

Natural Language Processing with Deep Learning

CS224N/Ling284



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Lecture 4: Backpropagation and
computation graphs

Lecture Plan

Lecture 4: Backpropagation and computation graphs

1. Matrix gradients for our simple neural net and some tips [15 mins]
2. Computation graphs and backpropagation [40 mins]
3. Stuff you should know [15 mins]
 - a. Regularization to prevent overfitting
 - b. Vectorization
 - c. Nonlinearities
 - d. Initialization
 - e. Optimizers
 - f. Learning rates

1. Derivative wrt a weight matrix

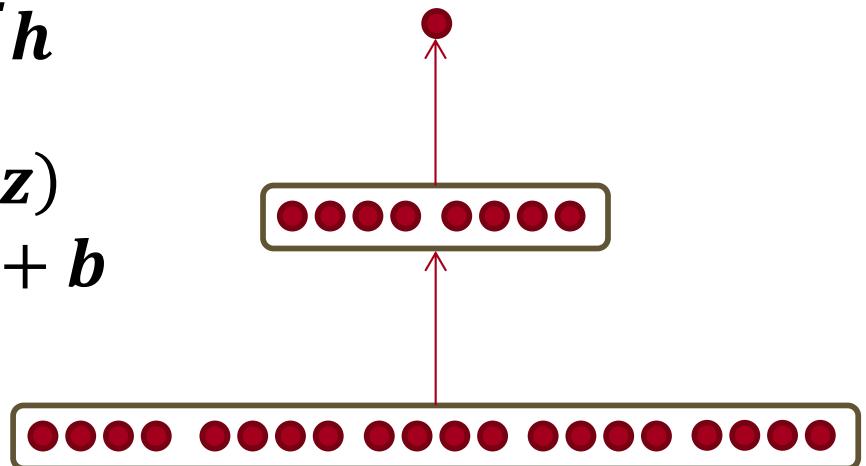
- Let's look carefully at computing $\frac{\partial s}{\partial W}$
 - Using the chain rule again:

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

计算过了，记作

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

$$\begin{aligned}\mathbf{h} &= f(\mathbf{z}) \\ \mathbf{z} &= \mathbf{Wx} + \mathbf{b}\end{aligned}$$



Deriving gradients for backprop

- For this function (following on from last time):

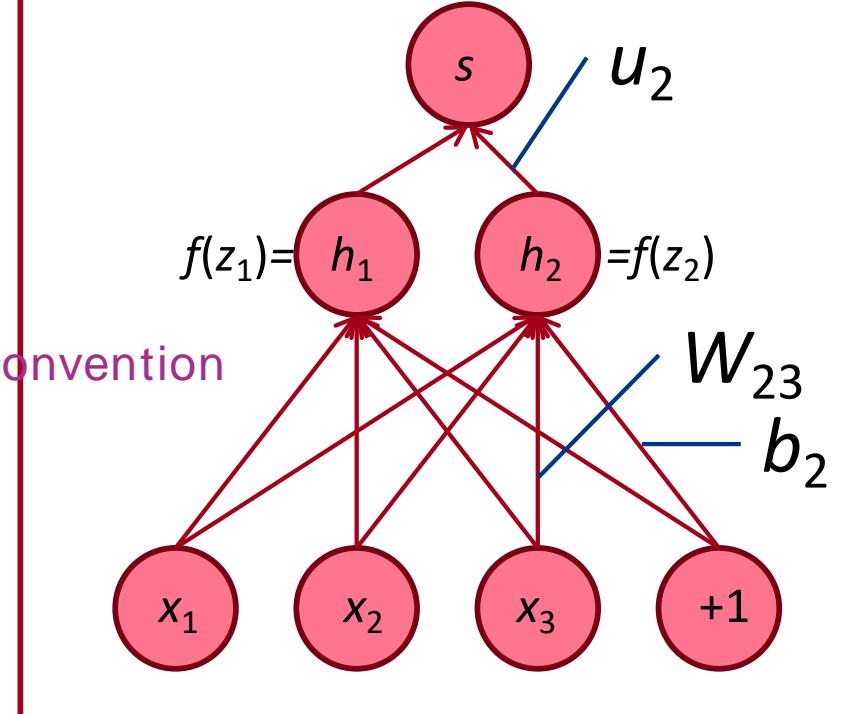
$$\frac{\partial s}{\partial W} = \delta \frac{\partial z}{\partial W} = \delta \frac{\partial}{\partial W} Wx + b$$

- 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

element-wise: 直接 ∂W 不直观，所以看元素 & shape convention

$$\begin{aligned}\frac{\partial z_i}{\partial W_{ij}} &= \frac{\partial}{\partial W_{ij}} W_{i \cdot} x + b_i \\ &= \frac{\partial}{\partial W_{ij}} \sum_{k=1}^d W_{ik} x_k = x_j\end{aligned}$$

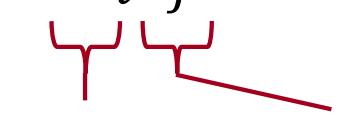
Wij: i是hidden layer的位置，j是input vector的一个下标



Deriving gradients for backprop

- So for derivative of single W_{ij} :

$$\frac{\partial s}{\partial W_{ij}} = \delta_i x_j$$


Error signal from above Local gradient signal

是之后也会一直出现的pattern

- We want gradient for full W – but each case is the same
- Overall answer: Outer product:

rewrite in matrix

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

看维度

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

Deriving gradients: Tips

- **Tip 1:** Carefully define your variables and keep track of their dimensionality!
- **Tip 2:** Chain rule! If $\mathbf{y} = f(\mathbf{u})$ and $\mathbf{u} = g(\mathbf{x})$, i.e., $\mathbf{y} = f(g(\mathbf{x}))$, then:

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial \mathbf{y}}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}}$$

Keep straight what variables feed into what computations

- **Tip 3:** For the top softmax part of a model: First consider the derivative wrt f_c when $c = y$ (the correct class), then consider derivative wrt f_c when $c \neq y$ (all the incorrect classes)
- **Tip 4:** Work out element-wise partial derivatives if you're getting confused by matrix calculus!
- **Tip 5:** Use Shape Convention. Note: The error message δ that arrives at a hidden layer has the same dimensionality as that hidden layer

Deriving gradients wrt words for window model

- The gradient that arrives at and updates the word vectors can simply be split up for each word vector:
- Let $\nabla_x J = W^T \delta = \delta_{x_{window}}$ word window matrix (稀疏) 的梯度
- With $x_{window} = [x_{museums} \quad x_{in} \quad x_{Paris} \quad x_{are} \quad x_{amazing}]$
- We have

$$\delta_{window} = \begin{bmatrix} \nabla x_{museums} \\ \nabla x_{in} \\ \nabla x_{Paris} \\ \nabla x_{are} \\ \nabla x_{amazing} \end{bmatrix} \in \mathbb{R}^{5d}$$

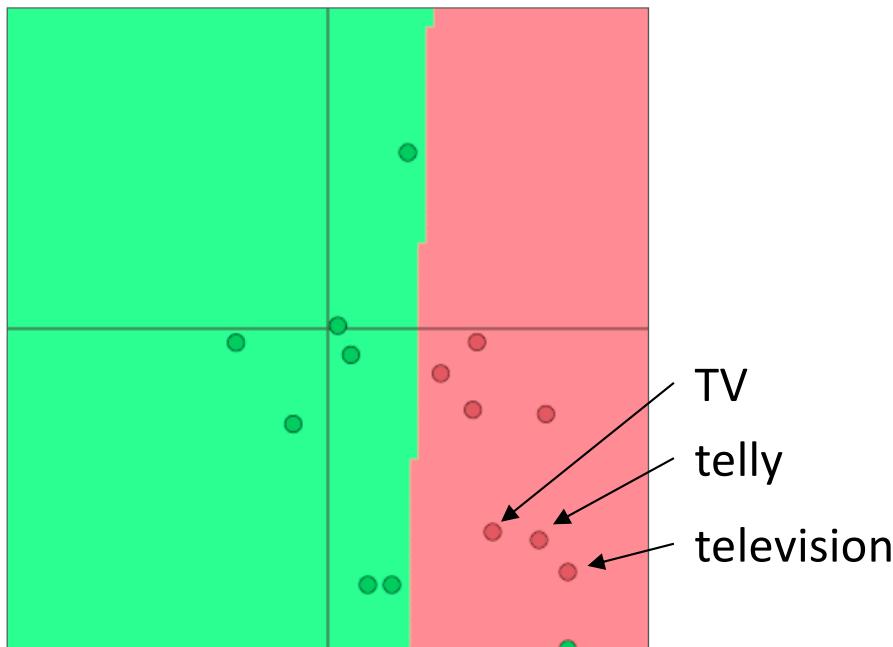
Updating word gradients in window model

相当于在extrinsic evaluation中tune词向量

- This will push word vectors around so that they will (in principle) be more helpful in determining named entities.
- For example, the model can learn that seeing x_{in} as the word just before the center word is indicative for the center word to be a location

A pitfall when retraining word vectors

- **Setting:** We are training a logistic regression classification model for movie review sentiment using single words.
- In the **training data** we have “TV” and “telly”
- In the **testing data** we have “television”
- The **pre-trained** word vectors have all three similar:

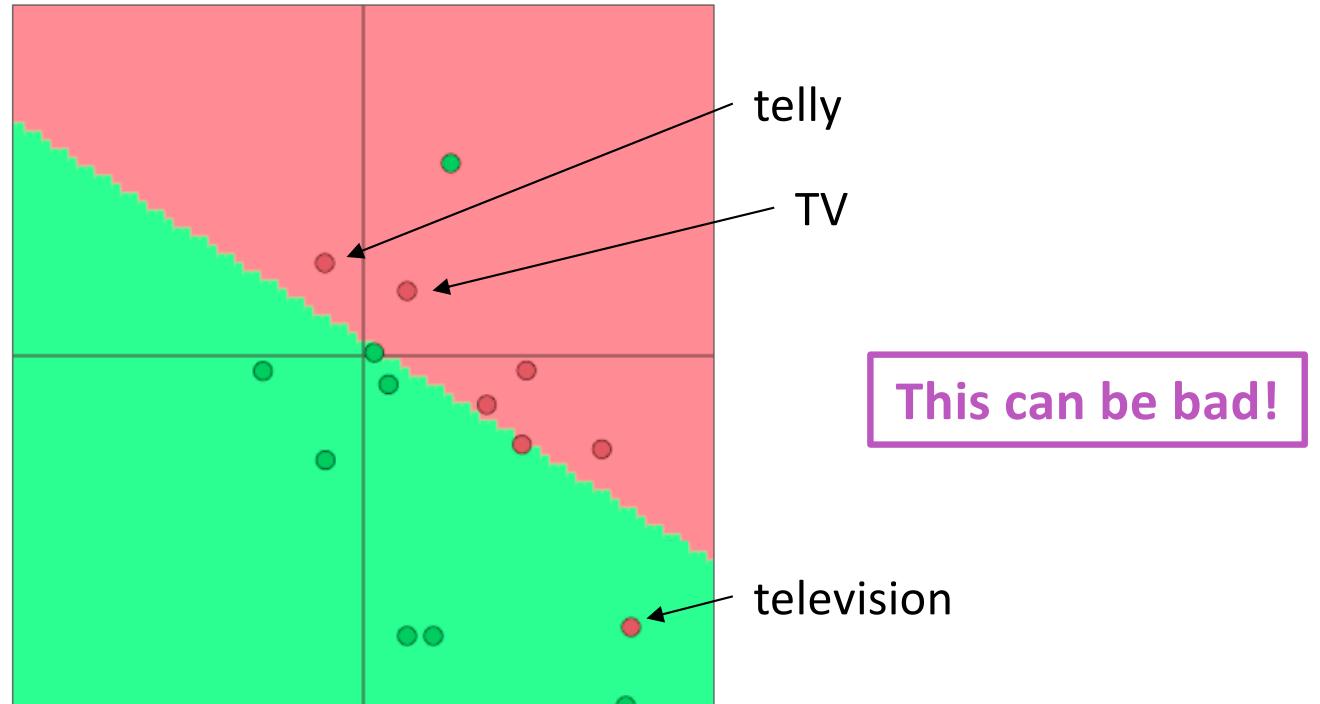


- **Question: What happens when we update the word vectors?**

A pitfall when retraining word vectors

- **Question:** What happens when we update the word vectors?
- **Answer:**
 - Those words that are **in** the training data **move around**
 - “TV” and “telly”
 - Words **not** in the training data **stay where they were**
 - “television”

dataset不够大，只移动了一部分词向量——不能保持 semantic relation in space



So what should I do?

- **Question:** Should I use available “pre-trained” word vectors

Answer:

- Almost always, yes!
 - They are trained on a huge amount of data, and so they will know about words not in your training data and will know more about words that are in your training data 例如机器翻译用到了巨多的words , 可以 randomly initialized
 - Have 100s of millions of words of data? Okay to start random
- **Question:** Should I update (“fine tune”) my own word vectors?
 - **Answer:**
 - If you only have a small training data set, don’t train the word vectors
 - If you have have a large dataset, it probably will work better to train = update = fine-tune word vectors to the task

Backpropagation

We've almost shown you backpropagation

It's taking derivatives and using the (generalized) chain rule

Other trick: we **re-use** derivatives computed for higher layers in computing derivatives for lower layers so as to minimize computation

2. Computation Graphs and Backpropagation

AST-抽象语法树

- We represent our neural net equations as a graph

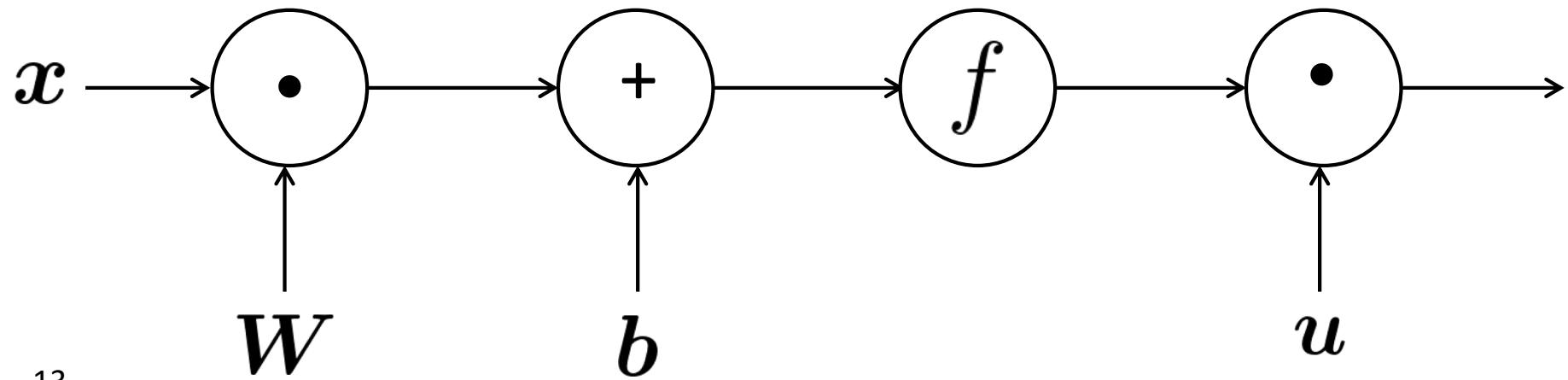
- Source nodes: inputs
- Interior nodes: operations

$$s = u^T h$$

$$h = f(z)$$

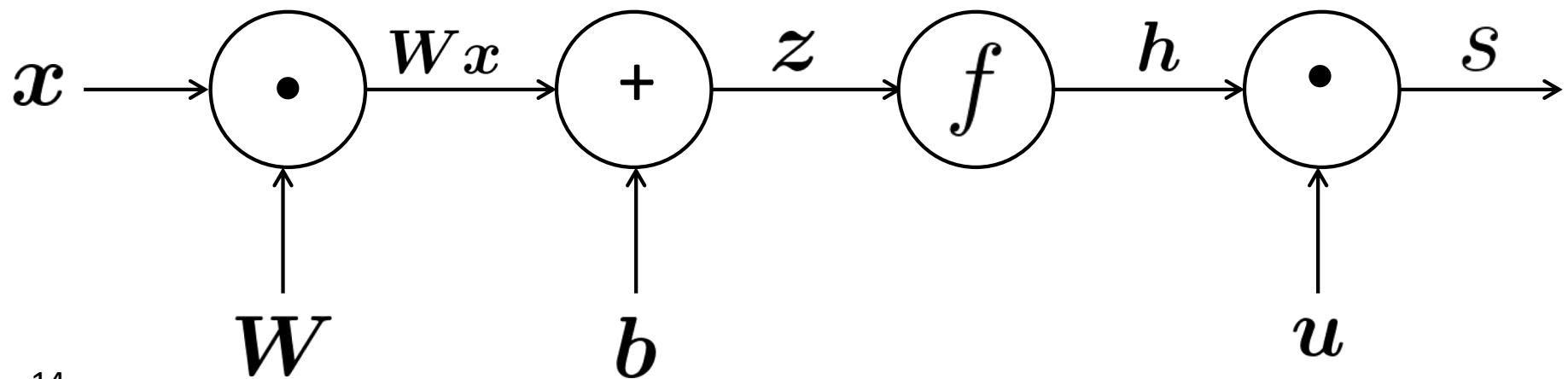
$$z = Wx + b$$

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



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



Computation Graphs and Backpropagation

- Representing our neural net equations as a graph

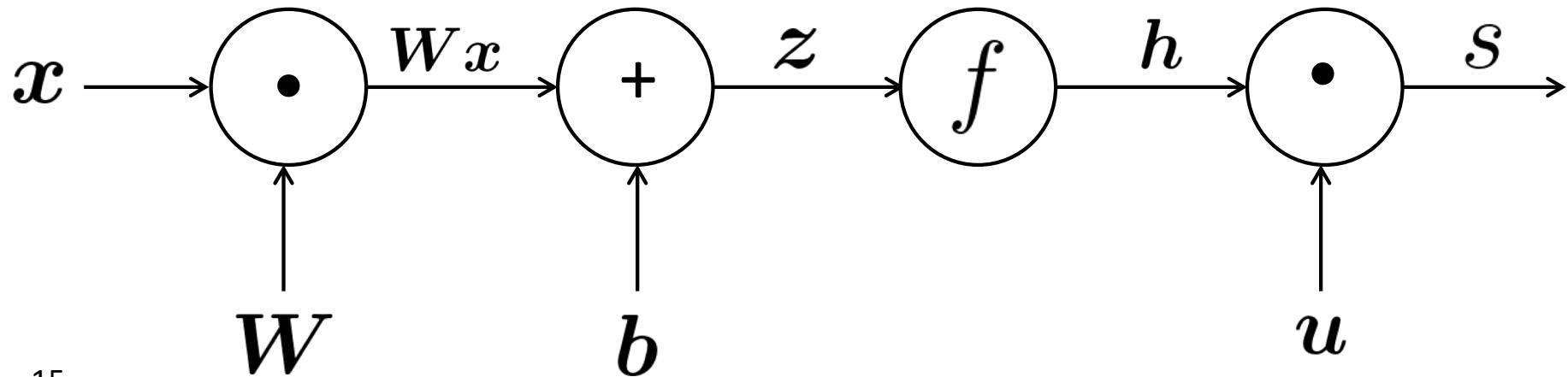
$$s = u^T h$$

$$h = f(z)$$

“Forward Propagation”

从左到右进行expression evaluation: $dz/dW * dh/dz * ds/dh = ds/dW$

operation



Backpropagation

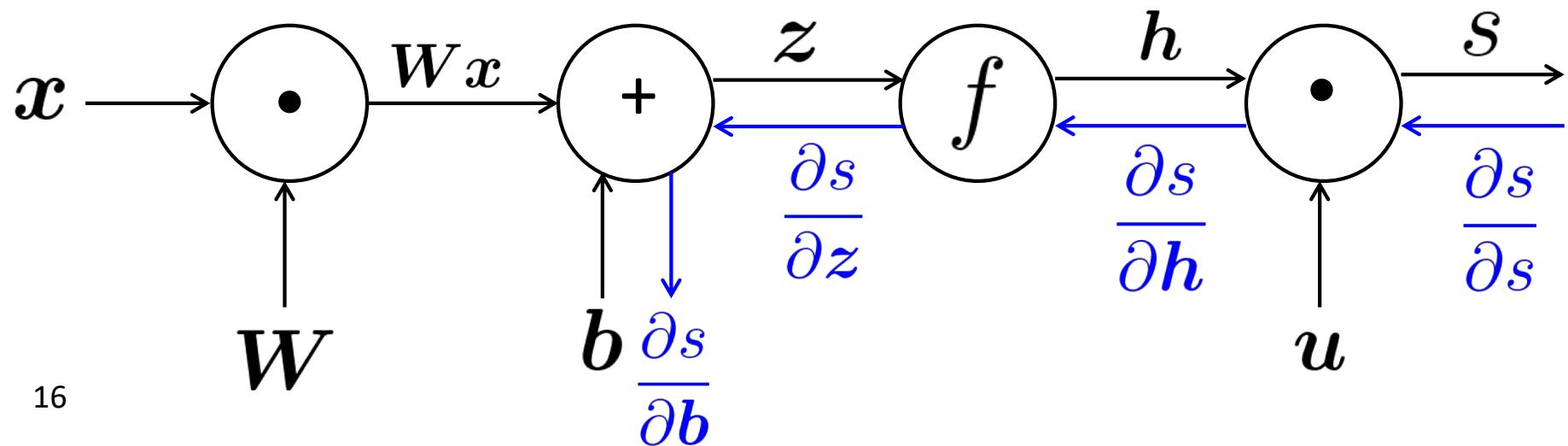
- Go backwards along edges
 - Pass along gradients

$$s = u^T h$$

$$h = f(z)$$

$$z = Wx + b$$

x (input)

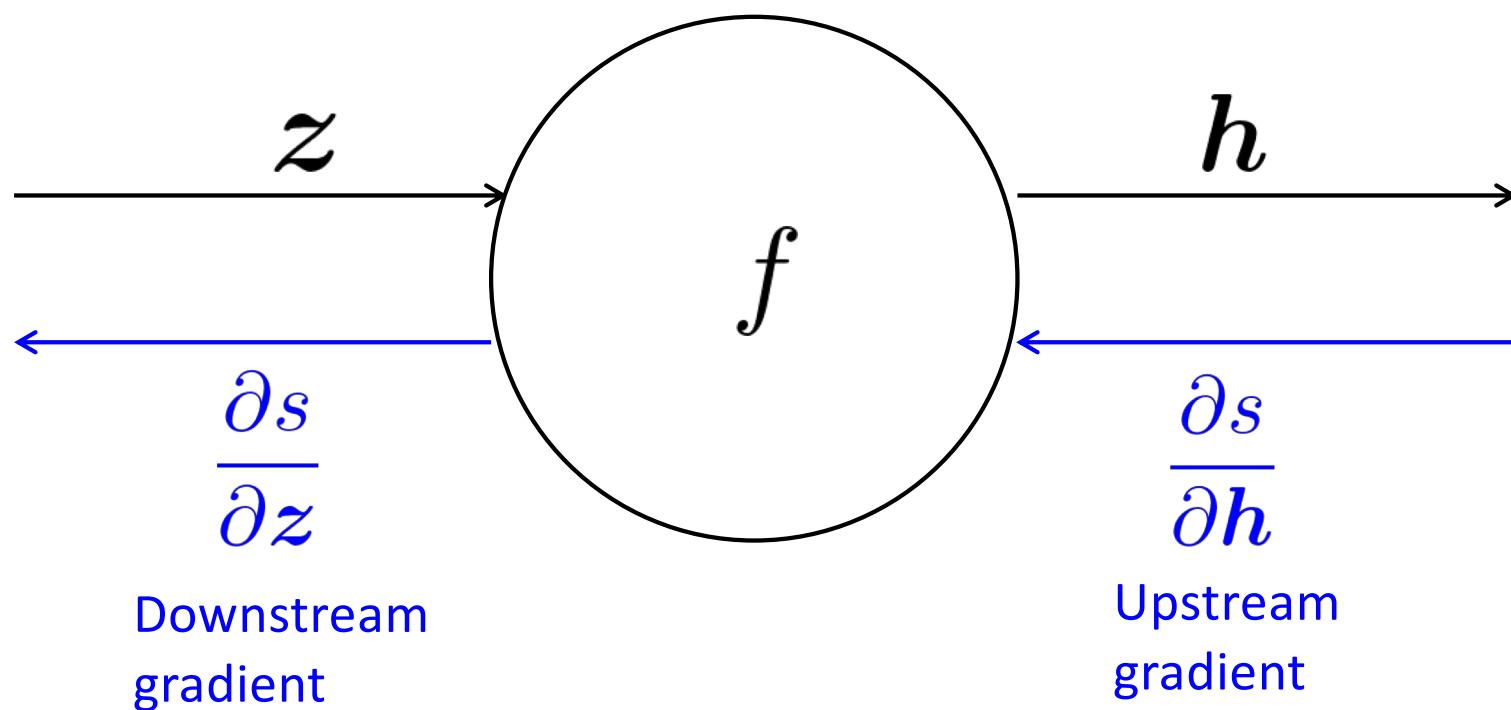


Backpropagation: Single Node

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

$$h = f(z)$$

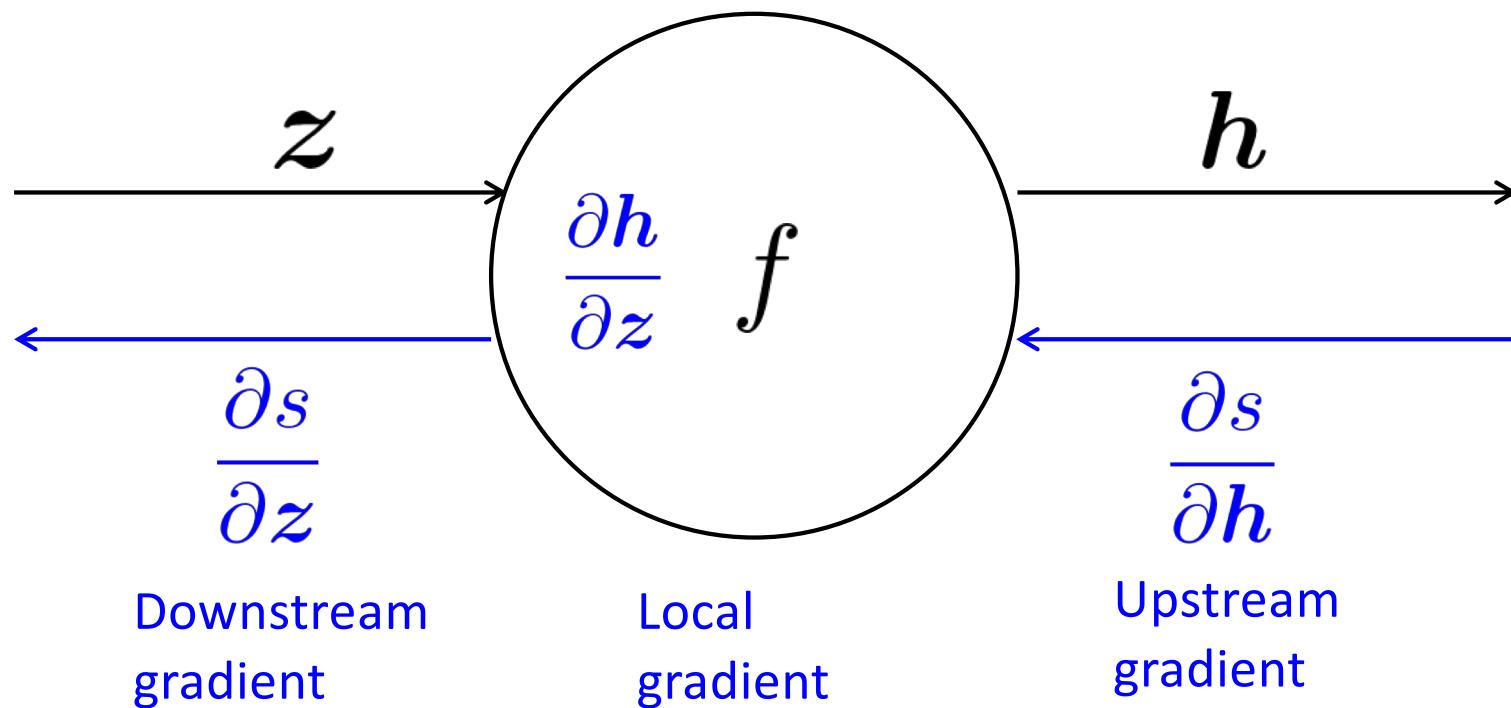
output



Backpropagation: Single Node

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

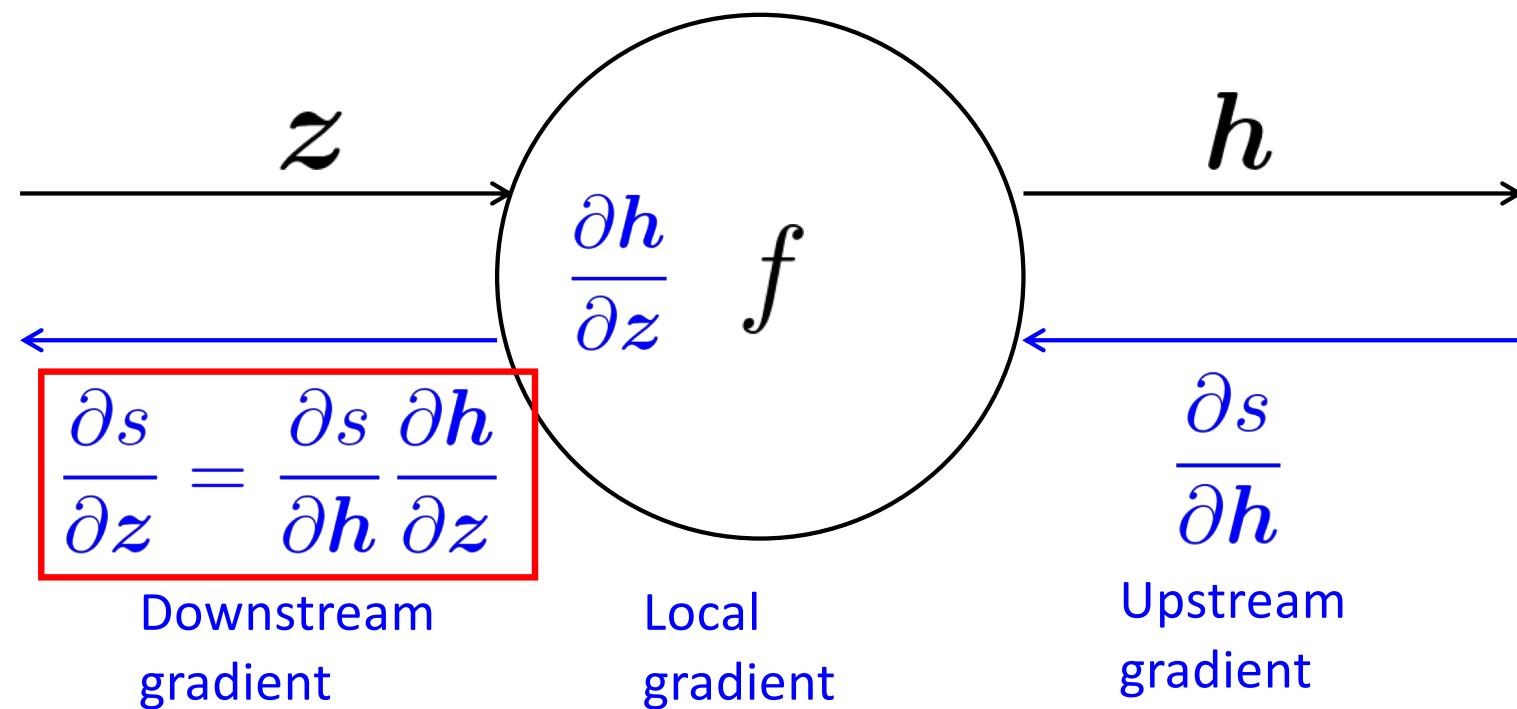
$$h = f(z)$$



Backpropagation: Single Node

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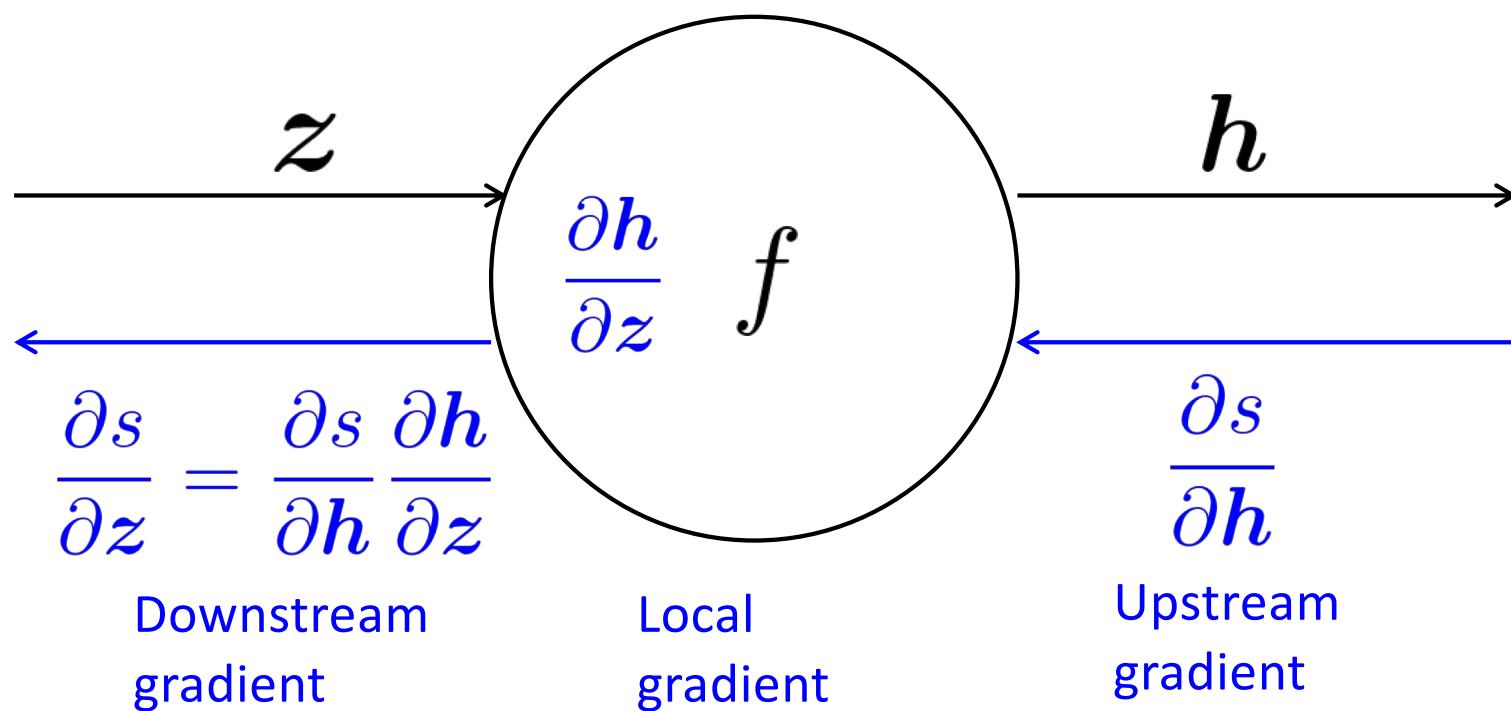
$$h = f(z)$$



Backpropagation: Single Node

- Each node has a **local gradient**
 - The gradient of it's output with respect to it's input
- [downstream gradient] = [upstream gradient] x [local gradient]

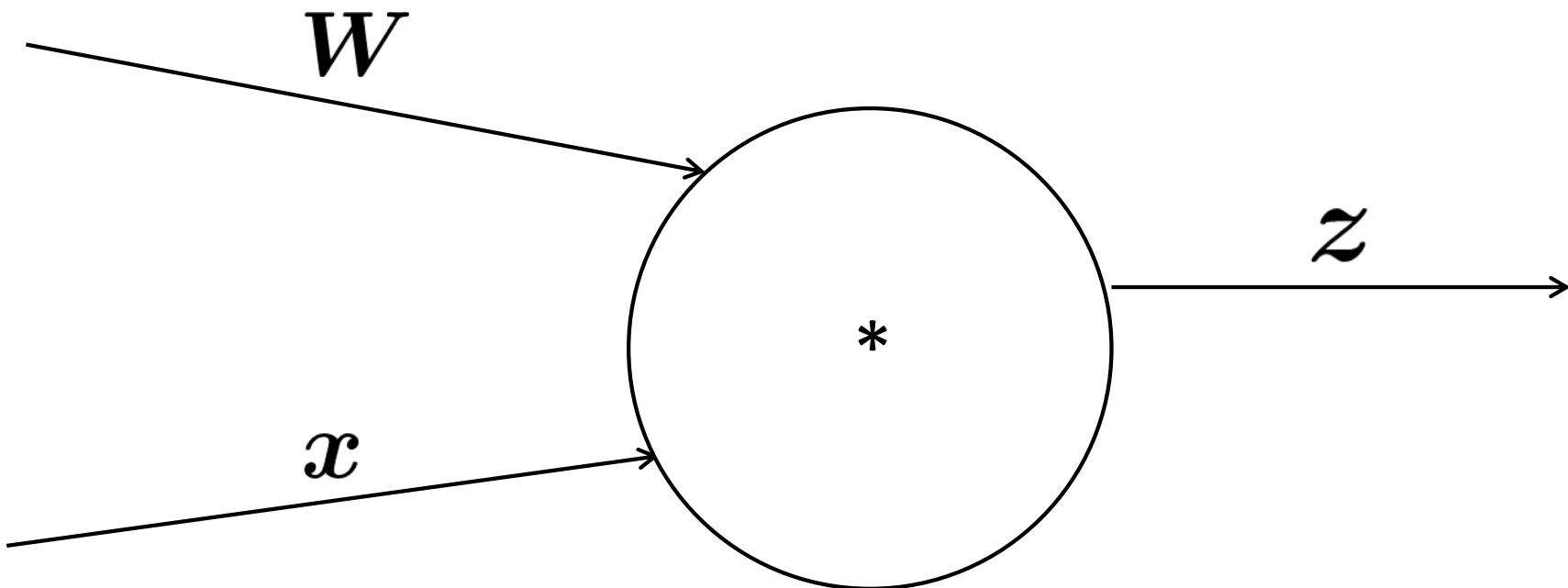
$$h = f(z)$$



Backpropagation: Single Node

- What about nodes with multiple inputs?

$$z = Wx$$

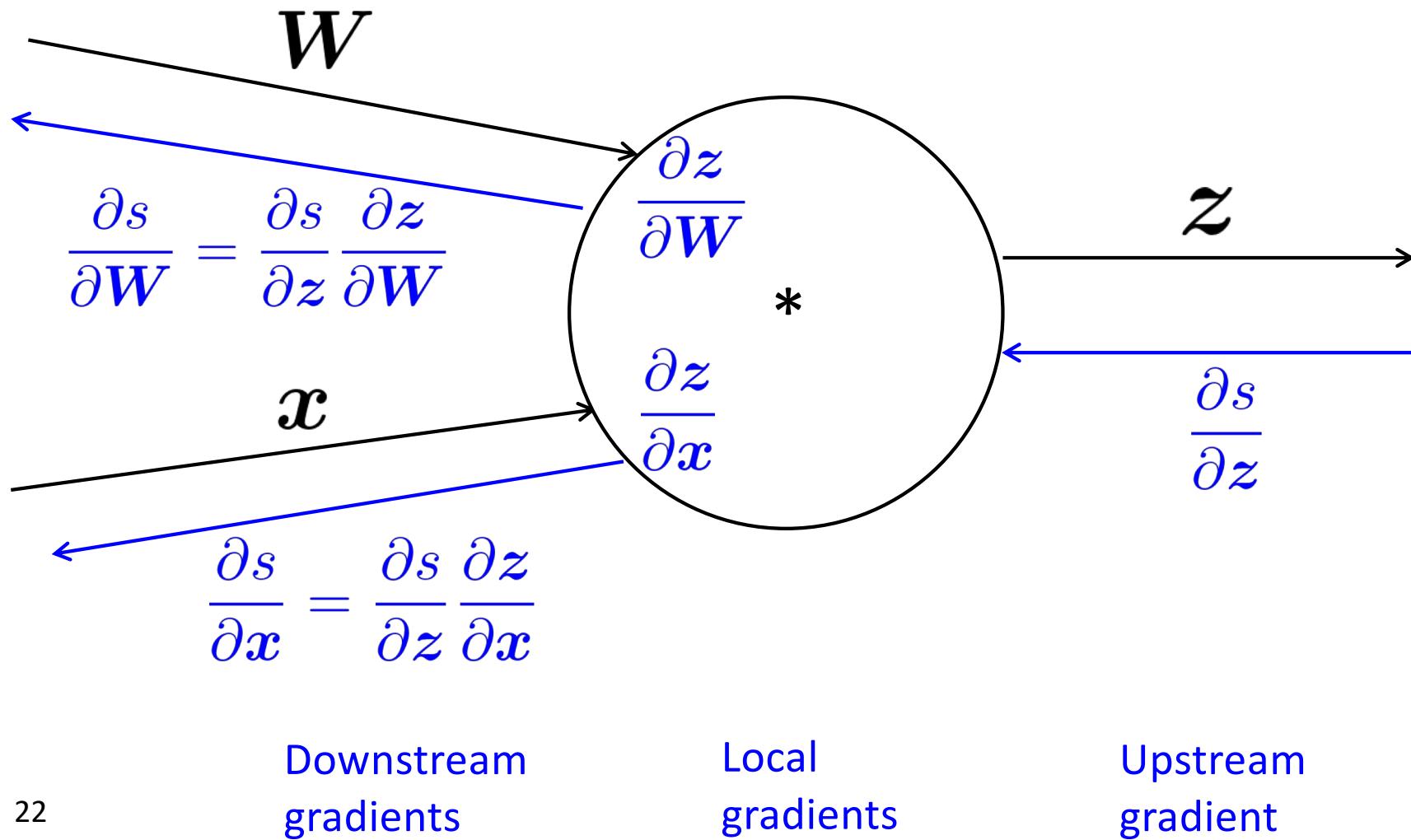


Backpropagation: Single Node

- Multiple inputs → multiple local gradients

forward时出现汇集，backprop时分别计算（分支）

$$z = Wx$$



An Example

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

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

An Example

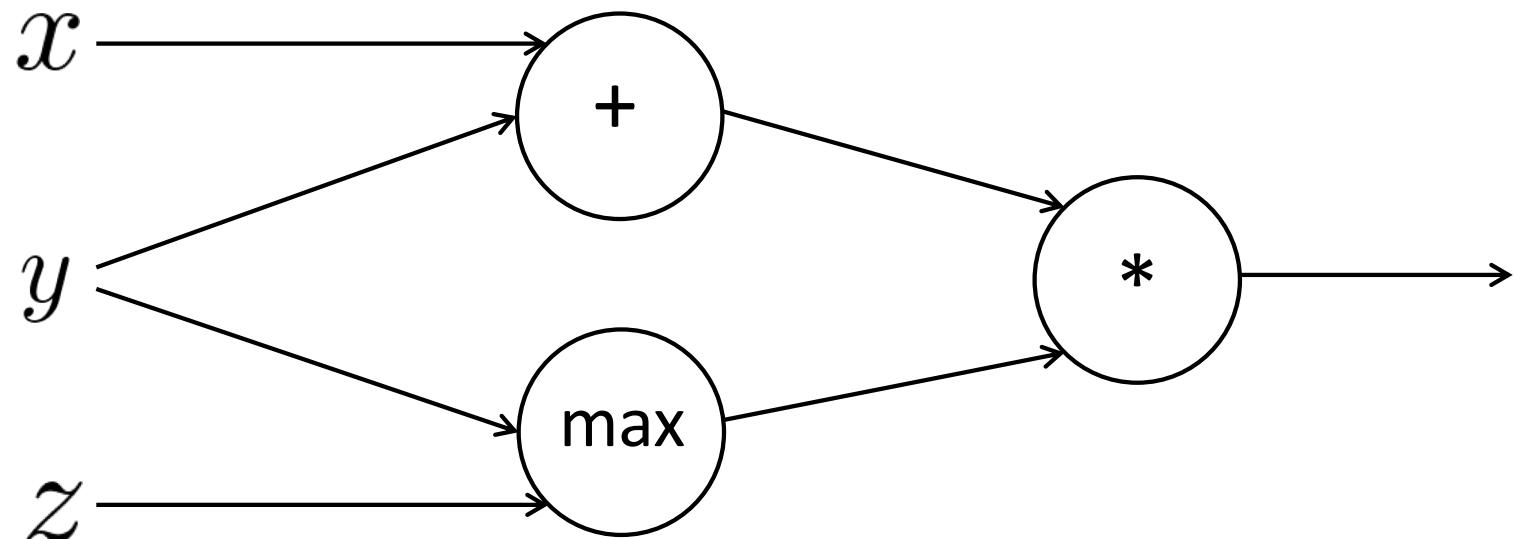
$$f(x, y, z) = (x + y) \max(y, z)$$
$$x = 1, y = 2, z = 0$$

Forward prop steps

$$a = x + y$$

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

$$f = ab$$



An Example

$$f(x, y, z) = (x + y) \max(y, z)$$
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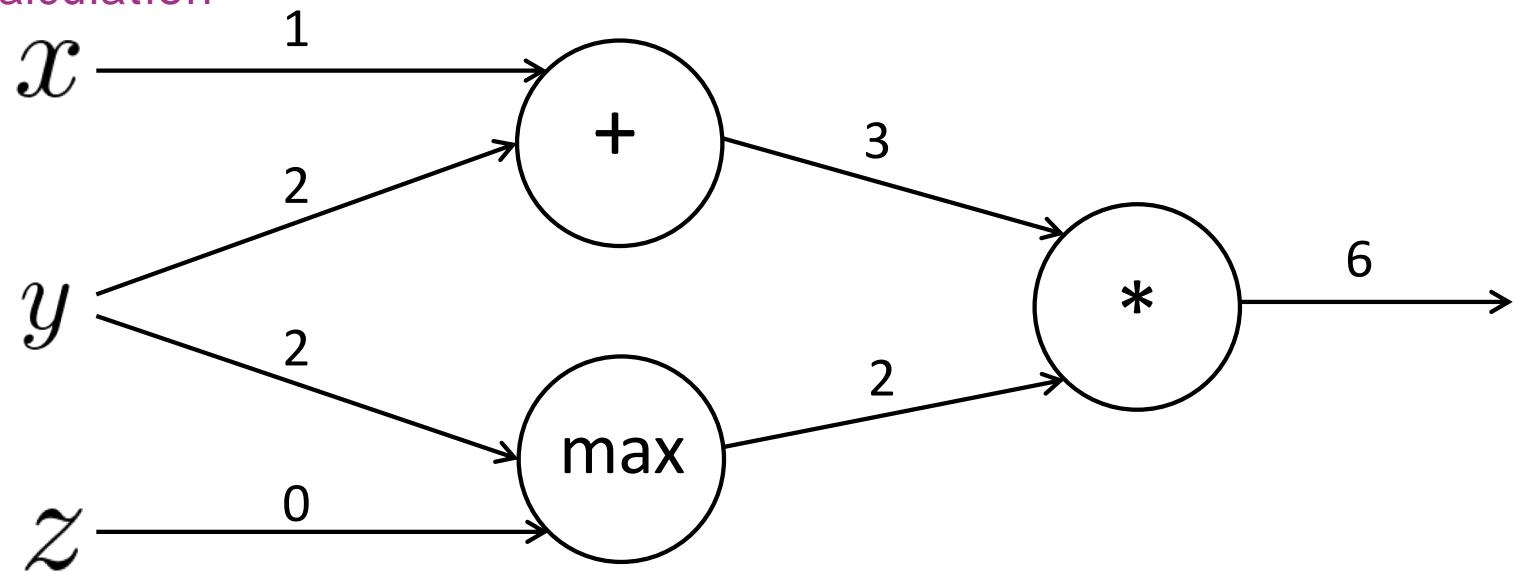
Forward prop steps

$$a = x + y$$

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

$$f = ab$$

Forward calculation



An Example

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

Forward prop steps

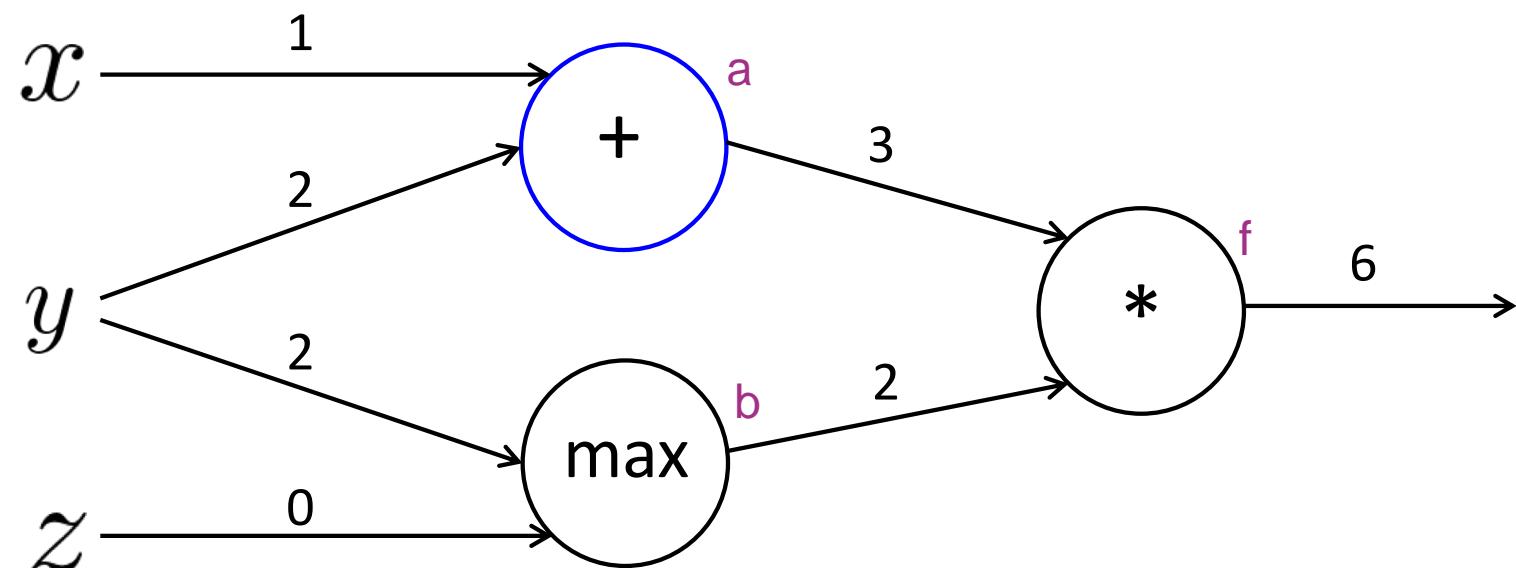
$$a = x + y$$

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Local gradients

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



An Example

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Forward prop steps

$$a = x + y$$

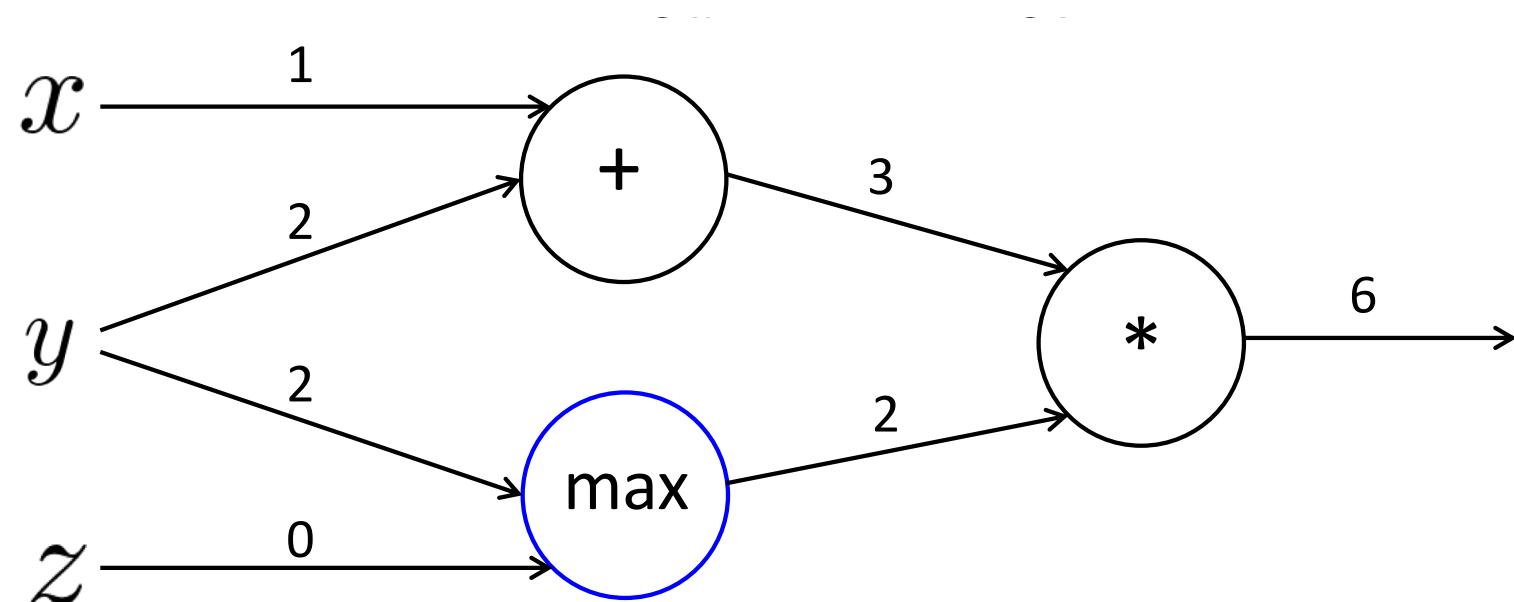
$$b = \max(y, z)$$

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Local gradients

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

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



An Example

$$f(x, y, z) = (x + y) \max(y, z)$$
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Forward prop steps

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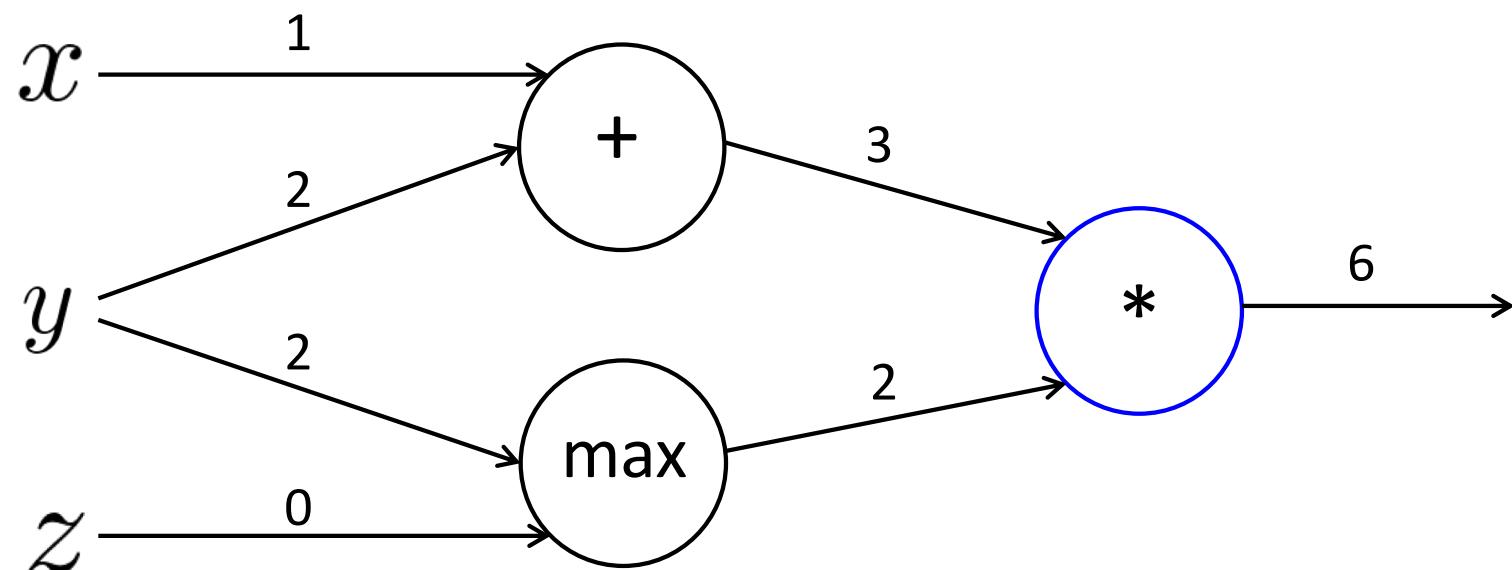
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$$\frac{\partial f}{\partial a} = b = 2 \quad \frac{\partial f}{\partial b} = a = 3$$



An Example

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Forward prop steps

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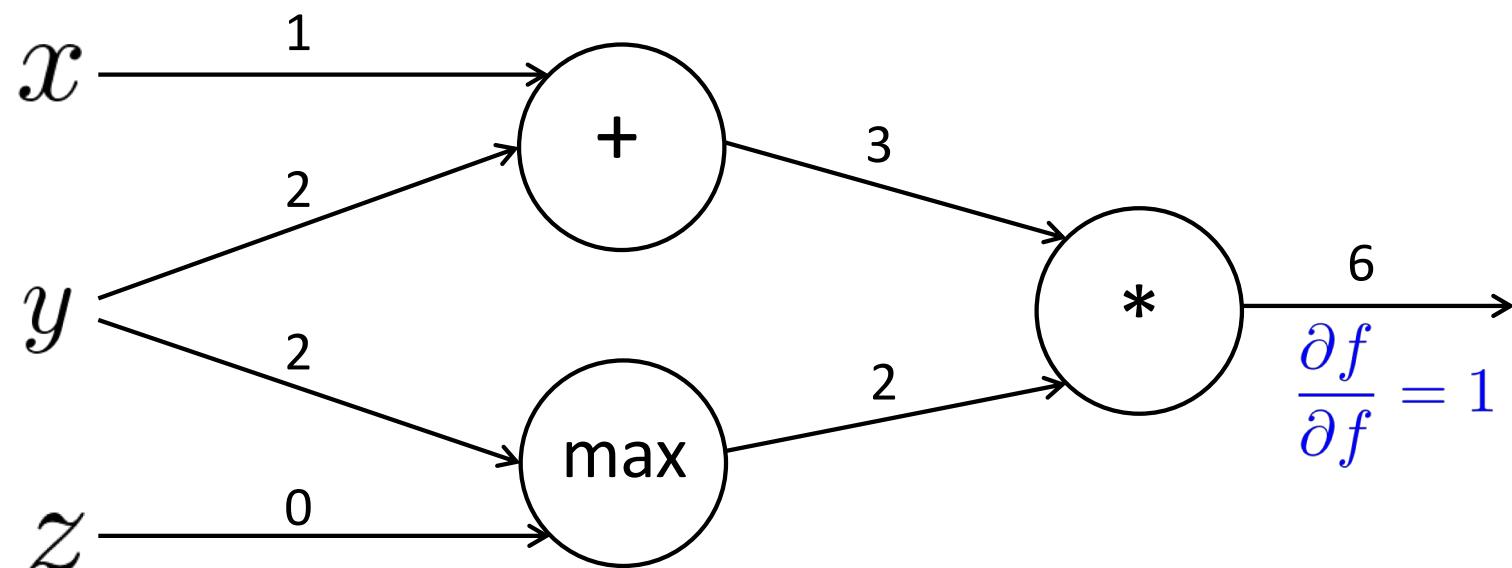
$$f = ab$$

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An Example

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Forward prop steps

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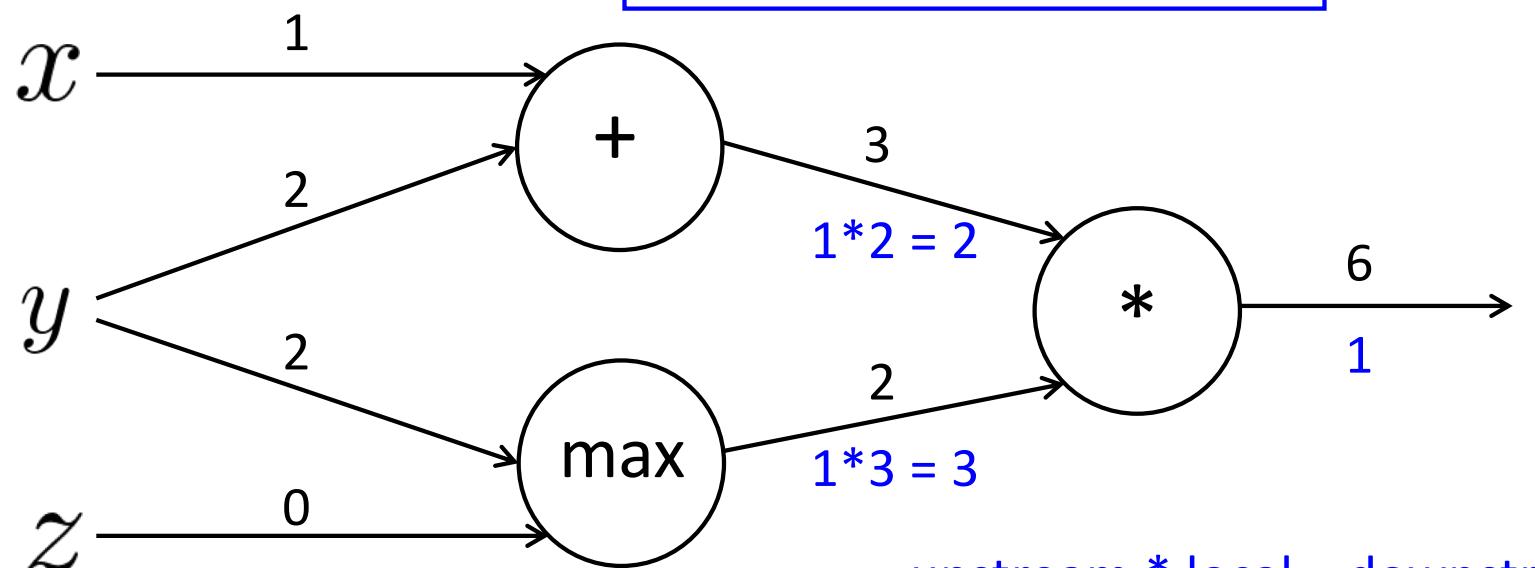
$$f = ab$$

Local gradients

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

$$\boxed{\frac{\partial f}{\partial a} = b = 2 \quad \frac{\partial f}{\partial b} = a = 3}$$



An Example

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Forward prop steps

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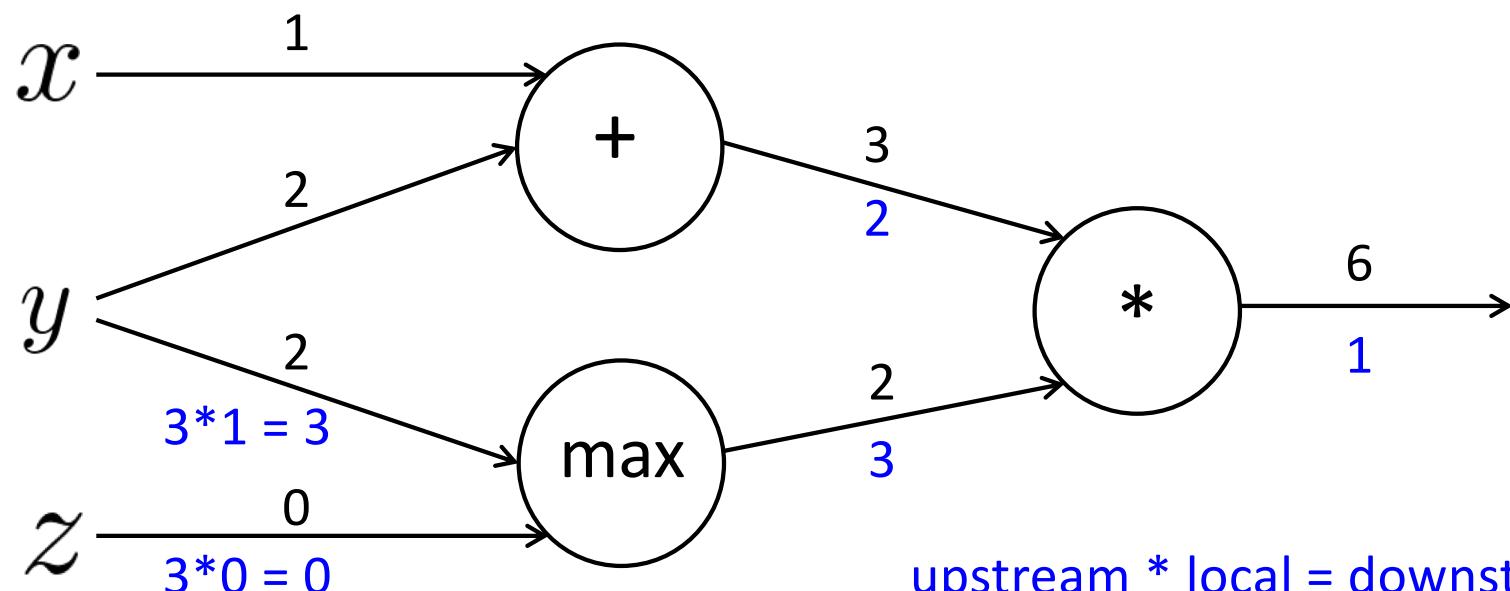
$$f = ab$$

Local gradients

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An Example

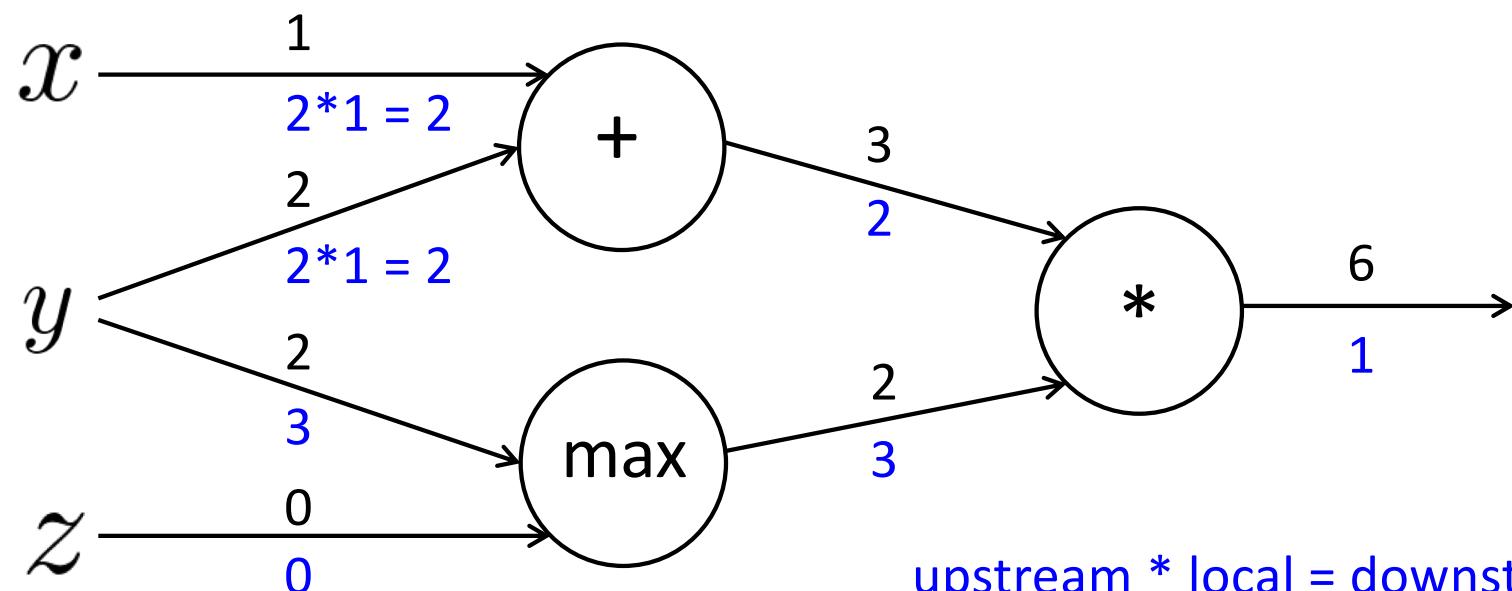
$$f(x, y, z) = (x + y) \max(y, z)$$
$$x = 1, y = 2, z = 0$$

Forward prop steps

$$a = x + y$$

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

$$f = ab$$



An Example

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

Forward prop steps

$$a = x + y$$

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

$$f = ab$$

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

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

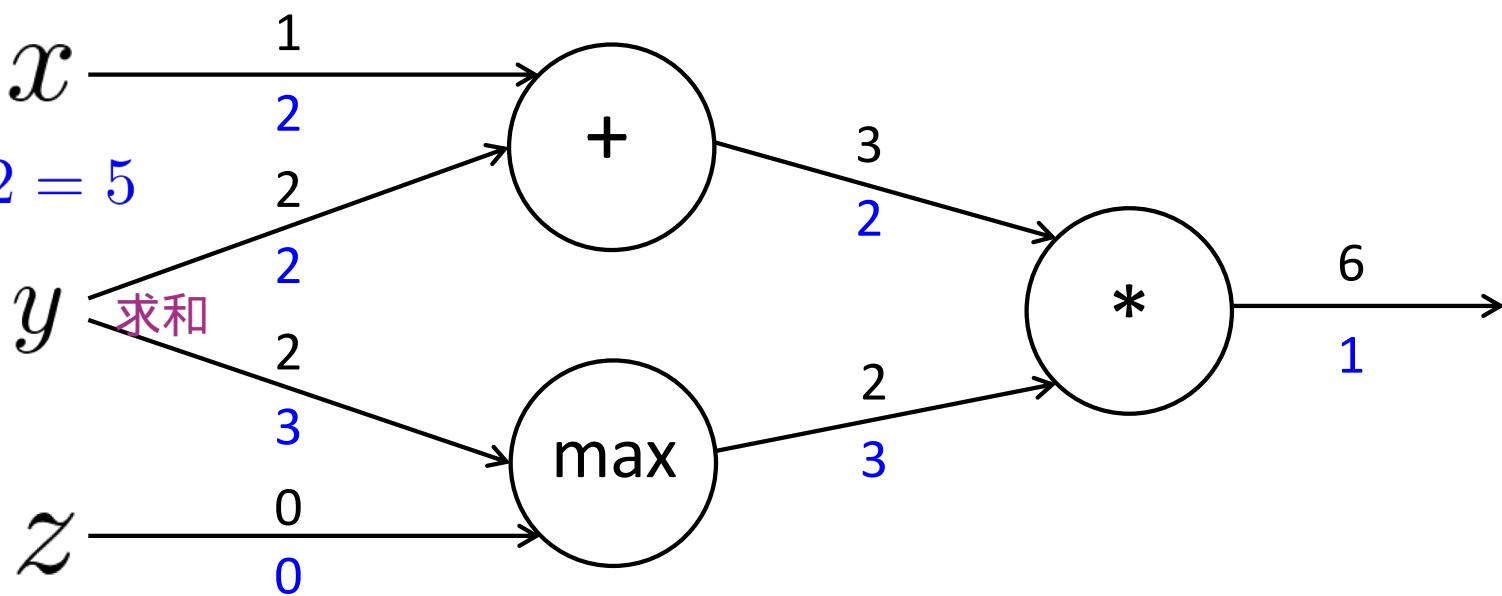
$$\frac{\partial f}{\partial z} = 0$$

Local gradients

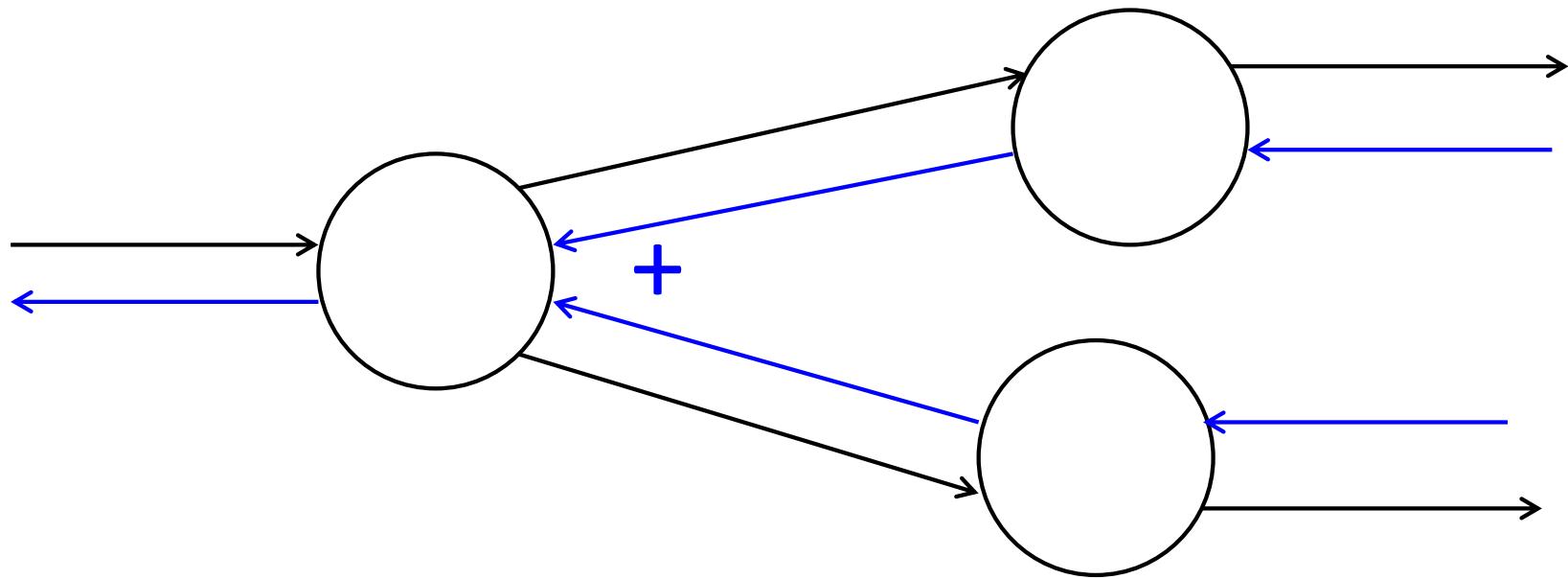
$$\frac{\partial a}{\partial x} = 1 \quad \frac{\partial a}{\partial y} = 1$$

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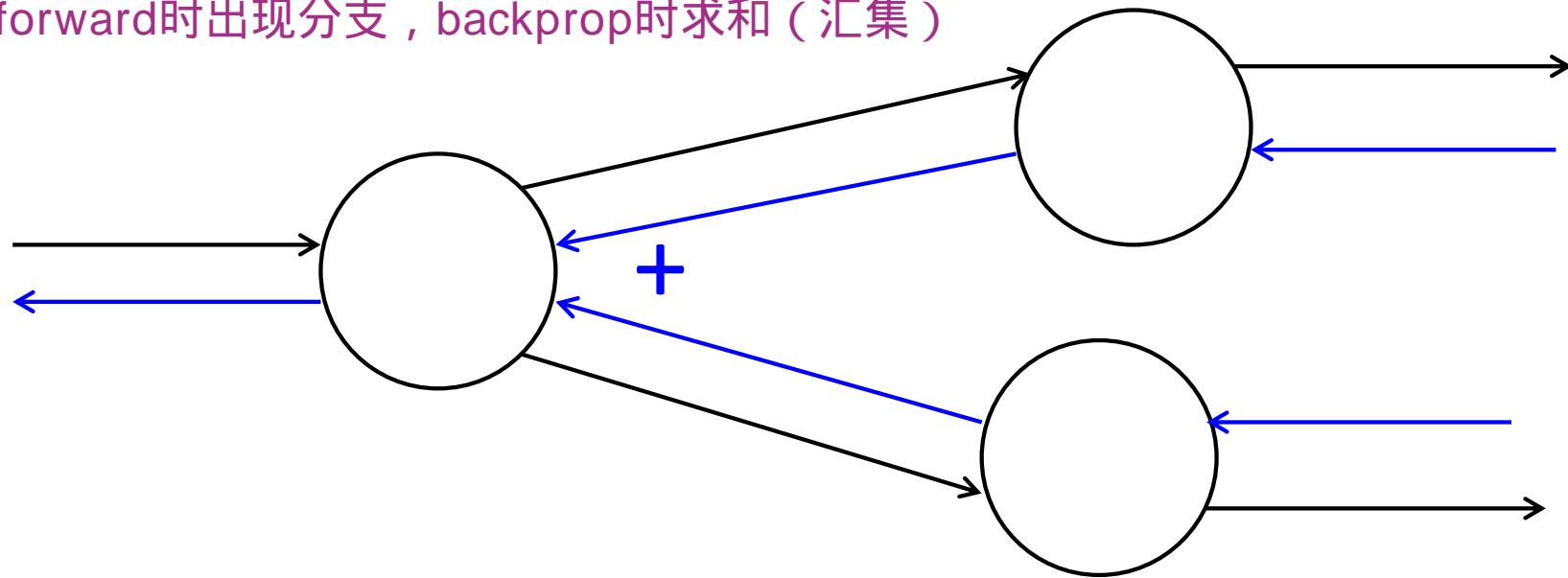


Gradients sum at outward branches



Gradients sum at outward branches

forward时出现分支，backprop时求和（汇集）



$$a = x + y$$

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

$$f = ab$$

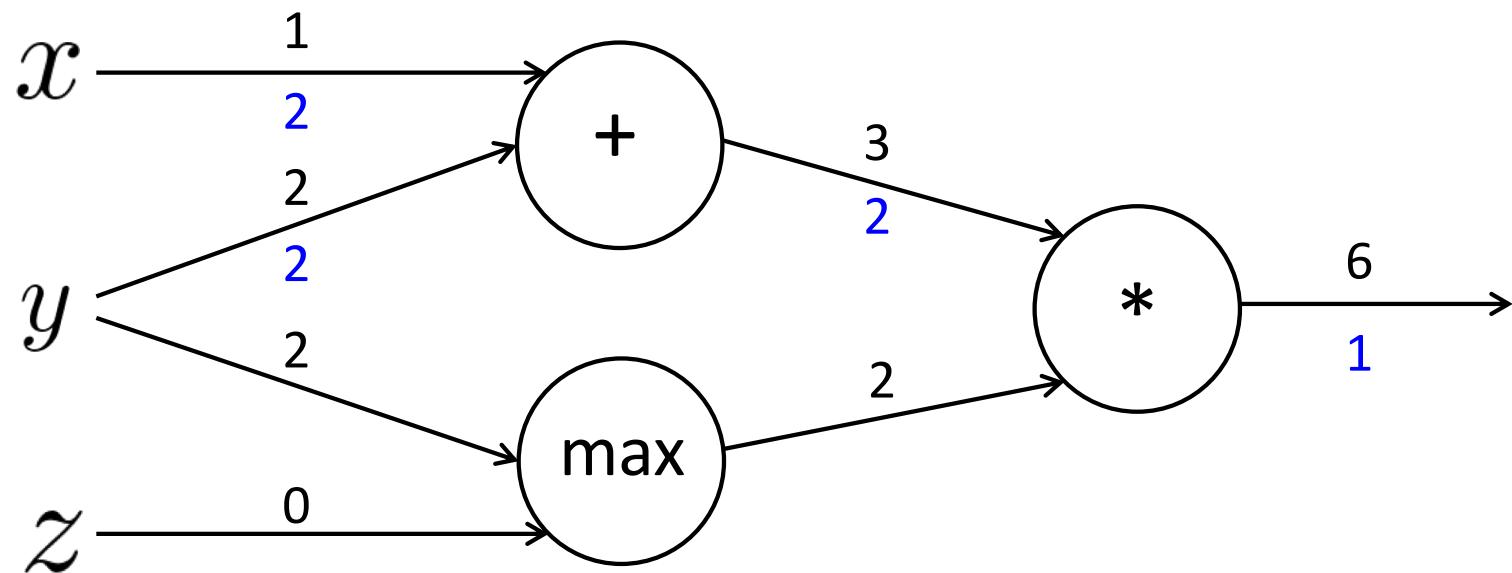
$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial a} \frac{\partial a}{\partial y} + \frac{\partial f}{\partial b} \frac{\partial b}{\partial y}$$

Node Intuitions

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

backprop时：

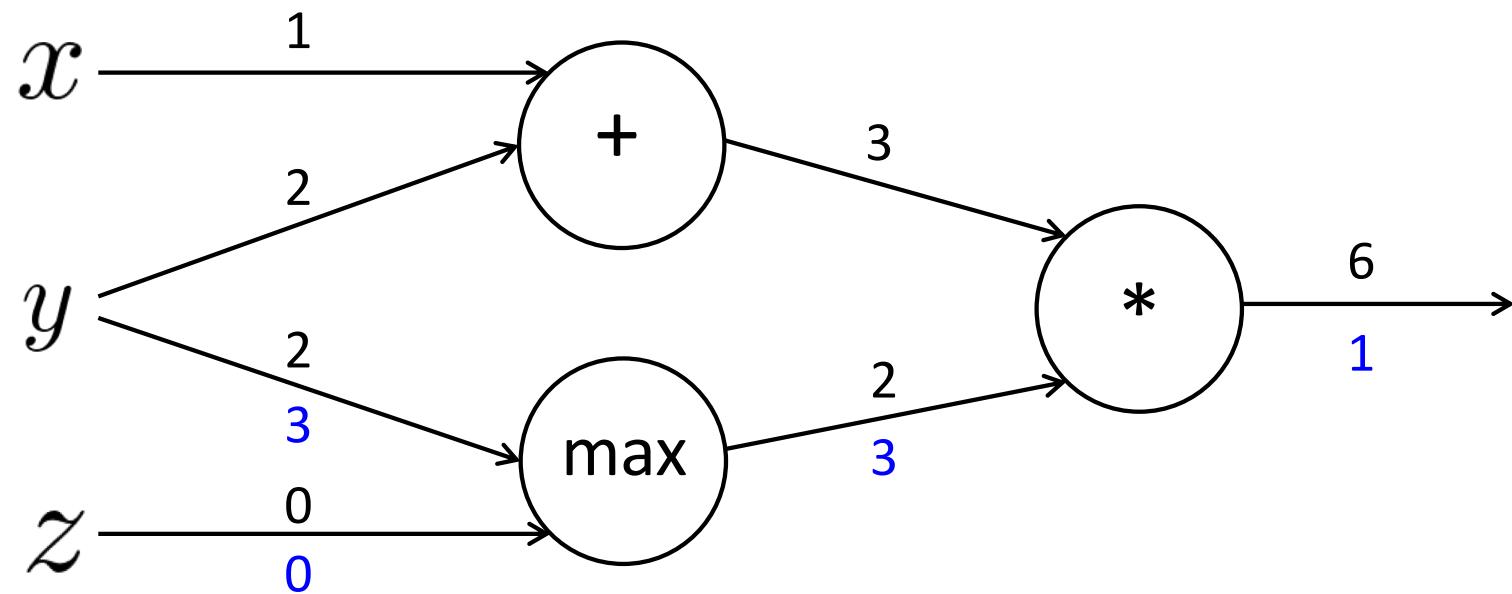
- + “**distributes**” the upstream gradient



Node Intuitions

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

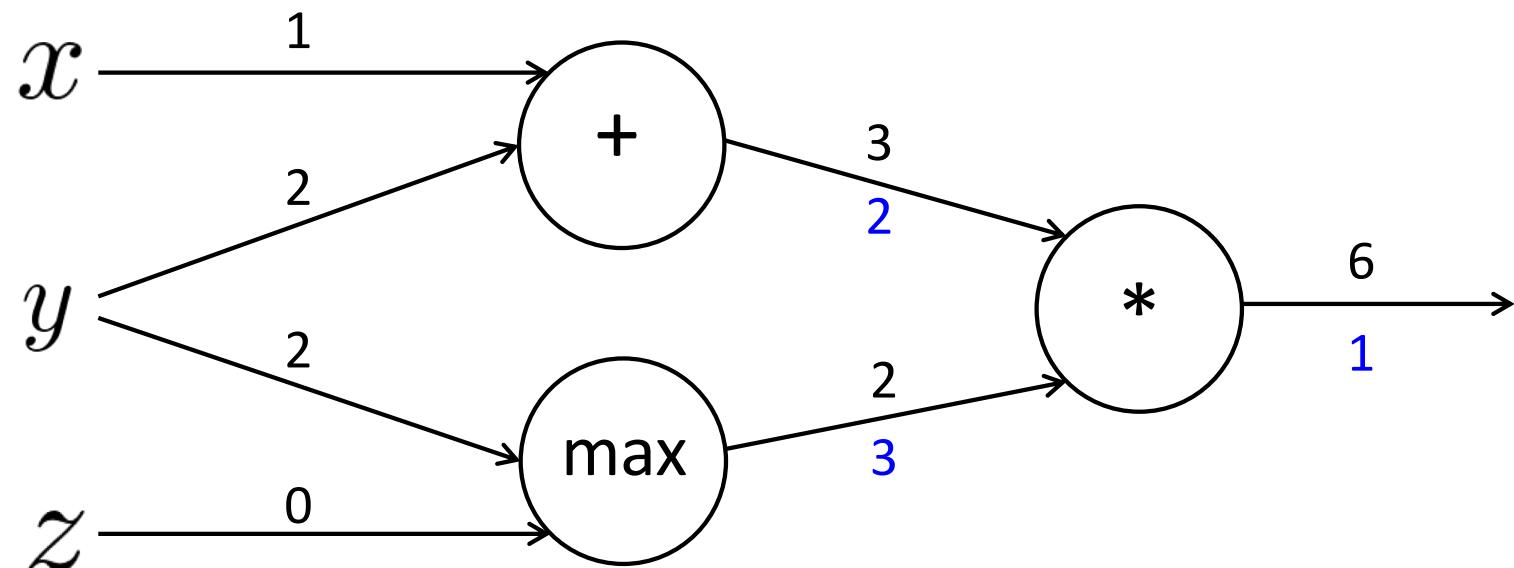
- $+$ “distributes” the upstream gradient to each summand
- \max “routes” the upstream gradient 只有一个梯度 0



Node Intuitions

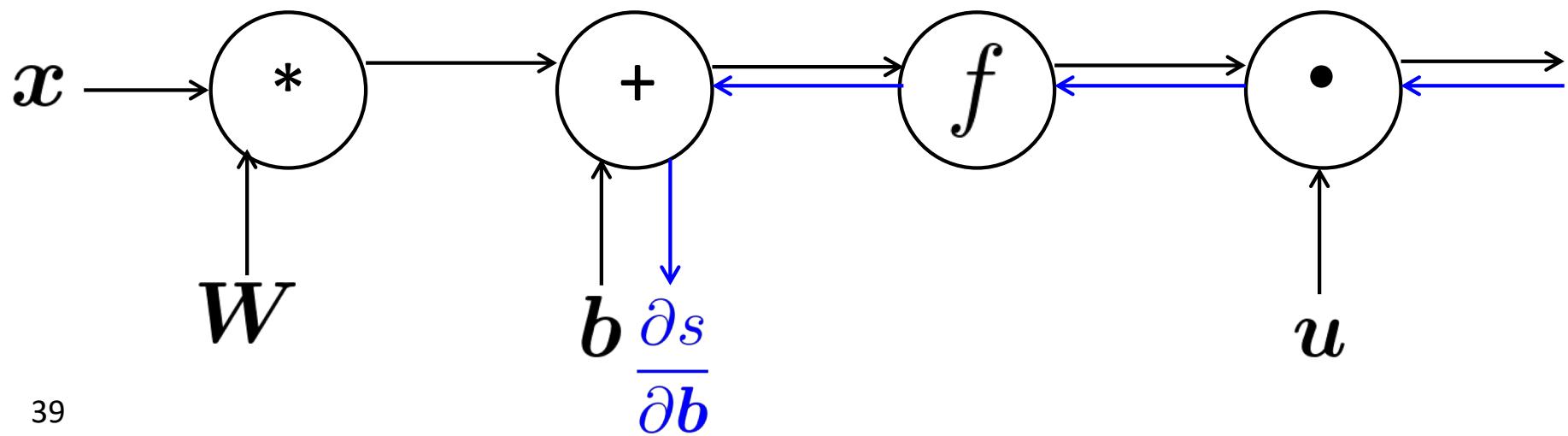
$$f(x, y, z) = (x + y) \max(y, z)$$
$$x = 1, y = 2, z = 0$$

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



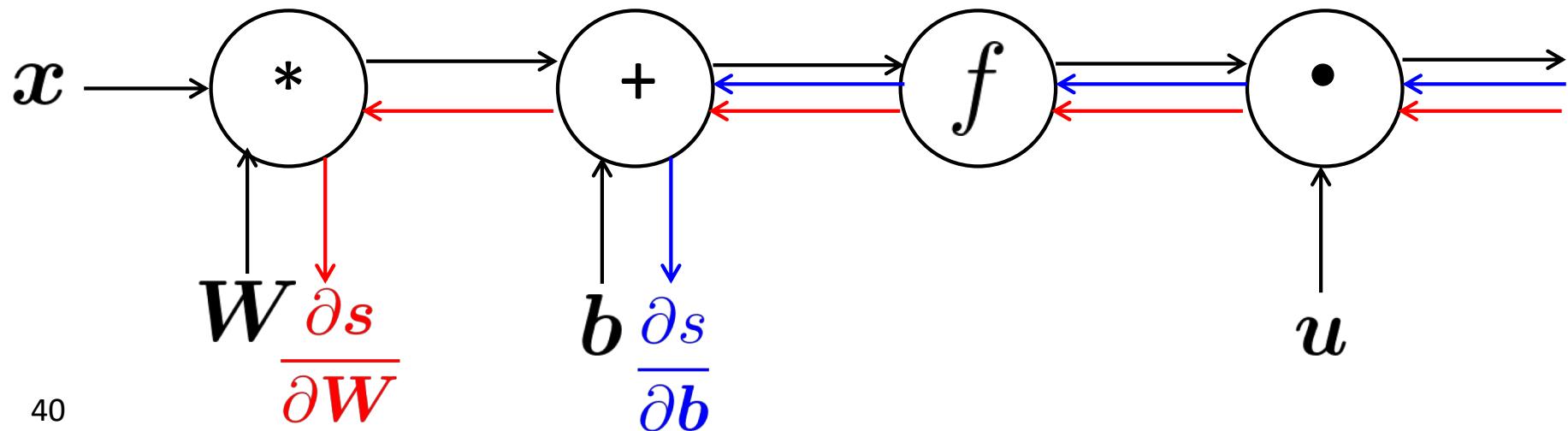
Efficiency: compute all gradients at once

- Incorrect way of doing backprop:
 - First compute $\frac{\partial s}{\partial b}$
- $$s = u^T h$$
- $$h = f(z)$$
- $$z = Wx + b$$
- $$x \quad (\text{input})$$



Efficiency: compute all gradients at once

- Incorrect way of doing backprop:
 - First compute $\frac{\partial s}{\partial b}$
 - Then independently compute $\frac{\partial s}{\partial W}$
 - Duplicated computation!
- $$s = u^T h$$
- $$h = f(z)$$
- $$z = Wx + b$$
- $$x \quad (\text{input})$$



Efficiency: compute all gradients at once

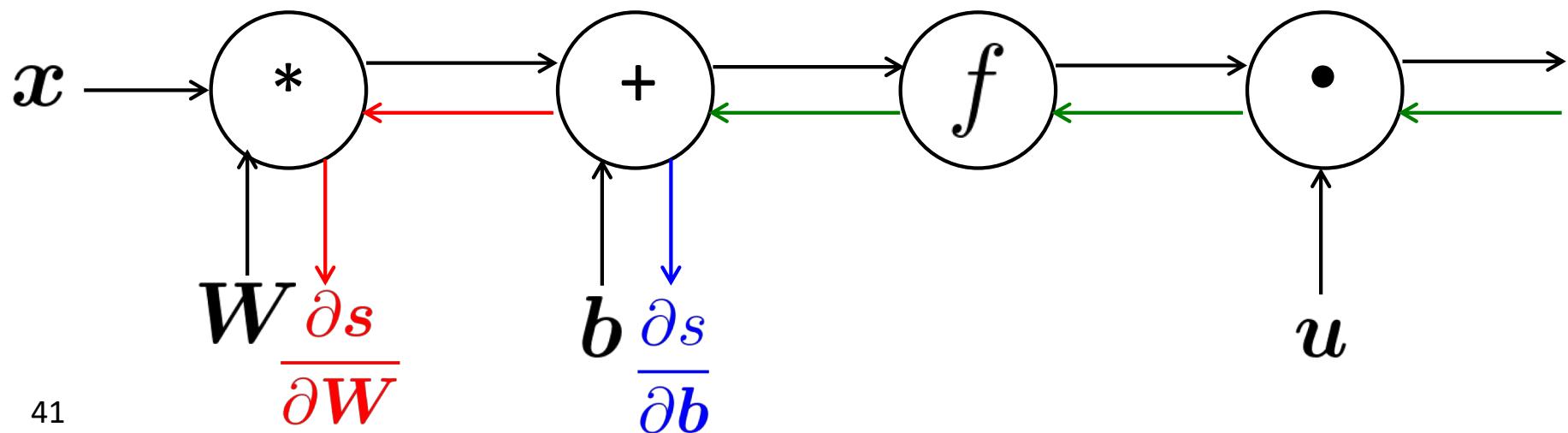
- Correct way:
 - Compute all the gradients at once
 - Analogous to using δ when we computed gradients by hand

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

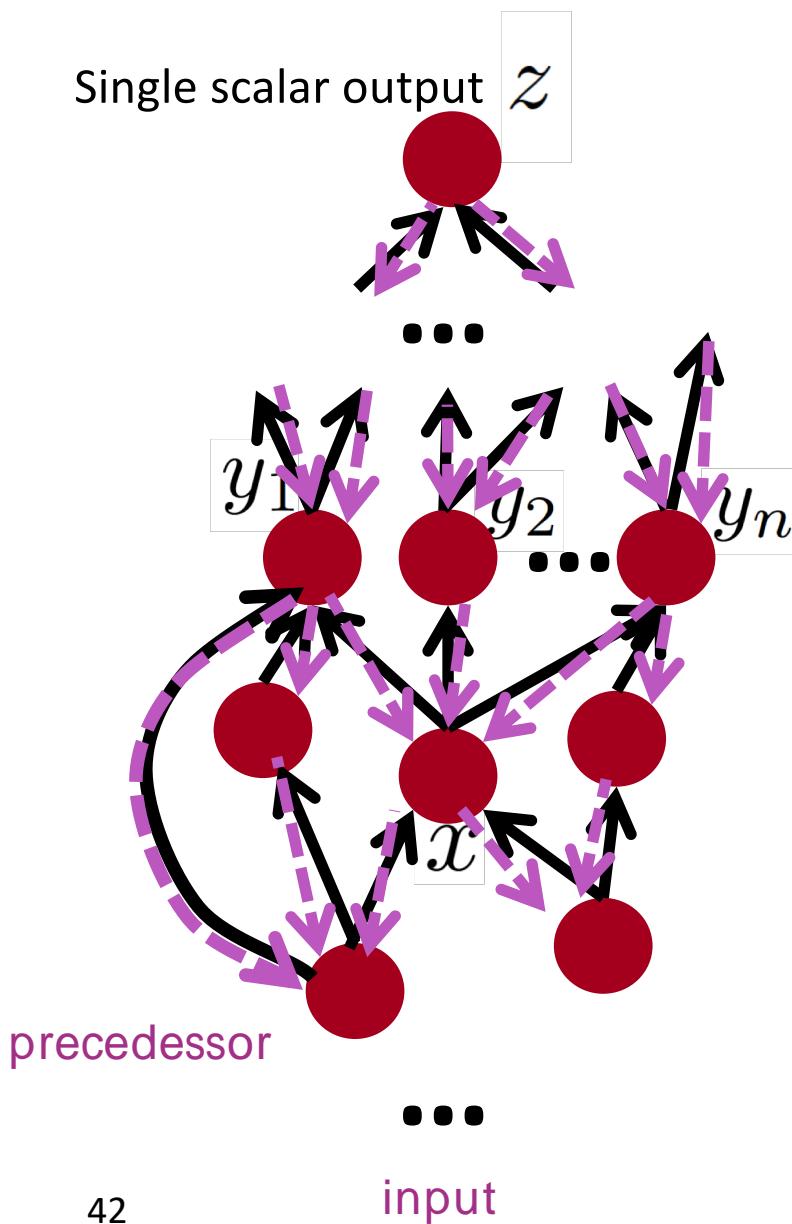
$$\mathbf{h} = f(\mathbf{z})$$

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

\mathbf{x} (input)



Back-Prop in General Computation Graph



- 需要保证不成环
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**
 $\{y_1, y_2, \dots, y_n\}$ = successors of x
above

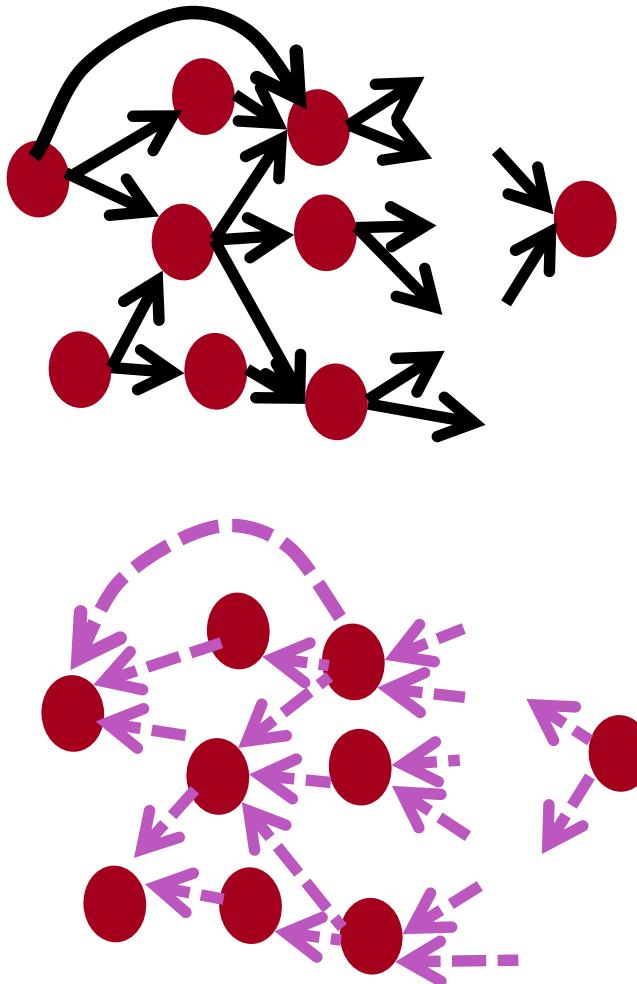
$$\frac{\partial z}{\partial x} = \sum_{i=1}^n \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x}$$

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...

vectorized gradients

Automatic Differentiation



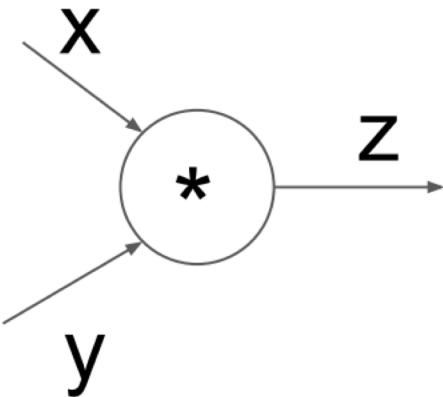
- The gradient computation can be automatically inferred from the **symbolic expression** of the fprop
- Each node type needs to know how to compute its output and how to compute the **gradient** wrt its inputs given the gradient wrt its output
- Modern DL frameworks (Tensorflow, PyTorch, etc.) do backpropagation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

Theano实现了完整的自动微分机制，但是PyTorch等需要自己写forward函数，然后它完成backward（节省了巨大的符号表示）

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)

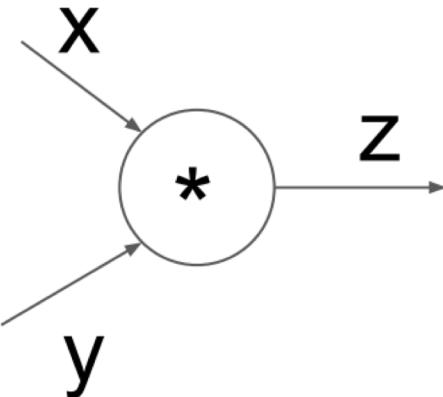
```
class MultiplyGate(object):  
    def forward(x,y):  
        z = x*y  
        return z  
    def backward(dz):  
        # dx = ... #todo  
        # dy = ... #todo  
        return [dx, dy]
```

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

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

Implementation: forward/backward API

DL框架要求实现的



(x, y, z are scalars)

记录inputs , self.x = x # must keep these around!
以便在 backprop中
计算local gradients

```
class MultiplyGate(object):  
    def forward(x,y):  
        z = x*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]
```

Gradient checking: Numeric Gradient

DL早期（2014以前）强调要用数值计算去检查梯度

- For small h ($\approx 1e-4$), $f'(x) \approx \frac{f(x + h) - f(x - h)}{2h}$
- Easy to implement correctly 做双向的梯度检查最好
- But approximate and **very slow**:
 - (属于forward计算=> f)
Have to recompute f for **every parameter** of our model
例如 W_{ij}
- Useful for checking your implementation
 - In the old days when we hand-wrote everything, it was key to do this everywhere.
 - Now much less needed, when throwing together layers

Summary

- We've mastered the core technology of neural nets!!!
- Backpropagation: recursively apply the chain rule along computation graph
 - $[\text{downstream gradient}] = [\text{upstream gradient}] \times [\text{local gradient}]$
- 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.
 - Understanding why is crucial for debugging and improving models
 - See Karpathy article (in syllabus):
 - <https://medium.com/@karpathy/yes-you-should-understand-backprop-e2f06eab496b>
 - Example in future lecture: exploding and vanishing gradients

后面是grab bag (一些技巧?)

3. We have models with many params! Regularization!

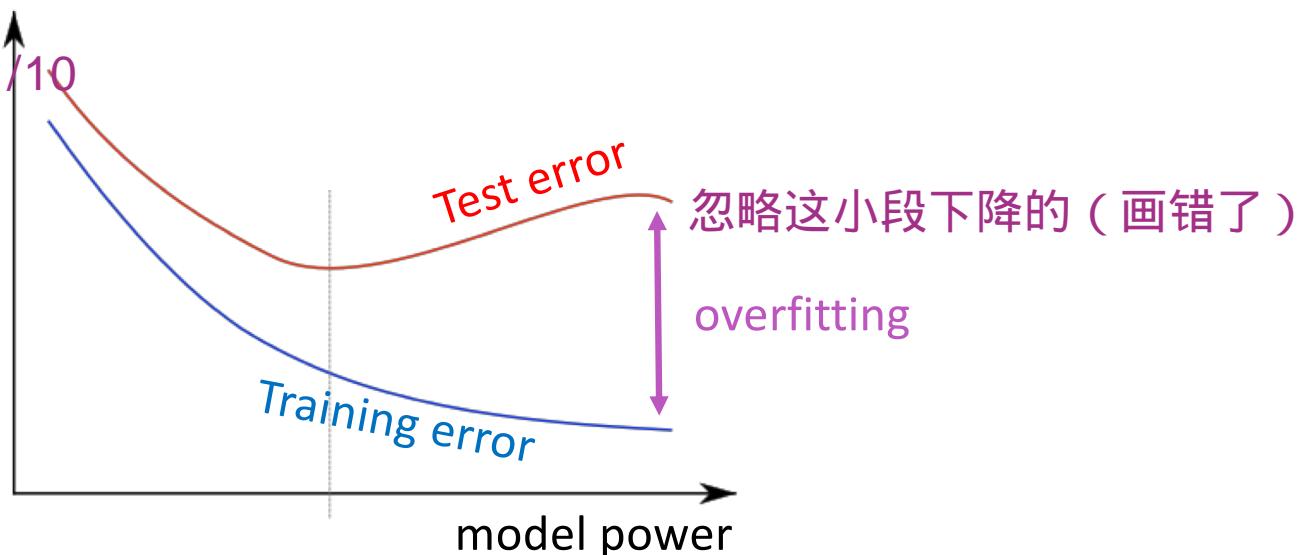
- Really a full loss function in practice includes **regularization** over all parameters θ , e.g., L2 regularization:

$$J(\theta) = \frac{1}{N} \sum_{i=1}^N -\log \left(\frac{e^{f_{y_i}}}{\sum_{c=1}^C e^{f_c}} \right) + \lambda \sum_k \theta_k^2$$

- Regularization (largely) prevents **overfitting** when we have a lot of features (or later a very powerful/deep model, ++)

应该保证：

param数量 < example数目的1/10



“Vectorization”

- E.g., looping over word vectors versus concatenating them all into one large matrix and then multiplying the softmax weights with that matrix

```
from numpy import random
N = 500 # number of windows to classify
d = 300 # dimensionality of each window
C = 5 # number of classes
W = random.rand(C,d)
wordvectors_list = [random.rand(d,1) for i in range(N)]
wordvectors_one_matrix = random.rand(d,N)

%timeit [W.dot(wordvectors_list[i]) for i in range(N)]
%timeit W.dot(wordvectors_one_matrix)
```

- 1000 loops, best of 3: **639 μs** per loop
10000 loops, best of 3: **53.8 μs** per loop

例子中好了一个数量级 (CPU)

而且GPU上只有vectorized才会更好 (?)

“Vectorization”

```
from numpy import random
N = 500 # number of windows to classify
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W = random.rand(C,d)
wordvectors_list = [random.rand(d,1) for i in range(N)]
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%timeit [W.dot(wordvectors_list[i]) for i in range(N)]
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```

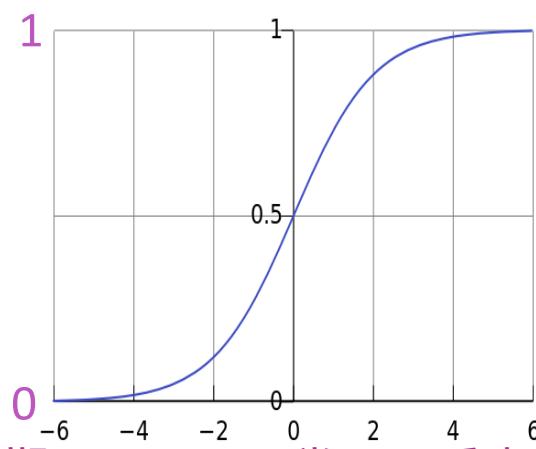
- The (10x) faster method is using a C x N matrix
- Always try to use vectors and matrices rather than for loops!
- You should speed-test your code a lot too!!
- tl;dr: Matrices are awesome!!!

affine layer

Non-linearities: The starting points

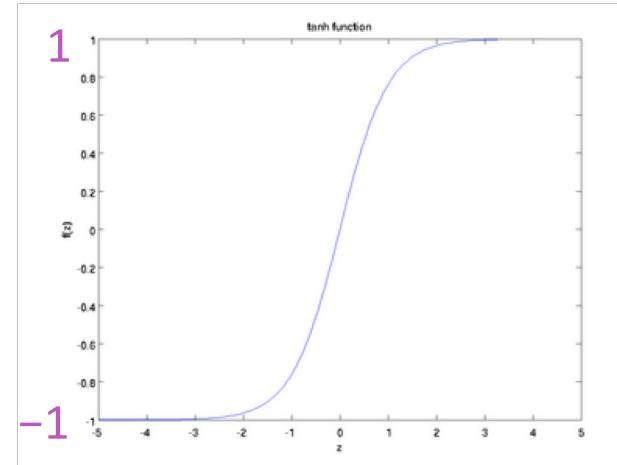
logistic (“sigmoid”)

$$f(z) = \frac{1}{1 + \exp(-z)}.$$



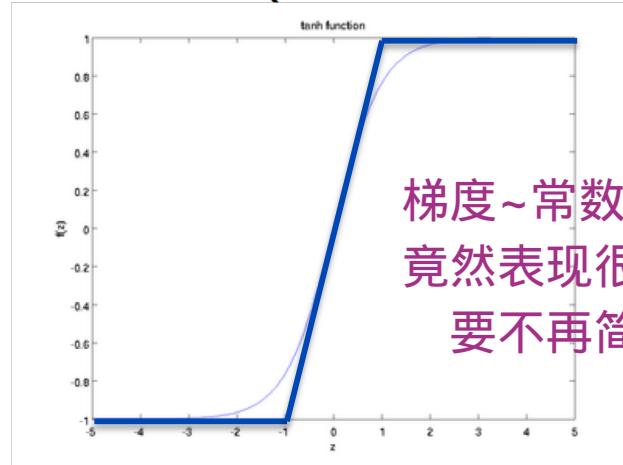
tanh

$$f(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}},$$



hard tanh

$$\text{HardTanh}(x) = \begin{cases} -1 & \text{if } x < -1 \\ x & \text{if } -1 \leq x \leq 1 \\ 1 & \text{if } x > 1 \end{cases}$$



梯度~常数
竟然表现很好
要不再简化点

早期 (80-90s) 常见，后来

几乎不用，只在gating (获得prob) 处

tanh is just a rescaled and shifted sigmoid ($2 \times$ as steep, $[-1, 1]$):

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

【！】就像 $\text{sgn}=2u-1$

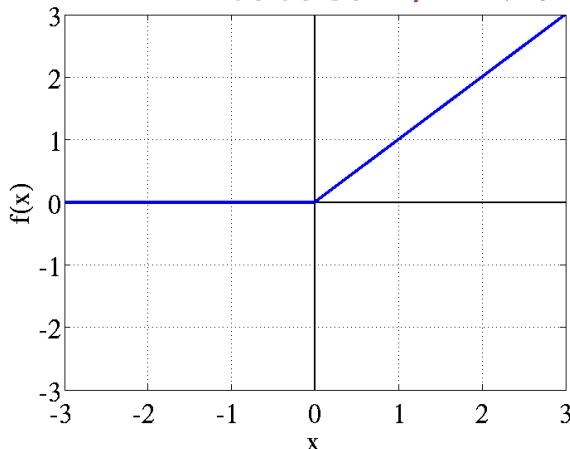
Both logistic and tanh are still used in particular uses, but are no longer the defaults for making deep networks

Non-linearities: The new world order

ReLU (rectified linear unit) hard tanh

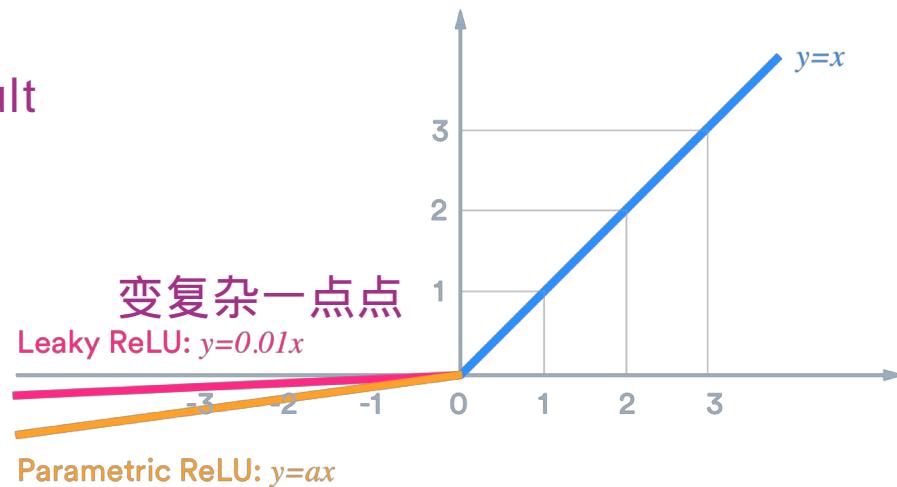
$$\text{rect}(z) = \max(z, 0)$$

hard tanh的再简化，表现更好成了default



Leaky ReLU

Parametric ReLU



可能的原因：梯度不会变化，这样不会长久停滞在一个梯度低的点，训练得更快

- For building a feed-forward deep network, the first thing you should try is ReLU — it trains quickly and performs well due to good gradient backflow

Parameter Initialization

W不可以全0开场，要破坏对称性，否则很可能同时变化

- You normally must initialize weights to small random values
 - To avoid symmetries that prevent learning/specialization
 - Initialize hidden layer biases to 0 and output (or reconstruction) biases to optimal value if weights were 0 (e.g., mean target or inverse sigmoid of mean target)
 - Initialize all other weights $\sim \text{Uniform}(-r, r)$, with r chosen so numbers get neither too big or too small
- PyTorch等推荐使用的
- Xavier initialization has variance inversely proportional to fan-in n_{in} (previous layer size) and fan-out n_{out} (next layer size):

$$\text{Var}(W_i) = \frac{2}{n_{\text{in}} + n_{\text{out}}}$$

Optimizers

- Usually, plain SGD will work just fine
 - However, getting good results will often require hand-tuning the learning rate (next slide)
- For more complex nets and situations, or just to avoid worry, you often do better with one of a family of more sophisticated “adaptive” optimizers that scale the parameter adjustment by an accumulated gradient.
 - These models give per-parameter learning rates
 - Adagrad 每个参数有自己的lr
 - RMSprop
 - Adam ← A fairly good, safe place to begin in many cases
 - SparseAdam
 - ...

Learning Rates

- You can just use a constant learning rate. Start around $lr = 0.001$?
 - It must be order of magnitude right – try powers of 10
 - Too big: model may diverge or not converge
 - Too small: your model may not have trained by the deadline
- Better results can generally be obtained by allowing learning rates to decrease as you train
 - By hand: halve the learning rate every k epochs
 - An epoch = a pass through the data (shuffled or sampled)
 - By a formula: $lr = lr_0 e^{-kt}$, for epoch t
 - There are fancier methods like cyclic learning rates (q.v.)
Ir时大时小，有助于绕开bad region
- Fancier optimizers still use a learning rate but it may be an initial rate that the optimizer shrinks – so may be able to start high