Computation Graphs & Backpropagation

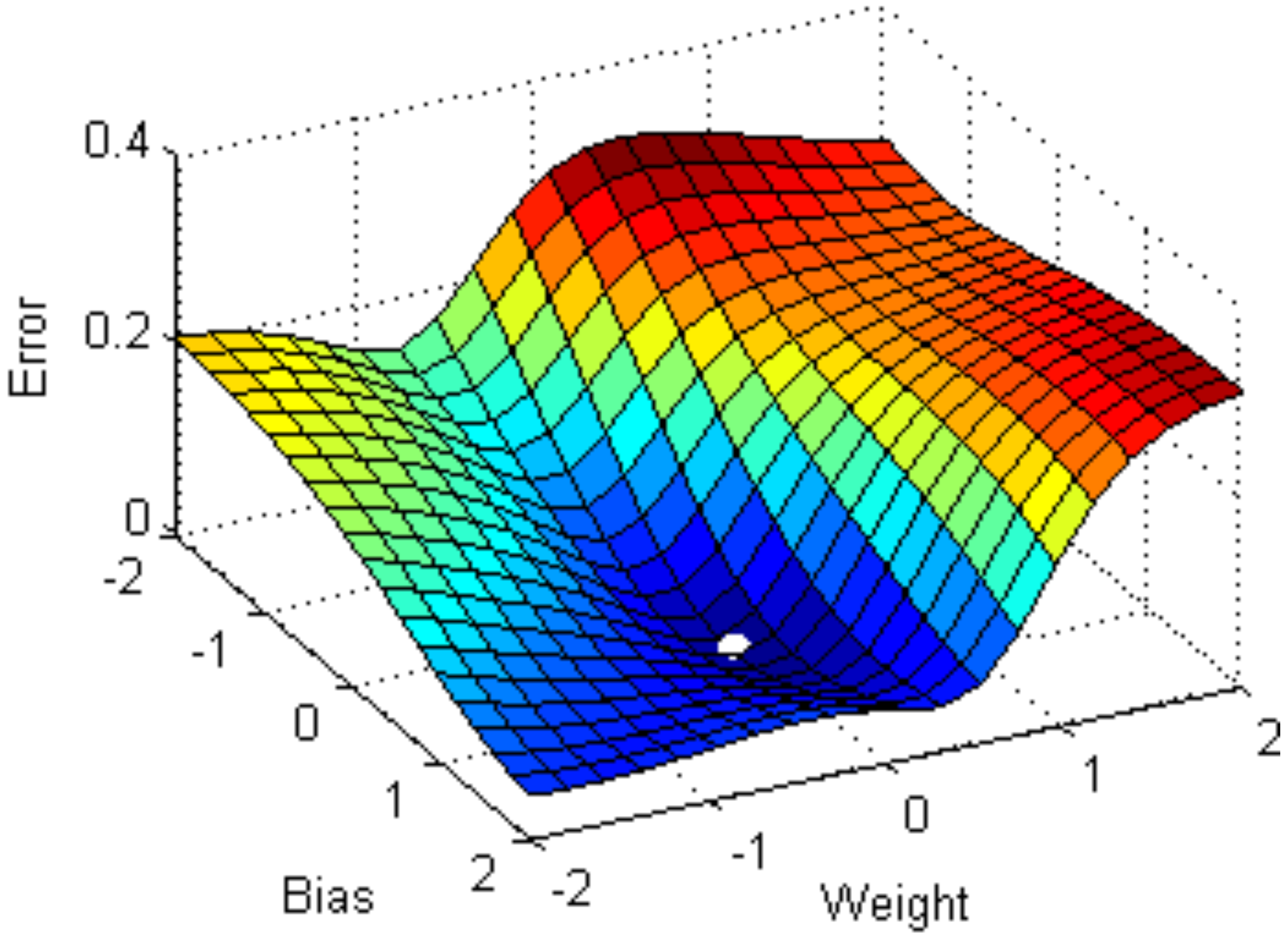
Ling 282/482: Deep Learning for Computational Linguistics

C.M. Downey

Fall 2025

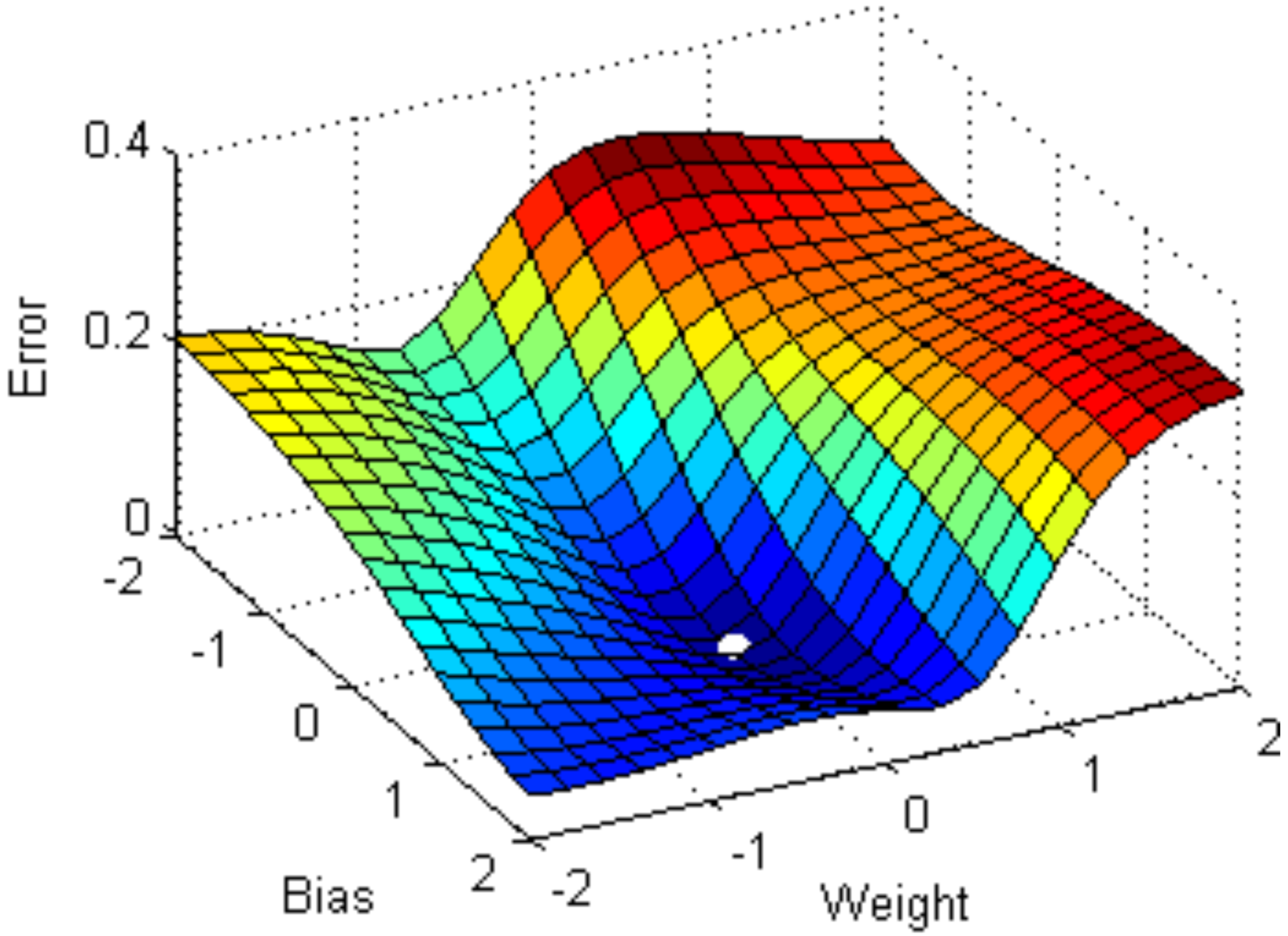
Last Time

- Last time: use **Gradient Descent** to **traverse the loss surface**
  - Finding optimal values for parameters θ
- This time: how do we **compute the gradients** for **complex models?**
  - i.e. from an **algorithmic** point of view
  - Solution: **computation graph** and **Backpropagation**



Last Time

- Last time: use **Gradient Descent** to **traverse the loss surface**
  - Finding optimal values for parameters θ
- This time: how do we **compute the gradients** for **complex models?**
  - i.e. from an **algorithmic** point of view
  - Solution: **computation graph** and **Backpropagation**



Computation Graphs

What is a computation graph?

What is a computation graph?

- The **descriptive language** of deep learning frameworks
  - e.g. PyTorch, TensorFlow

What is a computation graph?

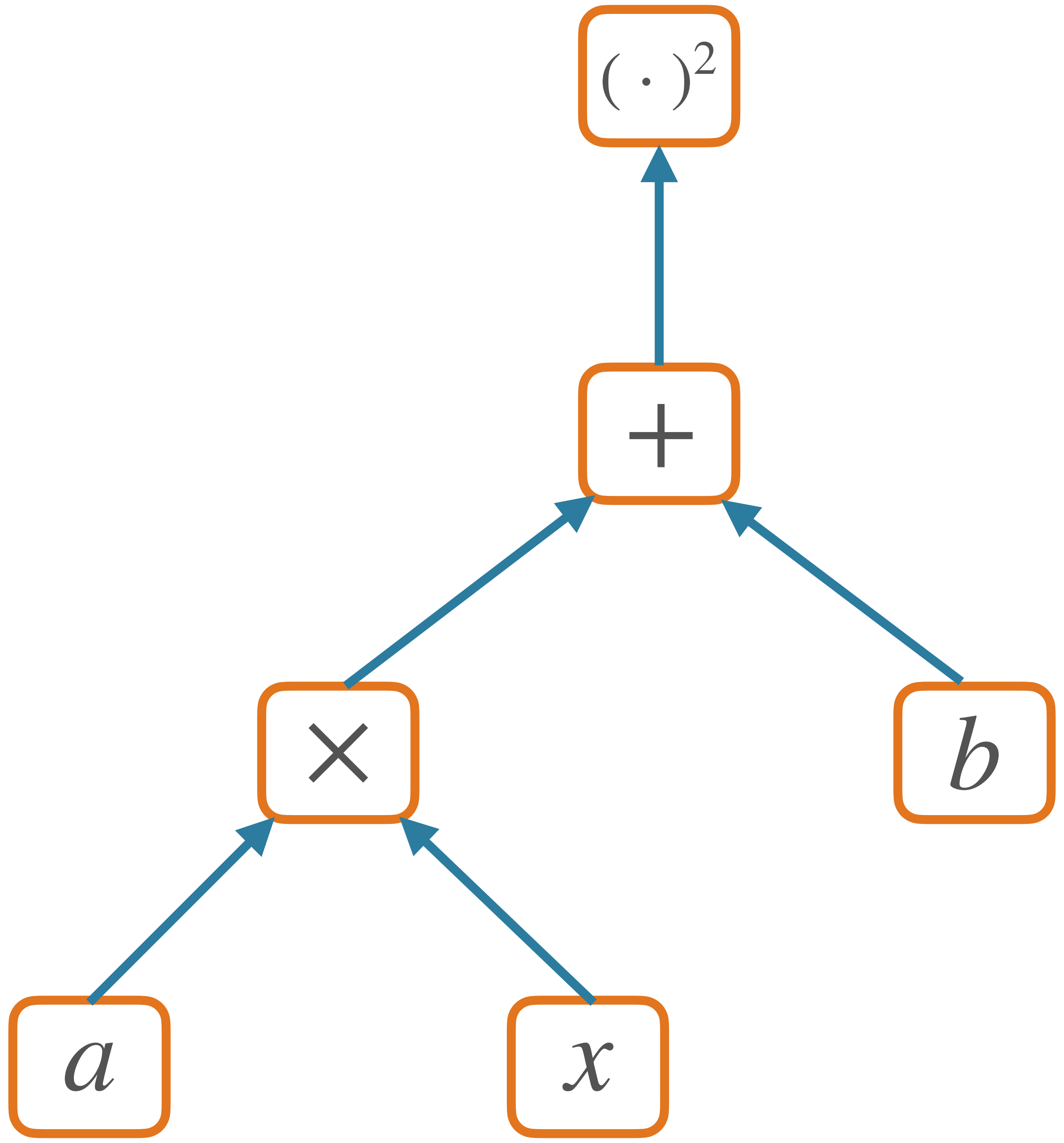
- The **descriptive language** of deep learning frameworks
  - e.g. PyTorch, TensorFlow
- Essentially, **parse trees** of mathematical expressions
  - Captures **dependence** between operations

What is a computation graph?

- The **descriptive language** of deep learning frameworks
  - e.g. PyTorch, TensorFlow
- Essentially, **parse trees** of mathematical expressions
  - Captures **dependence** between operations
- Two types of computation
  - **Forward**: compute **outputs** given inputs
  - **Backward**: compute **gradients**

Computation Graph Example

$$f(x; a, b) = (ax + b)^2$$



Forward Pass

Forward Pass

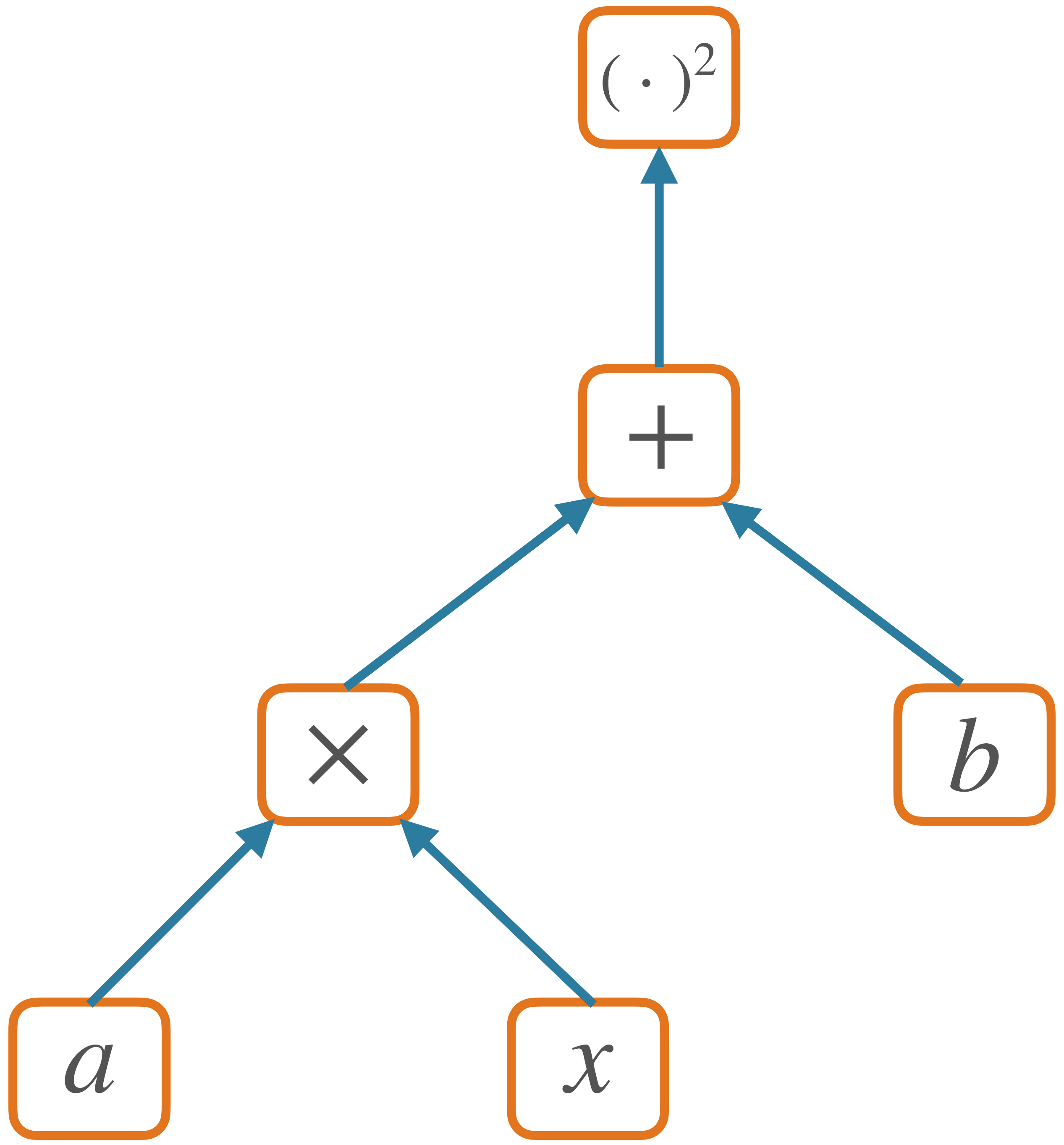
- Compute output(s) given inputs
  - **Inputs**: leaf nodes; need values
  - **Outputs**: those with no children

Forward Pass

- Compute output(s) given inputs
  - **Inputs**: leaf nodes; need values
  - **Outputs**: those with no children
- Forward computation
  - **Loop over nodes** in topological order (children after parents)
  - Compute **value of a node** given values of its parent nodes

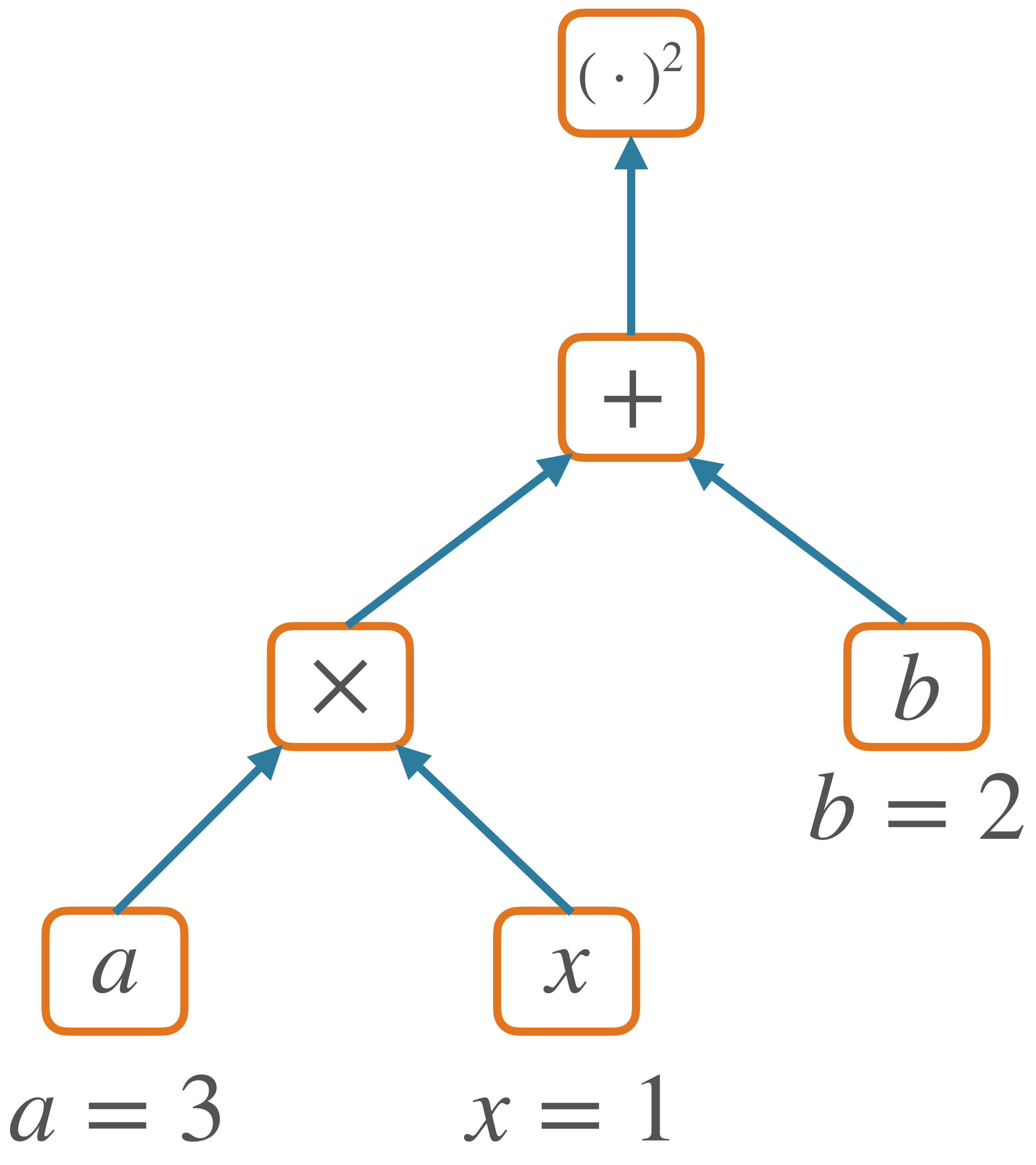
Computation Graph Example

$$f(x; a, b) = (ax + b)^2$$



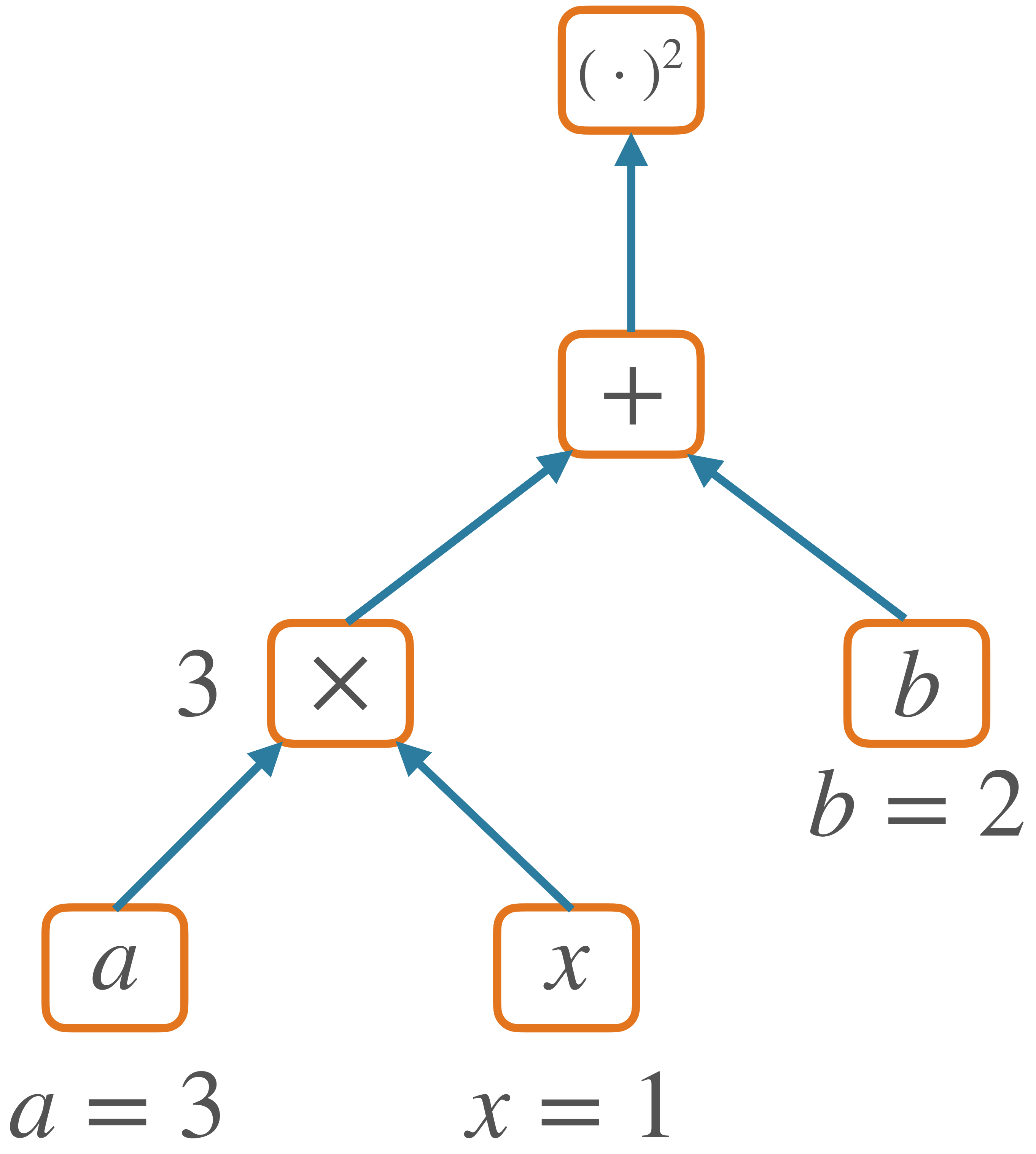
Computation Graph Example

$$f(x; a, b) = (ax + b)^2$$



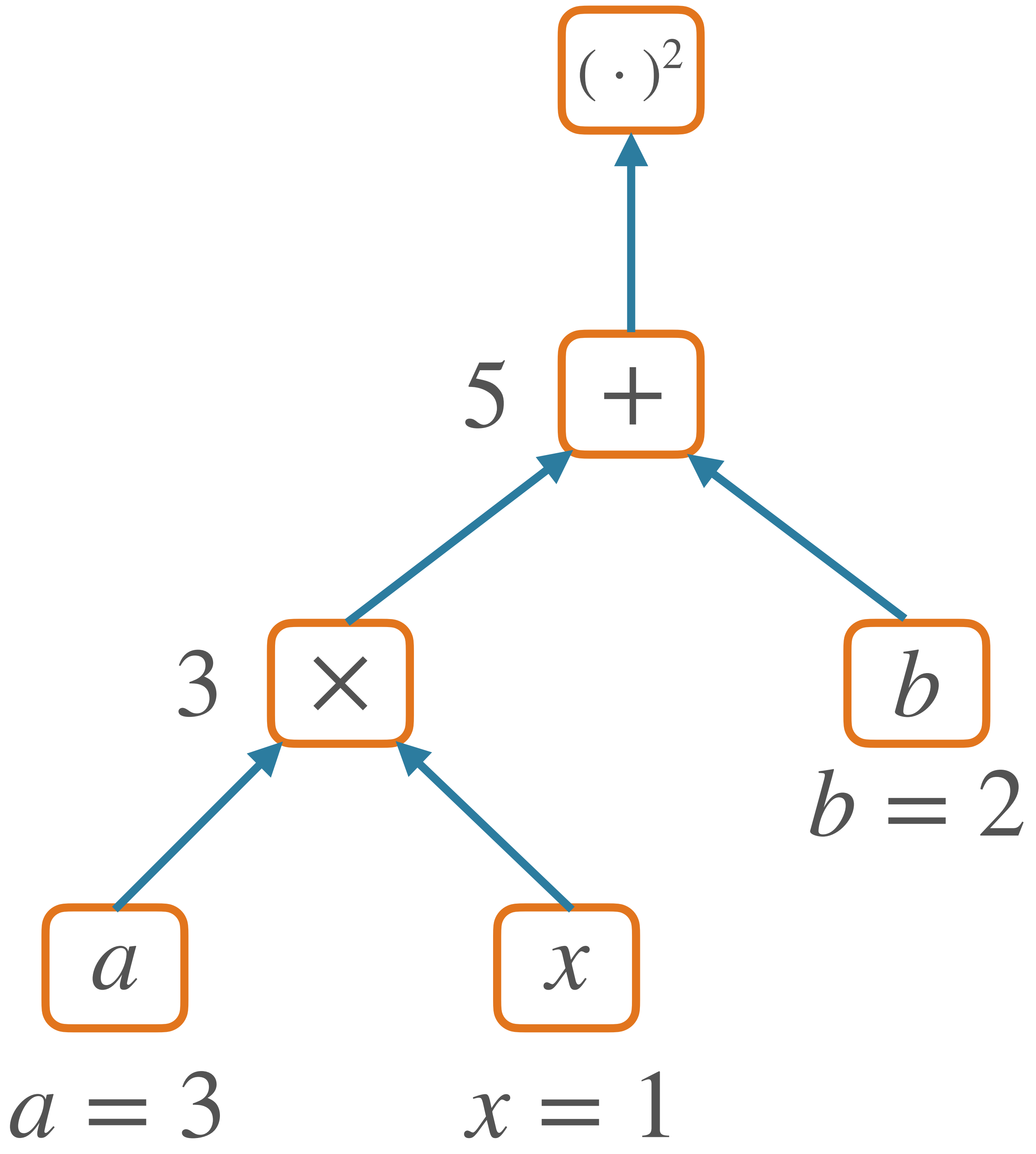
Computation Graph Example

$$f(x; a, b) = (ax + b)^2$$



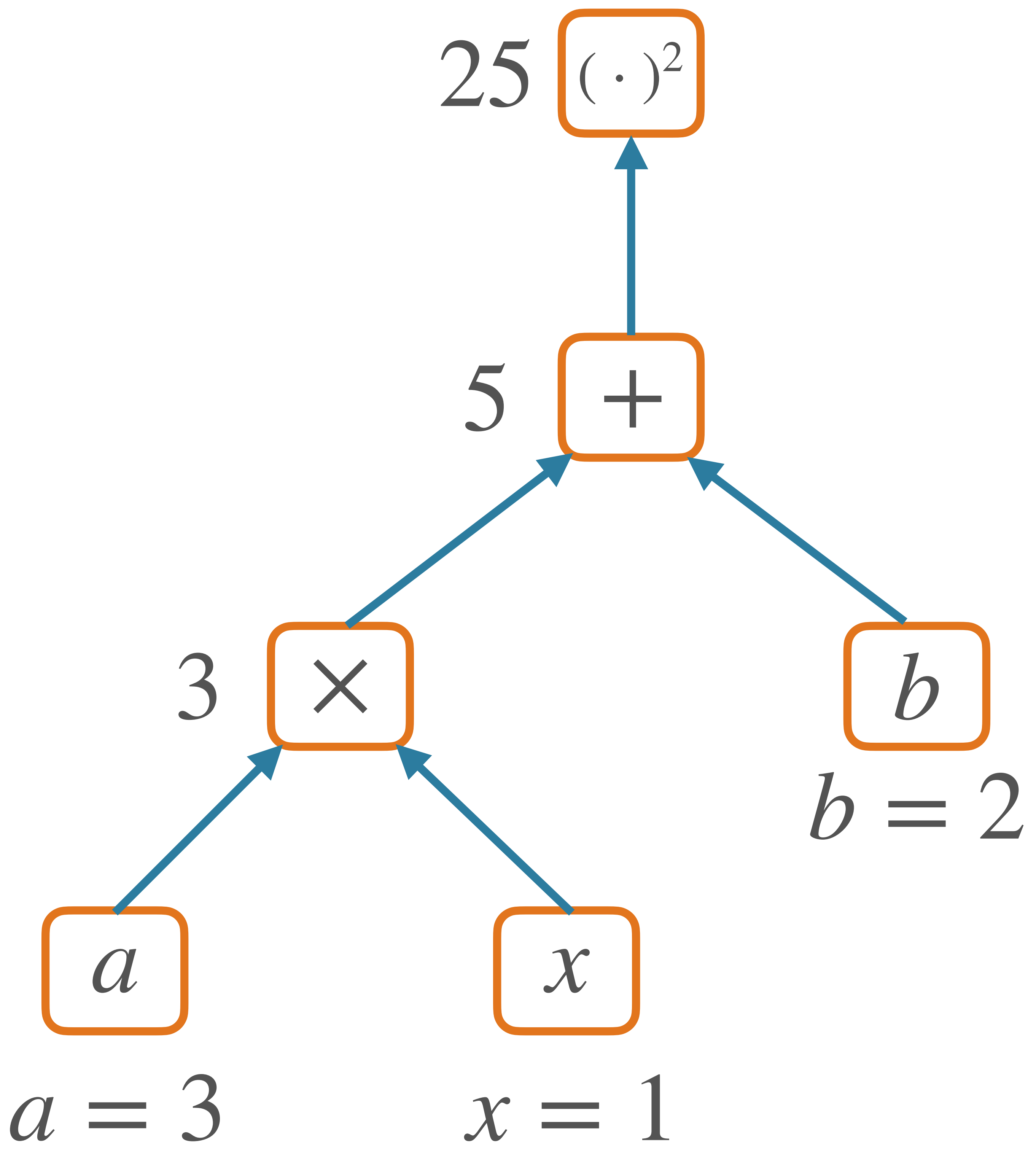
Computation Graph Example

$$f(x; a, b) = (ax + b)^2$$



Computation Graph Example

$$f(x; a, b) = (ax + b)^2$$

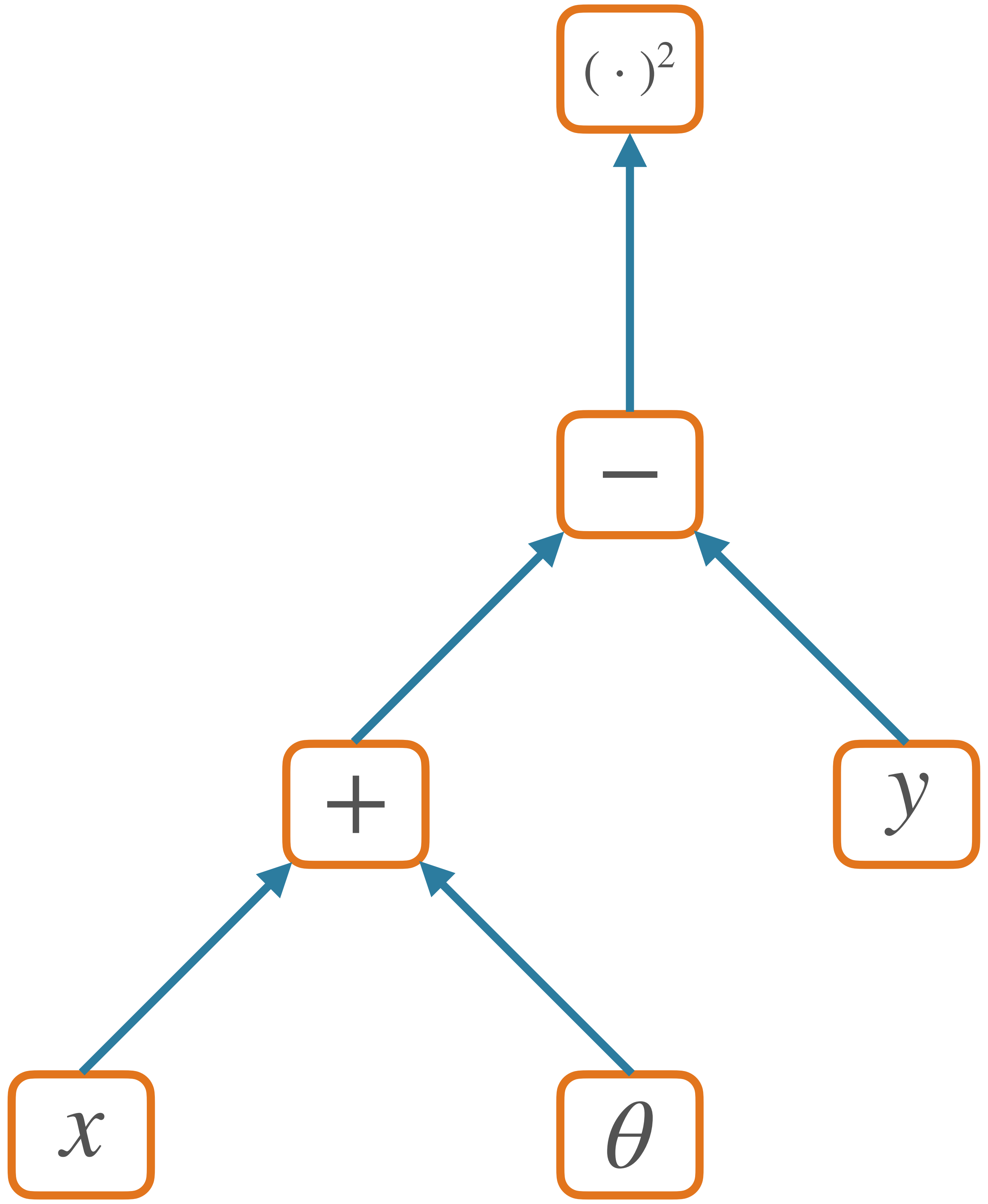


Nodes in a Graph

- Node: an **operation** yielding a **tensor value**
  - e.g. numpy ndarray; n-dimensional array of values
- Edge: operation **argument**
  - The value of a node is a **function of its parents' values**

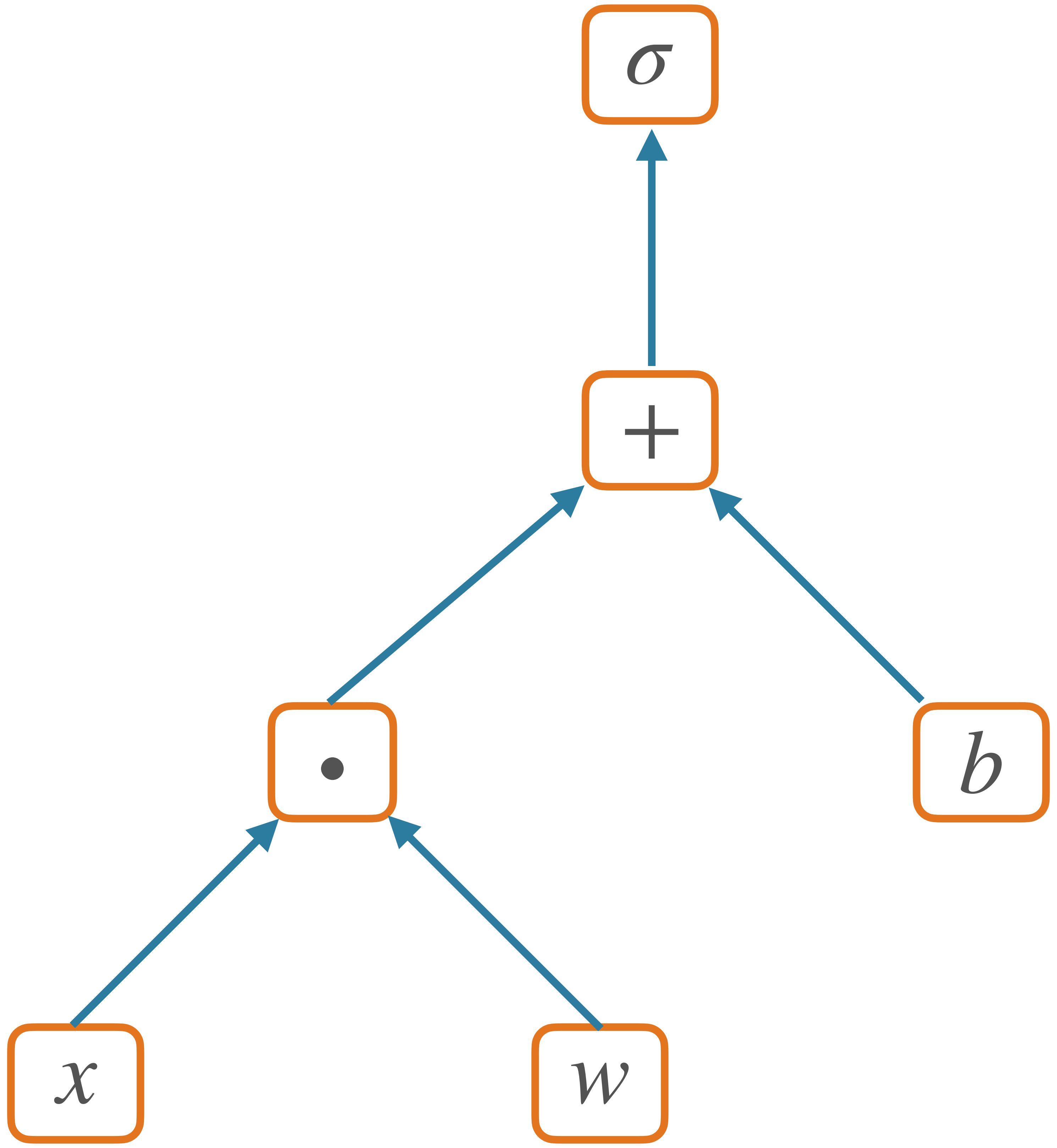
Secret Number Game Graph (Loss)

$$\mathcal{L}(\hat{y}, y) = (x + \theta - y)^2$$



Perceptron Graph

$$\hat{y} = \sigma(wx + b)$$



Backpropagation

So what?

So what?

- So far, this is just fancy re-writing of basic mathematical computation

So what?

- So far, this is just fancy re-writing of basic mathematical computation
- The real victory of the graph abstraction comes in **computing gradients**

So what?

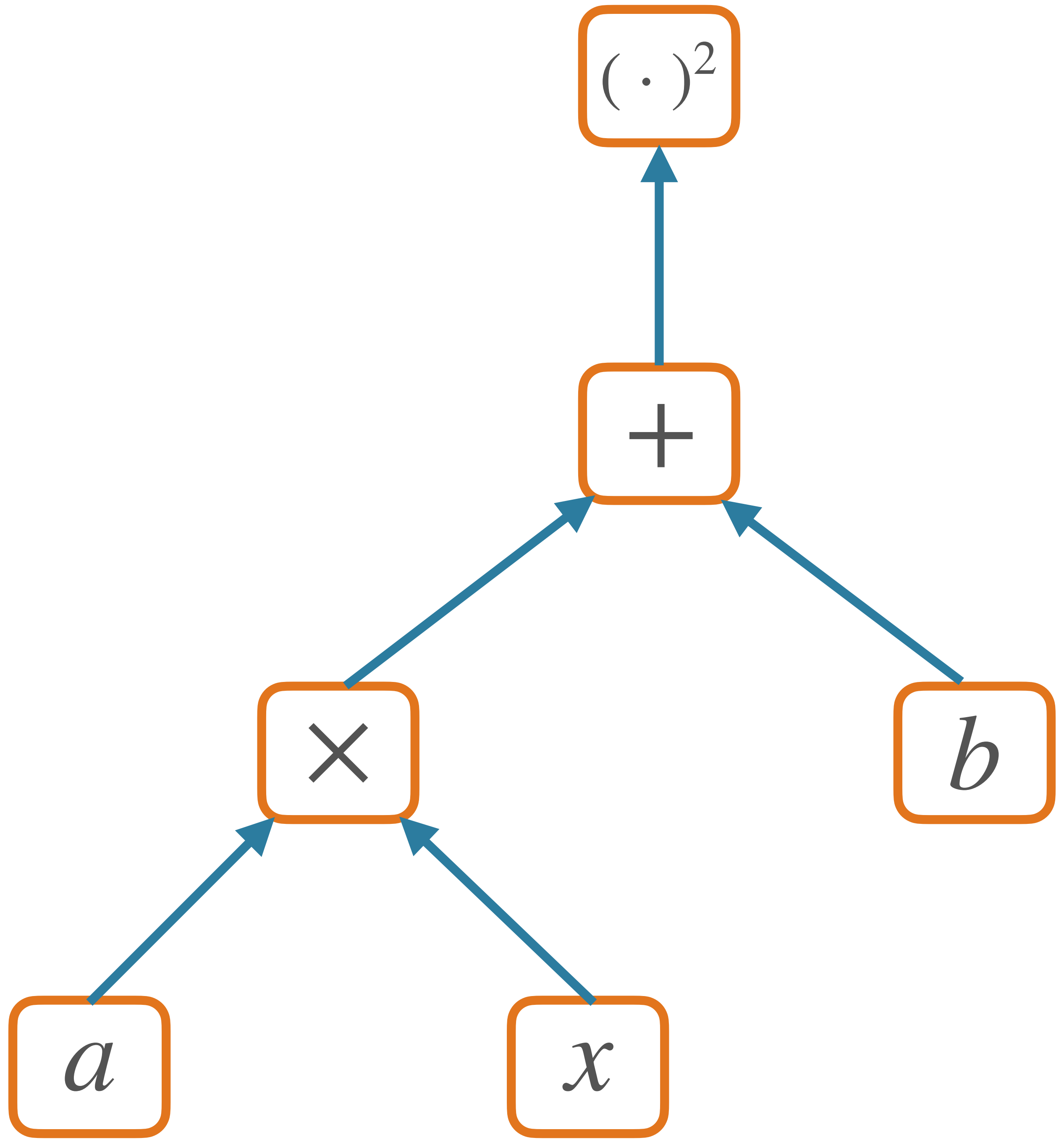
- So far, this is just fancy re-writing of basic mathematical computation
- The real victory of the graph abstraction comes in **computing gradients**
- Backpropagation
  - A **dynamic programming** algorithm on computation graphs
  - **Gradient** of an output to be computed **with respect to *every node*** in the graph

Chain Rule (of Calculus)

$$\frac{\partial}{\partial x} f(g(x)) = \frac{\partial f}{\partial g}\frac{\partial g}{\partial x}$$

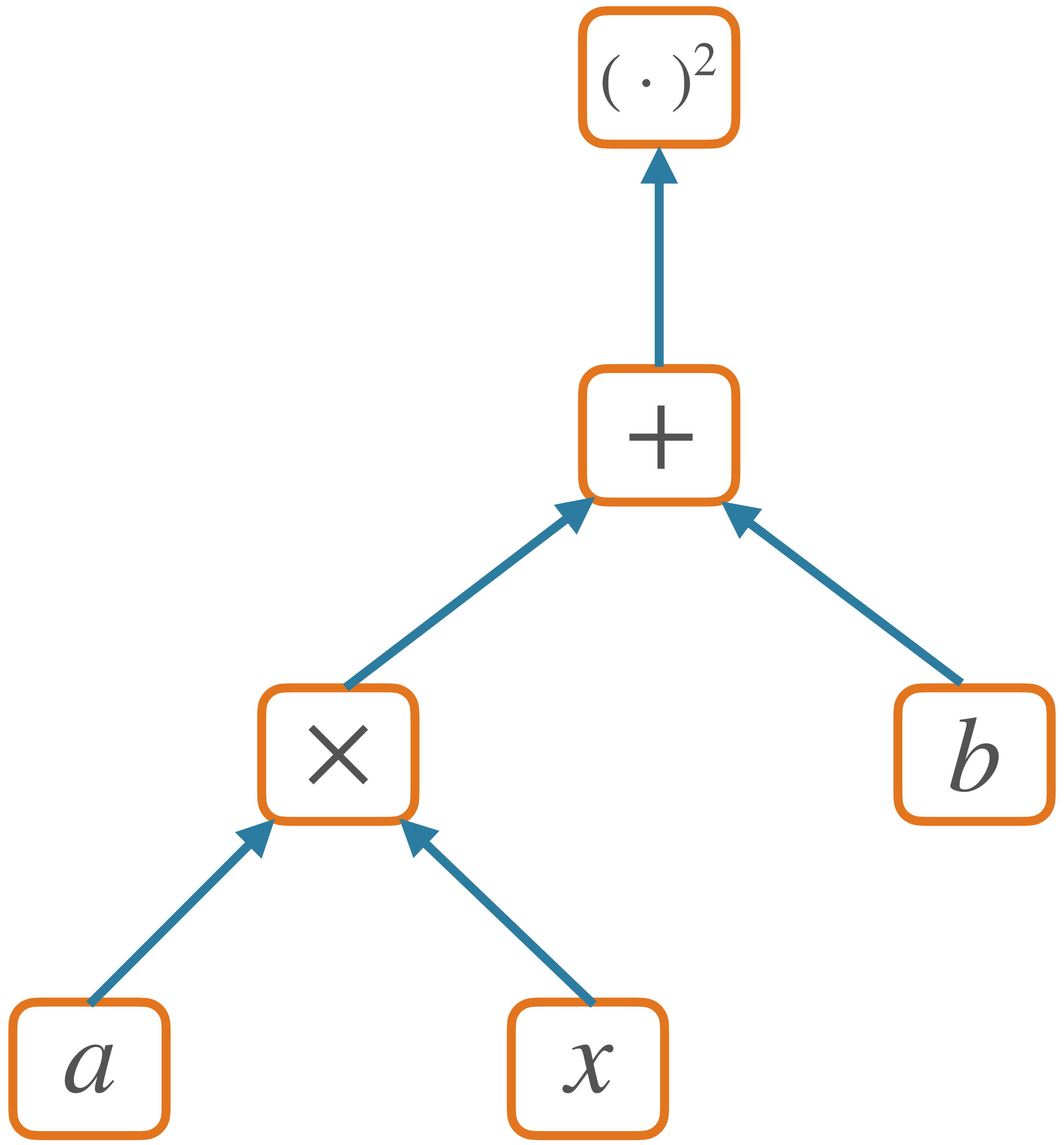
Computing Derivatives

$$f(x; a, b) = (ax + b)^2$$



Computing Derivatives

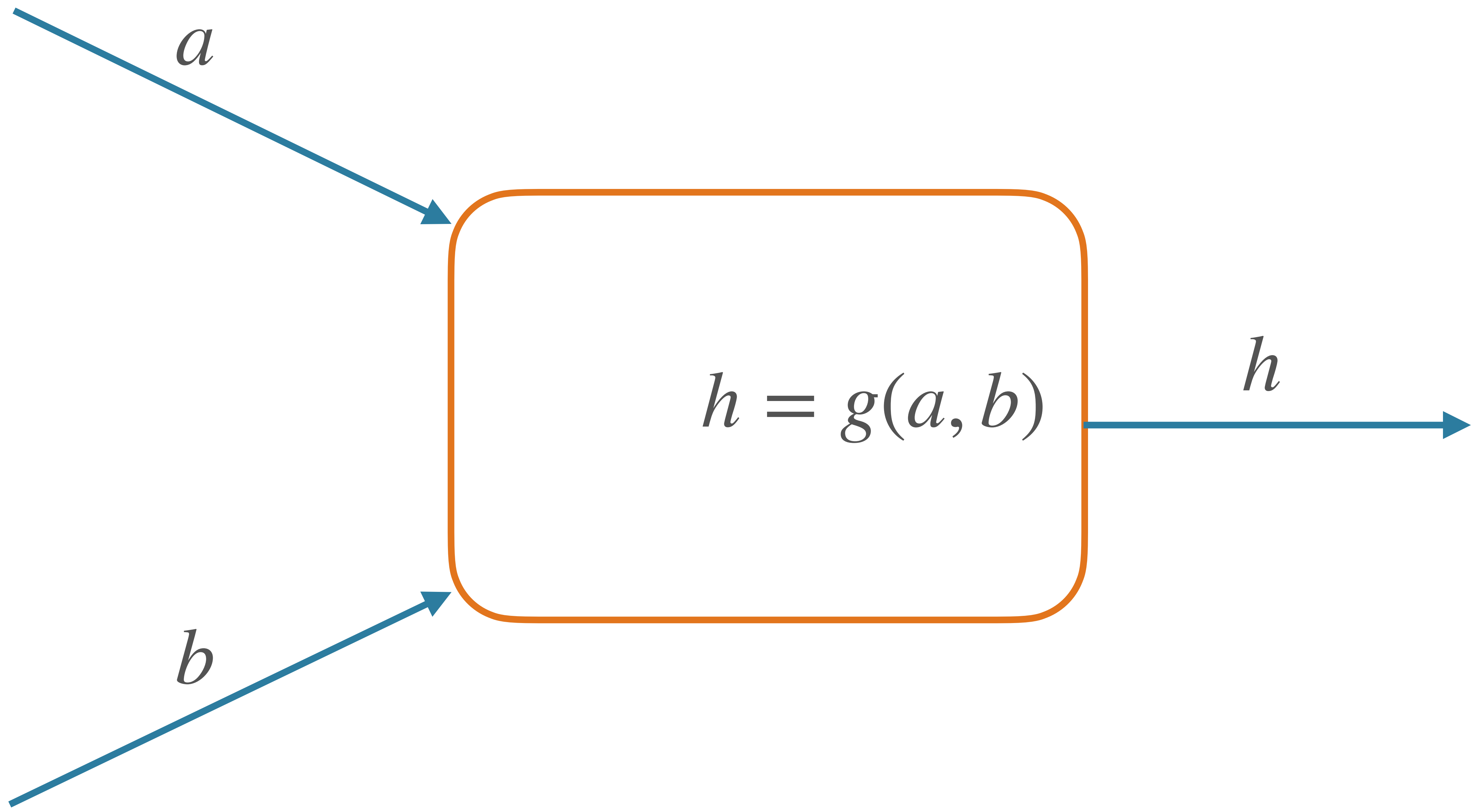
$$f(x; a, b) = (ax + b)^2$$



$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial (ax + b)} \frac{\partial (ax + b)}{\partial x}$$
$$= 2(ax + b)a$$
$$\frac{\partial f}{\partial a} = 2(ax + b)x$$
$$\frac{\partial f}{\partial b} = 2(ax + b)$$

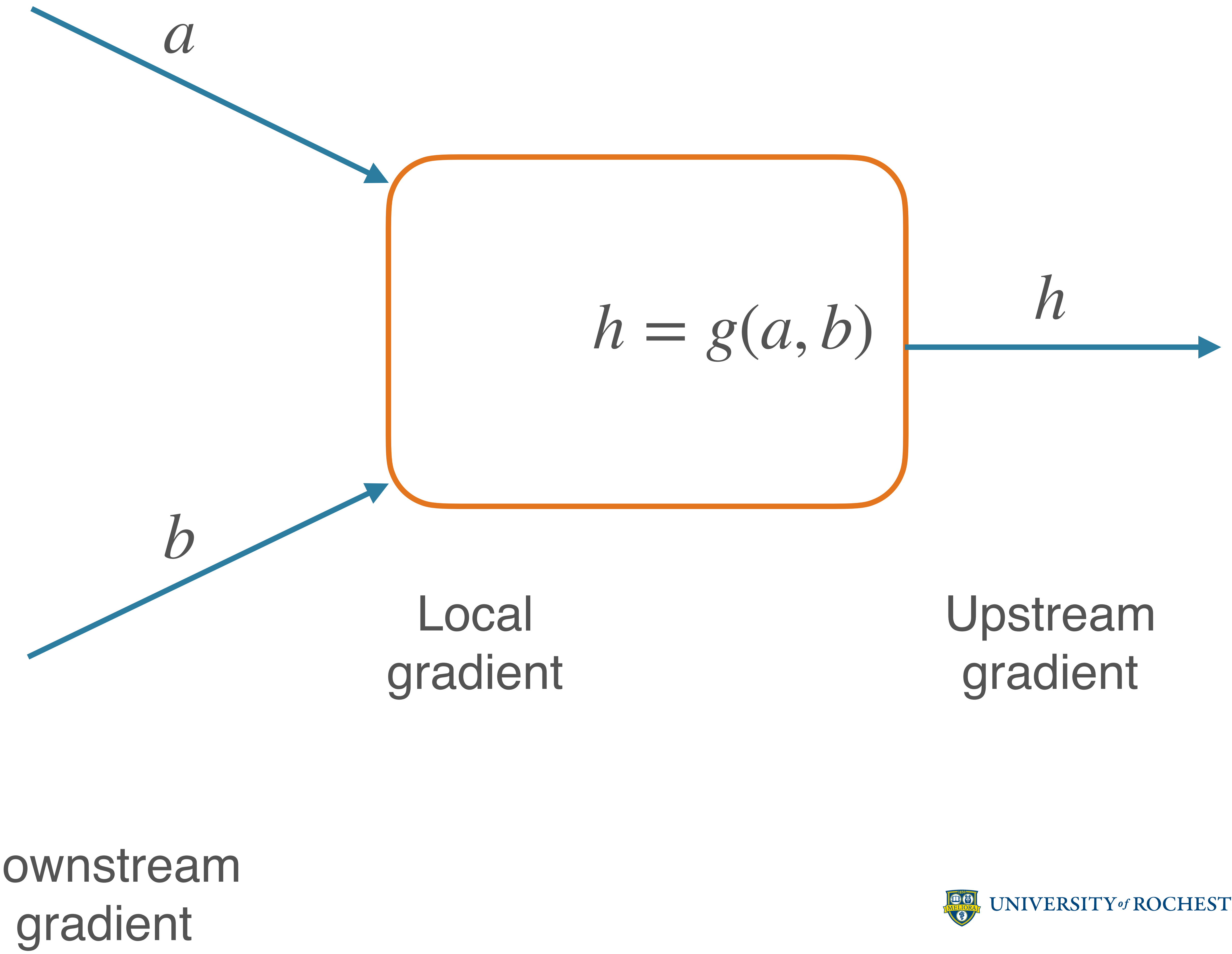
Nodes in Computational Graph

- Forward pass:
  - Compute **value** given **parents' values**
- Backward pass:
  - Compute **parents' gradients** given **children's**



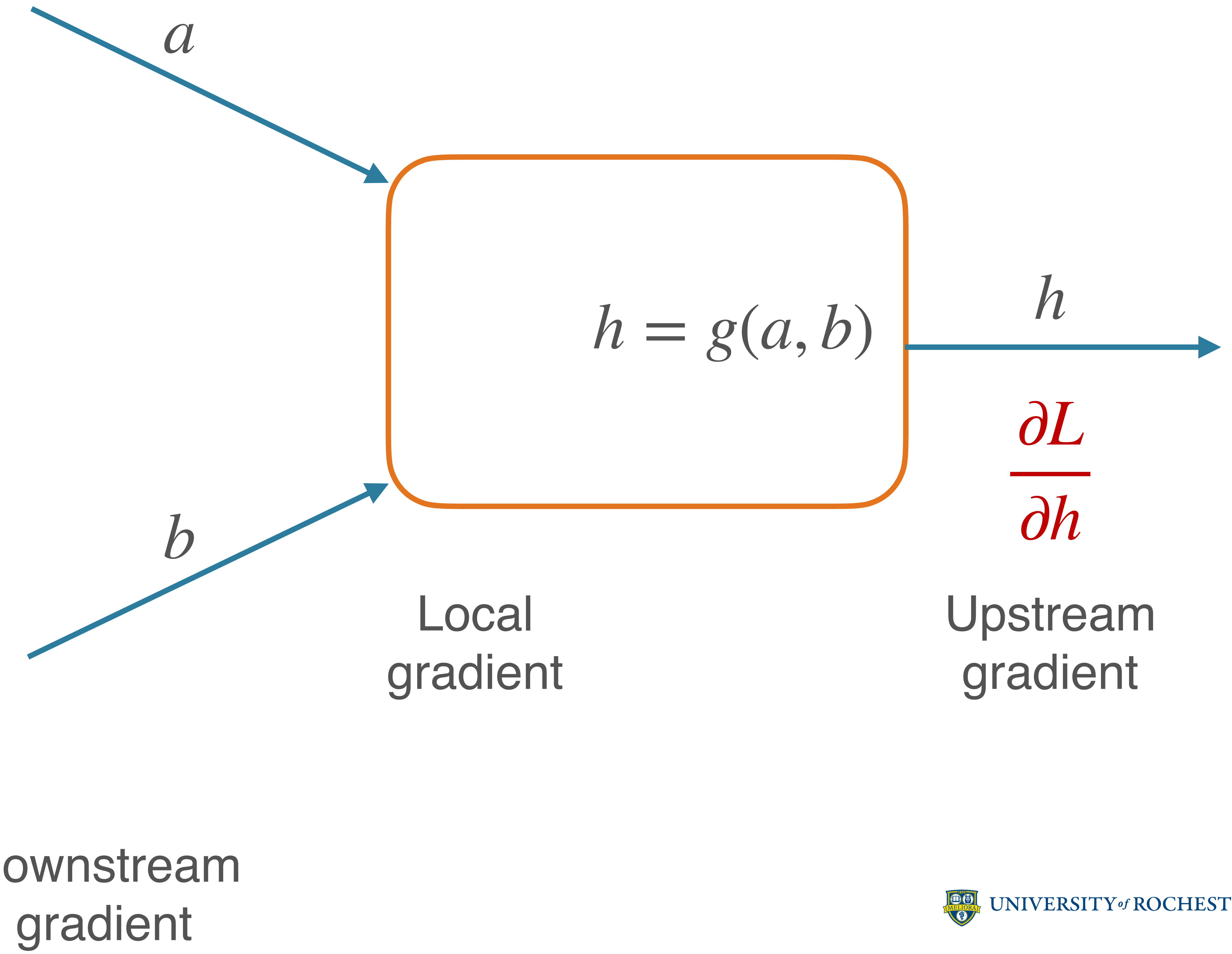
Nodes in Computational Graph

- Forward pass:
  - Compute **value** given **parents' values**
- Backward pass:
  - Compute **parents' gradients** given **children's**



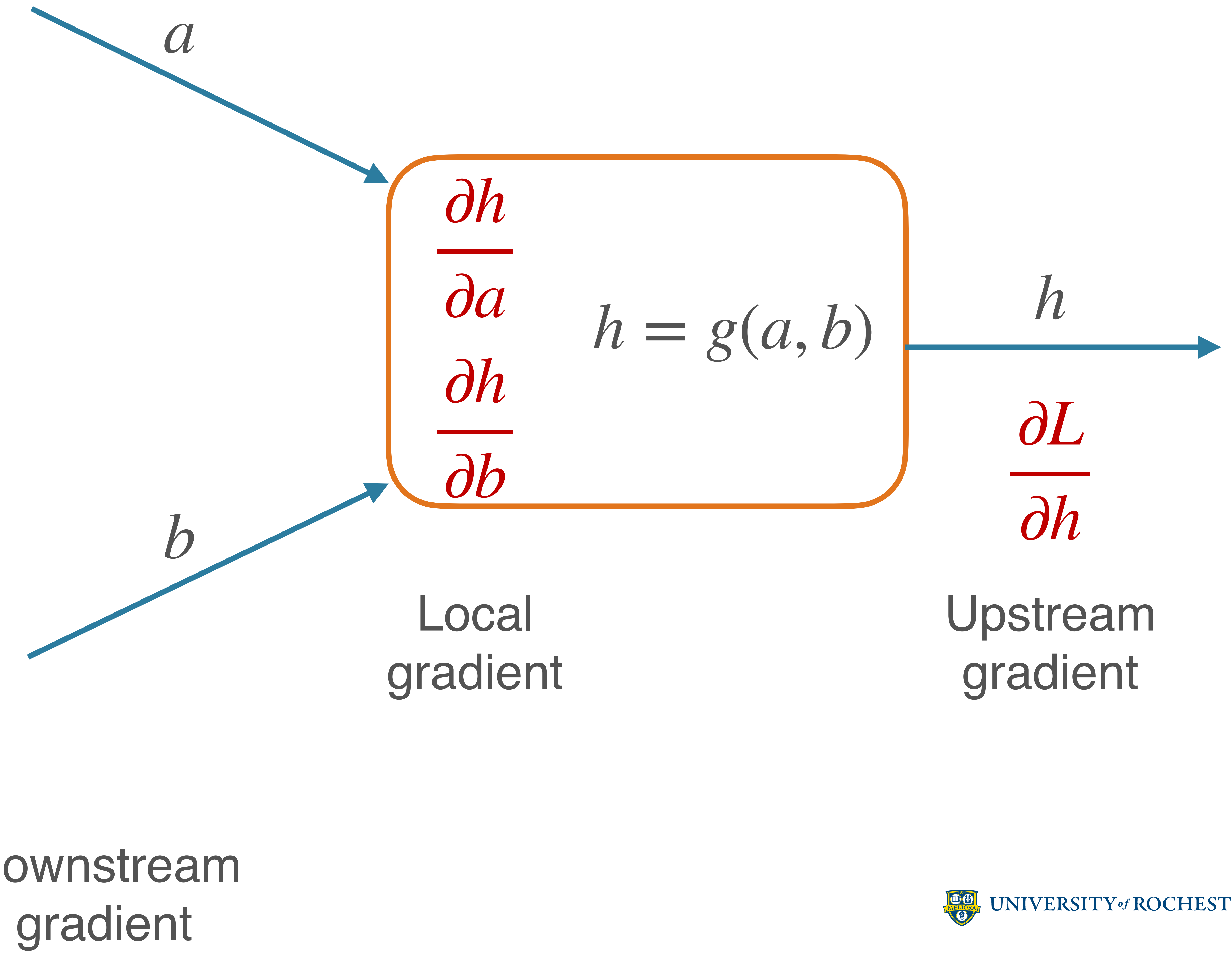
Nodes in Computational Graph

- Forward pass:
  - Compute **value** given **parents' values**
- Backward pass:
  - Compute **parents' gradients** given **children's**



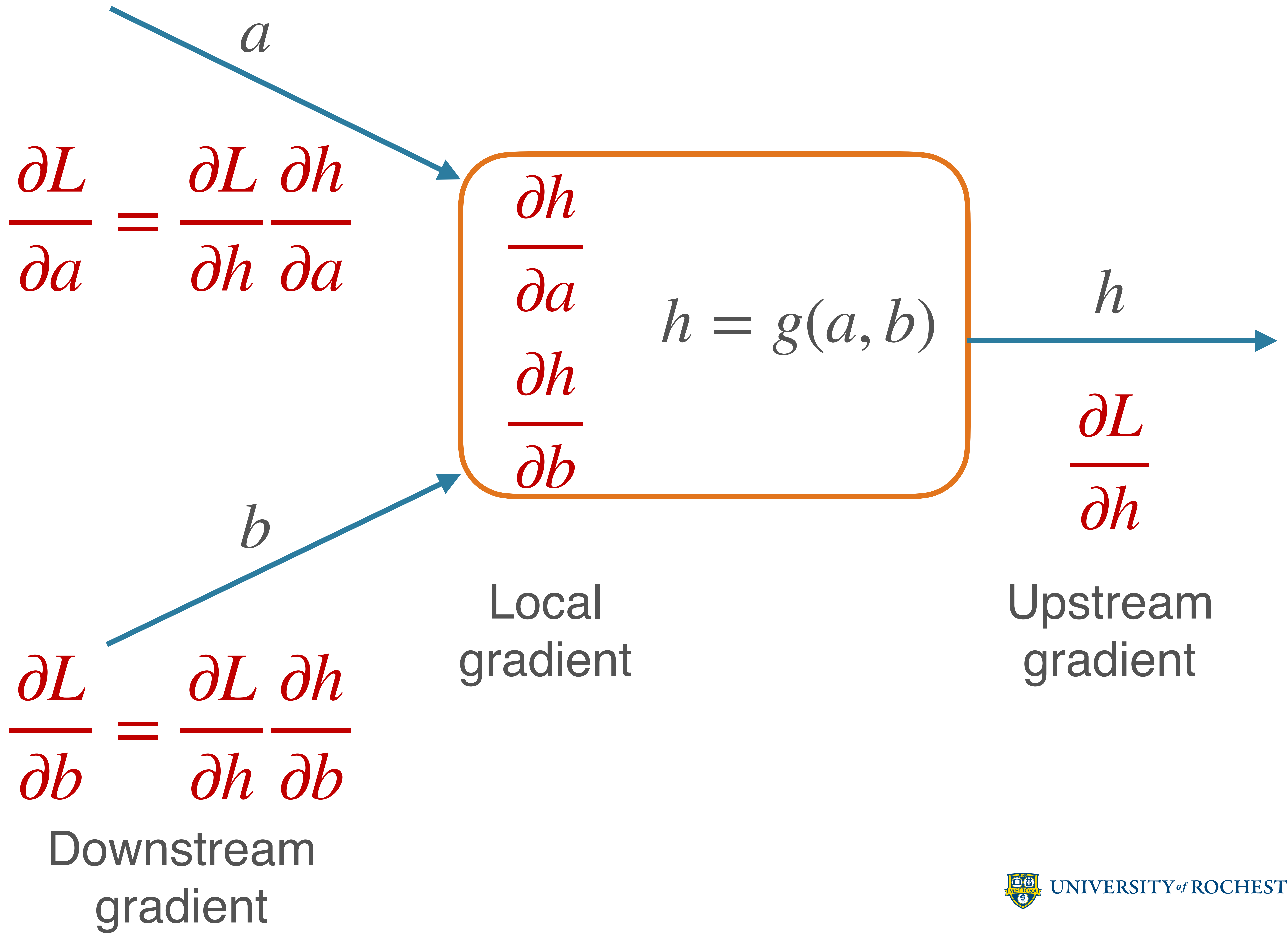
Nodes in Computational Graph

- Forward pass:
  - Compute **value** given **parents' values**
- Backward pass:
  - Compute **parents' gradients** given **children's**


a
b
$\frac{\partial h}{\partial a}$
$\frac{\partial h}{\partial b}$
$h = g(a, b)$
h
$\frac{\partial L}{\partial h}$
Local gradient
Upstream gradient
Downstream gradient

Nodes in Computational Graph

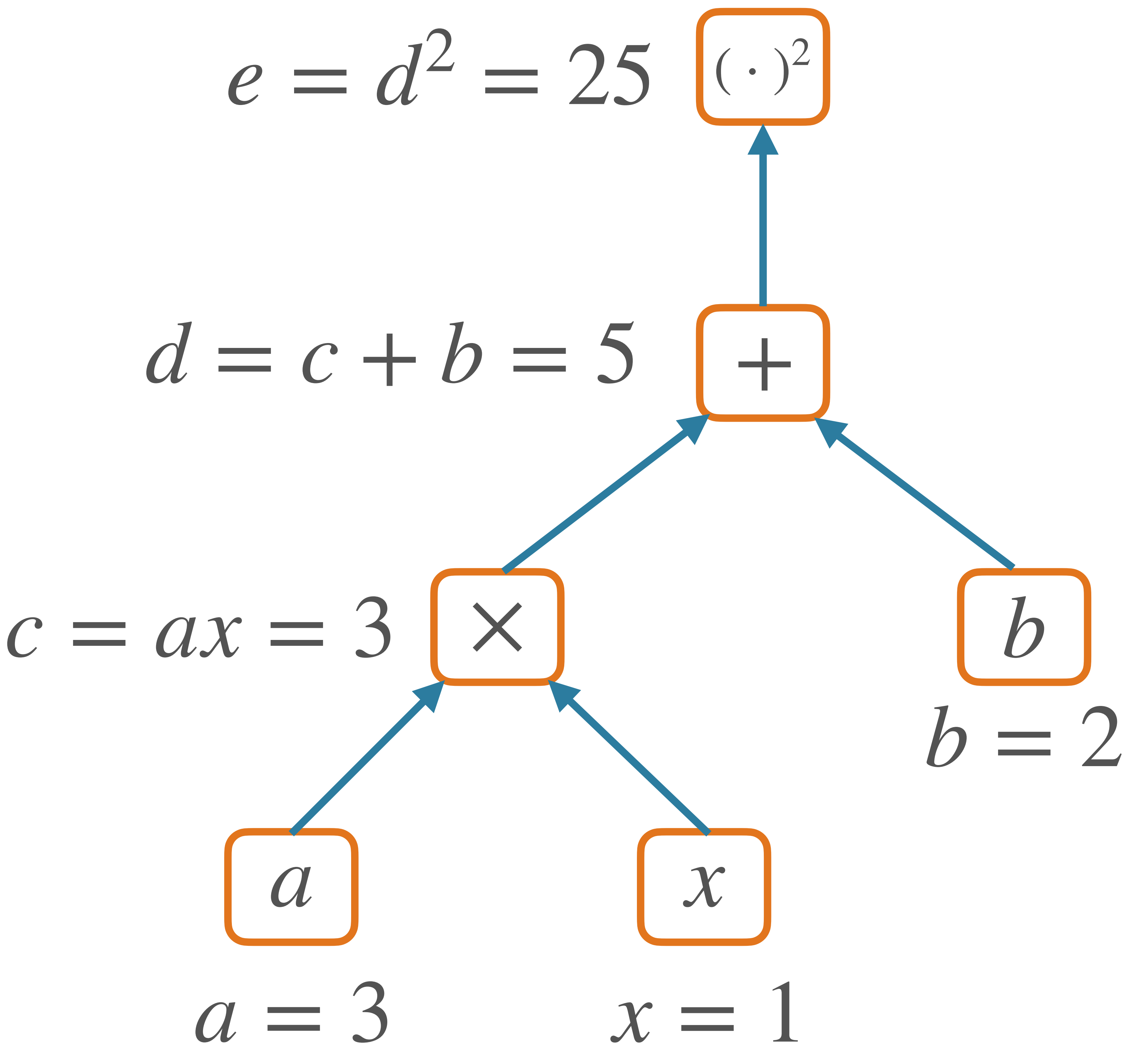
- Forward pass:
  - Compute **value** given **parents' values**
- Backward pass:
  - Compute **parents' gradients** given **children's**



a
$\frac{\partial L}{\partial a} = \frac{\partial L}{\partial h}\frac{\partial h}{\partial a}$
$\frac{\partial h}{\partial a}$
$h = g(a, b)$
$\frac{\partial h}{\partial b}$
h
$\frac{\partial L}{\partial h}$
b
$\frac{\partial L}{\partial b} = \frac{\partial L}{\partial h}\frac{\partial h}{\partial b}$
Local gradient
Upstream gradient
Downstream gradient

Backpropagation Example

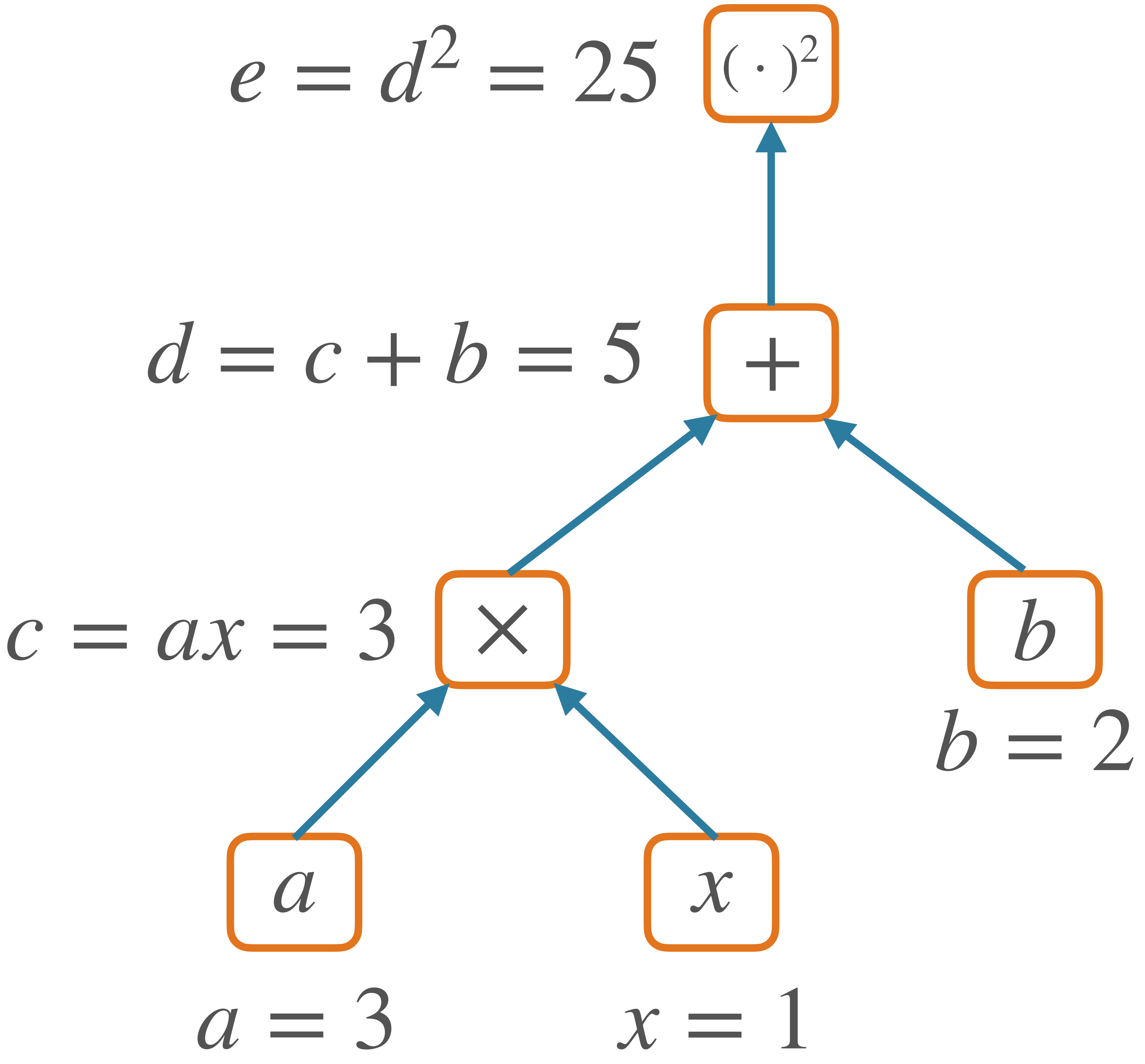
$$f(x; a, b) = (ax + b)^2$$



Backpropagation Example

$$\frac{\partial e}{\partial e} = 1$$

$$f(x; a, b) = (ax + b)^2$$



$e = d^2 = 25$

$d = c + b = 5$

$c = ax = 3$

$b = 2$

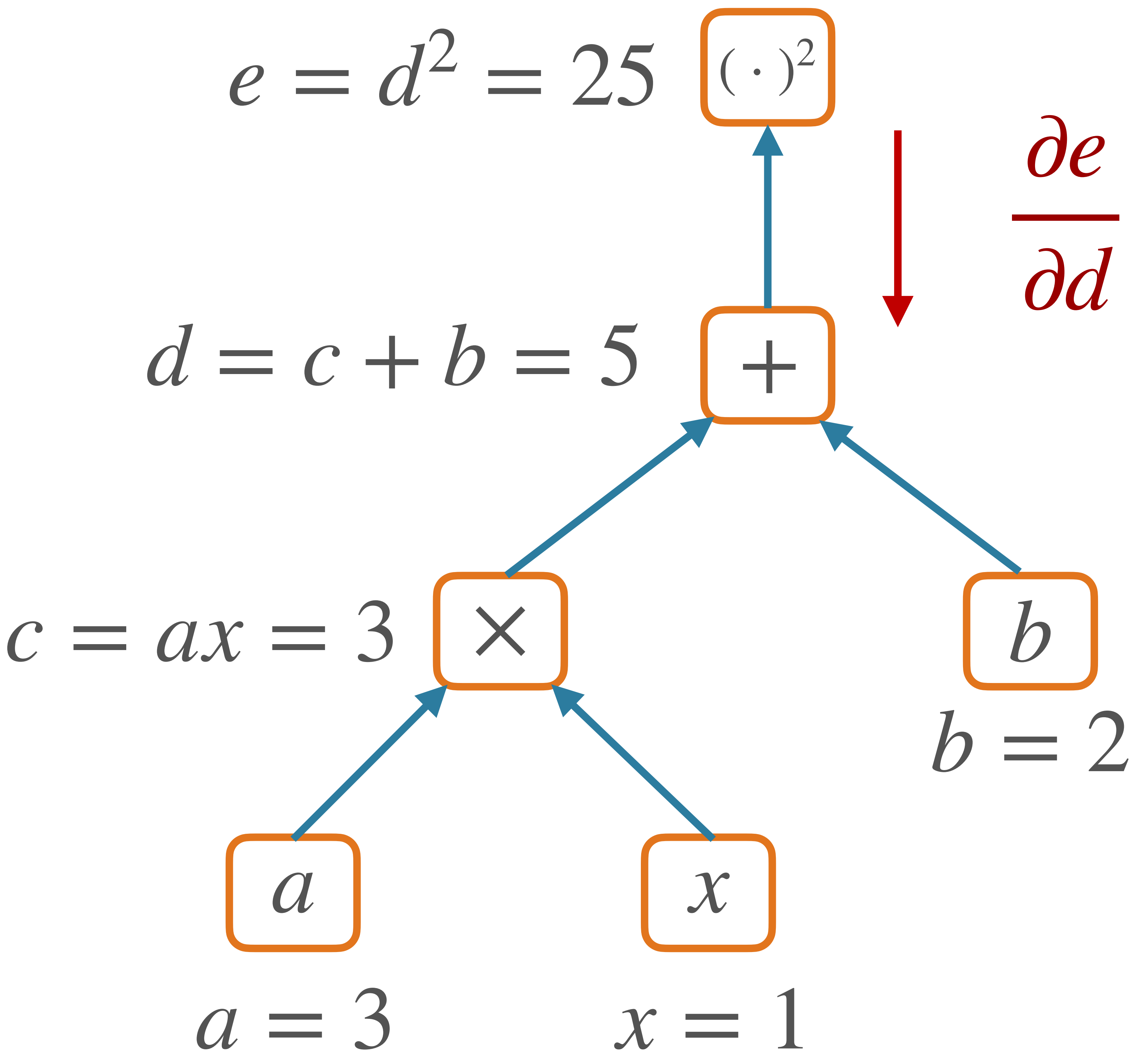
$a = 3$

$x = 1$

Backpropagation Example

$$\frac{\partial e}{\partial e} = 1$$

$$f(x; a, b) = (ax + b)^2$$

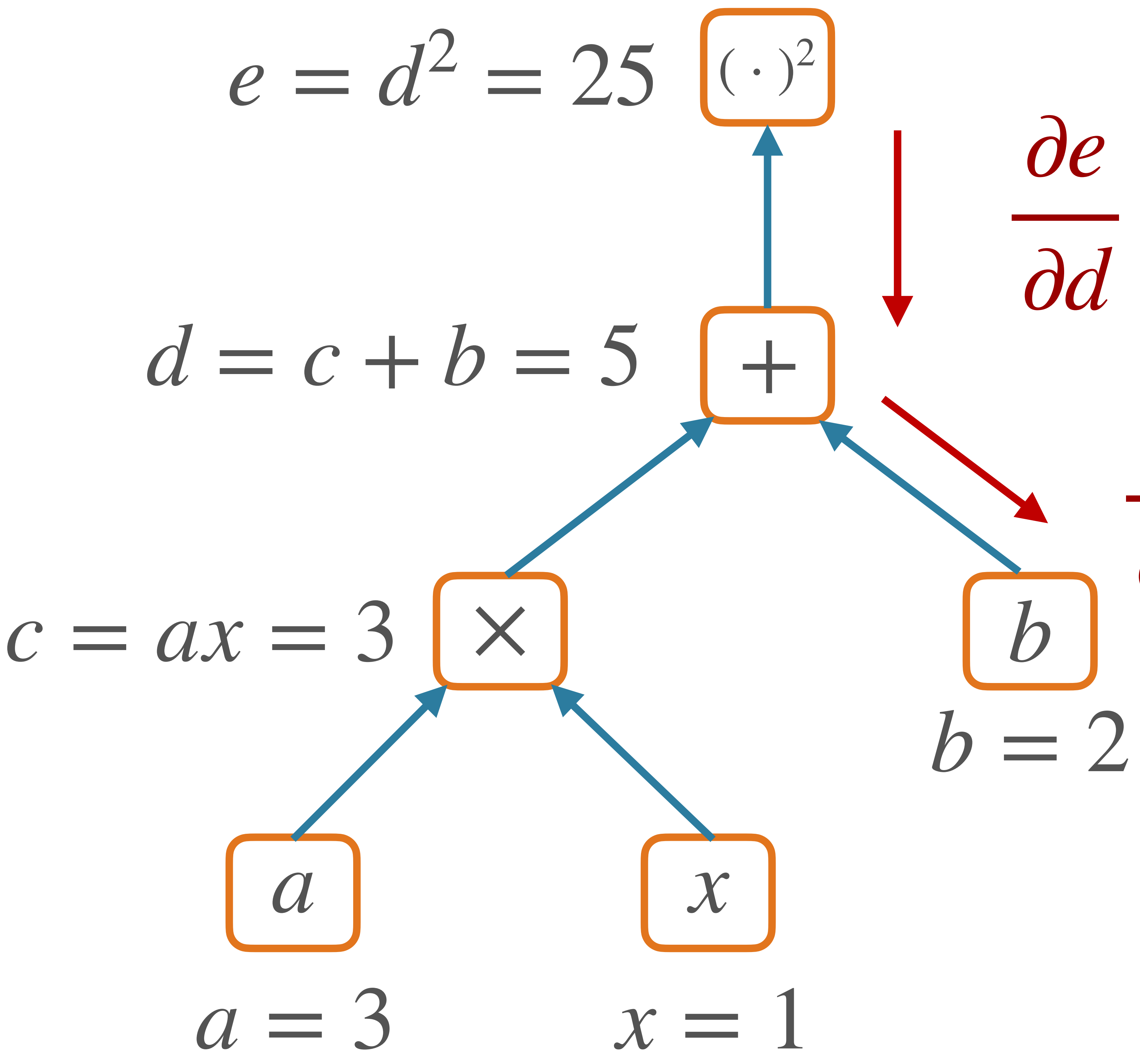


$$\frac{\partial e}{\partial d} = 2d\frac{\partial e}{\partial e} = 10$$

Backpropagation Example

$$\frac{\partial e}{\partial e} = 1$$

$$f(x; a, b) = (ax + b)^2$$



$e = d^2 = 25$

$(\cdot)^2$

$d = c + b = 5$

$+$

$c = ax = 3$

$\times$

b

$b = 2$

a

x

$a = 3$

$x = 1$

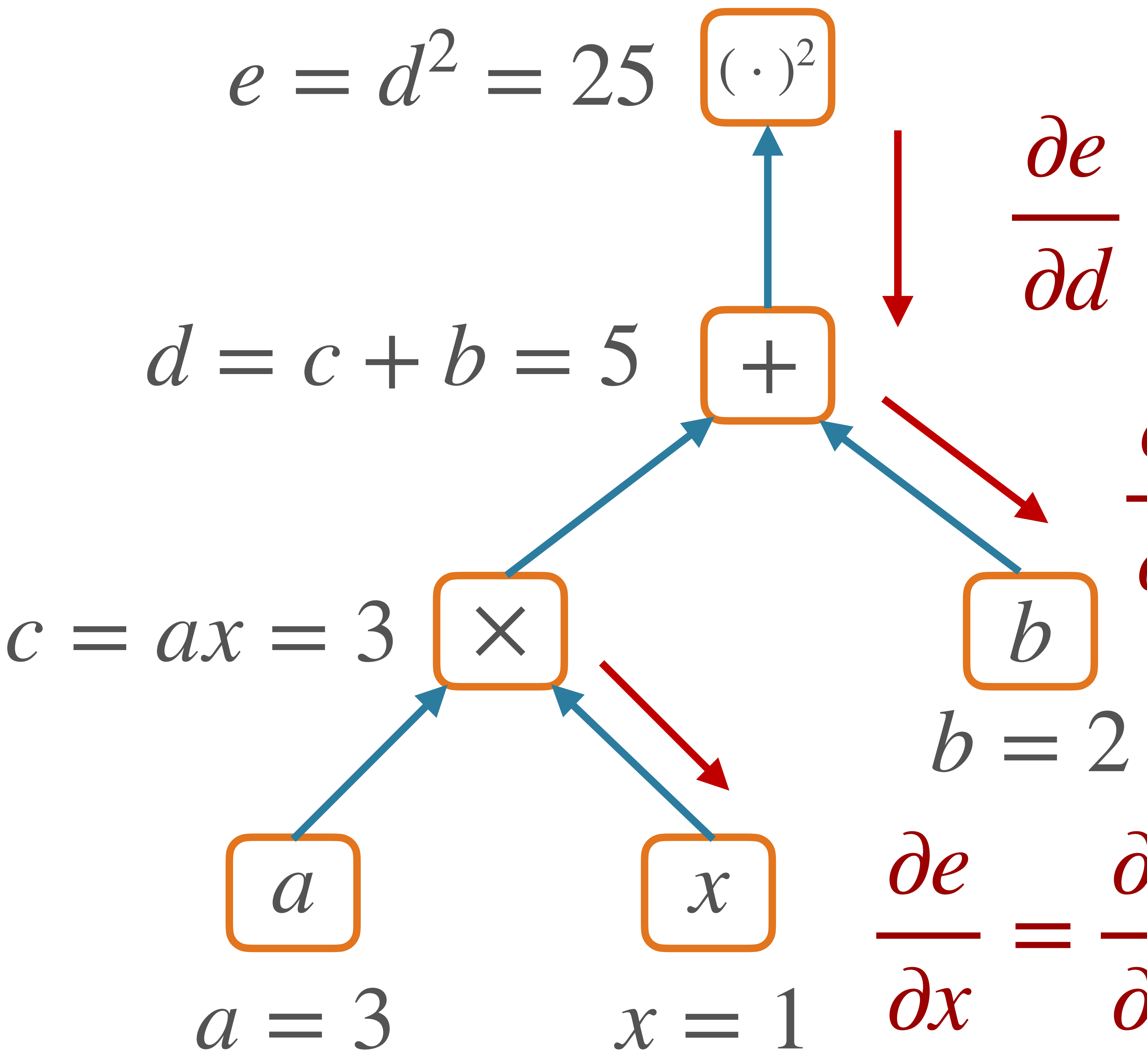
$$\frac{\partial e}{\partial d} = 2d\frac{\partial e}{\partial e} = 10$$

$$\frac{\partial e}{\partial b} = \frac{\partial e}{\partial d}\frac{\partial d}{\partial b} = 10\frac{\partial c + b}{\partial b} = 10$$

Backpropagation Example

$$\frac{\partial e}{\partial e} = 1$$

$$f(x; a, b) = (ax + b)^2$$



$e = d^2 = 25$ $\boxed{(\cdot)^2}$

$d = c + b = 5$ $\boxed{+}$

$c = ax = 3$ $\boxed{\times}$

$\boxed{b}$ $b = 2$

$\boxed{a}$ $a = 3$

$\boxed{x}$ $x = 1$

$$\frac{\partial e}{\partial d} = 2d\frac{\partial e}{\partial e} = 10$$

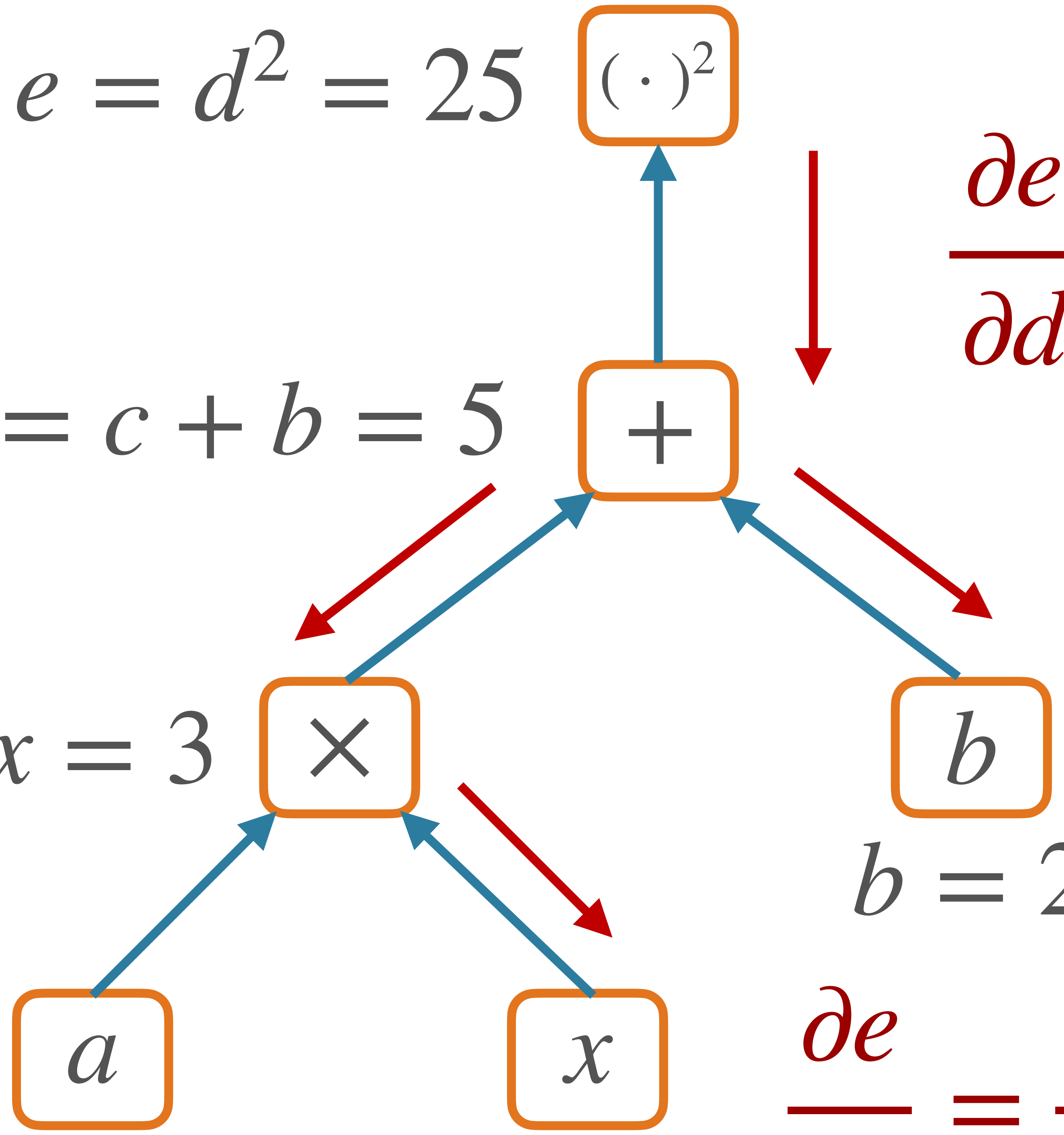
$$\frac{\partial e}{\partial b} = \frac{\partial e}{\partial d}\frac{\partial d}{\partial b} = 10\frac{\partial c + b}{\partial b} = 10$$

$$\frac{\partial e}{\partial x} = \frac{\partial e}{\partial c}\frac{\partial c}{\partial x} = 10a = 30$$

Backpropagation Example

$$\frac{\partial e}{\partial e} = 1$$

$$f(x; a, b) = (ax + b)^2$$



$$e = d^2 = 25$$

$$\frac{\partial e}{\partial d} = 2d\frac{\partial e}{\partial e} = 10$$

$$d = c + b = 5$$

$$\frac{\partial e}{\partial c} = \frac{\partial e}{\partial d}\frac{\partial d}{\partial c} = 10\frac{\partial c + b}{\partial c} = 10$$

$$\frac{\partial e}{\partial b} = \frac{\partial e}{\partial d}\frac{\partial d}{\partial b} = 10\frac{\partial c + b}{\partial b} = 10$$

$$c = ax = 3$$

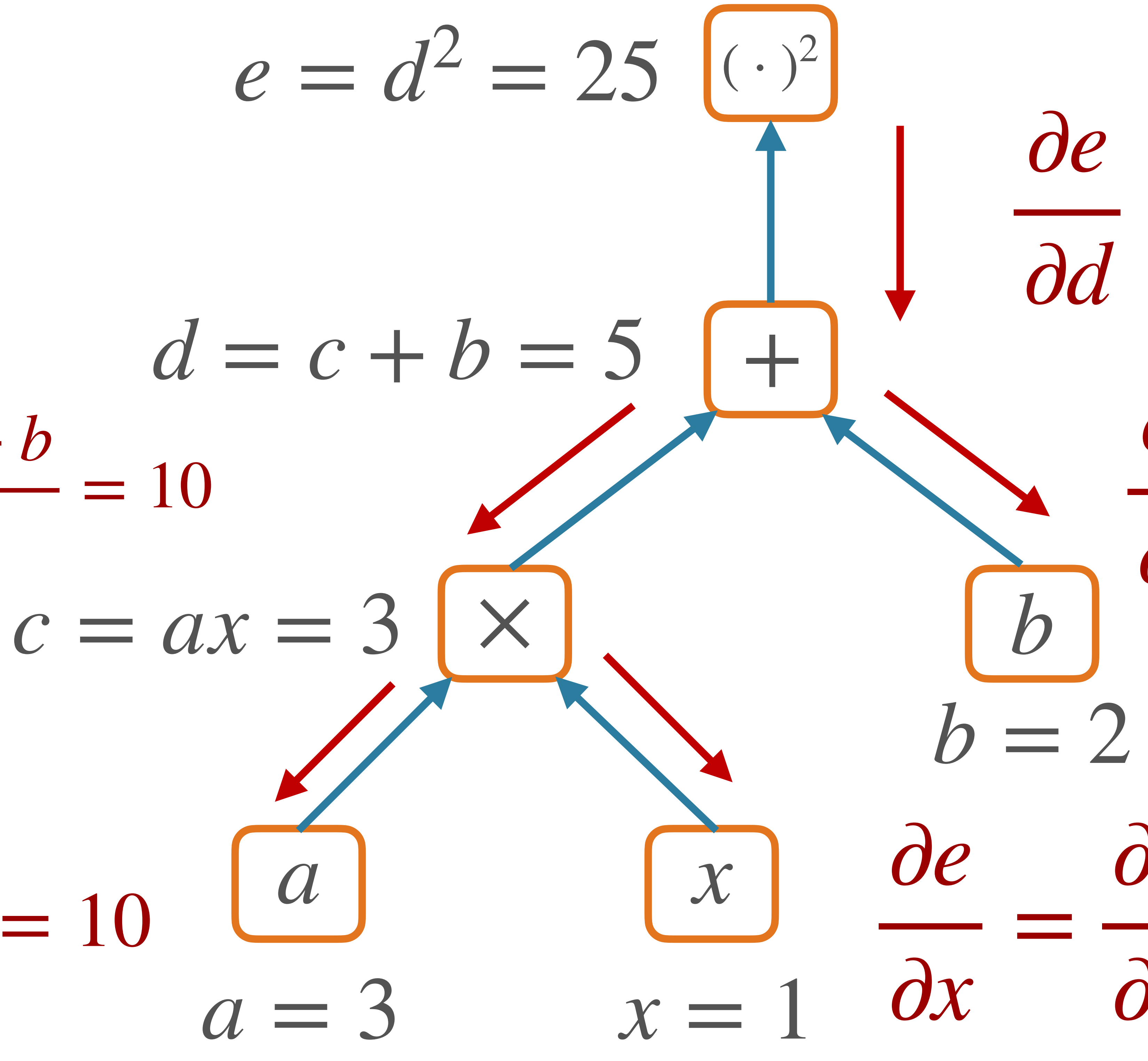
$$b = 2$$

$$\frac{\partial e}{\partial x} = \frac{\partial e}{\partial c}\frac{\partial c}{\partial x} = 10a = 30$$

$$a = 3 \qquad x = 1$$

Backpropagation Example

$$\frac{\partial e}{\partial e} = 1 \qquad f(x; a, b) = (ax + b)^2$$



$$e = d^2 = 25 \quad \boxed{(\cdot)^2}$$

$$\frac{\partial e}{\partial d} = 2d\frac{\partial e}{\partial e} = 10$$

$$d = c + b = 5 \quad \boxed{+}$$

$$\frac{\partial e}{\partial c} = \frac{\partial e}{\partial d}\frac{\partial d}{\partial c} = 10\frac{\partial c + b}{\partial c} = 10$$

$$\frac{\partial e}{\partial b} = \frac{\partial e}{\partial d}\frac{\partial d}{\partial b} = 10\frac{\partial c + b}{\partial b} = 10$$

$$c = ax = 3 \quad \boxed{\times}$$

$$\boxed{b} \quad b = 2$$

$$\frac{\partial e}{\partial a} = \frac{\partial e}{\partial c}\frac{\partial c}{\partial a} = 10x = 10$$

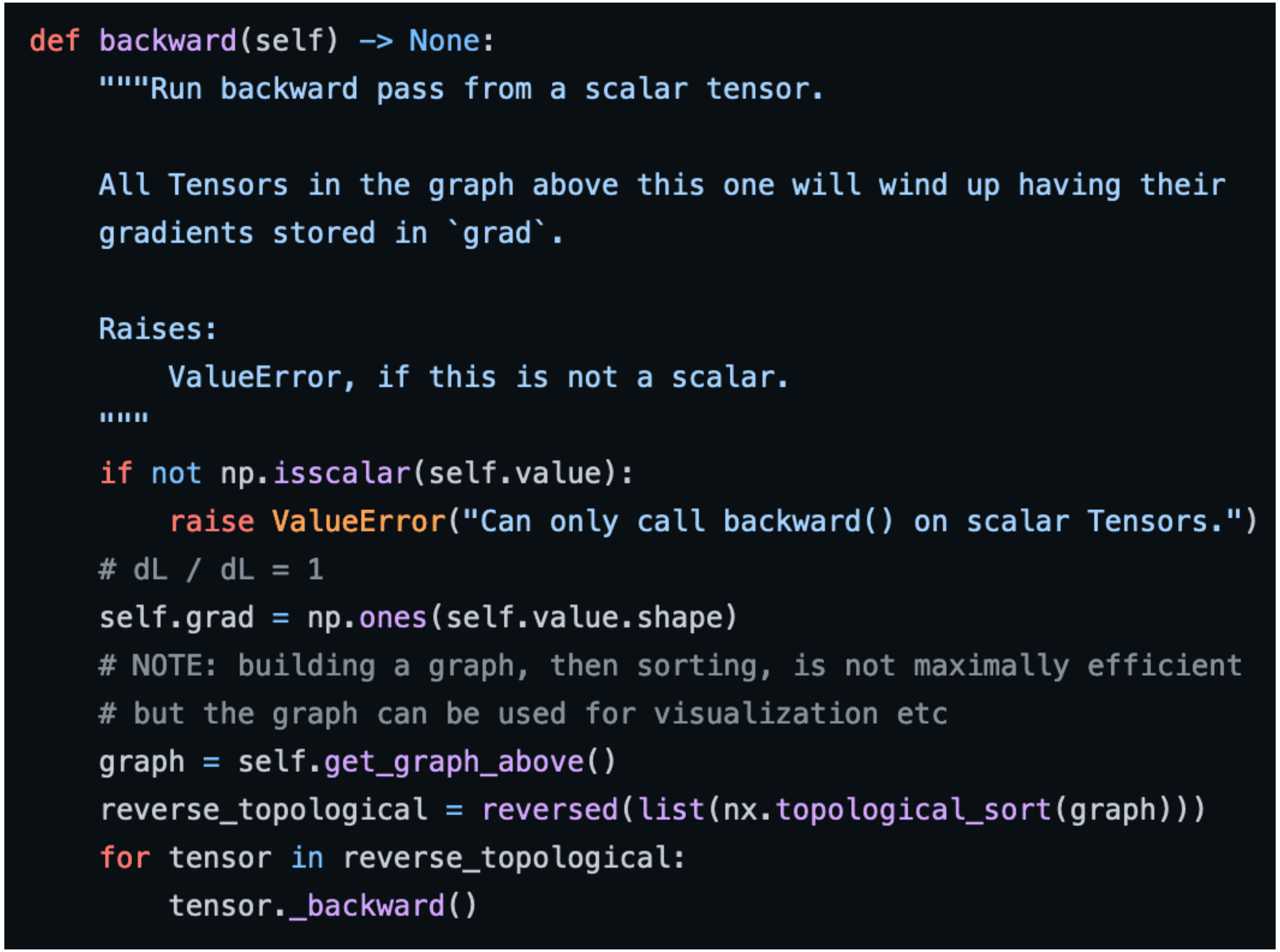
$$\boxed{a} \quad a = 3 \qquad \boxed{x} \quad x = 1$$

$$\frac{\partial e}{\partial x} = \frac{\partial e}{\partial c}\frac{\partial c}{\partial x} = 10a = 30$$

Backpropagation

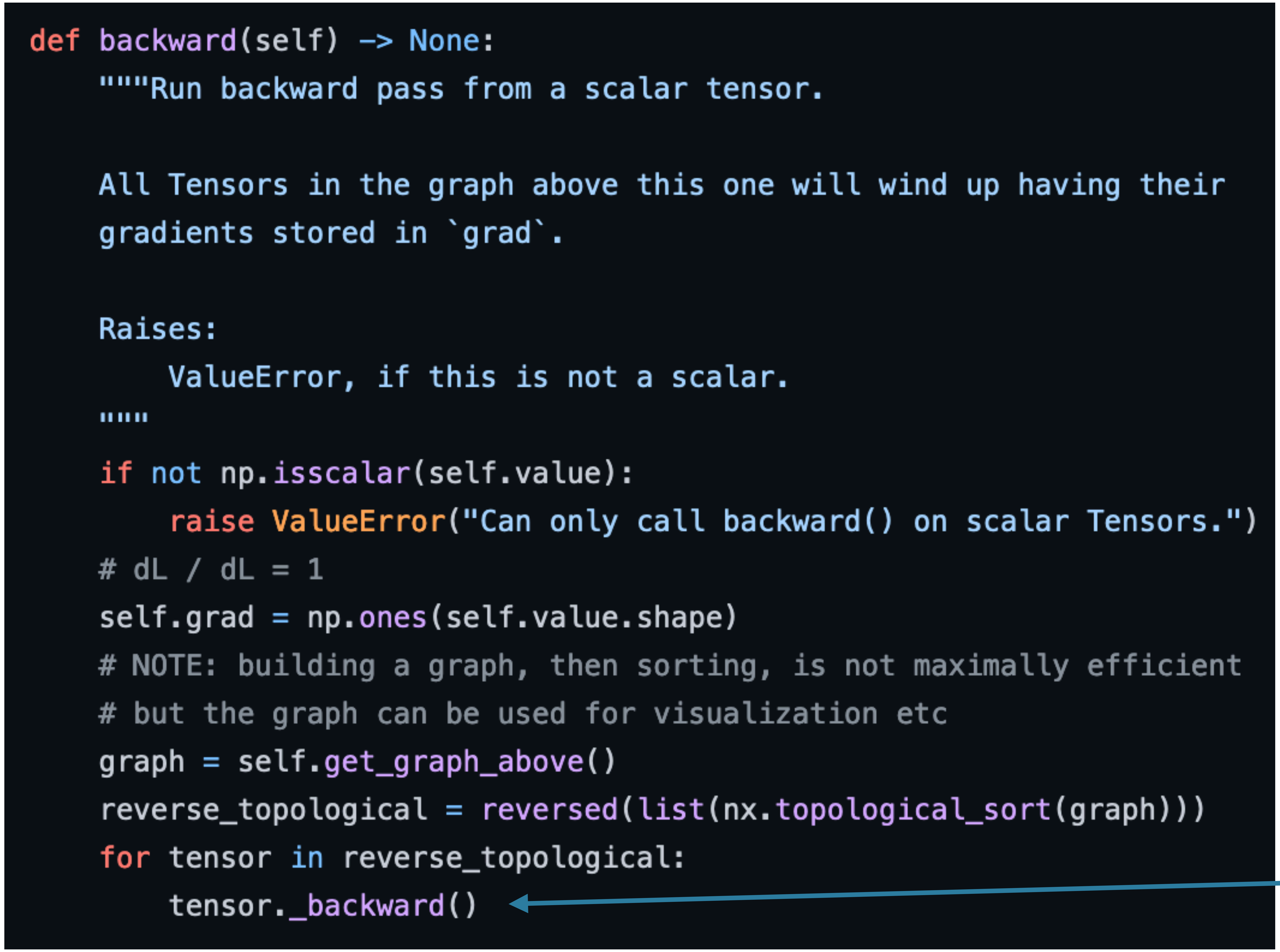
- **Initialize** gradient for **output node** f (df/df) to 1
  - (assuming that this output node is a *scalar)*
- **Loop over nodes** in graph in **reverse topological order**
  - (i.e. children come before parents)
  - Compute gradient of output node w/r/t this node, in terms of gradients w/r/t this node's children
    - Apply the chain rule!

Backpropagation Algorithm



```python
def backward(self) -> None:
    """Run backward pass from a scalar tensor.

    All Tensors in the graph above this one will wind up having their
    gradients stored in `grad`.

    Raises:
        ValueError, if this is not a scalar.
    """
    if not np.isscalar(self.value):
        raise ValueError("Can only call backward() on scalar Tensors.")
    # dL / dL = 1
    self.grad = np.ones(self.value.shape)
    # NOTE: building a graph, then sorting, is not maximally efficient
    # but the graph can be used for visualization etc
    graph = self.get_graph_above()
    reverse_topological = reversed(list(nx.topological_sort(graph)))
    for tensor in reverse_topological:
        tensor._backward()
```

Backpropagation Algorithm

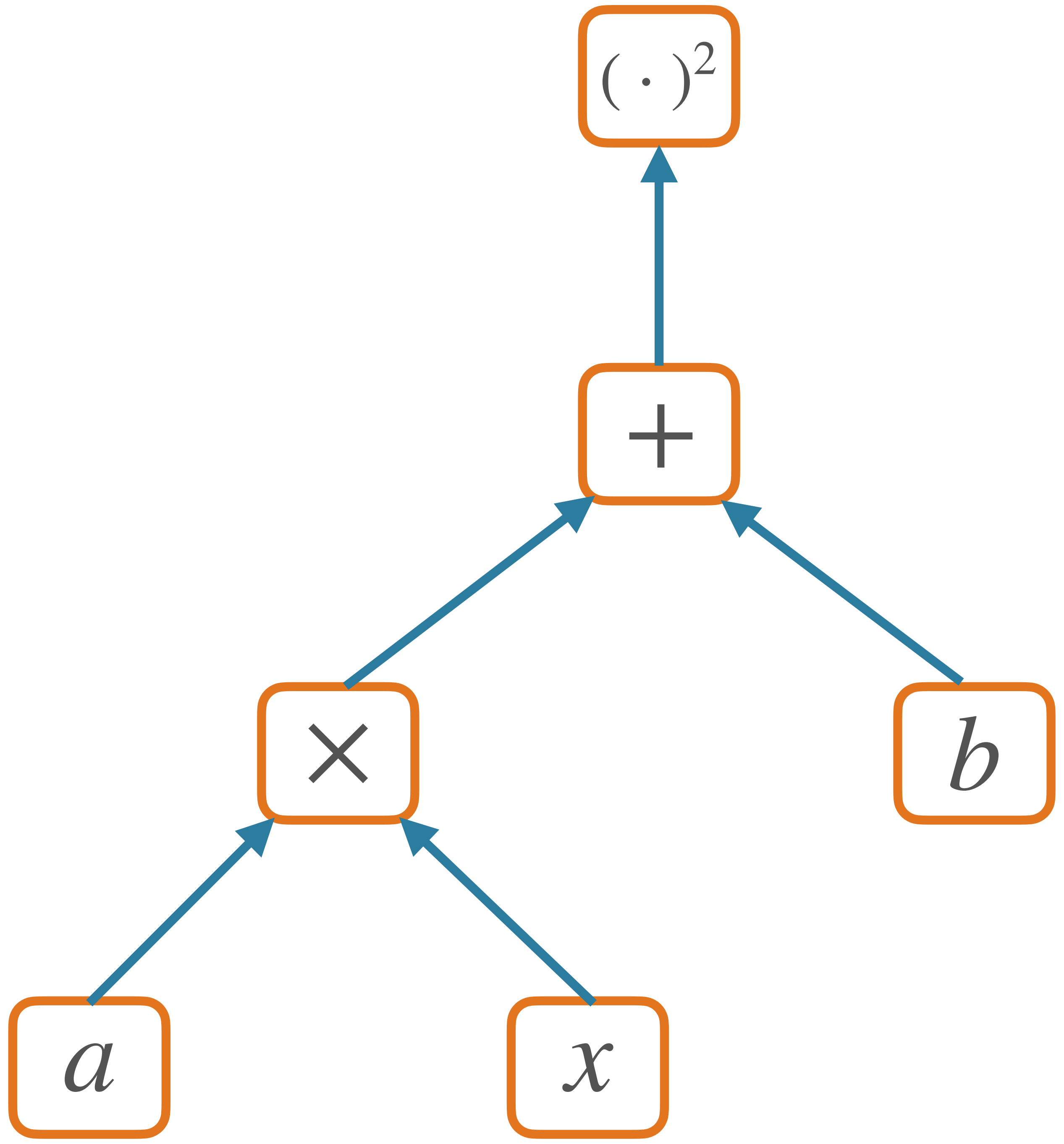


```python
def backward(self) -> None:
    """Run backward pass from a scalar tensor.

    All Tensors in the graph above this one will wind up having their
    gradients stored in `grad`.

    Raises:
        ValueError, if this is not a scalar.
    """
    if not np.isscalar(self.value):
        raise ValueError("Can only call backward() on scalar Tensors.")
    # dL / dL = 1
    self.grad = np.ones(self.value.shape)
    # NOTE: building a graph, then sorting, is not maximally efficient
    # but the graph can be used for visualization etc
    graph = self.get_graph_above()
    reverse_topological = reversed(list(nx.topological_sort(graph)))
    for tensor in reverse_topological:
        tensor._backward()
```

Local gradient + chain rule application

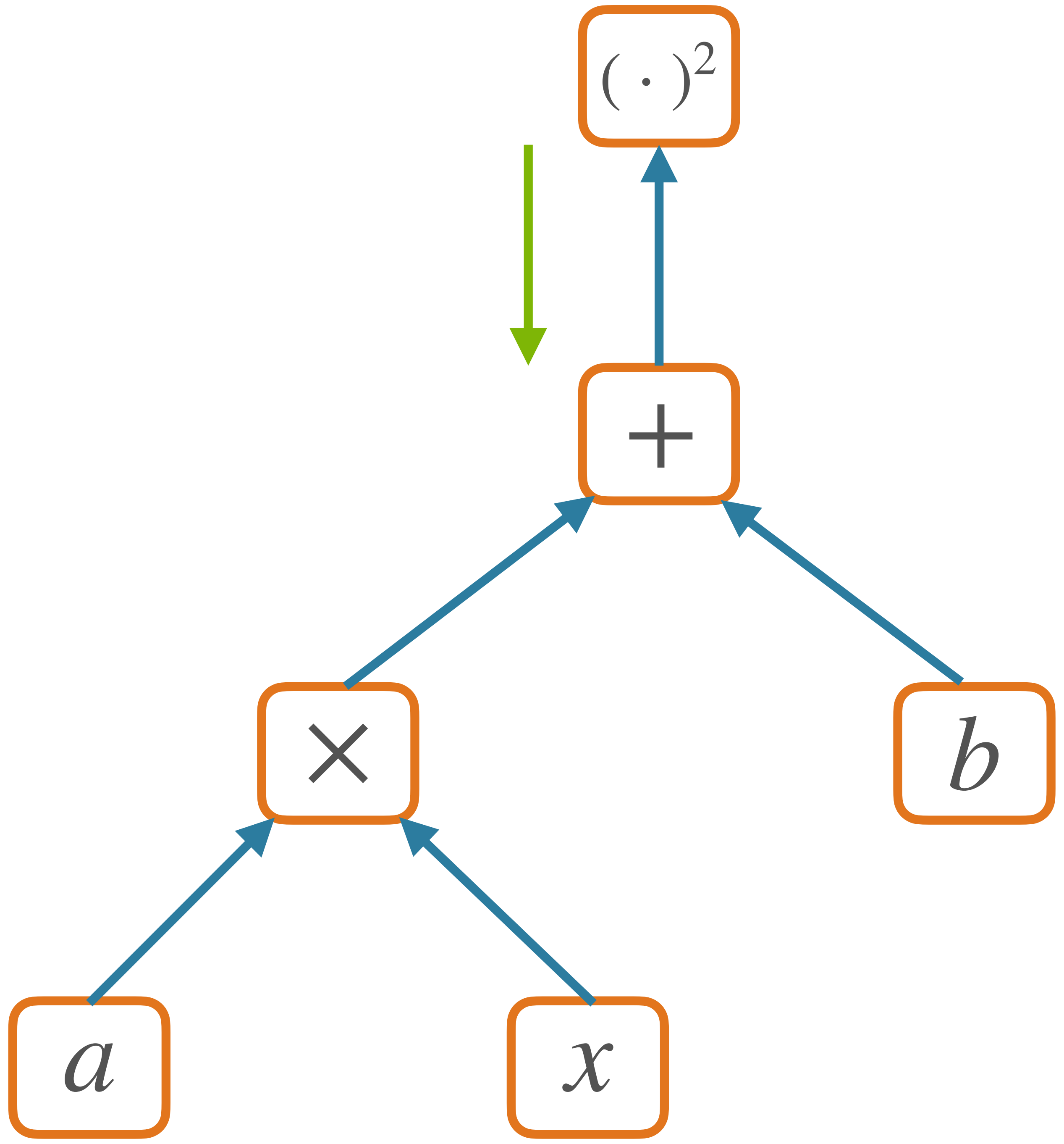
Why back-propagation?

- Efficient method for computing all gradients
  - Compute **once**
  - **Store and re-use** redundant computation
  - (The idea behind dynamic programming)
- Traverse each edge once, instead of once per dependency path



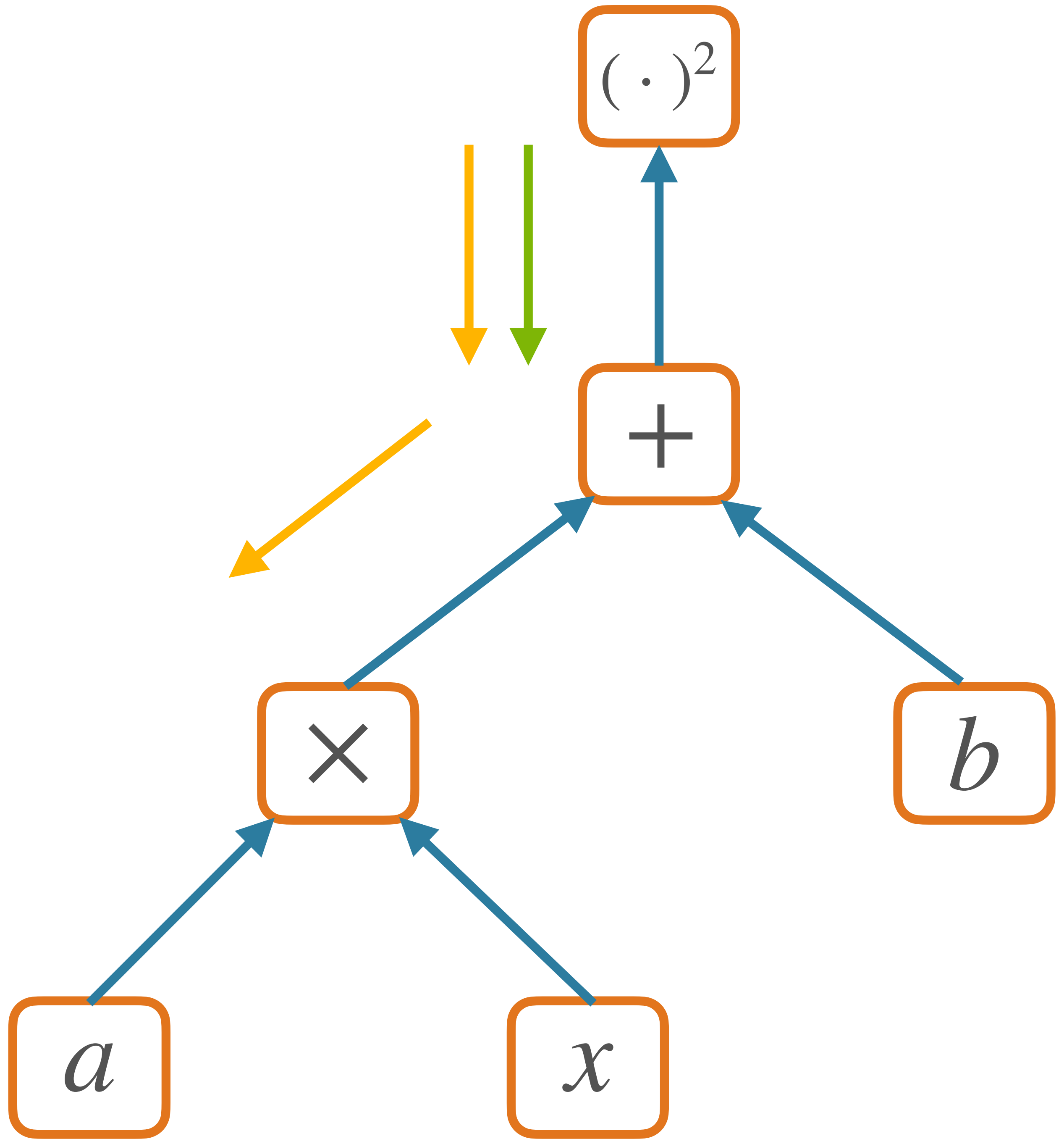
Why back-propagation?

- Efficient method for computing all gradients
    - Compute **once**
    - **Store and re-use** redundant computation
    - (The idea behind dynamic programming)
- Traverse each edge once, instead of once per dependency path



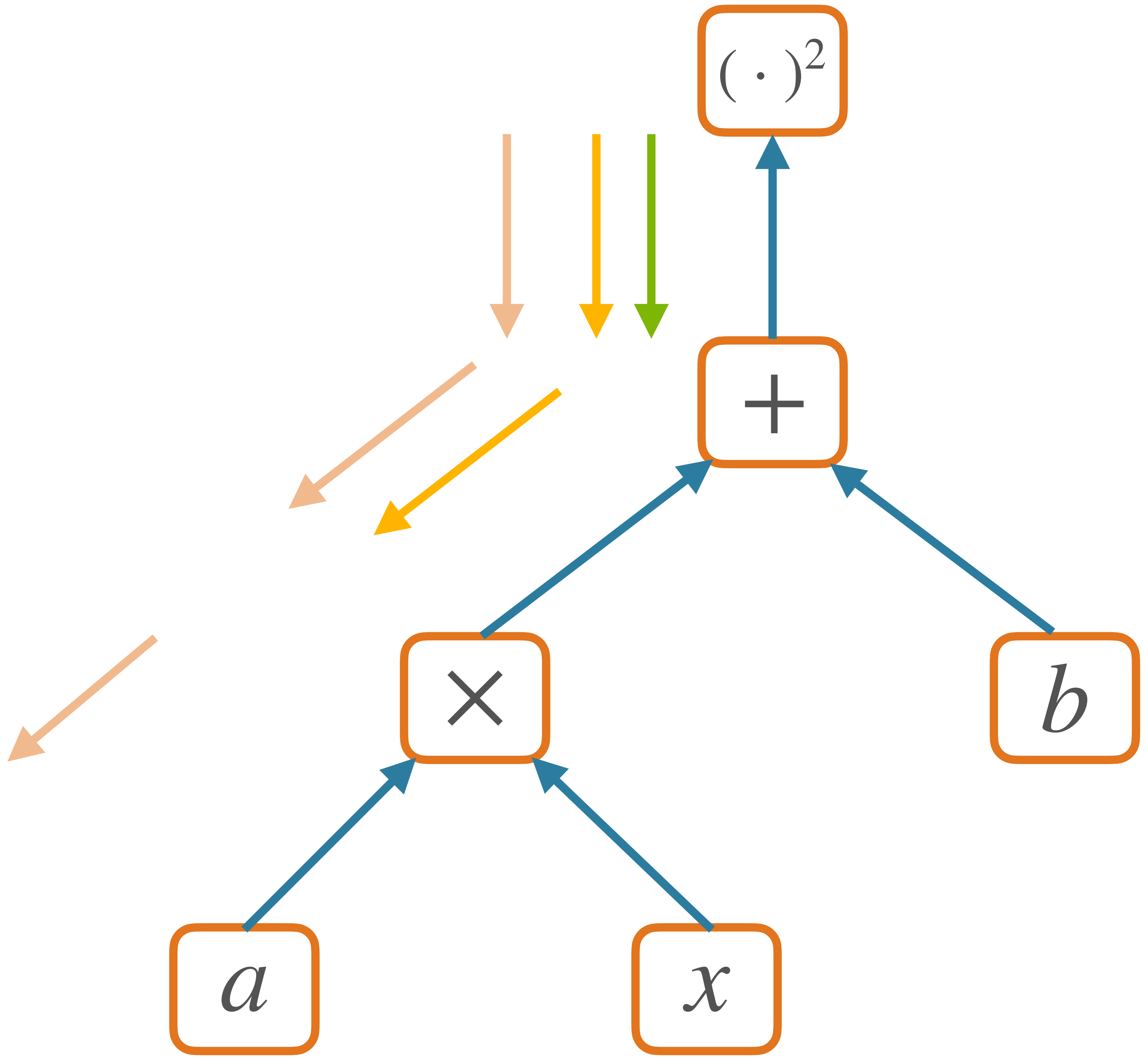
Why back-propagation?

- Efficient method for computing all gradients
  - Compute **once**
  - **Store and re-use** redundant computation
  - (The idea behind dynamic programming)
- Traverse each edge once, instead of once per dependency path



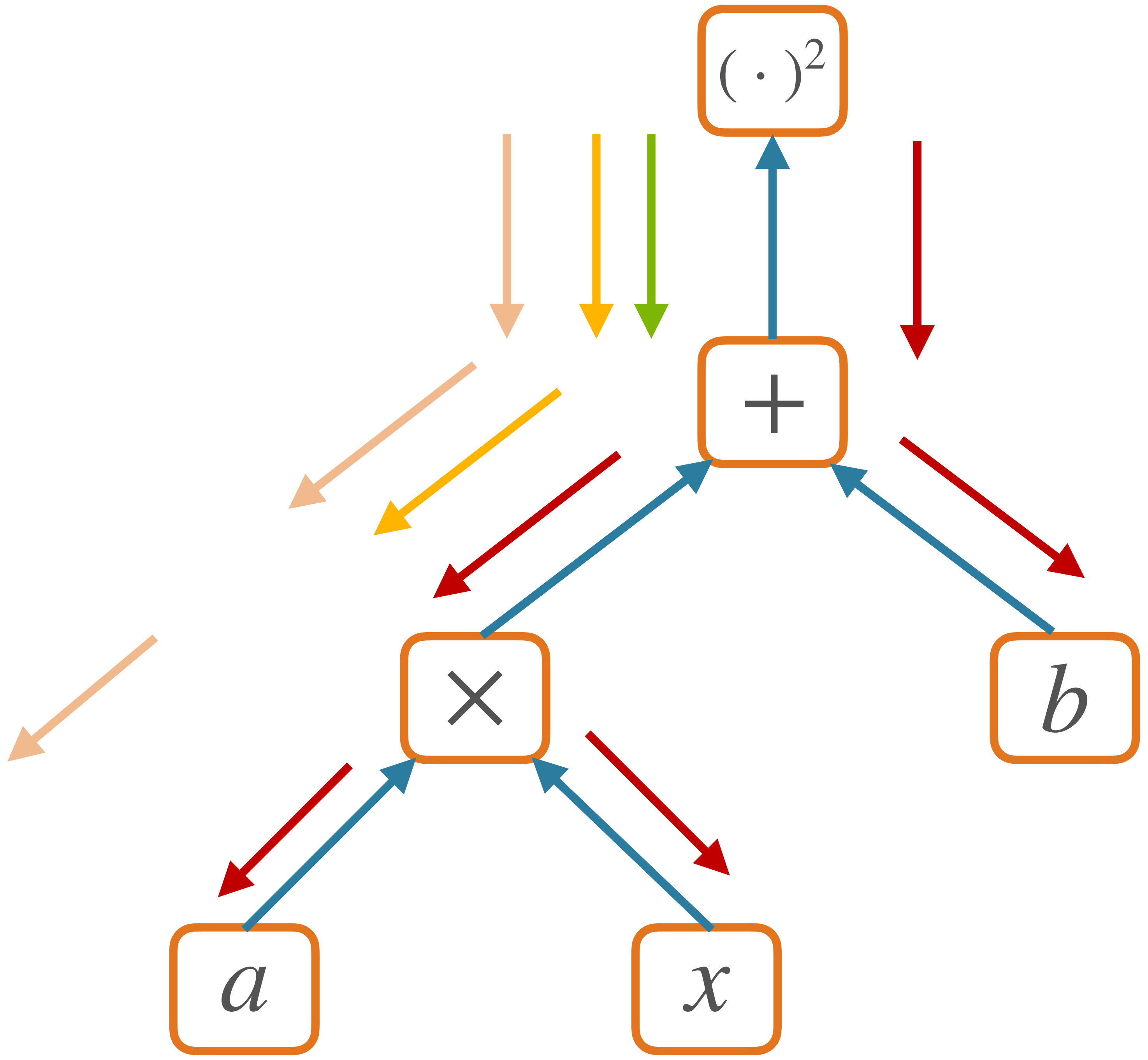
Why back-propagation?

- Efficient method for computing all gradients
  - Compute **once**
  - **Store and re-use** redundant computation
  - (The idea behind dynamic programming)
- Traverse each edge once, instead of once per dependency path



Why back-propagation?

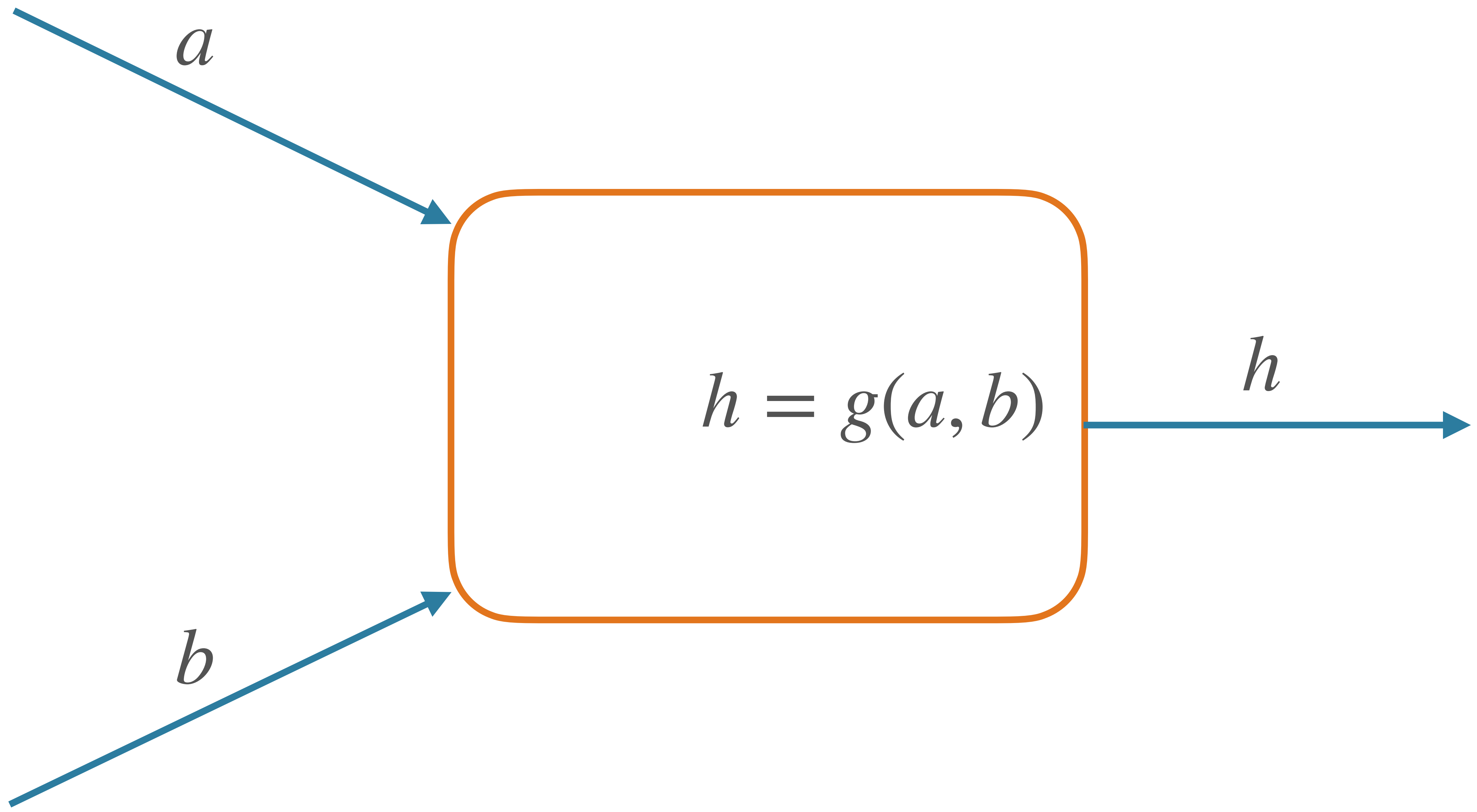
- Efficient method for computing all gradients
  - Compute **once**
  - **Store and re-use** redundant computation
  - (The idea behind dynamic programming)
- Traverse each edge once, instead of once per dependency path



Forward/backward API

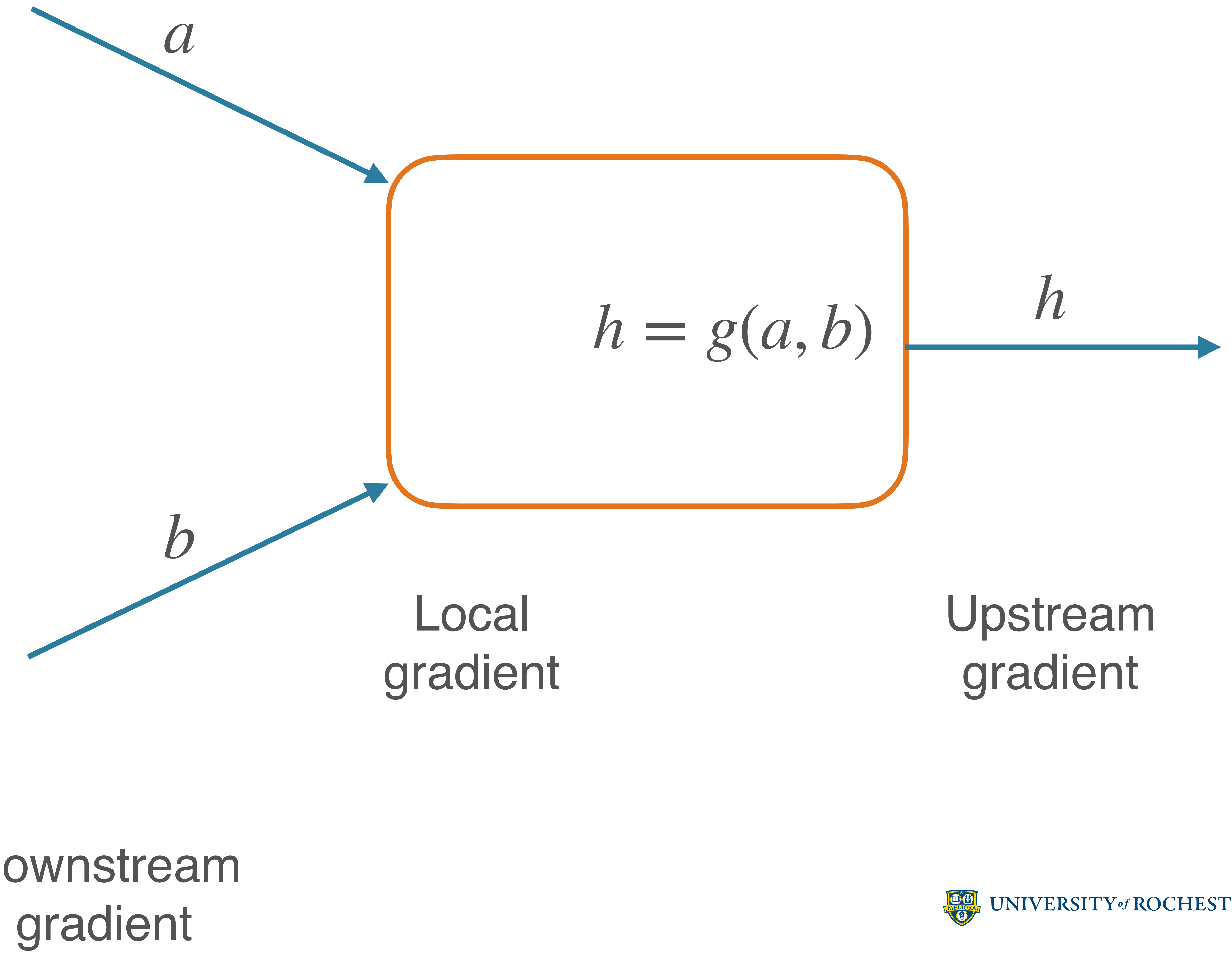
Nodes in Computational Graph

- Forward pass:
  - Compute **value** given **parents' values**
- Backward pass:
  - Compute **parents' gradients** given **children's**



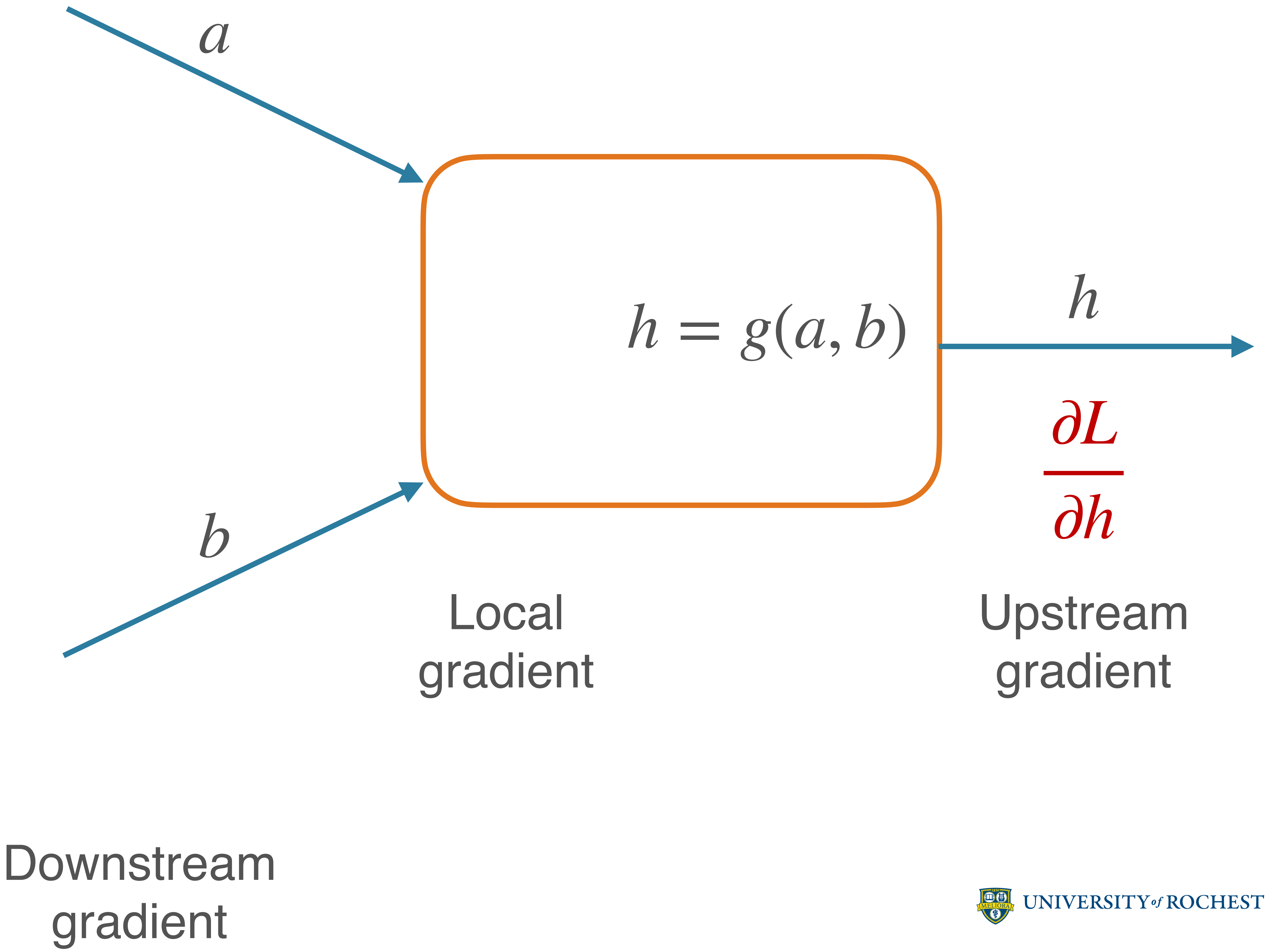
Nodes in Computational Graph

- Forward pass:
  - Compute **value** given **parents' values**
- Backward pass:
  - Compute **parents' gradients** given **children's**



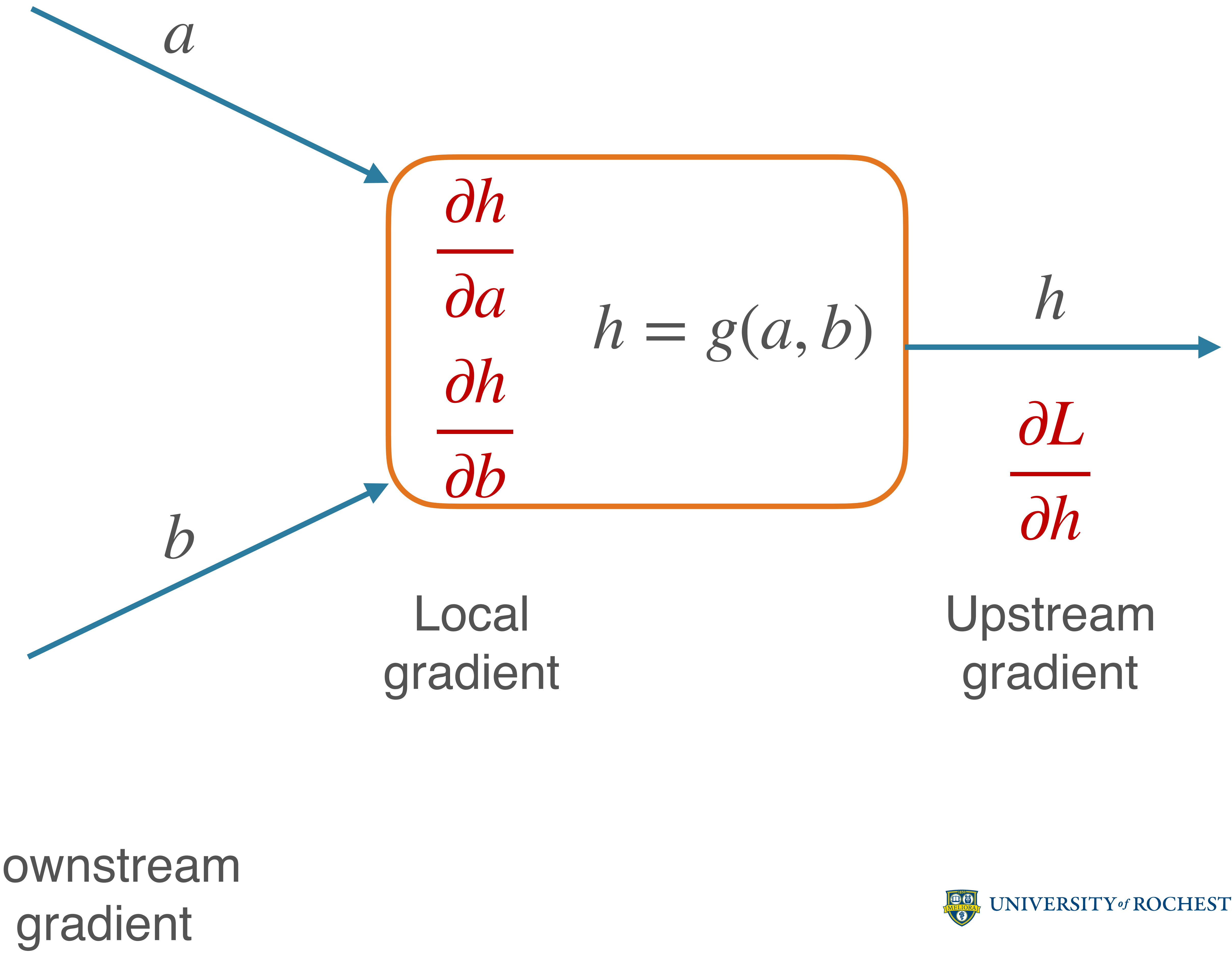
Nodes in Computational Graph

- Forward pass:
  - Compute **value** given **parents' values**
- Backward pass:
  - Compute **parents' gradients** given **children's**



Nodes in Computational Graph

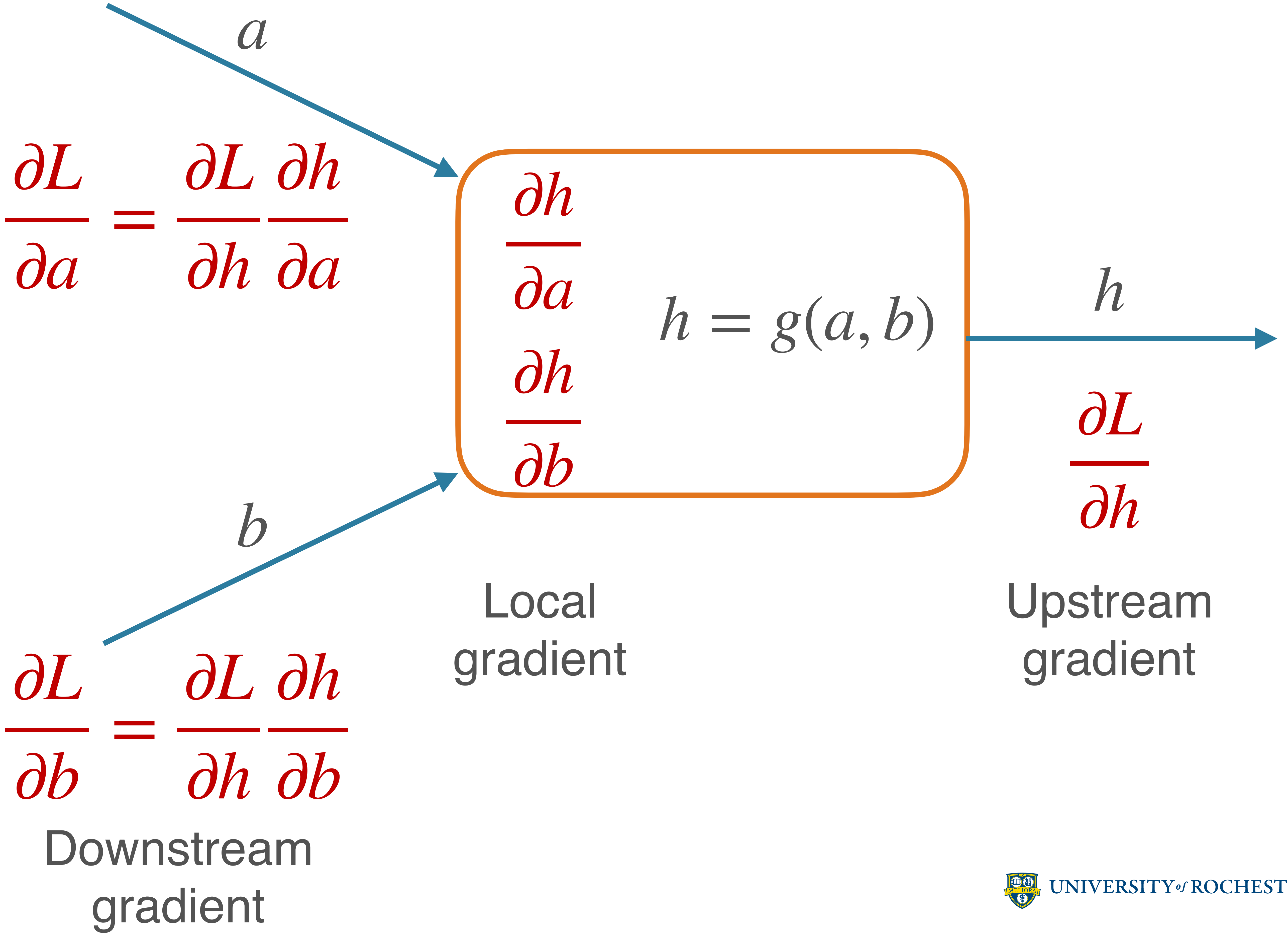
- Forward pass:
  - Compute **value** given **parents' values**
- Backward pass:
  - Compute **parents' gradients** given **children's**



a
b
$\frac{\partial h}{\partial a}$
$\frac{\partial h}{\partial b}$
$h = g(a, b)$
h
$\frac{\partial L}{\partial h}$
Local gradient
Upstream gradient
Downstream gradient

Nodes in Computational Graph

- Forward pass:
  - Compute **value** given **parents' values**
- Backward pass:
  - Compute **parents' gradients** given **children's**



a

b

$$\frac{\partial L}{\partial a} = \frac{\partial L}{\partial h}\frac{\partial h}{\partial a}$$

$$\frac{\partial L}{\partial b} = \frac{\partial L}{\partial h}\frac{\partial h}{\partial b}$$

Downstream gradient

$$\frac{\partial h}{\partial a} \qquad \frac{\partial h}{\partial b}$$

$$h = g(a, b)$$

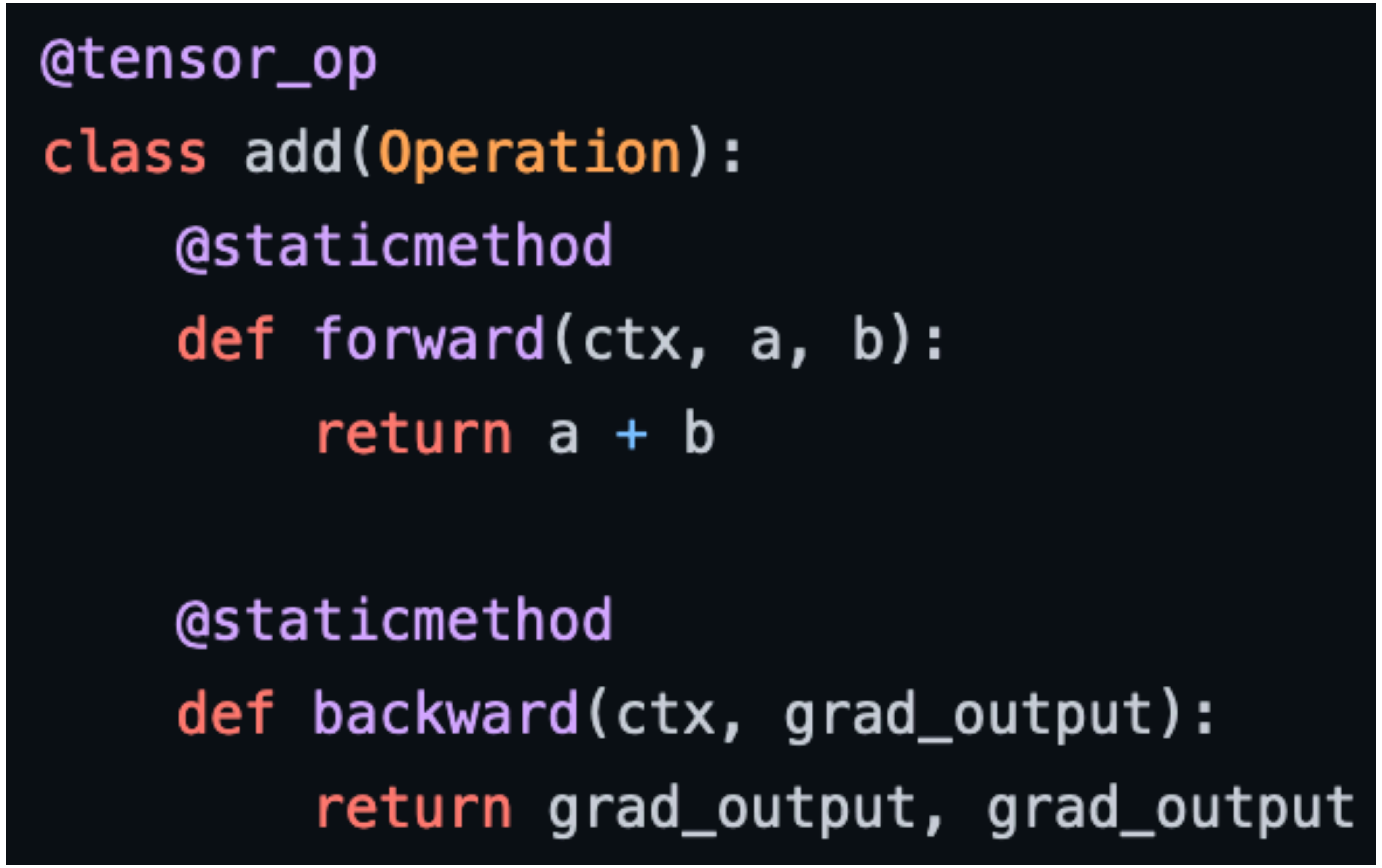
Local gradient

h

$$\frac{\partial L}{\partial h}$$

Upstream gradient

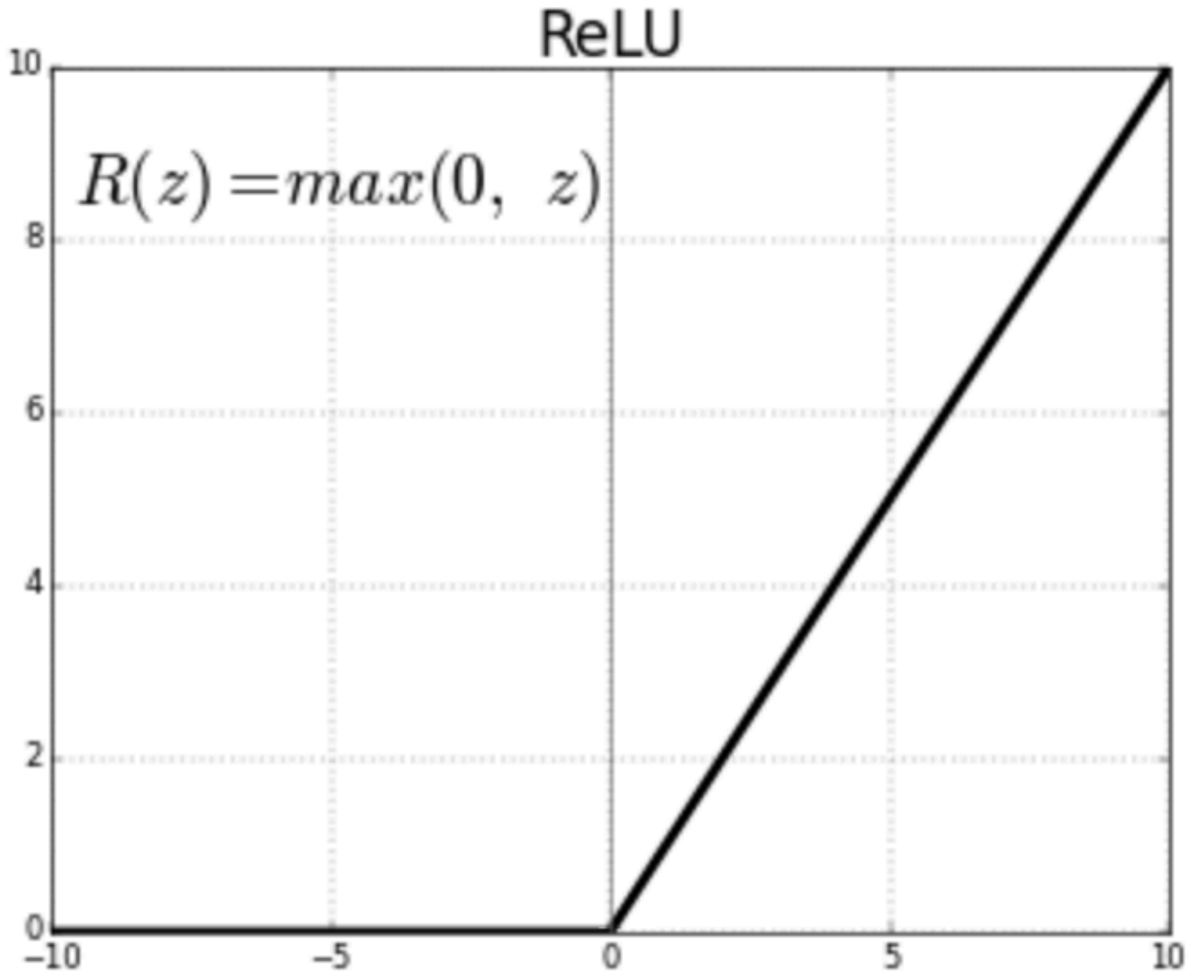
Example: Addition



```
@tensor_op
class add(Operation):
    @staticmethod
    def forward(ctx, a, b):
        return a + b

    @staticmethod
    def backward(ctx, grad_output):
        return grad_output, grad_output
```

$$\frac{\partial L}{\partial a} \qquad \frac{\partial L}{\partial b}$$

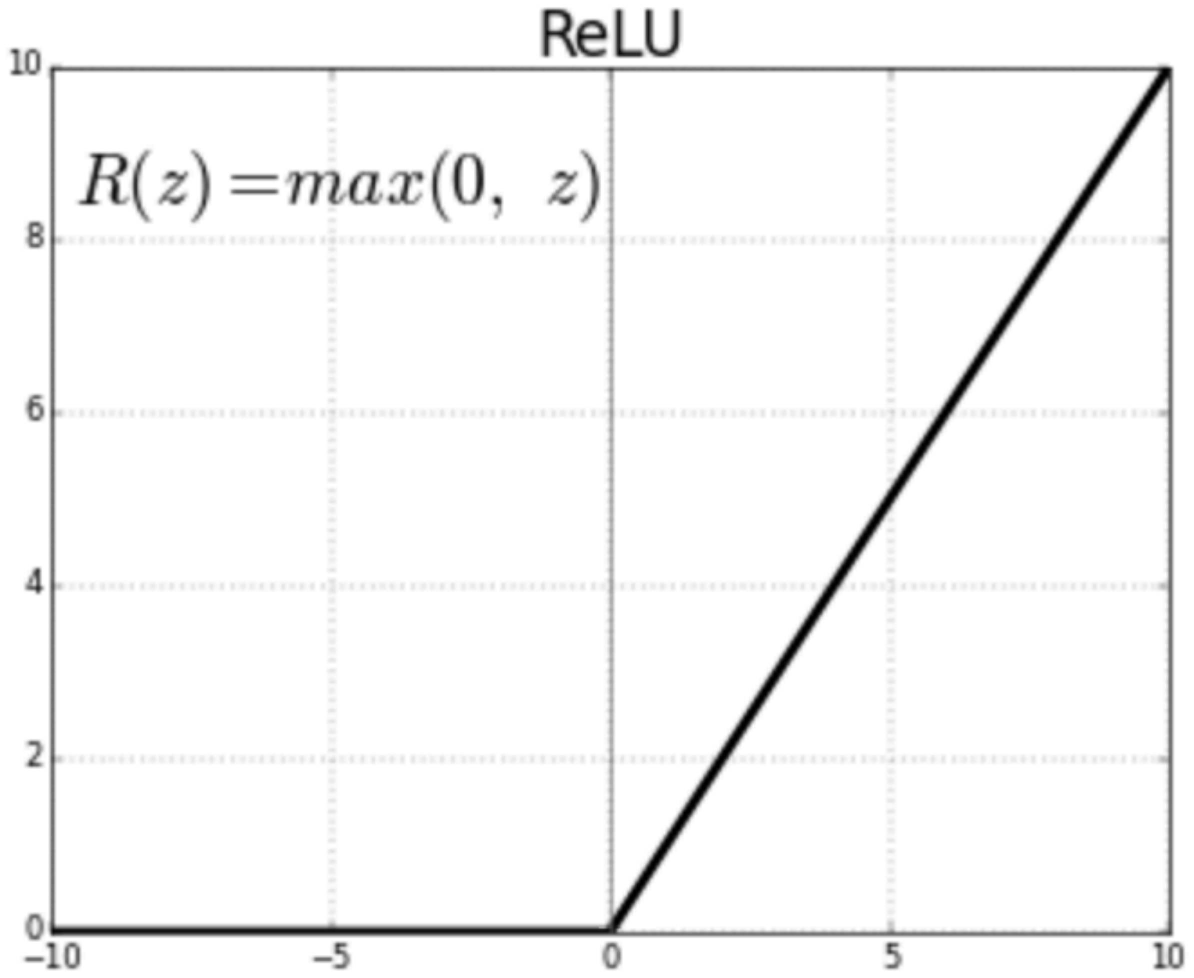
Example: ReLU



$$\text{ReLU}(x) = \max(0, x)$$

```
class relu(Operation):
 def forward(ctx, x):
  return np.maximum(0, x)

 def backward(ctx, grad_output):
```

Example: ReLU

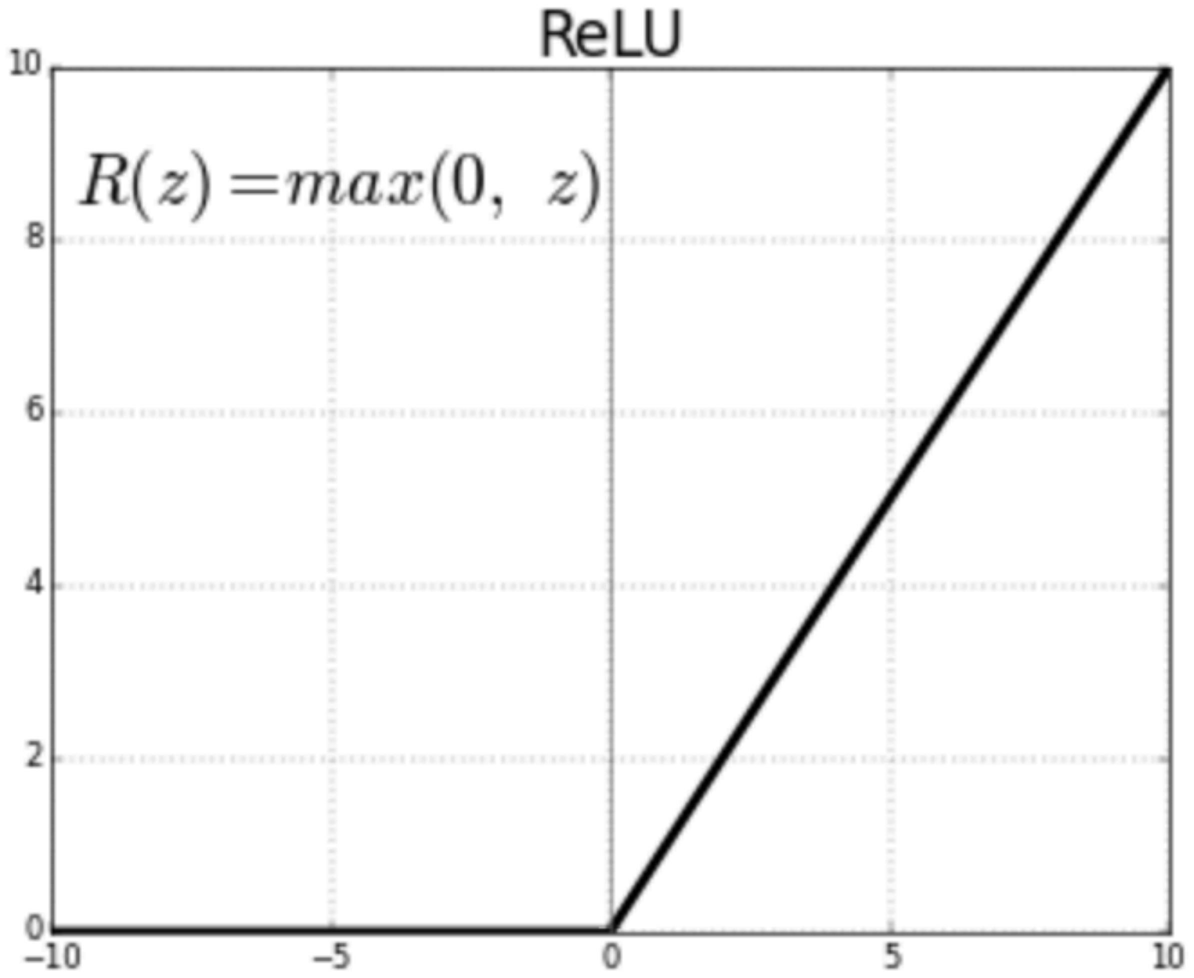


$$\text{ReLU}(x) = \max(0, x)$$

$$\frac{\partial R}{\partial x} = \begin{cases} 1 & x > 0 \\ 0 & \text{otherwise} \end{cases}$$

```
class relu(Operation):
 def forward(ctx, x):
  return np.maximum(0, x)

 def backward(ctx, grad_output):
```

Example: ReLU



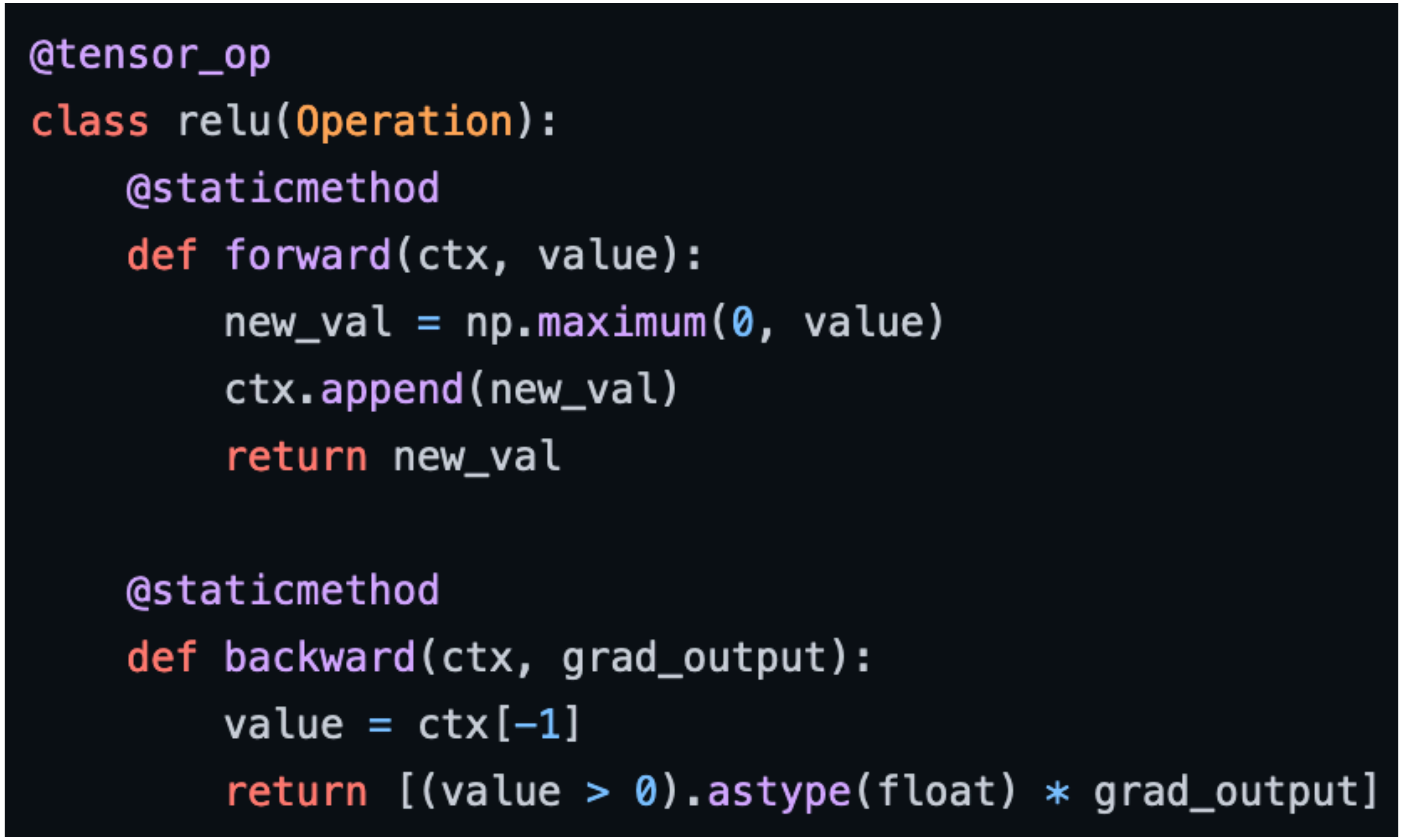
$$\mathrm{ReLU}(x) = \max(0, x)$$

$$\frac{\partial R}{\partial x} = \begin{cases} 1 & x > 0 \\ 0 & \text{otherwise} \end{cases}$$

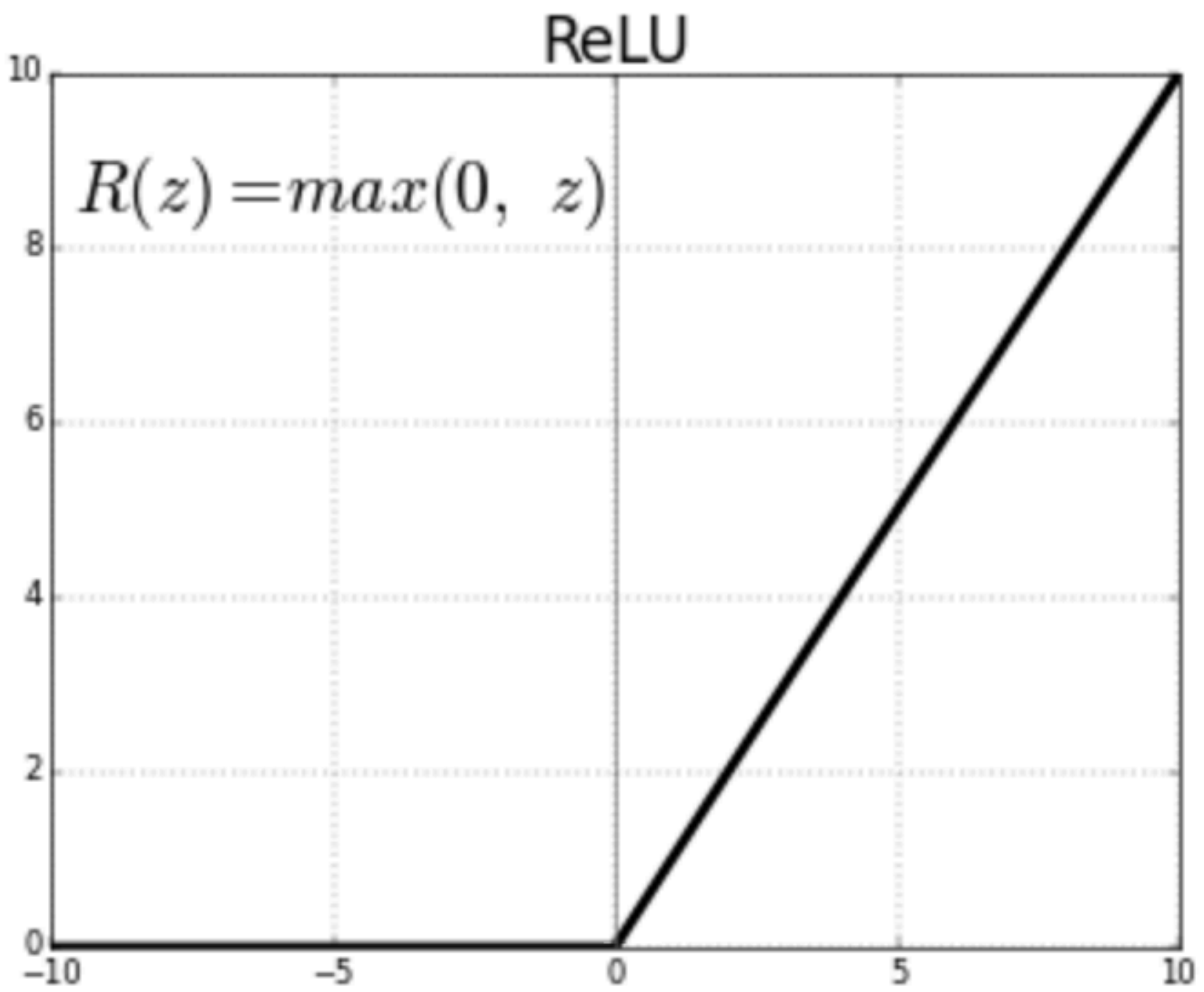
```
class relu(Operation):
  def forward(ctx, x):
    return np.maximum(0, x)

  def backward(ctx, grad_output):
```

🤔 where's x?

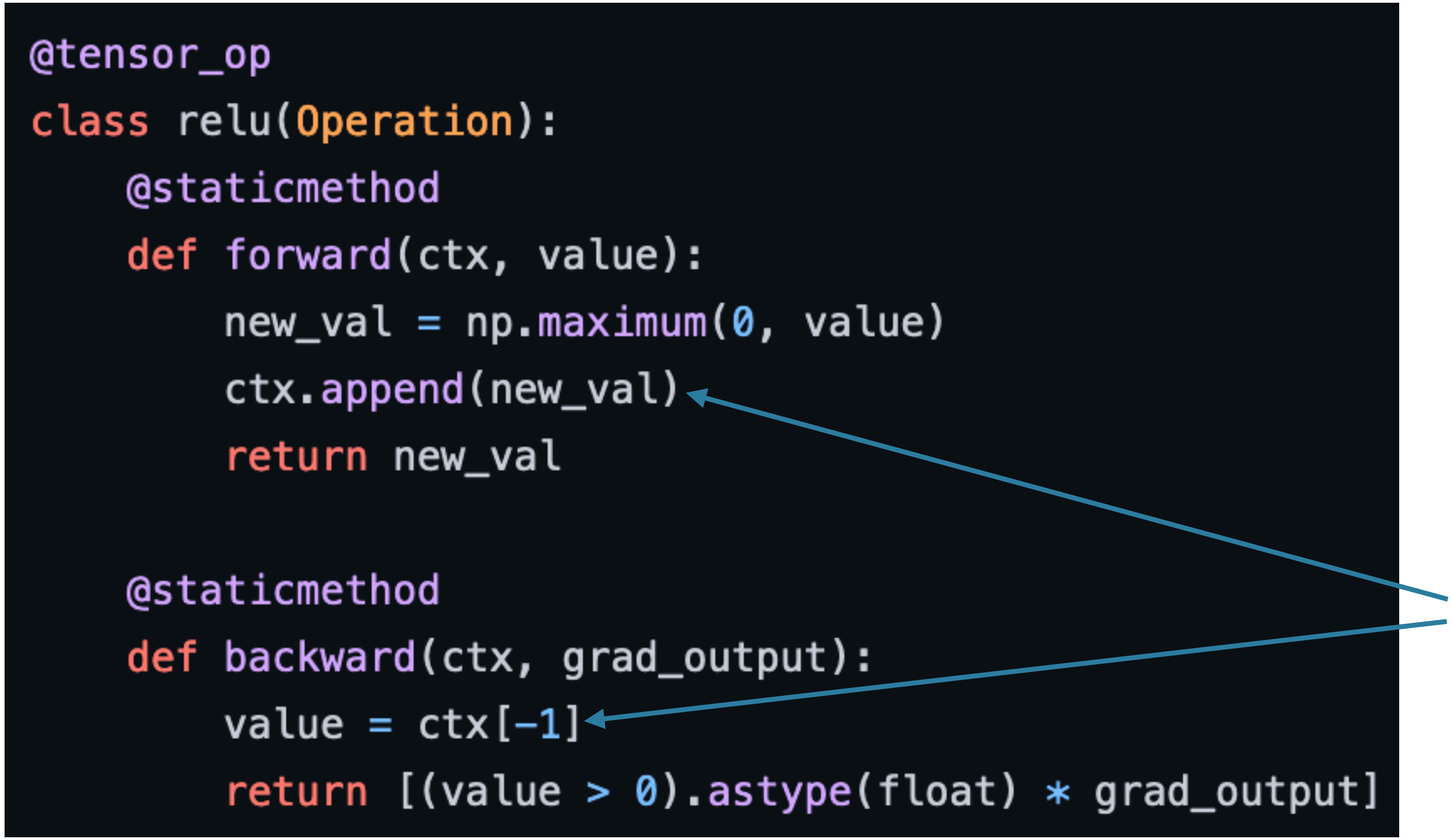
Example: ReLU



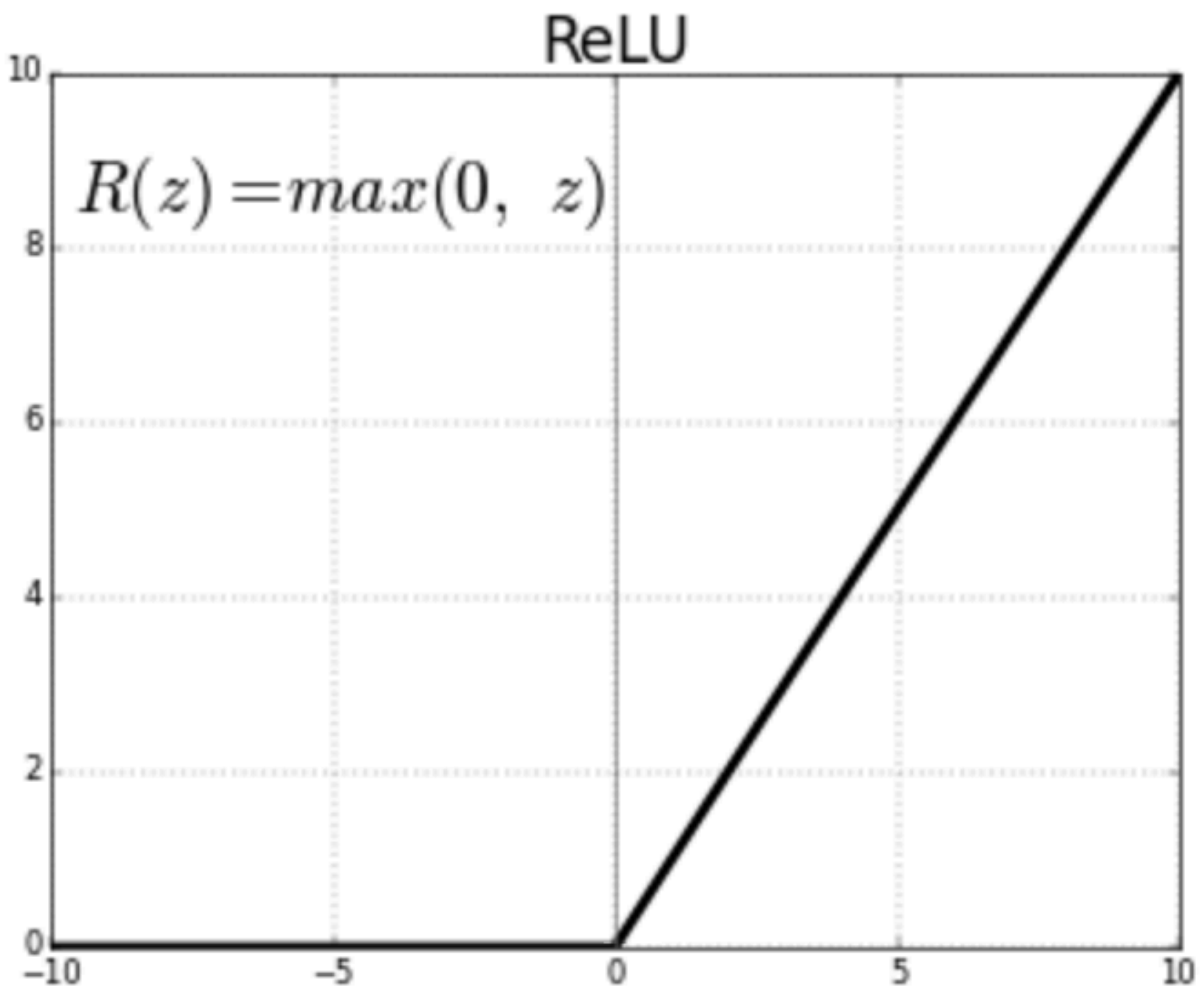
```
@tensor_op
class relu(Operation):
    @staticmethod
    def forward(ctx, value):
        new_val = np.maximum(0, value)
        ctx.append(new_val)
        return new_val

    @staticmethod
    def backward(ctx, grad_output):
        value = ctx[-1]
        return [(value > 0).astype(float) * grad_output]
```



Example: ReLU

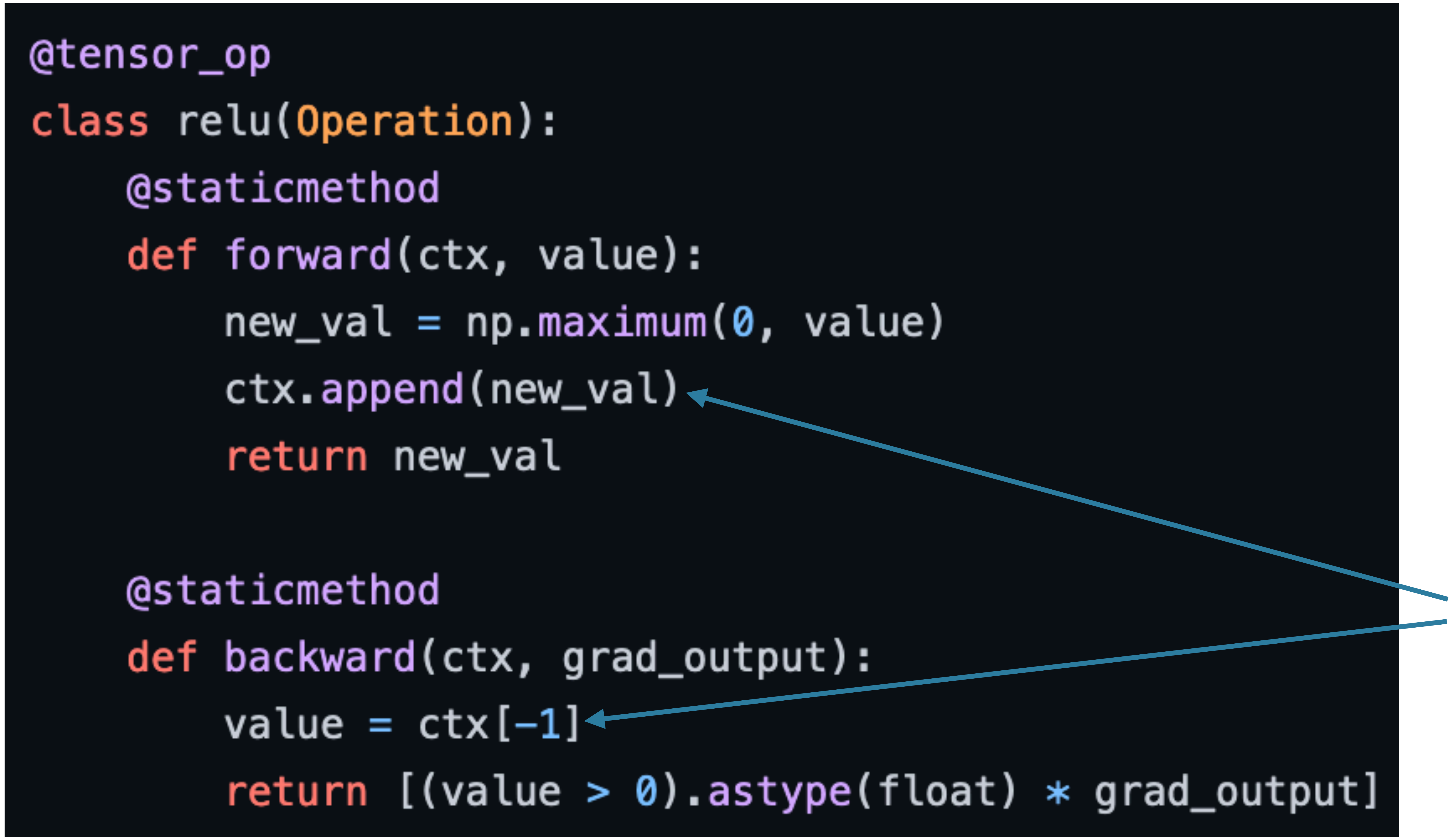


```
@tensor_op
class relu(Operation):
    @staticmethod
    def forward(ctx, value):
        new_val = np.maximum(0, value)
        ctx.append(new_val)
        return new_val

    @staticmethod
    def backward(ctx, grad_output):
        value = ctx[-1]
        return [(value > 0).astype(float) * grad_output]
```

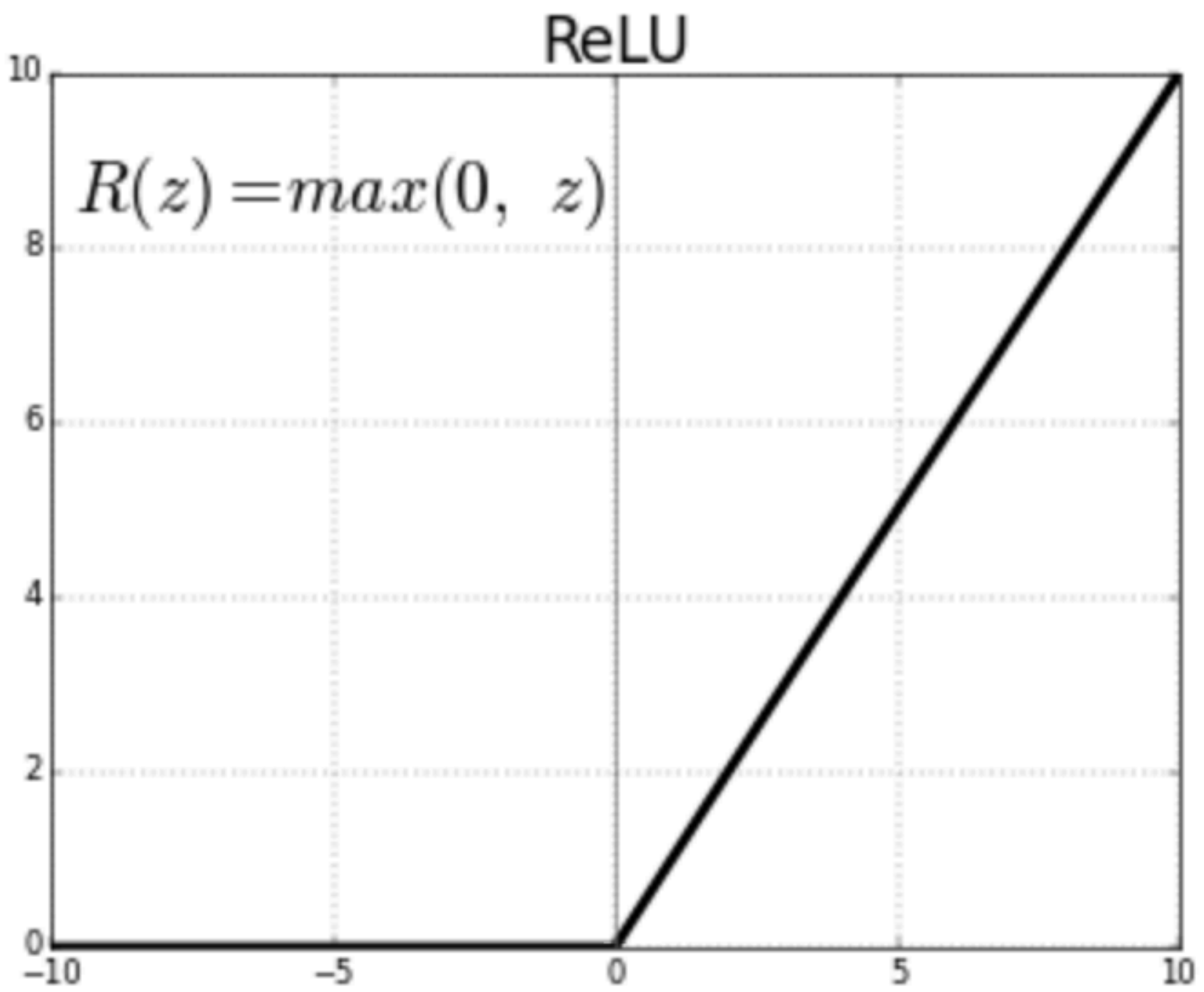


Save and retrieve the input value!

Example: ReLU



```
@tensor_op
class relu(Operation):
    @staticmethod
    def forward(ctx, value):
        new_val = np.maximum(0, value)
        ctx.append(new_val)
        return new_val

    @staticmethod
    def backward(ctx, grad_output):
        value = ctx[-1]
        return [(value > 0).astype(float) * grad_output]
```



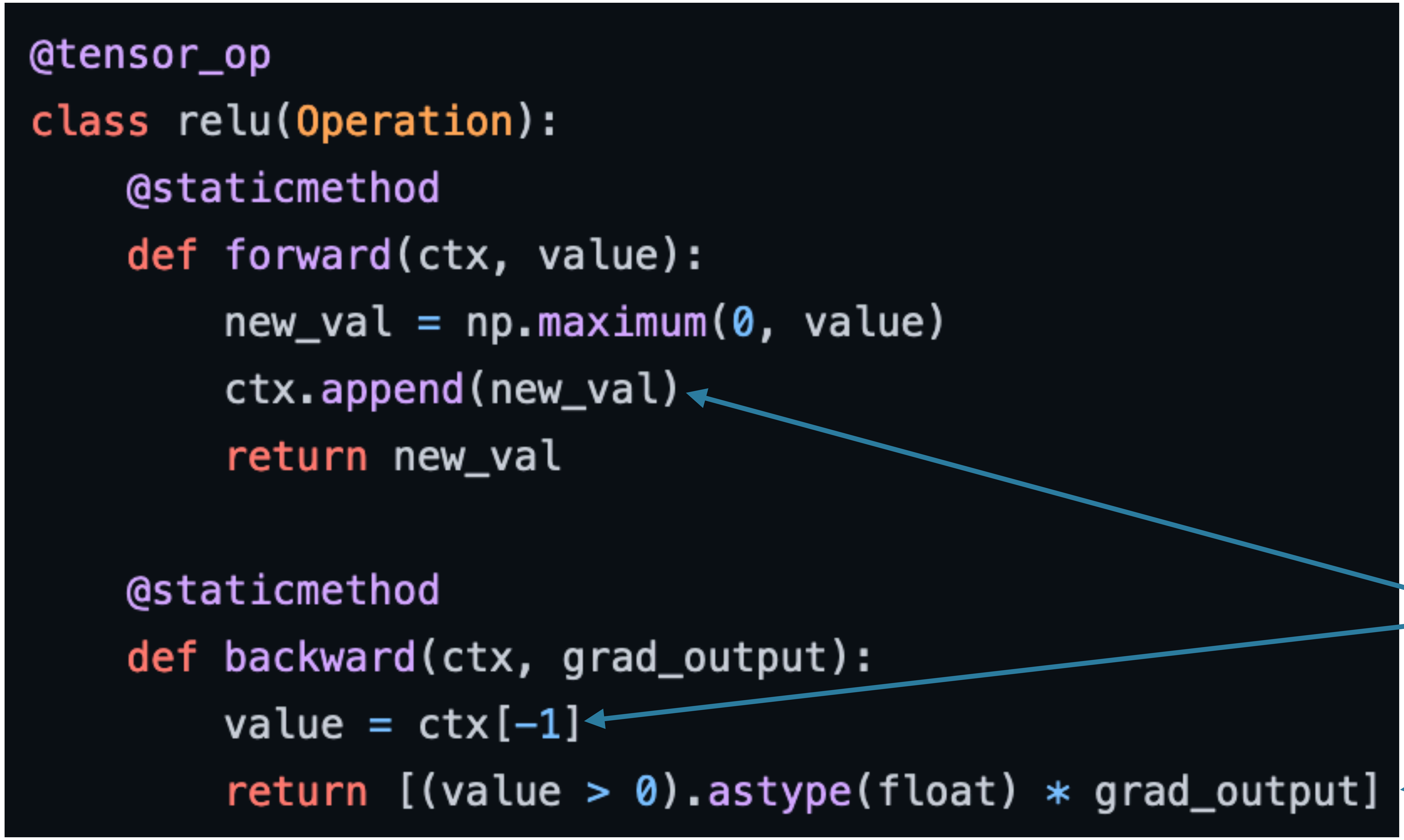
Save and retrieve the input value!

local gradient

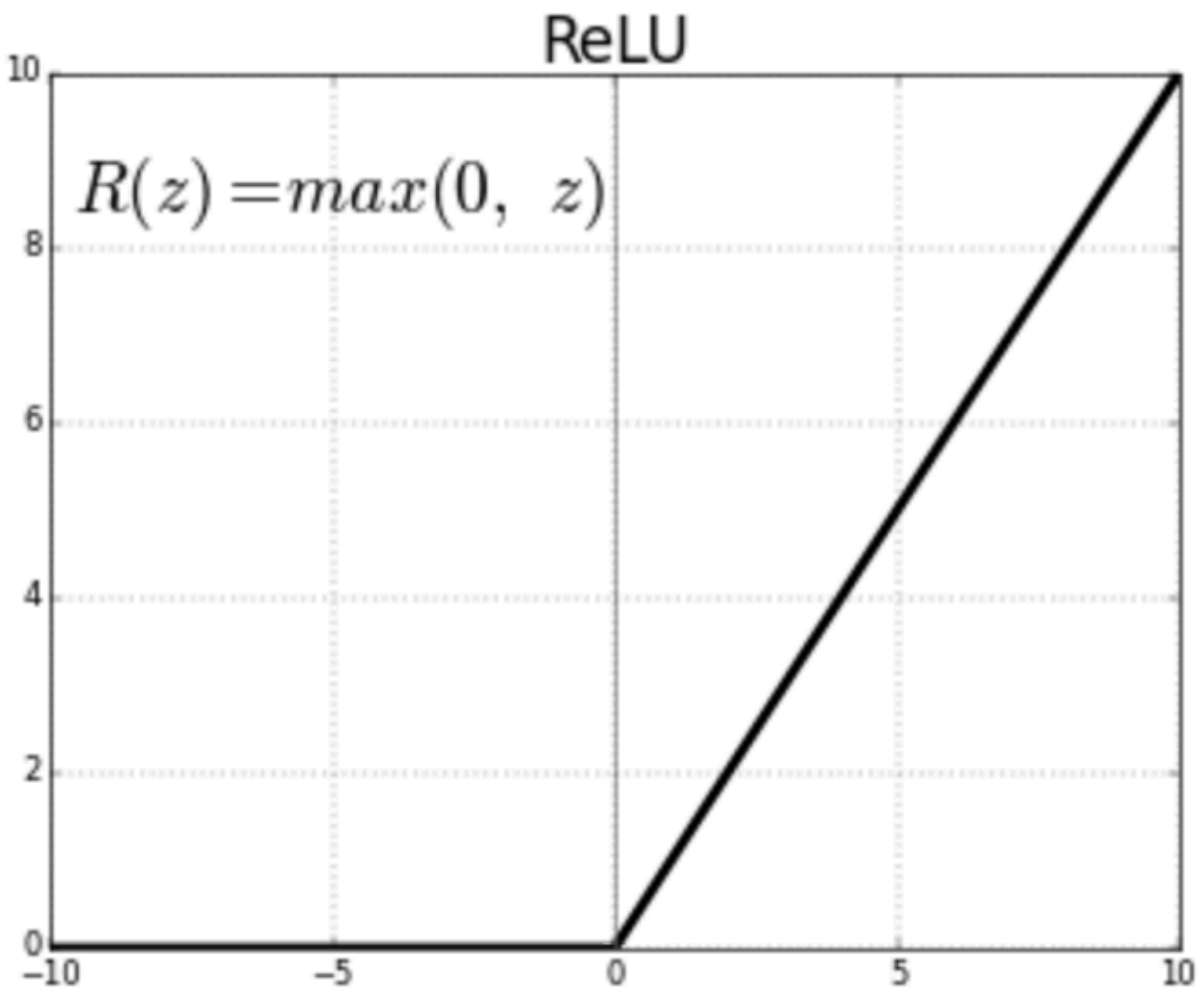
times

upstream gradient

Example: ReLU



```
@tensor_op
class relu(Operation):
    @staticmethod
    def forward(ctx, value):
        new_val = np.maximum(0, value)
        ctx.append(new_val)
        return new_val

    @staticmethod
    def backward(ctx, grad_output):
        value = ctx[-1]
        return [(value > 0).astype(float) * grad_output]
```



Save and retrieve the input value!

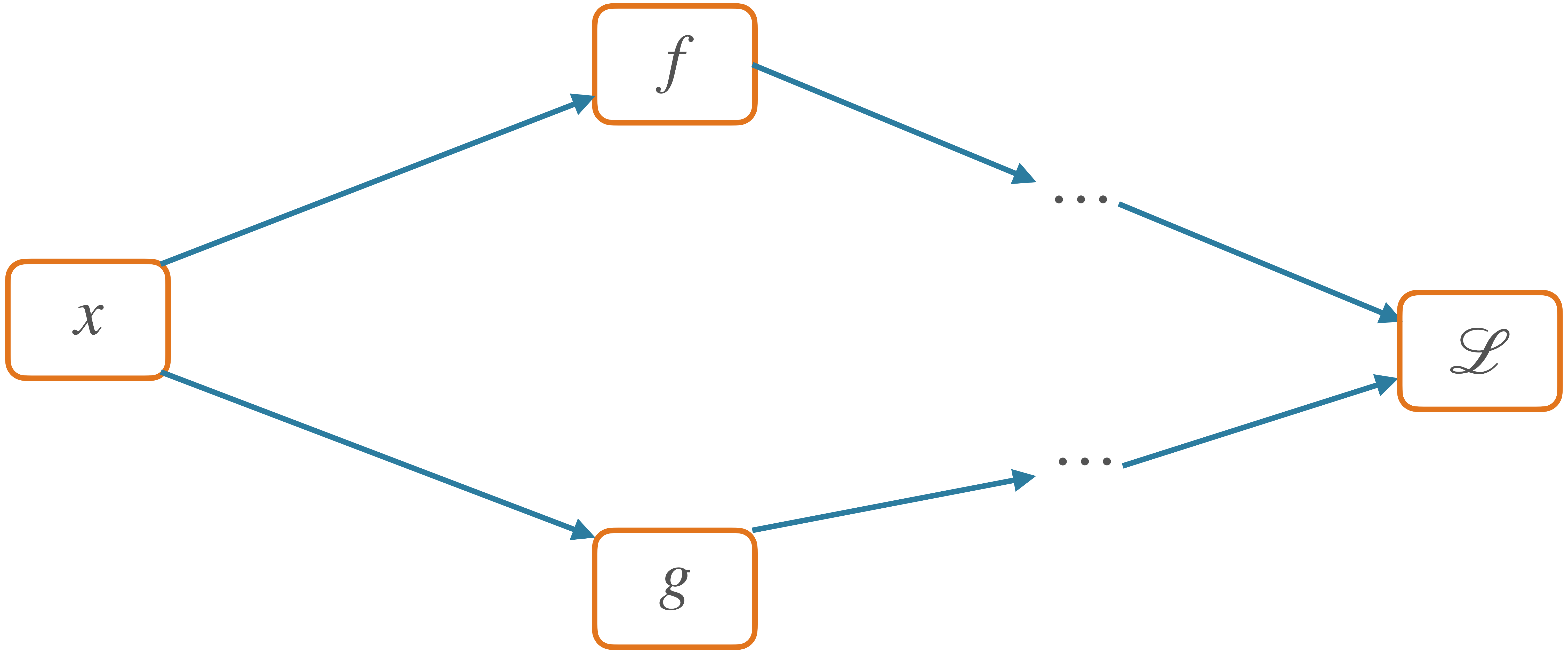
list, one downstream gradient per input (in this case, one)

local gradient

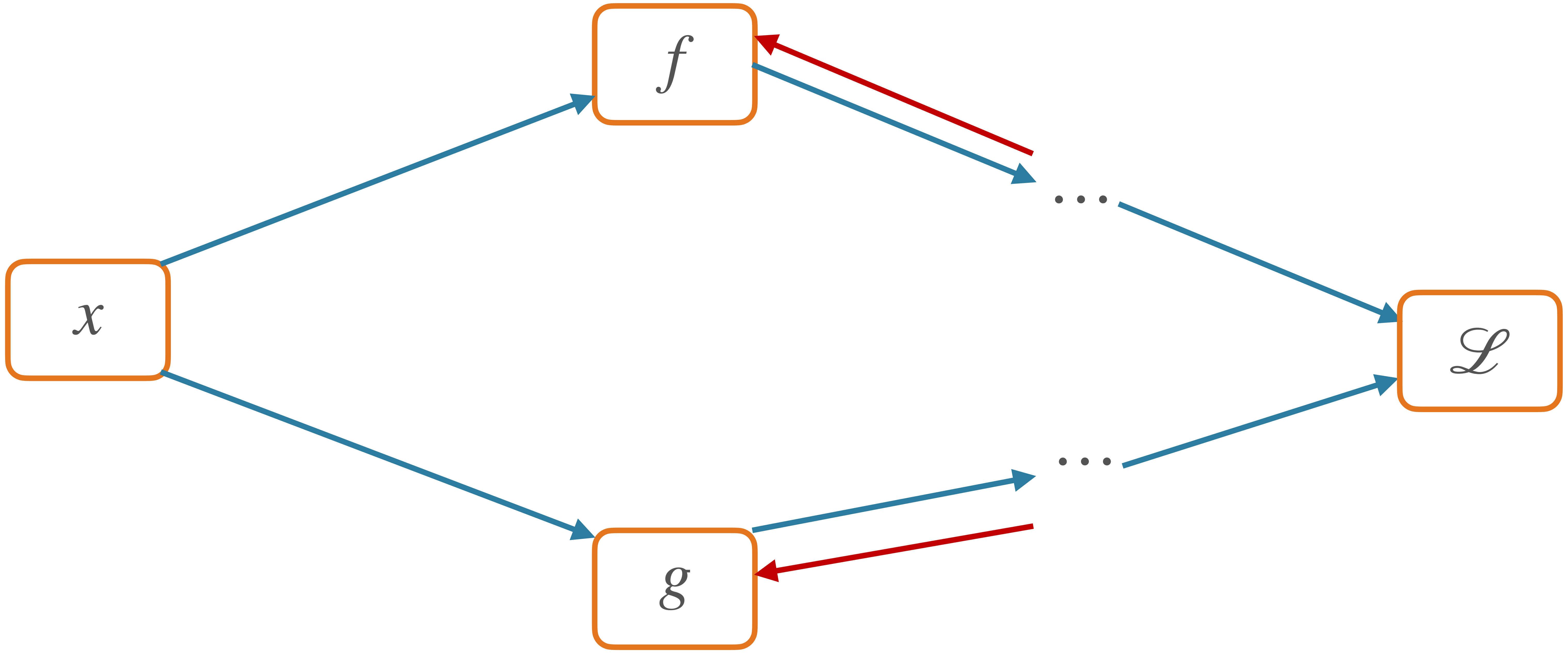
times

upstream gradient

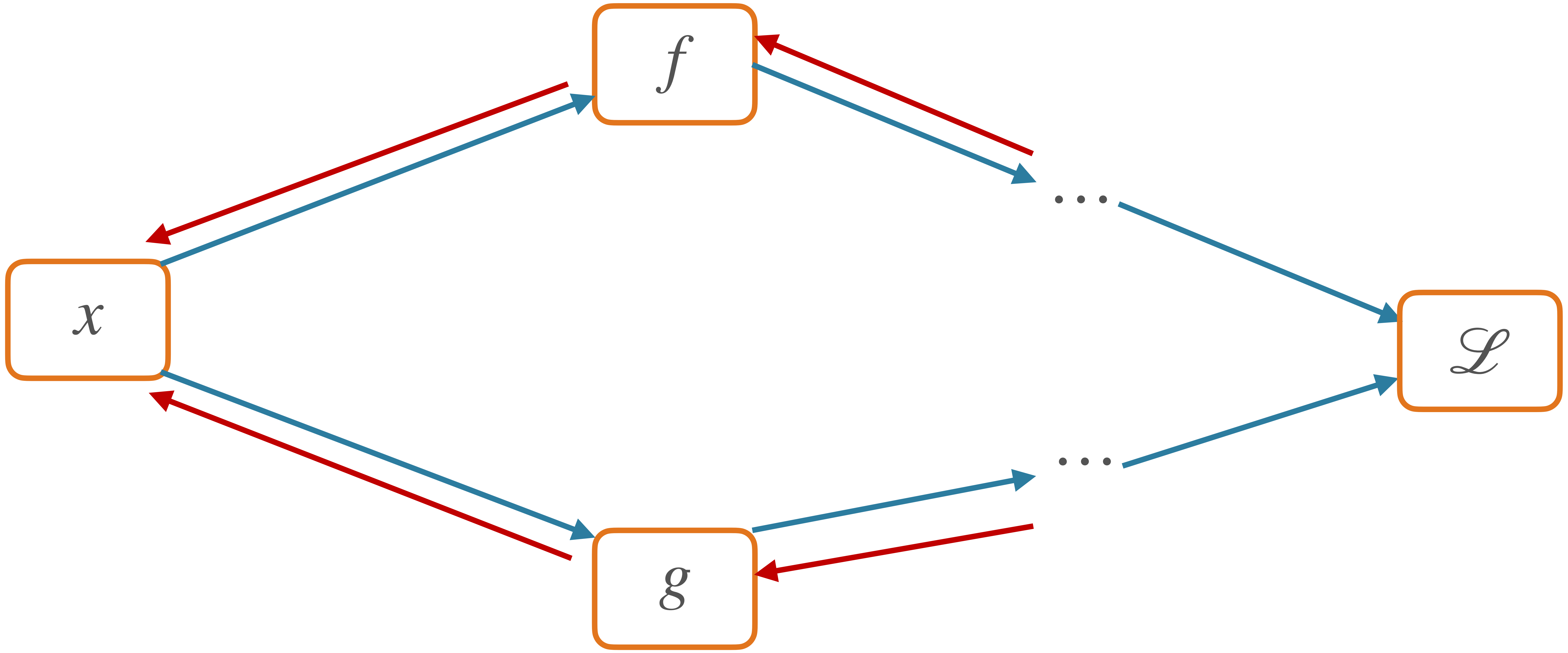
Adding Gradients with Multiple Outputs



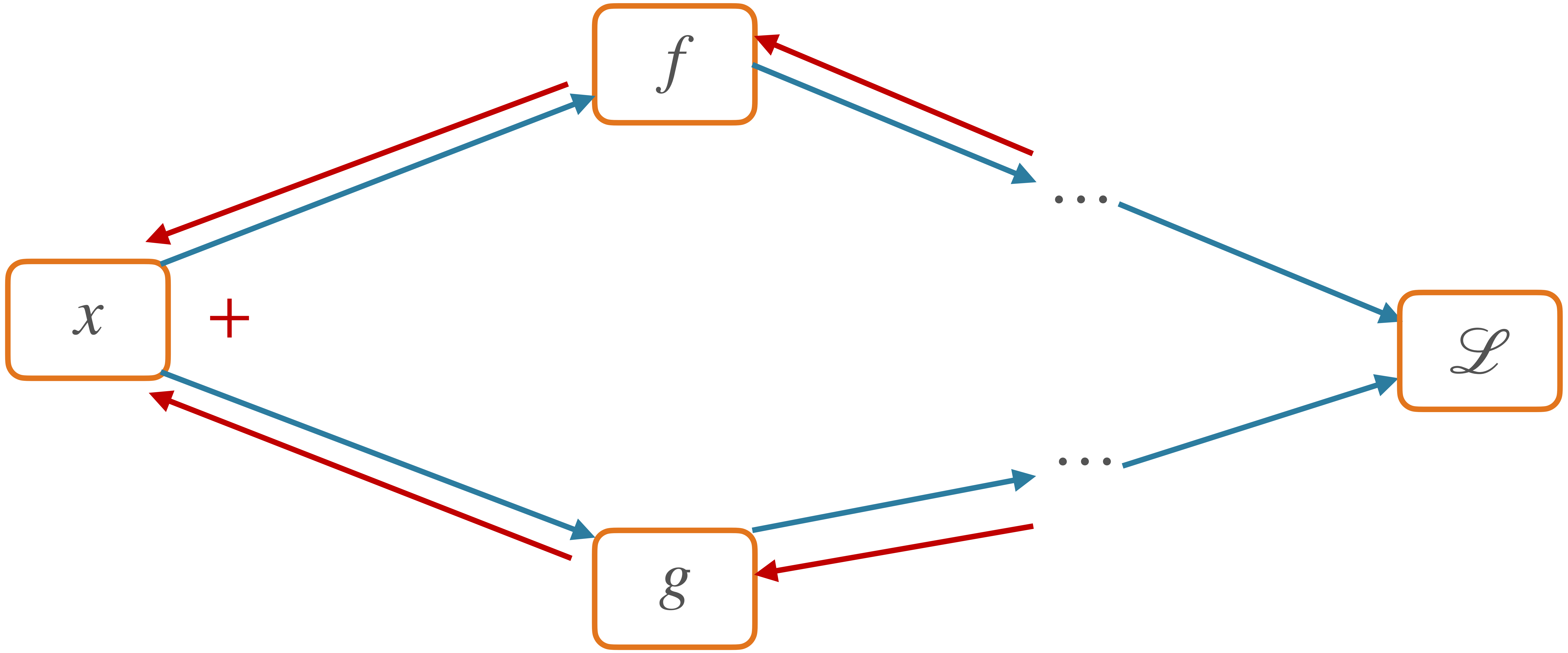
Adding Gradients with Multiple Outputs



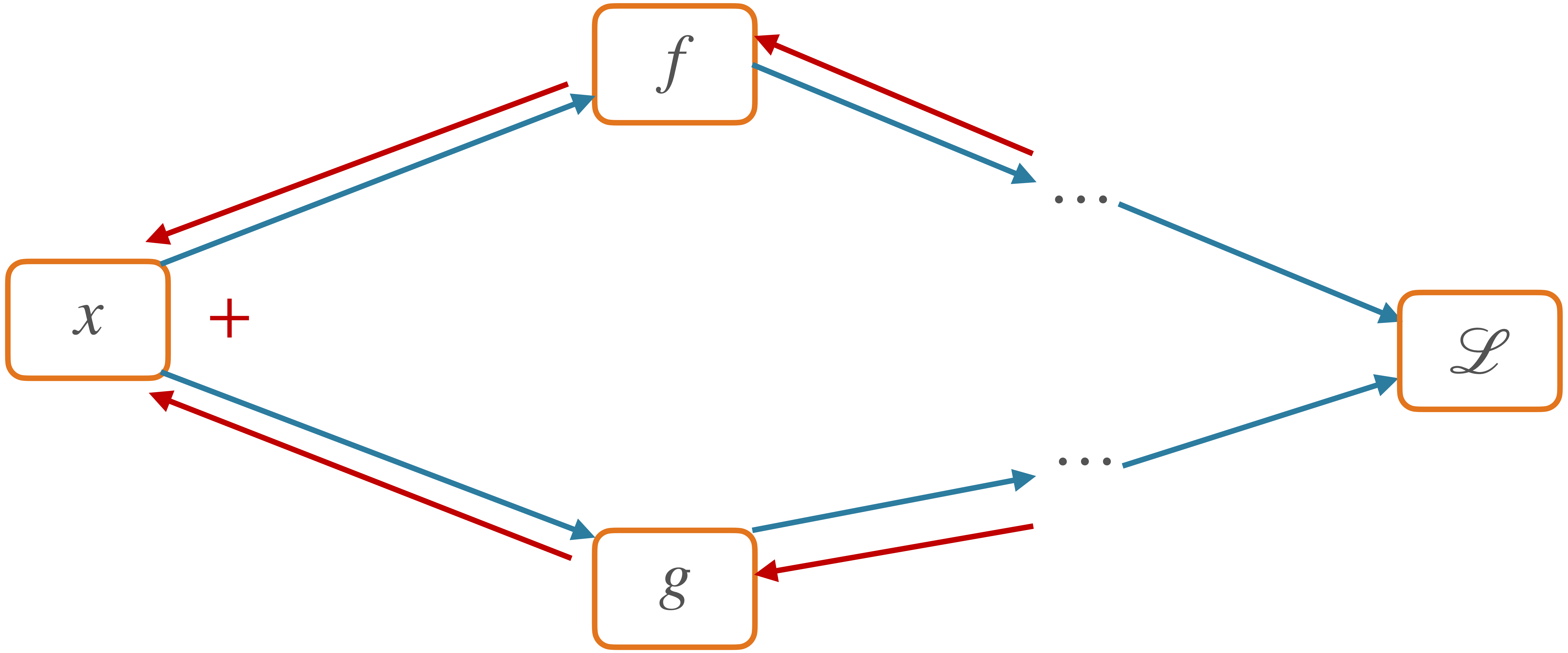
Adding Gradients with Multiple Outputs



Adding Gradients with Multiple Outputs



Adding Gradients with Multiple Outputs



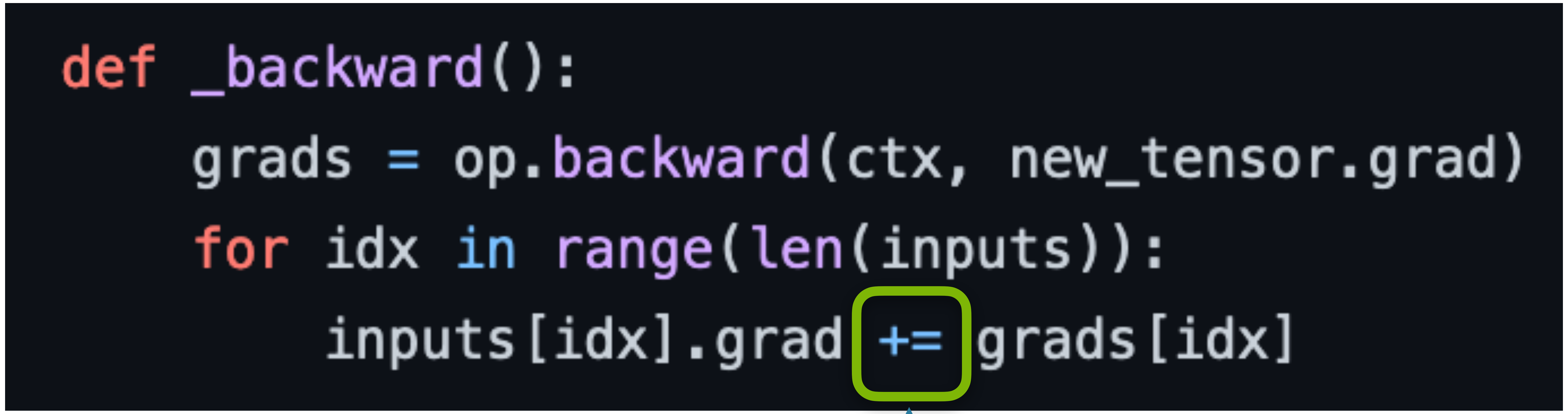
Multivariable chain rule: $\dfrac{\partial L}{\partial x} = \dfrac{\partial L}{\partial f}\dfrac{\partial f}{\partial x} + \dfrac{\partial L}{\partial g}\dfrac{\partial g}{\partial x}$

Adding Gradients with Multiple Outputs

Live demo and/or exercise!

$$f(x) = x^2 \times 3x$$

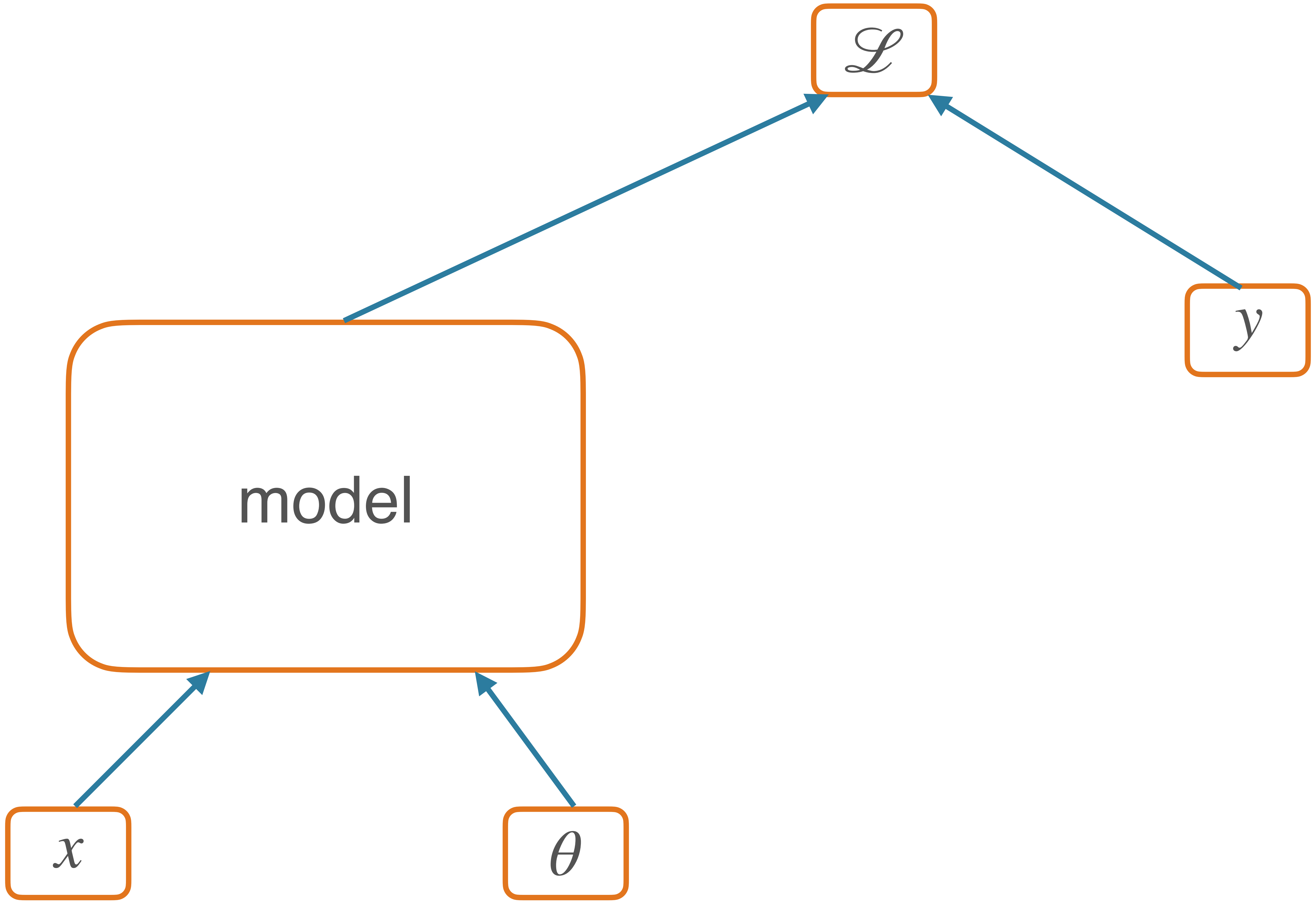
Adding Gradients with Multiple Outputs



```
def _backward():
    grads = op.backward(ctx, new_tensor.grad)
    for idx in range(len(inputs)):
        inputs[idx].grad += grads[idx]
```

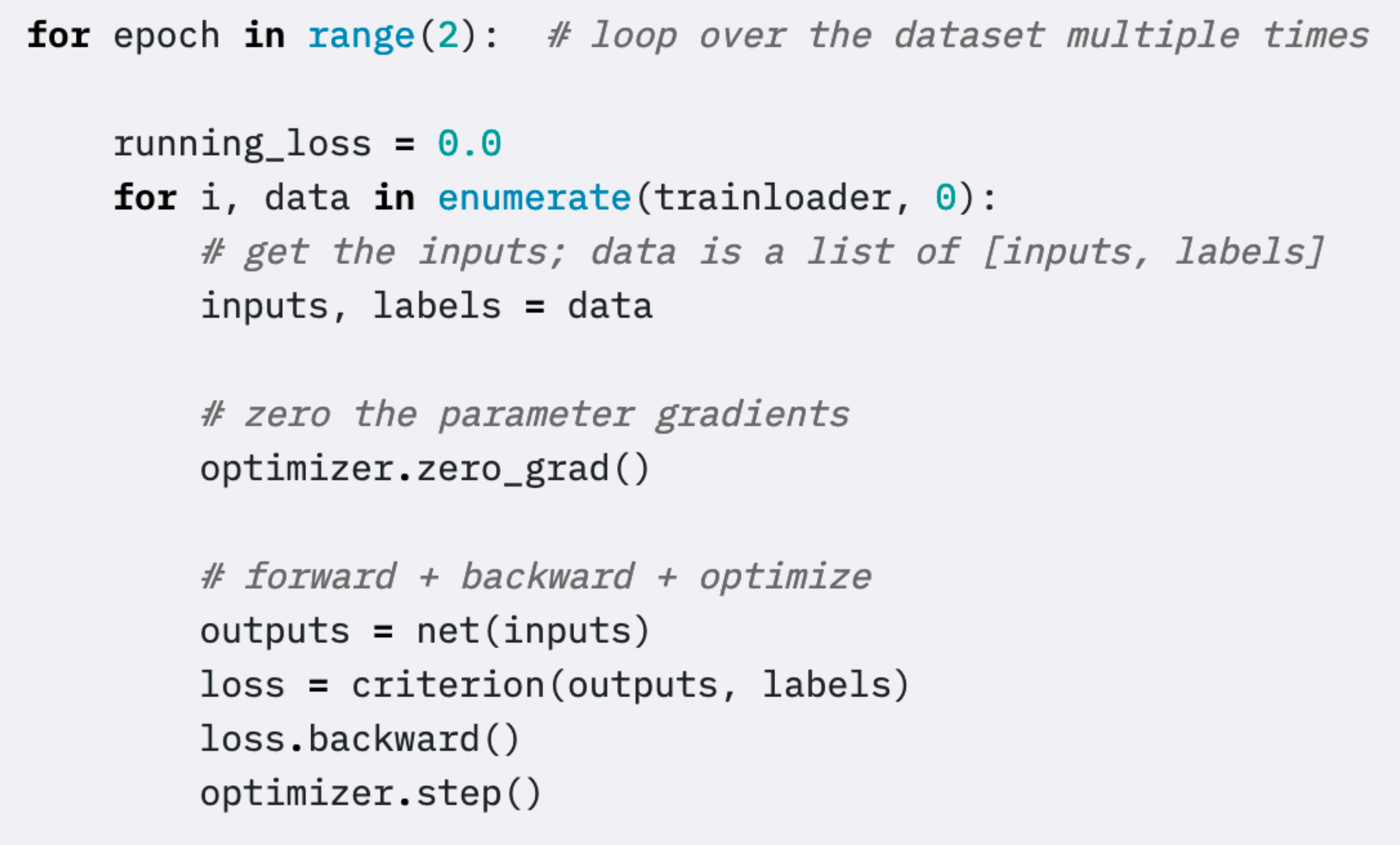
Adding over paths handled implicitly in auto-grad libraries;
more power to the forward/backward API

Schematic of Graph for Training



Training Loop

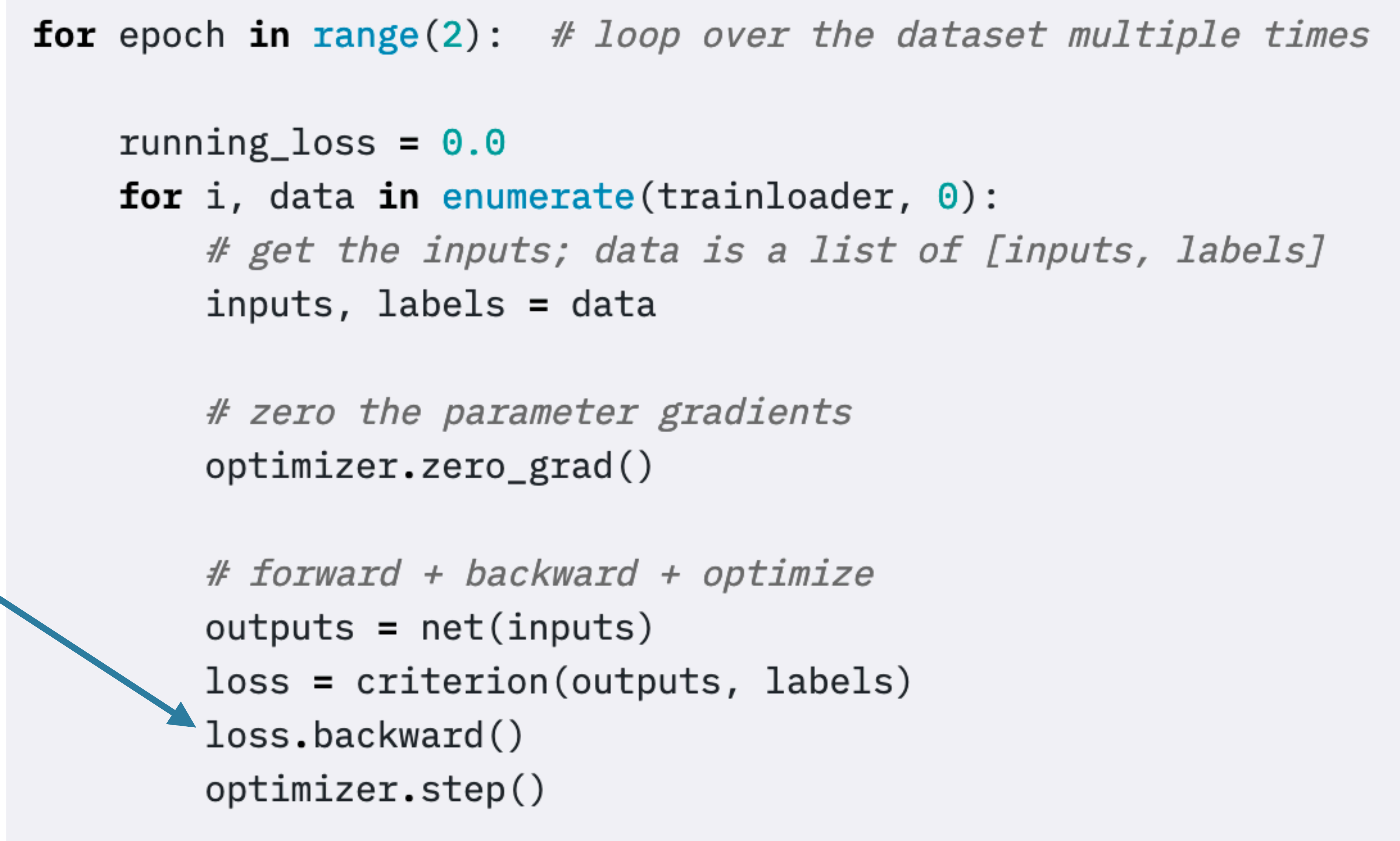
- Define (now, dynamically) computation graph, get backprop “automatically”



```
for epoch in range(2):  # loop over the dataset multiple times

    running_loss = 0.0
    for i, data in enumerate(trainloader, 0):
        # get the inputs; data is a list of [inputs, labels]
        inputs, labels = data

        # zero the parameter gradients
        optimizer.zero_grad()

        # forward + backward + optimize
        outputs = net(inputs)
        loss = criterion(outputs, labels)
        loss.backward()
        optimizer.step()
```

Training Loop

- Define (now, dynamically) computation graph, get backprop “automatically”

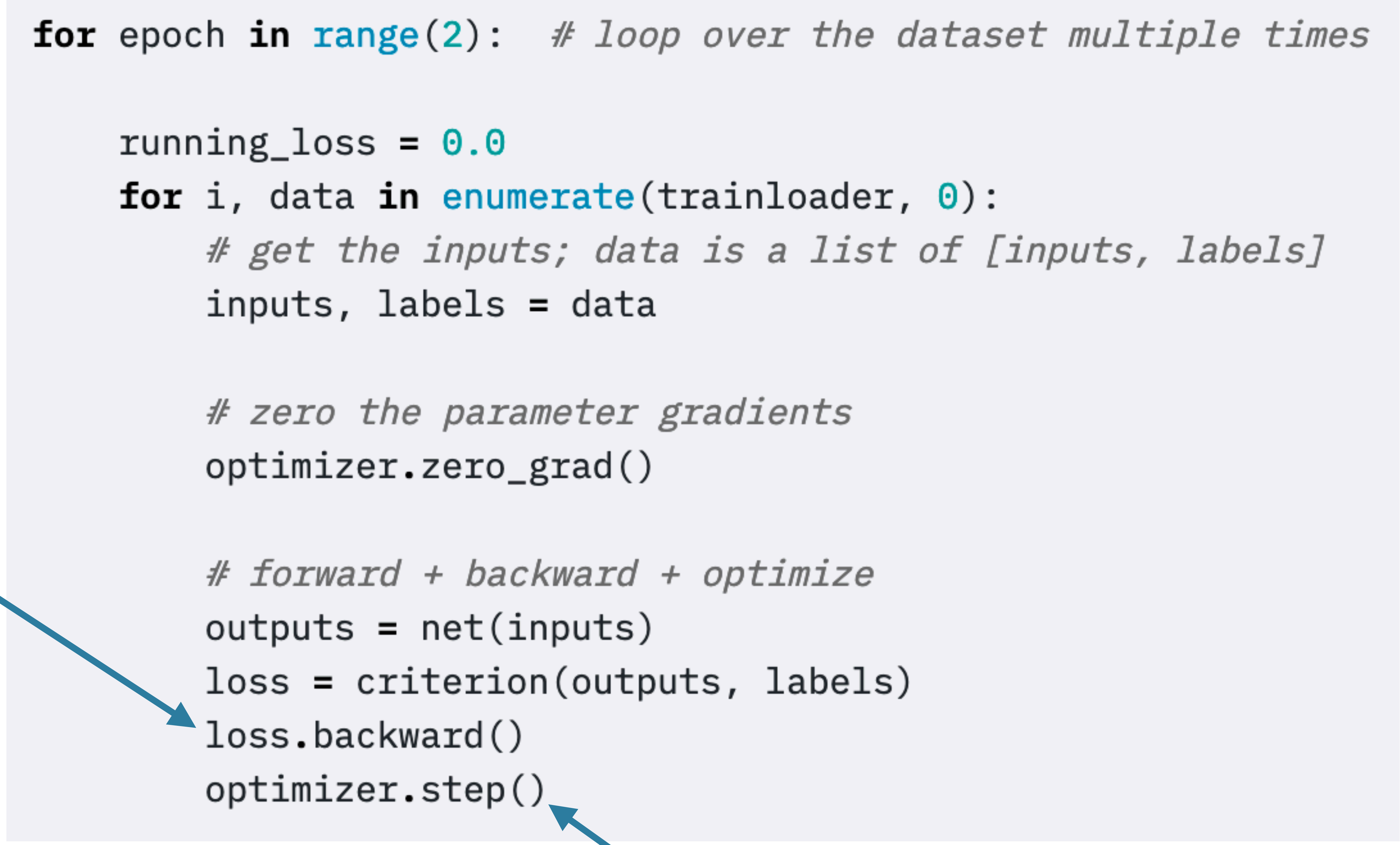


```
for epoch in range(2):  # loop over the dataset multiple times

    running_loss = 0.0
    for i, data in enumerate(trainloader, 0):
        # get the inputs; data is a list of [inputs, labels]
        inputs, labels = data

        # zero the parameter gradients
        optimizer.zero_grad()

        # forward + backward + optimize
        outputs = net(inputs)
        loss = criterion(outputs, labels)
        loss.backward()
        optimizer.step()
```

Backprop the loss

Training Loop

- Define (now, dynamically) computation graph, get backprop “automatically”



```
for epoch in range(2):  # loop over the dataset multiple times

    running_loss = 0.0
    for i, data in enumerate(trainloader, 0):
        # get the inputs; data is a list of [inputs, labels]
        inputs, labels = data

        # zero the parameter gradients
        optimizer.zero_grad()

        # forward + backward + optimize
        outputs = net(inputs)
        loss = criterion(outputs, labels)
        loss.backward()
        optimizer.step()
```

Backprop the loss

Update the parameters