ML/DL for Everyone with PYTORCH

Lecture 4: Back-propagation

Sung Kim <hunkim+ml@gmail.com> HKUST
Code: https://github.com/hunkim/PyTorchZeroToAll
Slides: http://bit.ly/PyTorchZeroAll
Videos: http://bit.ly/PyTorchVideo

Call for Comments

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Picture from http://www.tssablog.org/archives/3280

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Lecture 4: Back-propagation & Autograd

Sung Kim <hunkim+ml@gmail.com> HKUST

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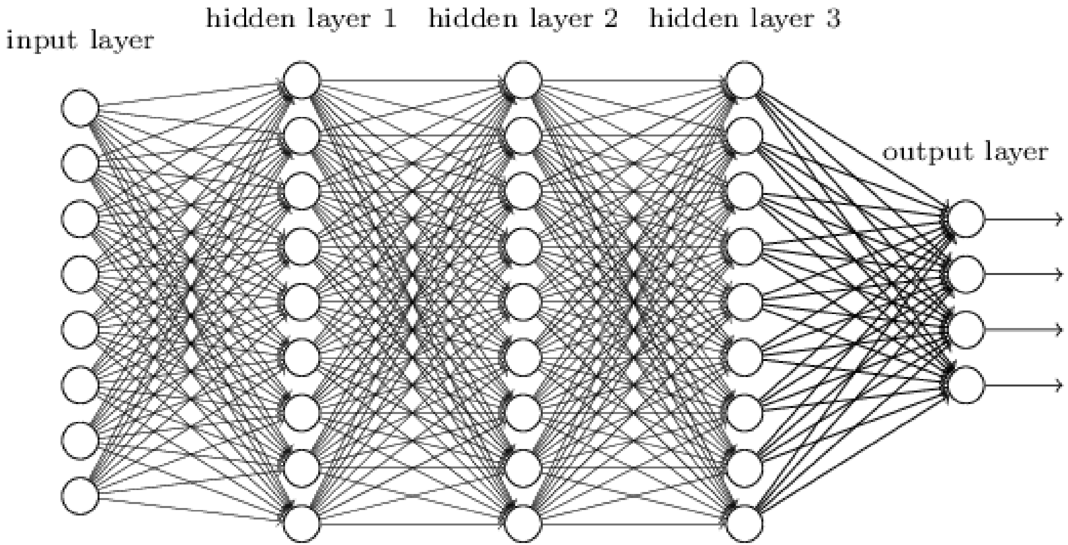
Computing gradient in simple network

Gradient of **loss** with respect to ***w***

$$\frac{\partial loss}{\partial w} = ?$$

```python
# compute gradient
def gradient(x, y):  # d_loss/d_w
    return 2 * x * (x * w - y)
```

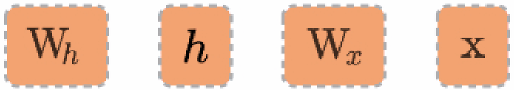
Complicated network?



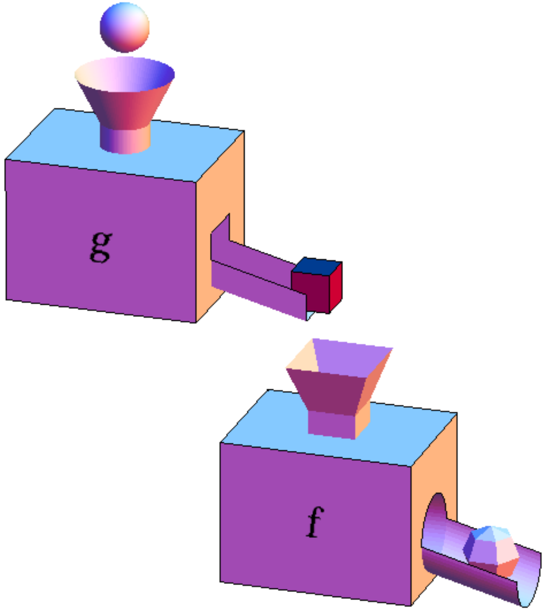
Gradient of **loss**
with respect to ***w***

$$\frac{\partial loss}{\partial w} = ?$$

Better way? Computational graph + chain rule



Chain Rule

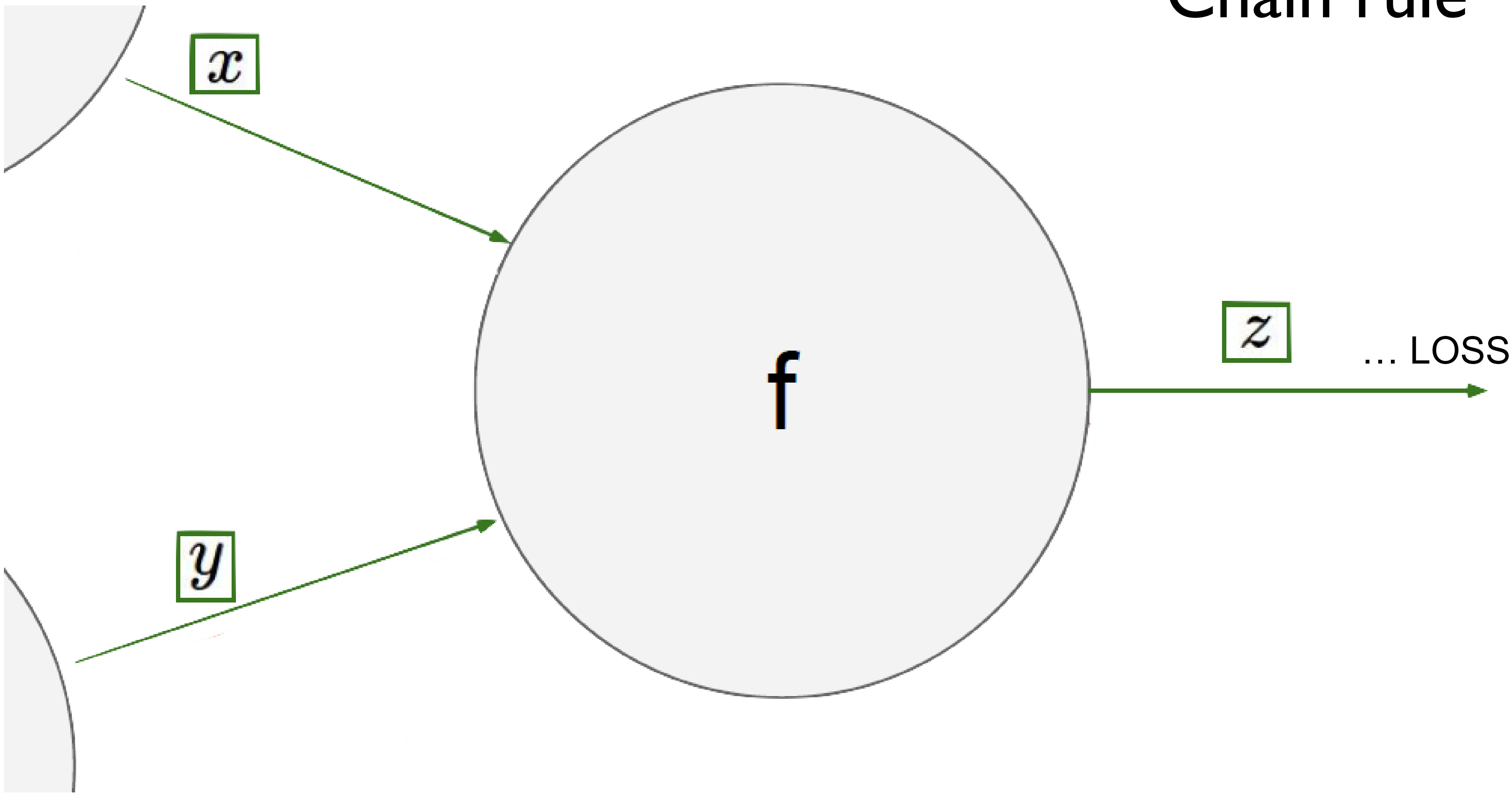


$$f = f(g)\ ;\quad g = g(x)$$

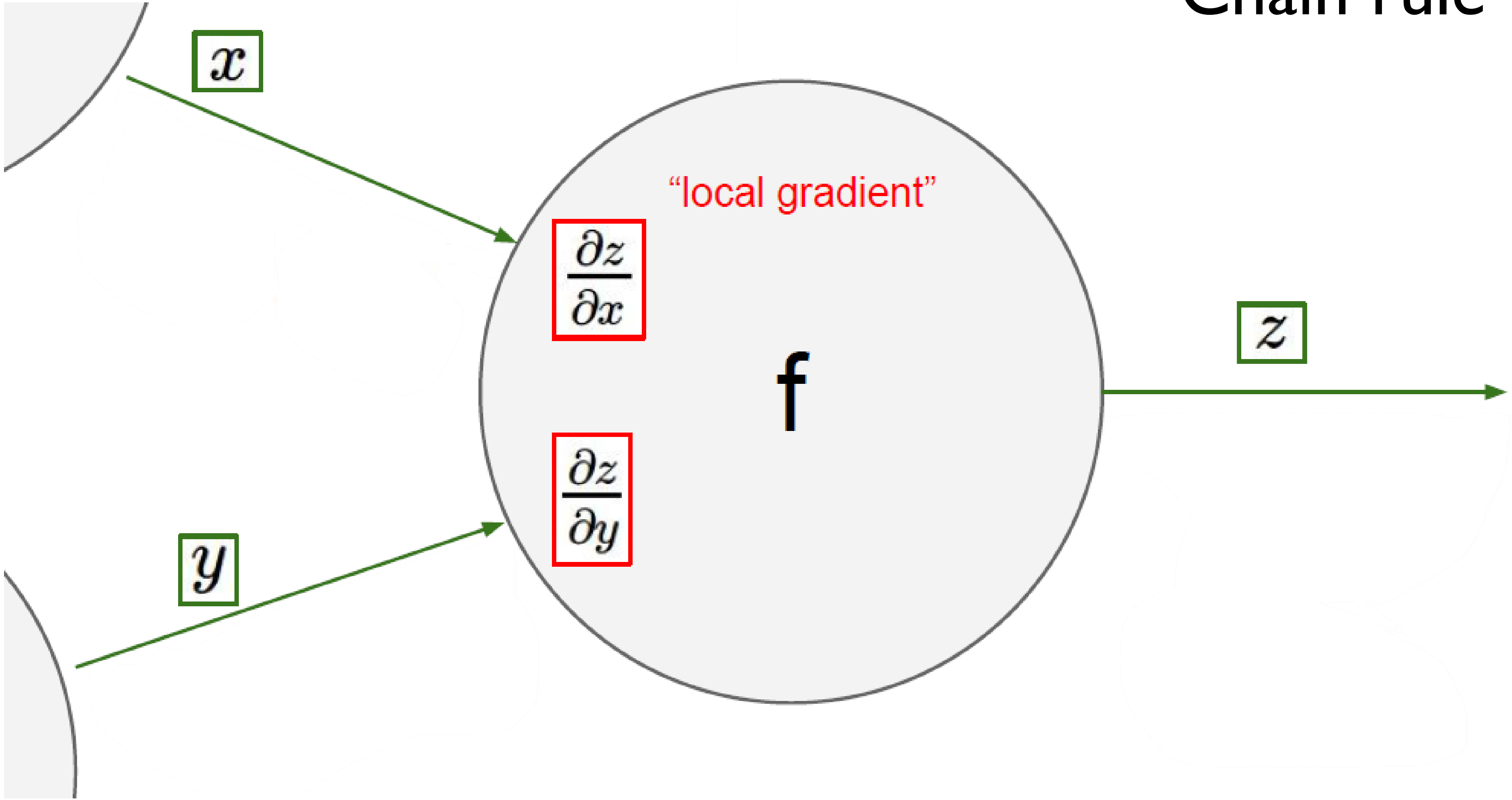
$$\frac{df}{dx} = \frac{df}{dg}\,\frac{dg}{dx}$$

http://mathinsight.org/image/function_machines_composed

Chain rule

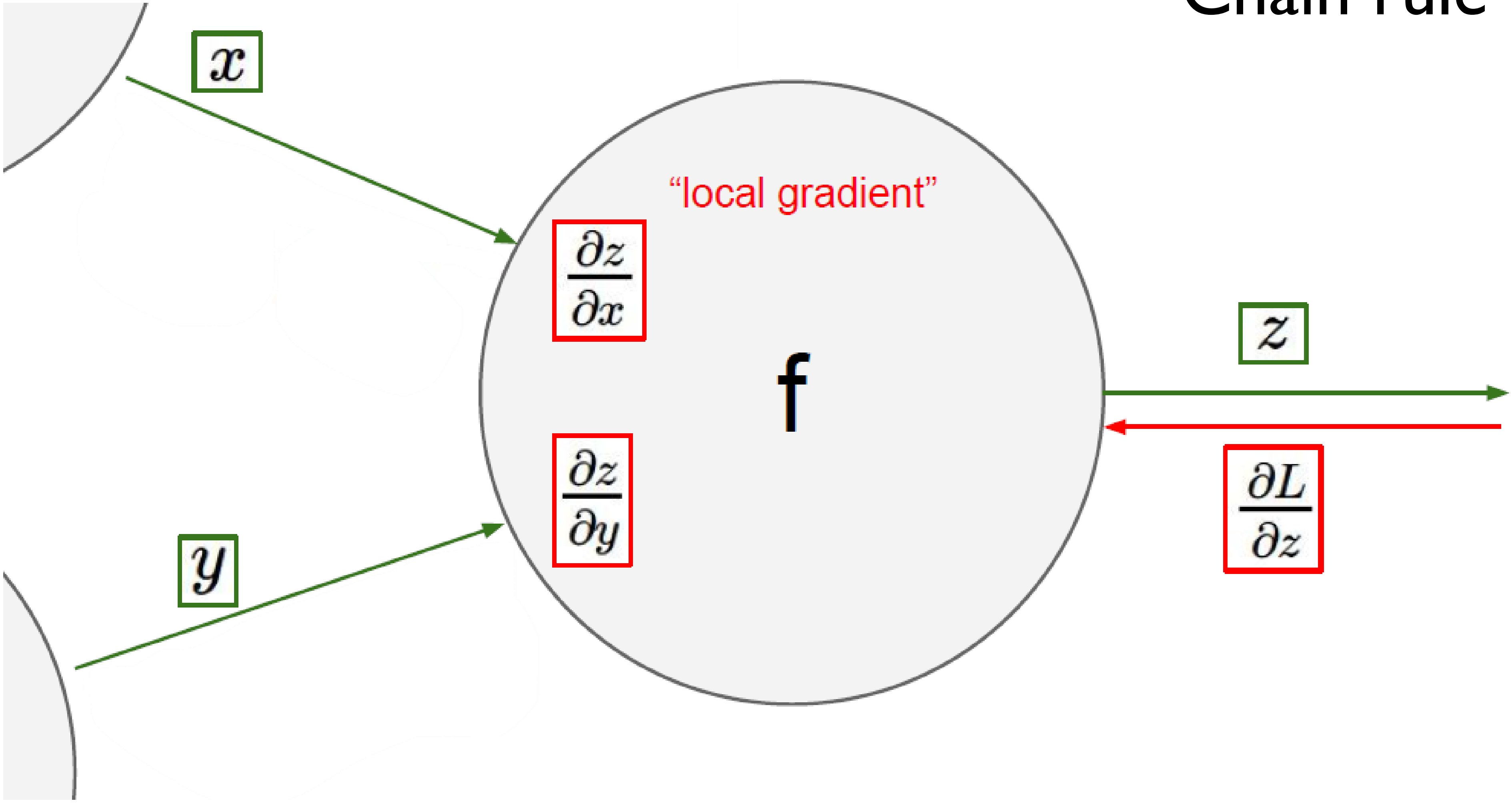


Chain rule



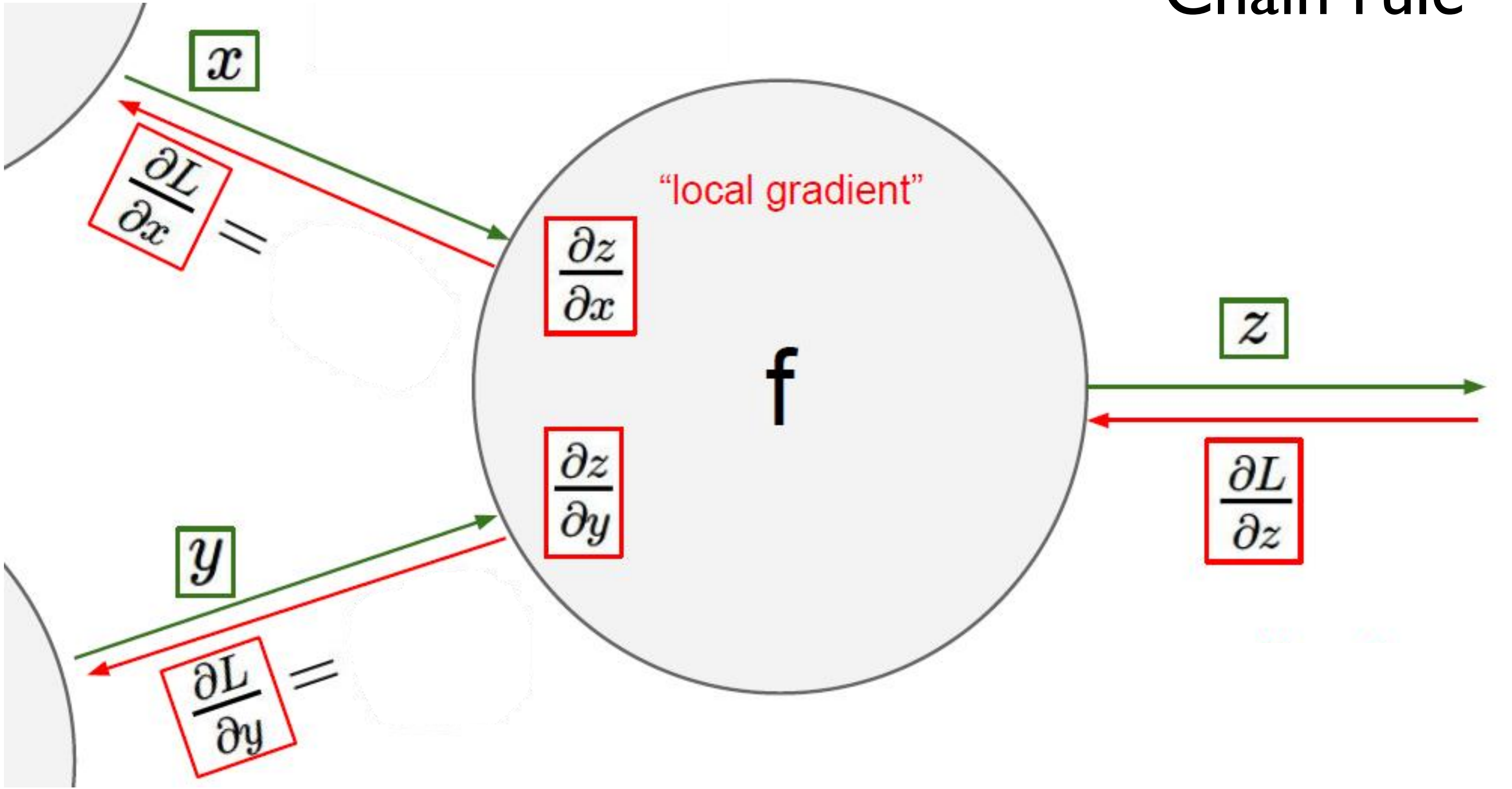
x
y
"local gradient"
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
z

Chain rule



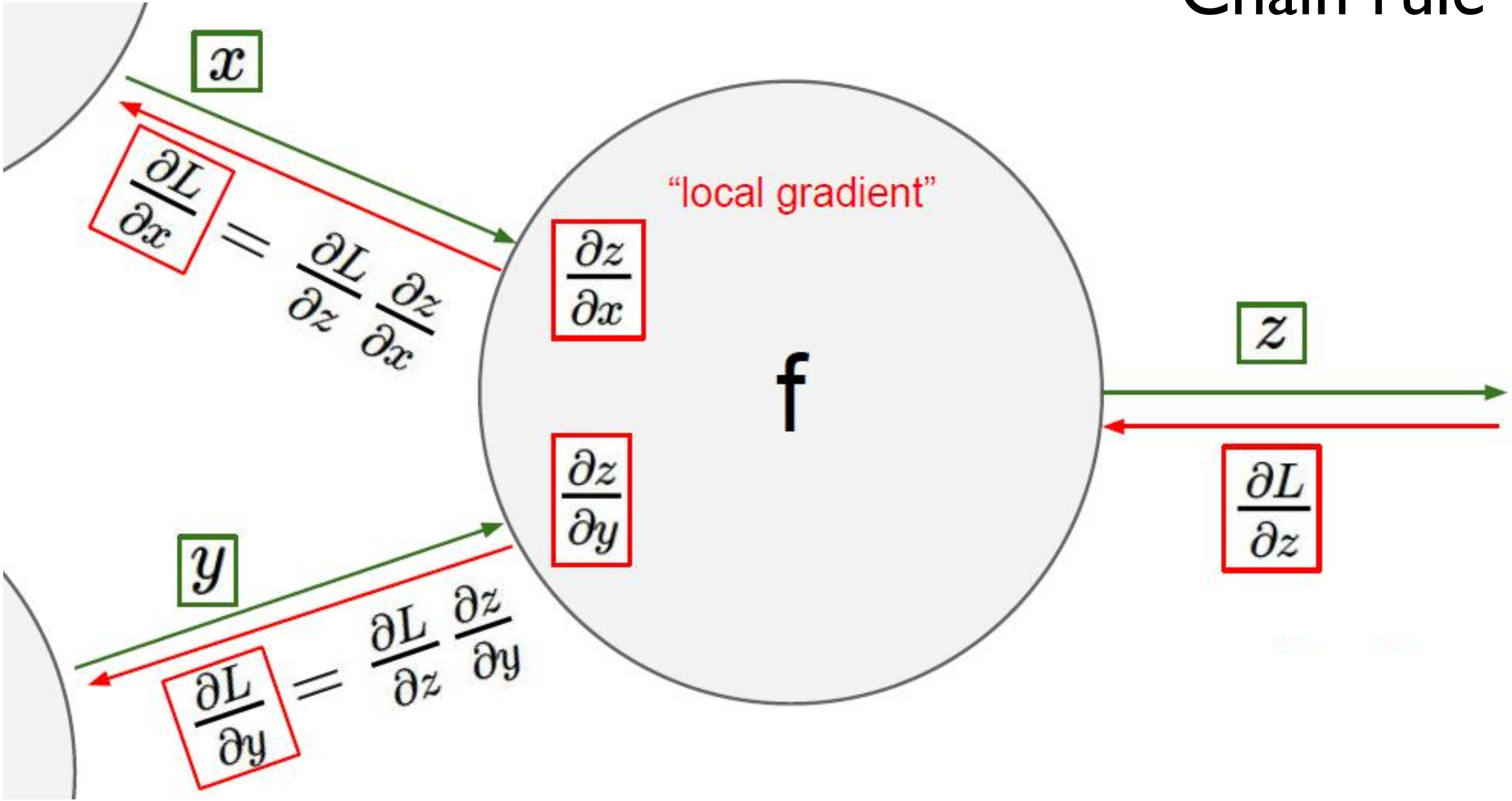
x
y
"local gradient"
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
z
$\frac{\partial L}{\partial z}$

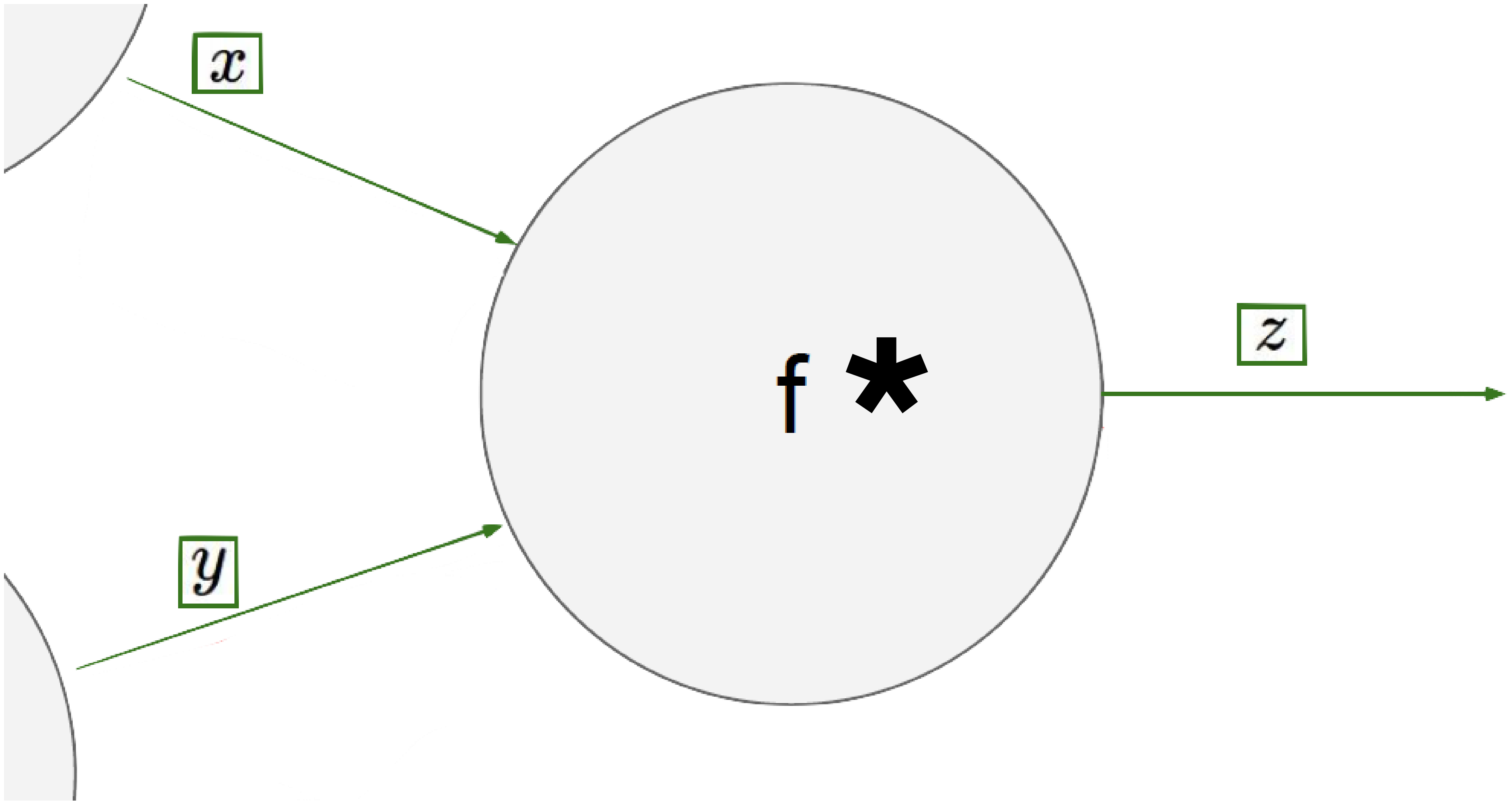
Chain rule



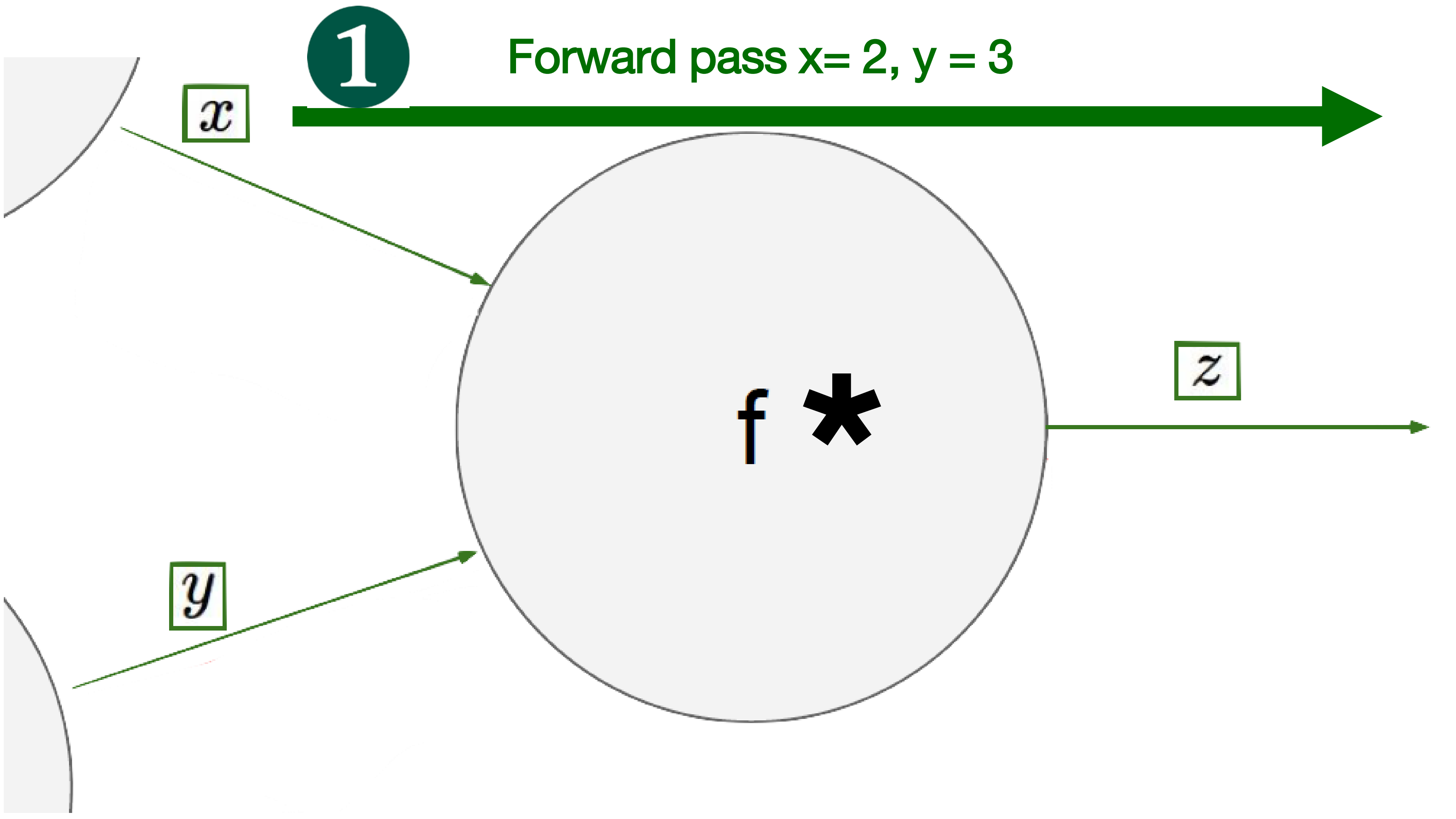
x
$\frac{\partial L}{\partial x}$ =
"local gradient"
$\frac{\partial z}{\partial x}$
z
f
$\frac{\partial z}{\partial y}$
$\frac{\partial L}{\partial z}$
y
$\frac{\partial L}{\partial y}$ =

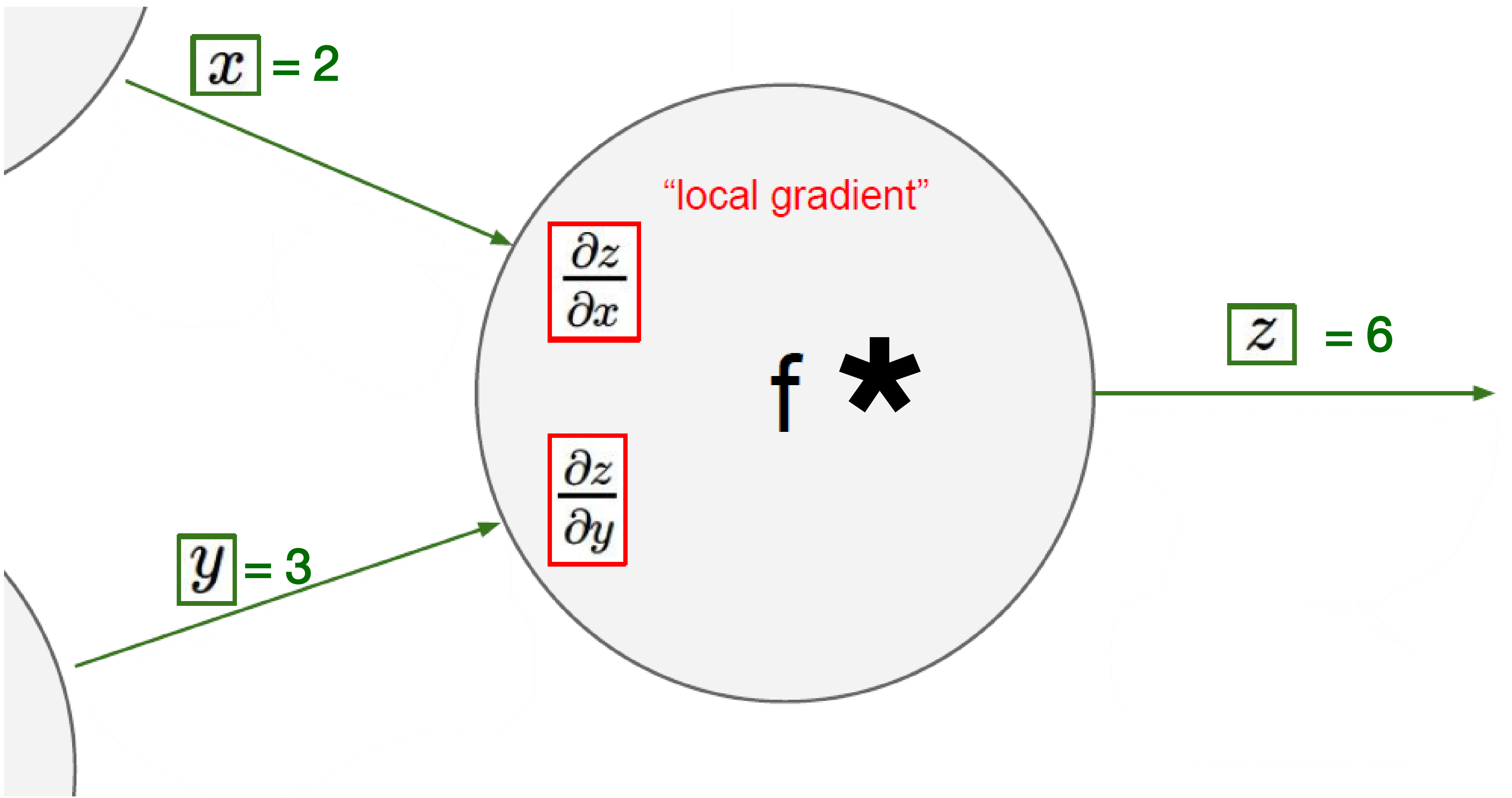
Chain rule


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

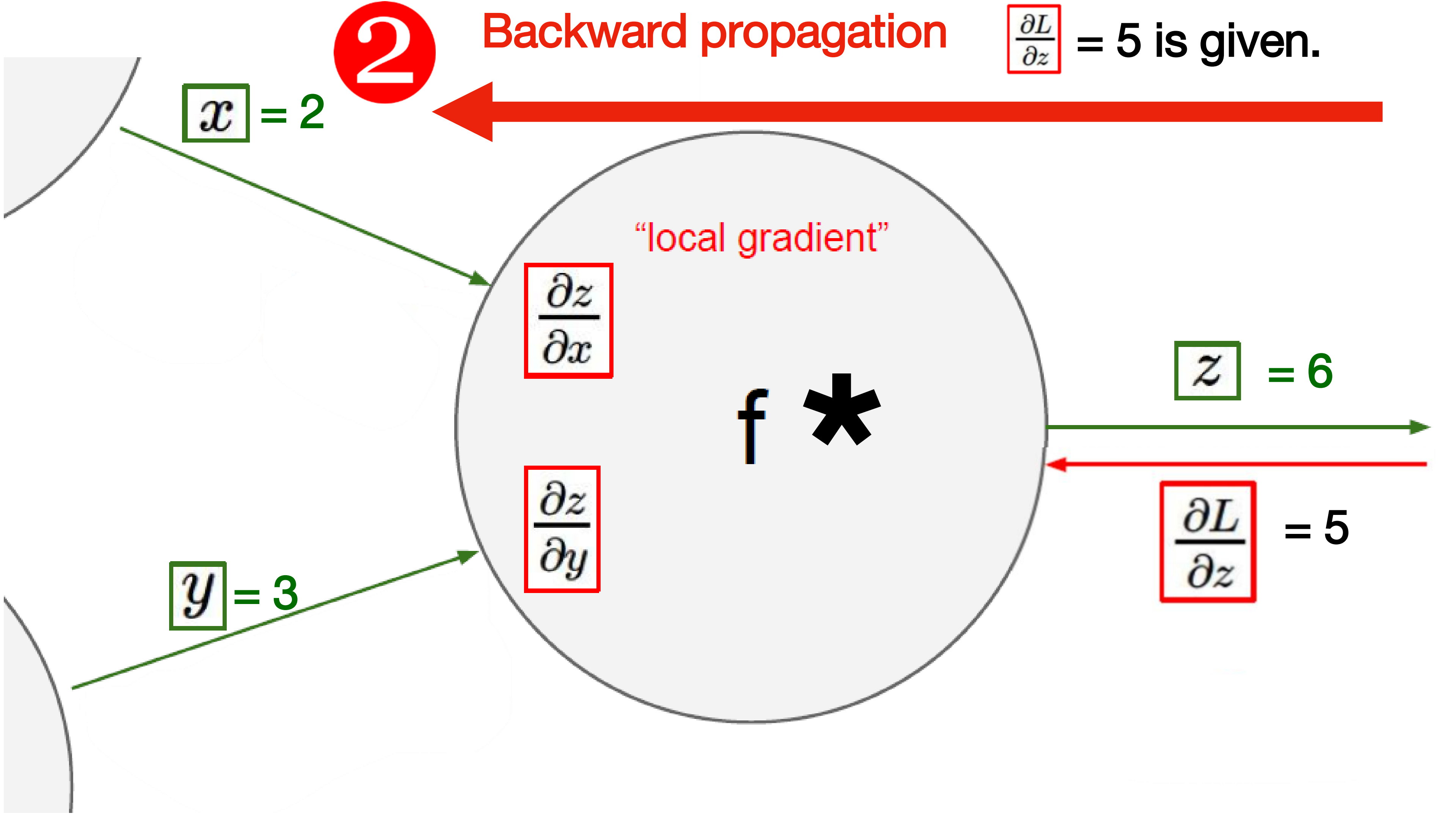


x
y
f *
z

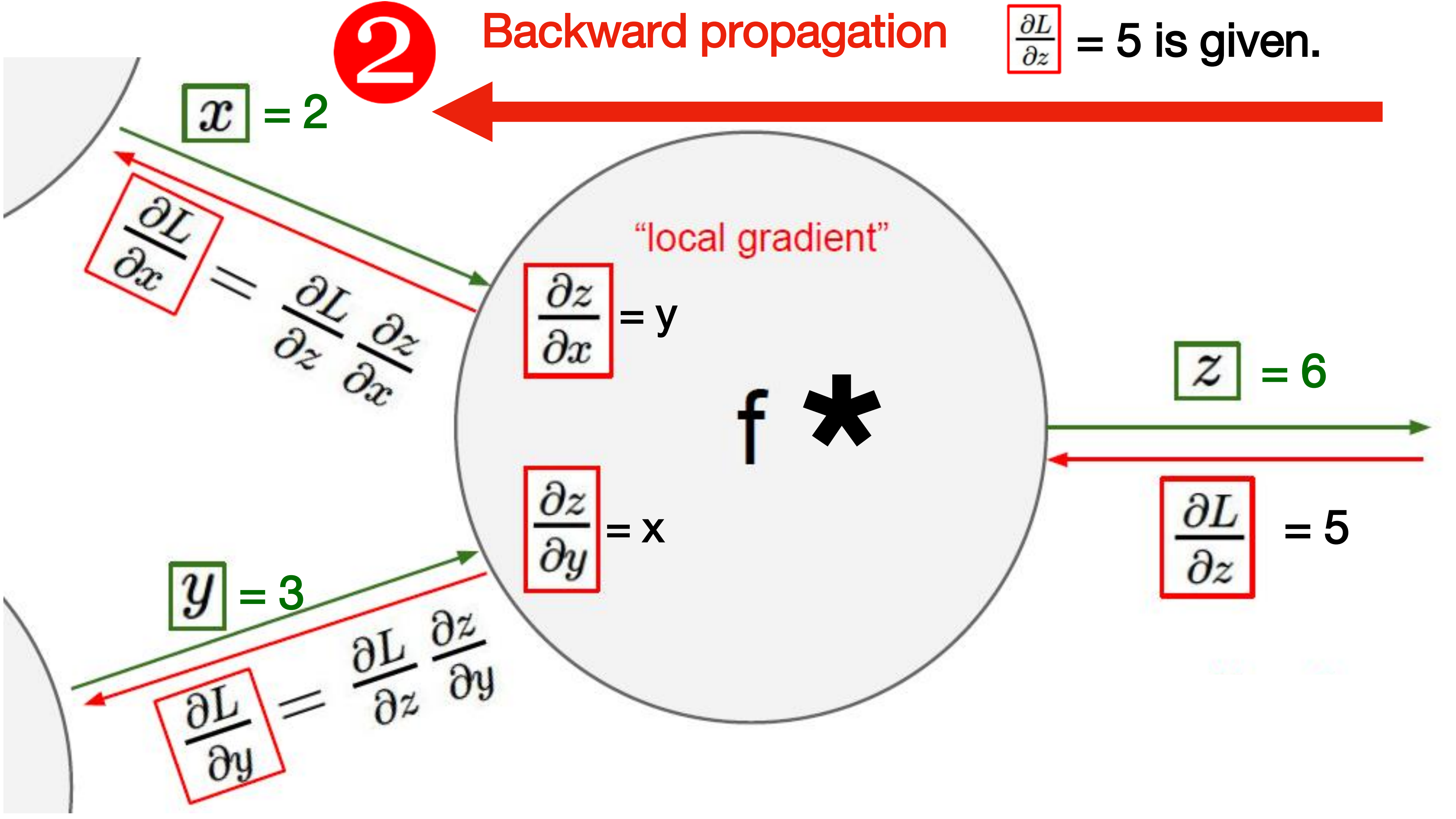

1
Forward pass x= 2, y = 3
x
y
z
f *



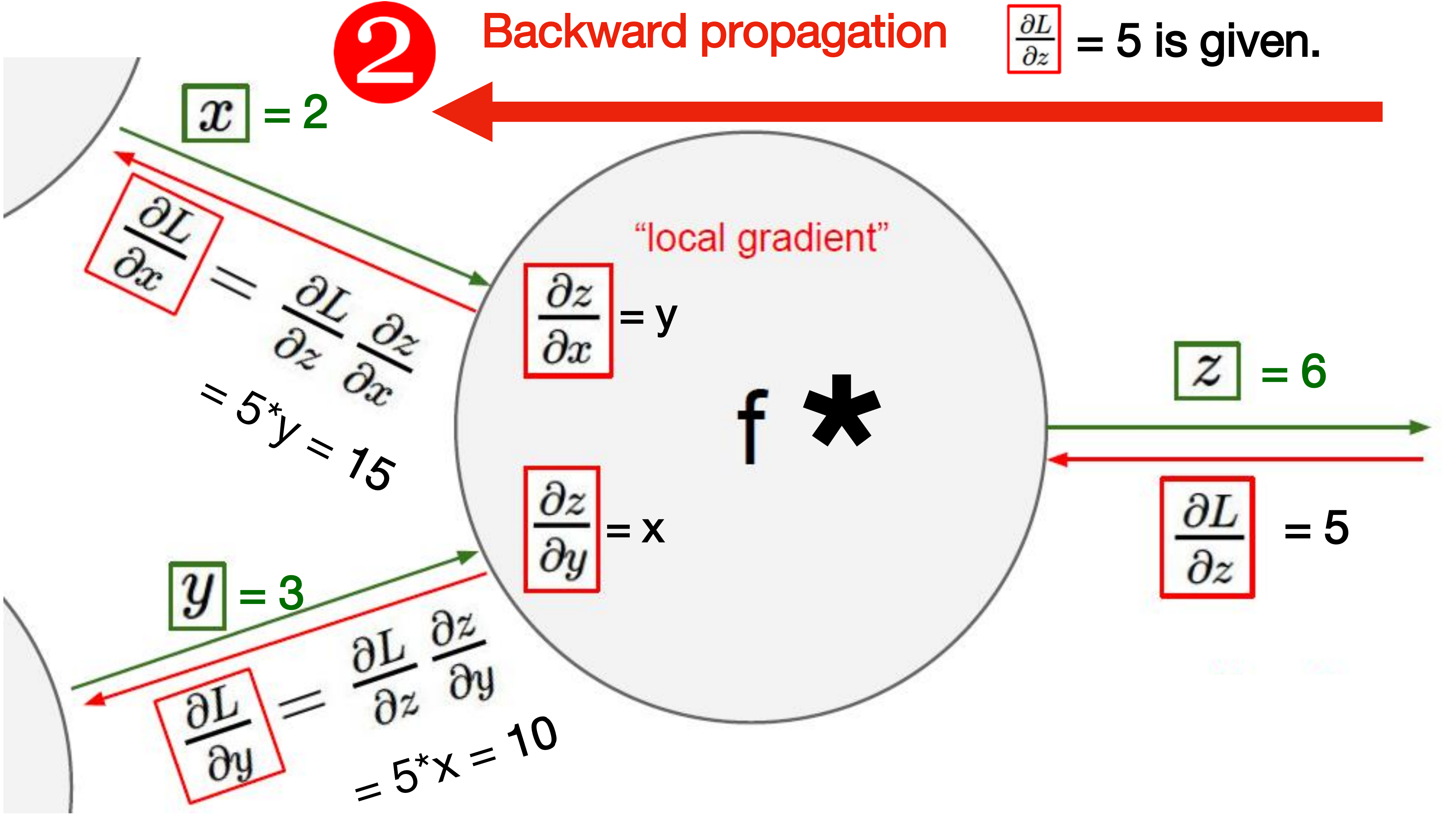
x = 2
"local gradient"
$\frac{\partial z}{\partial x}$
f *
z = 6
$\frac{\partial z}{\partial y}$
y = 3



2
Backward propagation
$\frac{\partial L}{\partial z}$ = 5 is given.
x = 2
y = 3
"local gradient"
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f *
z = 6
$\frac{\partial L}{\partial z}$ = 5



2
Backward propagation
$\frac{\partial L}{\partial z}$ = 5 is given.
x = 2
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"local gradient"
$\frac{\partial z}{\partial x}$ = y
f *
z = 6
$\frac{\partial z}{\partial y}$ = x
$\frac{\partial L}{\partial z}$ = 5
y = 3
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$



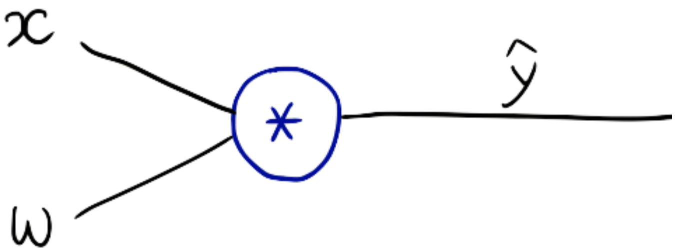
2
Backward propagation
$\frac{\partial L}{\partial z}$ = 5 is given.
x = 2
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
= 5*y = 15
"local gradient"
$\frac{\partial z}{\partial x}$ = y
f *
$\frac{\partial z}{\partial y}$ = x
z = 6
$\frac{\partial L}{\partial z}$ = 5
y = 3
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
= 5*x = 10

Computational graph

$$\hat{y} = x * w$$

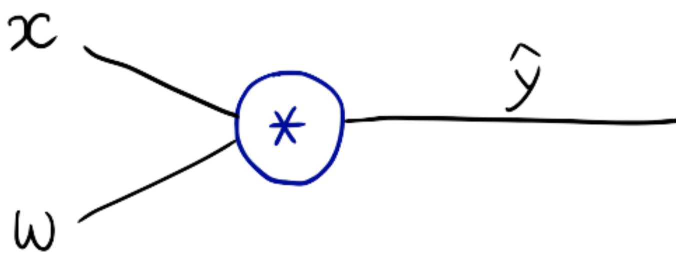
Computational graph

$$\hat{y} = x * w$$



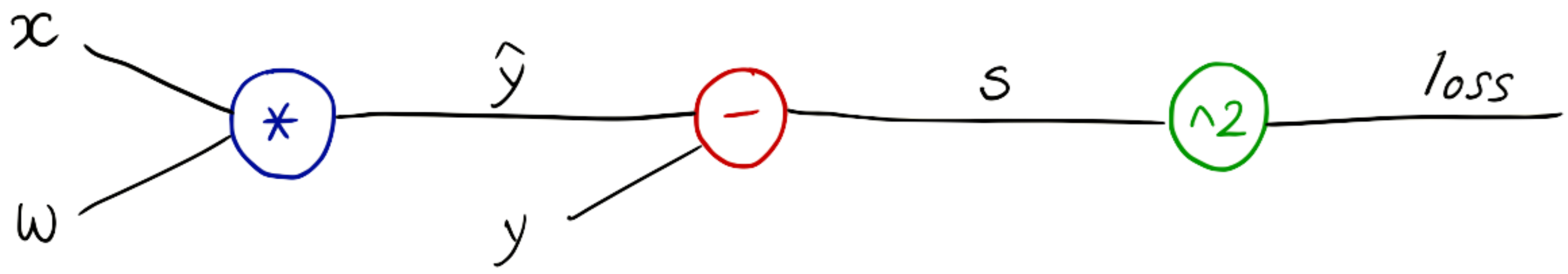
Computational graph

$$\hat{y} = x * w \qquad\qquad loss = (\hat{y} - y)^2 = (x * w - y)^2$$

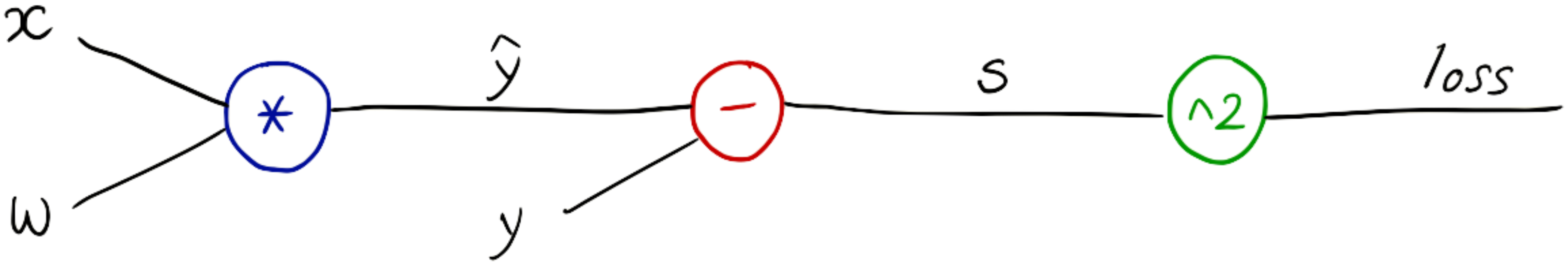


Computational graph

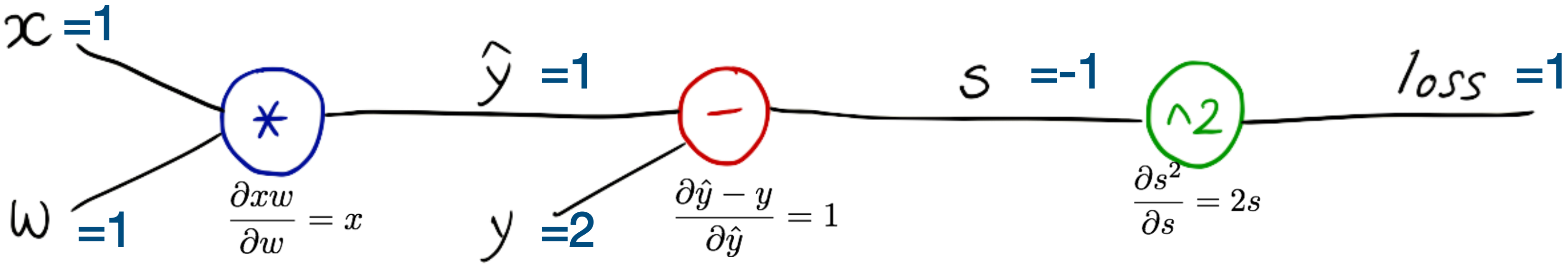
$$\hat{y} = x * w \qquad\qquad loss = (\hat{y} - y)^2 = (x * w - y)^2$$



1 Forward pass x=1, y = 2 where w=1



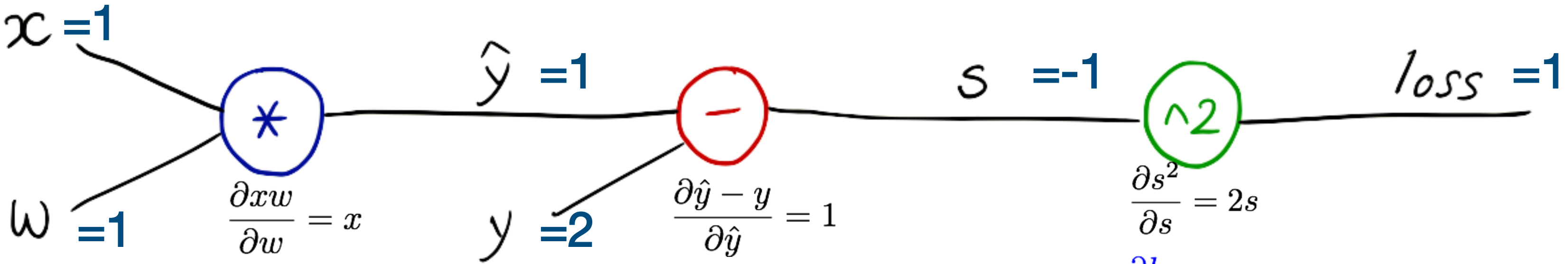
❷ Backward propagation



$$\frac{\partial loss}{\partial w} =$$

❷

Backward propagation



$$\frac{\partial xw}{\partial w} = x$$

$$\frac{\partial \hat{y} - y}{\partial \hat{y}} = 1$$

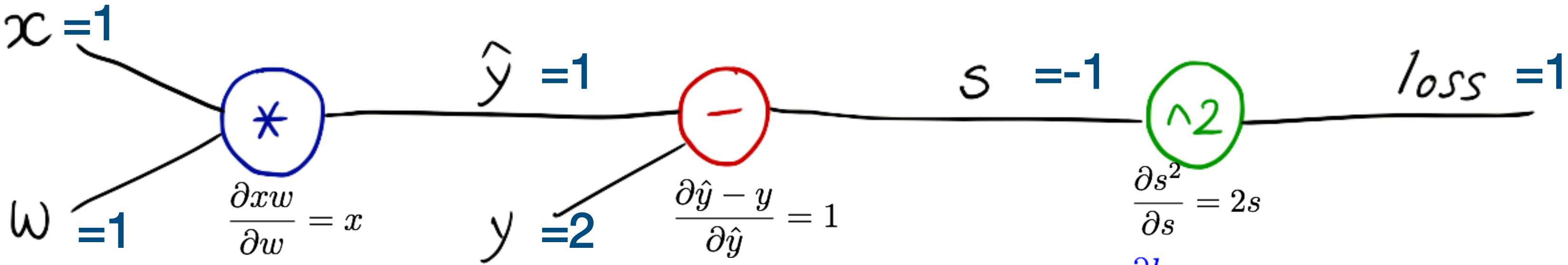
$$\frac{\partial s^2}{\partial s} = 2s$$

$$\frac{\partial loss}{\partial s} = 2s = -2$$

$$\frac{\partial loss}{\partial \hat{y}} = \frac{\partial loss}{\partial s}\frac{\partial s}{\partial \hat{y}} = -2 * 1 = -2$$

$$\frac{\partial loss}{\partial w} = \frac{\partial loss}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial w} = -2 * x = -2 * 1 = -2$$

❷ Backward propagation



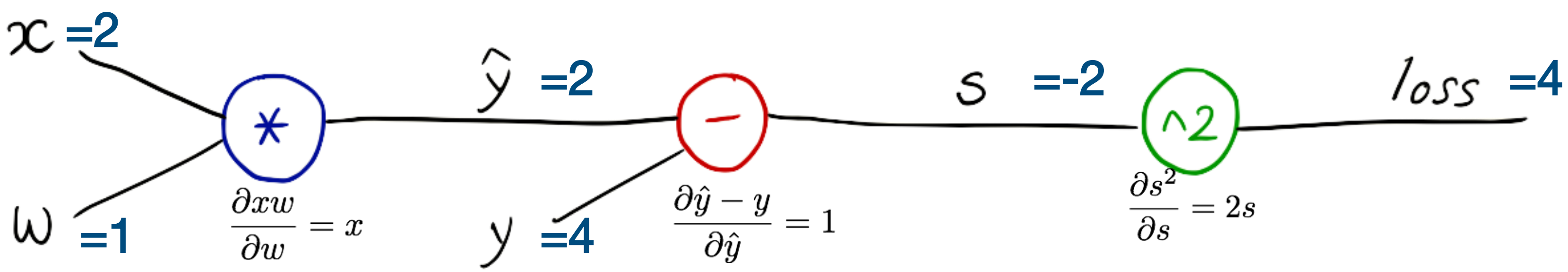
$$\frac{\partial loss}{\partial s} = 2s = -2$$

$$\frac{\partial loss}{\partial \hat{y}} = \frac{\partial loss}{\partial s}\frac{\partial s}{\partial \hat{y}} = -2 * 1 = -2$$

$$\frac{\partial loss}{\partial w} = \frac{\partial loss}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial w} = -2 * x = -2 * 1 = -2$$

```
	grad:  1.0 2.0 -2.0
	grad:  2.0 4.0 -7.84
	grad:  3.0 6.0 -16.2288
progress: 0 4.919240100095999
```

Exercise 4-1: x = 2, y=4, w=1

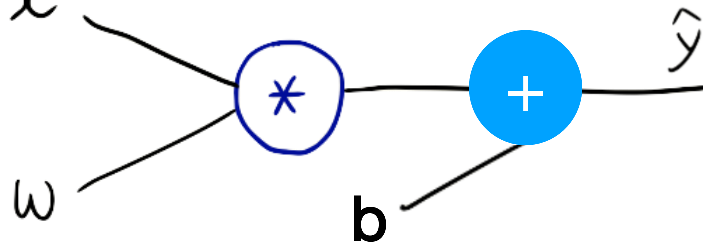


$$\frac{\partial loss}{\partial w} =$$

Exercise 4-2: x = 1, y=2, *w=1, b=2*

$$\hat{y} = x * w + b$$

$$loss = (\hat{y} - y)^2$$



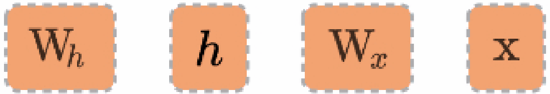
Data and **Variable**

```python
import torch
from torch.autograd import Variable

x_data = [1.0, 2.0, 3.0]
y_data = [2.0, 4.0, 6.0]

w = Variable(torch.Tensor([1.0]),  requires_grad=True)  # Any random value
```

http://pytorch.org/docs/master/notes/autograd.html?highlight=variable

Data and **Variable**

A graph is created on the fly




```python
from torch.autograd import Variable

x = Variable(torch.randn(1, 10))
prev_h = Variable(torch.randn(1, 20))
W_h = Variable(torch.randn(20, 20))
W_x = Variable(torch.randn(20, 10))
```

http://pytorch.org/docs/master/notes/autograd.html?highlight=variable

Model and Loss

```python
import torch
from torch.autograd import Variable

x_data = [1.0, 2.0, 3.0]
y_data = [2.0, 4.0, 6.0]

w = Variable(torch.Tensor([1.0]),  requires_grad=True)  # Any random value

# our model forward pass
def forward(x):
    return x * w

# Loss function
def loss(x, y):
    y_pred = forward(x)
    return (y_pred - y) * (y_pred - y)

# Before training
print("predict (before training)",  4, forward(4).data[0])
```

Training: forward, backward, and update weight

```python
# Training loop
for epoch in range(10):
    for x_val, y_val in zip(x_data, y_data):
        l = loss(x_val, y_val)
        l.backward()
        print("\tgrad: ", x_val, y_val, w.grad.data[0])
        w.data = w.data - 0.01 * w.grad.data

        # Manually zero the gradients after updating weights
        w.grad.data.zero_()

    print("progress:", epoch, l.data[0])

# After training
print("predict (after training)",  4, forward(4).data[0])
```

Output

```
# Training loop
for epoch in range(10):
    for x_val, y_val in zip(x_data, y_data):
        l = loss(x_val, y_val)
        l.backward()
        print("\tgrad: ", x_val, y_val, w.grad.data[0])
        w.data = w.data - 0.01 * w.grad.data

        # Manually zero the gradients after updating weights
        w.grad.data.zero_()

    print("progress:", epoch, l.data[0])

# After training
print("predict (after training)",  4, forward(4).data[0])
```

```
predict (before training) 4 4.0
	grad:  1.0 2.0 -2.0
	grad:  2.0 4.0 -7.840000152587891
	grad:  3.0 6.0 -16.228801727294922
progress: 0 7.315943717956543
	grad:  1.0 2.0 -1.478623867034912
	grad:  2.0 4.0 -5.796205520629883
	grad:  3.0 6.0 -11.998146057128906
progress: 1 3.9987640380859375
	grad:  1.0 2.0 -1.0931644439697266
	grad:  2.0 4.0 -4.285204887390137
	grad:  3.0 6.0 -8.870372772216797
progress: 2 2.1856532096862793
	grad:  1.0 2.0 -0.8081896305084229
	grad:  2.0 4.0 -3.1681032180786133
	grad:  3.0 6.0 -6.557973861694336
progress: 3 1.1946394443511963
	grad:  1.0 2.0 -0.5975041389465332
	grad:  2.0 4.0 -2.3422164916992188
	grad:  3.0 6.0 -4.848389625549316
progress: 4 0.6529689431190491
	grad:  1.0 2.0 -0.4417421817779541
	grad:  2.0 4.0 -1.7316293716430664
	grad:  3.0 6.0 -3.58447265625
progress: 5 0.35690122842788696
	grad:  1.0 2.0 -0.3265852928161621
	grad:  2.0 4.0 -1.2802143096923828
	grad:  3.0 6.0 -2.650045394897461
progress: 6 0.195076122879982
	grad:  1.0 2.0 -0.24144840240478516
	grad:  2.0 4.0 -0.9464778900146484
	grad:  3.0 6.0 -1.9592113494873047
progress: 7 0.10662525147199631
	grad:  1.0 2.0 -0.17850565910339355
	grad:  2.0 4.0 -0.699742317199707
	grad:  3.0 6.0 -1.4484672546386719
```

```
predict (before training) 4 4.0
	grad:  1.0 2.0 -2.0
	grad:  2.0 4.0 -7.84
	grad:  3.0 6.0 -16.2288
progress: 0 4.919240100095999
	grad:  1.0 2.0 -1.478624
	grad:  2.0 4.0 -5.796206079999999
	grad:  3.0 6.0 -11.998146585599997
progress: 1 2.688769240265834
	grad:  1.0 2.0 -1.093164466688
	grad:  2.0 4.0 -4.285204709416961
	grad:  3.0 6.0 -8.87037374849311
progress: 2 1.4696334962911515
	grad:  1.0 2.0 -0.8081896081960389
	grad:  2.0 4.0 -3.1681032641284723
	grad:  3.0 6.0 -6.557973756745939
progress: 3 0.8032755585999681
	grad:  1.0 2.0 -0.59750427561463
	grad:  2.0 4.0 -2.3422167604093502
	grad:  3.0 6.0 -4.848388694047353
progress: 4 0.43905614881022015
	grad:  1.0 2.0 -0.44174208101320334
	grad:  2.0 4.0 -1.7316289575717576
	grad:  3.0 6.0 -3.584471942173538
progress: 5 0.2399802903801062
	grad:  1.0 2.0 -0.3265852213980338
	grad:  2.0 4.0 -1.2802140678802925
	grad:  3.0 6.0 -2.650043120512205
progress: 6 0.1311689630744999
	grad:  1.0 2.0 -0.241448373202223
	grad:  2.0 4.0 -0.946477622952715
	grad:  3.0 6.0 -1.9592086795121197
progress: 7 0.07169462478267678
	grad:  1.0 2.0 -0.17850567968888198
	grad:  2.0 4.0 -0.6997422643804168
	grad:  3.0 6.0 -1.4484664872674653
progress: 8 0.03918700813247573
	grad:  1.0 2.0 -0.13197139106214673
	grad:  2.0 4.0 -0.5173278529636143
	grad:  3.0 6.0 -1.0708686556346834
progress: 9 0.021418922423117836
predict (after training) 4 7.804863933862125
```

Output

(from numeric gradient computation)

```python
# Before training
print("predict (before training)",  4, forward(4))

# Training loop
for epoch in range(10):
    for x, y in zip(x_data, y_data):
        grad = gradient(x, y)
        w = w - 0.01 * grad
        print("\tgrad: ", x, y, grad)
        l = loss(x, y)

    print ("progress:", epoch, l)

# After training
print("predict (after training)",  4, forward(4))
```

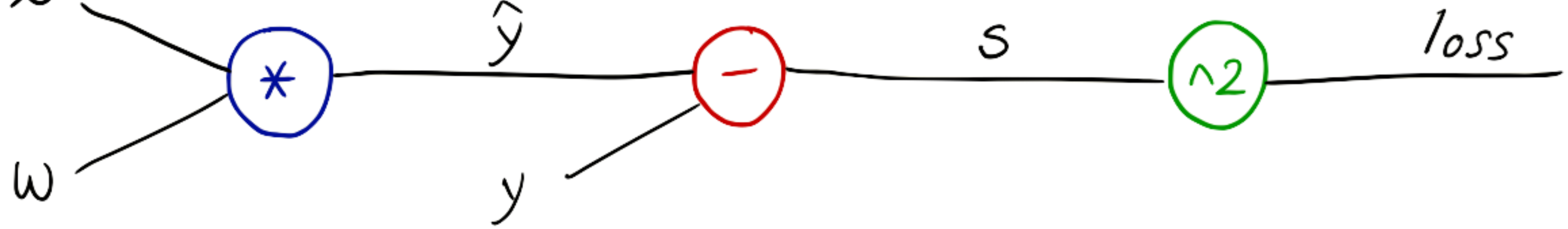
Output
(from numeric gradient computation)

```
predict (before training) 4 4.0
    grad:  1.0 2.0 -2.0
    grad:  2.0 4.0 -7.84
    grad:  3.0 6.0 -16.2288
progress: 0 4.919240100095999
    grad:  1.0 2.0 -1.478624
    grad:  2.0 4.0 -5.796206079999999
    grad:  3.0 6.0 -11.998146585599997
progress: 1 2.688769240265834
    grad:  1.0 2.0 -1.093164466688
    grad:  2.0 4.0 -4.285204709416961
    grad:  3.0 6.0 -8.87037374849311
progress: 2 1.4696334962911515
    grad:  1.0 2.0 -0.8081896081960389
    grad:  2.0 4.0 -3.1681032641284723
    grad:  3.0 6.0 -6.557973756745939
progress: 3 0.8032755585999681
    grad:  1.0 2.0 -0.59750427561463
    grad:  2.0 4.0 -2.3422167604093502
    grad:  3.0 6.0 -4.848388694047353
progress: 4 0.43905614881022015
    grad:  1.0 2.0 -0.44174208101320334
    grad:  2.0 4.0 -1.7316289575717576
    grad:  3.0 6.0 -3.584471942173538
progress: 5 0.2399802903801062
    grad:  1.0 2.0 -0.3265852213980338
    grad:  2.0 4.0 -1.2802140678802925
    grad:  3.0 6.0 -2.650043120512205
progress: 6 0.1311689630744999
    grad:  1.0 2.0 -0.241448373202223
    grad:  2.0 4.0 -0.946477622952715
    grad:  3.0 6.0 -1.9592086795121197
progress: 7 0.07169462478267678
    grad:  1.0 2.0 -0.17850567968888198
    grad:  2.0 4.0 -0.6997422643804168
```

Output
(computational graph)

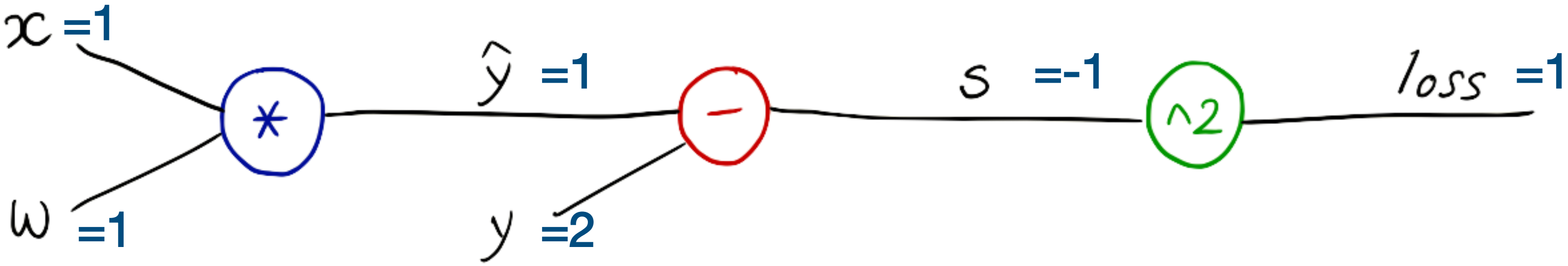

```
predict (before training) 4 4.0
    grad:  1.0 2.0 -2.0
    grad:  2.0 4.0 -7.84
    grad:  3.0 6.0 -16.2288
progress: 0 4.919240100095999
    grad:  1.0 2.0 -1.478624
    grad:  2.0 4.0 -5.796206079999999
    grad:  3.0 6.0 -11.998146585599997
progress: 1 2.688769240265834
    grad:  1.0 2.0 -1.093164466688
    grad:  2.0 4.0 -4.285204709416961
    grad:  3.0 6.0 -8.87037374849311
progress: 2 1.4696334962911515
    grad:  1.0 2.0 -0.8081896081960389
    grad:  2.0 4.0 -3.1681032641284723
    grad:  3.0 6.0 -6.557973756745939
progress: 3 0.8032755585999681
    grad:  1.0 2.0 -0.59750427561463
    grad:  2.0 4.0 -2.3422167604093502
    grad:  3.0 6.0 -4.848388694047353
progress: 4 0.43905614881022015
    grad:  1.0 2.0 -0.44174208101320334
    grad:  2.0 4.0 -1.7316289575717576
    grad:  3.0 6.0 -3.584471942173538
progress: 5 0.2399802903801062
    grad:  1.0 2.0 -0.3265852213980338
    grad:  2.0 4.0 -1.2802140678802925
    grad:  3.0 6.0 -2.650043120512205
progress: 6 0.1311689630744999
    grad:  1.0 2.0 -0.241448373202223
    grad:  2.0 4.0 -0.946477622952715
    grad:  3.0 6.0 -1.9592086795121197
progress: 7 0.07169462478267678
    grad:  1.0 2.0 -0.17850567968888198
    grad:  2.0 4.0 -0.6997422643804168
```

PyTorch forward/backward



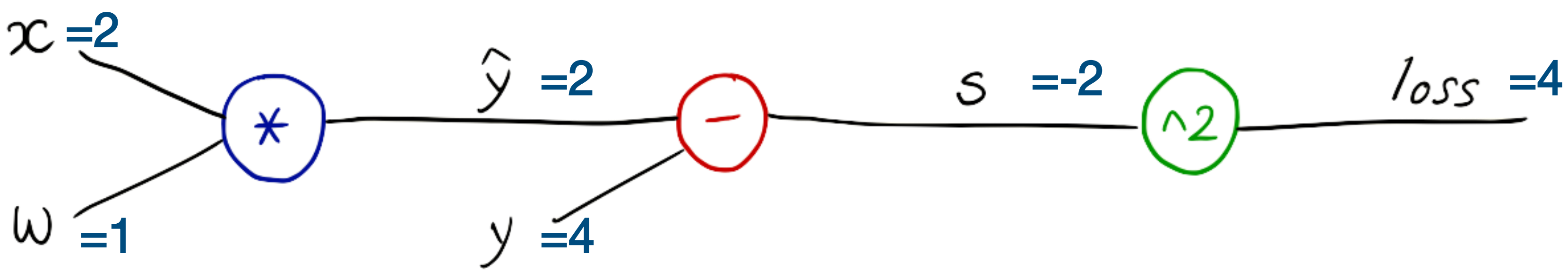
Forward pass

```python
# Any random value
w = Variable(torch.Tensor([1.0]),  requires_grad=True)
l = loss(x=1, y=2)
```



$$\frac{\partial loss}{\partial w} =$$

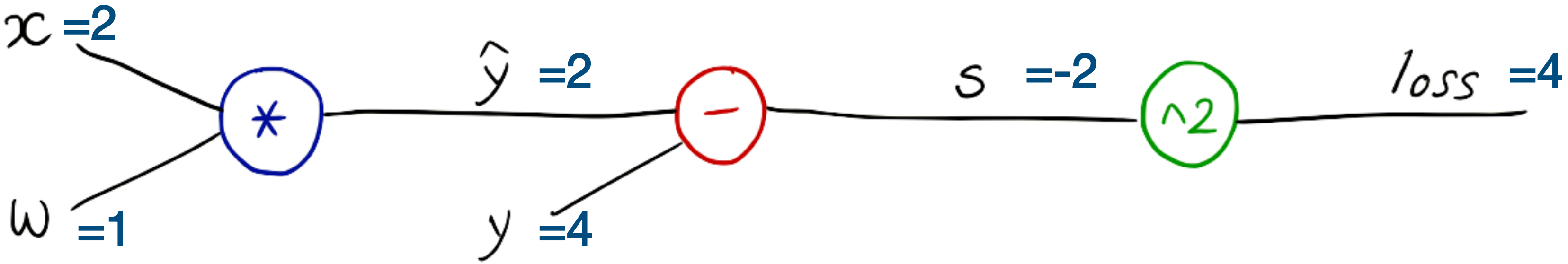
Back propagation: l.backward()



$$\frac{\partial loss}{\partial w} = \texttt{w.grad}$$

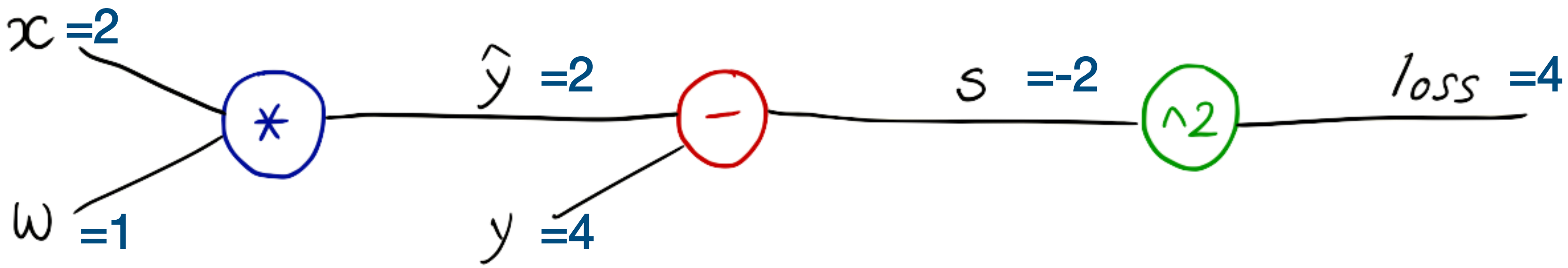
Weight update (step)

```
w.data = w.data - 0.01 * w.grad.data
```



$$\frac{\partial loss}{\partial w} = \texttt{w.grad}$$

Exercise 4-3: implement computational graph and backprop using NumPy



$$\frac{\partial loss}{\partial w} =$$

Exercise 4-4: Compute gradients using computational graph (manually)

$$\hat{y} = x^2 w_2 + x w_1 + b$$
$$loss = (\hat{y} - y)^2$$

$$\frac{\partial loss}{\partial w_1} = ?$$

$$\frac{\partial loss}{\partial w_2} = ?$$

Exercise 4-5: compute gradients using PyTorch

$$\hat{y} = x^2 w_2 + x w_1 + b$$
$$loss = (\hat{y} - y)^2$$

$$\frac{\partial loss}{\partial w_1} = ?$$

$$\frac{\partial loss}{\partial w_2} = ?$$

WHAT NEXT

Lecture 5: Linear regression in the PyTorch way