Lecture 4: Backpropagation and Neural Networks

Lecture 4: Backpropagation and Neural Networks

Administrative

Assignment 1 due **Thursday April 20**, 11:59pm on Canvas

Administrative

Project: TA specialities and some project ideas are posted on Piazza

Administrative

Google Cloud: All registered students will receive an email this week with instructions on how to redeem $100 in credits

Where we are...

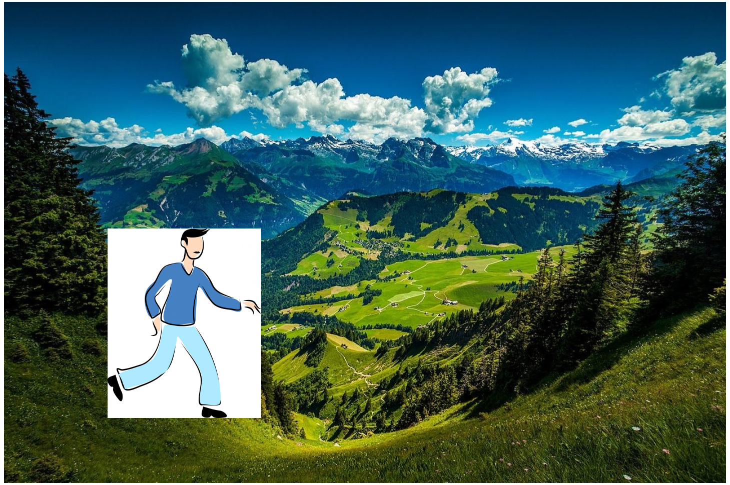
$$s = f(x; W) = Wx$$ scores function

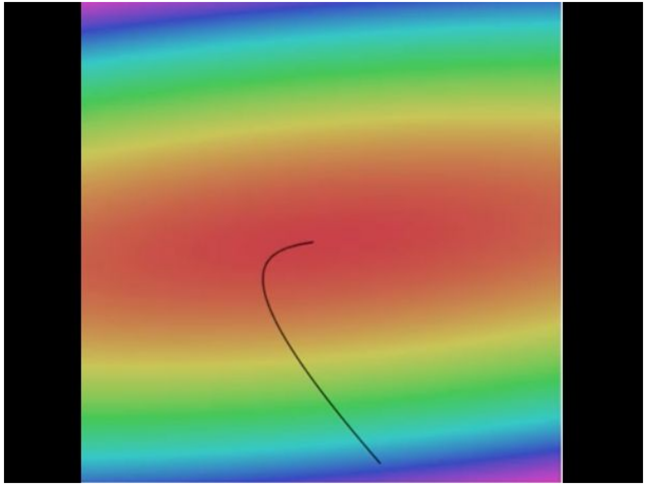
$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$ SVM loss

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i + \sum_k W_k^2$$ data loss + regularization

want $\boxed{\nabla_W L}$

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

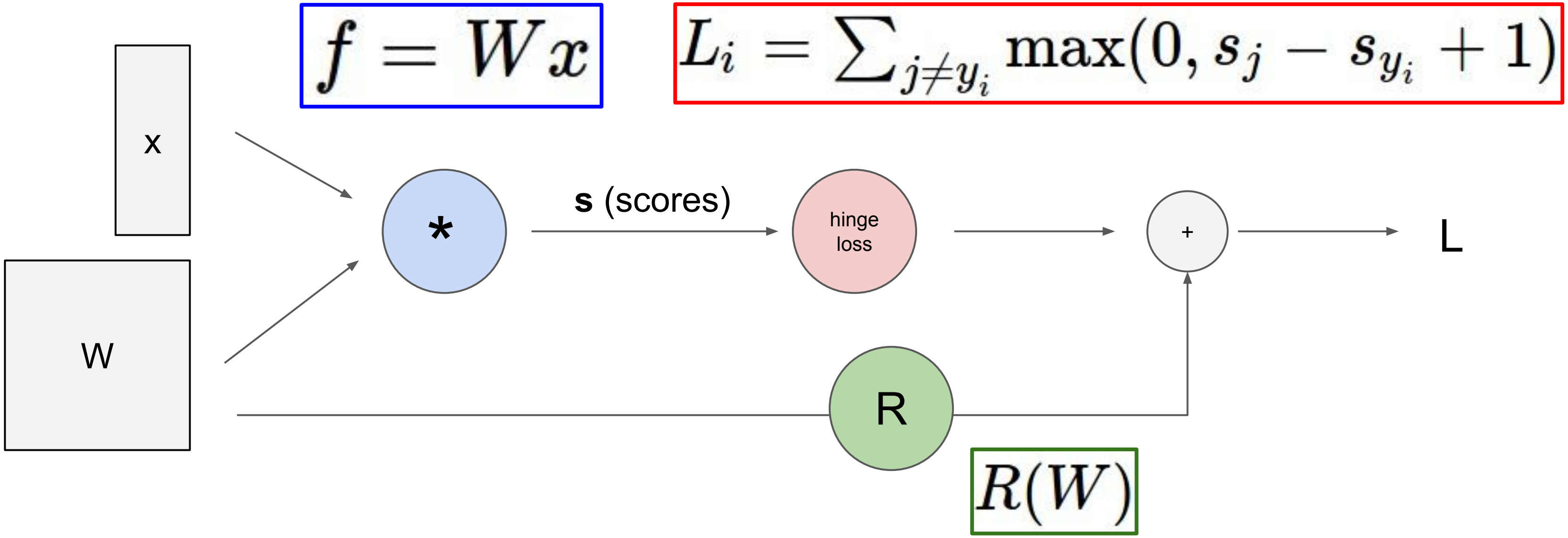
오늘은 임의의 복잡한 함수를 통해 어떻게 해석적미분을 계산하는지에 대해 이야기할 것입니다.

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

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

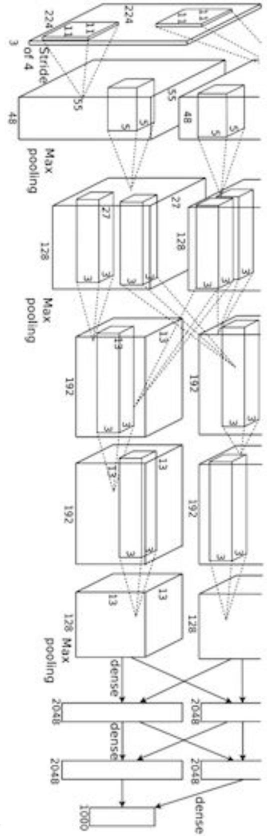


Convolutional network (AlexNet)

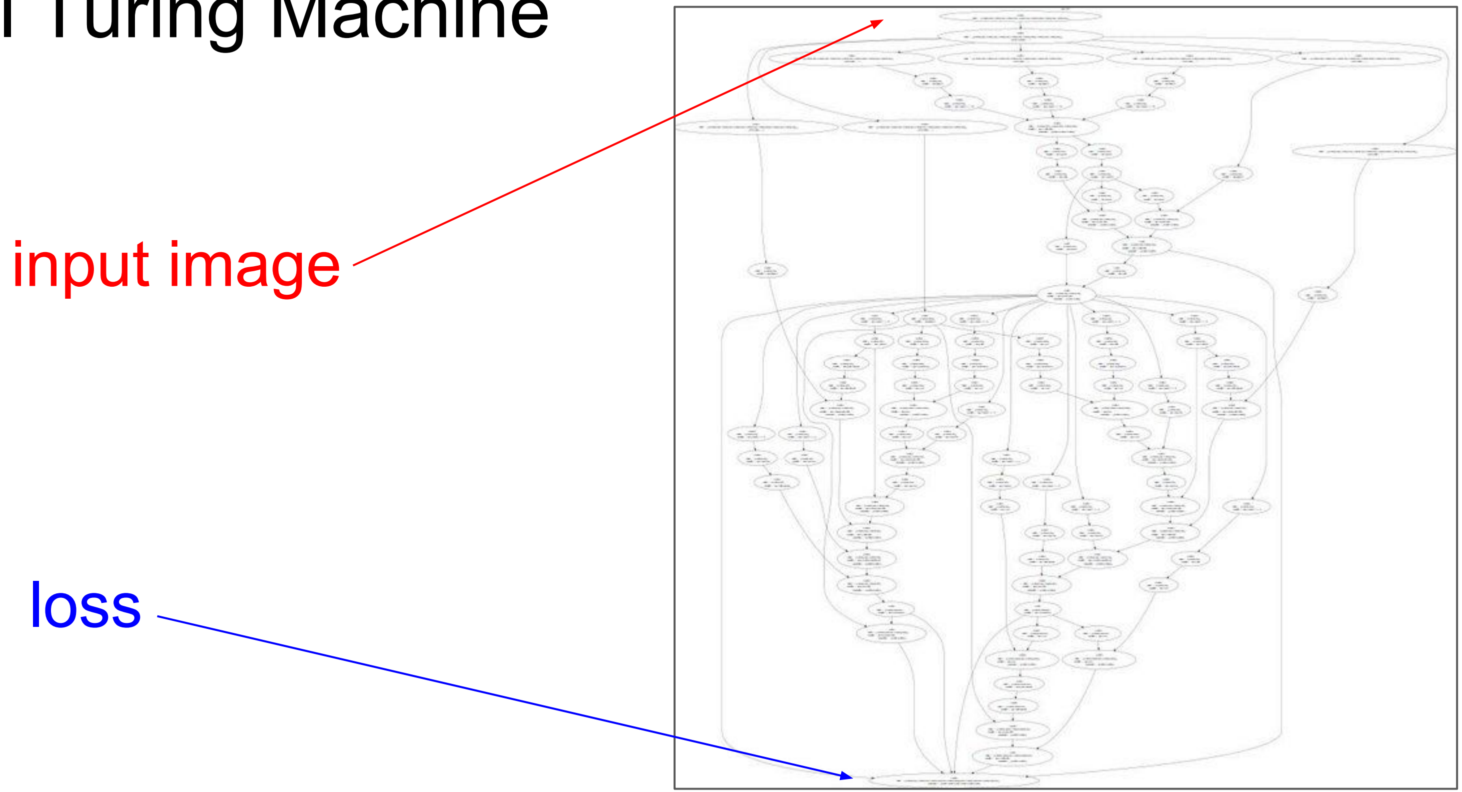
input image

weights

loss



Neural Turing Machine



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Neural Turing Machine

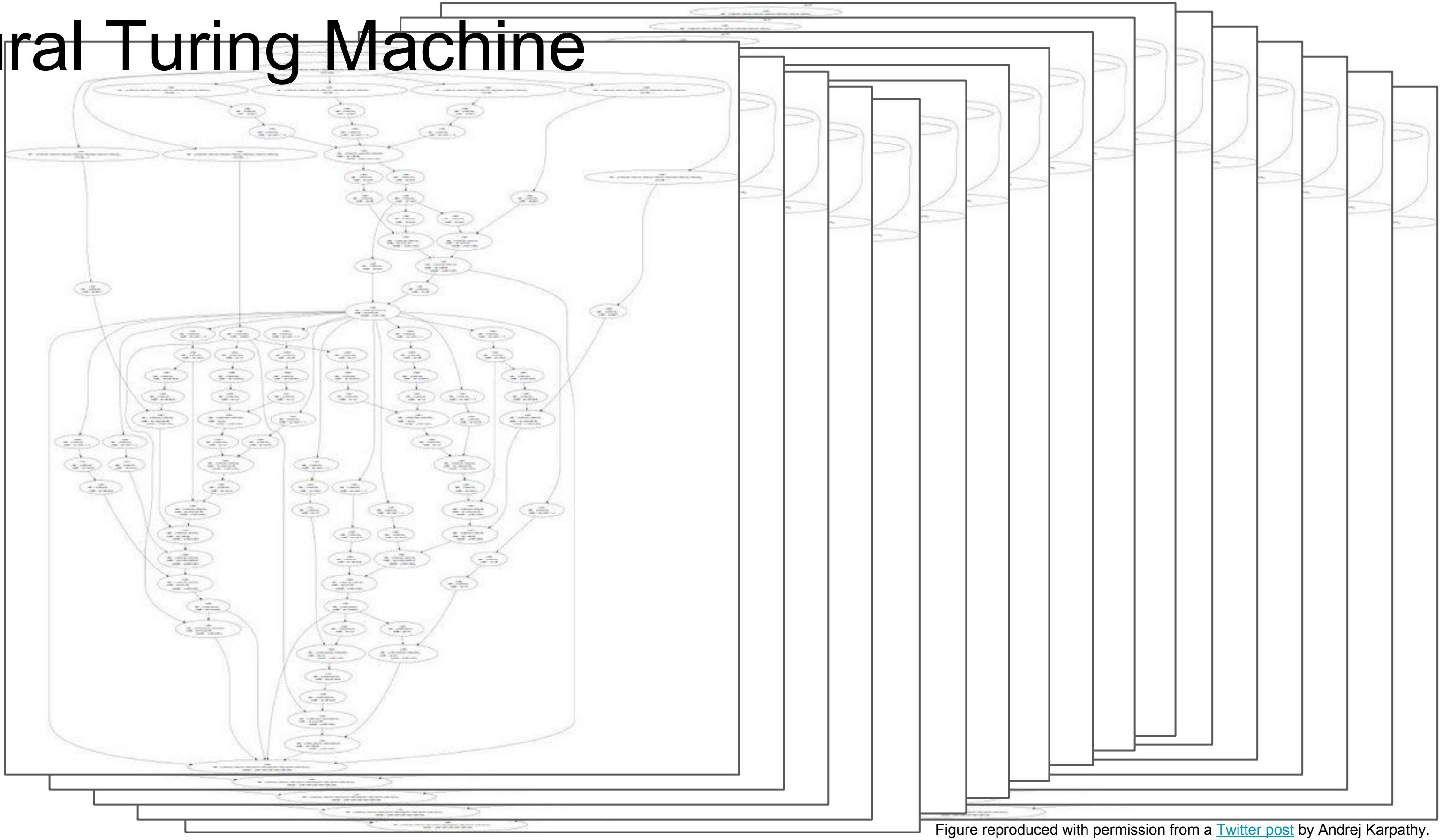
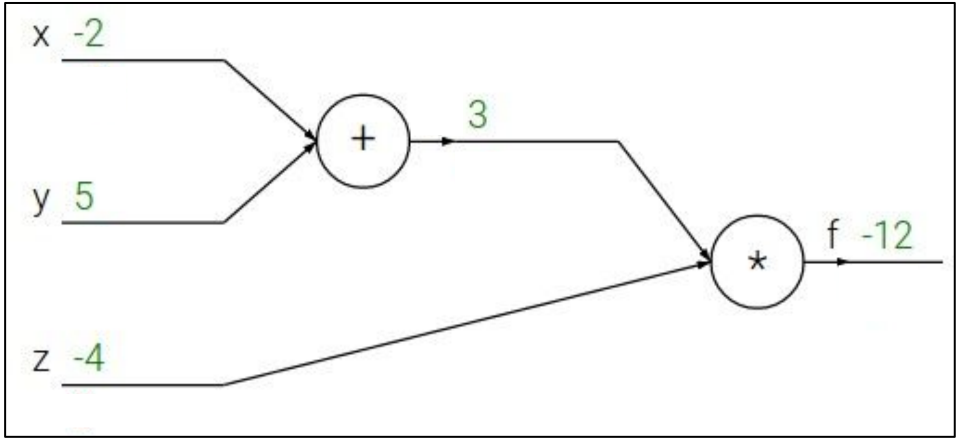


Figure reproduced with permission from a Twitter post by Andrej Karpathy.

Backpropagation: a simple example

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

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



역전파법은 어떻게 작동할까요? 먼저 간단한 예제를 봅시다.
첫번째단계는 해당함수를 이용해 계산그래프로 나타내는것입니다.

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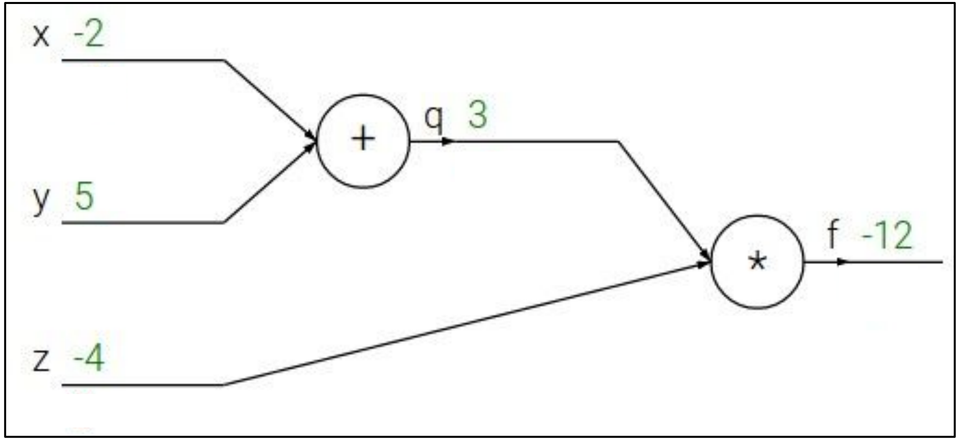
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



그다음 각 노드에 변수를 붙여주겠습니다. 여기서 덧셈노드에는 q를 명명하겠습니다.
우리가 찾기 원하는것은 x,y,z 각각에 대한 f의 기울기입니다.

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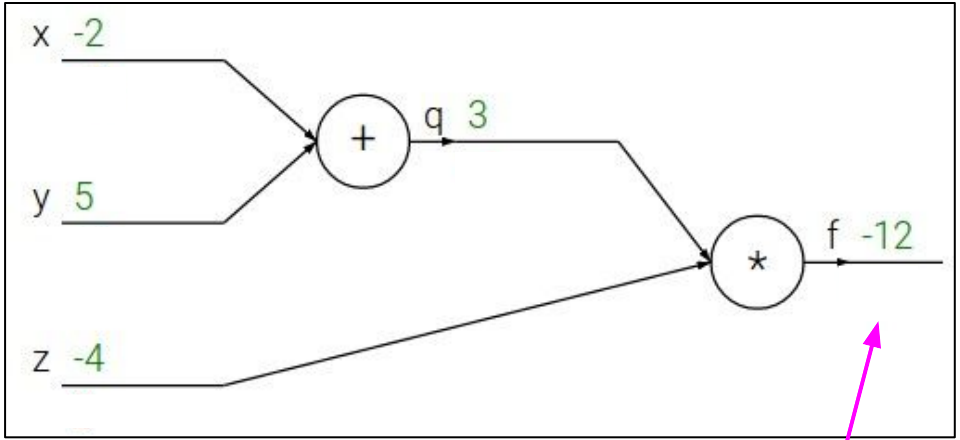

$$\frac{\partial f}{\partial f}$$

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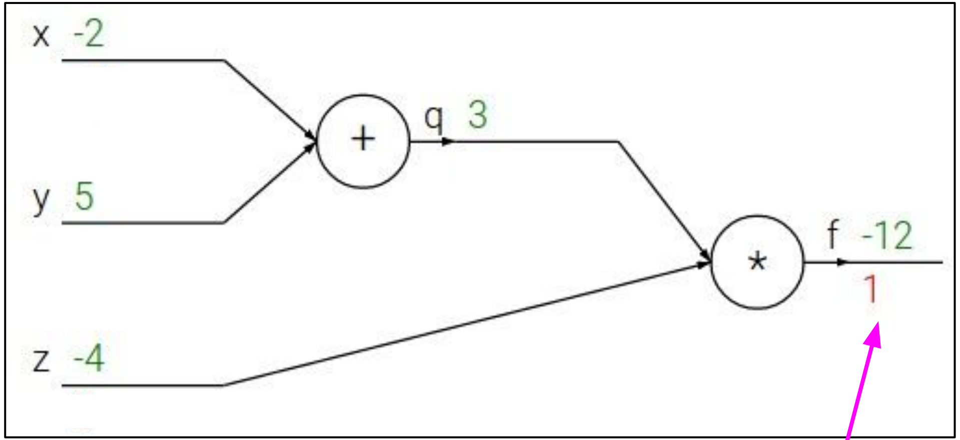

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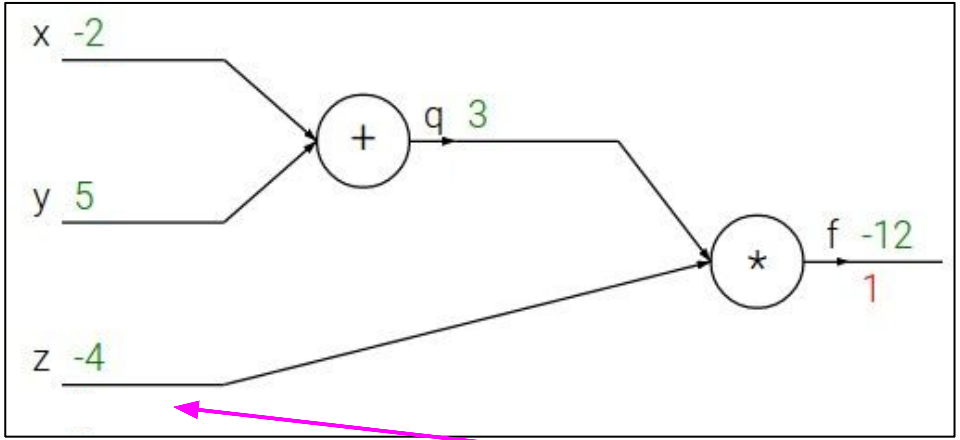

$$\frac{\partial f}{\partial z}$$

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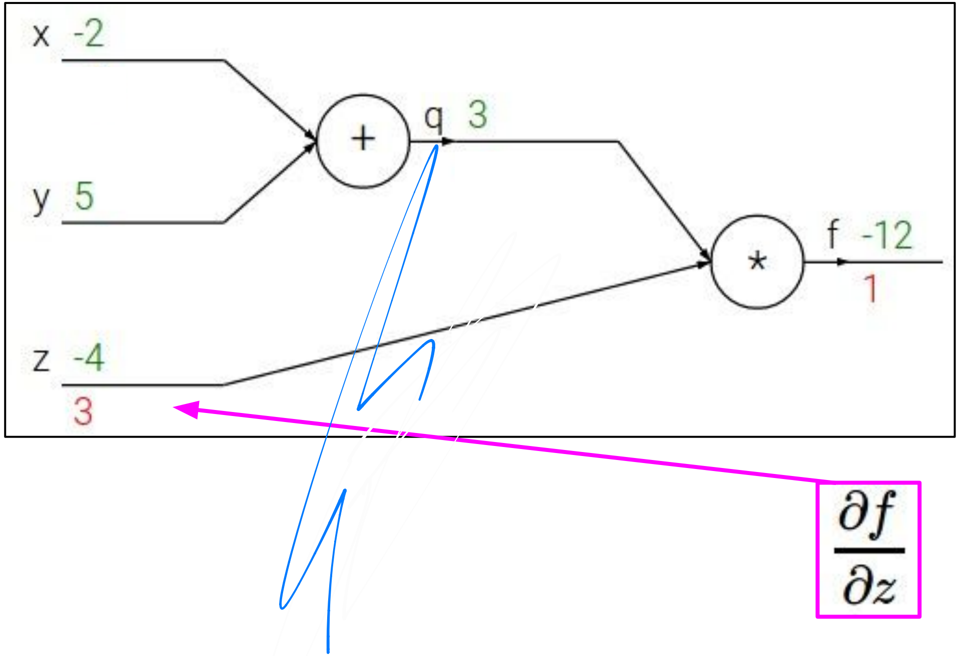

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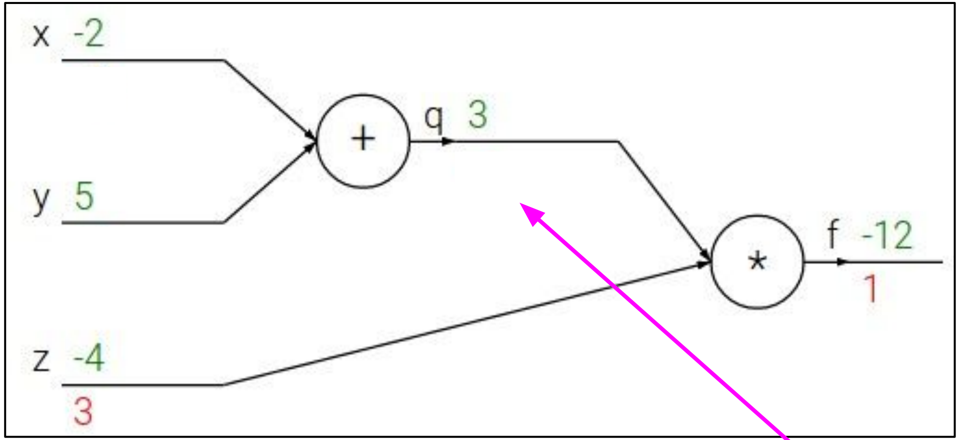

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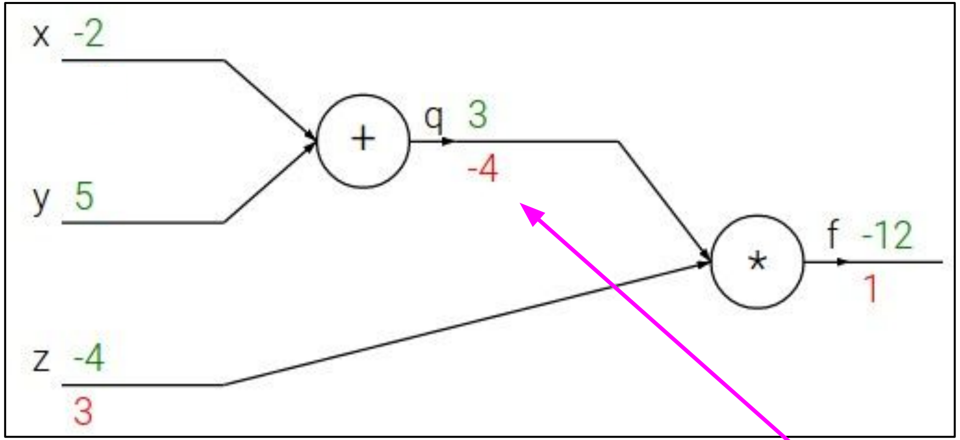

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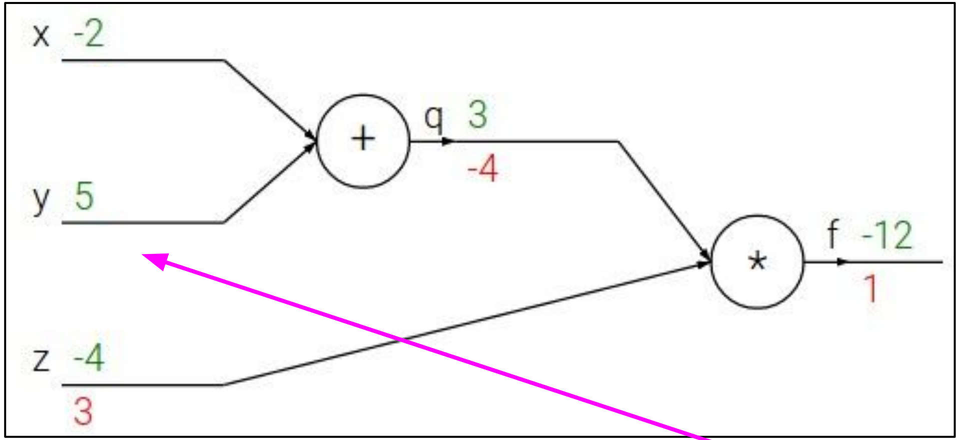

$$\frac{\partial f}{\partial y}$$

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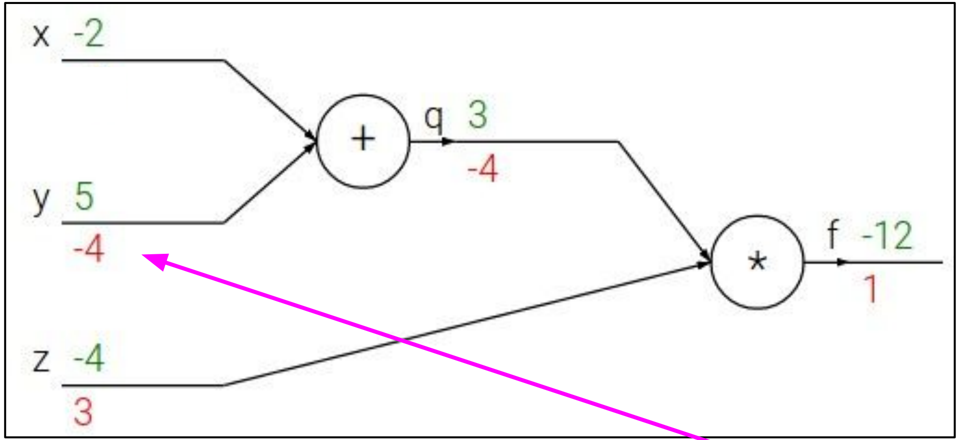

$$\frac{\partial f}{\partial y}$$

Chain rule:

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

Backpropagation: a simple example

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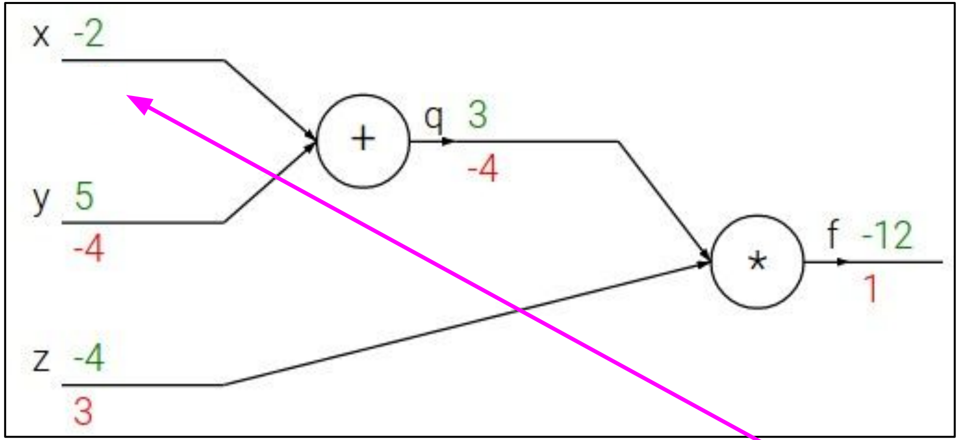

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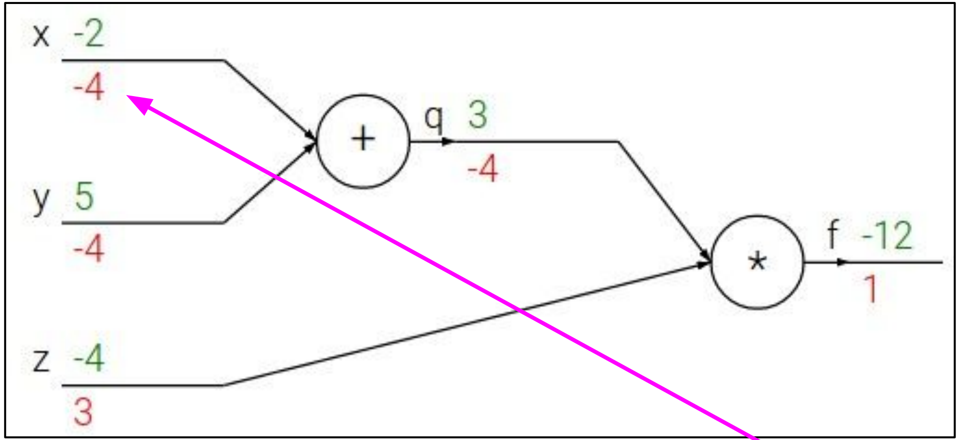

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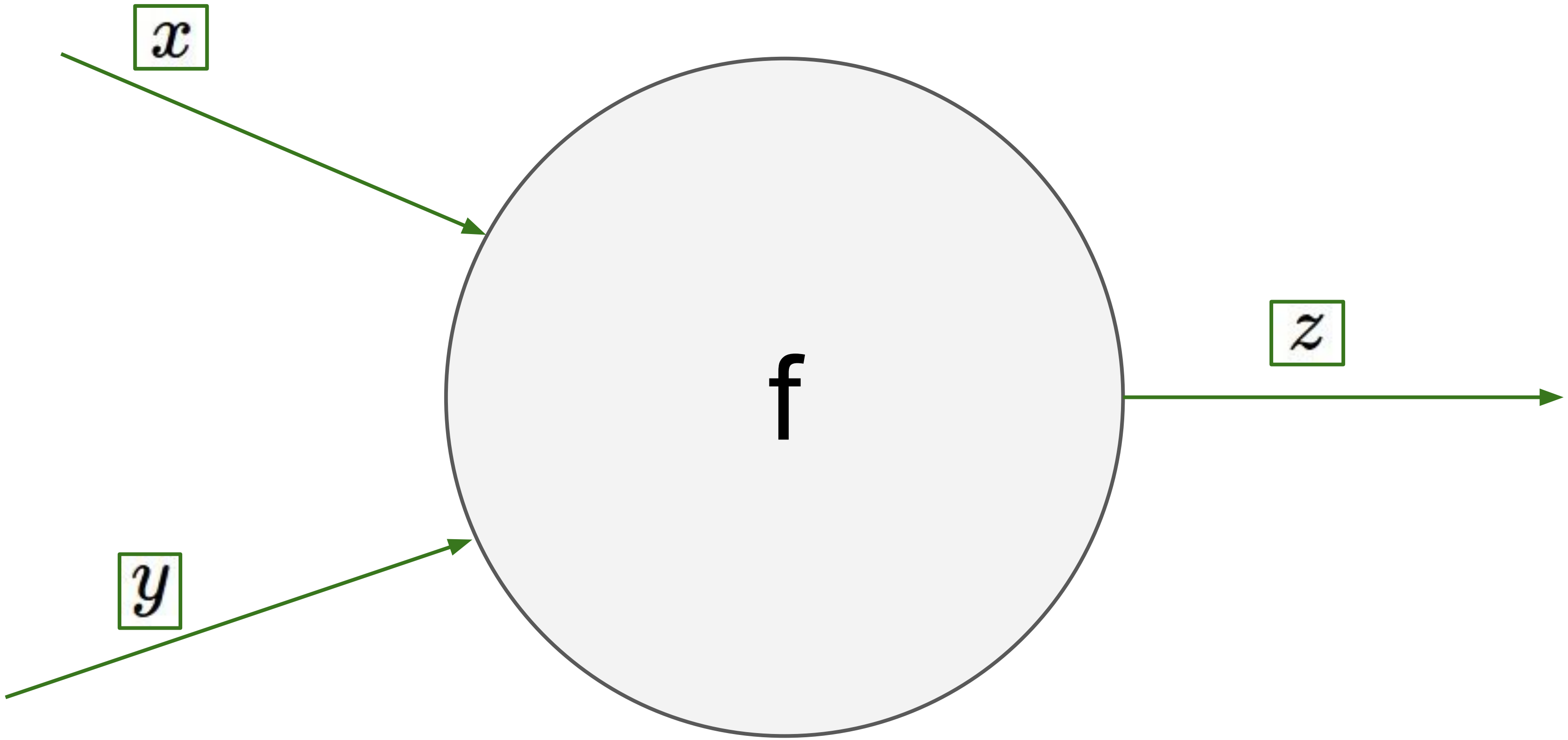
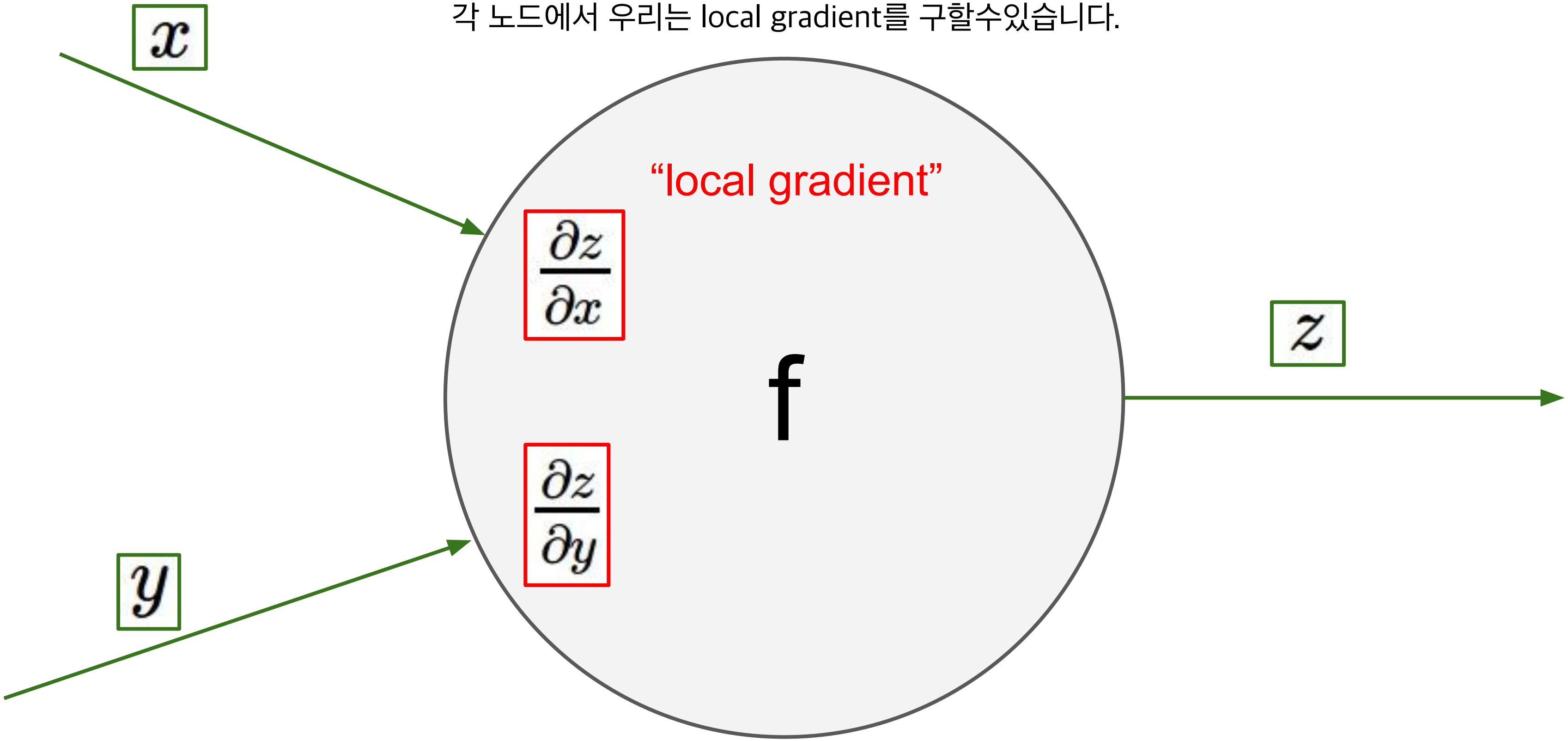
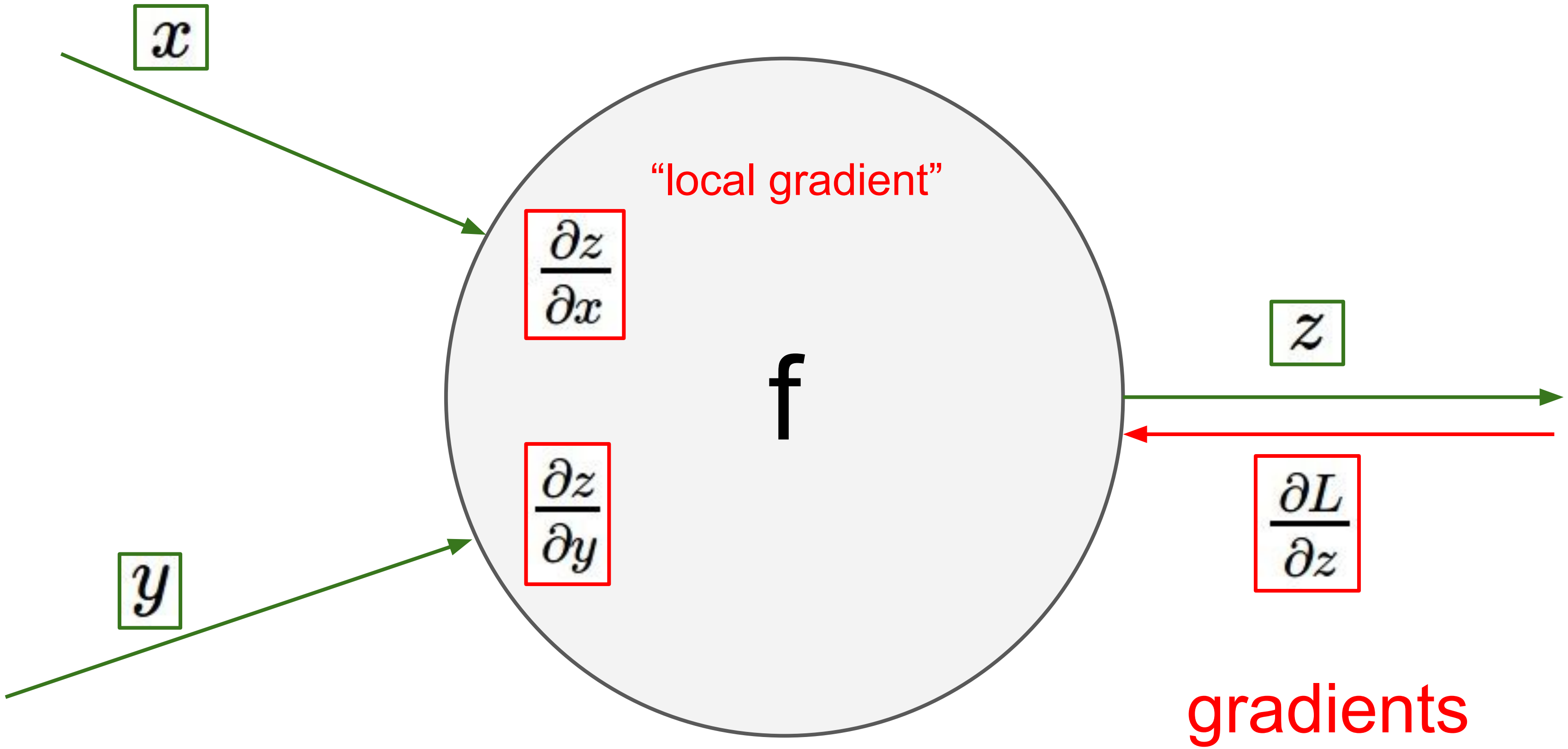

x
f
z
y

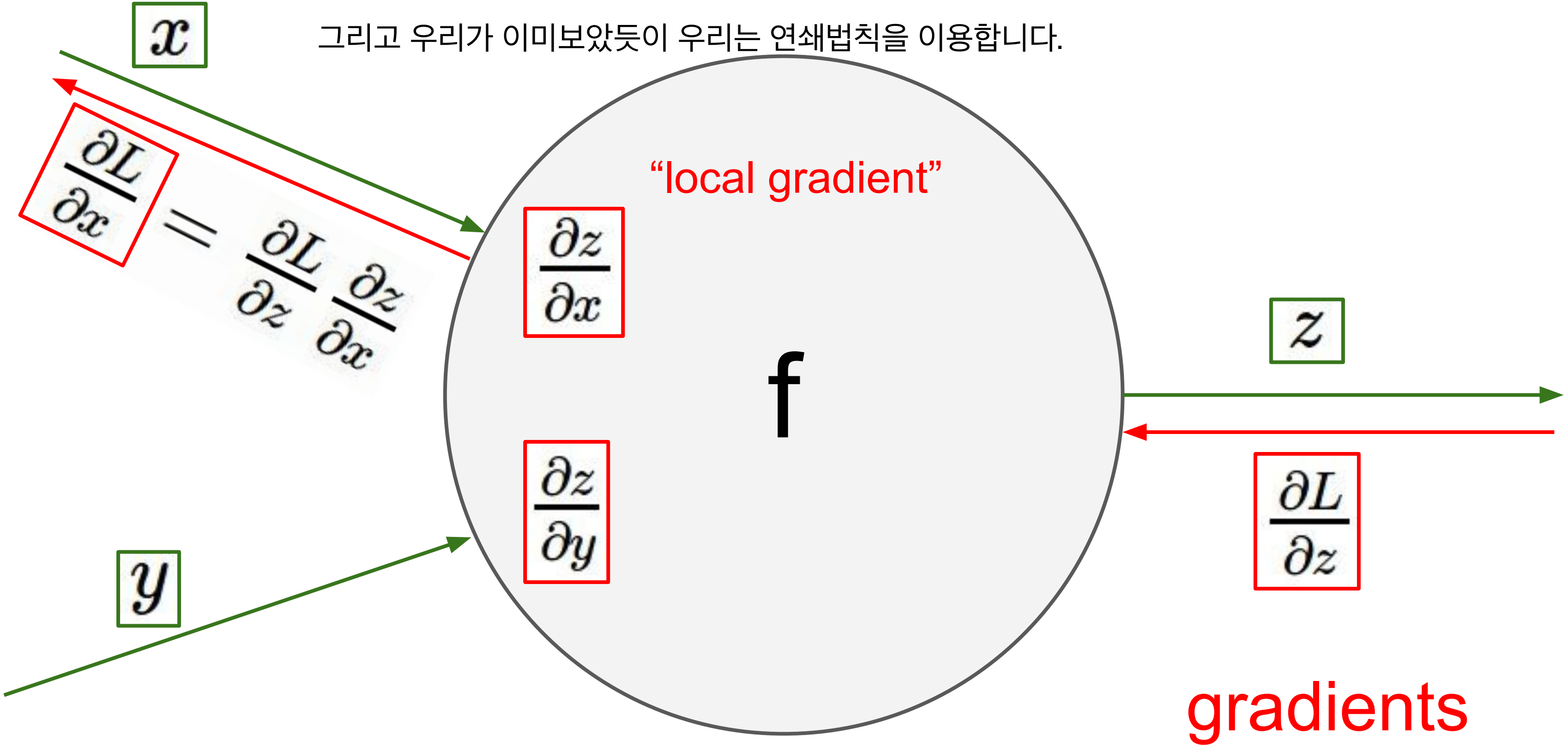
각 노드에서 우리는 local gradient를 구할수있습니다.

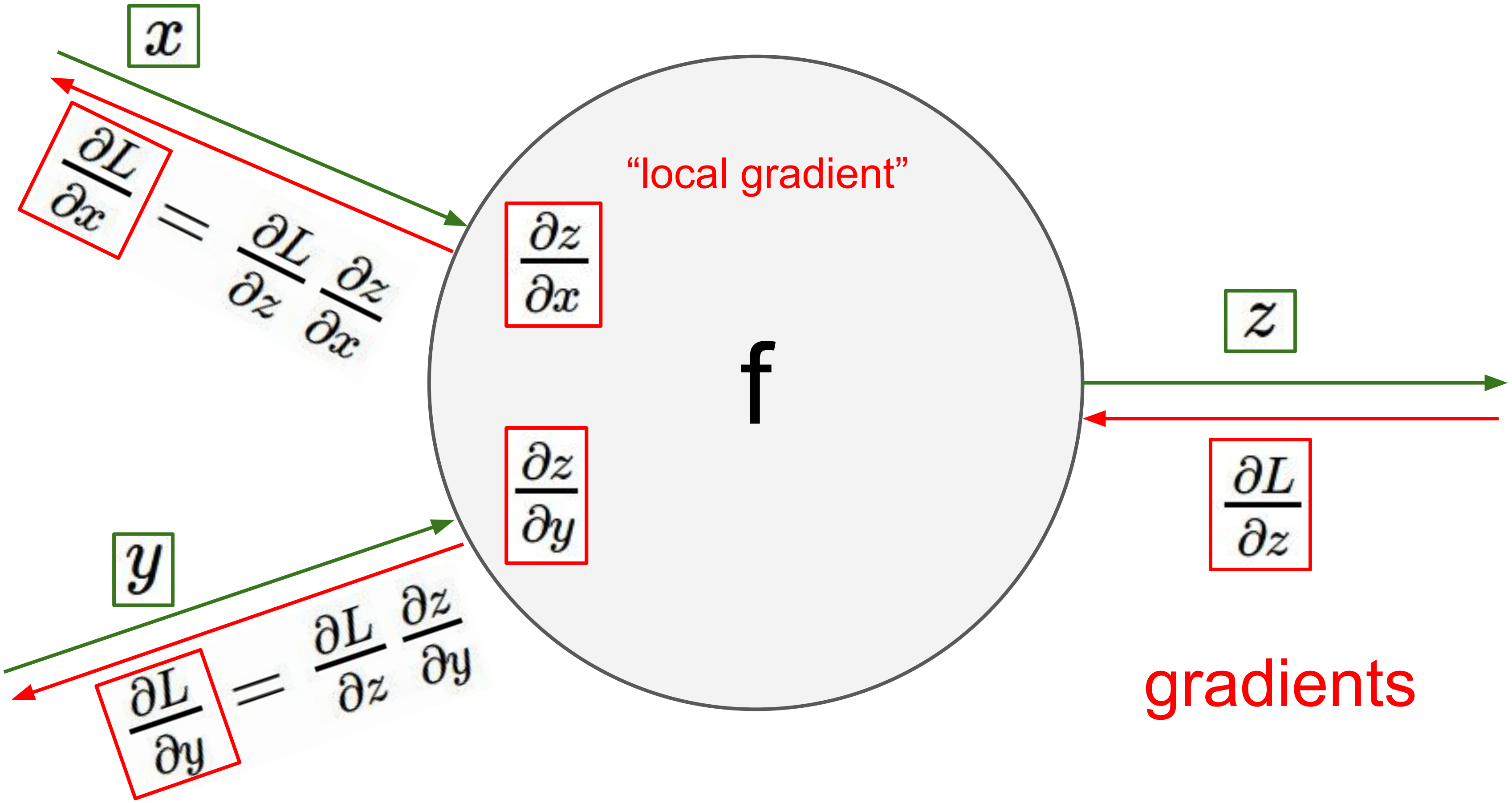



x
"local gradient"
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial z}{\partial y}$
$\frac{\partial L}{\partial z}$
y
gradients

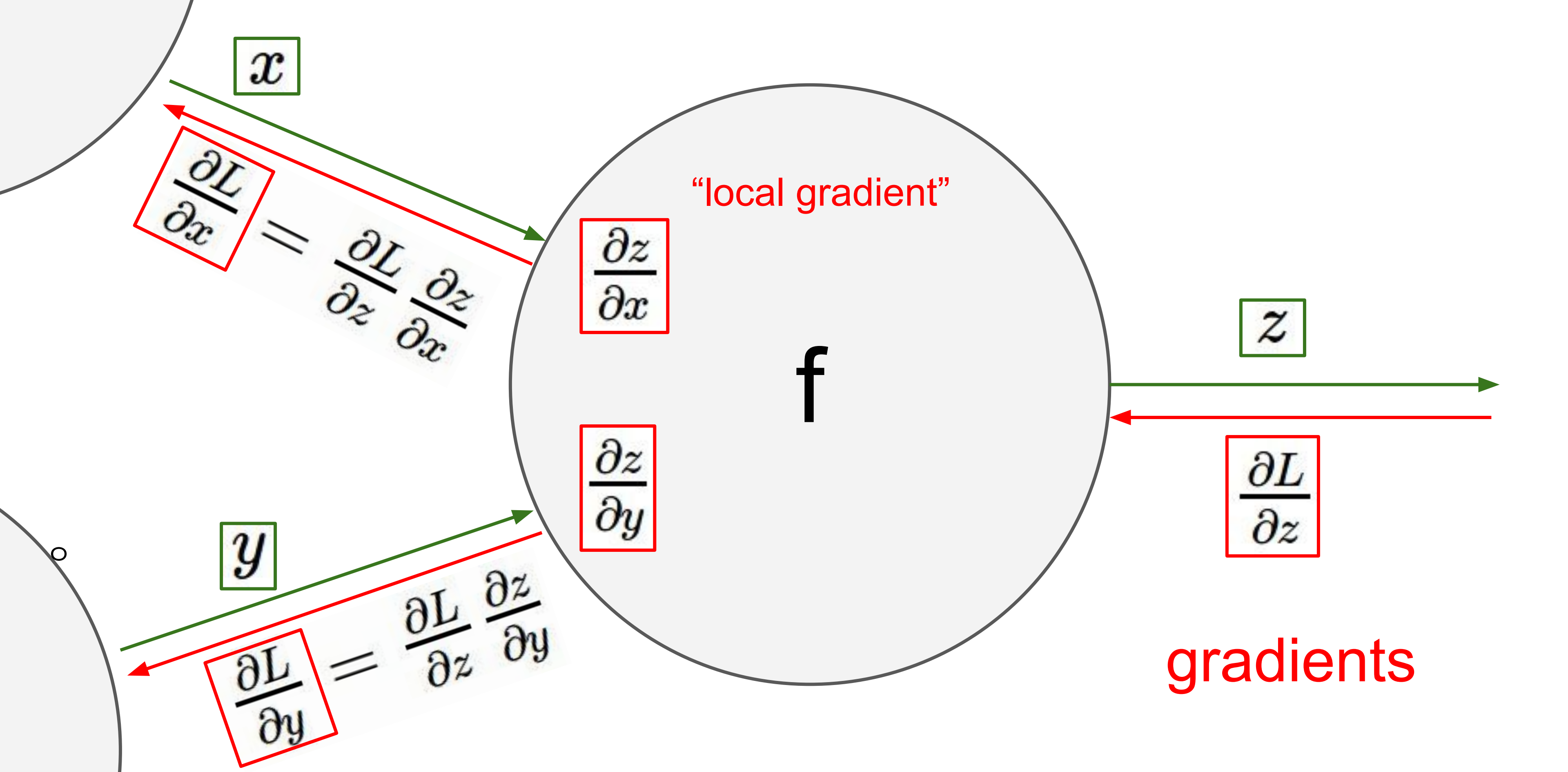
그럼 역전파법이 어떻게 동작하는지 알아봅시다.
먼저 우리는 그래프의 뒤에서부터 시작합니다. 그리고 이 노드에 도달할때까지 z에 대한 최종 loss L은 이미 계산되어져있습니다. 이제 우리는 x와y에 대한 바로 직전노드의 기울기를 찾고자합니다.

그리고 우리가 이미보았듯이 우리는 연쇄법칙을 이용합니다.



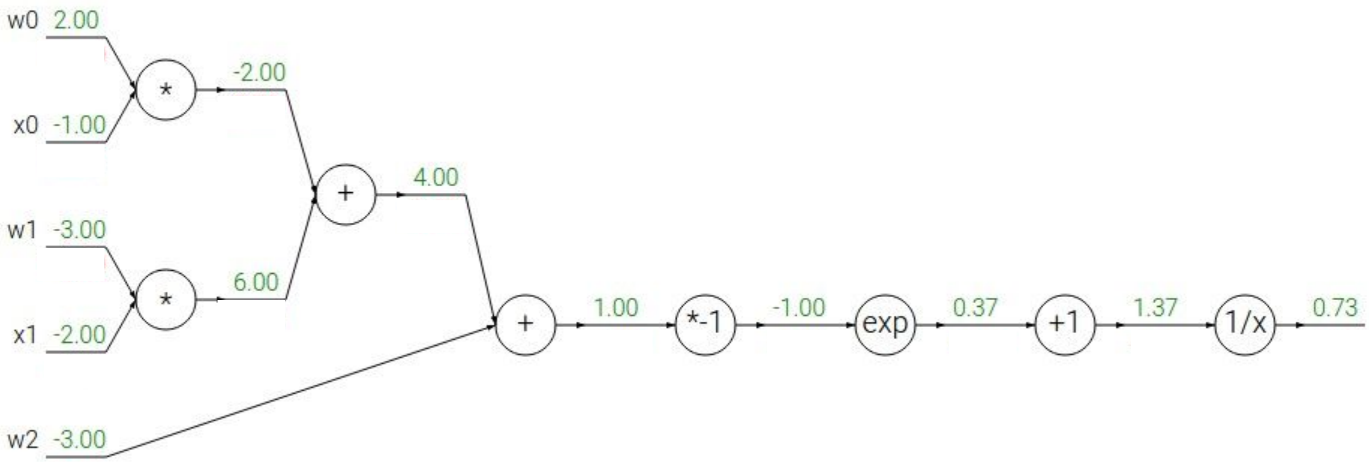


x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z} \frac{\partial z}{\partial x}$
"local gradient"
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial z}{\partial y}$
$\frac{\partial L}{\partial z}$
y
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z} \frac{\partial z}{\partial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


x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"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:

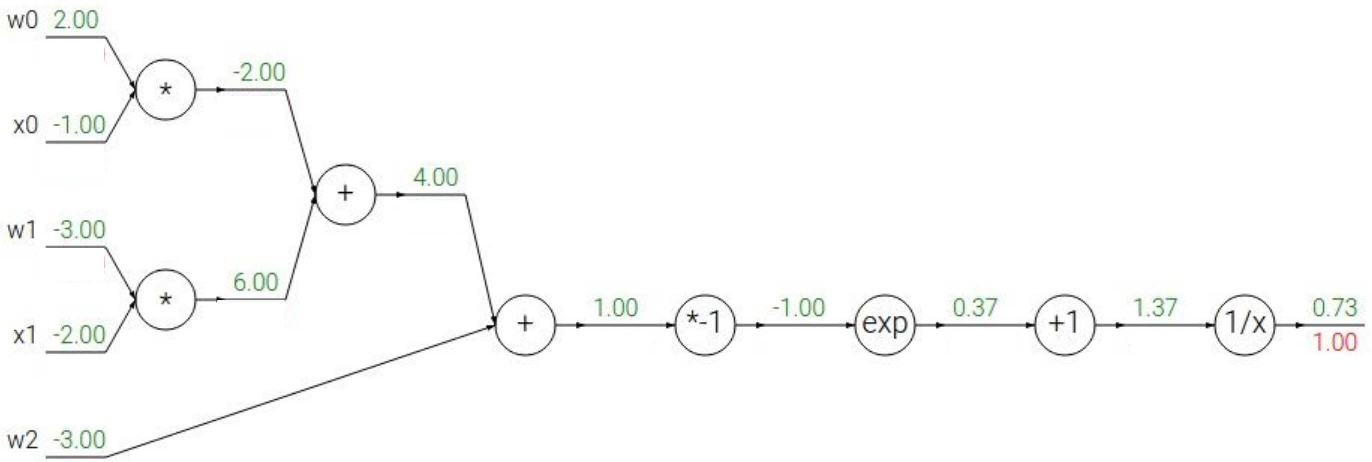
$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



이제부터 다른 예제를 살펴봅시다. 이전보다는 조금더 복잡해집니다. 다시말하지만, 첫번째과정은 식을 계산그래프로 나타내는것입니다.,

Another example:

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



$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

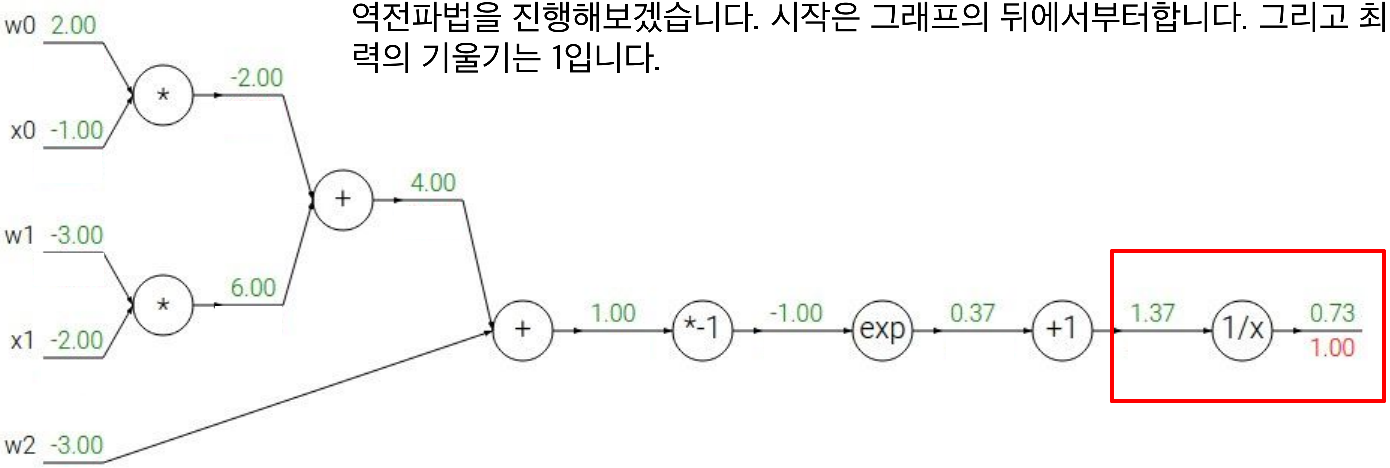
$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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

Another example:

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

역전파법을 진행해보겠습니다. 시작은 그래프의 뒤에서부터합니다. 그리고 최종변수에 대한 출력의 기울기는 1입니다.



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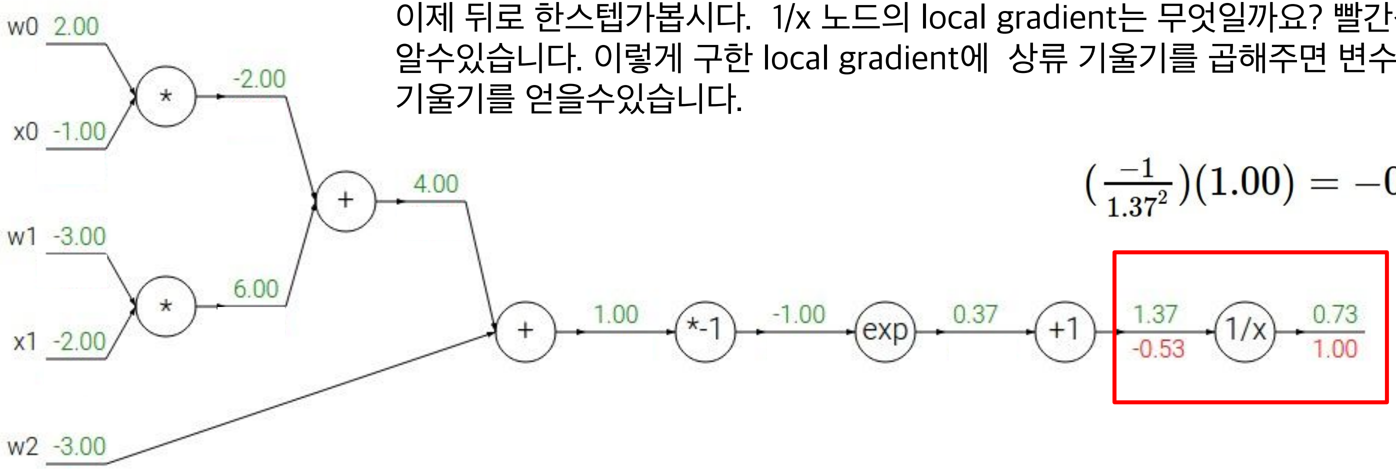
Another example:

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

이제 뒤로 한스텝가봅시다. 1/x 노드의 local gradient는 무엇일까요? 빨간색박스에서 알수있습니다. 이렇게 구한 local gradient에 상류 기울기를 곱해주면 변수1.37에대한 기울기를 얻을수있습니다.

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



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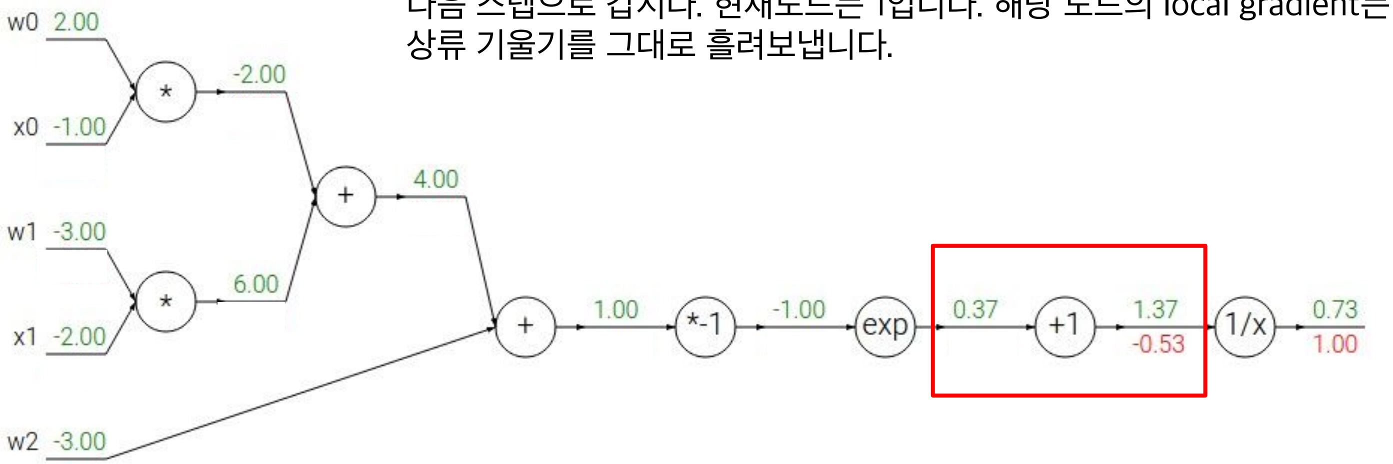
Another example:

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

다음 스텝으로 갑시다. 현재노드는 1입니다. 해당 노드의 local gradient는 1이기때문에 상류 기울기를 그대로 흘려보냅니다.



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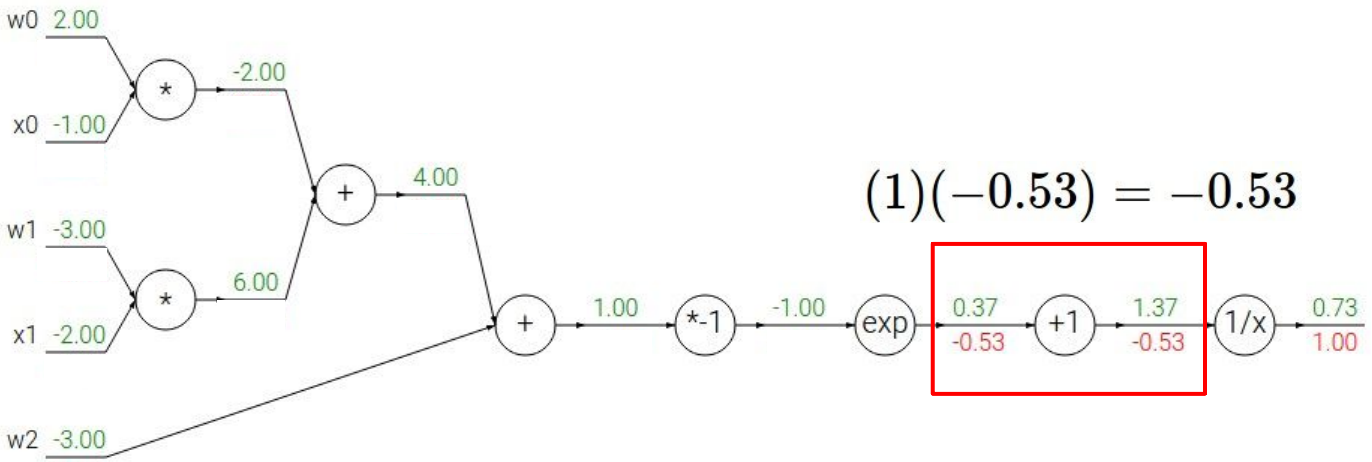

$$(1)(-0.53) = -0.53$$

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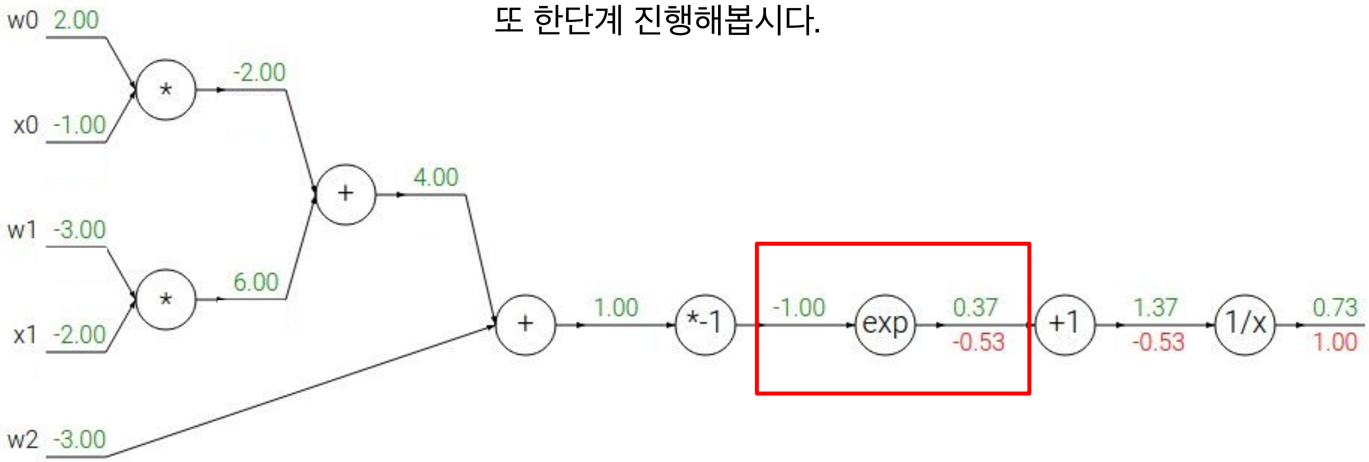
또 한단계 진행해봅시다.



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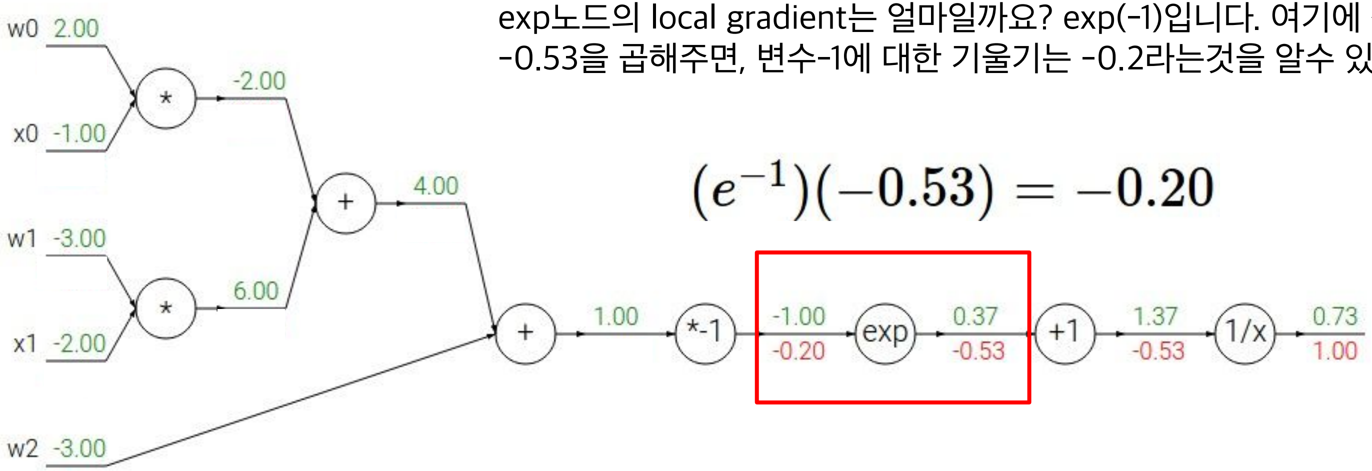
Another example: $f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$

exp노드의 local gradient는 얼마일까요? exp(-1)입니다. 여기에 상류 기울기인 -0.53을 곱해주면, 변수-1에 대한 기울기는 -0.2라는것을 알수 있습니다.

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



$$\boxed{f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x}$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

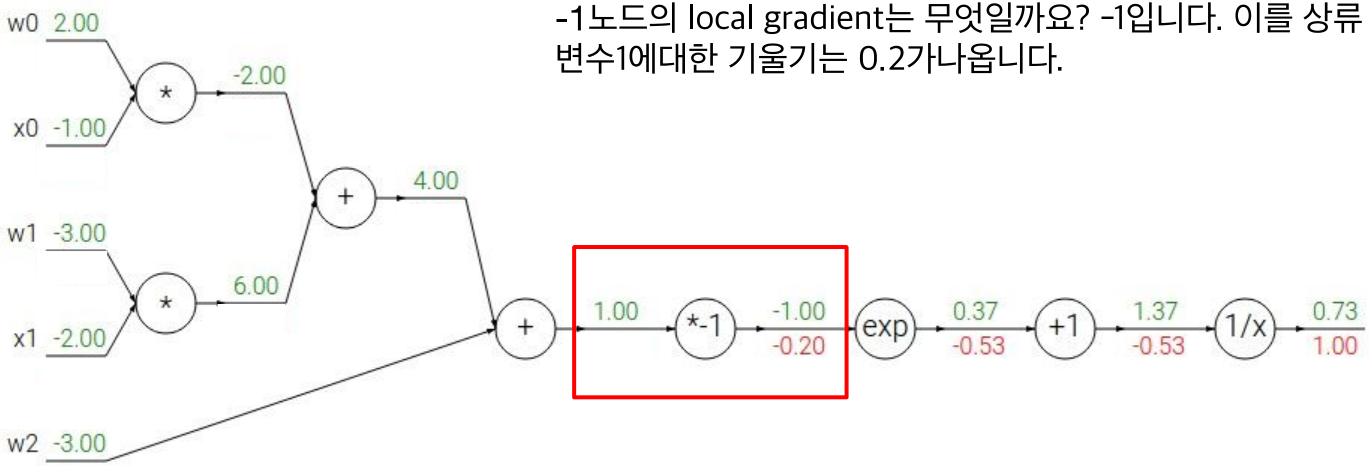
$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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

Another example:

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

-1노드의 local gradient는 무엇일까요? -1입니다. 이를 상류 기울기에 곱해주면 변수1에대한 기울기는 0.2가나옵니다.



$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

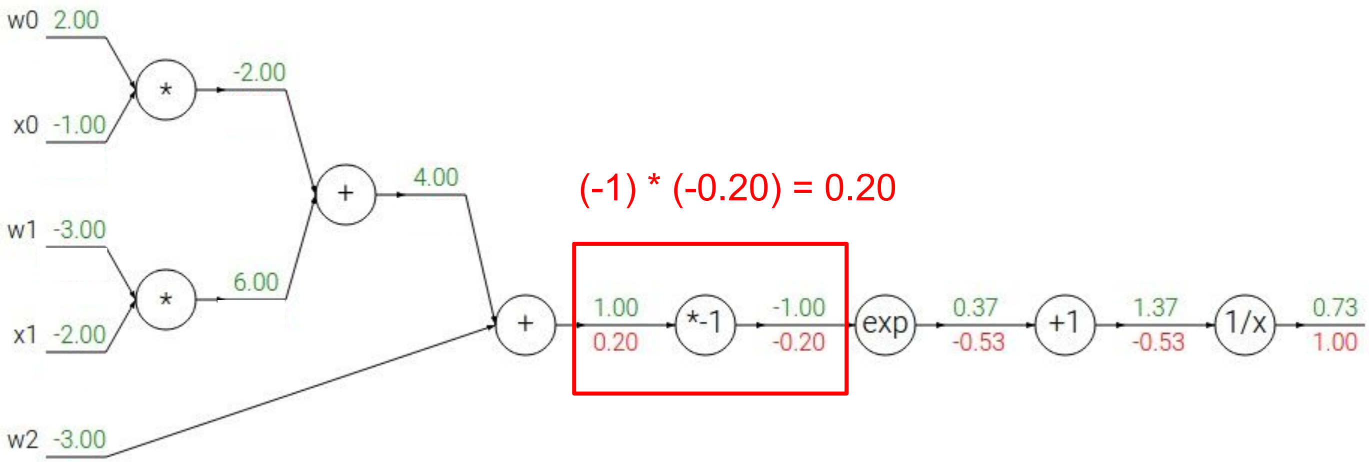
$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$\boxed{f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a}$$

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

Another example:

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



$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$\boxed{f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a}$$

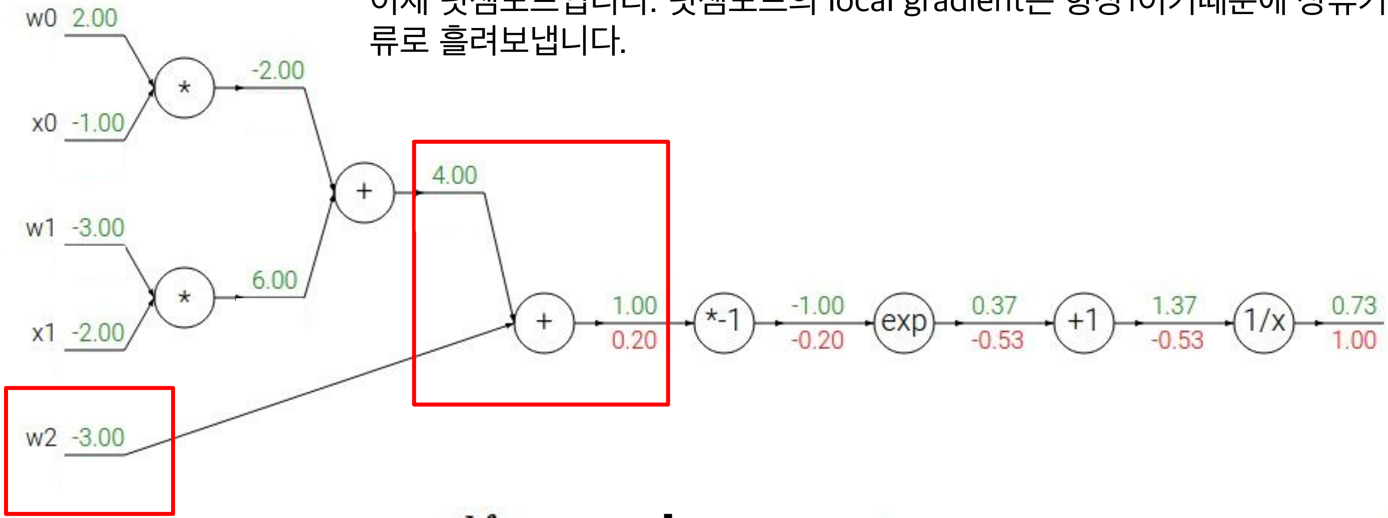
$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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

Another example:

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

이제 덧셈노드입니다. 덧셈노드의 local gradient는 항상1이기때문에 상류기울기를 그대로 하류로 흘려보냅니다.



$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

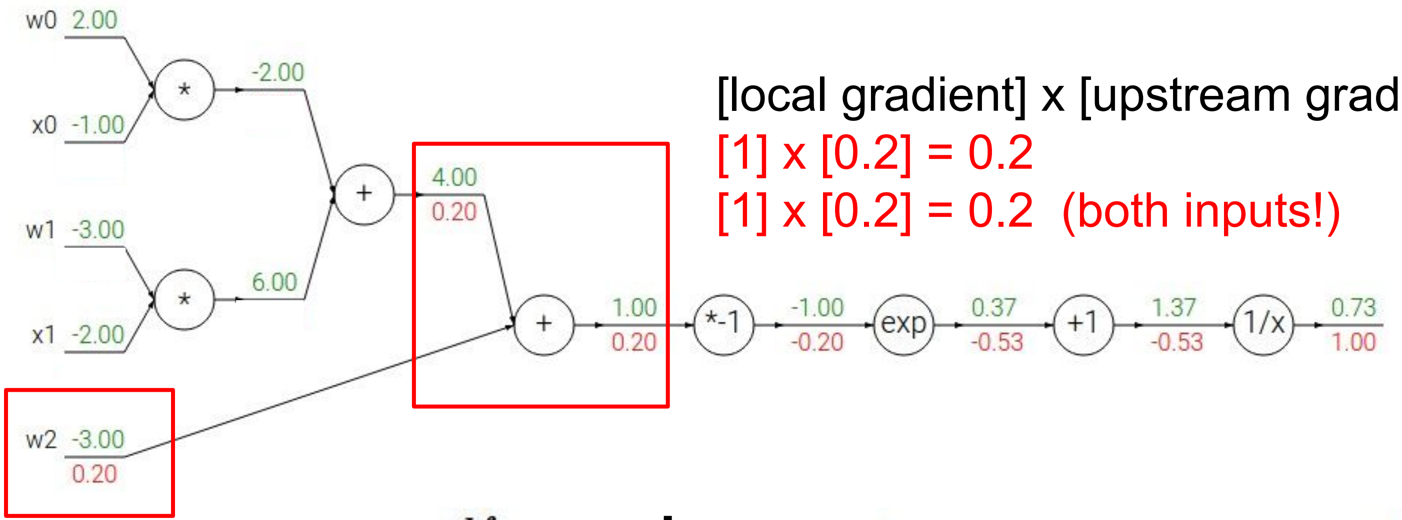
$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

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

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

Another example:

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



[local gradient] x [upstream gradient]

[1] x [0.2] = 0.2

[1] x [0.2] = 0.2 (both inputs!)

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

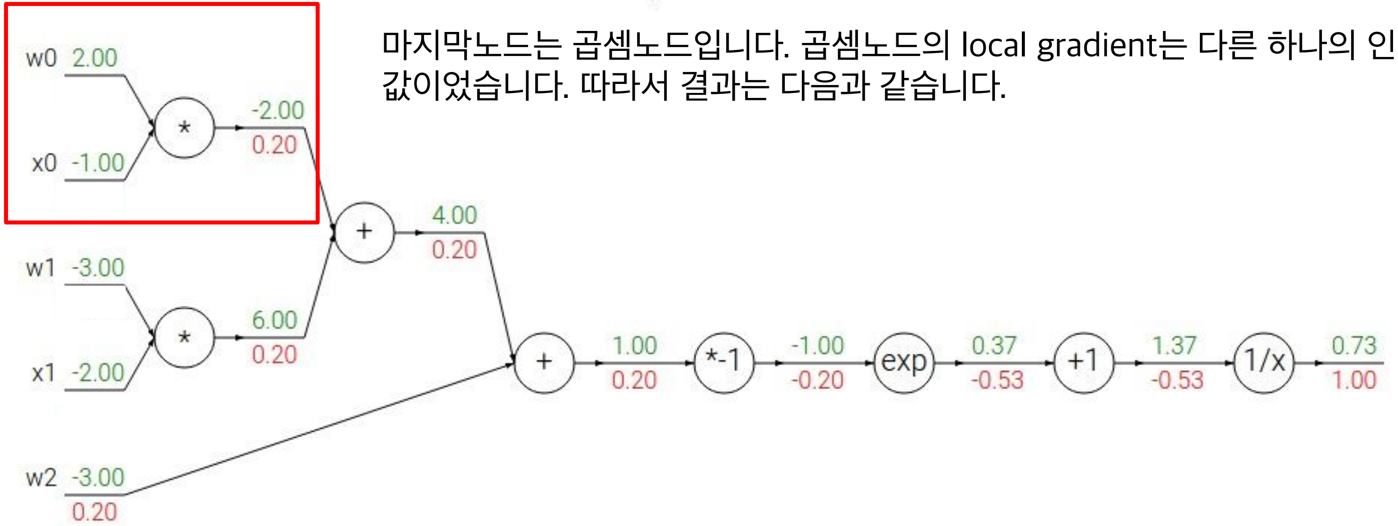
$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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

Another example:

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

마지막노드는 곱셈노드입니다. 곱셈노드의 local gradient는 다른 하나의 인풋값이었습니다. 따라서 결과는 다음과 같습니다.



$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

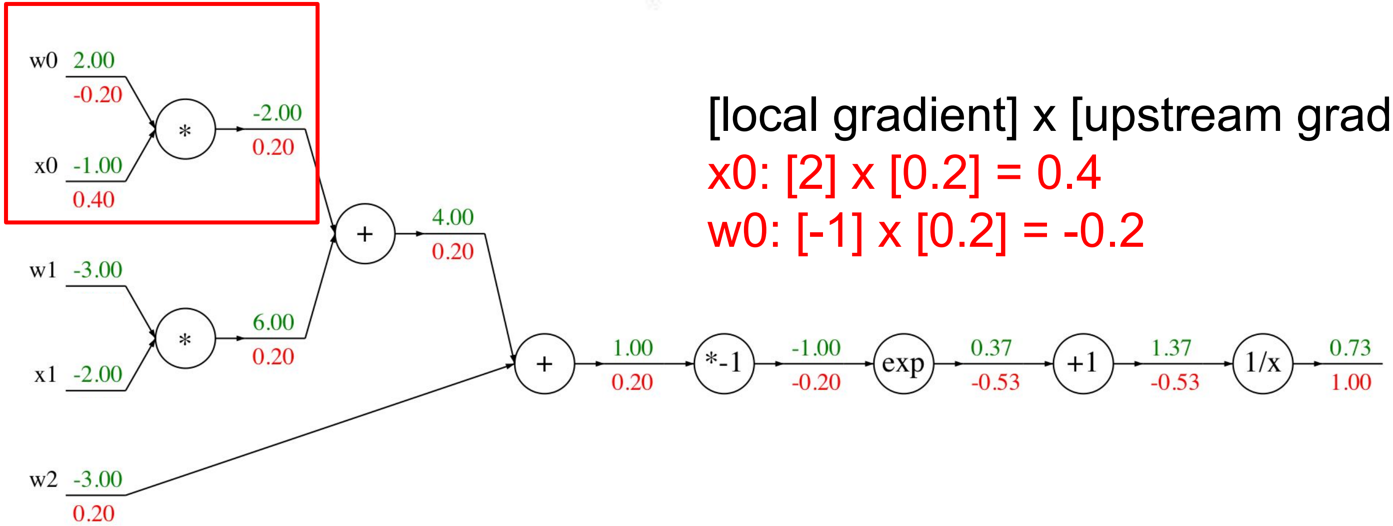
$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

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

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

Another example:

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



[local gradient] x [upstream gradient]

x0: [2] x [0.2] = 0.4

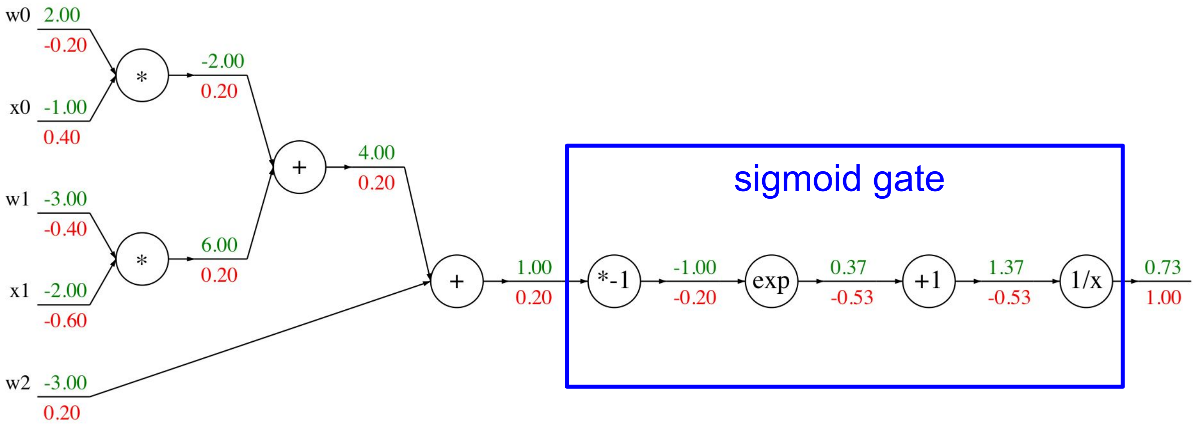
w0: [-1] x [0.2] = -0.2

$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$	$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$
$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$	$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$

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

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

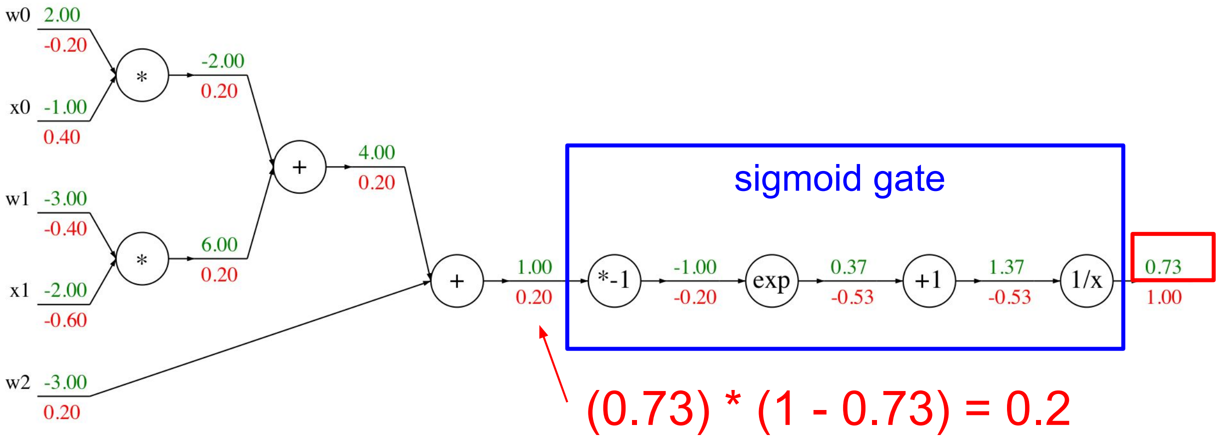
$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\sigma(x)$$



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

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

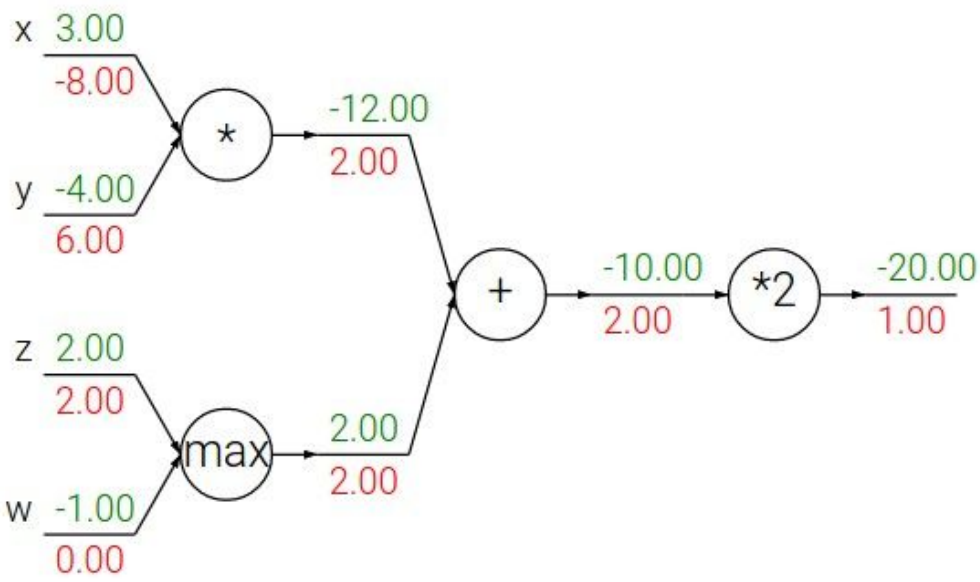
$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$



(0.73) * (1 - 0.73) = 0.2

Patterns in backward flow

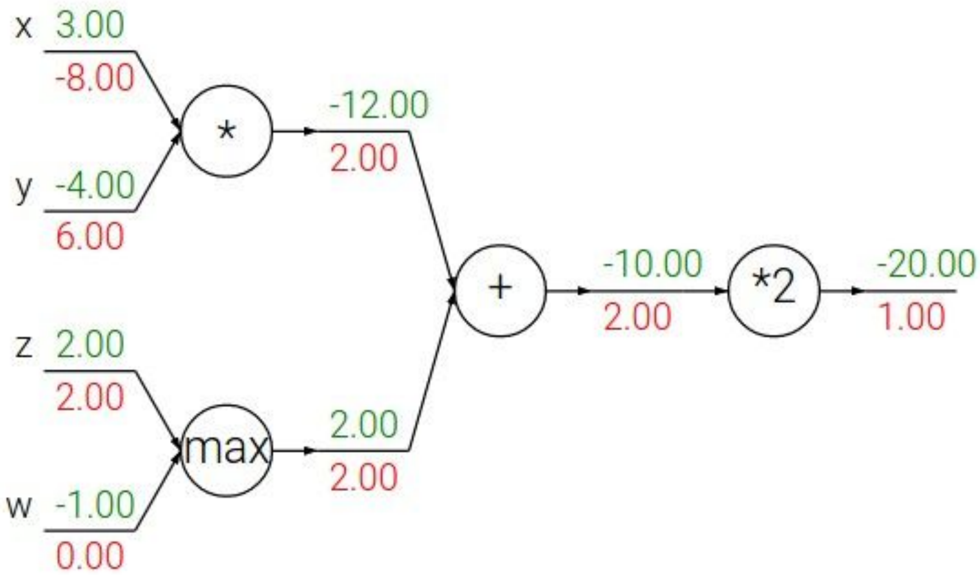
add gate: gradient distributor



Patterns in backward flow

add gate: gradient distributor

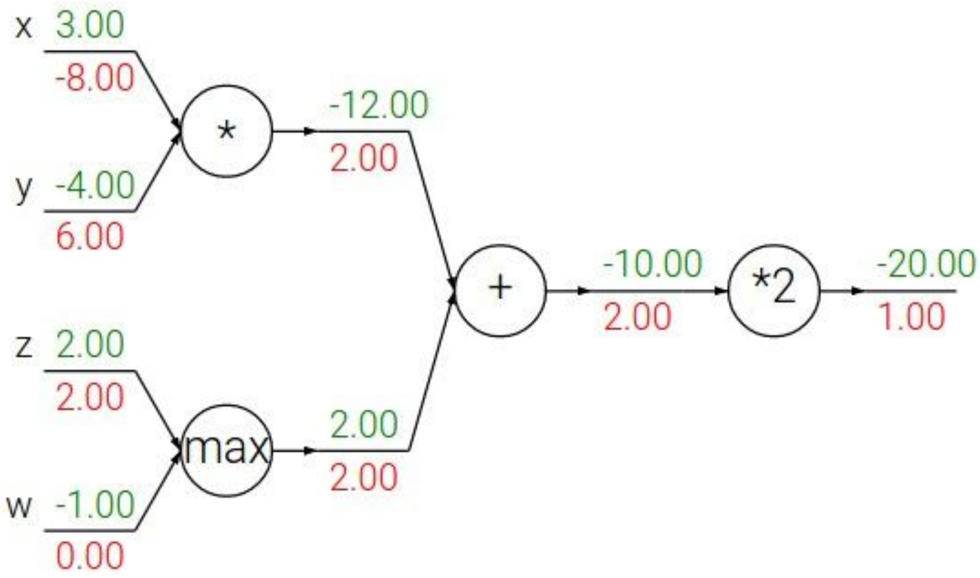
Q: What is a **max** gate?



Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

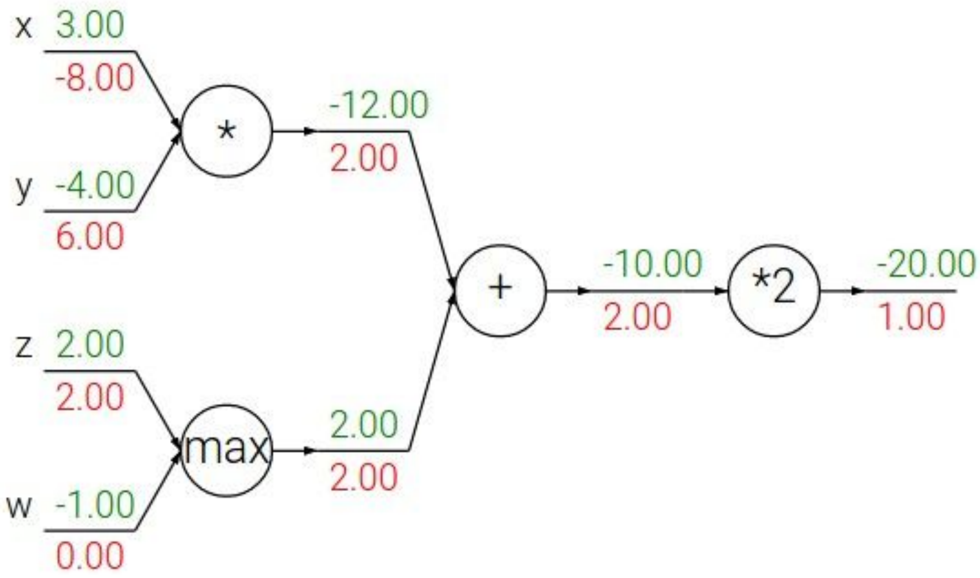


Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

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

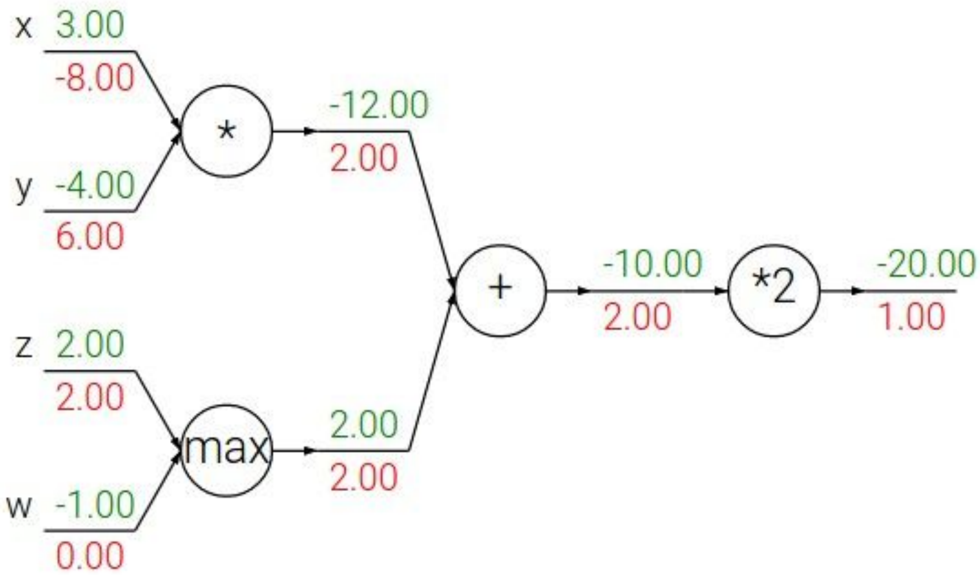


Patterns in backward flow

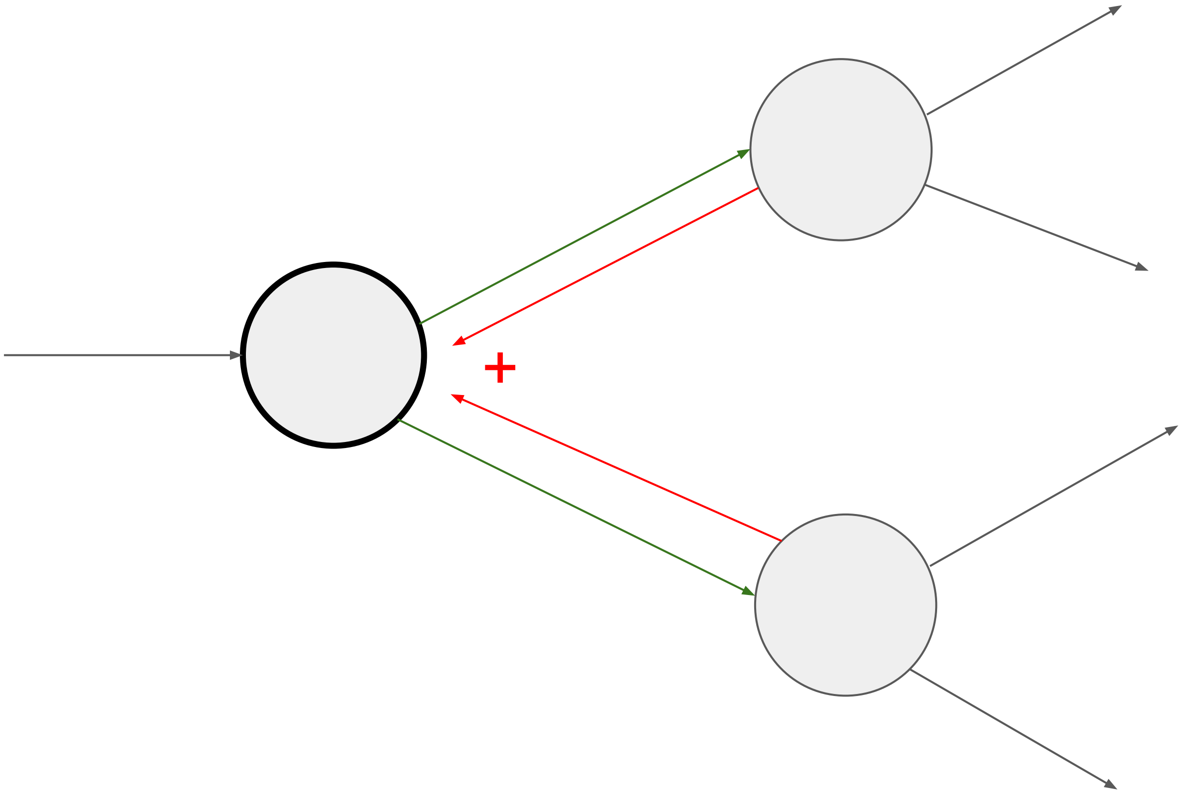
add gate: gradient distributor

max gate: gradient router

mul gate: gradient switcher

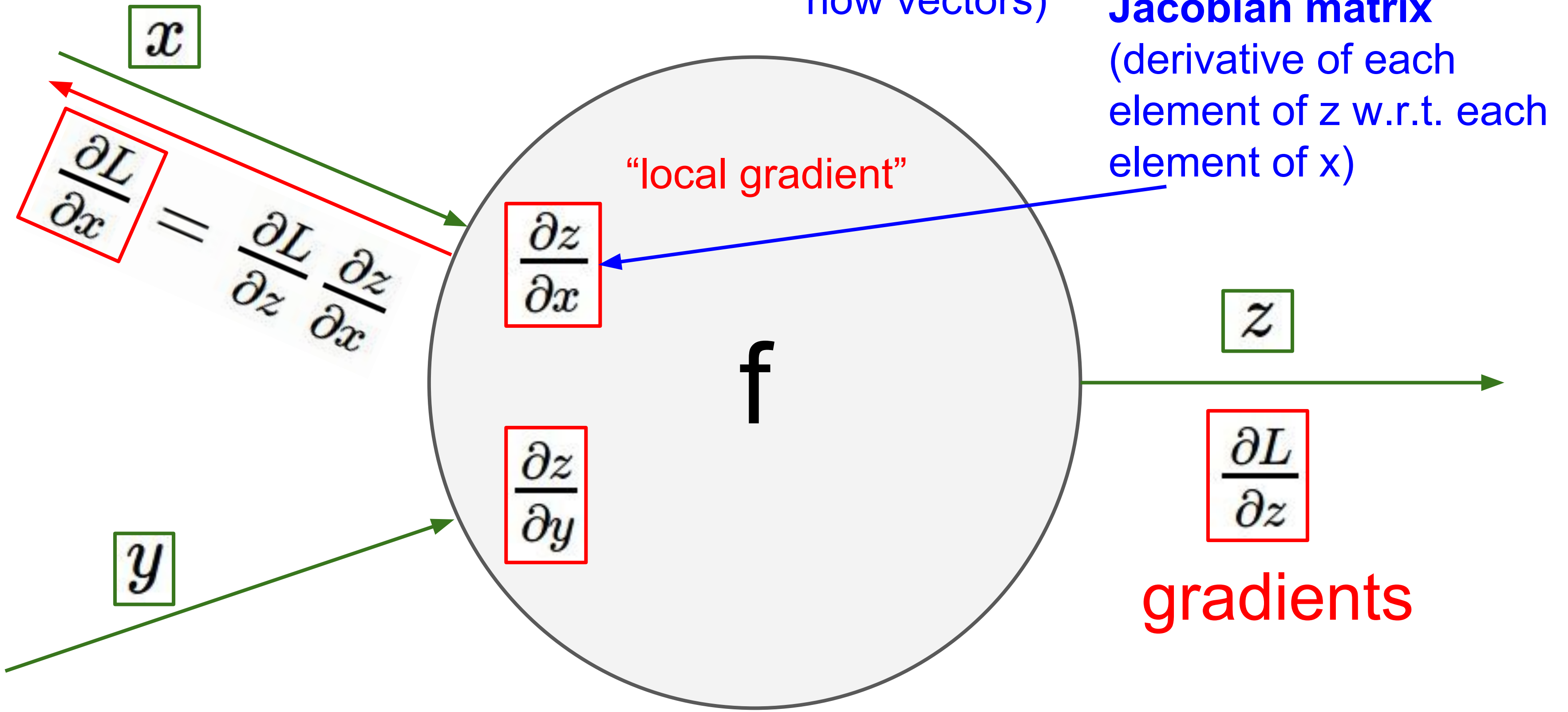


Gradients add at branches



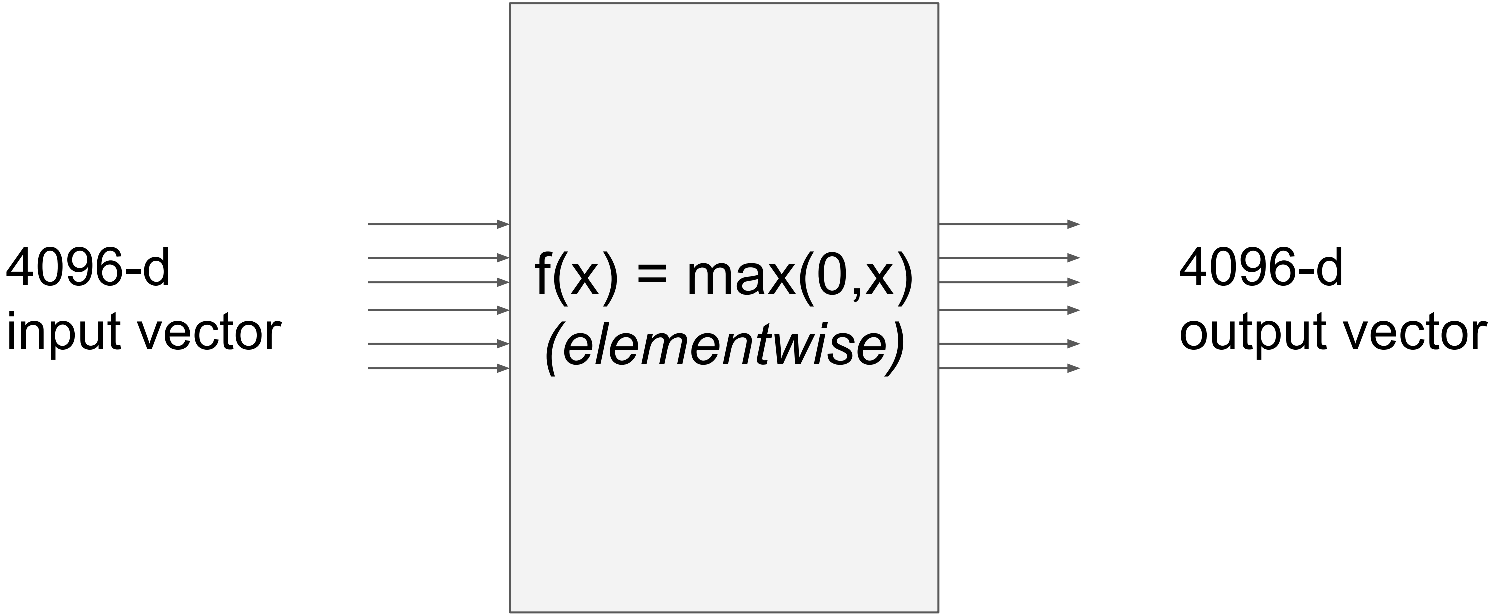
Gradients for vectorized code

(x,y,z are now vectors)



이제 우리의 변수 x,y,z에 대해서 숫자대신 벡터를 가지고 있다고 합시다.
모든 흐름은 정확히 같습니다. 차이점이라면 우리의 기울기는 자코비안 행렬이 될것입니다. 이는 각 요소의 미분을 포함하는 행렬입니다. 예를들어 x의 각원소에대해 z에대한 미분을 포함하는것입니다.

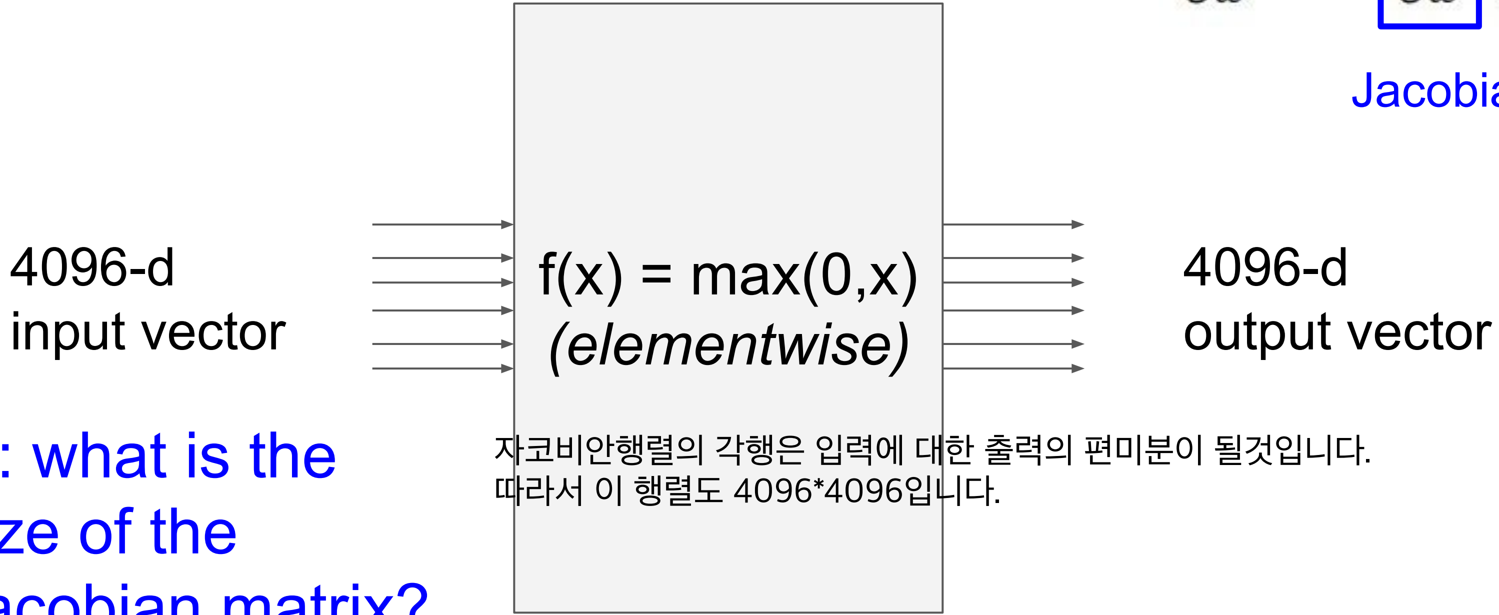
Vectorized operations



Vectorized operations

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

Jacobian matrix



Q: what is the size of the Jacobian matrix?

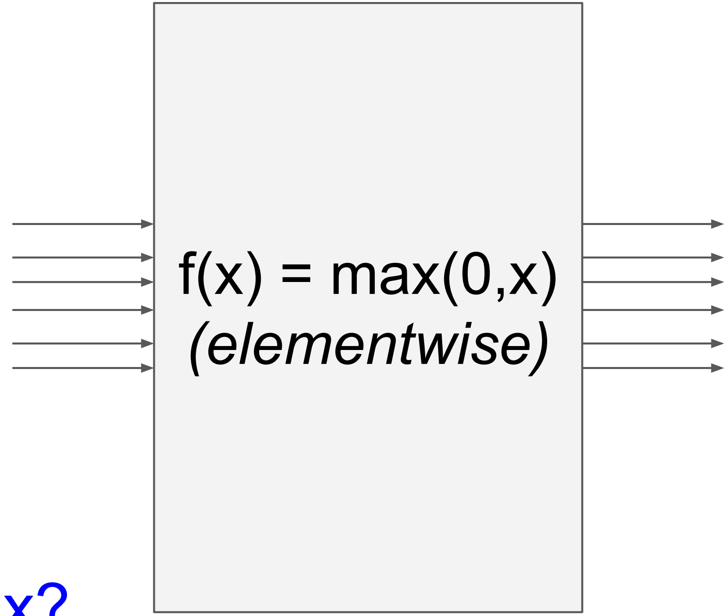
자코비안행렬의 각행은 입력에 대한 출력의 편미분이 될것입니다.
따라서 이 행렬도 4096*4096입니다.

Vectorized operations

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

Jacobian matrix

4096-d
input vector

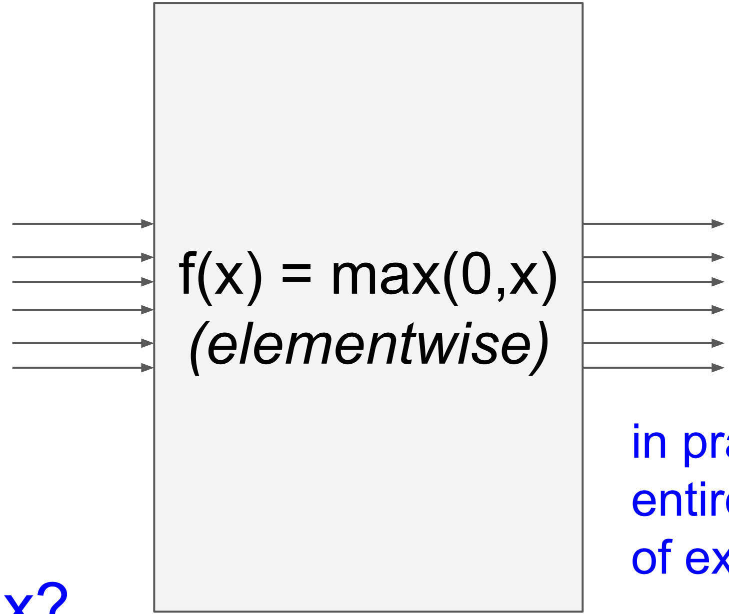


4096-d
output vector

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

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:

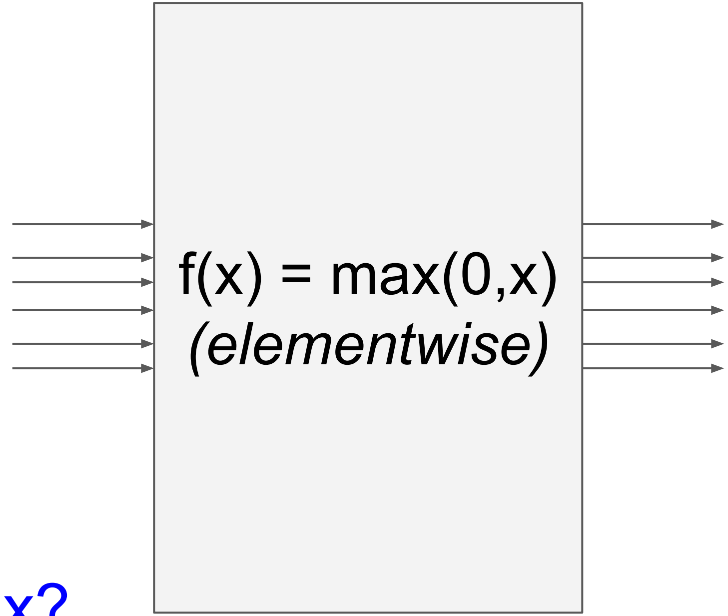
i.e. Jacobian would technically be a [409,600 x 409,600] matrix :\

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?

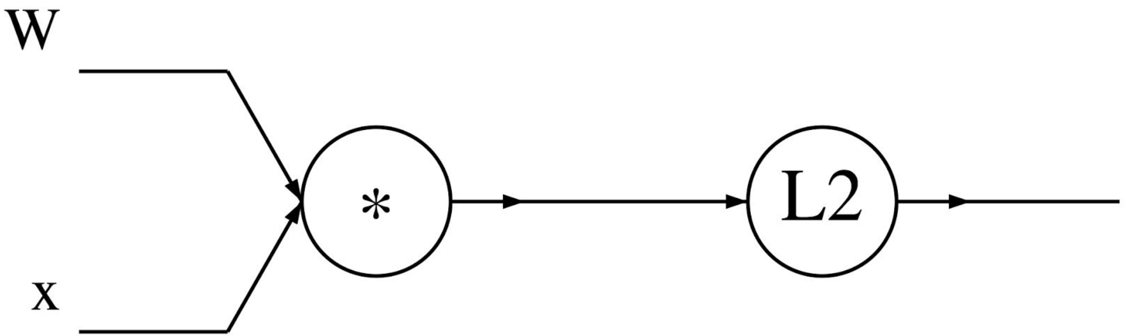
A vectorized example: $f(x,W) = ||W \cdot x||^2 = \sum_{i=1}^{n} (W \cdot x)_i^2$

그러면 이 자코비안행렬이 어떻게 생겨나게되었을까요? 만약 우리가 요소별로 최댓값을 갈는 여기에서 어떤일이 일어나는지 생각해본다면 입력의 어떤차원이 출력의 어떤 차원에 영향을 줍니까? 입력의 해당요소는 오직 출력의 해당요소에만 영향을 줍니다. 따라서 자코비안행렬은 대각행렬이 될것입니다.
좋습니다. 이제 계산그래프보다 구체적인 벡터화된 예제를 보겠습니다.

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

$\in \mathbb{R}^n \quad \in \mathbb{R}^{n \times n}$

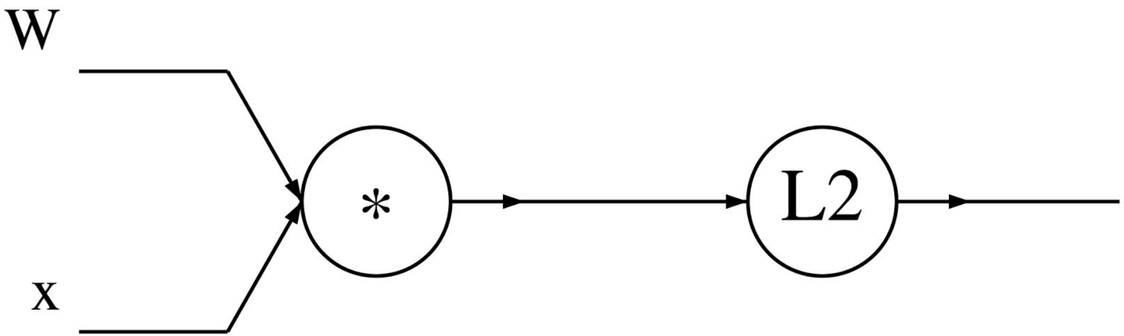
A vectorized example: $f(x, W) = ||W \cdot x||^2 = \sum_{i=1}^{n} (W \cdot x)_i^2$



여기서 x는 n차원 ,W는 n*n차원이라합시다.

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

$$\begin{bmatrix} 0.1 & 0.5 \\ -0.3 & 0.8 \end{bmatrix}$$



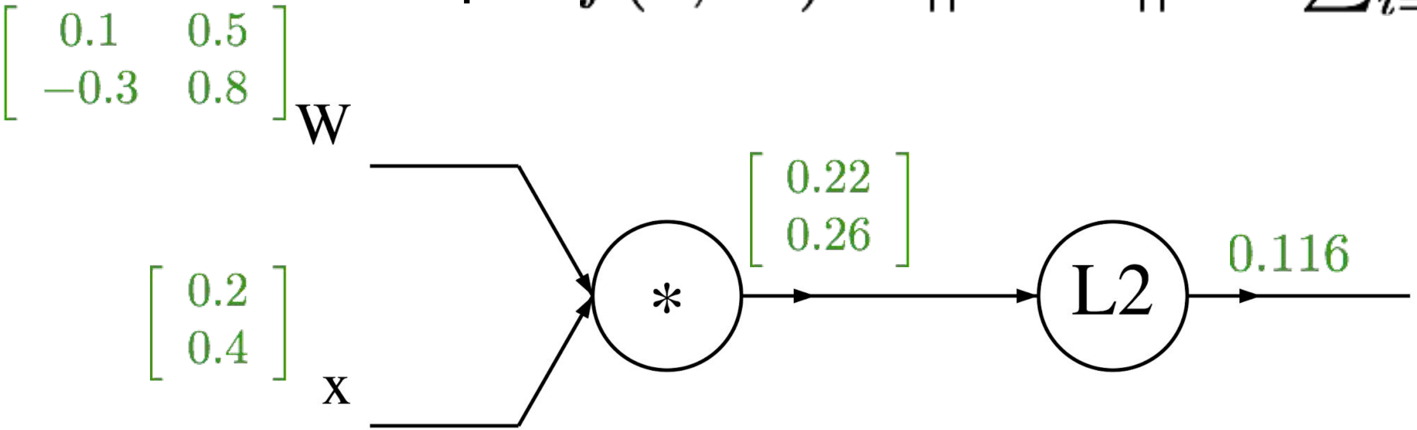
$$\begin{bmatrix} 0.2 \\ 0.4 \end{bmatrix}$$

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

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

해당 예는 x가 2차원벡터이고, W는 2*2행렬입니다. 이들의 곱인 q는 2*1행렬입니다. 이 q가 함수를 거치면 최종 값이 나옵니다.

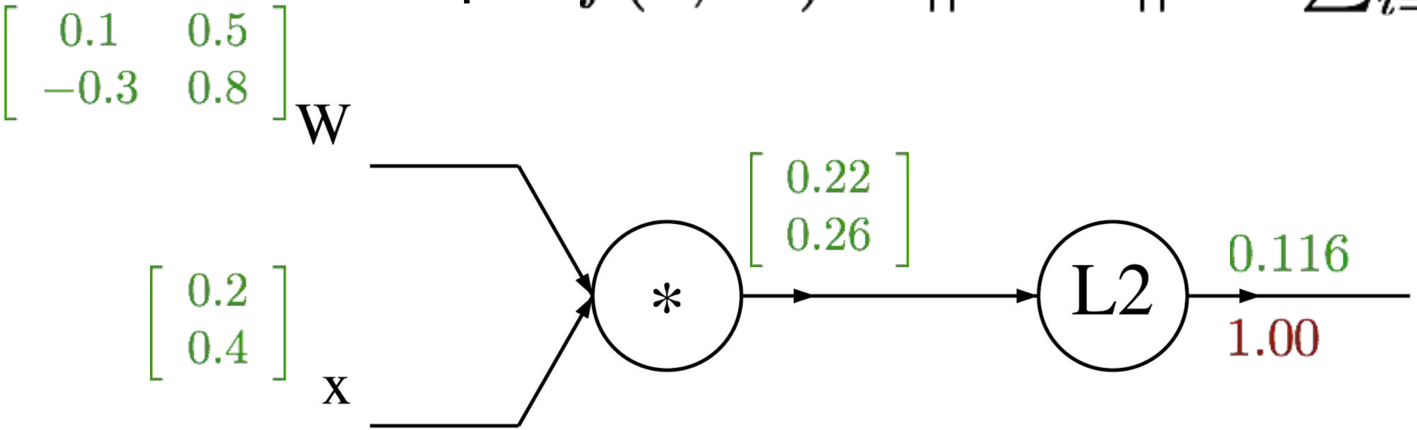
A vectorized example: $f(x, W) = ||W \cdot x||^2 = \sum_{i=1}^{n} (W \cdot x)_i^2$



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

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

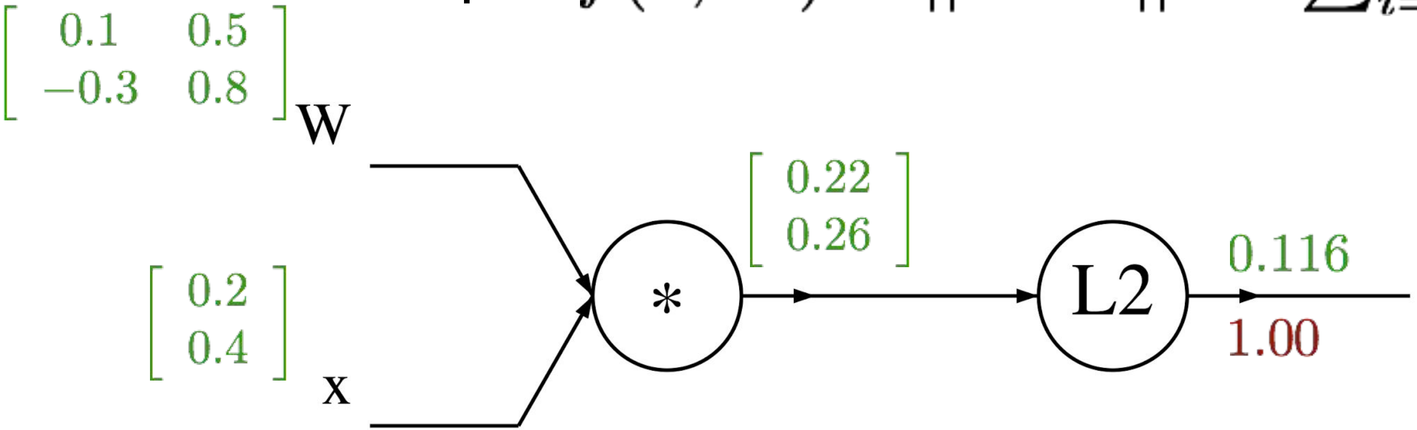
A vectorized example: $f(x, W) = ||W \cdot x||^2 = \sum_{i=1}^{n} (W \cdot x)_i^2$



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

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

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



이제 q에대한 f의 기울기 다음과같습니다.

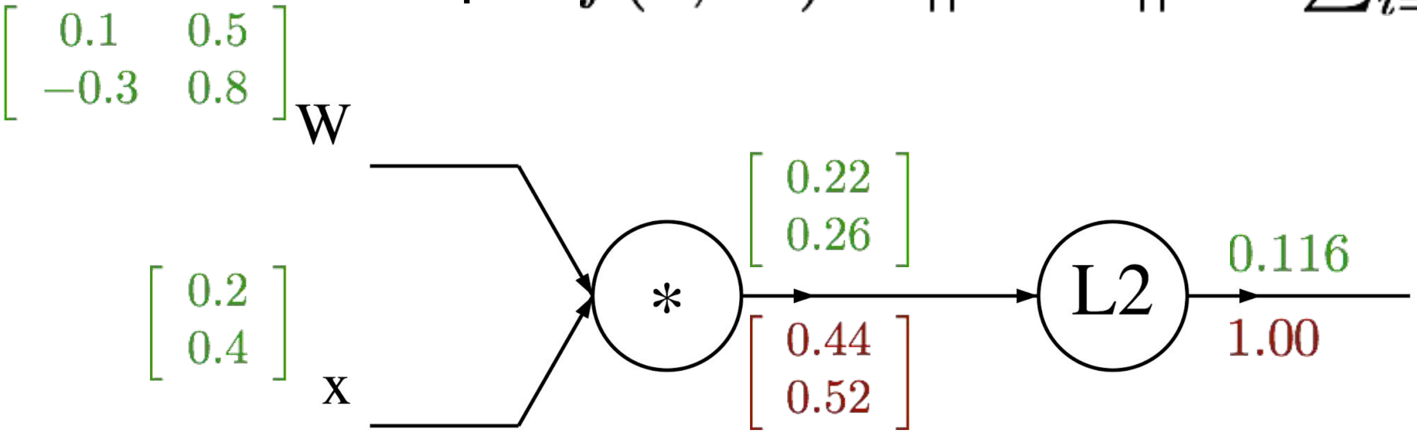
$$\frac{\partial f}{\partial q_i} = 2q_i$$

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

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

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

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



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

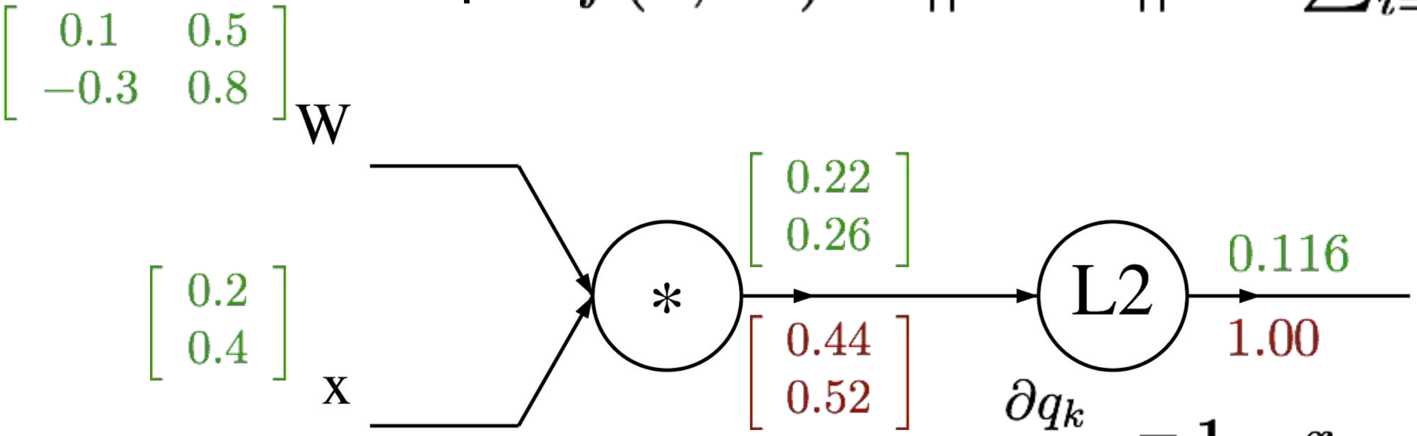
$$f(q) = ||q||^2 = q_1^2 + \cdots + q_n^2$$

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

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

이렇게 구한 함수의 local gradient에 상류기울기를 곱해줍니다.

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



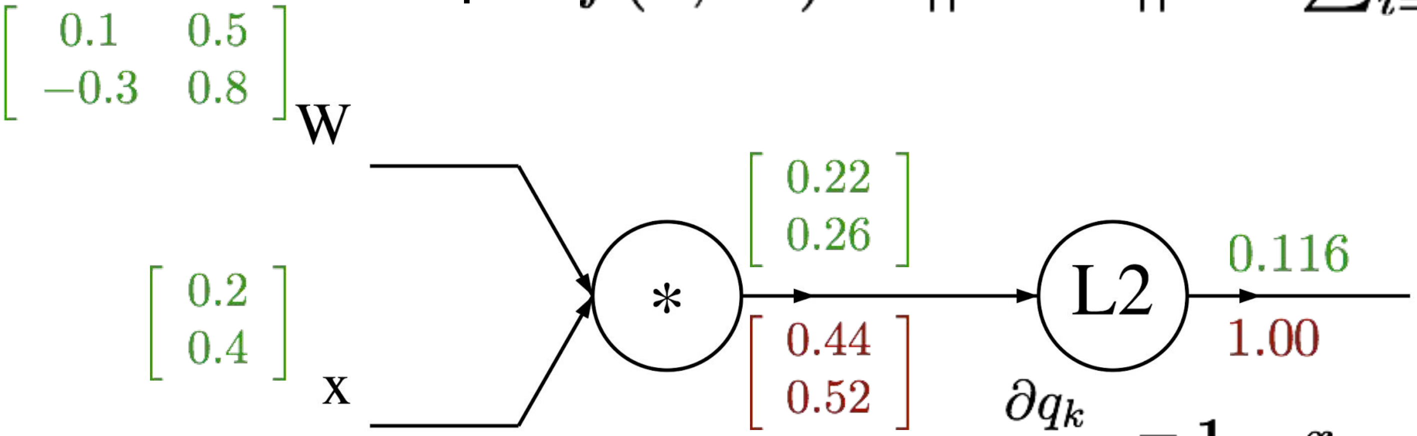
$$\frac{\partial q_k}{\partial W_{i,j}} = \mathbf{1}_{k=i} x_j$$

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

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

한걸음더 나아가봅시다. W의 기울기는 무엇입니까? 여기서 우리는 연쇄법칙을 다시 사용할것입니다.

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



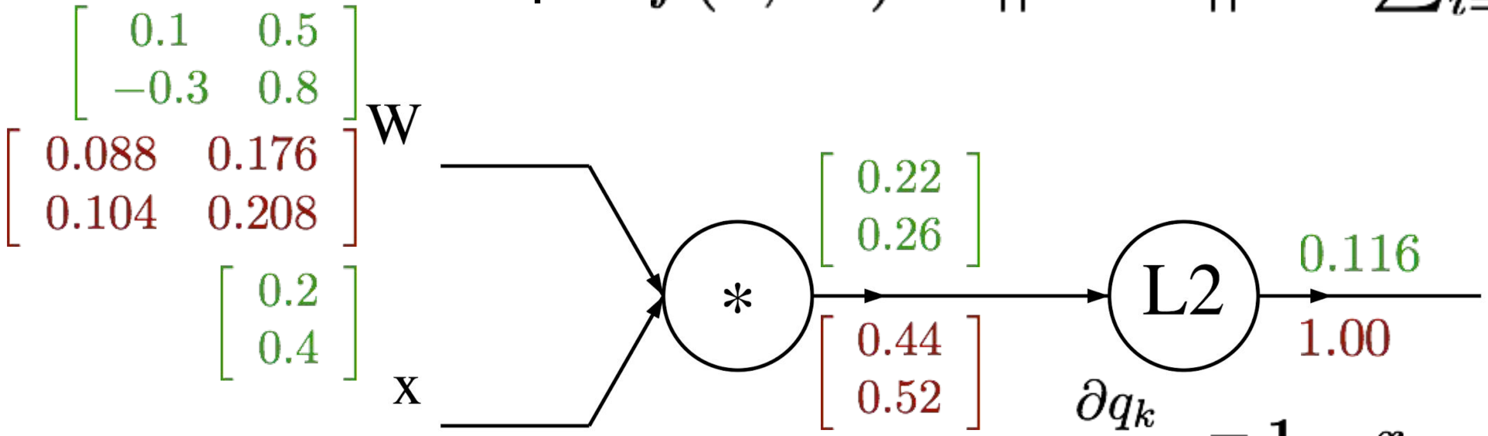
$$\frac{\partial q_k}{\partial W_{i,j}} = \mathbf{1}_{k=i} x_j$$

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

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

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

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



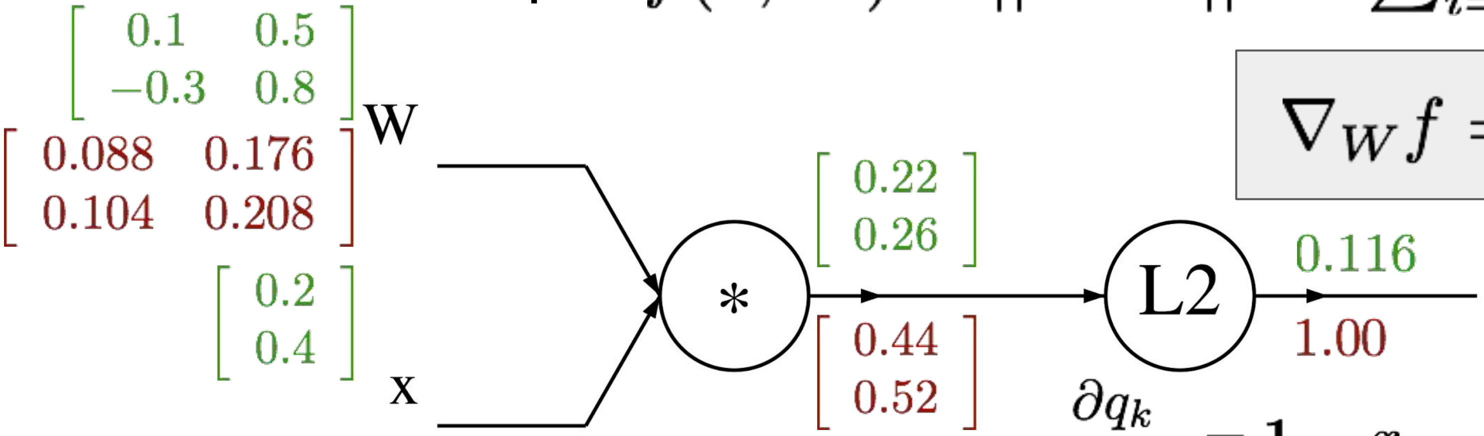
$$\frac{\partial q_k}{\partial W_{i,j}} = \mathbf{1}_{k=i} x_j$$

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

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

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

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



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

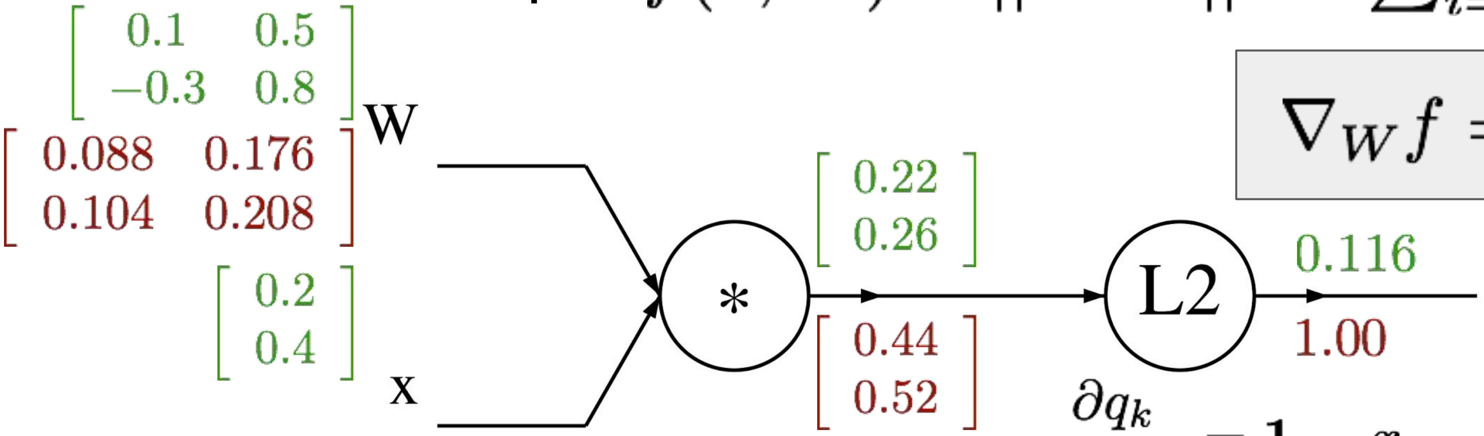
$$\frac{\partial q_k}{\partial W_{i,j}} = \mathbf{1}_{k=i} x_j$$

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

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

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

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



$$\nabla_W f = 2q \cdot x^T$$

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

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

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

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

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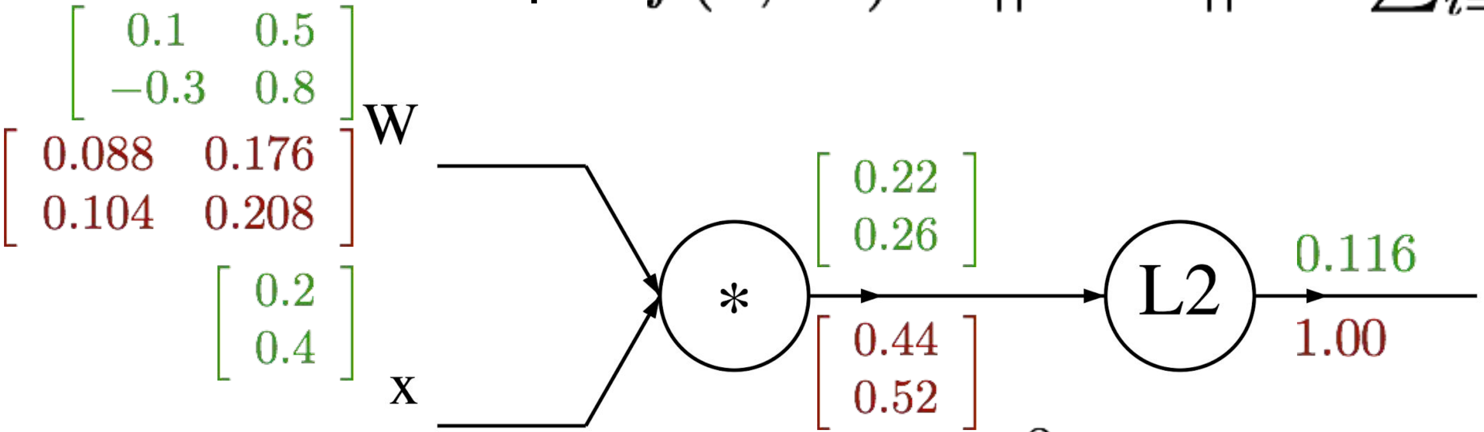
A vectorized example: $f(x, W) = ||W \cdot x||^2 = \sum_{i=1}^{n} (W \cdot x)_i^2$

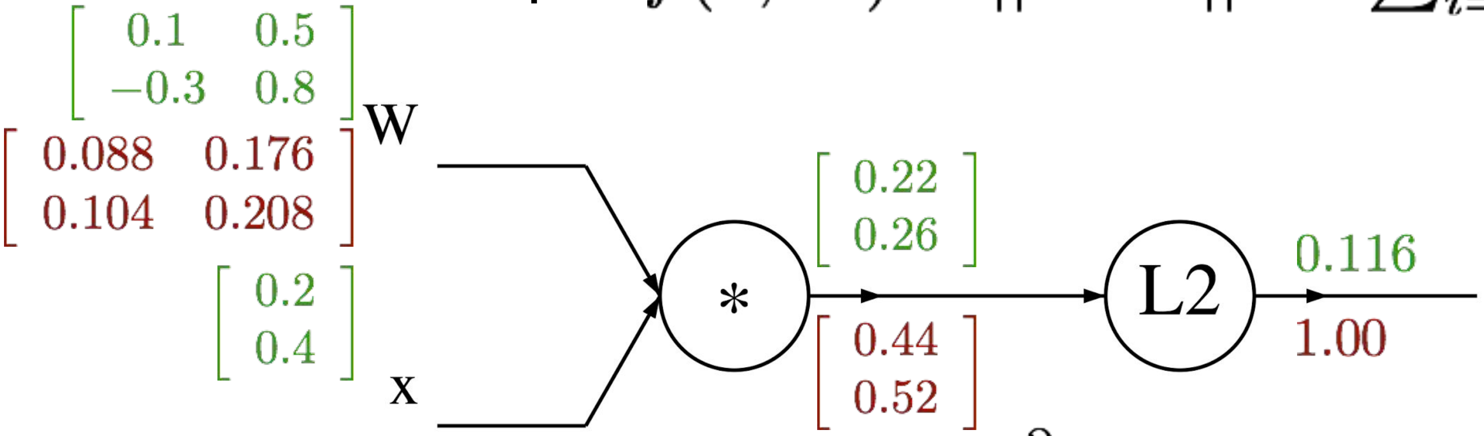


$$\frac{\partial q_k}{\partial x_i} = W_{k,i}$$

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

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

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



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

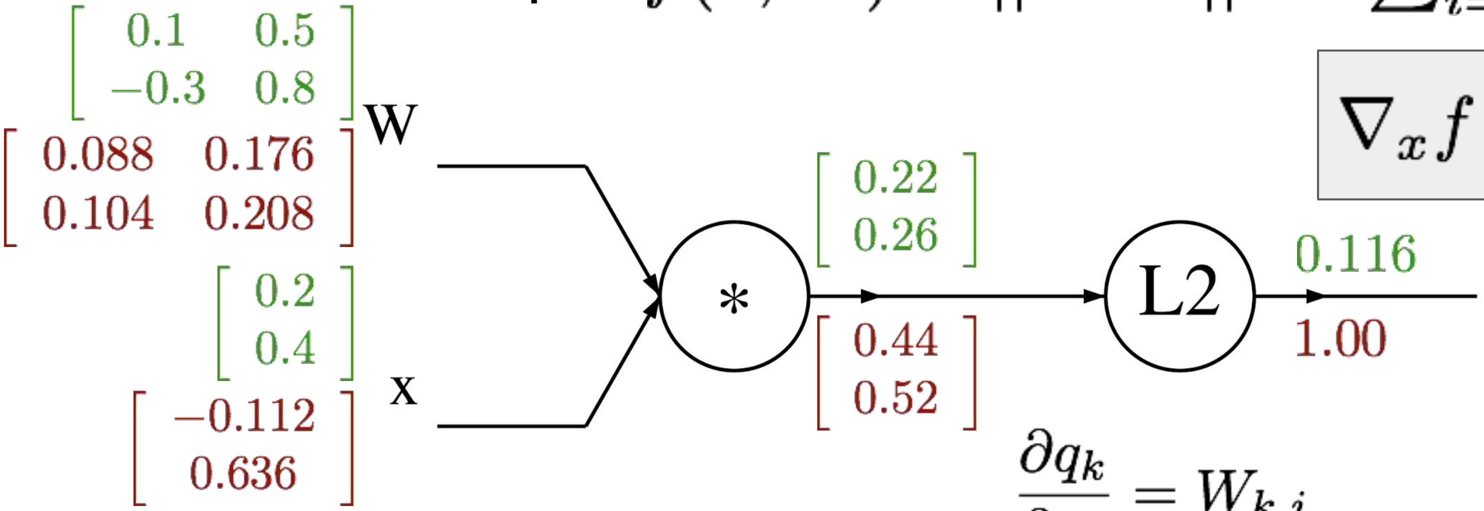
$$f(q) = ||q||^2 = q_1^2 + \cdots + q_n^2$$

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

$$\frac{\partial f}{\partial x_i} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial x_i}$$

$$= \sum_k 2 q_k W_{k,i}$$

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



$$\nabla_x f = 2W^T \cdot q$$

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

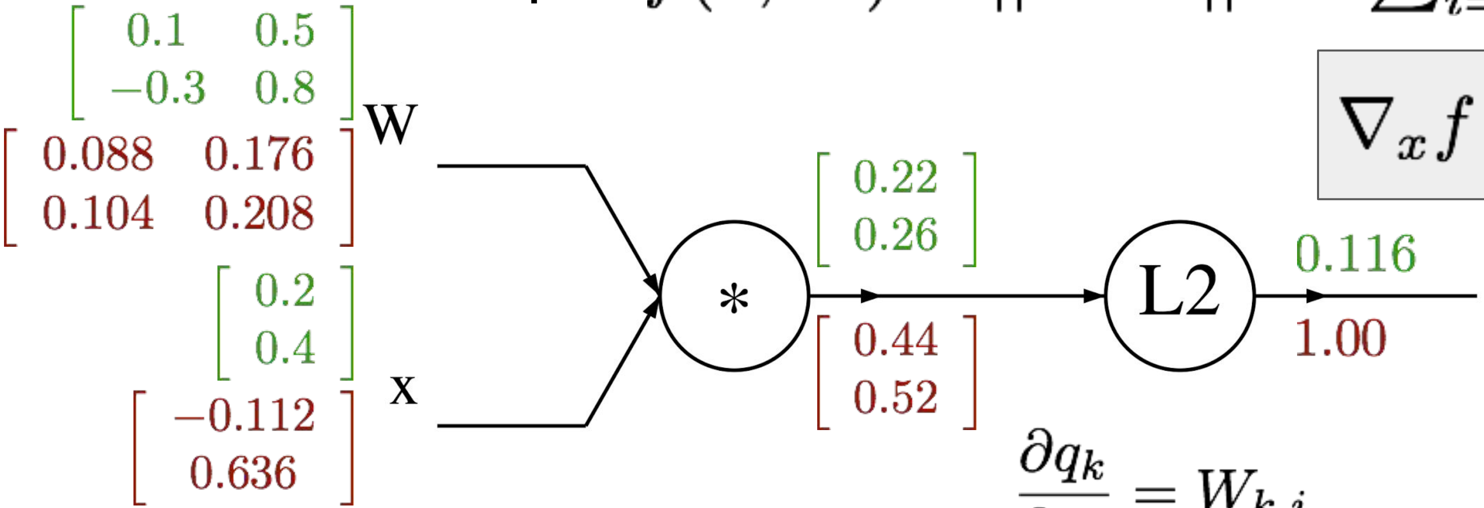
$$\frac{\partial f}{\partial x_i} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial x_i}$$

$$= \sum_k 2 q_k W_{k,i}$$

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

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

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



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

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

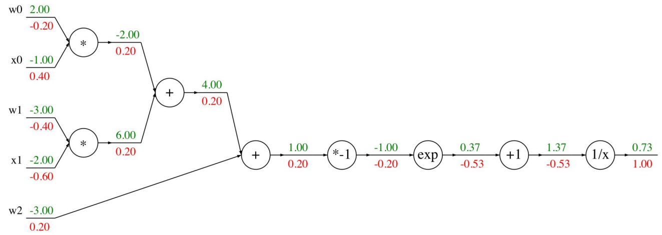
$$\frac{\partial f}{\partial x_i} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial x_i}$$

$$= \sum_k 2 q_k W_{k,i}$$

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

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

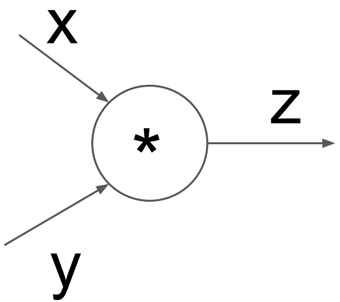
Modularized implementation: forward / backward API



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



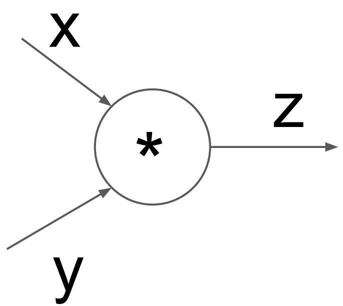
(x,y,z are scalars)

```
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]
```

Example: Caffe layers

Branch: master ▾ caffe / src / caffe / layers / | Create new file | Upload files | Find file | History

shelhamer committed on GitHub Merge pull request #4630 from BlGene/load_hdf5_fix … Latest commit e687a71 21 days ago

..		
absval_layer.cpp	dismantle layer headers	a year ago
absval_layer.cu	dismantle layer headers	a year ago
accuracy_layer.cpp	dismantle layer headers	a year ago
argmax_layer.cpp	dismantle layer headers	a year ago
base_conv_layer.cpp	enable dilated deconvolution	a year ago
base_data_layer.cpp	Using default from proto for prefetch	3 months ago
base_data_layer.cu	Switched multi-GPU to NCCL	3 months ago
batch_norm_layer.cpp	Add missing spaces besides equal signs in batch_norm_layer.cpp	4 months ago
batch_norm_layer.cu	dismantle layer headers	a year ago
batch_reindex_layer.cpp	dismantle layer headers	a year ago
batch_reindex_layer.cu	dismantle layer headers	a year ago
bias_layer.cpp	Remove incorrect cast of gemm int arg to Dtype in BiasLayer	a year ago
bias_layer.cu	Separation and generalization of ChannelwiseAffineLayer into BiasLayer	a year ago
bnll_layer.cpp	dismantle layer headers	a year ago
bnll_layer.cu	dismantle layer headers	a year ago
concat_layer.cpp	dismantle layer headers	a year ago
concat_layer.cu	dismantle layer headers	a year ago
contrastive_loss_layer.cpp	dismantle layer headers	a year ago
contrastive_loss_layer.cu	dismantle layer headers	a year ago
conv_layer.cpp	add support for 2D dilated convolution	a year ago
conv_layer.cu	dismantle layer headers	a year ago
crop_layer.cpp	remove redundant operations in Crop layer (#5138)	2 months ago
crop_layer.cu	remove redundant operations in Crop layer (#5138)	2 months ago
cudnn_conv_layer.cpp	dismantle layer headers	a year ago
cudnn_conv_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago

cudnn_lcn_layer.cpp	dismantle layer headers	a year ago
cudnn_lcn_layer.cu	dismantle layer headers	a year ago
cudnn_lrn_layer.cpp	dismantle layer headers	a year ago
cudnn_lrn_layer.cu	dismantle layer headers	a year ago
cudnn_pooling_layer.cpp	dismantle layer headers	a year ago
cudnn_pooling_layer.cu	dismantle layer headers	a year ago
cudnn_relu_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_relu_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_sigmoid_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_sigmoid_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_softmax_layer.cpp	dismantle layer headers	a year ago
cudnn_softmax_layer.cu	dismantle layer headers	a year ago
cudnn_tanh_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_tanh_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
data_layer.cpp	Switched multi-GPU to NCCL	3 months ago
deconv_layer.cpp	enable dilated deconvolution	a year ago
deconv_layer.cu	dismantle layer headers	a year ago
dropout_layer.cpp	supporting N-D Blobs in Dropout layer Reshape	a year ago
dropout_layer.cu	dismantle layer headers	a year ago
dummy_data_layer.cpp	dismantle layer headers	a year ago
eltwise_layer.cpp	dismantle layer headers	a year ago
eltwise_layer.cu	dismantle layer headers	a year ago
elu_layer.cpp	ELU layer with basic tests	a year ago
elu_layer.cu	ELU layer with basic tests	a year ago
embed_layer.cpp	dismantle layer headers	a year ago
embed_layer.cu	dismantle layer headers	a year ago
euclidean_loss_layer.cpp	dismantle layer headers	a year ago
euclidean_loss_layer.cu	dismantle layer headers	a year ago
exp_layer.cpp	Solving issue with exp layer with base e	a year ago
exp_layer.cu	dismantle layer headers	a year ago

Caffe Sigmoid Layer

```
#include <cmath>
#include <vector>

#include "caffe/layers/sigmoid_layer.hpp"

namespace caffe {

template <typename Dtype>
inline Dtype sigmoid(Dtype x) {
  return 1. / (1. + exp(-x));
}

template <typename Dtype>
void SigmoidLayer<Dtype>::Forward_cpu(const vector<Blob<Dtype>*>& bottom,
    const vector<Blob<Dtype>*>& top) {
  const Dtype* bottom_data = bottom[0]->cpu_data();
  Dtype* top_data = top[0]->mutable_cpu_data();
  const int count = bottom[0]->count();
  for (int i = 0; i < count; ++i) {
    top_data[i] = sigmoid(bottom_data[i]);
  }
}

template <typename Dtype>
void SigmoidLayer<Dtype>::Backward_cpu(const vector<Blob<Dtype>*>& top,
    const vector<bool>& propagate_down,
    const vector<Blob<Dtype>*>& bottom) {
  if (propagate_down[0]) {
    const Dtype* top_data = top[0]->cpu_data();
    const Dtype* top_diff = top[0]->cpu_diff();
    Dtype* bottom_diff = bottom[0]->mutable_cpu_diff();
    const int count = bottom[0]->count();
    for (int i = 0; i < count; ++i) {
      const Dtype sigmoid_x = top_data[i];
      bottom_diff[i] = top_diff[i] * sigmoid_x * (1. - sigmoid_x);
    }
  }
}

#ifdef CPU_ONLY
STUB_GPU(SigmoidLayer);
#endif

INSTANTIATE_CLASS(SigmoidLayer);


}  // namespace caffe
```

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

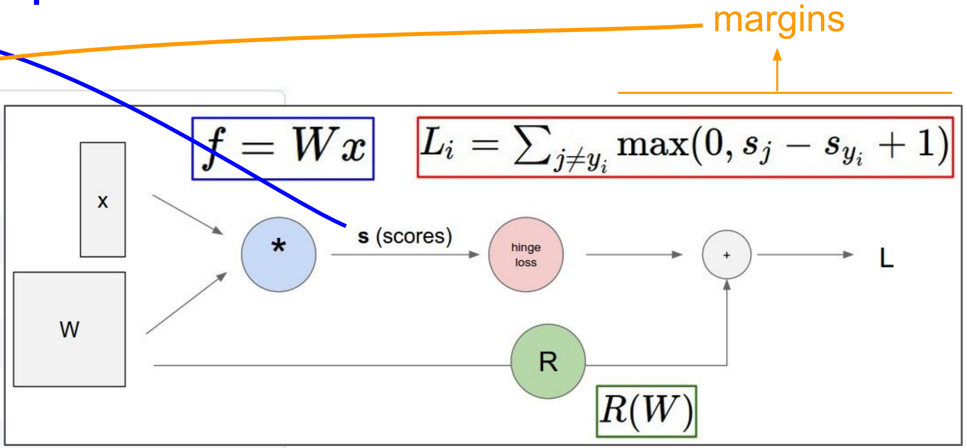
$$\boxed{(1-\sigma(x))\sigma(x)}$$ * top_diff (chain rule)

In Assignment 1: Writing SVM / Softmax

Stage your forward/backward computation!

E.g. for the SVM:

```
# receive W (weights), X (data)
# forward pass (we have 8 lines)
scores = #...
margins = #...
data_loss = #...
reg_loss = #...
loss = data_loss + reg_loss
# backward pass (we have 5 lines)
dmargins = # ... (optionally, we go direct to dscores)
dscores = #...
dW = #...
```



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

Next: Neural Networks

Neural networks: without the brain stuff

(**Before**) Linear score function: $f = Wx$

Neural networks: without the brain stuff

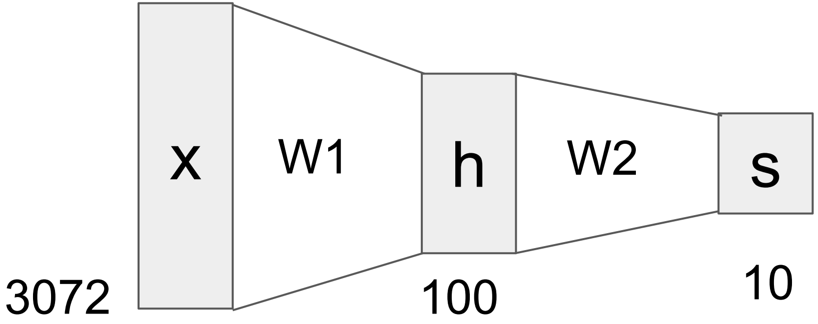
(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

Neural networks: without the brain stuff

(**Before**) Linear score function: $f = Wx$

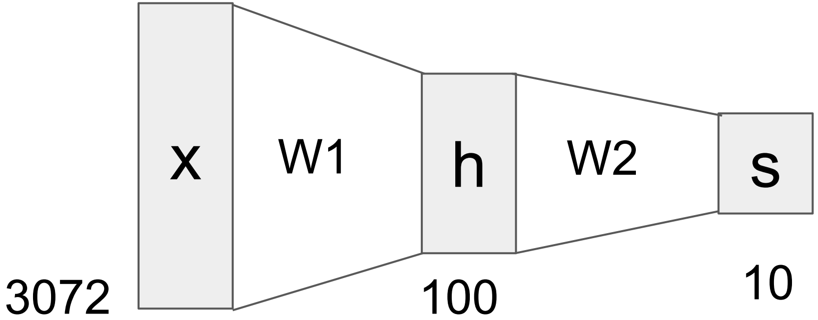
(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

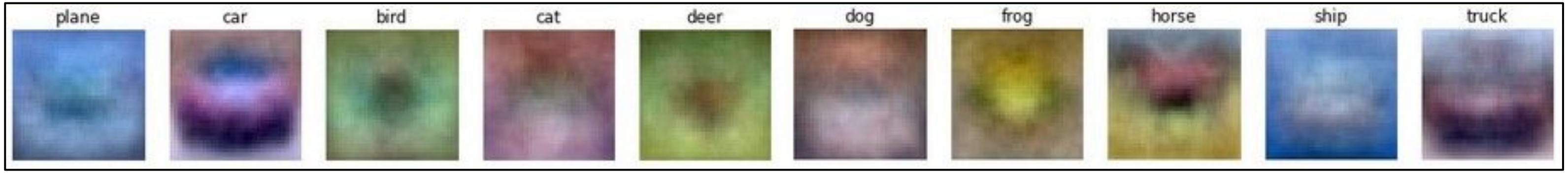


Neural networks: without the brain stuff

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$





Neural networks: without the brain stuff

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$
or 3-layer Neural Network

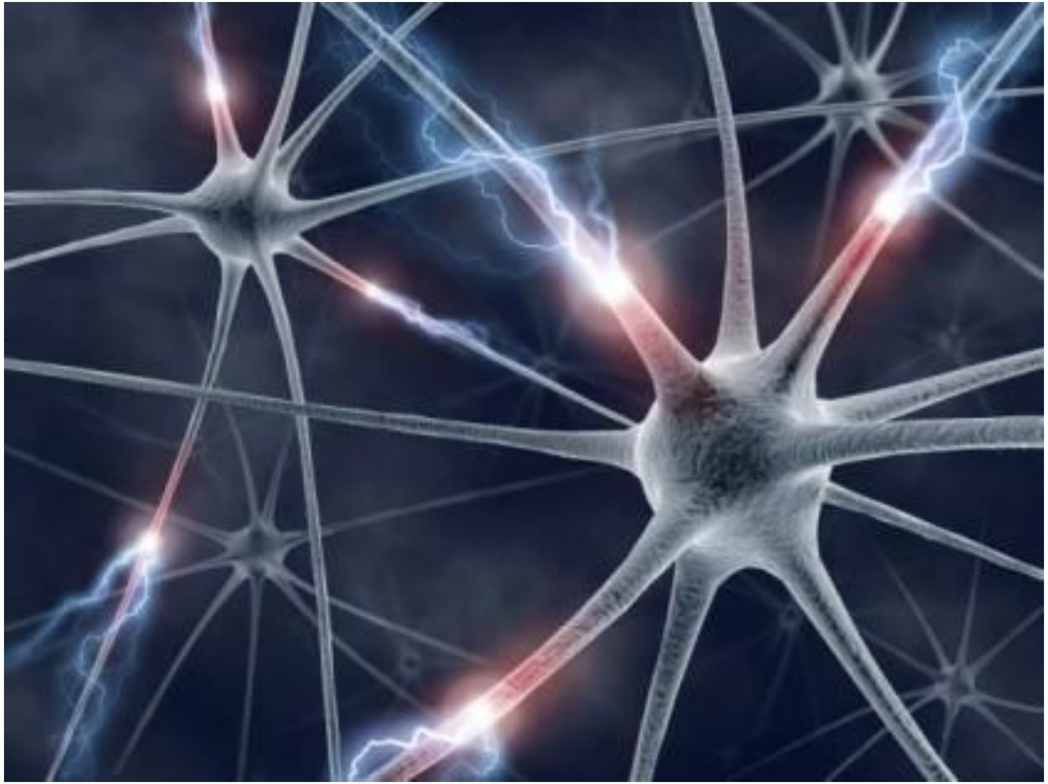
$$f = W_3 \max(0, W_2 \max(0, W_1 x))$$

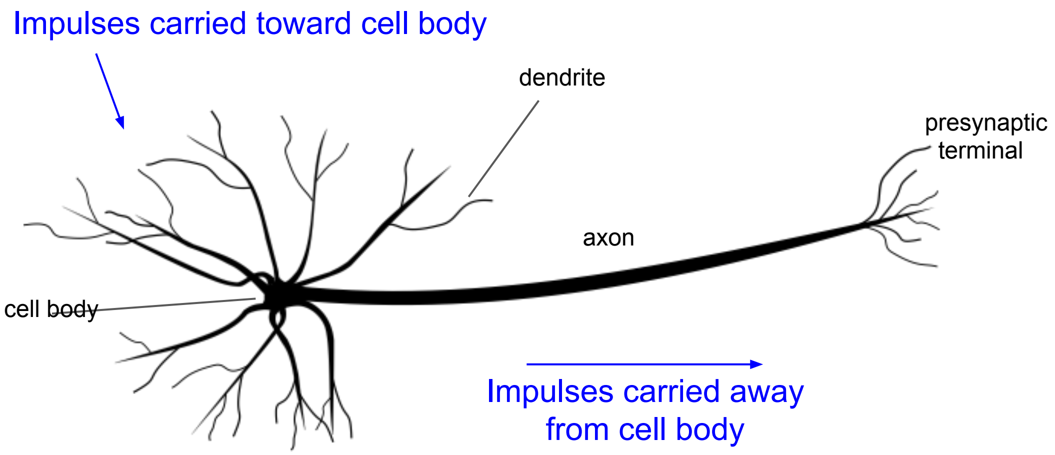
Full implementation of training a 2-layer Neural Network needs ~20 lines:

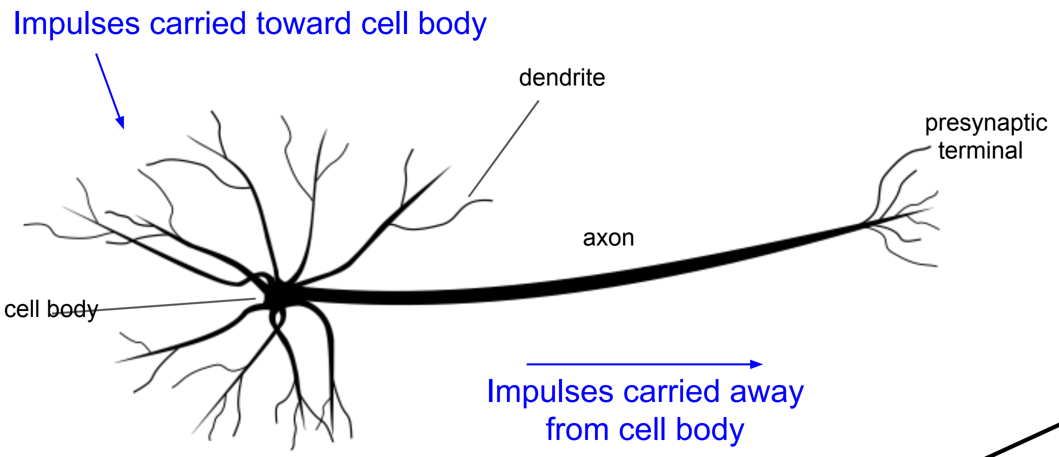
```python
import numpy as np
from numpy.random import randn

N, D_in, H, D_out = 64, 1000, 100, 10
x, y = randn(N, D_in), randn(N, D_out)
w1, w2 = randn(D_in, H), randn(H, D_out)

for t in range(2000):
  h = 1 / (1 + np.exp(-x.dot(w1)))
  y_pred = h.dot(w2)
  loss = np.square(y_pred - y).sum()
  print(t, loss)

  grad_y_pred = 2.0 * (y_pred - y)
  grad_w2 = h.T.dot(grad_y_pred)
  grad_h = grad_y_pred.dot(w2.T)
  grad_w1 = x.T.dot(grad_h * h * (1 - h))

  w1 -= 1e-4 * grad_w1
  w2 -= 1e-4 * grad_w2
```

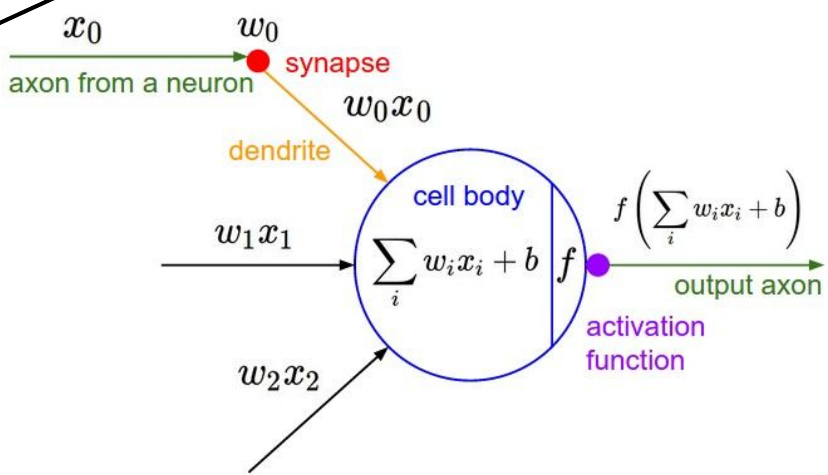
In Assignment 2: Writing a 2-layer net

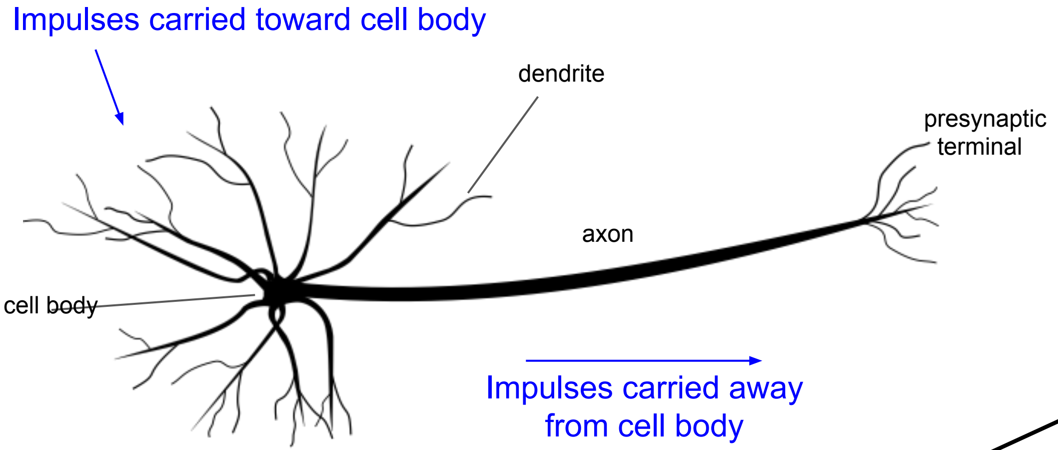
```
# receive W1,W2,b1,b2 (weights/biases), X (data)
# forward pass:
h1 = #... function of X,W1,b1
scores = #... function of h1,W2,b2
loss = #... (several lines of code to evaluate Softmax loss)
# backward pass:
dscores = #...
dh1,dW2,db2 = #...
dW1,db1 = #...
```

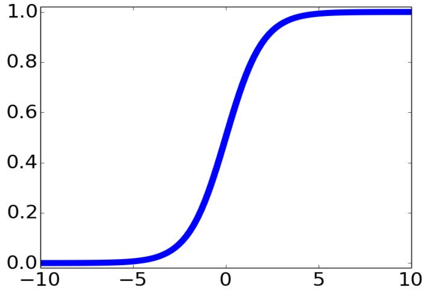



Impulses carried toward cell body
dendrite
presynaptic terminal
axon
cell body
Impulses carried away from cell body


Impulses carried toward cell body
dendrite
presynaptic
terminal
axon
cell body
Impulses carried away
from cell body

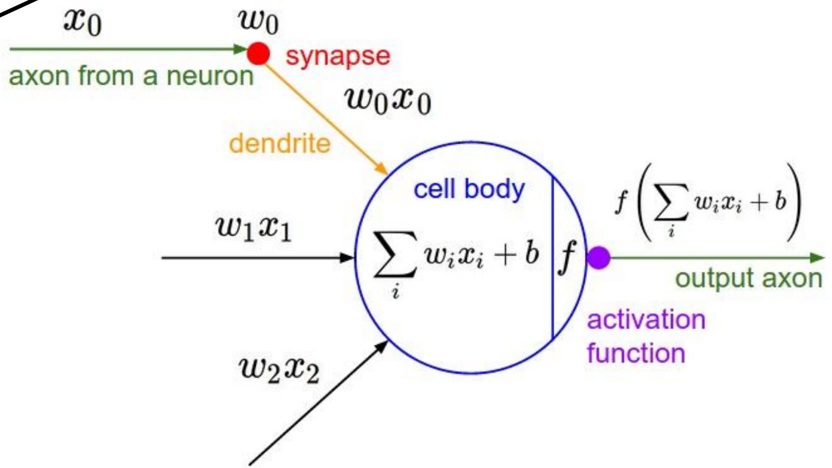

x_0
w_0
synapse
axon from a neuron
$w_0 x_0$
dendrite
cell body
$f\left(\sum_i w_i x_i + b\right)$
$w_1 x_1$
$\sum_i w_i x_i + b$
f
output axon
activation
function
$w_2 x_2$

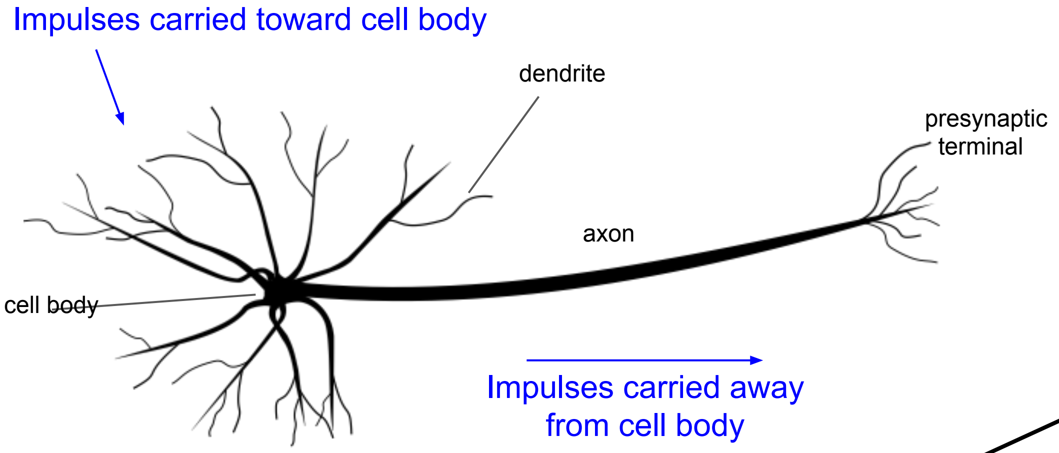


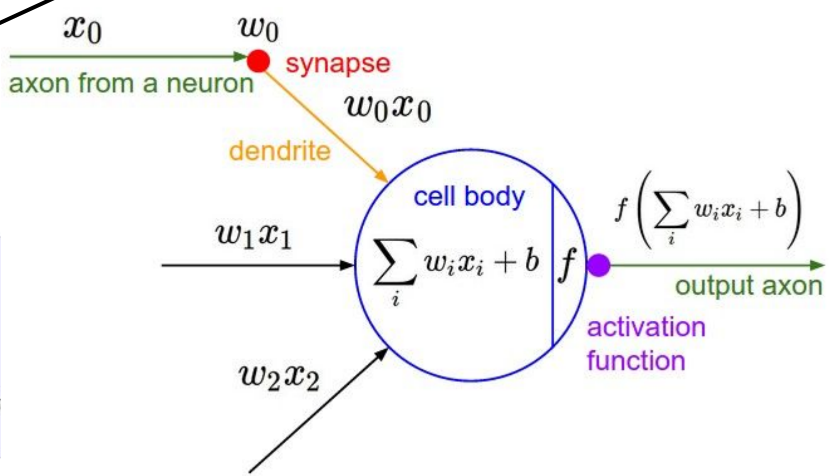


sigmoid activation function

$$\frac{1}{1+e^{-x}}$$








```python
class Neuron:
  # ...
  def neuron_tick(inputs):
    """ assume inputs and weights are 1-D numpy arrays and bias is a number """
    cell_body_sum = np.sum(inputs * self.weights) + self.bias
    firing_rate = 1.0 / (1.0 + math.exp(-cell_body_sum)) # sigmoid activation func
    return firing_rate
```

Be very careful with your brain analogies!

Biological Neurons:

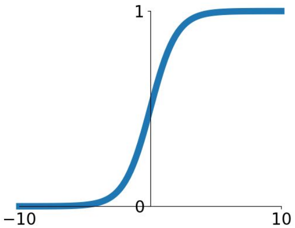
- Many different types
- Dendrites can perform complex non-linear computations
- Synapses are not a single weight but a complex non-linear dynamical system
- Rate code may not be adequate

[Dendritic Computation. London and Hausser]

Activation functions

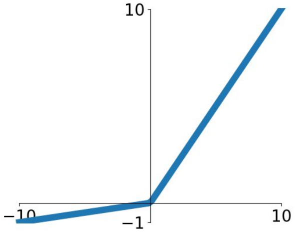
Sigmoid

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



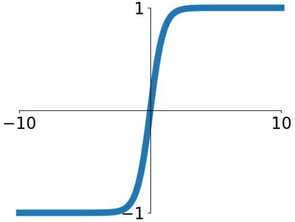
Leaky ReLU

$$\max(0.1x, x)$$



tanh

$$\tanh(x)$$

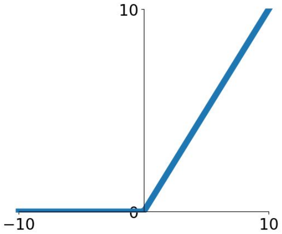


Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

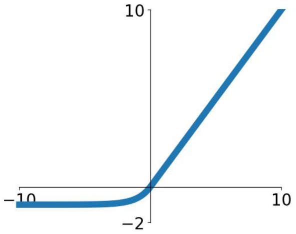
ReLU

$$\max(0, x)$$

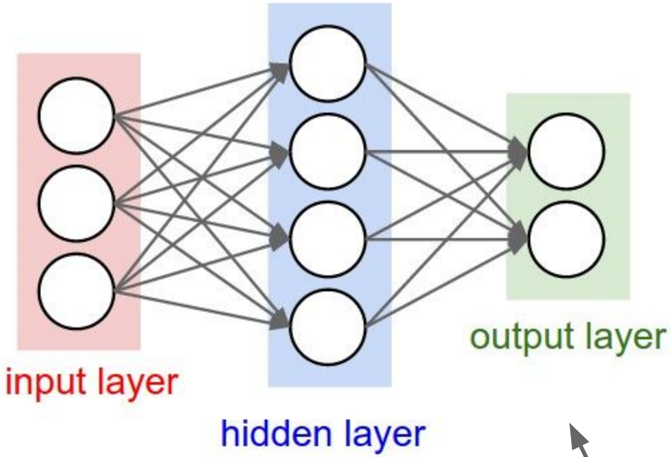


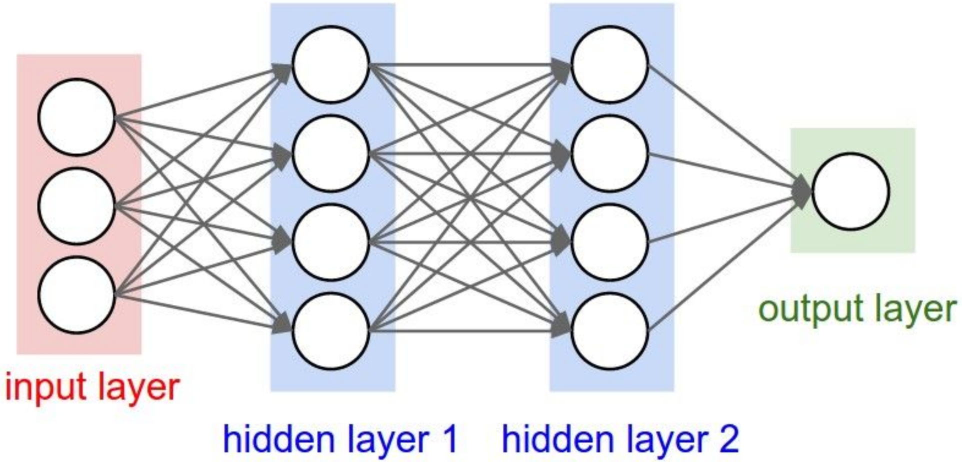
ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Neural networks: Architectures





"2-layer Neural Net", or
"1-hidden-layer Neural Net"

"3-layer Neural Net", or
"2-hidden-layer Neural Net"

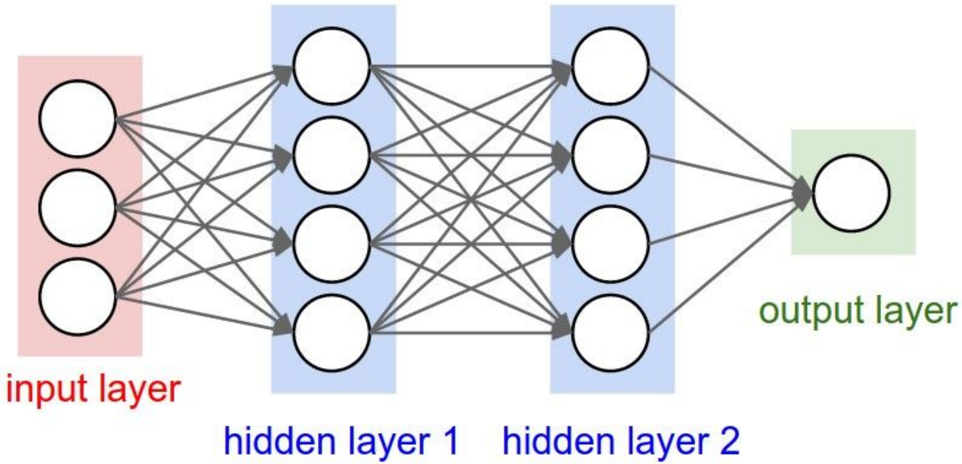
"Fully-connected" layers

Example feed-forward computation of a neural network

```python
class Neuron:
  # ...
  def neuron_tick(inputs):
    """ assume inputs and weights are 1-D numpy arrays and bias is a number """
    cell_body_sum = np.sum(inputs * self.weights) + self.bias
    firing_rate = 1.0 / (1.0 + math.exp(-cell_body_sum)) # sigmoid activation function
    return firing_rate
```

We can efficiently evaluate an entire layer of neurons.

Example feed-forward computation of a neural network




```
# forward-pass of a 3-layer neural network:
f = lambda x: 1.0/(1.0 + np.exp(-x)) # activation function (use sigmoid)
x = np.random.randn(3, 1) # random input vector of three numbers (3x1)
h1 = f(np.dot(W1, x) + b1) # calculate first hidden layer activations (4x1)
h2 = f(np.dot(W2, h1) + b2) # calculate second hidden layer activations (4x1)
out = np.dot(W3, h2) + b3 # output neuron (1x1)
```

Summary

- We arrange neurons into fully-connected layers
- The abstraction of a **layer** has the nice property that it allows us to use efficient vectorized code (e.g. matrix multiplies)
- Neural networks are not really *neural*
- Next time: Convolutional Neural Networks