CS-671: Deep Learning and its Applications
Lecture: 09
Backpropagation and Neural Networks

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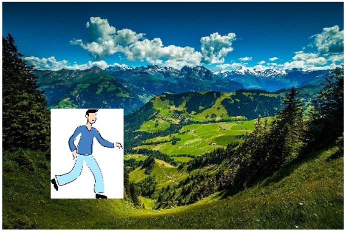
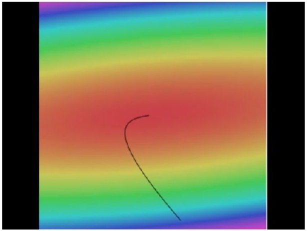
Presentation for CS-671@IIT Mandi (7 March, 2019)
(*Slides Credit : Stanford University CS231n, Spring 2017)
https://www.youtube.com/watch?v=vT1JzLTH4G4&list=PLC1qU-LWwrF64f4QKQT-Vg5Wr4qEE1Zxk

February - May, 2019

Optimization





Landscape image is CC0 1.0 public domain
Walking man image is CC0 1.0 public domain

```
# Vanilla Gradient Descent

while True:
  weights_grad = evaluate_gradient(loss_fun, data, weights)
  weights += - step_size * weights_grad # perform parameter update
```

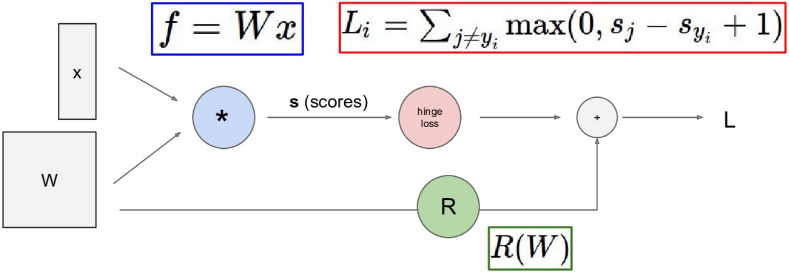
Gradient descent

$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Numerical gradient: slow :(, approximate :(, easy to write :)
Analytic gradient: fast :), exact :), error-prone :(

In practice: Derive analytic gradient, check your implementation with numerical gradient

Computational graphs

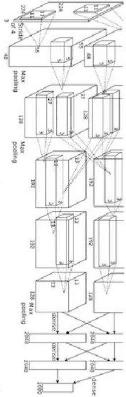


Convolutional network (AlexNet)

input image

weights

loss



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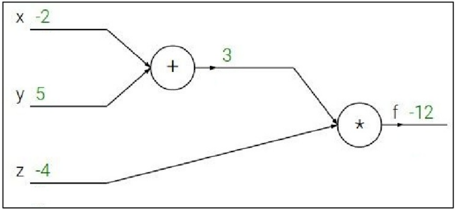
Backpropagation: a simple example

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

e.g. x = -2, y = 5, z = -4



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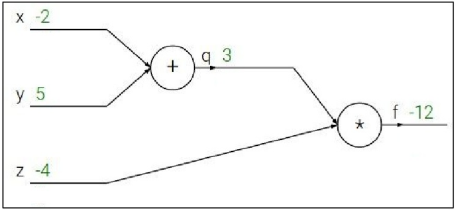
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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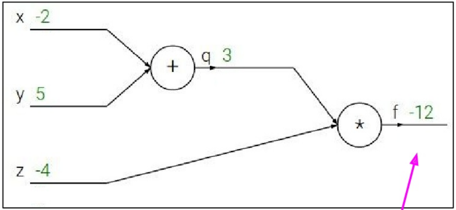

$\frac{\partial f}{\partial f}$

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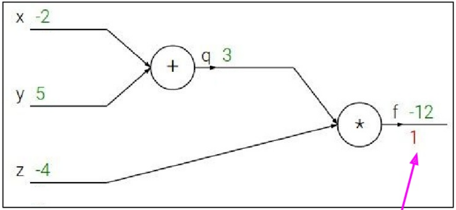

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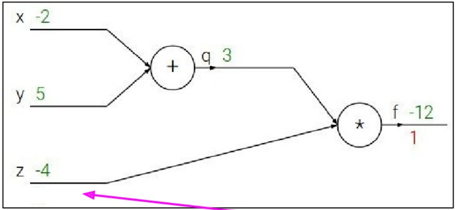

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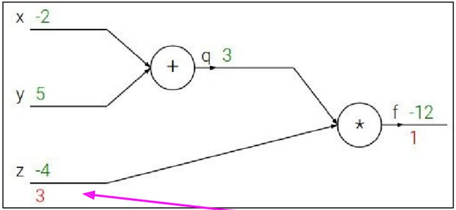

$$\boxed{\frac{\partial f}{\partial z}}$$

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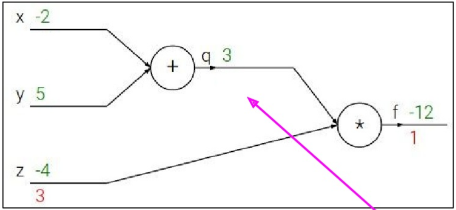

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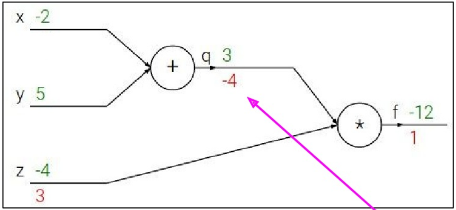

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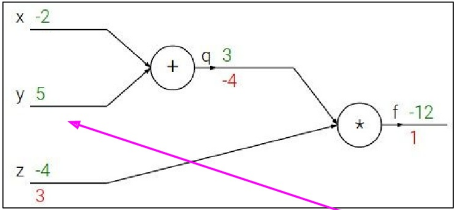

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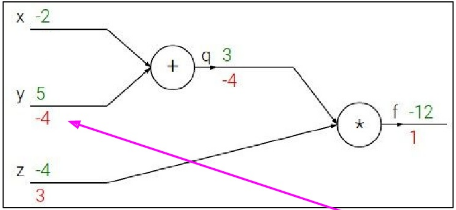

Chain rule:

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial y}$$

$$\frac{\partial f}{\partial y}$$

Backpropagation: a simple example

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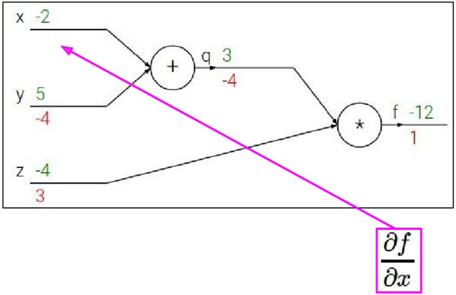

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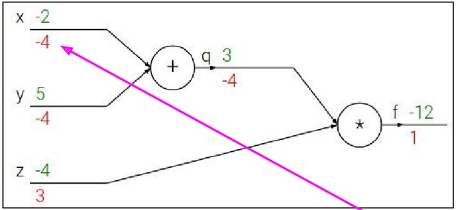
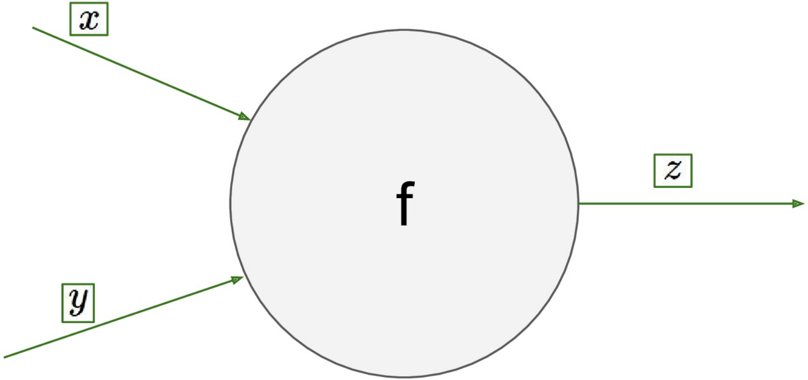


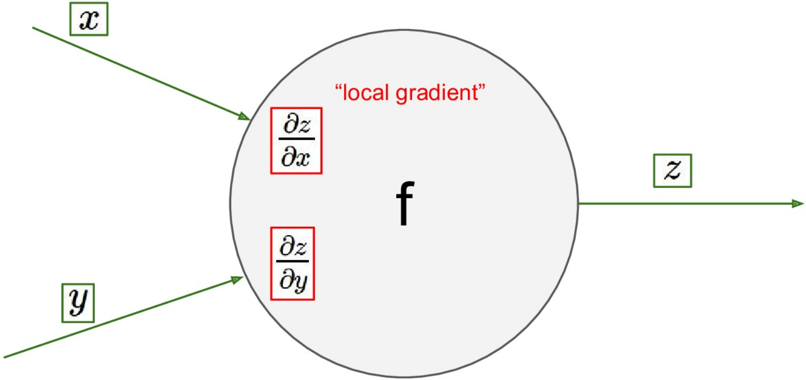
$$\boxed{\frac{\partial f}{\partial x}}$$

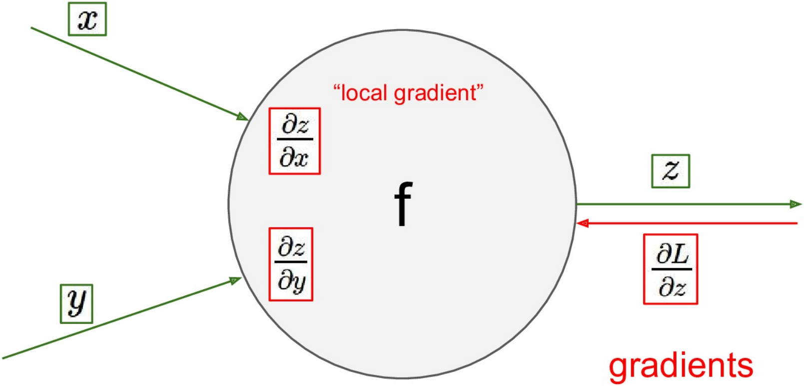
Chain rule:

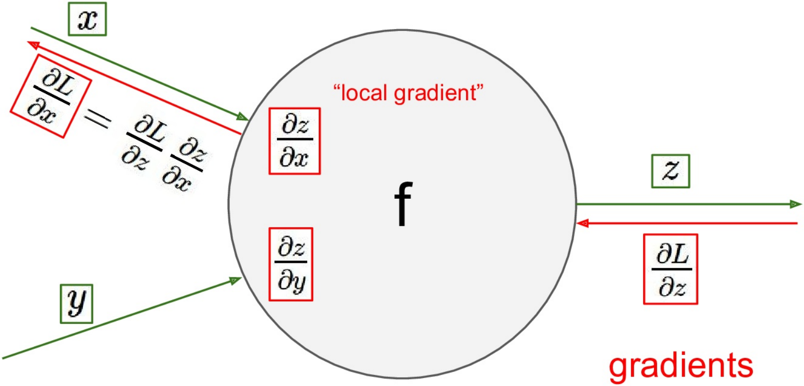
$$\boxed{\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial x}}$$



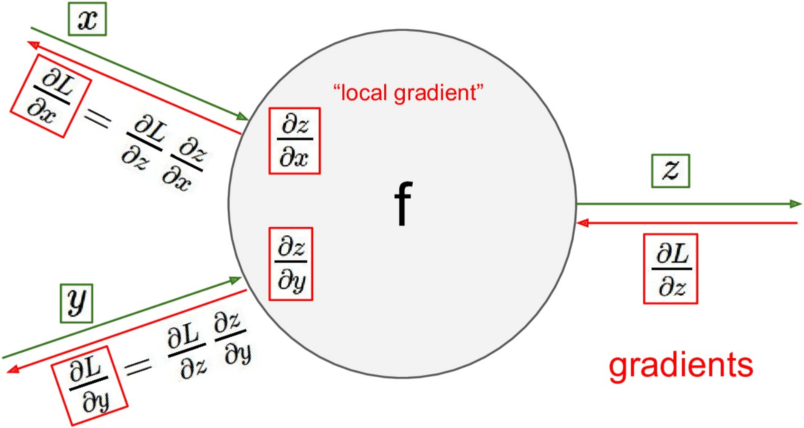
x
y
f
z


x
"local gradient"
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial z}{\partial y}$
y


x
"local gradient"
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial z}{\partial y}$
$\frac{\partial L}{\partial z}$
y
gradients



x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"local gradient"
$\frac{\partial z}{\partial x}$
f
$\frac{\partial z}{\partial y}$
y
z
$\frac{\partial L}{\partial z}$
gradients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$\frac{\partial L}{\partial z}$
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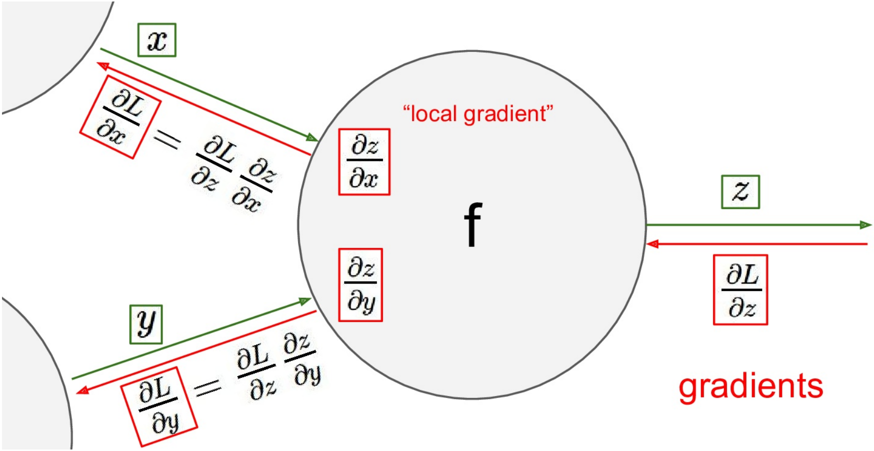
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
gradients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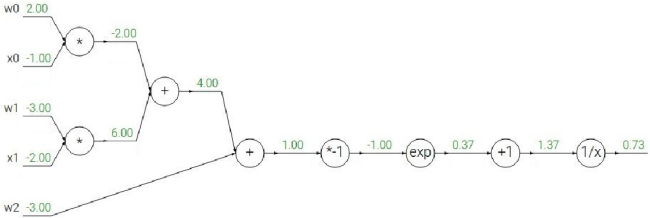
"local gradient"
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial z}{\partial y}$
$\frac{\partial L}{\partial z}$
y
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
gradients

Another example: $$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



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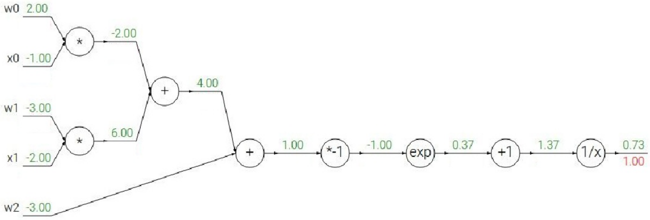

$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$ | $f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$

$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$ | $f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$

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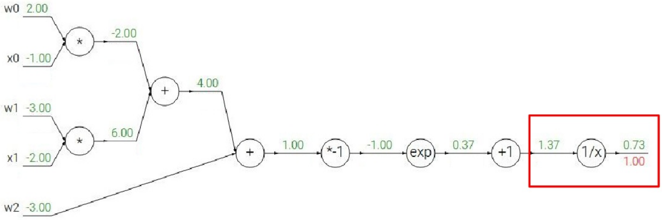

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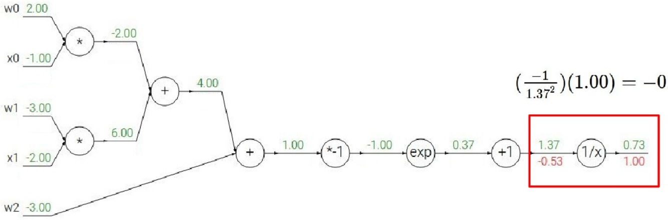
Another example: $f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$

$$\left(\frac{-1}{1.37^2}\right)(1.00) = -0.53$$



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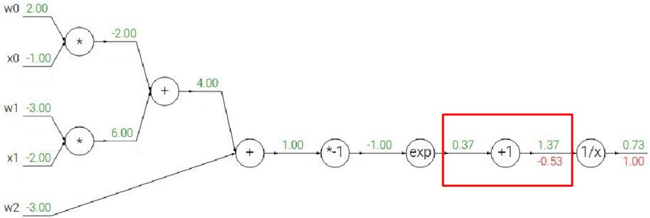

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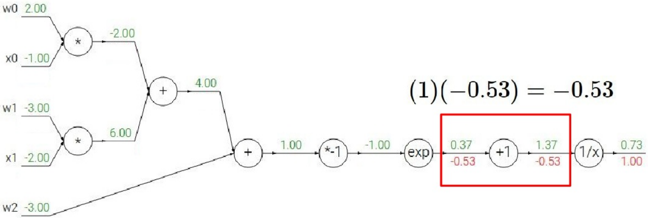
Another example: $f(w,x) = \dfrac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$

$$(1)(-0.53) = -0.53$$



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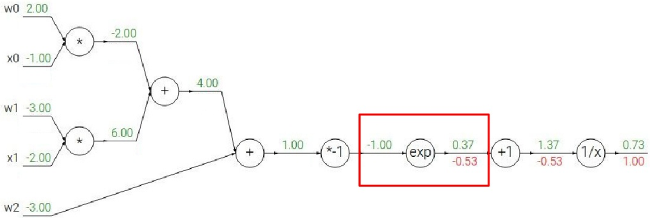

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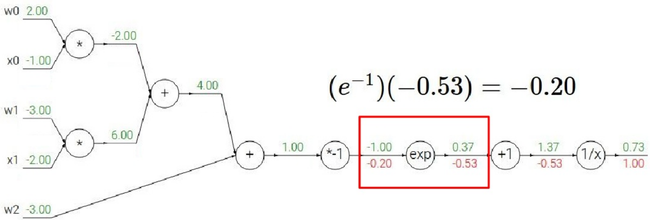

$$(e^{-1})(-0.53) = -0.20$$

$\boxed{f(x) = e^x}$	$\rightarrow$	$\boxed{\dfrac{df}{dx} = e^x}$	$f(x) = \dfrac{1}{x}$	$\rightarrow$	$\dfrac{df}{dx} = -1/x^2$
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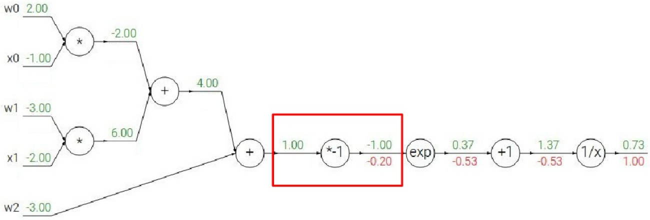

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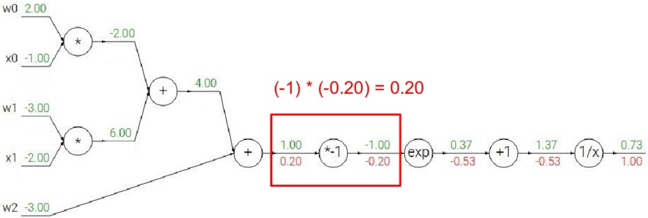

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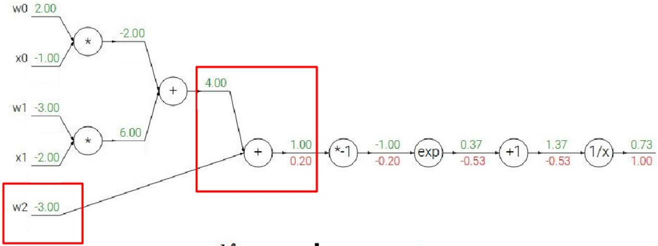

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Another example:

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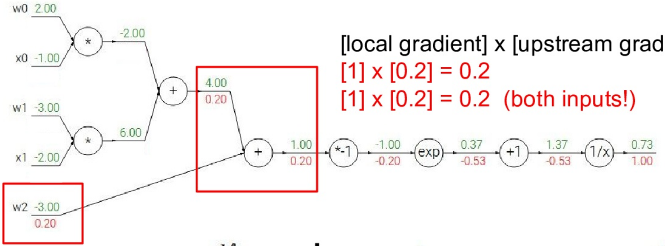
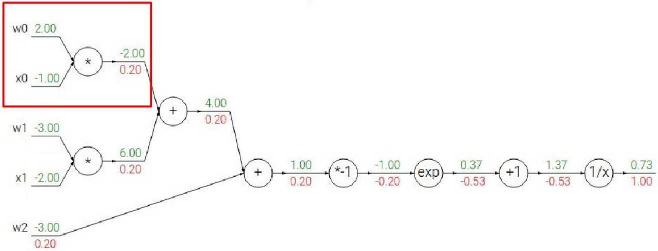


[local gradient] x [upstream gradient]
[1] x [0.2] = 0.2
[1] x [0.2] = 0.2 (both inputs!)

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x \qquad\qquad f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a \qquad\qquad f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

Another example: $f(w,x) = \dfrac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$



$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x \qquad \Bigg| \qquad f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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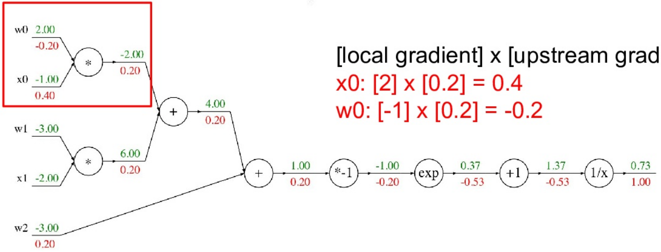


[local gradient] x [upstream gradient]

x0: [2] x [0.2] = 0.4

w0: [-1] x [0.2] = -0.2

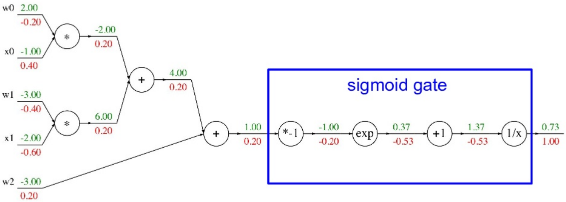
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x \qquad\qquad f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a \qquad\qquad f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

$$\boxed{\sigma(x) = \frac{1}{1+e^{-x}}}$$ sigmoid function

$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$



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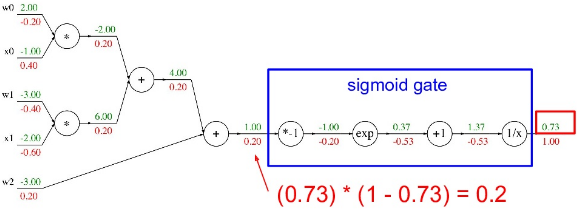
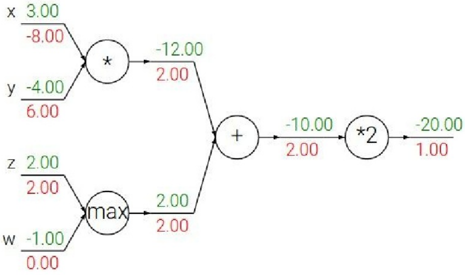


Patterns in backward flow

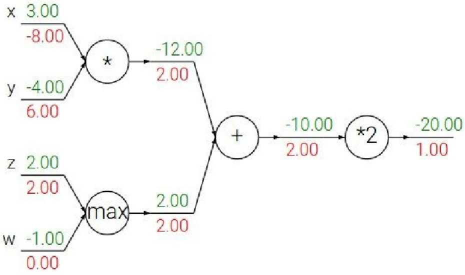
add gate: gradient distributor



Patterns in backward flow

add gate: gradient distributor

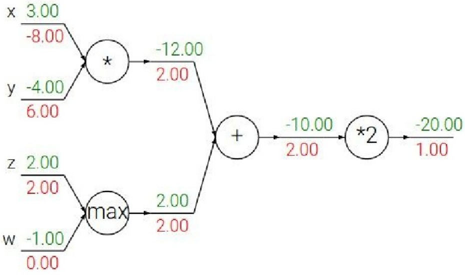
Q: What is a **max** gate?



Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

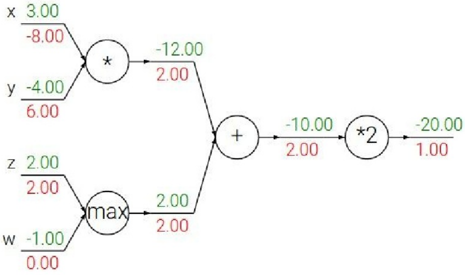


Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

Q: What is a **mul** gate?

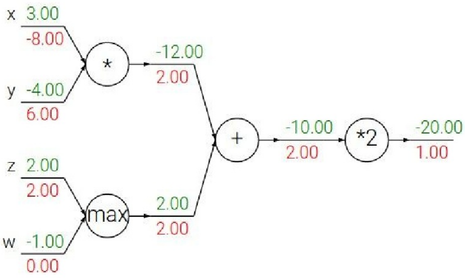


Patterns in backward flow

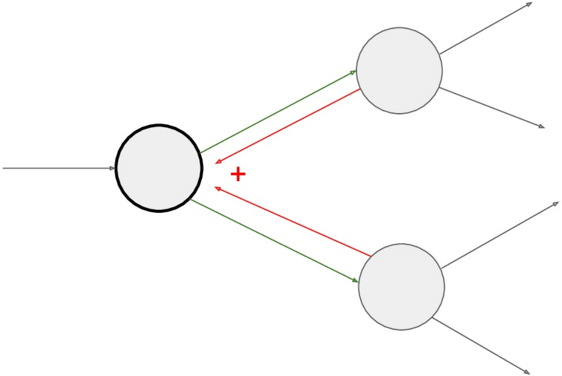
add gate: gradient distributor

max gate: gradient router

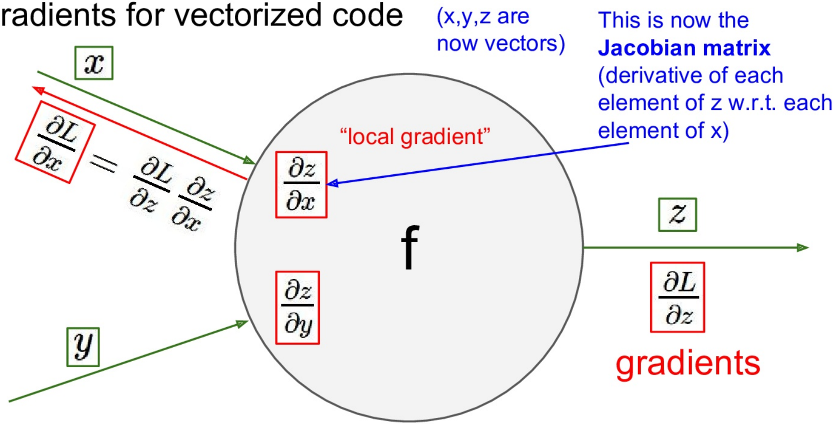
mul gate: gradient switcher



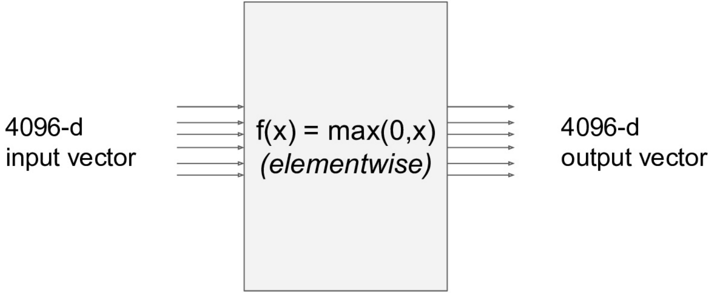
Gradients add at branches



Gradients for vectorized code



Vectorized operations

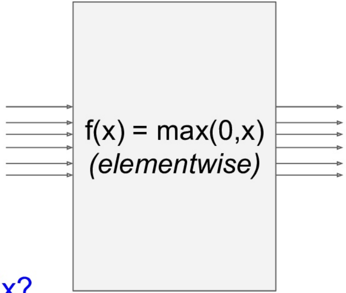


Vectorized operations

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

Jacobian matrix

4096-d
input vector



4096-d
output vector

Q: what is the size of the Jacobian matrix?

Vectorized operations

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Jacobian matrix

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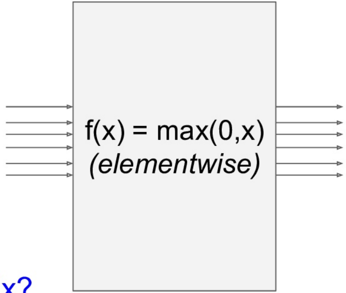
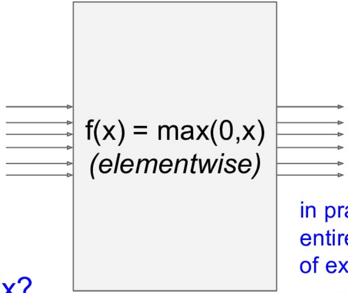


4096-d
output vector

Q: what is the size of the Jacobian matrix?
[4096 x 4096!]

Vectorized operations

4096-d
input vector



4096-d
output vector

Q: what is the size of the Jacobian matrix? [4096 x 4096!]

in practice we process an entire minibatch (e.g. 100) of examples at one time:

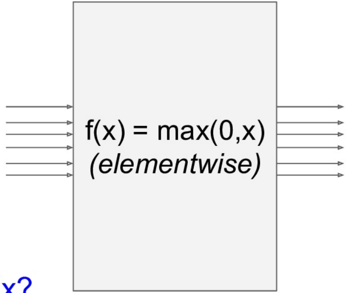
i.e. Jacobian would technically be a [409,600 x 409,600] matrix :\

Vectorized operations

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

Jacobian matrix

4096-d
input vector



4096-d
output vector

Q: what is the size of the Jacobian matrix?
[4096 x 4096!]

Q2: what does it look like?

A vectorized example: $f(x, W) = ||W \cdot x||^2 = \sum_{i=1}^{n} (W \cdot x)_i^2$

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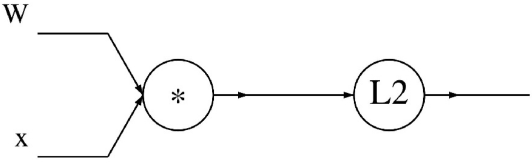
$$\underset{\in \mathbb{R}^n}{x} \quad \underset{\in \mathbb{R}^{n \times n}}{W}$$

A vectorized example: $f(x, W) = ||W \cdot x||^2 = \sum_{i=1}^{n} (W \cdot x)_i^2$



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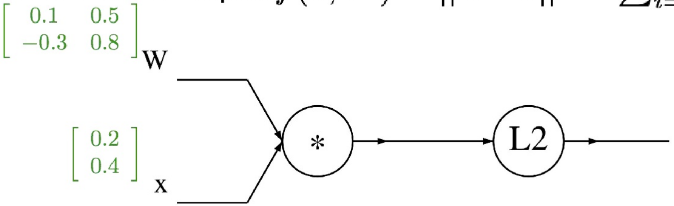

$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \cdots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \cdots + W_{n,n}x_n \end{pmatrix}$$

$$f(q) = ||q||^2 = q_1^2 + \cdots + q_n^2$$

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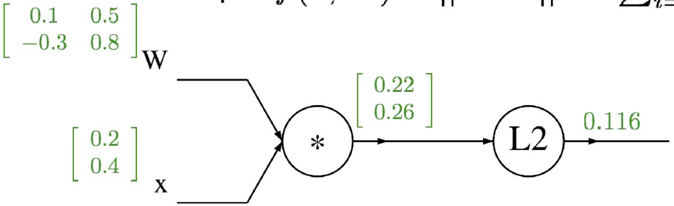

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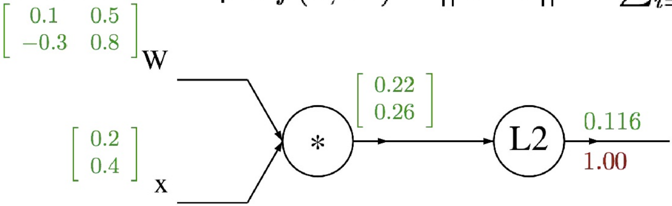

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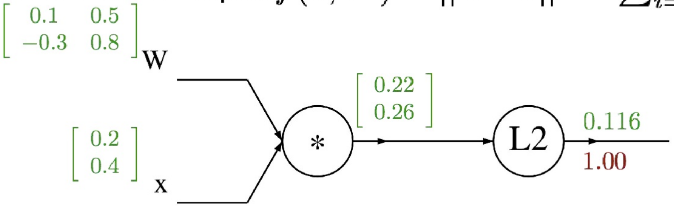

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$$\frac{\partial f}{\partial q_i} = 2q_i$$

$$\boxed{\nabla_q f = 2q}$$

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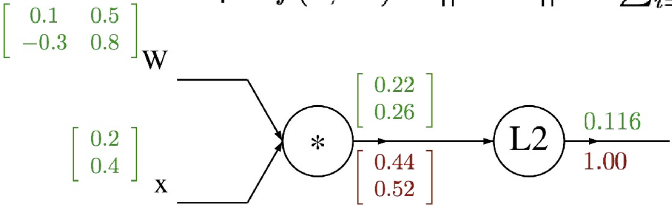

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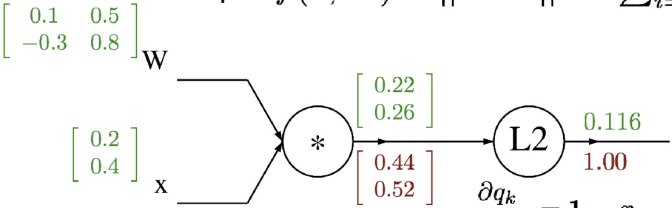

$$\frac{\partial q_k}{\partial W_{i,j}} = \mathbf{1}_{k=i} x_j$$

$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \cdots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \cdots + W_{n,n}x_n \end{pmatrix}$$

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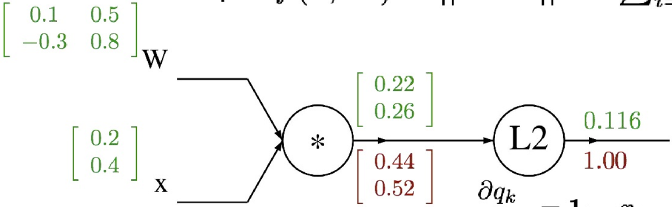

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$$\frac{\partial f}{\partial W_{i,j}} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial W_{i,j}}$$

$$= \sum_k (2q_k)(\mathbf{1}_{k=i} x_j)$$

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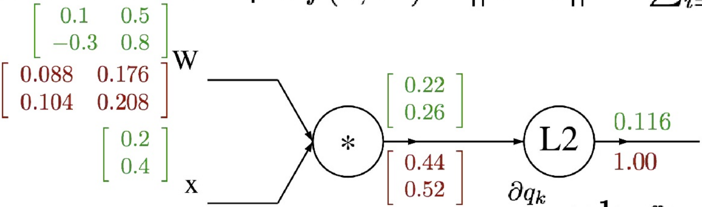

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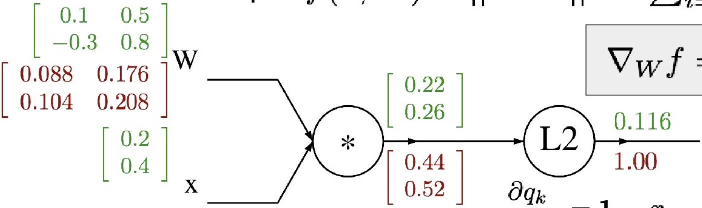
$$\begin{aligned} \frac{\partial f}{\partial W_{i,j}} &= \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial W_{i,j}} \\ &= \sum_k (2q_k)(\mathbf{1}_{k=i} x_j) \\ &= 2q_i x_j \end{aligned}$$

A vectorized example: $f(x, W) = ||W \cdot x||^2 = \sum_{i=1}^{n} (W \cdot x)_i^2$

$$\boxed{\nabla_W f = 2q \cdot x^T}$$



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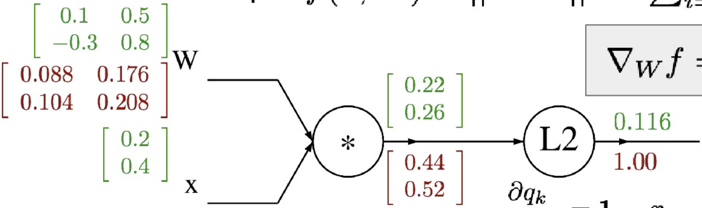

$$\boxed{\nabla_W f = 2q \cdot x^T}$$

Always check: The gradient with respect to a variable should have the same shape as the variable

$$\frac{\partial q_k}{\partial W_{i,j}} = \mathbf{1}_{k=i} x_j$$

$$\frac{\partial f}{\partial W_{i,j}} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial W_{i,j}} = \sum_k (2q_k)(\mathbf{1}_{k=i} x_j) = 2q_i x_j$$

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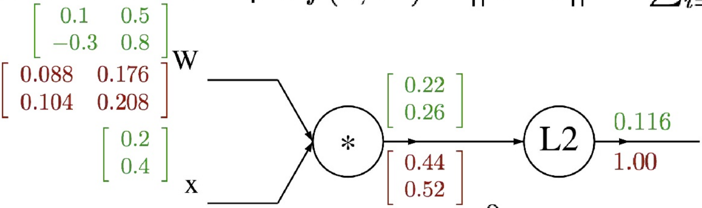

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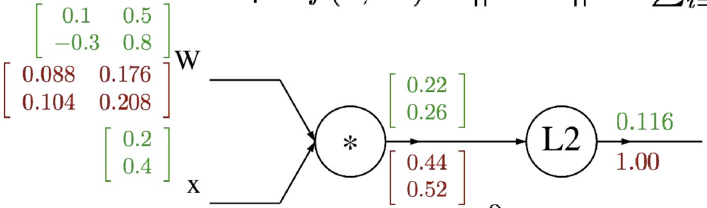

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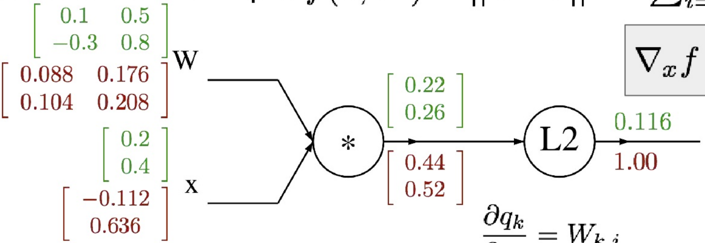
$$\boxed{\nabla_x f = 2W^T \cdot q}$$



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$$\frac{\partial q_k}{\partial x_i} = W_{k,i}$$

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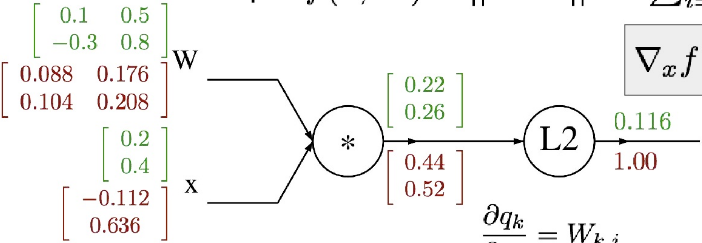

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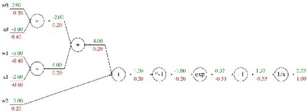
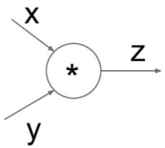
Modularized implementation: forward / backward API



Graph (or Net) object *(rough psuedo code)*

```
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
```

Modularized implementation: forward / backward API



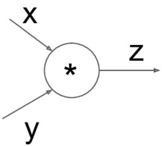
(x,y,z are scalars)

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

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

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

Modularized implementation: forward / backward API



(x,y,z are scalars)

```python
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]
```

Summary so far...

- neural nets will be very large: impractical to write down gradient formula by hand for all parameters
- **backpropagation** = recursive application of the chain rule along a computational graph to compute the gradients of all inputs/parameters/intermediates
- implementations maintain a graph structure, where the nodes implement the **forward**() / **backward**() API
- **forward**: compute result of an operation and save any intermediates needed for gradient computation in memory
- **backward**: apply the chain rule to compute the gradient of the loss function with respect to the inputs