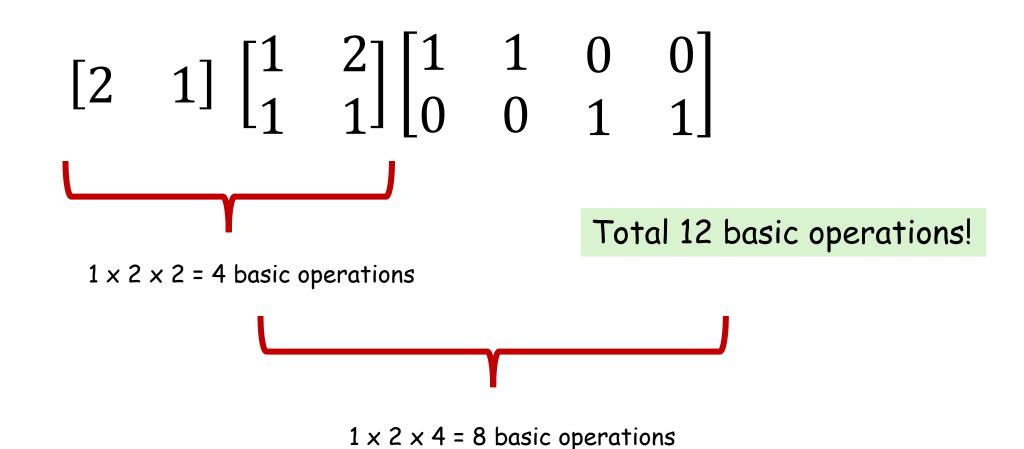
If we have a sequence of matrix multiplications like bellow, where would you start in order to be efficient?

$$\begin{bmatrix} 2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}$$

If we have a sequence of matrix multiplications like bellow, where would you start in order to be efficient?



If we have a sequence of matrix multiplications like bellow, where would you start in order to be efficient?



## Automatic Differentiation: Reverse Mode AD

$$h_1 = f_1(x, W_1)$$

$$h_2 = f_2(h_1, W_2)$$

$$\vdots$$

$$h_l = f_l(h_{l-1}, W_l)$$

Because matrix multiplication is associative, we can perform the computations in any order. In Forward-AD, we proceeded from the right to the left, since it corresponds to the ordering in which the primitive functions were executed. However, we can do better by noting two interesting aspects:

#### What we want to compute:

$$\frac{\partial h_{l}}{\partial W_{1}} = \frac{\partial h_{l}}{\partial h_{l-1}} \cdot \frac{\partial h_{l-1}}{\partial h_{l-2}} \dots \cdot \frac{\partial h_{2}}{\partial h_{1}} \cdot \frac{\partial h_{1}}{\partial W_{1}}$$
$$\frac{\partial h_{l}}{\partial W_{2}} = \frac{\partial h_{l}}{\partial h_{l-1}} \cdot \frac{\partial h_{l-1}}{\partial h_{l-2}} \dots \frac{\partial h_{2}}{\partial W_{2}}$$

The leftmost term is a product between a vector and a matrix (which is a consequence of having a scalar term in output), which is computationally better than a product between two matrices.

:

$$h_1 = f_1(x, W_1)$$

$$h_2 = f_2(h_1, W_2)$$

$$\vdots$$

$$h_l = f_l(h_{l-1}, W_l)$$

Because matrix multiplication is associative, we can perform the computations in any order. In Forward-AD, we proceeded from the right to the left, since it corresponds to the ordering in which the primitive functions were executed. However, we can do better by noting two interesting aspects:

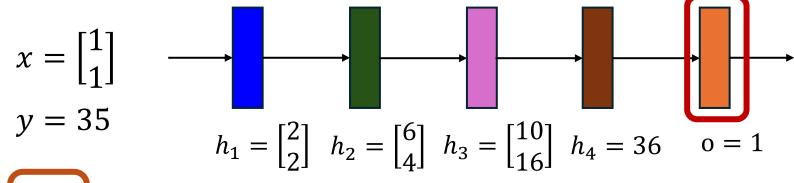
#### What we want to compute:

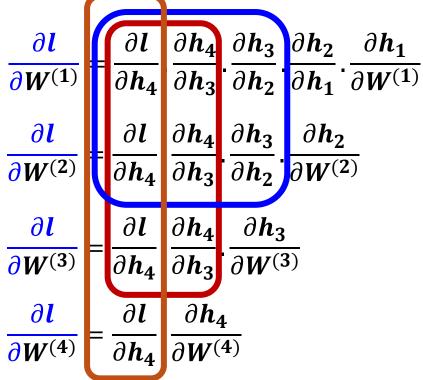
$$\frac{\partial h_{l}}{\partial W_{1}} = \begin{bmatrix} \partial h_{l} & \partial h_{l-1} \\ \partial h_{l-1} & \partial h_{l-2} \end{bmatrix} \dots \frac{\partial h_{2}}{\partial h_{1}} \cdot \frac{\partial h_{1}}{\partial W_{1}}$$

$$\frac{\partial h_{l}}{\partial W_{2}} = \begin{bmatrix} \partial h_{l} & \partial h_{l-1} \\ \partial h_{1} & \partial h_{l-2} \end{bmatrix} \dots \frac{\partial h_{2}}{\partial W_{2}}$$

The leftmost term is a product between a vector and a matrix (which is a consequence of having a scalar term in output), which is computationally better than a product between two matrices.

:





Ini adalah contoh bagian yang cukup dikomputasi sekali lalu disimpan dan digabung untuk komputasi selanjutnya.

$$\boldsymbol{h_1} = f_1(\boldsymbol{x}, \boldsymbol{W_1})$$

$$\boldsymbol{h_2} = f_2(\boldsymbol{h_1}, \boldsymbol{W_2})$$

:

$$h_{l-1} = f_{l-1}(h_{l-2}, W_{l-1})$$

$$L = l(h_{l-1}, W_l)$$

#### Step 1: Forward Pass

Differently from F-AD, we start by executing the entire program to be differentiated, storing all intermediate outputs.

#### Step 2: Backward Pass

Initialize a vector 
$$\tilde{h} = \frac{\partial L}{\partial h_{l-1}}$$

For index i ranging in l, l-1, l-2, ..., 2, 1:

$$\partial_{W^{(i)}}L = \widetilde{h} \times \frac{\partial h_i}{\partial W^{(i)}}$$

$$\rightarrow \widetilde{h} \leftarrow \widetilde{h} \times \frac{\partial h_i}{\partial h_{i-1}}$$

We update our "back-propagated" input Jacobian.

$$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$y = 35$$

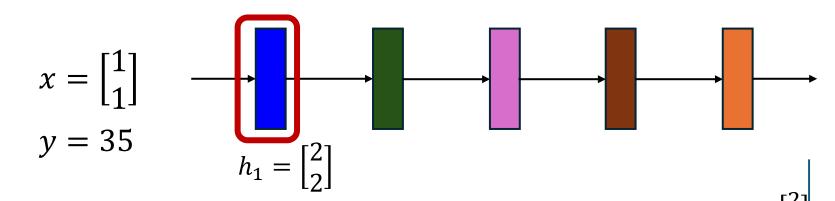
$$h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$$
Storage: [

$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial W^{(1)}}$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial W^{(2)}}$$

$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial W^{(3)}}$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial W^{(4)}}$$



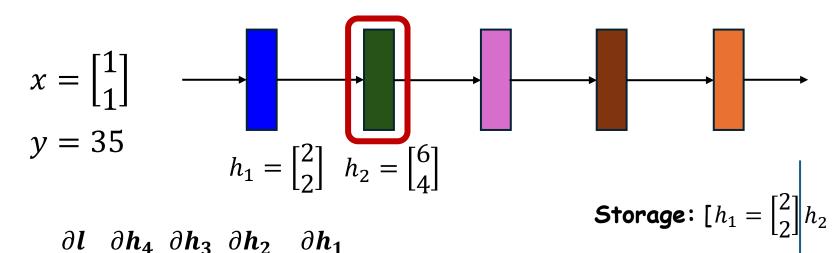
$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial W^{(1)}}$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial W^{(2)}}$$

$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial W^{(3)}}$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial W^{(4)}}$$

Storage:  $[h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$ 



Forward Pass

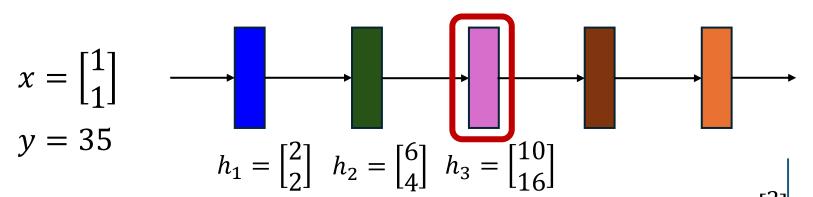
$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial W^{(1)}}$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial W^{(2)}}$$

$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial W^{(3)}}$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial W^{(4)}}$$

Storage:  $[h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix} h_2 = \begin{bmatrix} 6 \\ 4 \end{bmatrix}$ 



Forward Pass

$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial W^{(1)}}$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial W^{(2)}}$$

$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial W^{(3)}}$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial W^{(4)}}$$

Storage:  $\begin{bmatrix} h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix} h_2 = \begin{bmatrix} 6 \\ 4 \end{bmatrix} h_3 = \begin{bmatrix} 10 \\ 16 \end{bmatrix}$ 

$$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$y = 35$$

$$h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix} \quad h_2 = \begin{bmatrix} 6 \\ 4 \end{bmatrix} \quad h_3 = \begin{bmatrix} 10 \\ 16 \end{bmatrix} \quad h_4 = 36$$

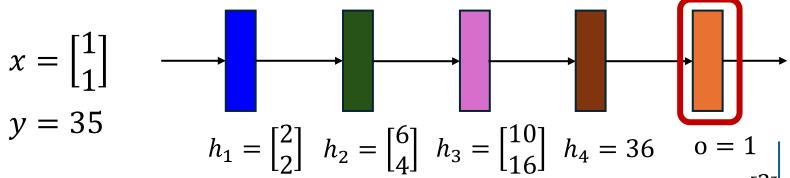
$$\partial \mathbf{h}_4 \quad \partial \mathbf{h}_3 \quad \partial \mathbf{h}_2 \quad \partial \mathbf{h}_1$$
Storage: 
$$[h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix}] \quad h_2 = \begin{bmatrix} 6 \\ 4 \end{bmatrix} \quad h_3 = \begin{bmatrix} 10 \\ 16 \end{bmatrix} \quad h_4 = 36$$

$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial W^{(1)}}$$

$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial W^{(2)}}$$

$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial W^{(3)}}$$

$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial W^{(4)}}$$



#### Forward Pass

$$\frac{\partial l}{\partial W^{(1)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial W^{(1)}}$$

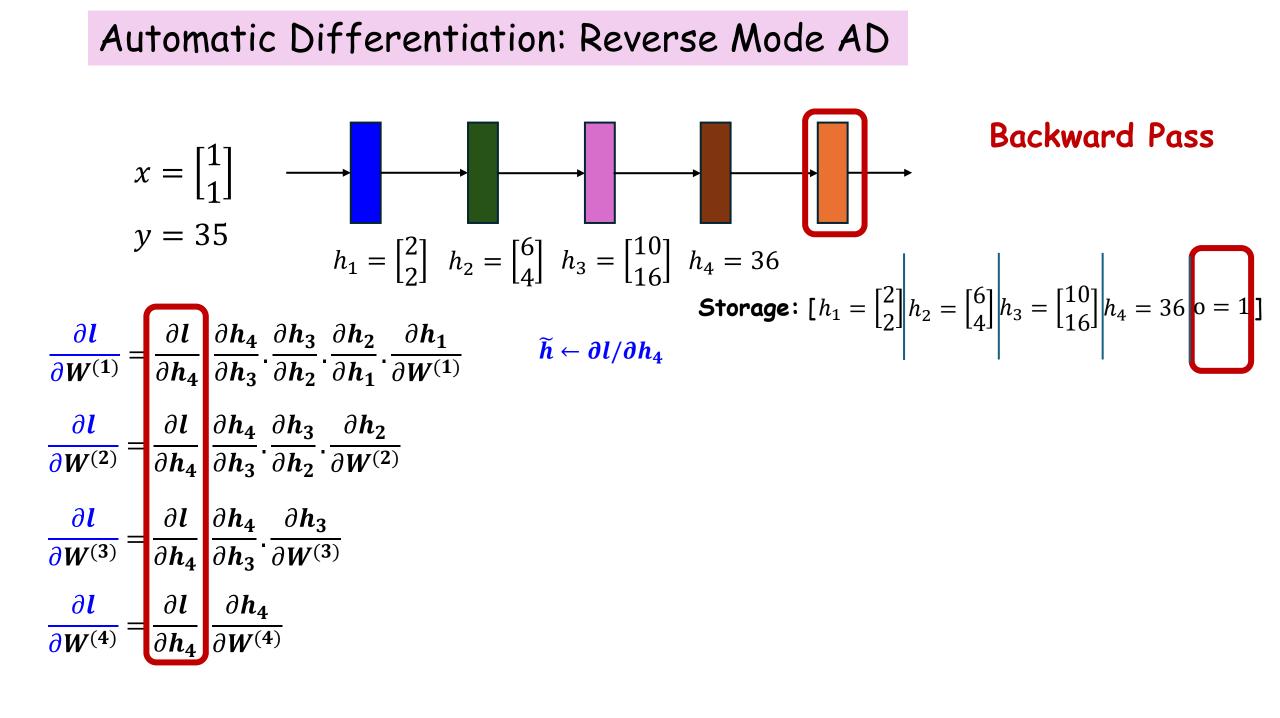
$$\frac{\partial l}{\partial W^{(2)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial W^{(2)}}$$

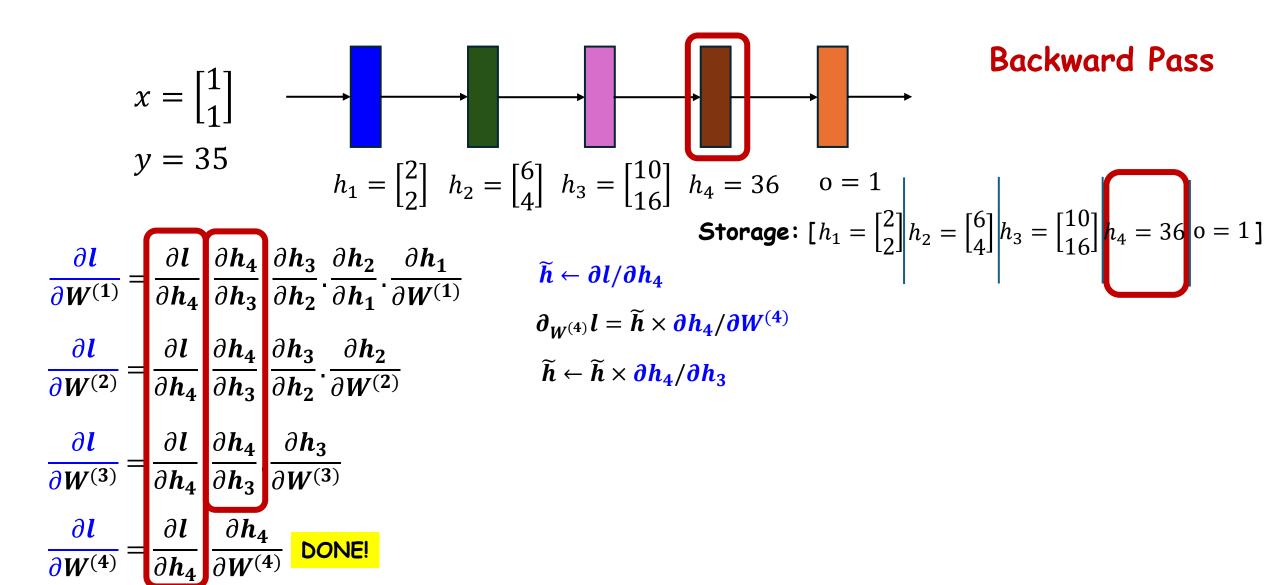
$$\frac{\partial l}{\partial W^{(3)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial h_3} \cdot \frac{\partial h_3}{\partial W^{(3)}}$$

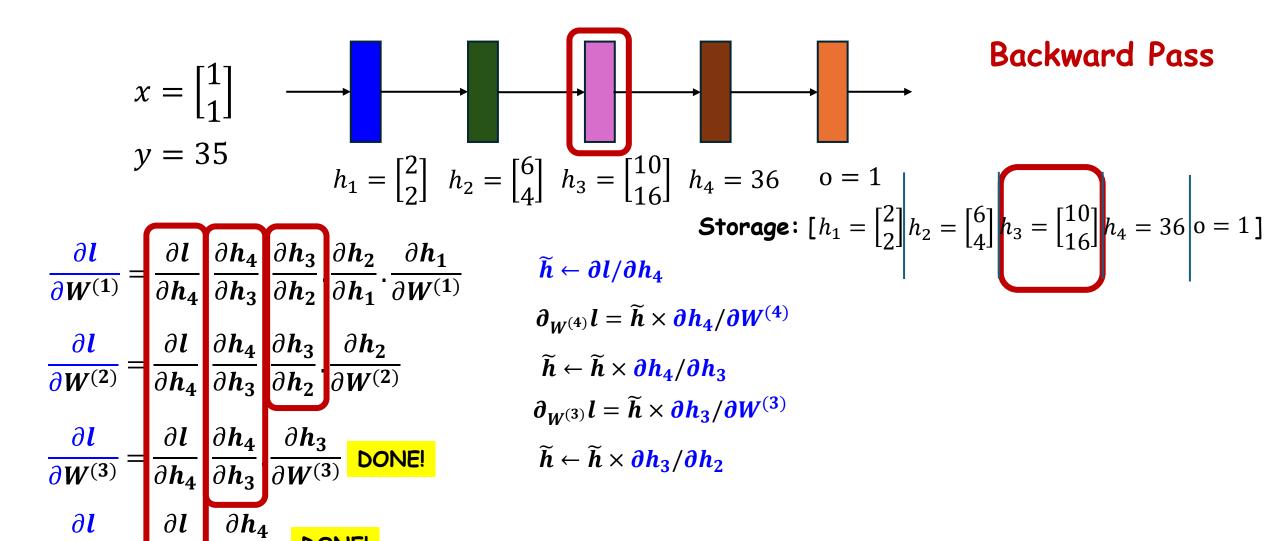
$$\frac{\partial l}{\partial W^{(4)}} = \frac{\partial l}{\partial h_4} \cdot \frac{\partial h_4}{\partial W^{(4)}}$$

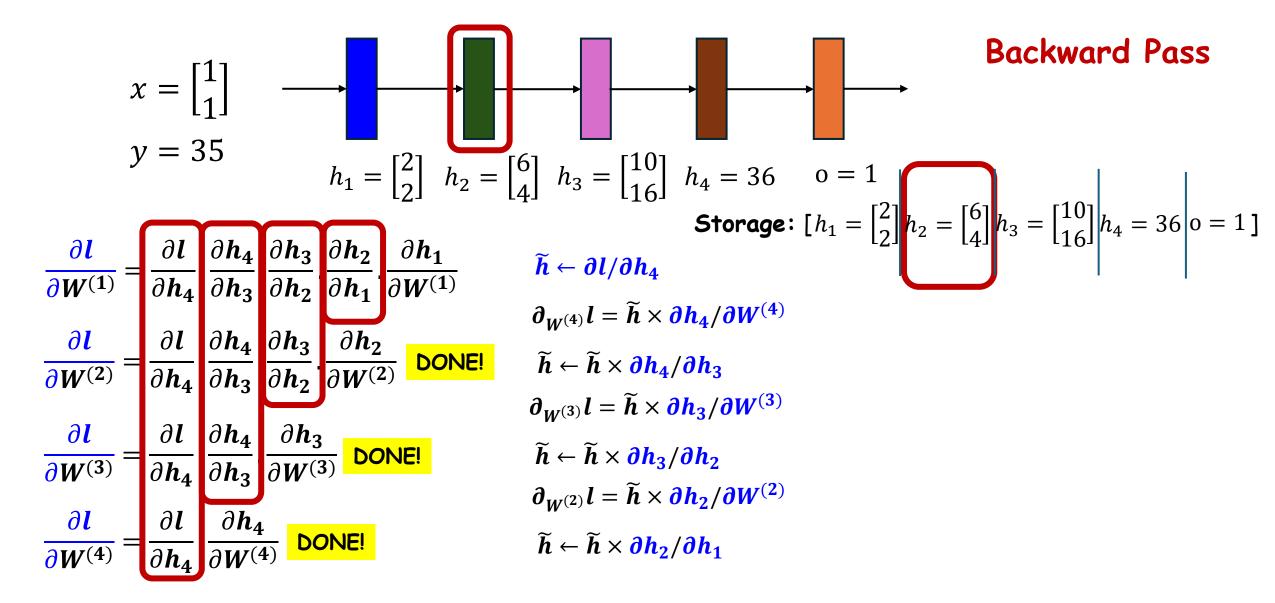
$$h_{1} = \begin{bmatrix} 2 \\ 2 \end{bmatrix} \quad h_{2} = \begin{bmatrix} 6 \\ 4 \end{bmatrix} \quad h_{3} = \begin{bmatrix} 10 \\ 16 \end{bmatrix} \quad h_{4} = 36 \quad \text{o} = 1$$

$$\text{Storage: } [h_{1} = \begin{bmatrix} 2 \\ 2 \end{bmatrix}] \quad h_{2} = \begin{bmatrix} 6 \\ 4 \end{bmatrix} \quad h_{3} = \begin{bmatrix} 10 \\ 16 \end{bmatrix} \quad h_{4} = 36 \quad \text{o} = 1 \end{bmatrix}$$

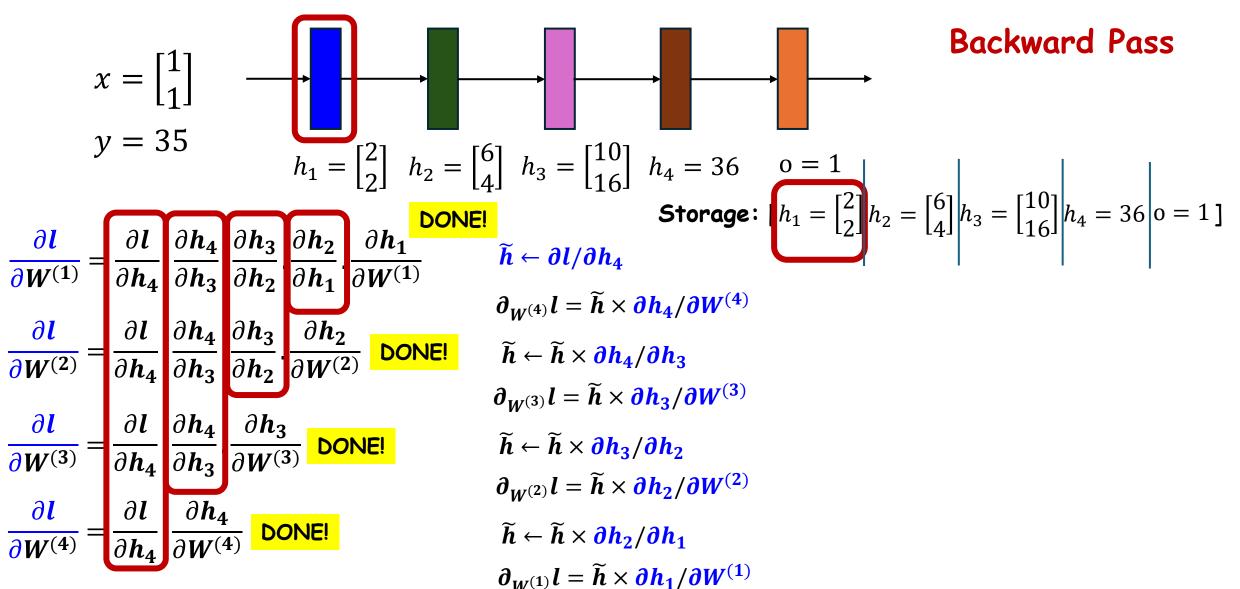








#### **Backward Pass**



#### **Backward Pass**

$$h_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix} h_2 = \begin{bmatrix} 6 \\ 4 \end{bmatrix} h_3 = \begin{bmatrix} 10 \\ 16 \end{bmatrix} h_4 = 36 \text{ o} = 1 \text{ J}$$

#### Automatic Differentiation

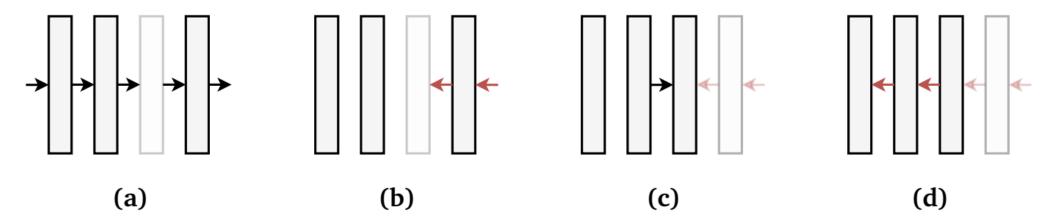
Computationally, Reverse-Mode AD is significantly more efficient than Forward-Mode AD.

In particular, both operations in backward steps at Reverse-Mode AD are vector-matrix products scaling only linearly in all shape quantities.

The tradeoff is that executing Reverse-Mode AD requires a large amount of memory, since all intermediate values of the primal program must be stored on disk with a suitable strategy

#### Automatic Differentiation

Specific techniques, such as gradient checkpointing, can be used to improve on this tradeoff by increasing computations and partially reducing the memory requirements.



**Figure F.6.1:** An example of **gradient checkpointing**. (a) We execute a forward pass, but we only store the outputs of the first, second, and fourth blocks (**checkpoints**). (b) The backward pass (red arrows) stops at the third block, whose activations are not available. (c) We run a second forward pass starting from the closest checkpoint to materialize again the activations. (d) We complete the forward pass. Compared to a standard backward pass, this requires 1.25x more computations. In general, the less checkpoints are stored, the higher the computational cost of the backward pass.

#### Vector-Jacobian Products

Looking at the backward step in the R-AD algorithm, we can make an interesting observation: the only operation we need is a product between a row vector  $\mathbf{v}$  and a Jacobian of  $\mathbf{f}$  (either the input or the weight Jacobian). We call these two operations the vector-Jacobian products  $(\mathbf{VJPs})$  of  $\mathbf{f(x)}$ .

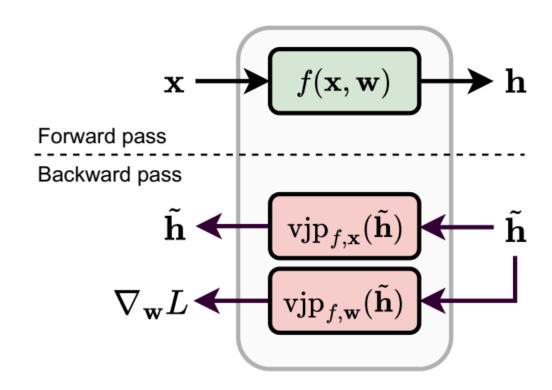
**Definition D.6.2 (Vector-Jacobian product (VJP))** Given a function  $\mathbf{y} = f(\mathbf{x})$ , with  $\mathbf{x} \sim (c)$  and  $\mathbf{y} \sim (c')$ , its VJP is another function defined as:

$$vjp_f(\mathbf{v}) = \mathbf{v}^{\top} \partial f(\mathbf{x})$$
 (E.6.4)

where  $\mathbf{v} \sim (c')$ . If f has multiple parameters  $f(\mathbf{x}_1, \dots, \mathbf{x}_n)$ , we can define n individual VJPs denoted as  $vjp_{f,\mathbf{x}_1}(\mathbf{v})$ , ...,  $vjp_{f,\mathbf{x}_n}(\mathbf{v})$ .

# Vector-Jacobian Products: How to implement R-AD?

**Figure F.6.2:** For performing R-AD, primitives must be augmented with two VJP operations to be able to perform a backward pass, corresponding to the input VJP (E.6.5) and the weight VJP (E.6.6). One call for each is sufficient to perform the backward pass through the primitive, corresponding to (E.6.7)-(E.6.8).



$$vjp_{f,\mathbf{x}}(\mathbf{v}) = \mathbf{v}^{\top} \partial_{\mathbf{x}} f(\mathbf{x}, \mathbf{w})$$
$$vjp_{f,\mathbf{w}}(\mathbf{v}) = \mathbf{v}^{\top} \partial_{\mathbf{w}} f(\mathbf{x}, \mathbf{w})$$

# Contoh implementasi sederhana Reverse-Mode AD

Contoh kode dari A. Karpathy <a href="https://github.com/karpathy/micrograd">https://github.com/karpathy/micrograd</a>

$$f(a,b) = a^2 + 2ab + b^2$$



$$g(a,b) = a + b$$

$$h(g) = g^2$$

$$f(a,b) = h(g(a,b))$$

$$\frac{\partial f(a,b)}{\partial a} = 2a + 2b$$

$$\frac{\partial f(a,b)}{\partial b} = 2a + 2b$$

$$\frac{\partial f(a,b)}{\partial a} = \frac{\partial h}{\partial a} = \frac{\partial h}{\partial g} \cdot \frac{\partial g}{\partial a}$$

$$\frac{\partial f(a,b)}{\partial b} = \frac{\partial h}{\partial b} = \frac{\partial h}{\partial g} \cdot \frac{\partial g}{\partial b}$$

$$f(a,b) = a^2 + 2ab + b^2$$

```
a = Value(...)
b = Value(...)
c = a + b
d = c ** 2
d.backward()
print(a.grad) # ∂d/∂a
print(b.grad) # ∂d/∂b
```

# https://github.com/karpathy/micrograd

```
class Value:
    """ stores a single scalar value and its gradient """
    def __init__(self, data, _children=()):
        self.data = data
        self.grad = 0
       # internal variables used for autograd graph construction
        self. backward = lambda: None
        self._prev = set(_children)
    def __add__(self, other):
        other = other if isinstance(other, Value) else Value(other)
        out = Value(self.data + other.data, (self, other), '+')
       def _backward():
            self.grad += out.grad
            other.grad += out.grad
       out. backward = backward
        return out
```

# https://github.com/karpathy/micrograd

```
def __mul__(self, other):
    other = other if isinstance(other, Value) else Value(other)
   out = Value(self.data * other.data, (self, other))
   def _backward():
        self.grad += other.data * out.grad
        other.grad += self.data * out.grad
   out._backward = _backward
    return out
def __pow__(self, other):
    assert isinstance(other, (int, float)), "only supporting int/float powers for now"
   out = Value(self.data**other, (self,))
   def backward():
        self.grad += (other * self.data**(other-1)) * out.grad
   out. backward = backward
   return out
```

# https://github.com/karpathy/micrograd

```
def backward(self):
    # topological order all of the children in the graph
    topo = []
    visited = set()
    def build_topo(v):
        if v not in visited:
            visited.add(v)
            for child in v._prev:
                build_topo(child)
            topo.append(v)
    build_topo(self)
    # go one variable at a time and apply the chain rule to get its gradient
    self.grad = 1
    for v in reversed(topo):
        v._backward()
```

$$f(a,b) = a^2 + 2ab + b^2$$

```
a = Value(2)
b = Value(3)
c = a + b
d = c ** 2
d.backward()
print(a.grad) # ∂d/∂a
print(b.grad) # ∂d/∂b
```

$$f(a,b) = a^2 + 2ab + b^2$$

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a = Value(2)
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d.backward()
print(a.grad) # ∂d/∂a
print(b.grad) # ∂d/∂b
```

```
_prev = ()
data = 2
grad = 0
_backward =
lambda: None
```

$$f(a,b) = a^2 + 2ab + b^2$$

```
a = Value(2)

b = Value(3)

c = a + b

d = c ** 2

d.backward()

print(a.grad) # \partial d/\partial a

print(b.grad) # \partial d/\partial b
```

```
_prev = ()
data = 2
grad = 0
_backward =
lambda: None
```

```
_prev = ()
data = 3
grad = 0
_backward =
lambda: None
```

$$f(a,b) = a^2 + 2ab + b^2$$

```
a = Value(2)

b = Value(3)

c = a + b

d = c ** 2

d.backward()

print(a.grad) # \partial d/\partial a

print(b.grad) # \partial d/\partial b
```

```
_{prev} = ()
                             prev = ()
                             data = 3
data = 2
                             grad = 0
grad = 0
                             backward =
backward =
                                 lambda: None
    lambda: None
           prev = (a, b)
          data = a.data + b.data = 2 + 3 = 5
          grad = 0
          backward =
              lambda: a.grad += self.grad
                       b.grad += self.grad
```

$$f(a,b) = a^2 + 2ab + b^2$$

```
a = Value(2)
b = Value(3)
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                             prev = ()
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                            grad = 0
grad = 0
                            backward =
backward =
                                lambda: None
    lambda: None
          prev = (a, b)
          data = a.data + b.data = 2 + 3 = 5
          grad = 0
          backward =
              lambda: a.grad += self.grad
                      b.grad += self.grad
    prev = (c)
    data = c ** 2 = 5 ** 2 = 25
    grad = 0
    backward =
      lambda: c.grad =
                (2 * c.data ** 1) * self.grad
```

$$f(a,b) = a^2 + 2ab + b^2$$

```
a = Value(2)

b = Value(3)

c = a + b

d = c ** 2

d.backward()

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print(b.grad) # \partial d/\partial b
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                              prev = ()
                              data = 3
data = 2
                              grad = 0
grad = 0
                              backward =
backward =
                                  lambda: None
    lambda: None
           prev = (a, b)
           data = a.data + b.data = 2 + 3 = 5
          grad = 10 \rightarrow \partial d/\partial c
           _backward =
               lambda: a.grad += self.grad
                       b.grad += self.grad
     prev = (c)
    data = c ** 2 = 5 ** 2 = 25
    grad = 1
     backward =
      lambda: c.grad = (2 * 5 ** 1) * 1 = 10
                 (2 * c.data ** 1) * self.grad
```

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data = 2
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                                 backward =
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      backward =
       lambda: c.grad = (2 * 5 ** 1) * 1 = 10
                   (2 * c.data ** 1) * self.grad
```