Gradients

- Given a function with 1 output and 1 input

$$f(x) = x^3$$

- It's gradient (slope) is its derivative

$$\frac{df}{dx} = 3x^2$$

"How much will the output change if we change the input a bit?"

Gradients

- Given a function with 1 output and *n* inputs

$$f(\boldsymbol{x}) = f(x_1, x_2, ..., x_n)$$

- Its gradient is a vector of partial derivatives with respect to each input

$$\frac{\partial f}{\partial \boldsymbol{x}} = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, ..., \frac{\partial f}{\partial x_n}\right]$$

Jacobian Matrix: Generalization of the Gradient

- Given a function with ***m* outputs** and *n* inputs

$$\boldsymbol{f}(\boldsymbol{x}) = [f_1(x_1, x_2, ..., x_n), ..., f_m(x_1, x_2, ..., x_n)]$$

- It's Jacobian is an ***m* x *n* matrix** of partial derivatives

$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

$$\left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right)_{ij} = \frac{\partial f_i}{\partial x_j}$$

Chain Rule

- For one-variable functions: **multiply derivatives**

$$z = 3y$$

$$y = x^2$$

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx} = (3)(2x) = 6x$$

- For multiple variables at once: **multiply Jacobians**

$$\boldsymbol{h} = f(\boldsymbol{z})$$

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

$$\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}}\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}} = \ldots$$

Example Jacobian: Elementwise activation Function

$$\boldsymbol{h} = f(\boldsymbol{z}), \text{what is } \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}}? \qquad \boldsymbol{h}, \boldsymbol{z} \in \mathbb{R}^n$$

$$h_i = f(z_i)$$

Slides were taken from Manning's course "NLP with Deep Learning" at Stanford University

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Function has *n* outputs and *n* inputs → *n* by *n* Jacobian

Example Jacobian: Elementwise activation Function

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$$\left(\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}}\right)_{ij} = \frac{\partial h_i}{\partial z_j} = \frac{\partial}{\partial z_j} f(z_i) \qquad \text{definition of Jacobian}$$

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$$= \begin{cases} f'(z_i) & \text{if } i = j \\ 0 & \text{if otherwise} \end{cases} \qquad \text{regular 1-variable derivative}$$

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$$\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} = \begin{pmatrix} f'(z_1) & & 0 \\ & \ddots & \\ 0 & & f'(z_n) \end{pmatrix} = \operatorname{diag}(\boldsymbol{f}'(\boldsymbol{z}))$$

Other Jacobians

$$\frac{\partial}{\partial \boldsymbol{x}}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) = \boldsymbol{W}$$

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$$\frac{\partial}{\partial \boldsymbol{x}}(\boldsymbol{W}\boldsymbol{x}+\boldsymbol{b})=\boldsymbol{W}$$

$$\frac{\partial}{\partial \boldsymbol{b}}(\boldsymbol{W}\boldsymbol{x}+\boldsymbol{b})=\boldsymbol{I}\ \ \text{(Identity matrix)}$$

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$$\frac{\partial}{\partial \boldsymbol{u}}(\boldsymbol{u}^T\boldsymbol{h}) = \boldsymbol{h}^{\boldsymbol{T}}$$

Fine print: This is the correct Jacobian. Later we discuss the “shape convention”; using it the answer would be ***h***.

Other Jacobians

$$\frac{\partial}{\partial \boldsymbol{x}}(\boldsymbol{W}\boldsymbol{x}+\boldsymbol{b}) = \boldsymbol{W}$$

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$$\frac{\partial}{\partial \boldsymbol{u}}(\boldsymbol{u}^T\boldsymbol{h}) = \boldsymbol{h}^{\boldsymbol{T}}$$

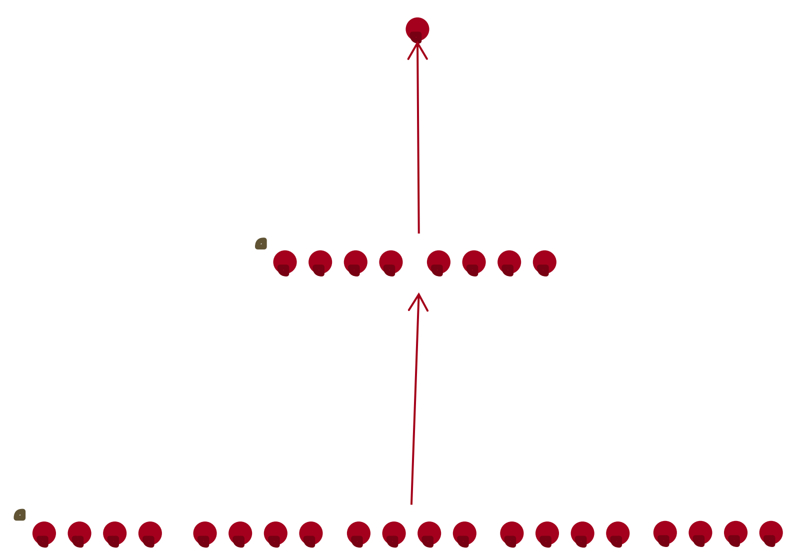
- Compute these at home for practice!
  - Check your answers with the lecture notes

Back to our Neural Net!

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$$

$$\boldsymbol{x} \quad \text{(input)}$$



$$x = [\; x_{museums} \quad x_{in} \quad x_{Paris} \quad x_{are} \quad x_{amazing} \;]$$

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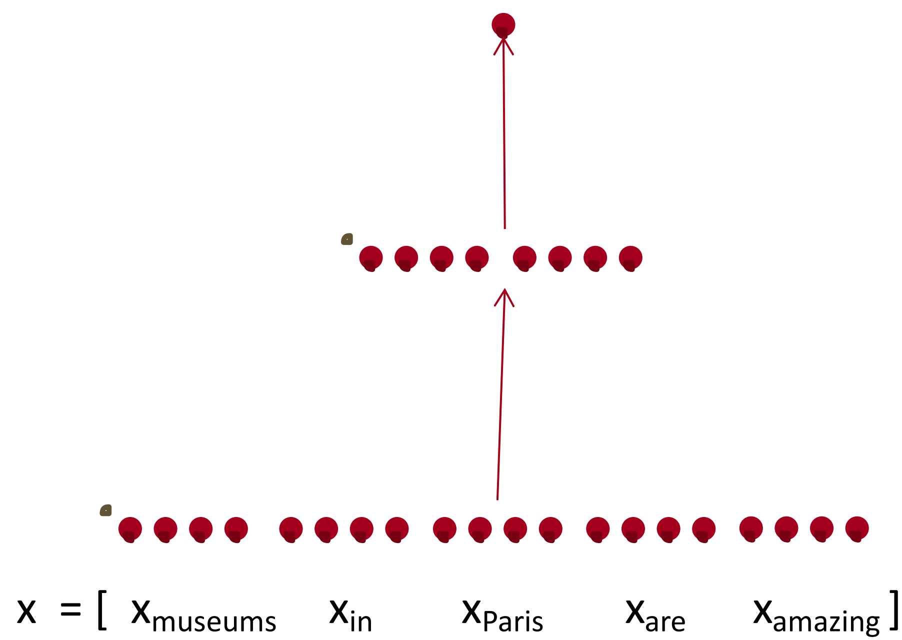
Back to our Neural Net!

- Let's find $\dfrac{\partial s}{\partial \boldsymbol{b}}$
  - Really, we care about the gradient of the loss, but we will compute the gradient of the score for simplicity

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$$

$$\boldsymbol{x} \quad \text{(input)}$$



1. Break up equations into simple pieces

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$$

$$\boldsymbol{x} \quad \text{(input)}$$

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{z})$$

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

$$\boldsymbol{x} \quad \text{(input)}$$

2. Apply the chain rule

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{z})$$

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

$$\boldsymbol{x} \quad \text{(input)}$$

$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

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$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

3. Write out the Jacobians

$$\boldsymbol{s} = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$

$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \quad \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \quad \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

- Useful Jacobians from previous slide

$$\frac{\partial}{\partial \boldsymbol{u}}(\boldsymbol{u}^T \boldsymbol{h}) = \boldsymbol{h}^T$$
$$\frac{\partial}{\partial \boldsymbol{z}}(f(\boldsymbol{z})) = \text{diag}(f'(\boldsymbol{z}))$$
$$\frac{\partial}{\partial \boldsymbol{b}}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) = \boldsymbol{I}$$

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$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
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$$\boldsymbol{u}^T \text{diag}(f'(\boldsymbol{z}))$$

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$$\frac{\partial s}{\partial \boldsymbol{b}} = \underbrace{\frac{\partial s}{\partial \boldsymbol{h}}}_{\boldsymbol{u}^T} \; \underbrace{\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}}}_{\text{diag}(f'(\boldsymbol{z}))} \; \underbrace{\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}}_{\boldsymbol{I}}$$

$$= \boldsymbol{u}^T \text{diag}(f'(\boldsymbol{z}))\boldsymbol{I}$$

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3. Write out the Jacobians

$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$

$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \quad \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \quad \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

$$= \boldsymbol{u}^T \operatorname{diag}(f'(\boldsymbol{z}))\boldsymbol{I}$$

$$= \boldsymbol{u}^T \circ f'(\boldsymbol{z})$$

- Useful Jacobians from previous slide

$$\frac{\partial}{\partial \boldsymbol{u}}(\boldsymbol{u}^T \boldsymbol{h}) = \boldsymbol{h}^T$$

$$\frac{\partial}{\partial \boldsymbol{z}}(f(\boldsymbol{z})) = \operatorname{diag}(f'(\boldsymbol{z}))$$

$$\frac{\partial}{\partial \boldsymbol{b}}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) = \boldsymbol{I}$$

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Re-using Computation

- Suppose we now want to compute $\frac{\partial s}{\partial \boldsymbol{W}}$
  - Using the chain rule again:

$$\frac{\partial s}{\partial \boldsymbol{W}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{W}}$$

Re-using Computation

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$$\frac{\partial s}{\partial \boldsymbol{W}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{W}}$$

$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

The same! Let's avoid duplicated computation…

Re-using Computation

- Suppose we now want to compute $\frac{\partial s}{\partial \boldsymbol{W}}$
  - Using the chain rule again:

$$\frac{\partial s}{\partial \boldsymbol{W}} = \boldsymbol{\delta} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{W}}$$

$$\frac{\partial s}{\partial \boldsymbol{b}} = \boldsymbol{\delta} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}} = \boldsymbol{\delta}$$

$$\boldsymbol{\delta} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} = \boldsymbol{u}^T \circ f'(\boldsymbol{z})$$

δ is local error signal

Derivative with respect to Matrix: Output shape

- What does $\frac{\partial s}{\partial \boldsymbol{W}}$ look like? $\boldsymbol{W} \in \mathbb{R}^{n \times m}$
- 1 output, *nm* inputs: 1 by *nm* Jacobian?
  - Inconvenient to do $\theta^{new} = \theta^{old} - \alpha \nabla_\theta J(\theta)$

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Derivative with respect to Matrix: Output shape

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- 1 output, *nm* inputs: 1 by *nm* Jacobian?
  - Inconvenient to do $\theta^{new} = \theta^{old} - \alpha \nabla_\theta J(\theta)$

- Instead we use **shape convention**: the shape of the gradient is the shape of the parameters
  - So $\frac{\partial s}{\partial \boldsymbol{W}}$ is *n* by *m*: $\begin{bmatrix} \frac{\partial s}{\partial W_{11}} & \cdots & \frac{\partial s}{\partial W_{1m}} \\ \vdots & \ddots & \vdots \\ \frac{\partial s}{\partial W_{n1}} & \cdots & \frac{\partial s}{\partial W_{nm}} \end{bmatrix}$

Derivative with respect to Matrix

- Remember $\dfrac{\partial s}{\partial \boldsymbol{W}} = \boldsymbol{\delta} \dfrac{\partial \boldsymbol{z}}{\partial \boldsymbol{W}}$
  - $\boldsymbol{\delta}$ is going to be in our answer
  - The other term should be $\boldsymbol{x}$ because $\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$

- Answer is: $\dfrac{\partial s}{\partial \boldsymbol{W}} = \boldsymbol{\delta}^T \boldsymbol{x}^T$

δ is local error signal at z

x is local input signal

Why the Transposes?

$$\frac{\partial s}{\partial \boldsymbol{W}} = \boldsymbol{\delta}^T \quad \boldsymbol{x}^T$$

$$[n \times m] \quad [n \times 1][1 \times m]$$

- Hacky answer: this makes the dimensions work out!
  - Useful trick for checking your work!
- Full explanation in the lecture notes; intuition next
  - Each input goes to each output – you get outer product

Why the Transposes?

$$\frac{\partial s}{\partial \boldsymbol{W}} = \boldsymbol{\delta}^T \boldsymbol{x}^T = \begin{bmatrix} \delta_1 \\ \vdots \\ \delta_n \end{bmatrix} [x_1, ..., x_m] = \begin{bmatrix} \delta_1 x_1 & \dots & \delta_1 x_m \\ \vdots & \ddots & \vdots \\ \delta_n x_1 & \dots & \delta_n x_m \end{bmatrix}$$

3. Backpropagation

We've almost shown you backpropagation

It's taking derivatives and using the (generalized, multivariate, or matrix) chain rule

Other trick:

We **re-use** derivatives computed for higher layers in computing derivatives for lower layers to minimize computation

Computation Graphs and Backpropagation

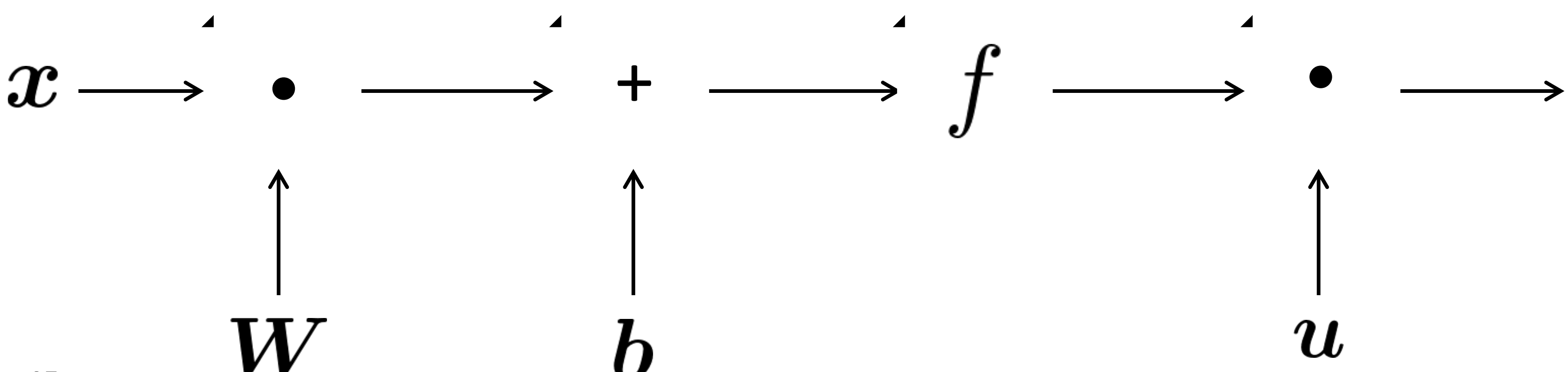
- We represent our neural net equations as a graph
  - Source nodes: inputs
  - Interior nodes: operations

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{z})$$

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

$$\boldsymbol{x} \quad \text{(input)}$$



Computation Graphs and Backpropagation

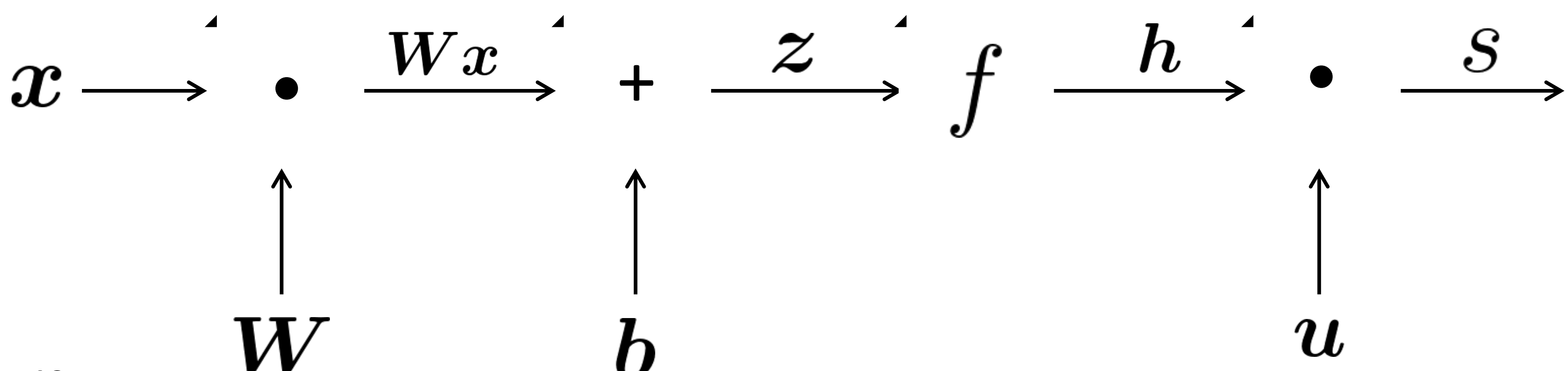
- We represent our neural net equations as a graph
  - Source nodes: inputs
  - Interior nodes: operations
  - Edges pass along result of the operation

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{z})$$

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

$$\boldsymbol{x} \quad \text{(input)}$$



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Computation Graphs and Backpropagation

- Representing our neural net equations as a graph

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

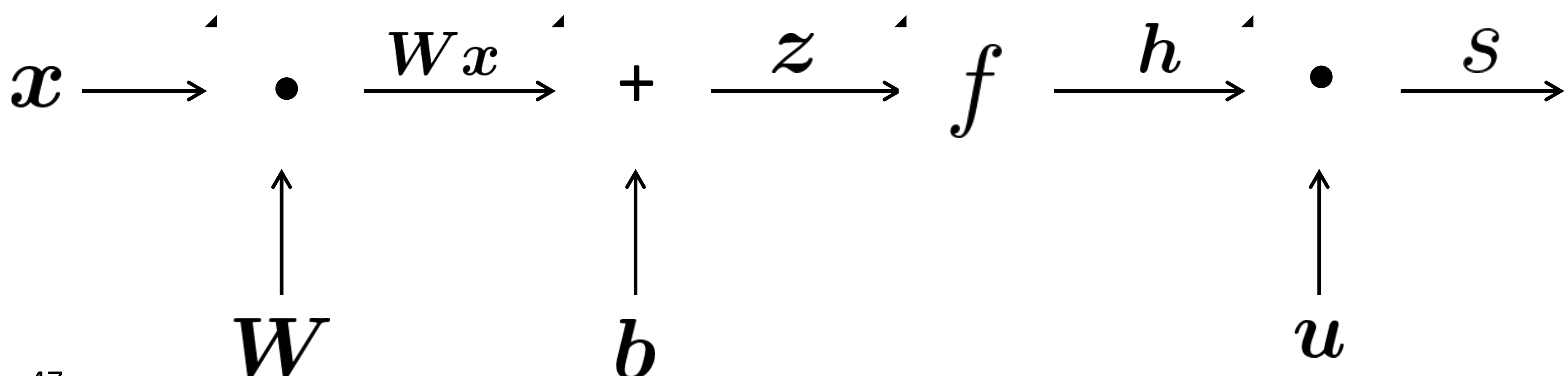
$$\boldsymbol{h} = f(\boldsymbol{z})$$

$c + \boldsymbol{b}$

ut)

"Forward Propagation"

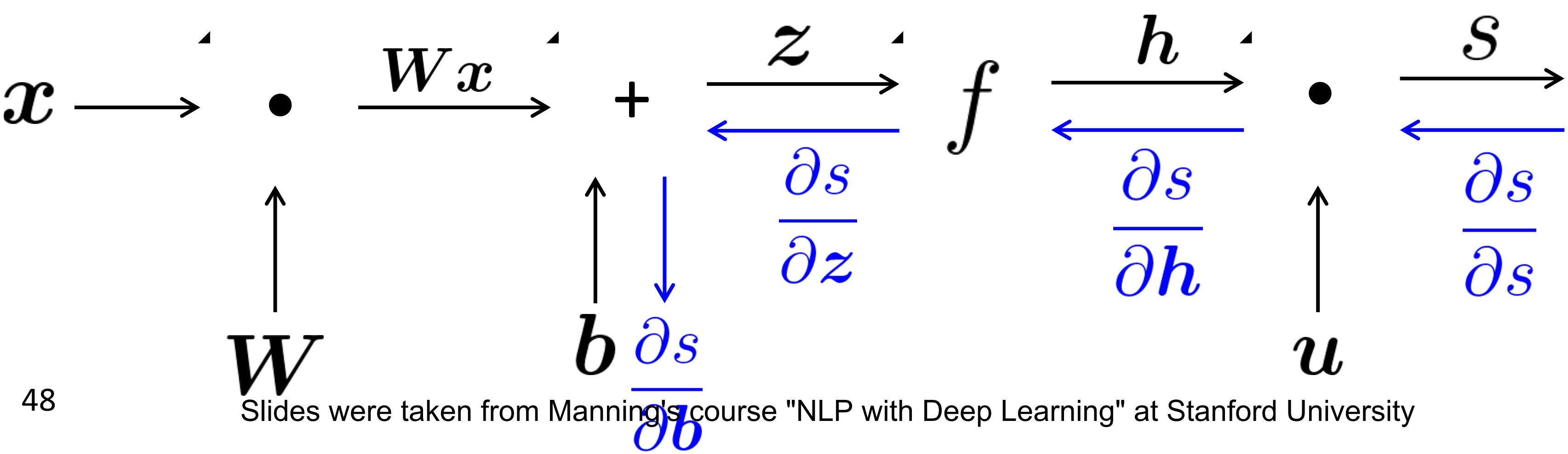
operation



Backpropagation

- Go backwards along edges
  - Pass along **gradients**

$$
\begin{aligned}
s &= \boldsymbol{u}^T \boldsymbol{h} \\
\boldsymbol{h} &= f(\boldsymbol{z}) \\
\boldsymbol{z} &= \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b} \\
\boldsymbol{x} & \quad \text{(input)}
\end{aligned}
$$



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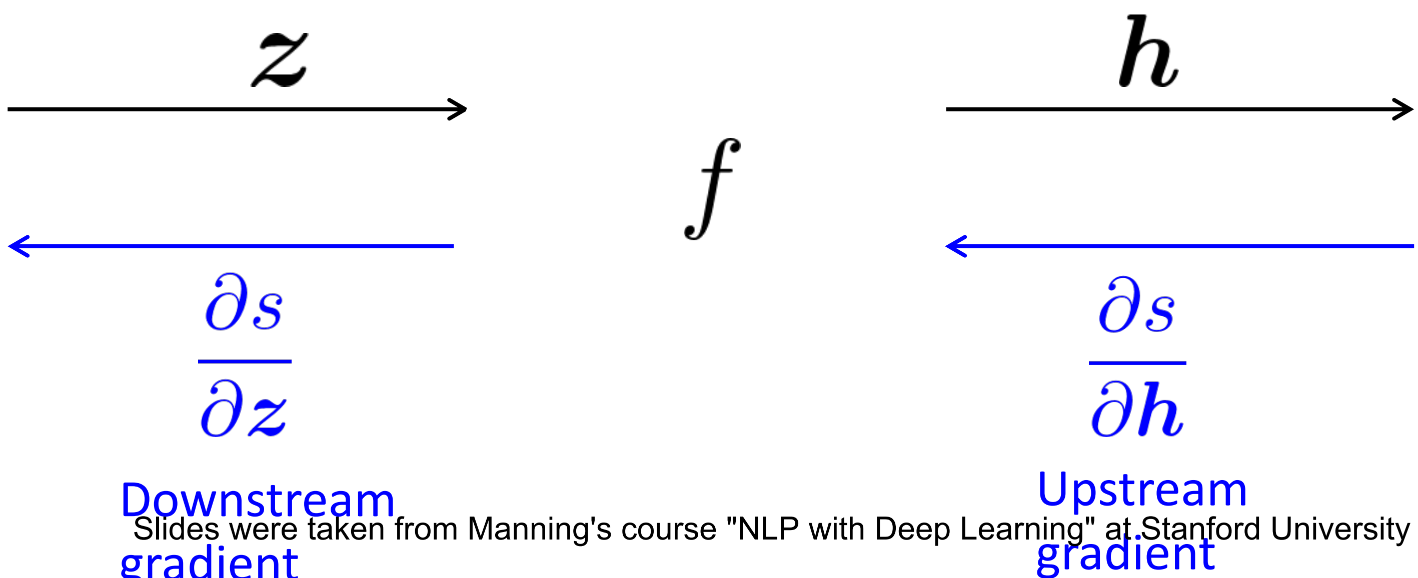
Backpropagation: Single Node

- Node receives an “upstream gradient”
- Goal is to pass on the correct “downstream gradient”

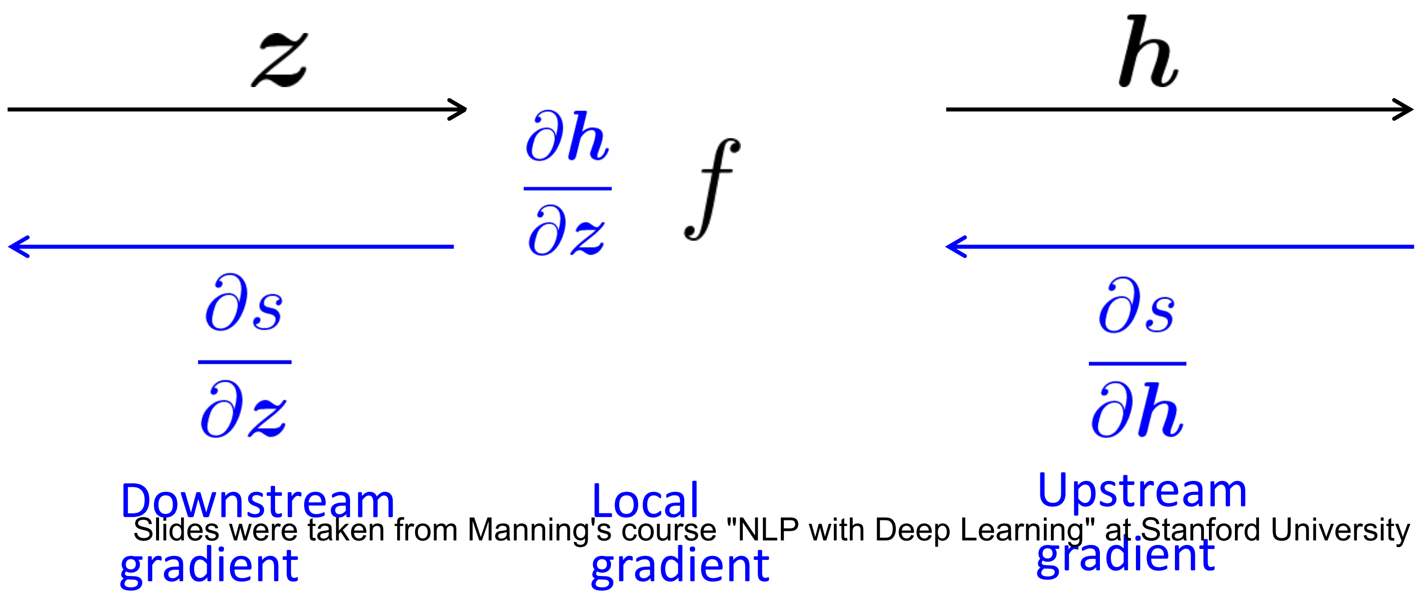
$$\boldsymbol{h} = f(\boldsymbol{z})$$



Backpropagation: Single Node

- Each node has a **local gradient**
  - The gradient of its output with respect to its input

$$h = f(z)$$



Backpropagation: Single Node

- Each node has a **local gradient**
  - The gradient of its output with respect to its input

$$\boldsymbol{h} = f(\boldsymbol{z})$$

$$\xrightarrow{\boldsymbol{z}} \quad \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \quad f \quad \xrightarrow{\boldsymbol{h}}$$

Chain rule!

$$\frac{\partial s}{\partial \boldsymbol{z}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \qquad \frac{\partial s}{\partial \boldsymbol{h}}$$

Downstream gradient

Local gradient

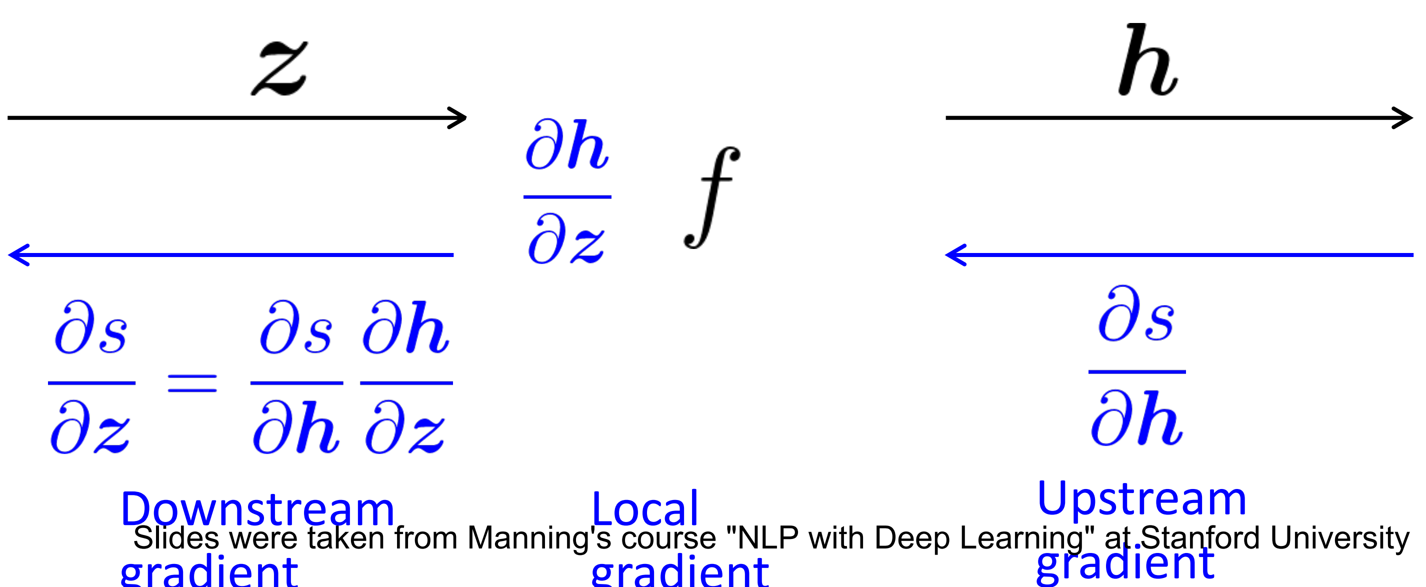
Upstream gradient

Backpropagation: Single Node

- Each node has a **local gradient**
  - The gradient of it's output with respect to it's input

$$\boldsymbol{h} = f(\boldsymbol{z})$$

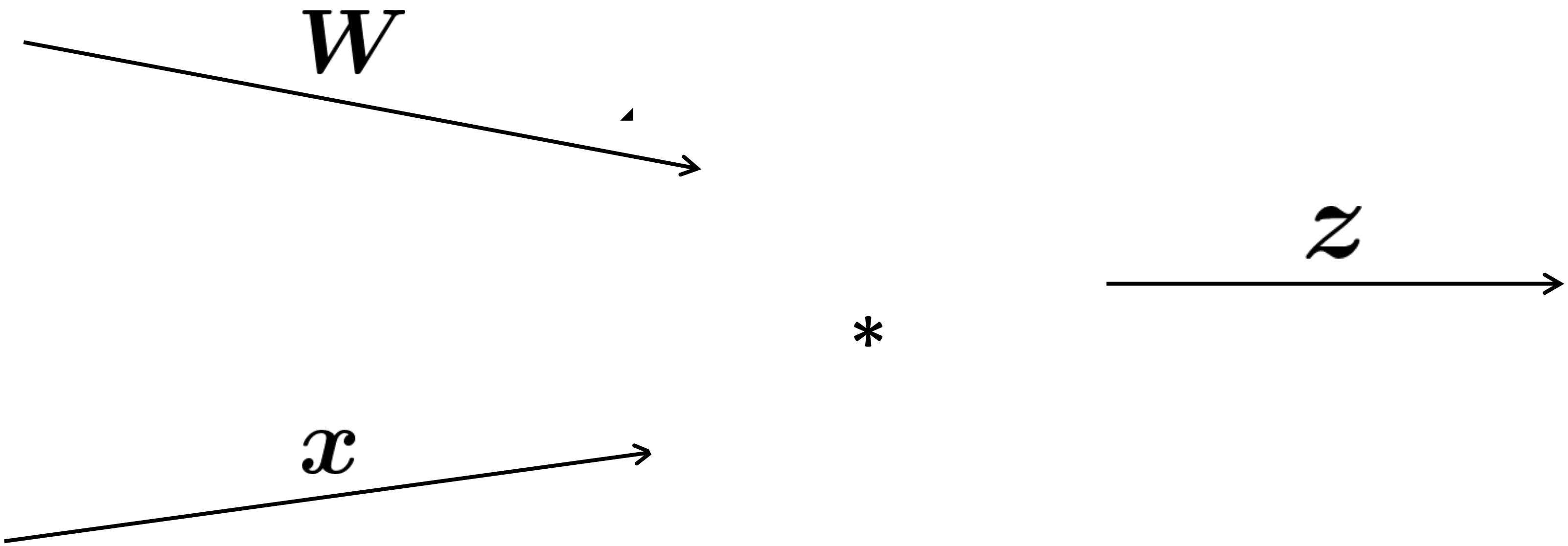
- [downstream gradient] = [upstream gradient] x [local gradient]



Backpropagation: Single Node

- What about nodes with multiple inputs?

$$z = \boldsymbol{W}\boldsymbol{x}$$



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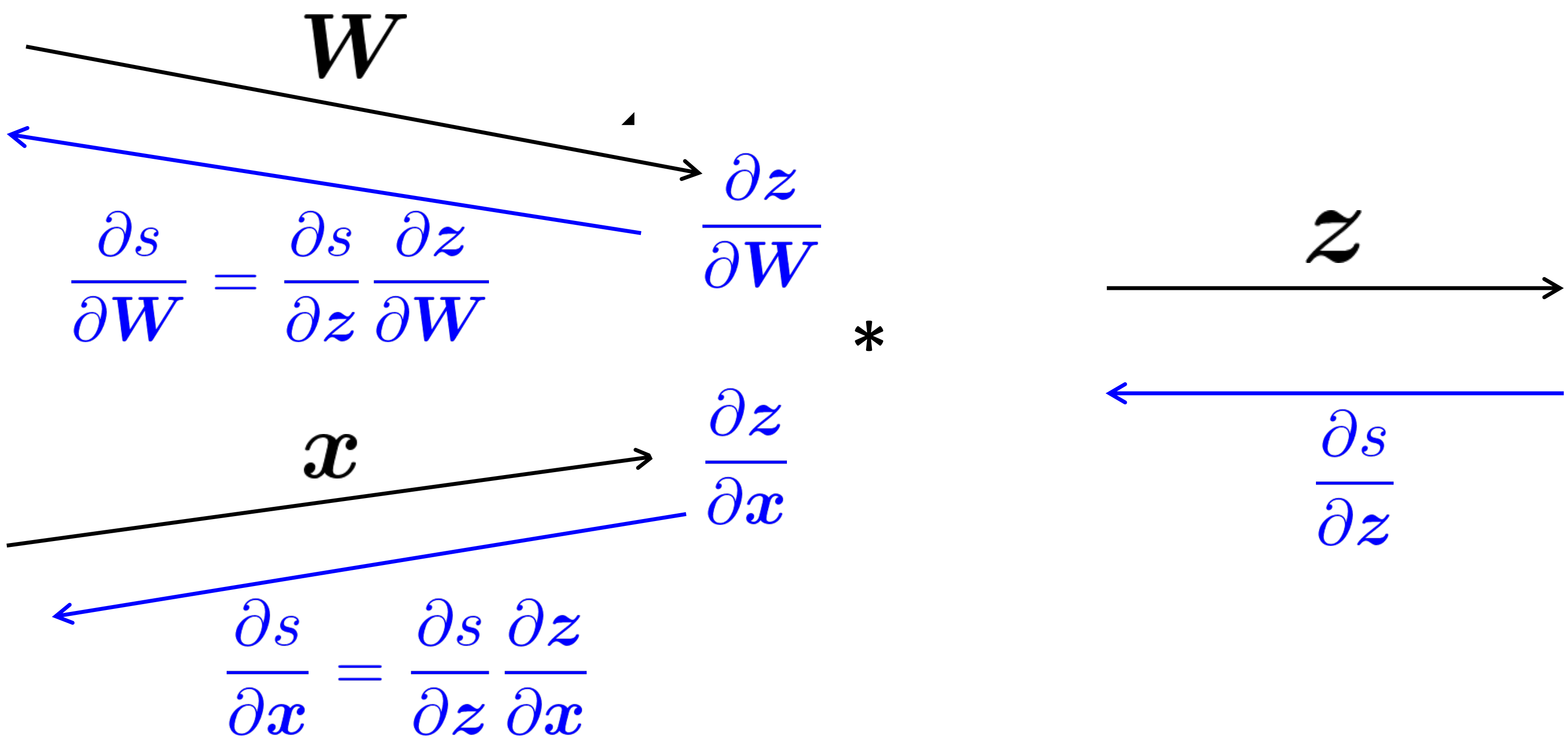
Backpropagation: Single Node

- Multiple inputs → multiple local gradients $\quad \boldsymbol{z} = \boldsymbol{W}\boldsymbol{x}$



Downstream gradients

Local gradients

Upstream gradient

An Example

- $$f(x, y, z) = (x + y)\max(y, z)$$
  $$x = 1, y = 2, z = 0$$

An Example

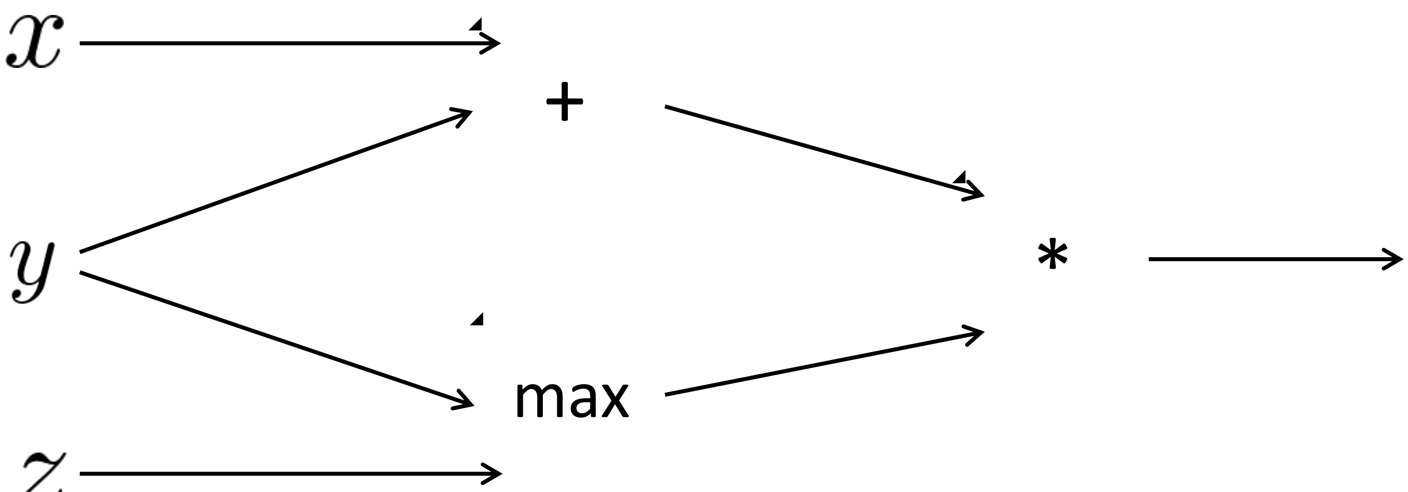
$$f(x, y, z) = (x + y)\max(y, z)$$
$$x = 1, y = 2, z = 0$$

Forward prop steps

$$a = x + y$$

$$b = \max(y, z)$$

$$f = ab$$



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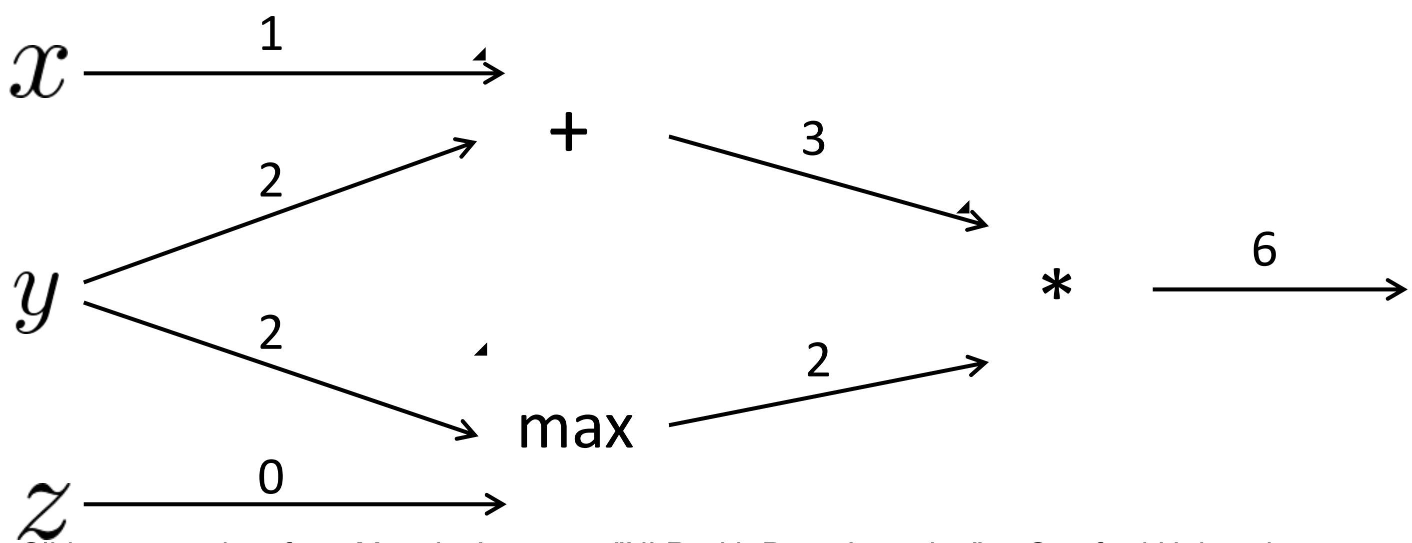

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An Example

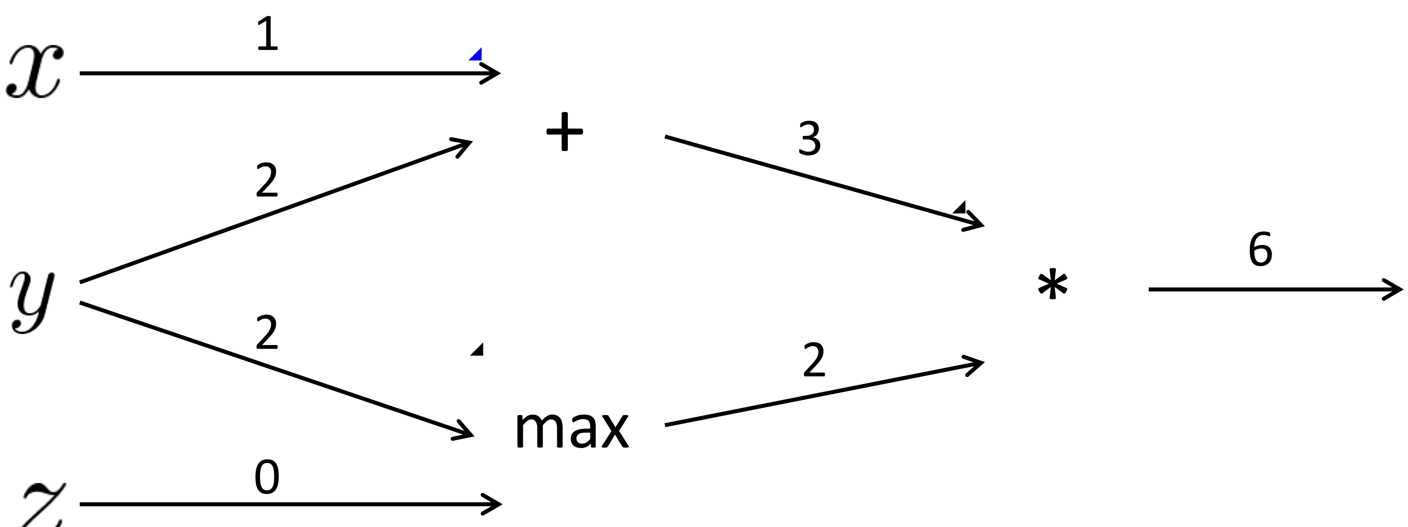
$$f(x,y,z) = (x+y)\max(y,z)$$
$$x = 1, y = 2, z = 0$$

Forward prop steps

$$a = x + y$$
$$b = \max(y,z)$$
$$f = ab$$

Local gradients

$$\frac{\partial a}{\partial x} = 1 \quad \frac{\partial a}{\partial y} = 1$$



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An Example

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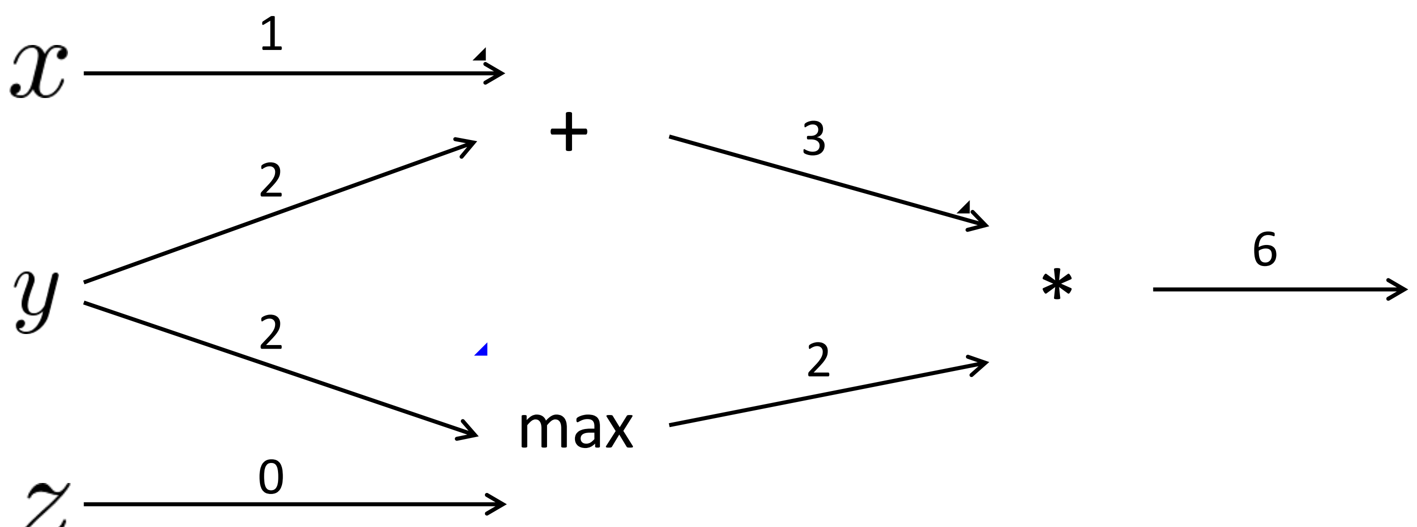
$$x = 1, y = 2, z = 0$$

Forward prop steps

$$a = x + y$$
$$b = \max(y, z)$$
$$f = ab$$

Local gradients

$$\frac{\partial a}{\partial x} = 1 \quad \frac{\partial a}{\partial y} = 1$$
$$\frac{\partial b}{\partial y} = \mathbf{1}(y > z) = 1 \quad \frac{\partial b}{\partial z} = \mathbf{1}(z > y) = 0$$



Slides were taken from Manning's course "NLP with Deep Learning" at Stanford University

An Example

$$f(x, y, z) = (x + y)\max(y, z)$$
$$x = 1, y = 2, z = 0$$

Forward prop steps

$$a = x + y$$
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$$f = ab$$

Local gradients

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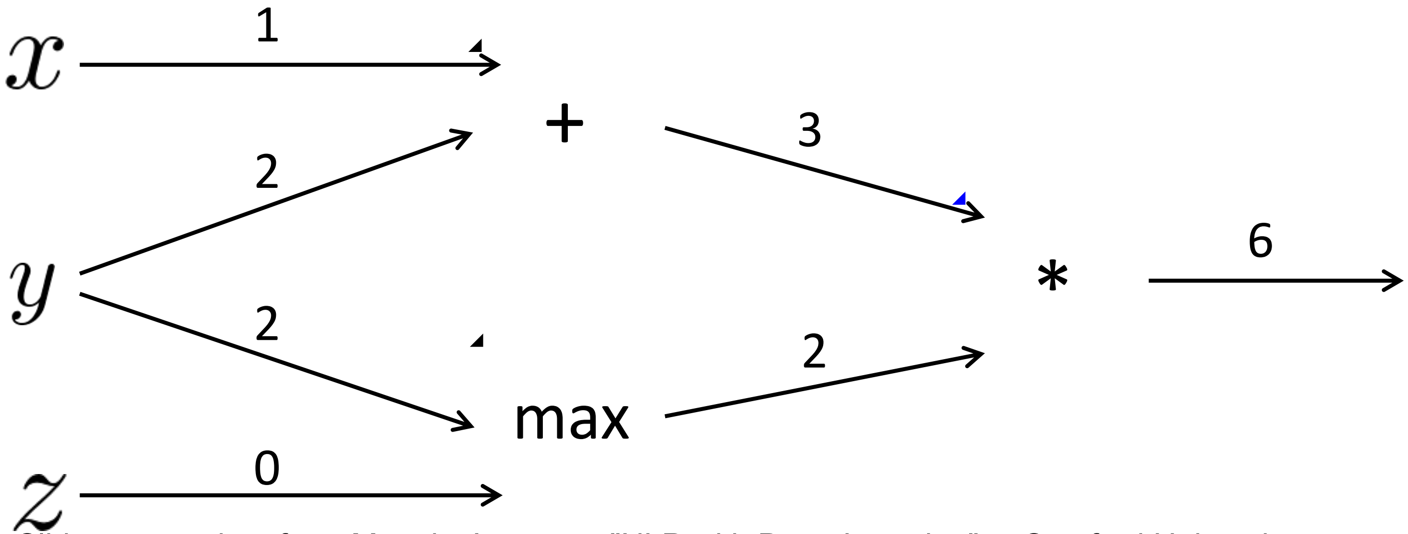

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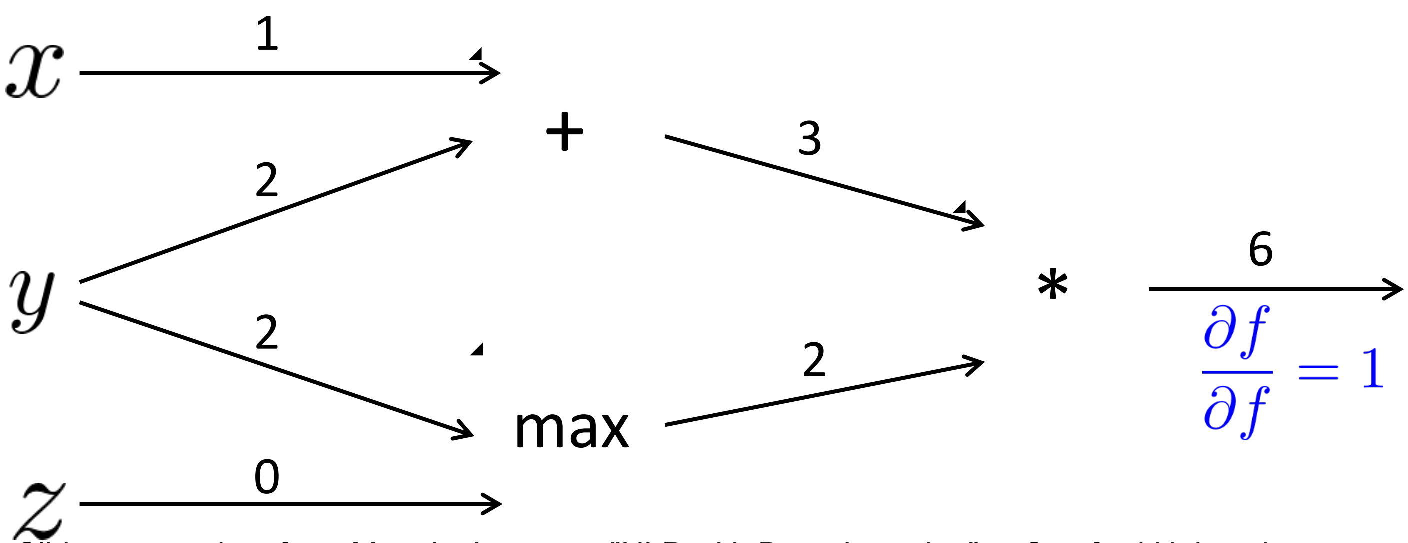

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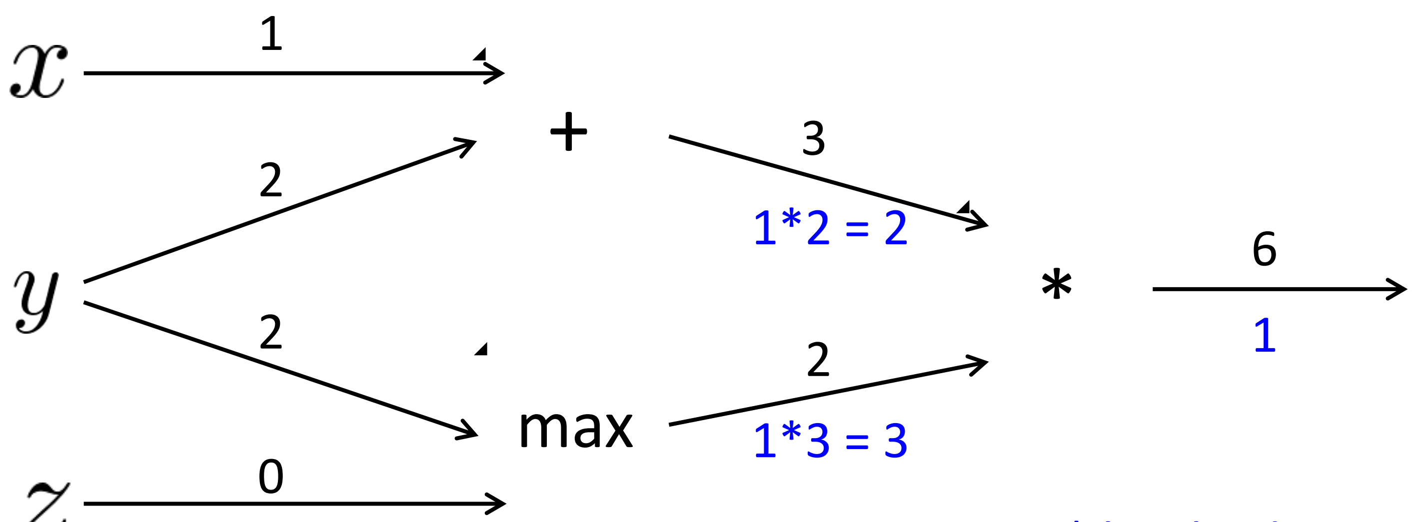

upstream * local = downstream

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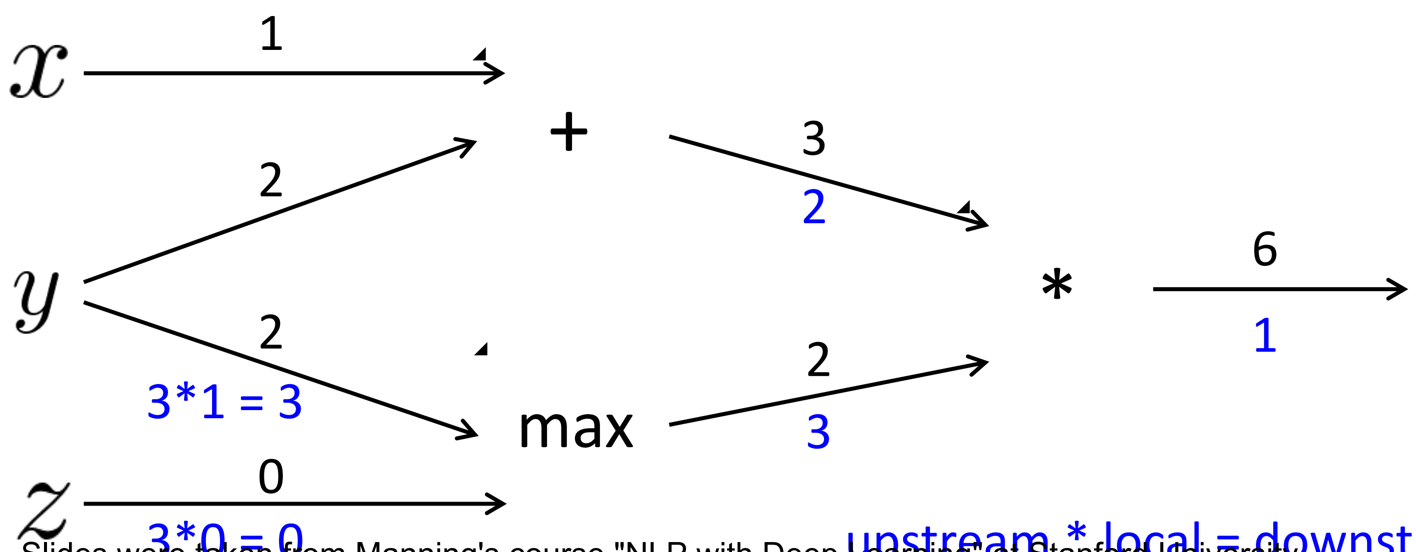

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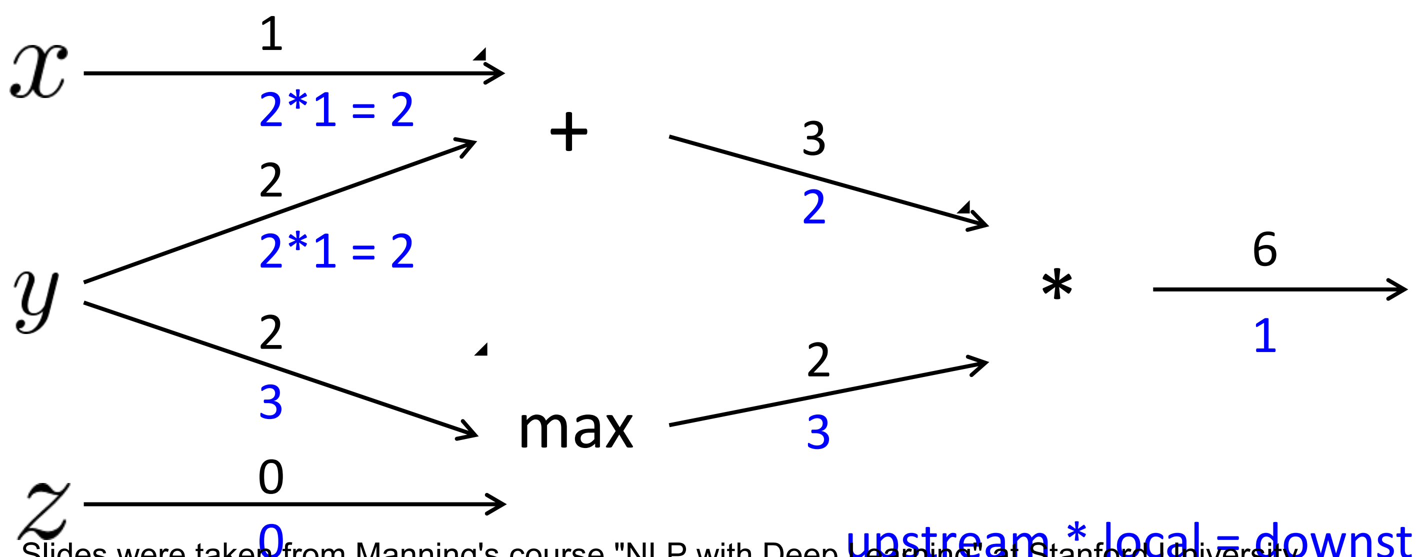

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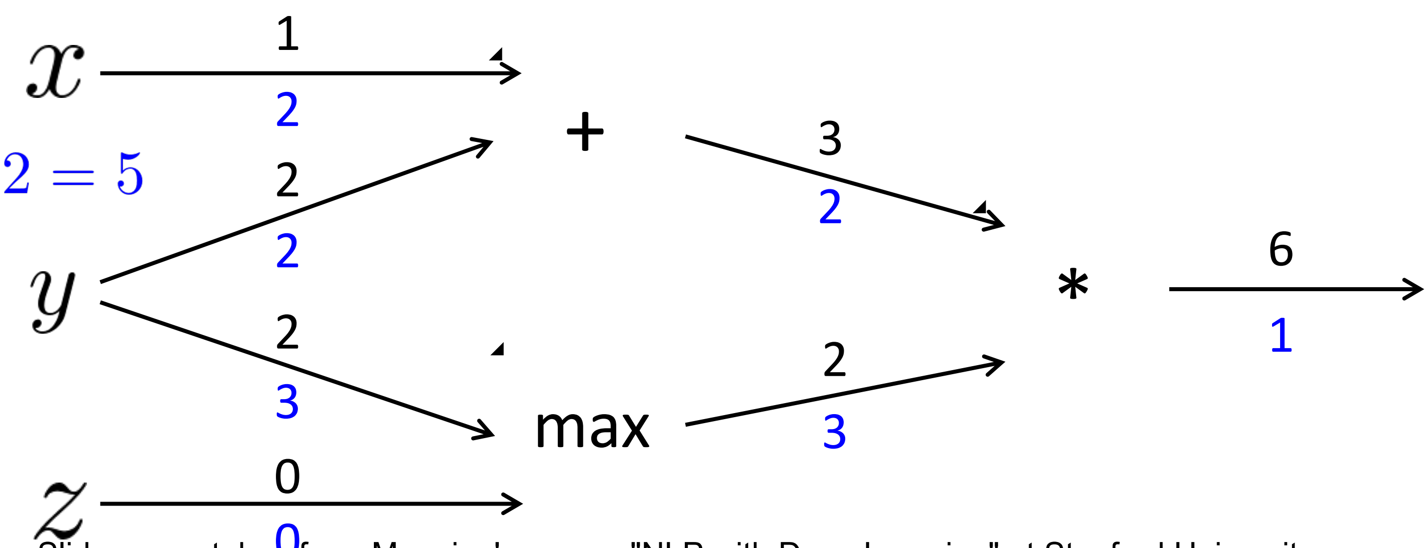
$$\frac{\partial f}{\partial x} = 2$$
$$\frac{\partial f}{\partial y} = 3 + 2 = 5$$
$$\frac{\partial f}{\partial z} = 0$$



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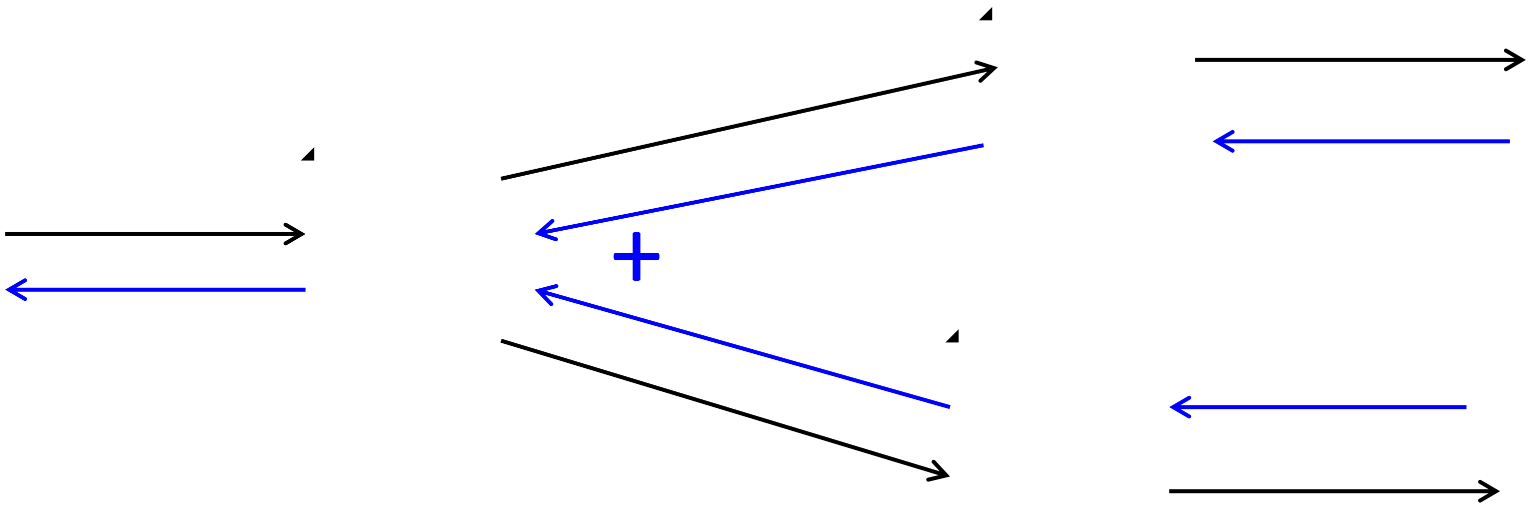
Gradients sum at outward branches



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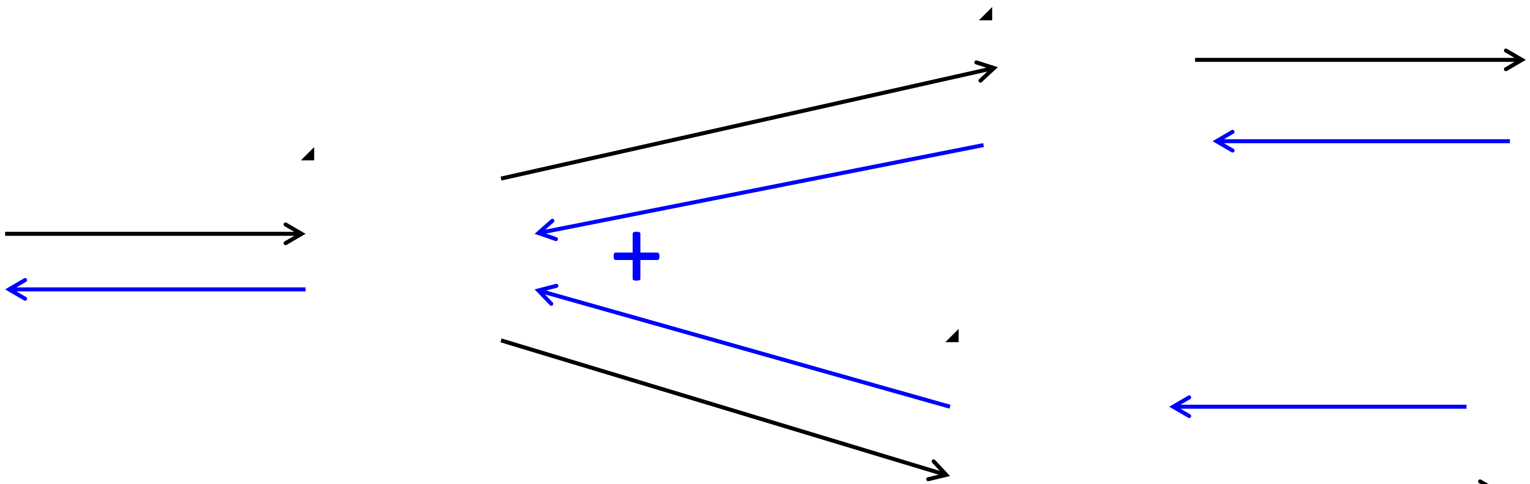
Gradients sum at outward branches



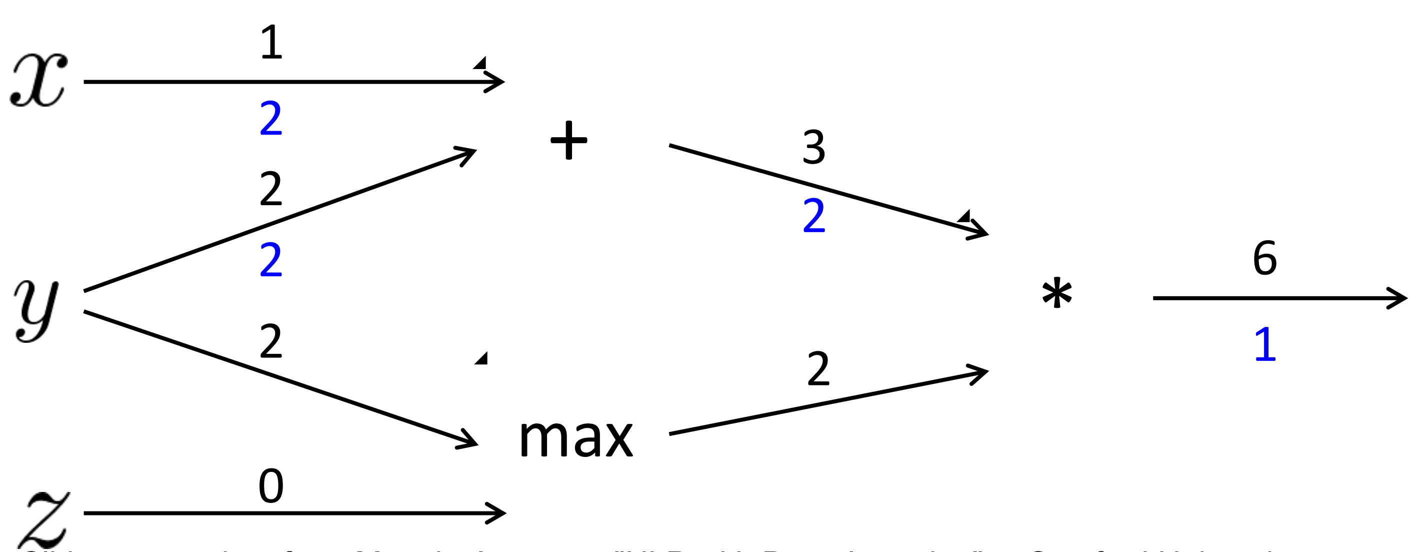
$$a = x + y$$
$$b = \max(y, z)$$
$$f = ab$$

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial a}\frac{\partial a}{\partial y} + \frac{\partial f}{\partial b}\frac{\partial b}{\partial y}$$

Node Intuitions

$$f(x, y, z) = (x + y) \max(y, z)$$
$$x = 1, y = 2, z = 0$$

- \+ “distributes” the upstream gradient to each summand



Node Intuitions

$$f(x, y, z) = (x + y)\max(y, z)$$
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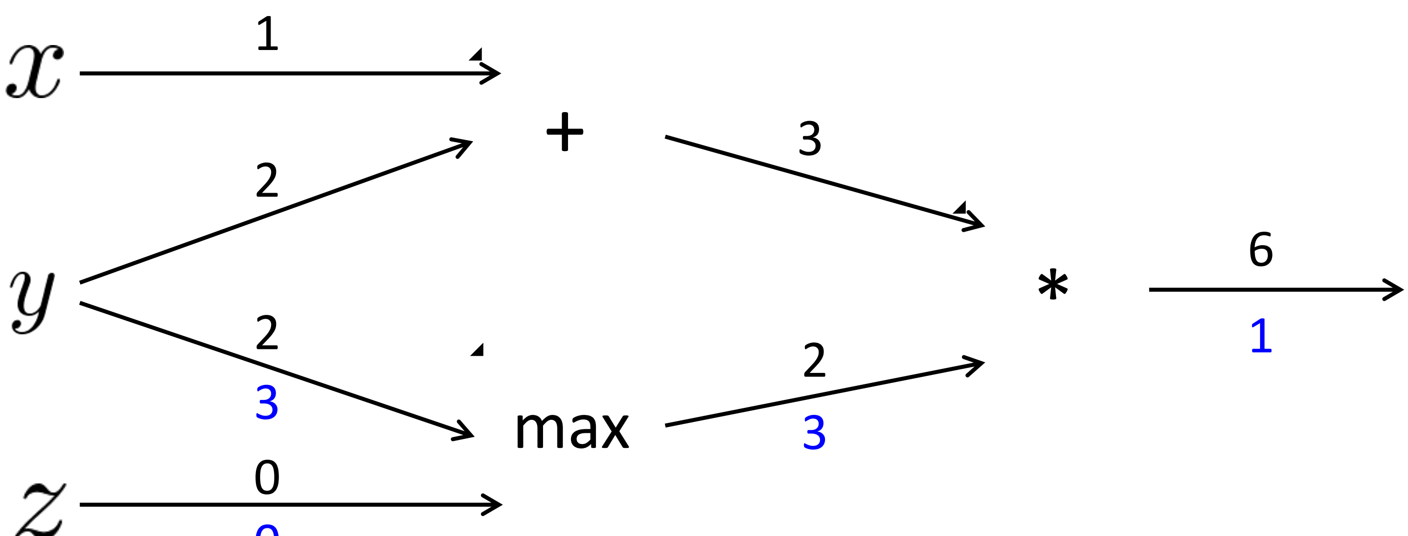
- + “distributes” the upstream gradient to each summand
- max “routes” the upstream gradient



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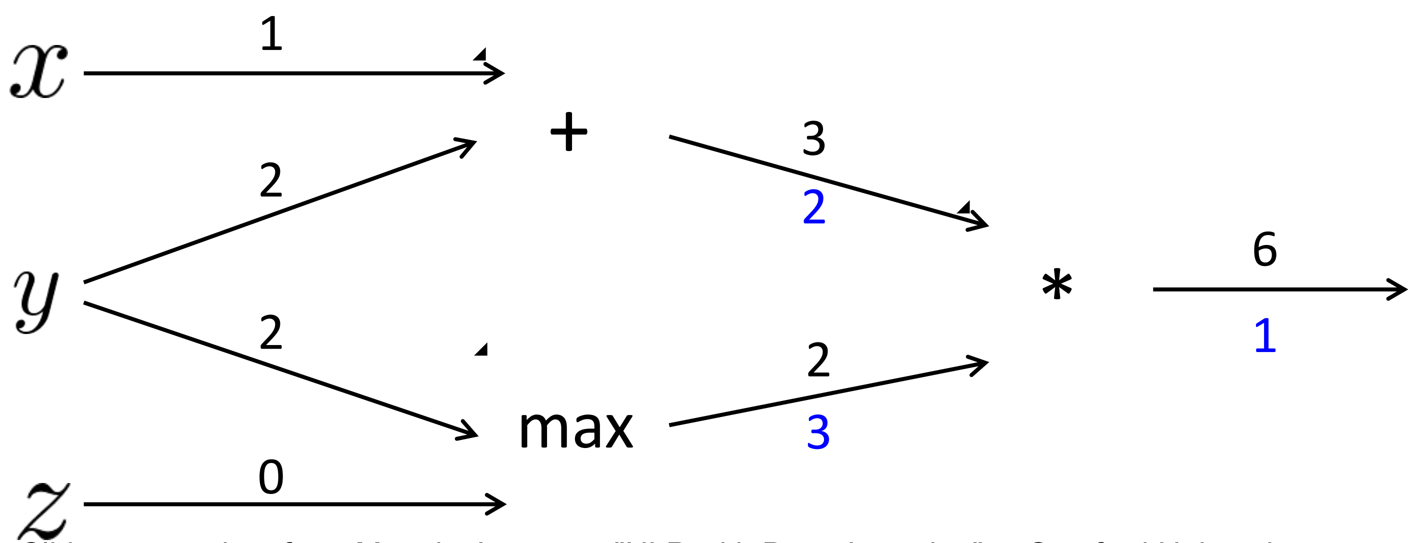
Node Intuitions

$$f(x, y, z) = (x + y)\max(y, z)$$
$$x = 1, y = 2, z = 0$$

- + “distributes” the upstream gradient
- max “routes” the upstream gradient
- * “switches” the upstream gradient



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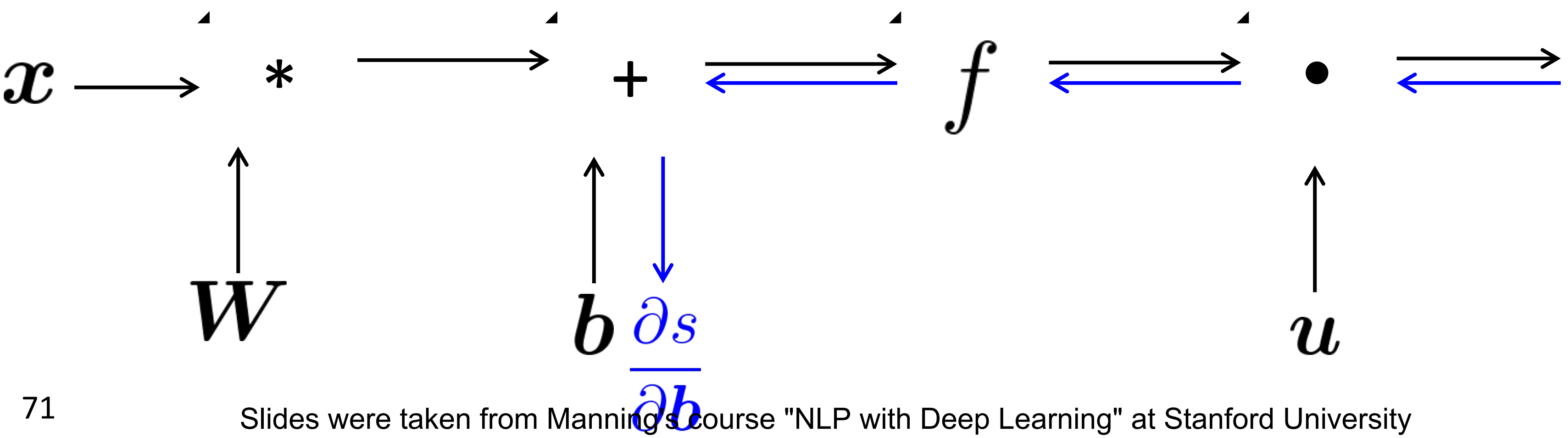
Efficiency: compute all gradients at once

- Incorrect way of doing backprop:
  - First compute $\frac{\partial s}{\partial \boldsymbol{b}}$

$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$



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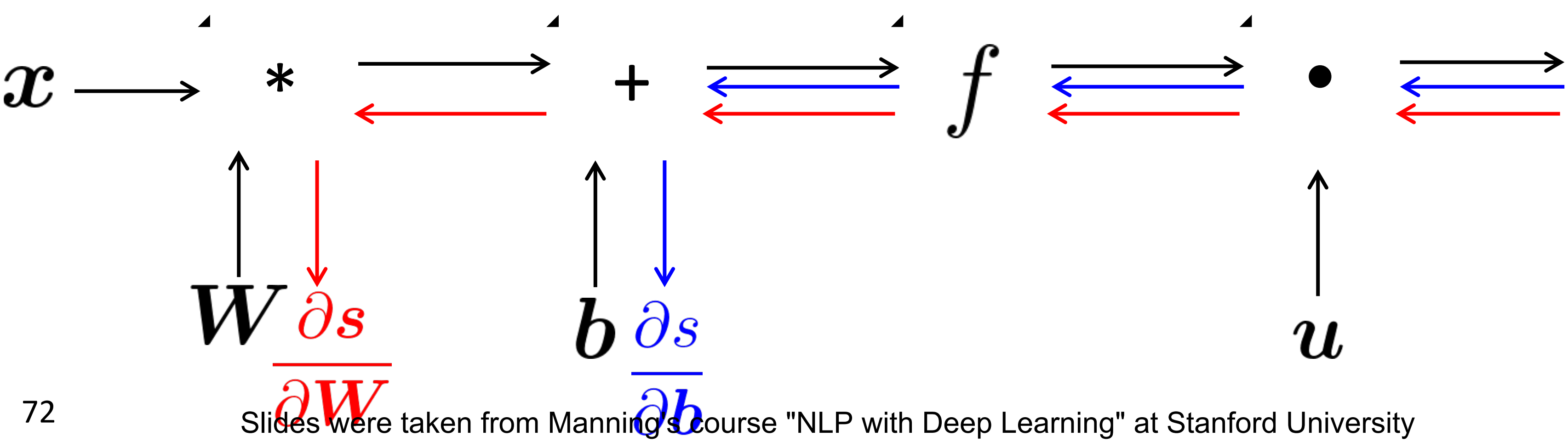
Efficiency: compute all gradients at once

- Incorrect way of doing backprop:
  - First compute $\frac{\partial s}{\partial \boldsymbol{b}}$
  - Then independently compute $\frac{\partial s}{\partial \boldsymbol{W}}$
  - Duplicated computation!

$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$



Efficiency: compute all gradients at once

- Correct way:
  - Compute all the gradients at once
  - Analogous to using $\boldsymbol{\delta}$ when we computed gradients by hand

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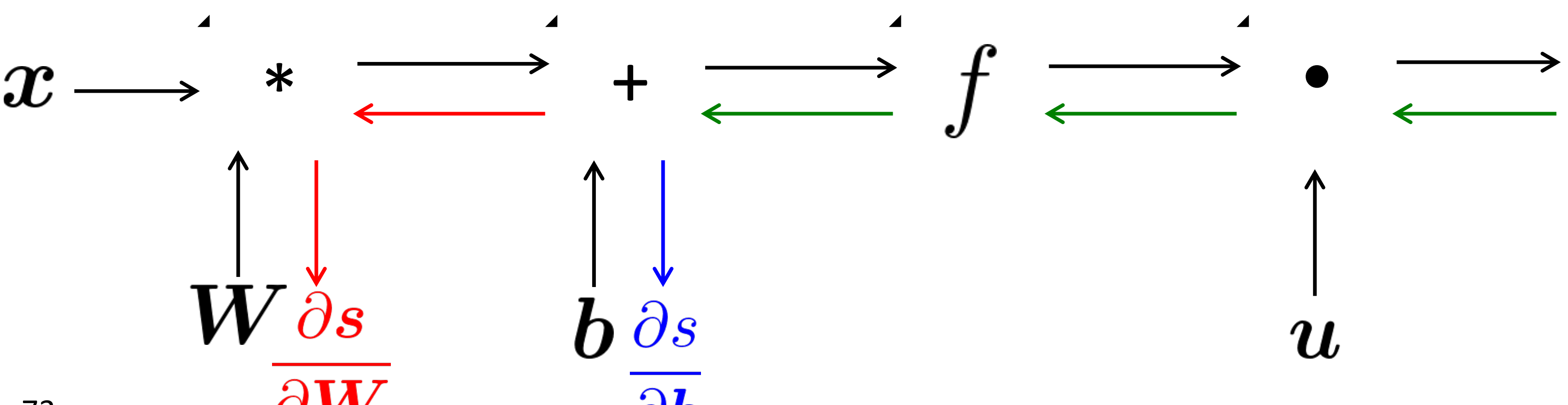
$$\boldsymbol{x} \quad (\text{input})$$



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