Computational Natural Language Processing

Neural Networks: Gradients and Backpropagation

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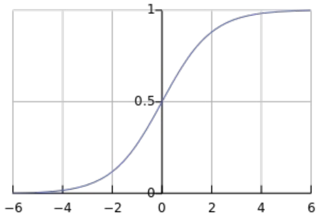
Binary classification for center word being location

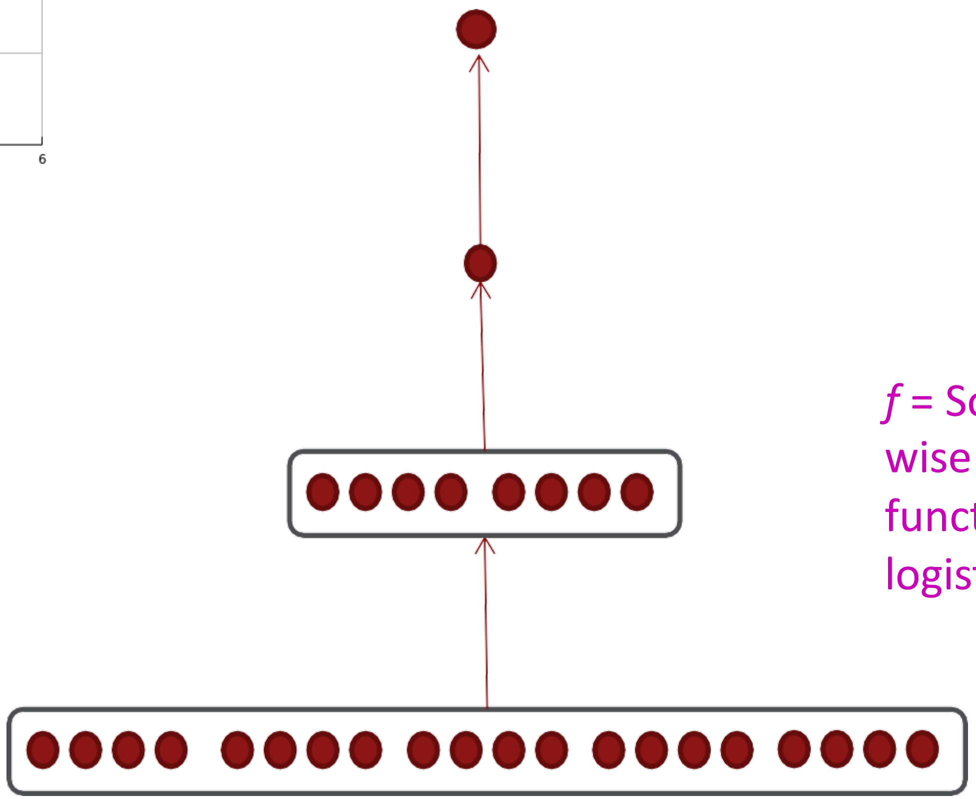
- We do supervised training and want high score if it's a location

$$J_t(\theta) = \sigma(s) = \frac{1}{1 + e^{-s}}$$

predicted model probability of class



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



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

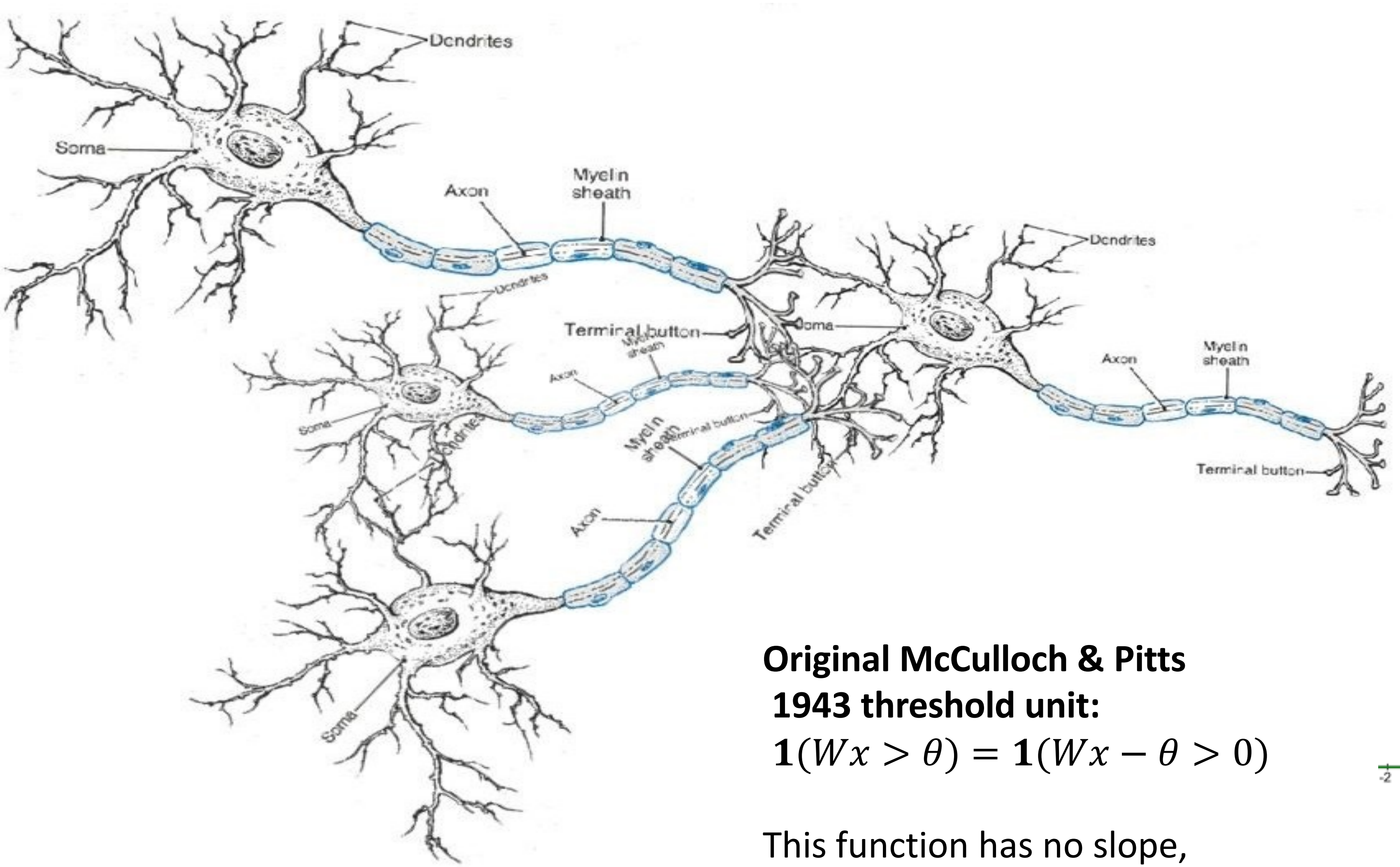
f = Some element-wise non-linear function, e.g., logistic, tanh, ReLU

$$\boldsymbol{x} \quad \text{(input)} \in \mathrm{R}^{5d}$$

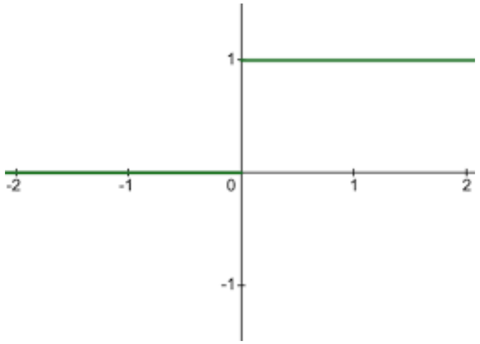
$x = [\ x_{museums} \quad x_{in} \quad x_{Paris} \quad x_{are} \quad x_{amazing}\ ]$

Embedding of 1-hot words

Neural computation



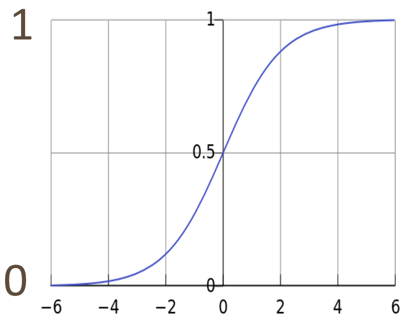
Original McCulloch & Pitts
1943 threshold unit:
$\mathbf{1}(Wx > \theta) = \mathbf{1}(Wx - \theta > 0)$

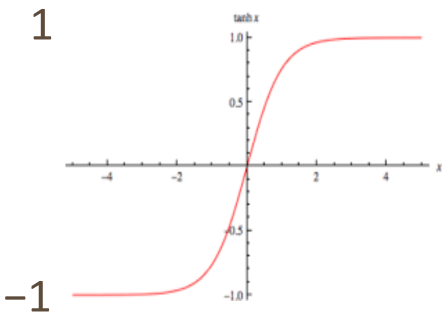


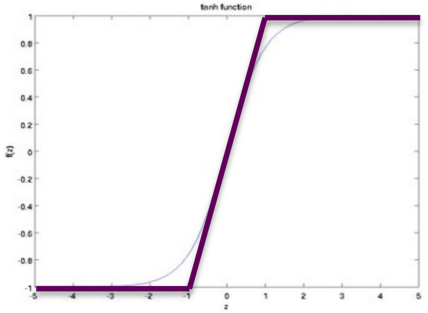
This function has no slope,
so, no gradient-based learning

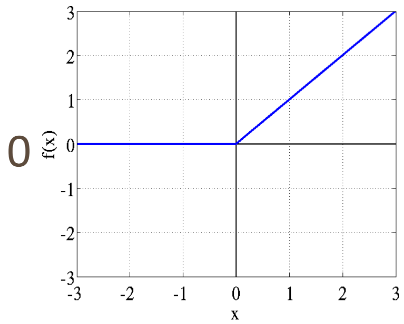
Non-linearities, old and new

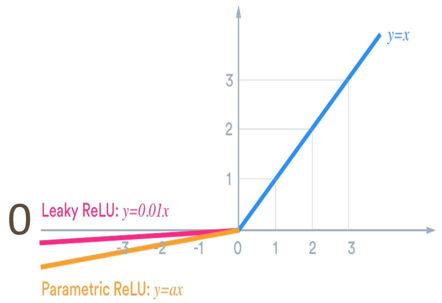
logistic ("sigmoid")	tanh	hard tanh	(Rectified Linear Unit) ReLU	Leaky ReLU / Parametric ReLU
$f(z) = \dfrac{1}{1+\exp(-z)}$	$\tanh(z) = \dfrac{e^z - e^{-z}}{e^z + e^{-z}}$	$\mathrm{HardTanh}(x) = \begin{cases} -1 & \text{if } x < -1 \\ x & \text{if } -1 <= x <= 1 \\ 1 & \text{if } x > 1 \end{cases}$	$\mathrm{ReLU}(z) = \max(z, 0)$	











tanh is just a rescaled and shifted sigmoid (2 × as steep, [−1,1]):

$$\tanh(z) = 2\,\mathrm{logistic}(2z) - 1$$

Logistic and tanh are still used (e.g., logistic to get a probability)

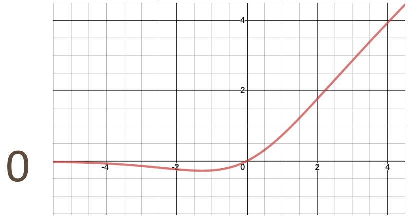
However, now, for deep networks, the first thing to try is ReLU: it trains quickly and performs well due to good gradient backflow.

ReLU has a negative "dead zone" that recent proposals mitigate

GELU is frequently used with Transformers (BERT, RoBERTa, etc.)

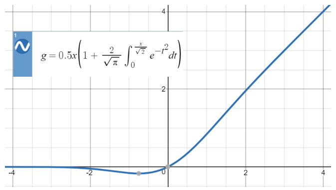
Swish [arXiv:1710.05941](https://arxiv.org/abs/1710.05941)

$\mathrm{swish}(x) = x \,.\, \mathrm{logistic}(x)$



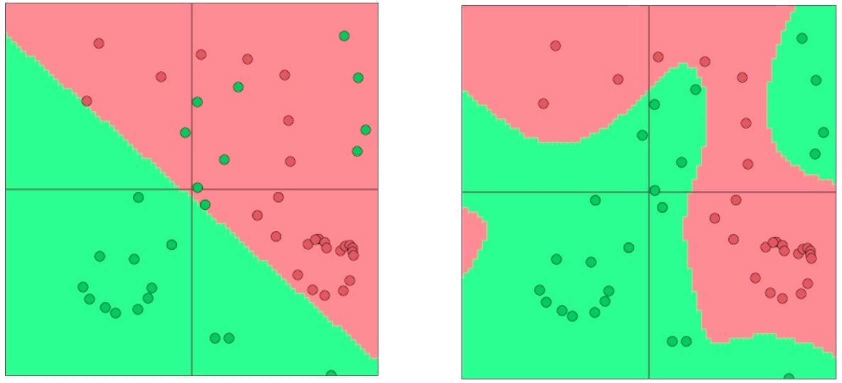
GELU [arXiv:1606.08415](https://arxiv.org/abs/1606.08415)

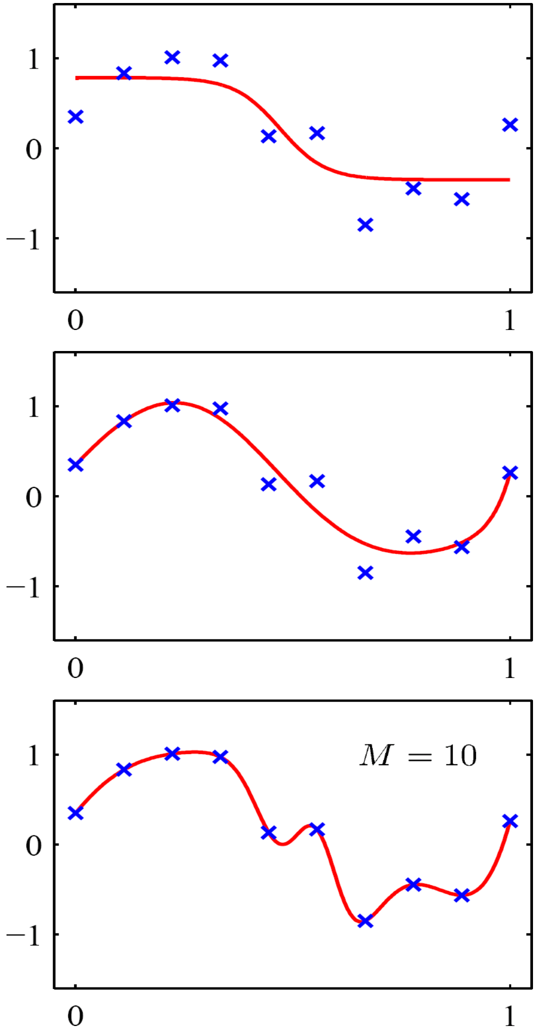
$\mathrm{GELU}(x)$
$= x \,.\, P(X \le x), X \sim N(0,1)$
$\approx x \,.\, \mathrm{logistic}(1.702x)$



Non-linearities (i.e., “*f*” on previous slide): Why they’re needed

- Neural networks do function approximation, e.g., regression or classification
  - Without non-linearities, deep neural networks can’t do anything more than a linear transform
  - Extra layers could just be compiled down into a single linear transform: $W_1 W_2 x = Wx$
  - But, with more layers that include non-linearities, they can approximate any complex function!





Training with "cross entropy loss" – you use this in PyTorch!

- Until now, our objective was stated as to maximize the probability of the correct class *y* or equivalently we can minimize the negative log probability of that class
- Now restated in terms of cross entropy, a concept from information theory
- Let the true probability distribution be *p; l*et our computed model probability be *q*
- The cross entropy is:

$$H(p,q) = -\sum_{c=1}^{C} p(c) \log q(c)$$

- Assuming a ground truth (or true or gold or target) probability distribution that is 1 at the right class and 0 everywhere else, *p* = [0, …, 0, 1, 0, …, 0], then:
- **Because of one-hot *p*, the only term left is the negative log probability of the true class y_i:** $-\log p(y_i|x_i)$

Cross entropy can be used in other ways with a more interesting *p,* but for now just know that you'll want to use it as the loss in PyTorch

Remember: Stochastic Gradient Descent

Update equation:

$$\theta^{new} = \theta^{old} - \alpha \nabla_{\theta} J(\theta)$$

α = *step size or learning rate*

i.e., for each parameter: $\theta_j^{new} = \theta_j^{old} - \alpha \frac{\partial J(\theta)}{\partial \theta_j^{old}}$

In deep learning, θ includes the data representation (e.g., word vectors) too!

How can we compute $\nabla_{\theta} J(\theta)$?

1. By hand
2. Algorithmically: the backpropagation algorithm

Lecture Plan

Gradients

1. Introduction
2. Matrix calculus
3. Backpropagation

Computing Gradients by Hand

- **Matrix calculus:** Fully vectorized gradients
  - “Multivariable calculus is just like single-variable calculus if you use matrices”
  - Much faster and more useful than non-vectorized gradients
  - But doing a non-vectorized gradient can be good for intuition; recall the first lecture for an example

Gradients

- Given a function with 1 output and 1 input

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

- It's gradient (slope) is its derivative

  $$\frac{d\,\mathrm{f}}{dx} = 3x^2$$

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

  At *x* = 1 it changes about 3 times as much: $1.01^3 = 1.03$

  At x = 4 it changes about 48 times as much: $4.01^3 = 64.48$

Gradients

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

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

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

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

Jacobian Matrix: Generalization of the Gradient

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

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

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

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

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

Chain Rule

- For composition of 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 functions: **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

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

$$h_i = f(z_i)$$

Example Jacobian: Elementwise activation Function

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

$$h_i = f(z_i)$$

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

Example Jacobian: Elementwise activation Function

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$$h_i = f(z_i)$$

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

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definition of Jacobian

$$= \begin{cases} f'(z_i) & \text{if } i = j \\ 0 & \text{if otherwise} \end{cases}$$

regular 1-variable derivative

Example Jacobian: Elementwise activation Function

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

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

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

Other Jacobians

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

Other Jacobians

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

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

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

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

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

Other Jacobians

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

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

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

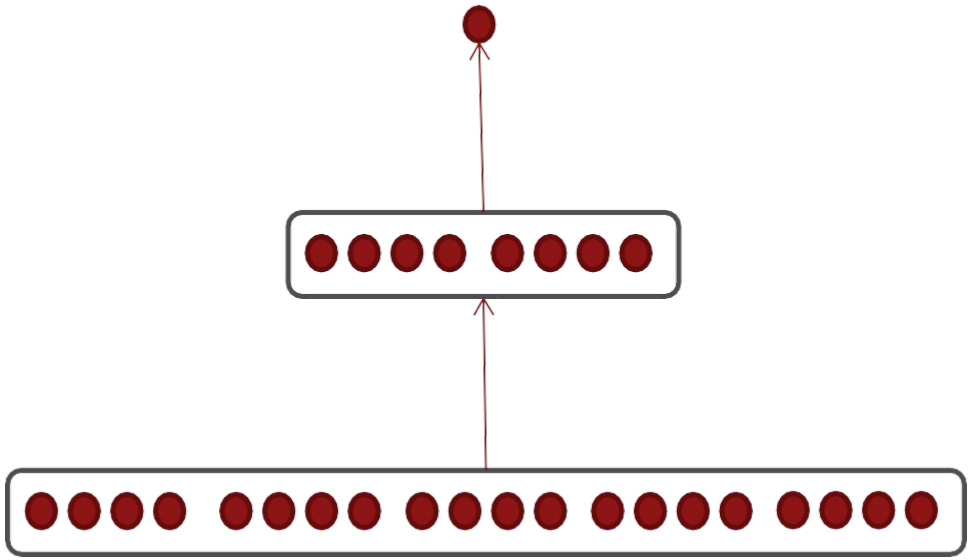
- Compute these at home for practice!

Back to our Neural Net!

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

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

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



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

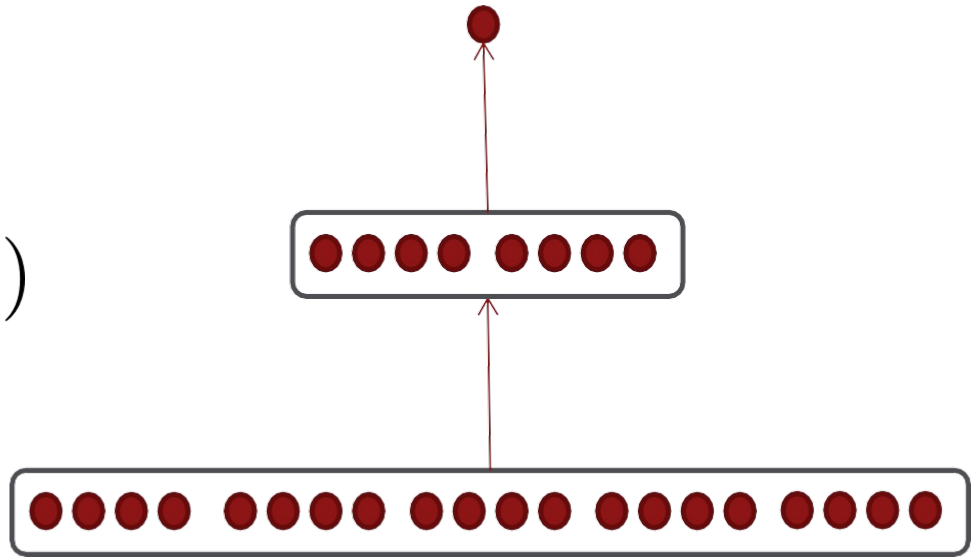
Back to our Neural Net!

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

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

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

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



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

1. Break up equations into simple pieces

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

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

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

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

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

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

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

Carefully define your variables and keep track of their dimensionality!

2. Apply the chain rule

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

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

2. Apply the chain rule

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

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

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

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

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

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

3. Write out the Jacobians

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

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

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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$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$

$$\frac{\partial s}{\partial \boldsymbol{b}} = \underset{\displaystyle \downarrow \atop \displaystyle \boldsymbol{u}^T}{\frac{\partial s}{\partial \boldsymbol{h}}} \quad \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \quad \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

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

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

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$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$
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$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \quad \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \quad \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$
$$= \boldsymbol{u}^T \operatorname{diag}(f'(\boldsymbol{z}))\boldsymbol{I}$$
$$= \boldsymbol{u}^T \circ f'(\boldsymbol{z})$$

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

$\odot$ = Hadamard product = element-wise multiplication of 2 vectors to give vector

Re-using Computation

- Suppose we now want to compute $\dfrac{\partial s}{\partial \boldsymbol{W}}$
  - 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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$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

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 the upstream gradient ("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 then do $\theta^{new} = \theta^{old} - \alpha \nabla_\theta J(\theta)$

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  - Inconvenient to then do $\theta^{new} = \theta^{old} - \alpha \nabla_\theta J(\theta)$

- Instead, we leave pure math and use the **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

- What is $\dfrac{\partial s}{\partial \boldsymbol{W}} = \boldsymbol{\delta} \dfrac{\partial \boldsymbol{z}}{\partial \boldsymbol{W}}$
  - $\boldsymbol{\delta}$ 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 upstream gradient (“error signal”) at z
x is local input signal

Why the Transposes?

$$\underset{[n \times m]}{\frac{\partial s}{\partial \boldsymbol{W}}} = \underset{[n \times 1]}{\boldsymbol{\delta}^T} \underset{[1 \times m]}{\boldsymbol{x}^T}$$

$$= \begin{bmatrix} \delta_1 \\ \vdots \\ \delta_n \end{bmatrix} [x_1, ..., x_m] = \begin{bmatrix} \delta_1 x_1 & \dots & \delta_1 x_m \\ \vdots & \ddots & \vdots \\ \delta_n x_1 & \dots & \delta_n x_m \end{bmatrix}$$

- Hacky answer: this makes the dimensions work out!
  - Useful trick for checking your work!
- Full explanation in the Goodflow book
  - Each input goes to each output – you want to get outer product

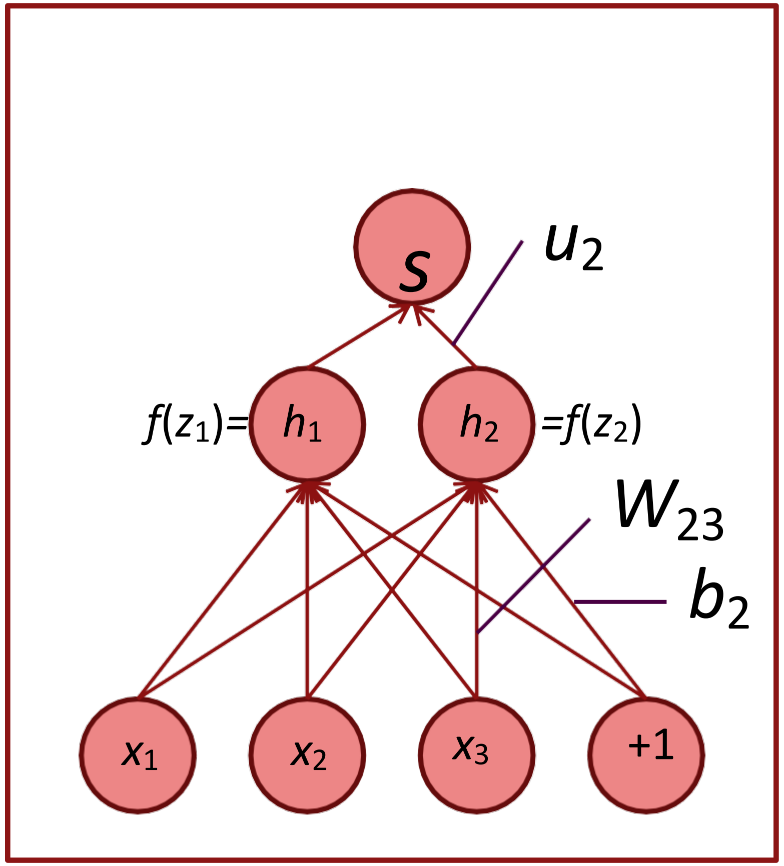
Deriving local input gradient in backprop

- For $\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{W}}$ in our equation:

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

- Let's consider the derivative of a single weight W_{ij}
- W_{ij} only contributes to z_i
  - For example: W_{23} is only used to compute z_2 not z_1

$$\frac{\partial z_i}{\partial W_{ij}} = \frac{\partial}{\partial W_{ij}} \boldsymbol{W}_{i\cdot}\boldsymbol{x} + b_i$$
$$= \frac{\partial}{\partial W_{ij}} \sum_{k=1}^{d} W_{ik} x_k = x_j$$



3. Backpropagation

We’ve almost shown you backpropagation

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

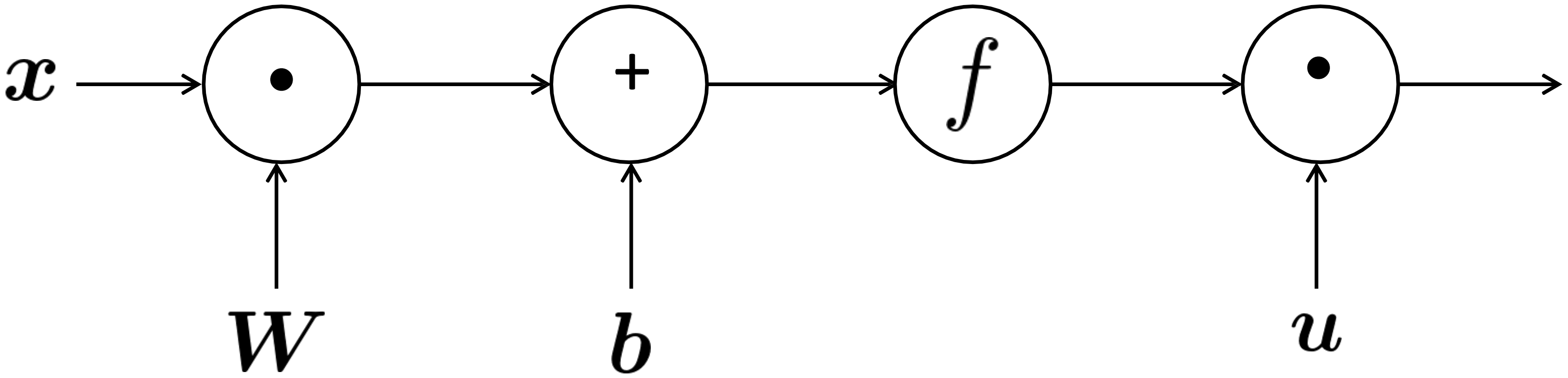
Other trick:

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

Computation Graphs and Backpropagation

- Software represents 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

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

$$s = \boldsymbol{u}^T \boldsymbol{h}$$
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$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
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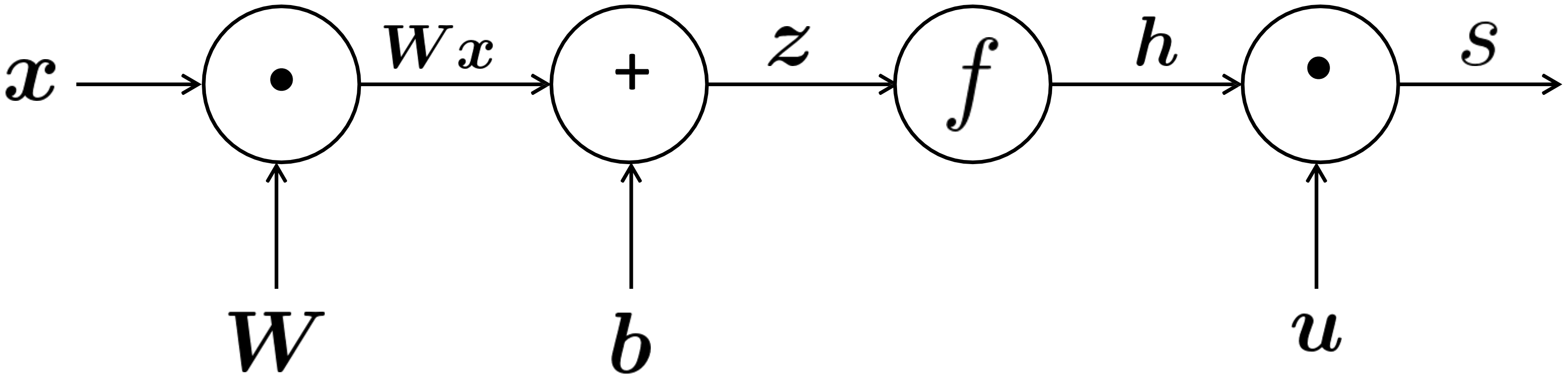


Computation Graphs and Backpropagation

- Software represents our neural net equations as a graph

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

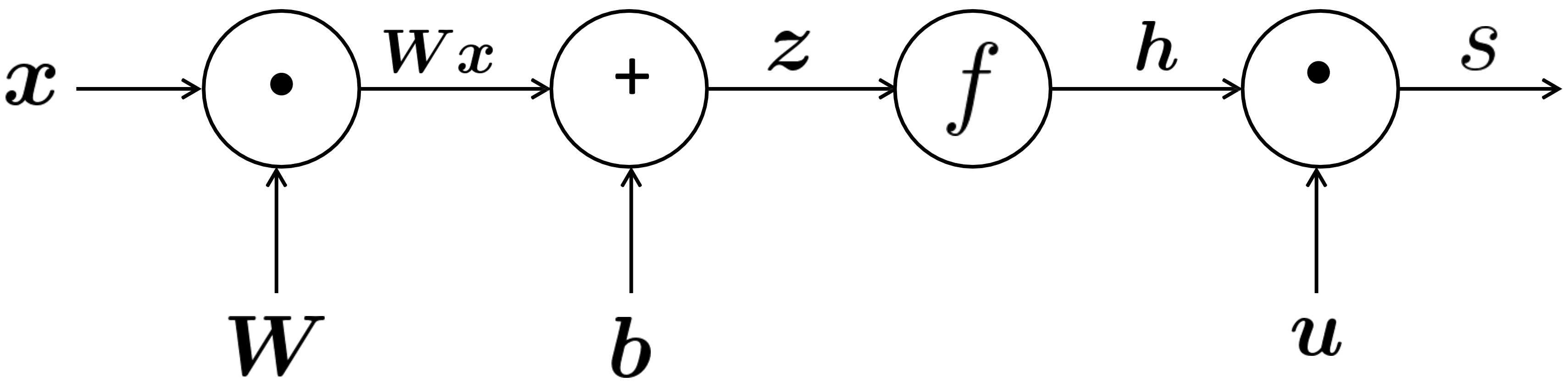
$$\boldsymbol{h} = f(\boldsymbol{z})$$

$$\ldots x + \boldsymbol{b}$$

…ut)

"Forward Propagation"

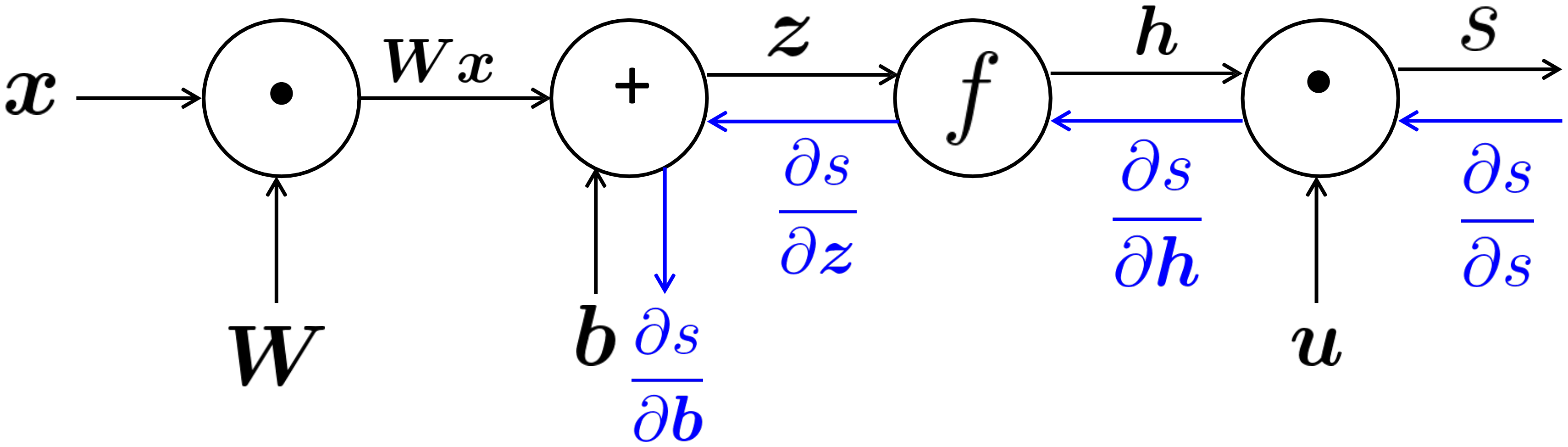
operation



Backpropagation

- Then go backwards along edges
  - Pass along **gradients**

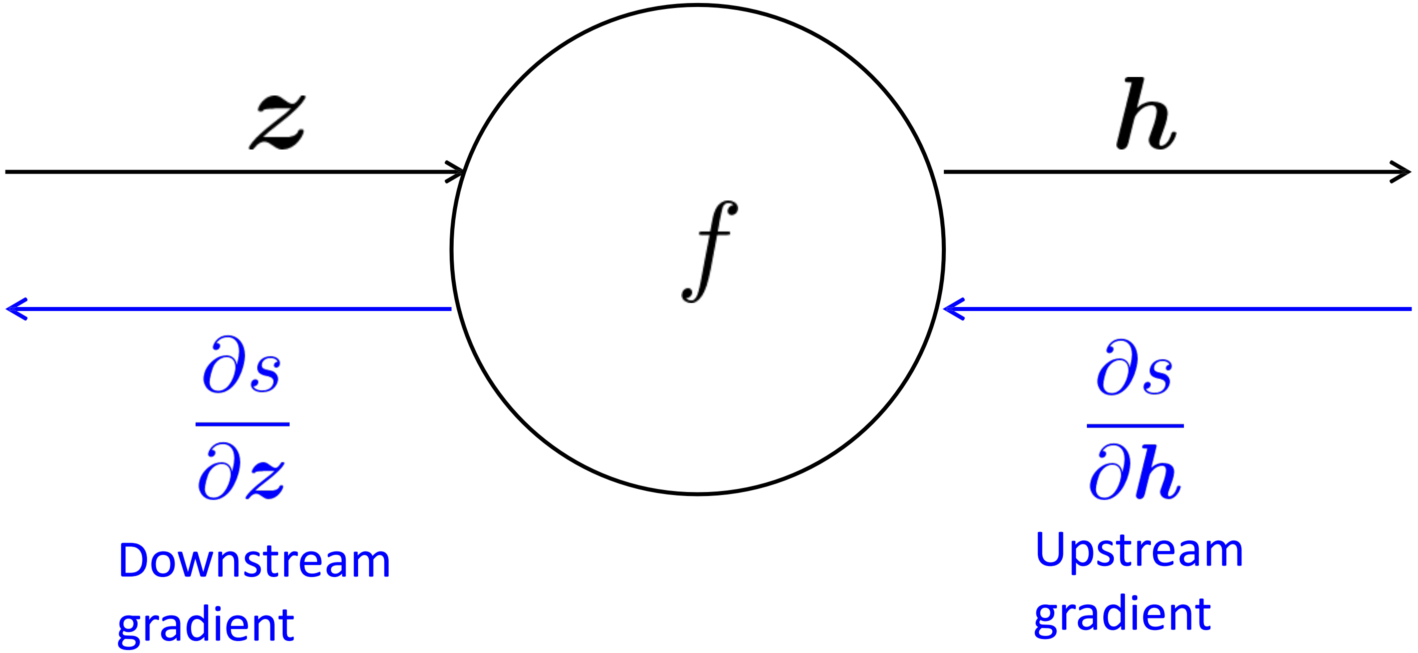
$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$



Backpropagation: Single Node

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

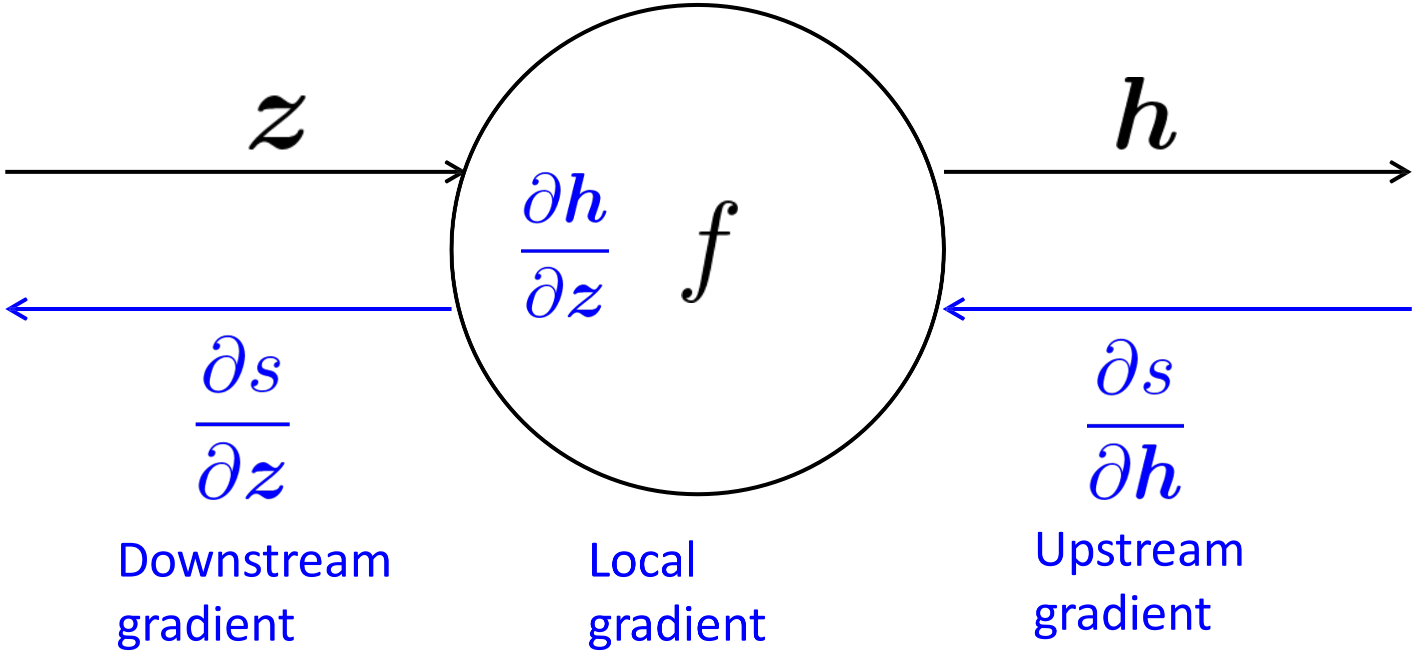
$$\boxed{\boldsymbol{h} = f(\boldsymbol{z})}$$



Backpropagation: Single Node

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

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



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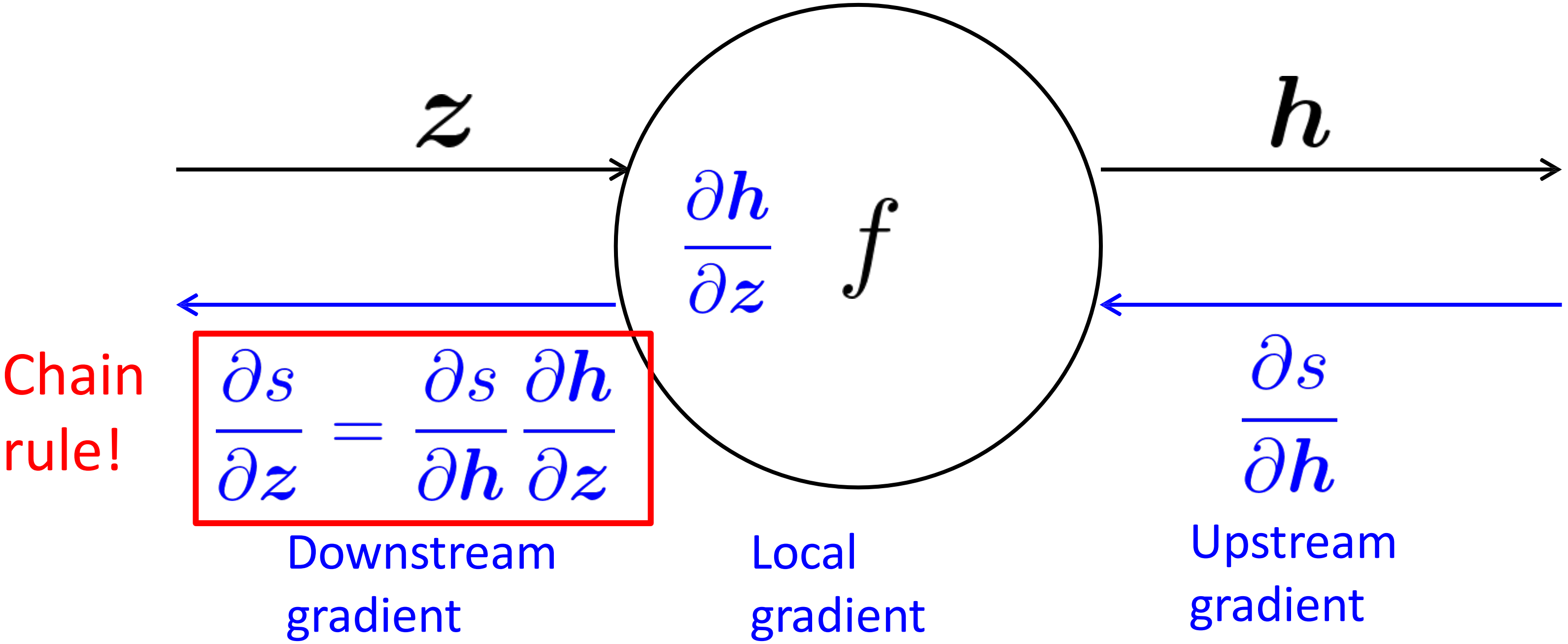
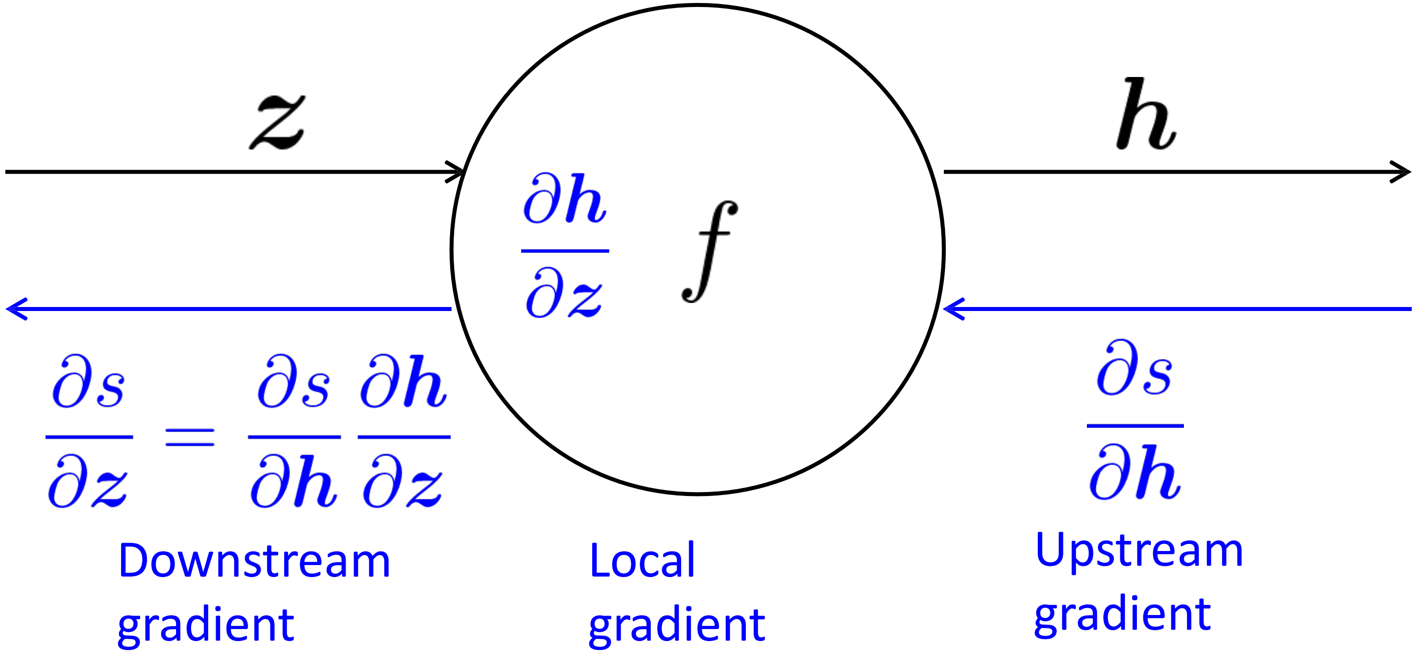


Backpropagation: Single Node

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

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

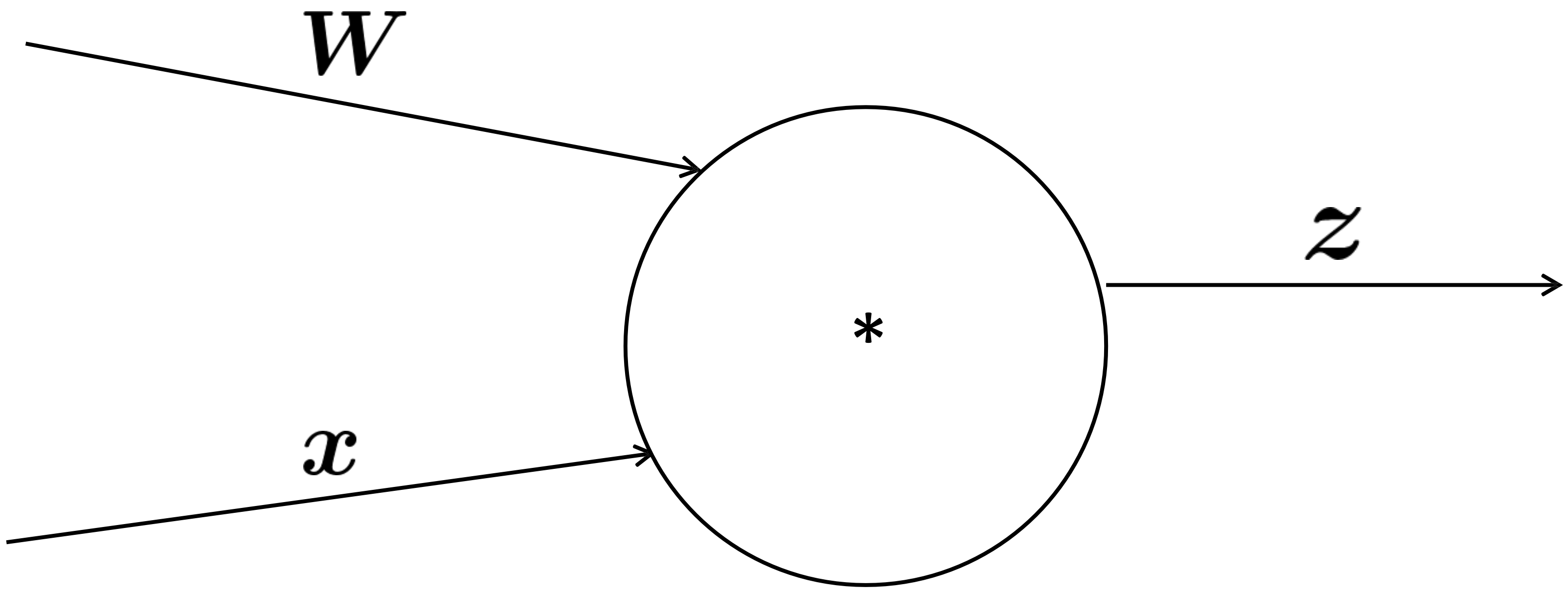
- [downstream gradient] = [upstream gradient] x [local gradient]



Backpropagation: Single Node

- What about nodes with multiple inputs?

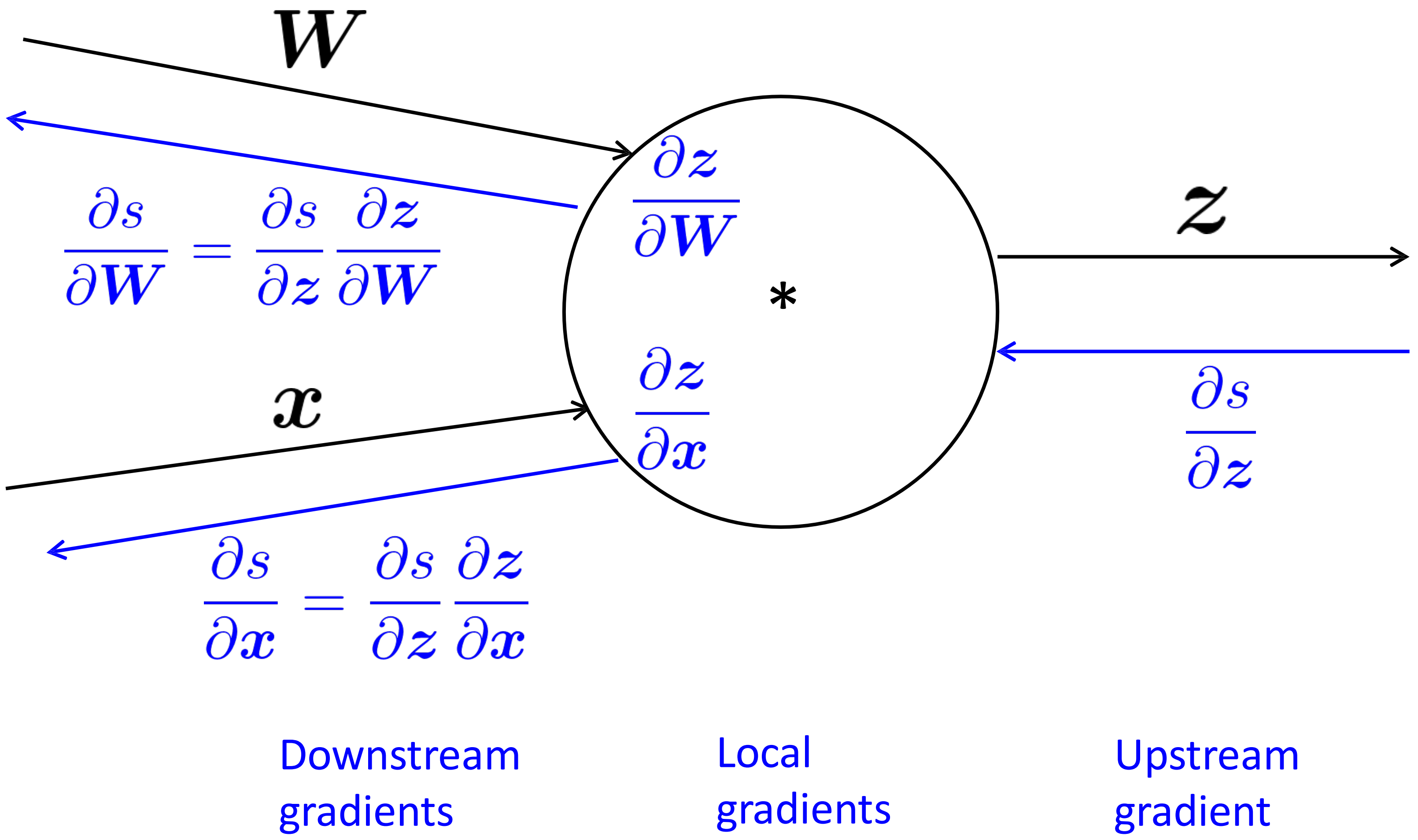
$$\boxed{z = \boldsymbol{W}\boldsymbol{x}}$$



Backpropagation: Single Node

- Multiple inputs → multiple local gradients

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



An Example

$$\boxed{\begin{aligned}&f(x,y,z) = (x+y)\max(y,z)\\&x=1, y=2, z=0\end{aligned}}$$

An Example

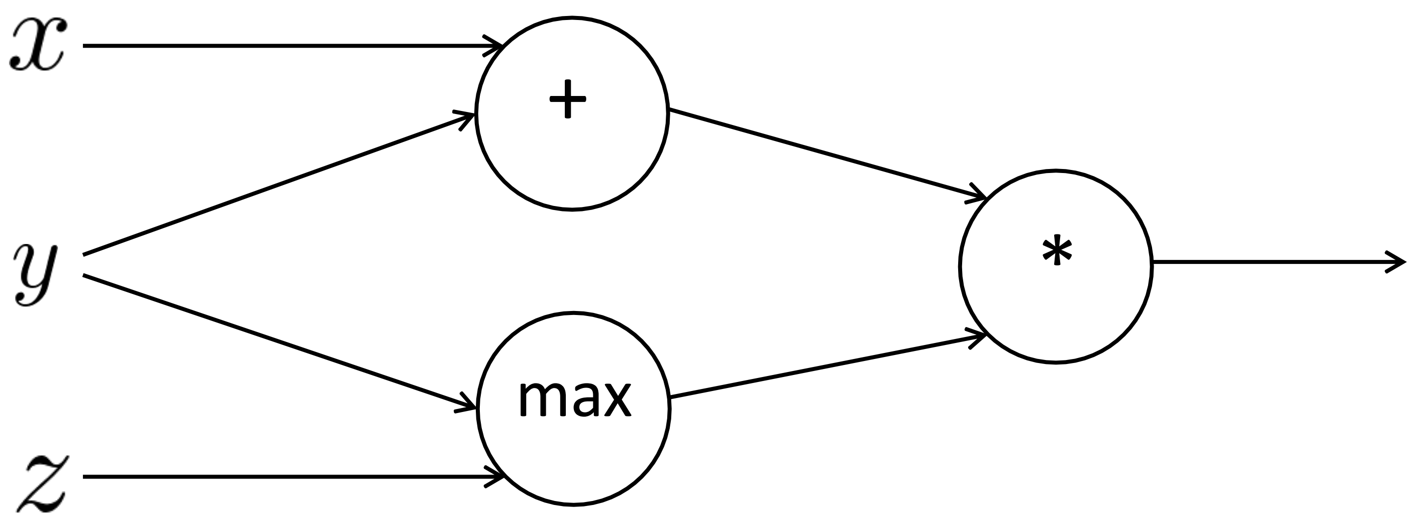
$$f(x, y, z) = (x + y)\max(y, z)$$
$$x = 1, y = 2, z = 0$$

Forward prop steps

$$a = x + y$$

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

$$f = ab$$



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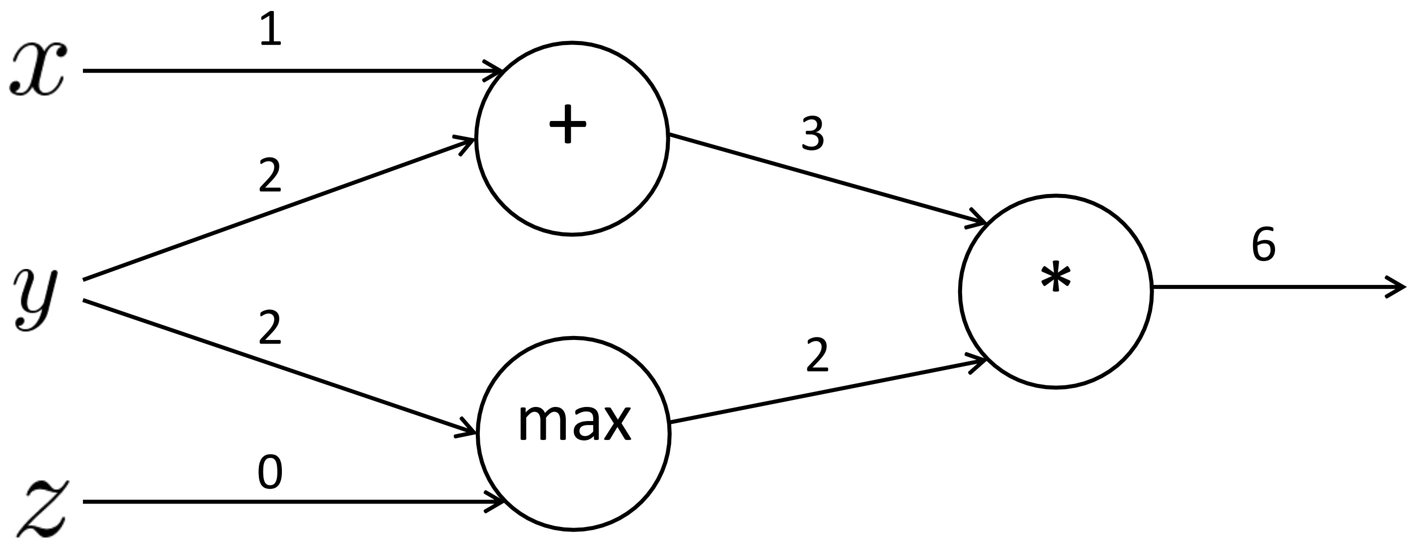

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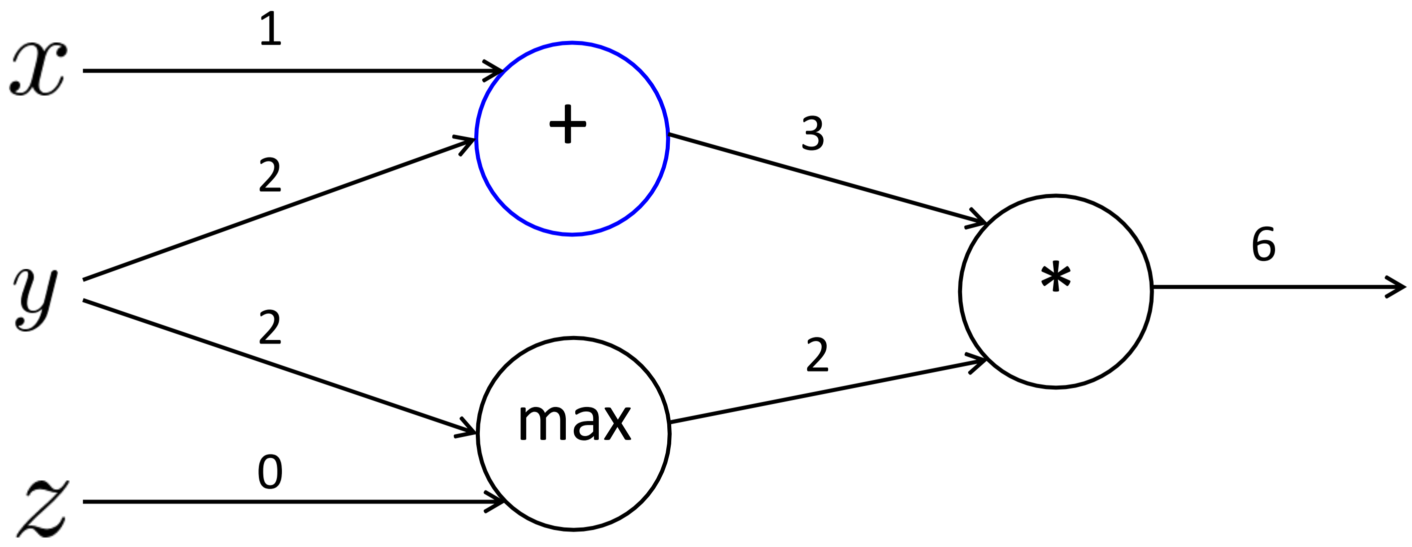

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$$\frac{\partial a}{\partial x} = 1 \quad \frac{\partial a}{\partial y} = 1$$
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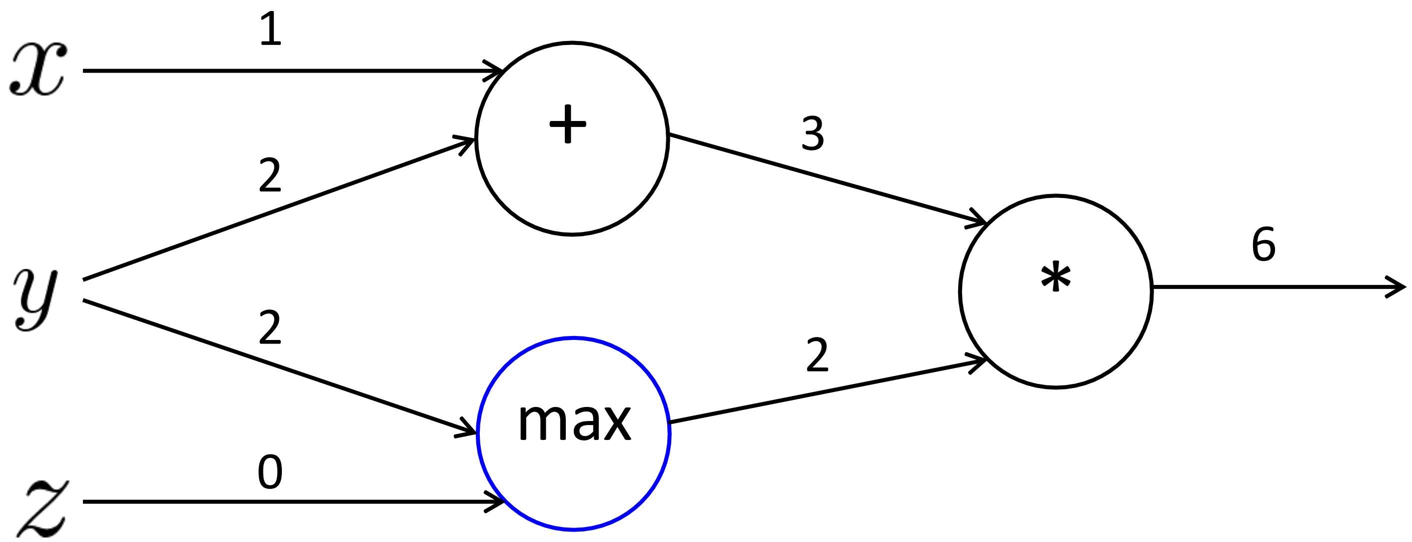

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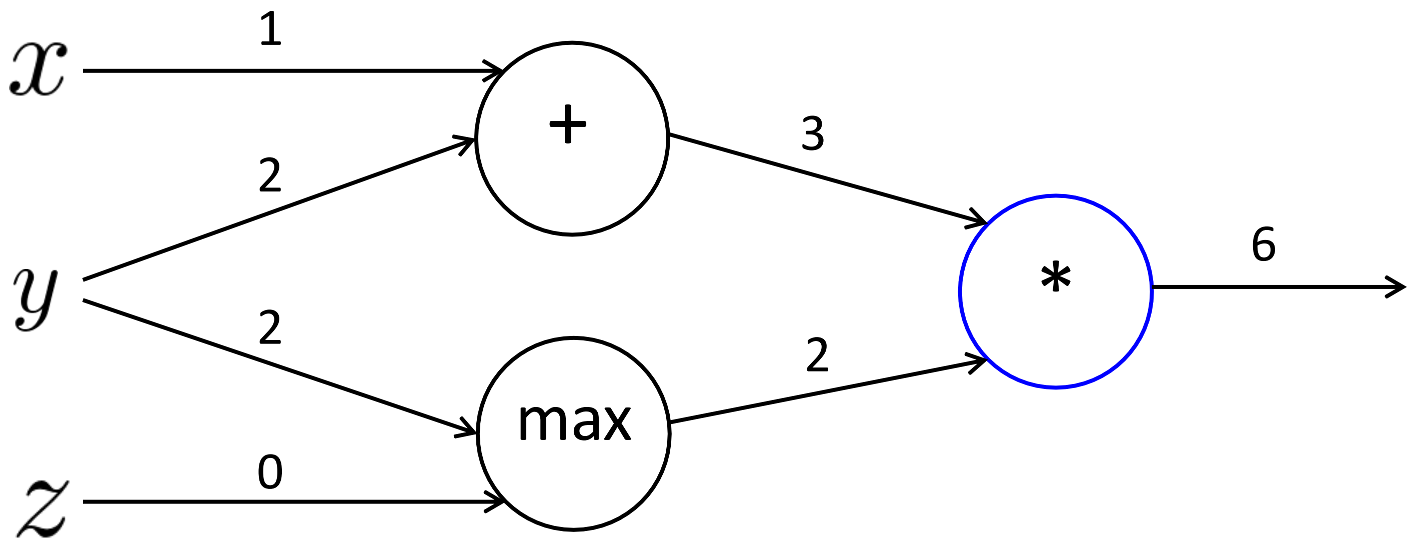

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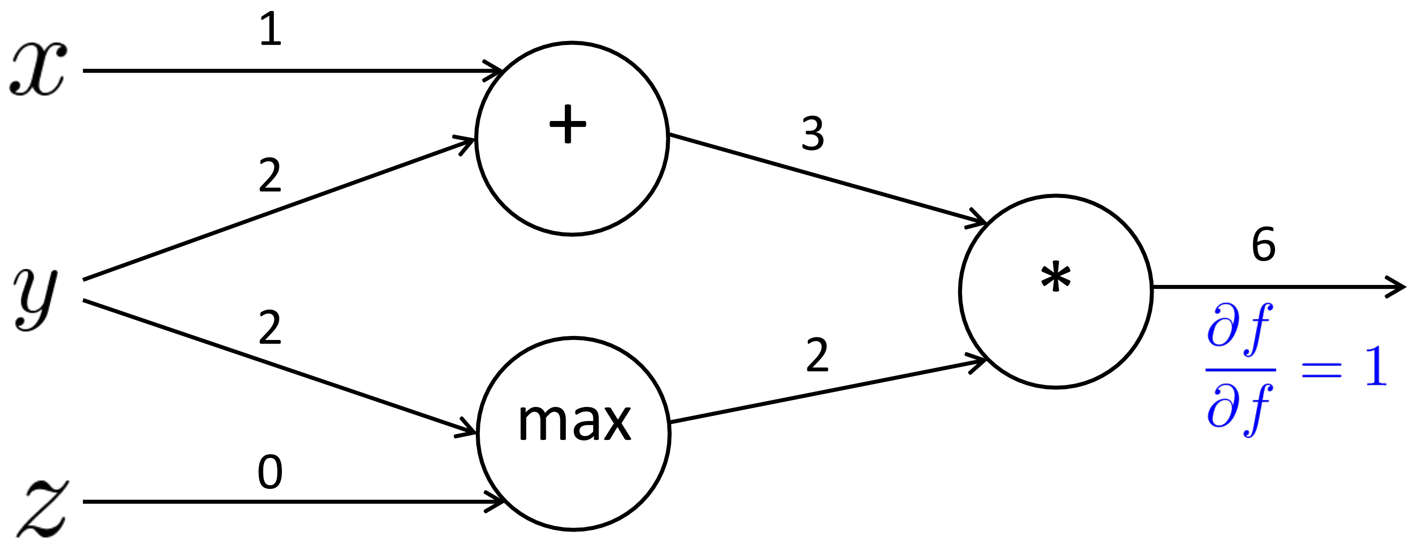

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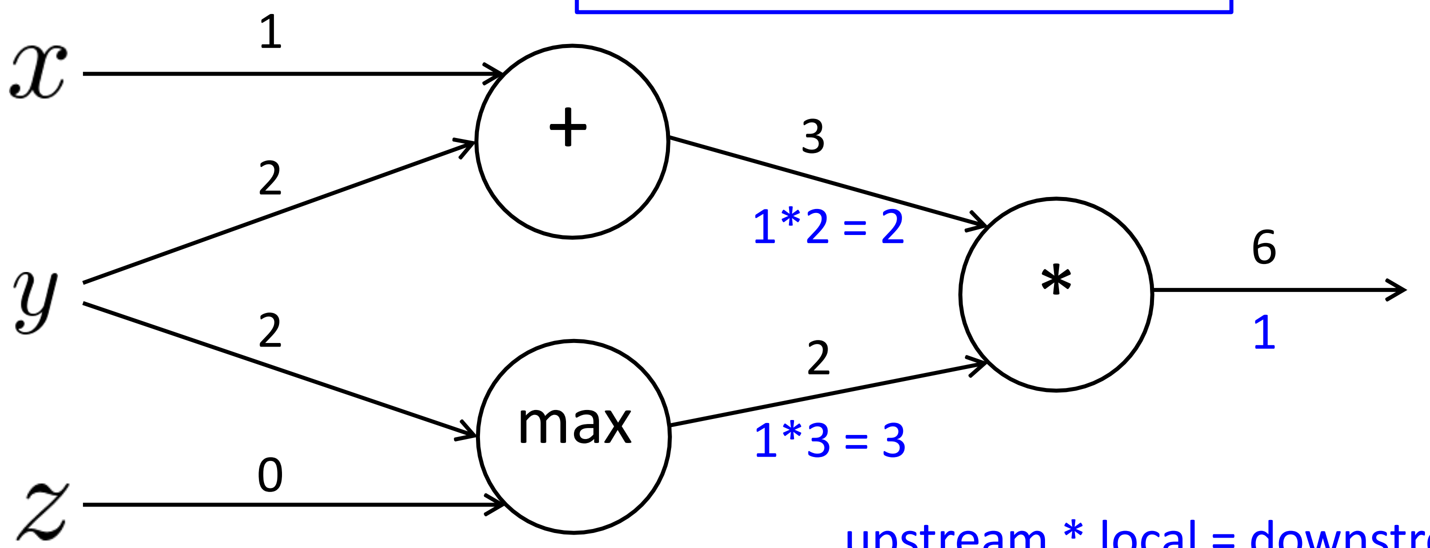

upstream * local = downstream

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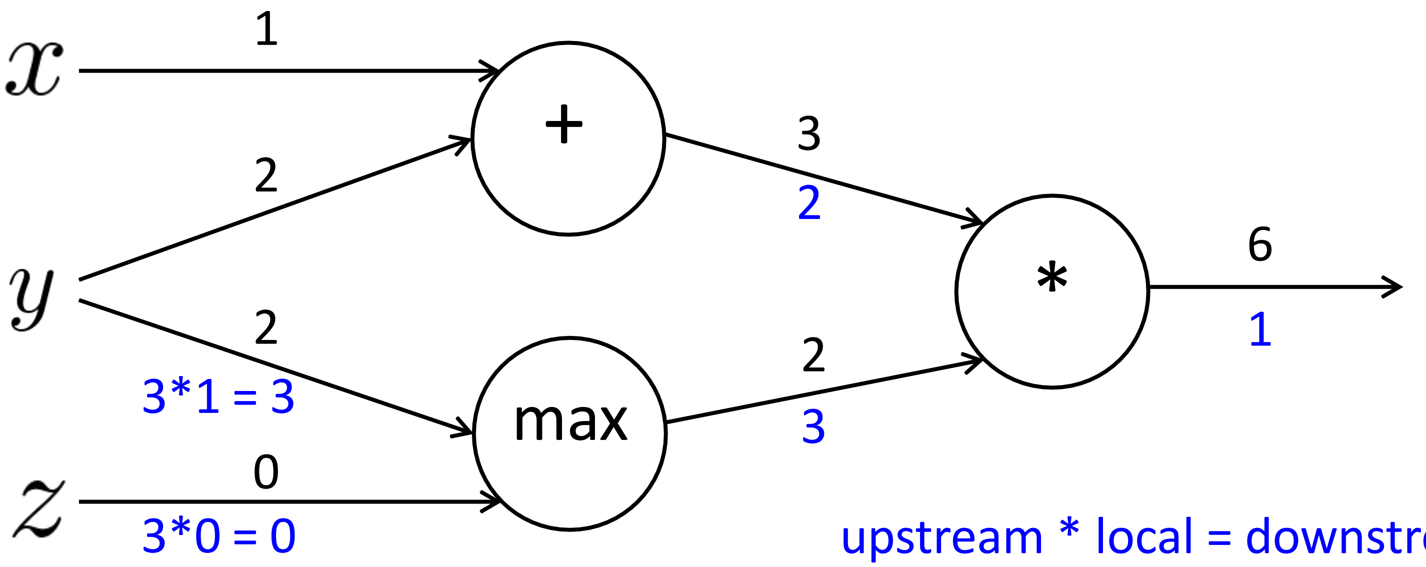

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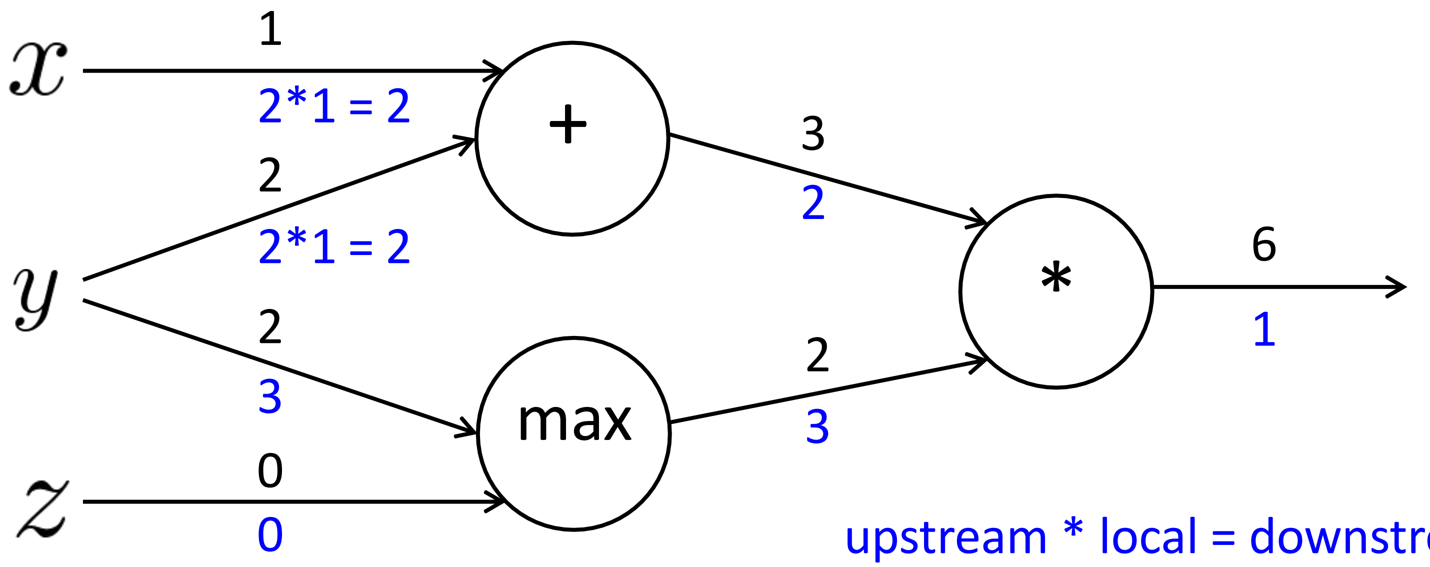

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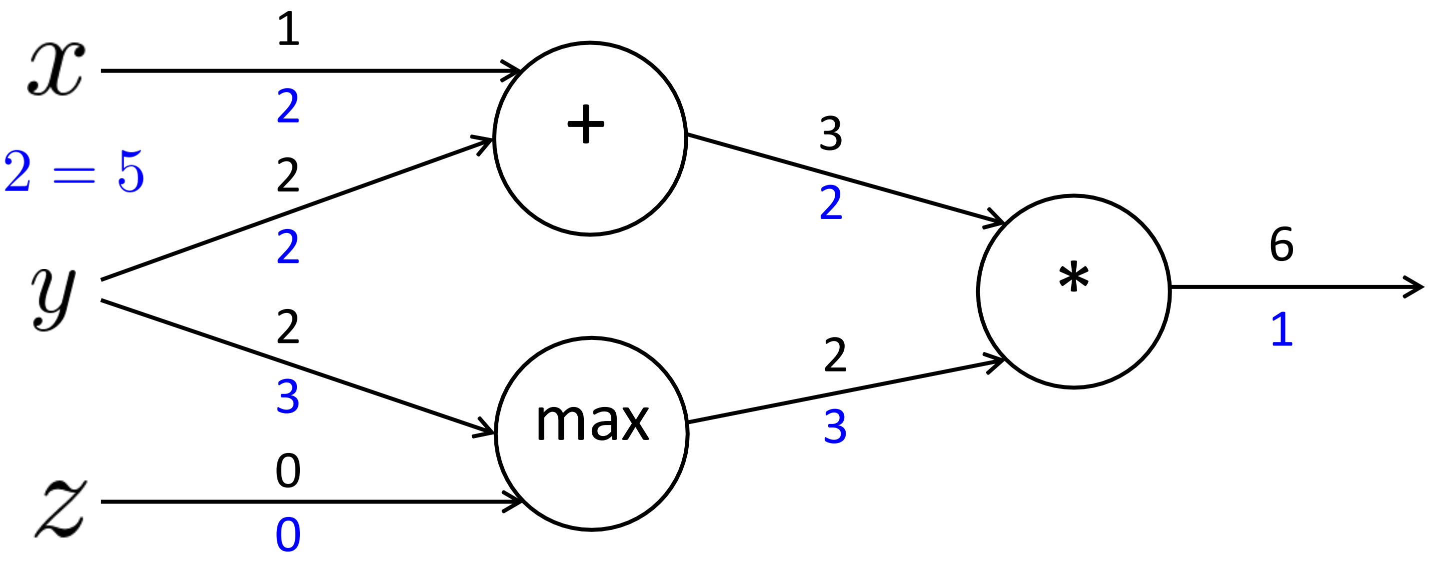
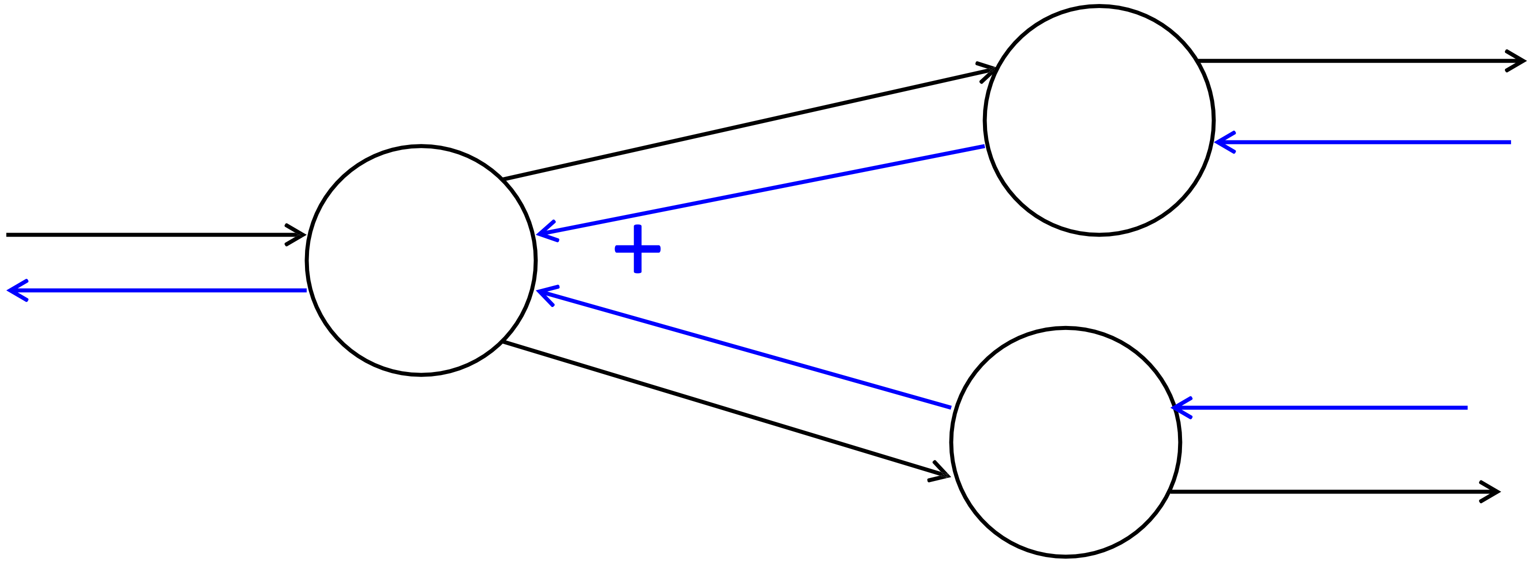
$$\frac{\partial f}{\partial x} = 2$$

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

$$\frac{\partial f}{\partial z} = 0$$



Gradients sum at outward branches



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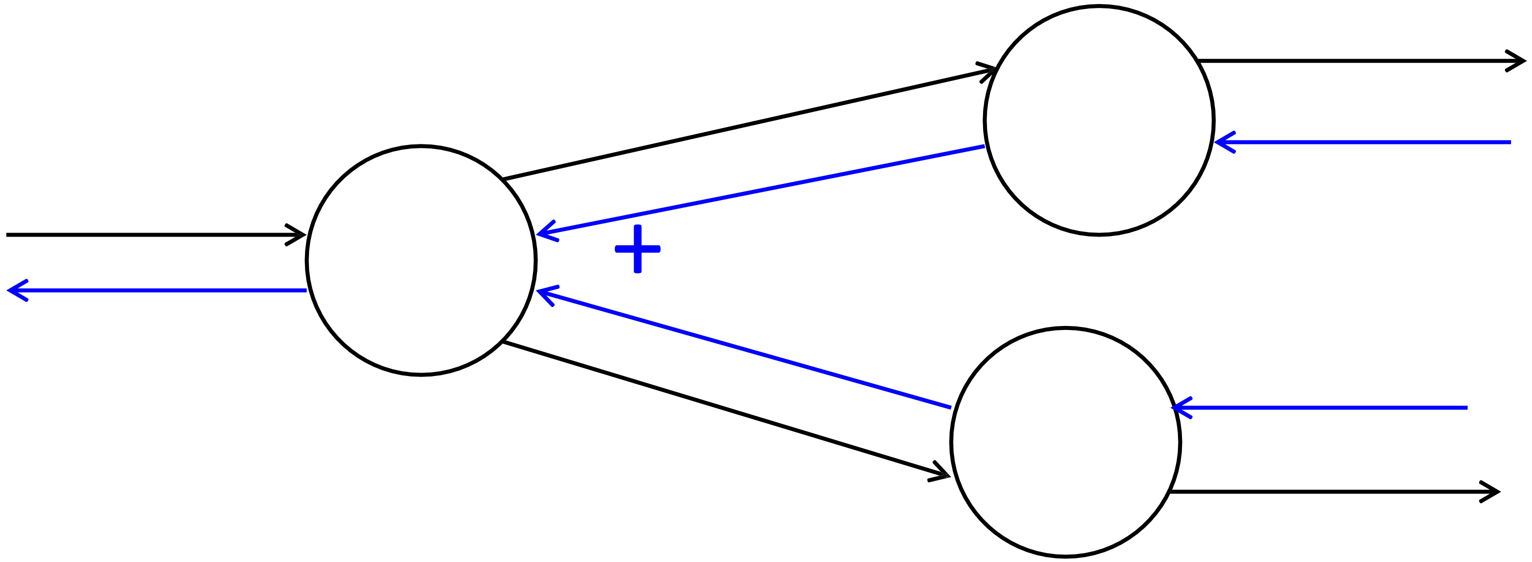


$$a = x + y$$

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

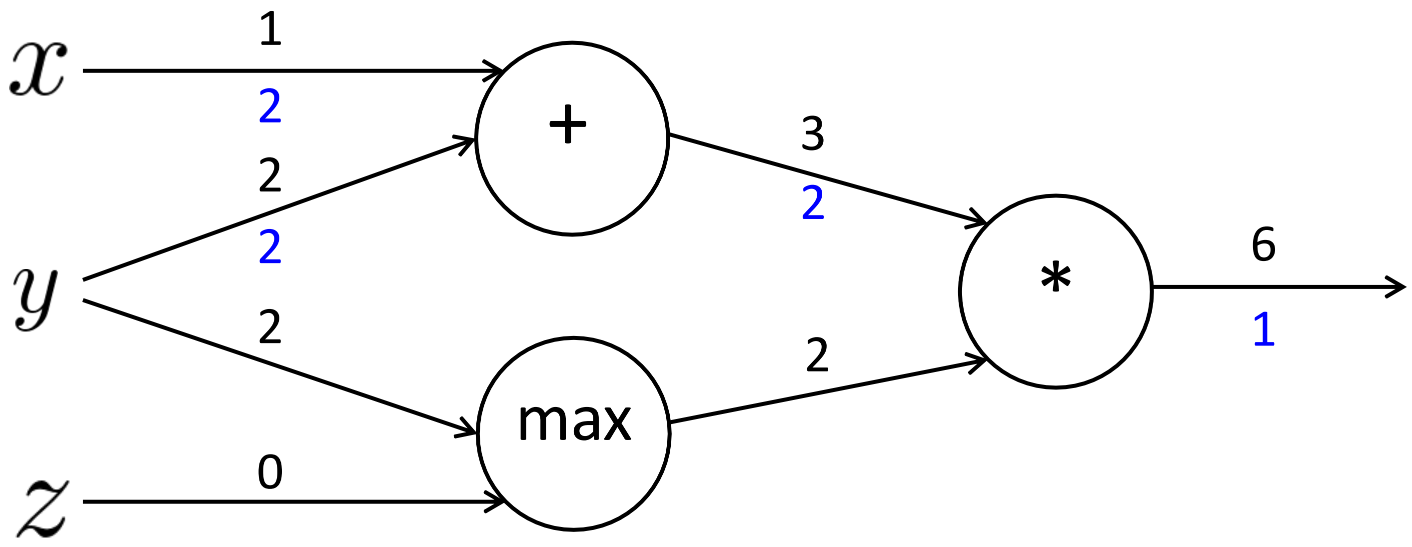
$$f = ab$$

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

Node Intuitions

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

- + "distributes" the upstream gradient to each summand



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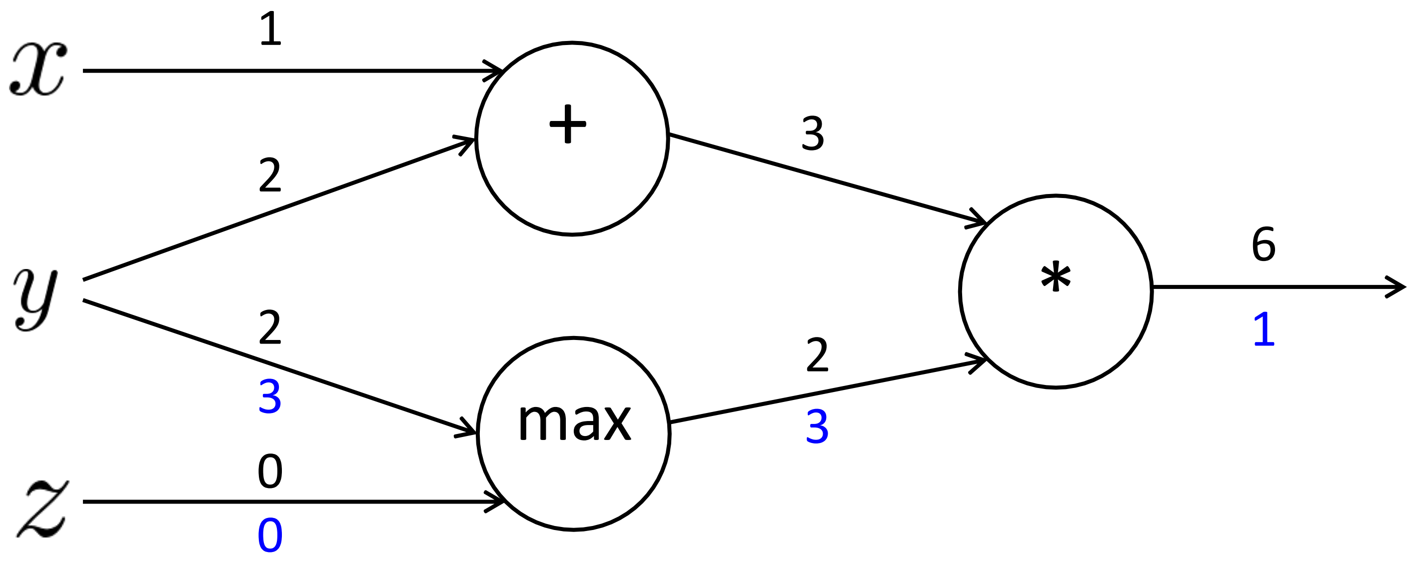
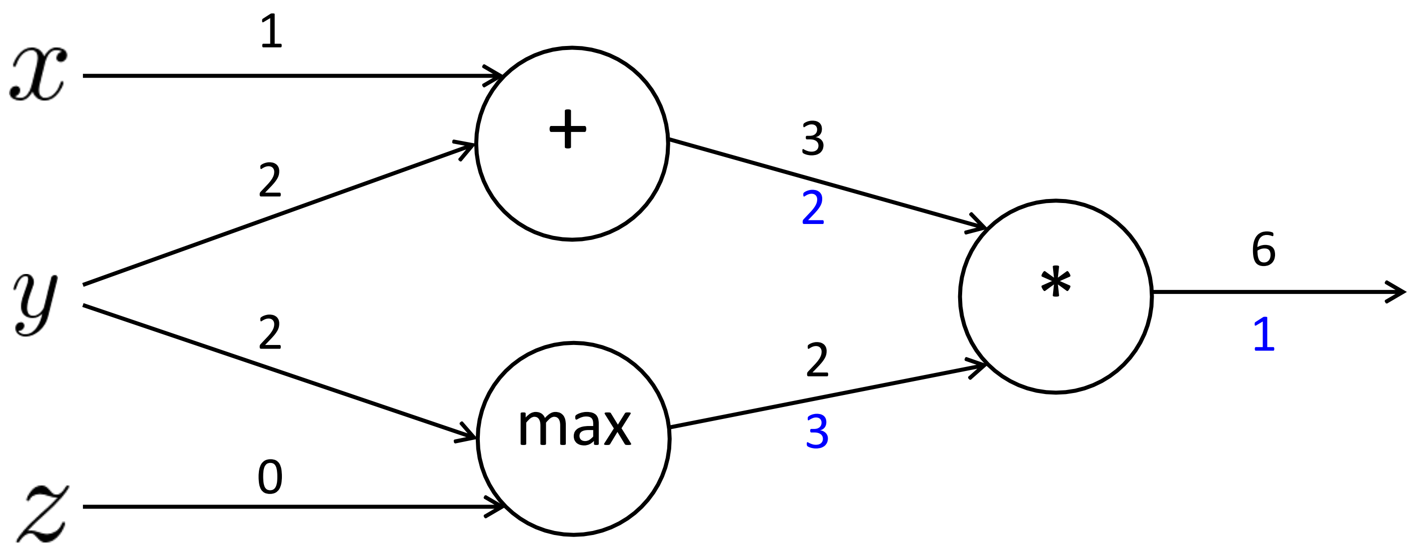
- + "distributes" the upstream gradient to each summand
- max "routes" the upstream gradient



Node Intuitions

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

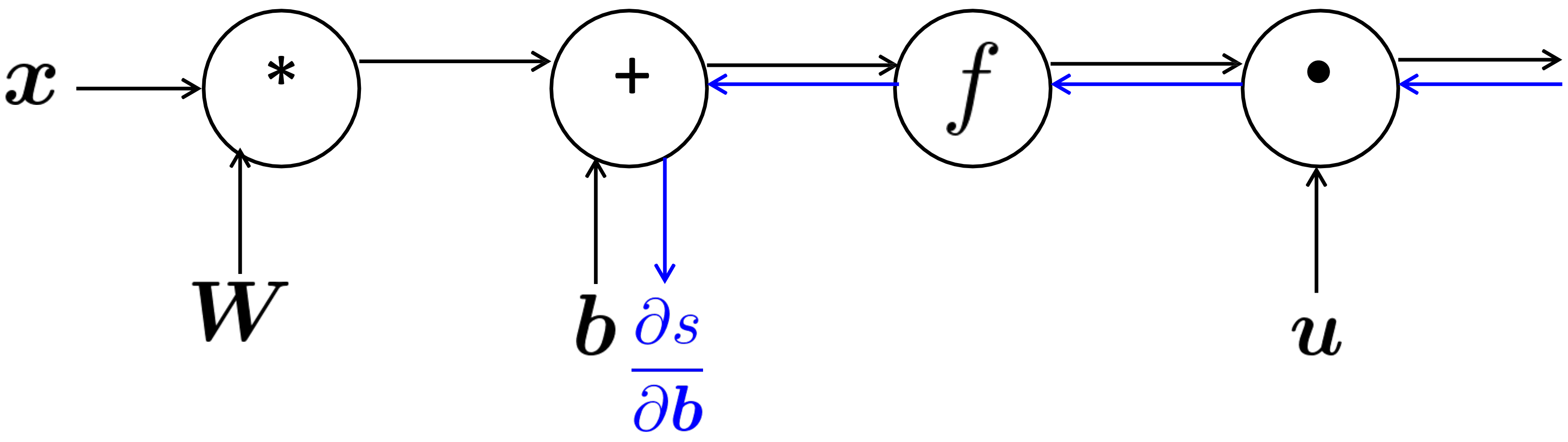
- + “distributes” the upstream gradient
- max “routes” the upstream gradient
- * “switches” the upstream gradient



Efficiency: compute all gradients at once

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

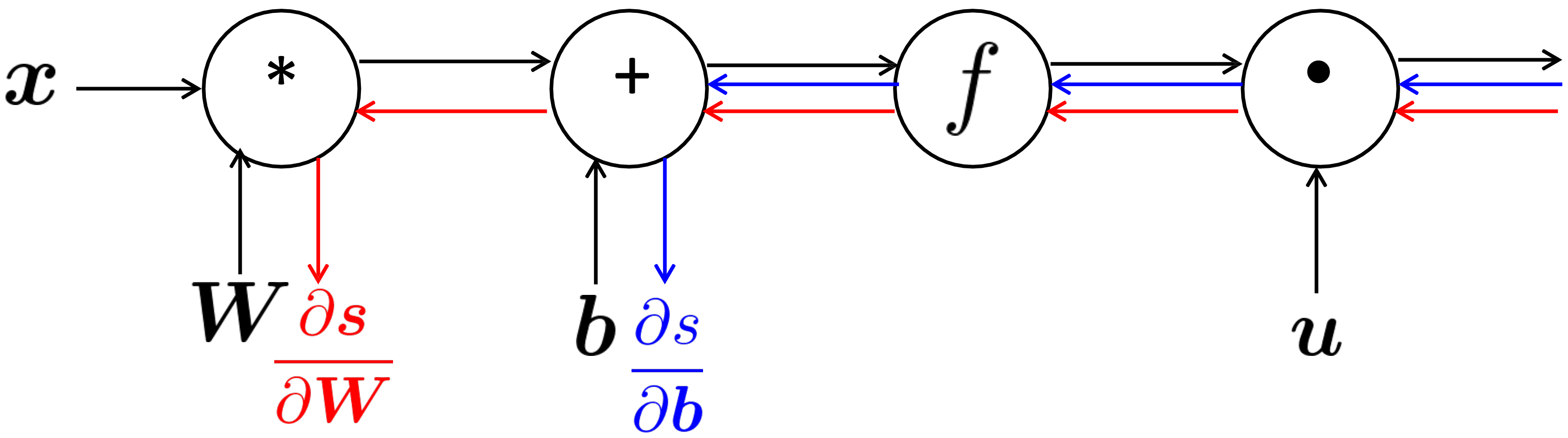
$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$



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!

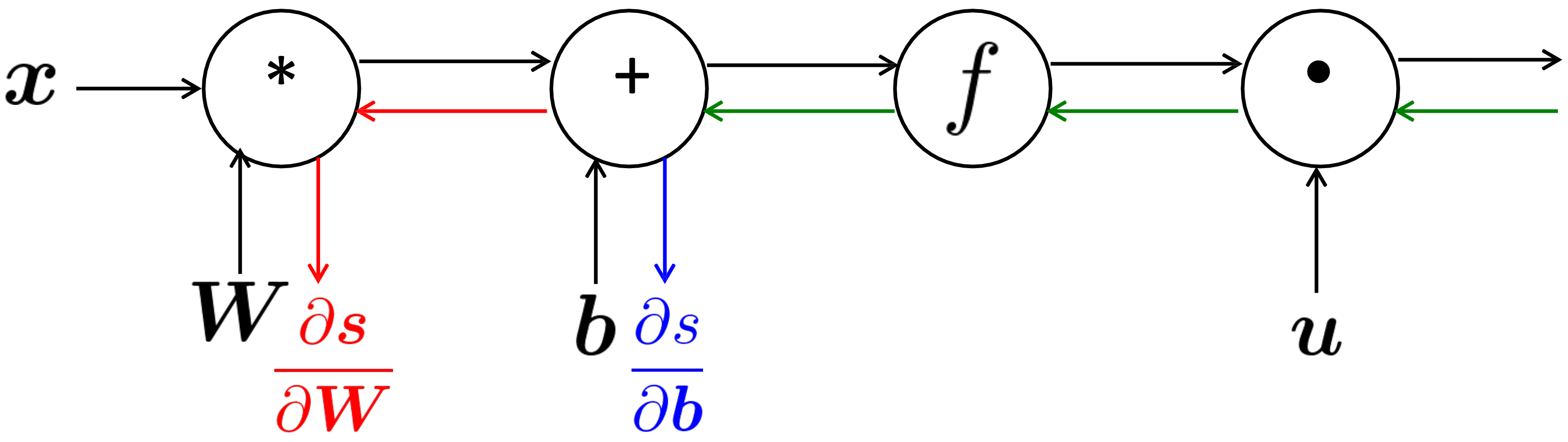
$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$



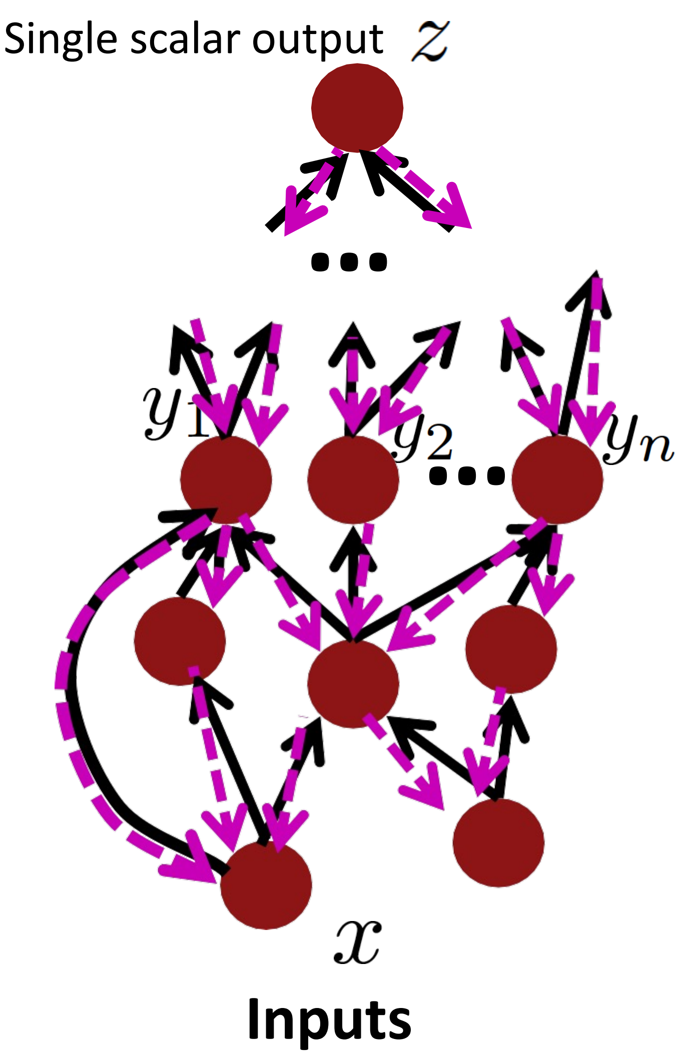
Efficiency: compute all gradients at once

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

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



Back-Prop in General Computation Graph



1. Fprop: visit nodes in topological sort order
   - Compute value of node given predecessors
2. Bprop:
   - initialize output gradient = 1
   - visit nodes in reverse order:
   Compute gradient wrt each node using gradient wrt successors

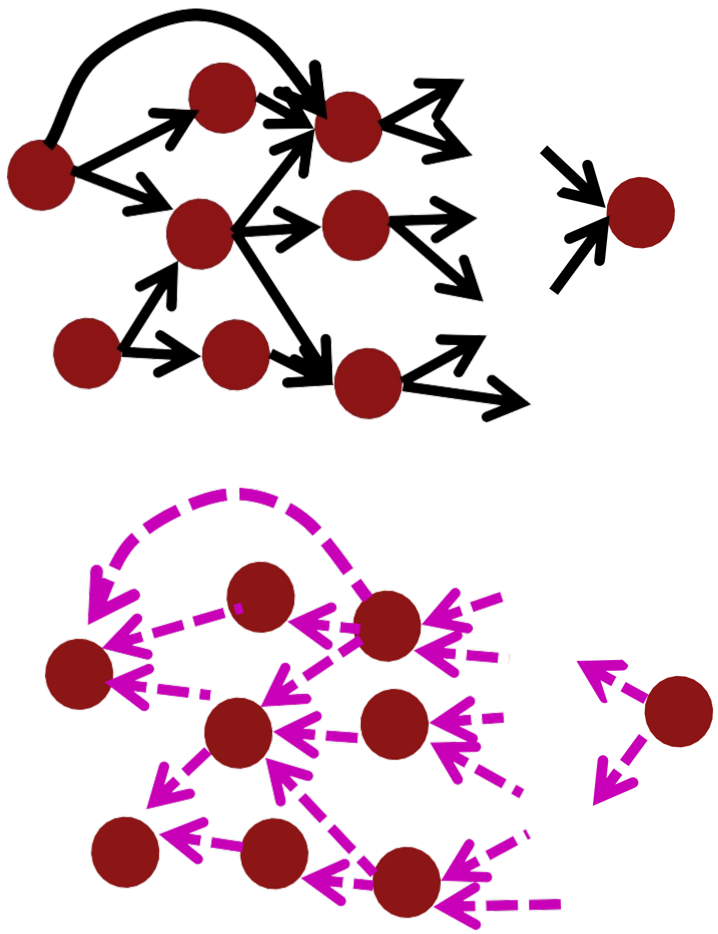
$\{y_1, y_2, \ldots y_n\}$ = successors of x

$$\frac{\partial z}{\partial x} = \sum_{i=1}^{n} \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x}$$

Done correctly, big O() complexity of fprop and bprop is **the same**

In general, our nets have regular layer-structure and so we can use matrices and Jacobians…

Automatic Differentiation

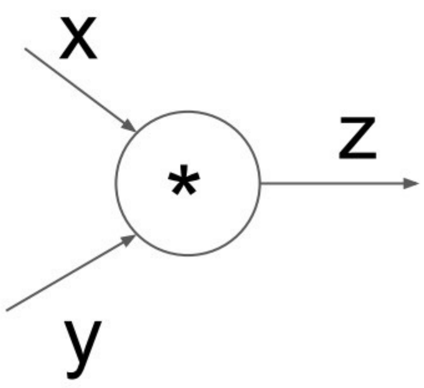


- The gradient computation can be automatically inferred from the symbolic expression of the fprop
- Each node type needs to know how to compute its output and how to compute the gradient wrt its inputs given the gradient wrt its output
- Modern DL frameworks (Tensorflow, PyTorch, etc.) do backpropagation for you but mainly leave layer/node writer to hand-calculate the local derivative

Backprop Implementations

```
class ComputationalGraph(object):
    #...
    def forward(inputs):
        # 1. [pass inputs to input gates...]
        # 2. forward the computational graph:
        for gate in self.graph.nodes_topologically_sorted():
            gate.forward()
        return loss # the final gate in the graph outputs the loss
    def backward():
        for gate in reversed(self.graph.nodes_topologically_sorted()):
            gate.backward() # little piece of backprop (chain rule applied)
        return inputs_gradients
```

Implementation: forward/backward API



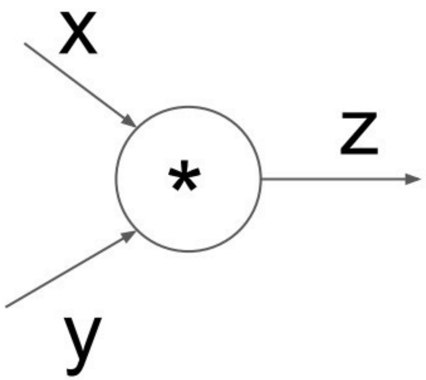
(x,y,z are scalars)

```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        return z
    def backward(dz):
        # dx = ... #todo
        # dy = ... #todo
        return [dx, dy]
```

$$\boxed{\frac{\partial L}{\partial z}}$$

$$\boxed{\frac{\partial L}{\partial x}}$$

Implementation: forward/backward API



(x,y,z are scalars)

```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        self.x = x # must keep these around!
        self.y = y
        return z
    def backward(dz):
        dx = self.y * dz # [dz/dx * dL/dz]
        dy = self.x * dz # [dz/dy * dL/dz]
        return [dx, dy]
```

Manual Gradient checking: Numeric Gradient

- For small *h* (≈ 1e-4), $$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$
- Easy to implement correctly
- But approximate and **very** slow:
  - You have to recompute *f* for **every parameter** of our model
- Useful for checking your implementation
  - In the old days, we hand-wrote everything, doing this everywhere was the key test
  - Now much less needed; you can use it to check layers are correctly implemented

Summary

We've mastered the core technology of neural nets! 🎉 🎉🎉🎉🎉

- **Backpropagation:** recursively (and hence efficiently) apply the chain rule along computation graph
  - [downstream gradient] = [upstream gradient] x [local gradient]
- **Forward pass:** compute results of operations and save intermediate values
- **Backward pass:** apply chain rule to compute gradients

Why learn all these details about gradients?

- **Modern deep learning frameworks compute gradients for you!**

- But why take a class on compilers or systems when they are implemented for you?
  - Understanding what is going on under the hood is useful!

- Backpropagation doesn't always work perfectly out of the box
  - Understanding why is crucial for debugging and improving models
  - See Karpathy article:
    - https://medium.com/@karpathy/yes-you-should-understand-backprop-e2f06eab496b
  - Example in future lecture: exploding and vanishing gradients