Computation Graphs + Backpropagation

Ling 282/482: Deep Learning for Computational Linguistics

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Fall 2025

Computation Graphs

What is a computation graph?

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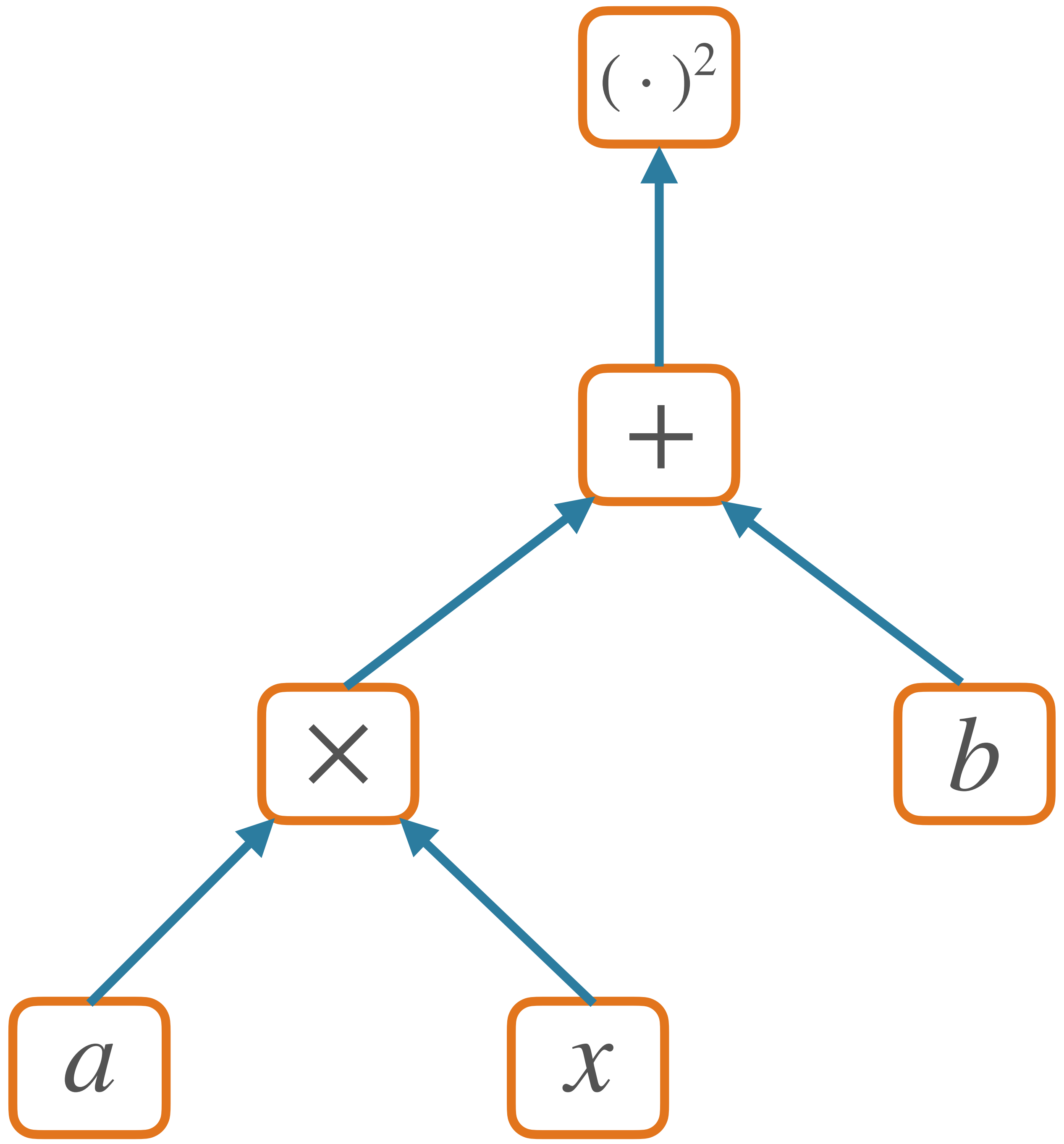
- The **descriptive language** of deep learning frameworks
  - e.g. TensorFlow, PyTorch
- Essentially, **parse trees** of mathematical expressions
  - Captures **dependence** between operations
- Two types of computation
  - **Forward**: compute **outputs** given inputs
  - **Backward**: compute **gradients**

Computation Graph Example

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



Forward Pass

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  - **Inputs**: leaf nodes; need values
  - **Outputs**: those with no children

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  - **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

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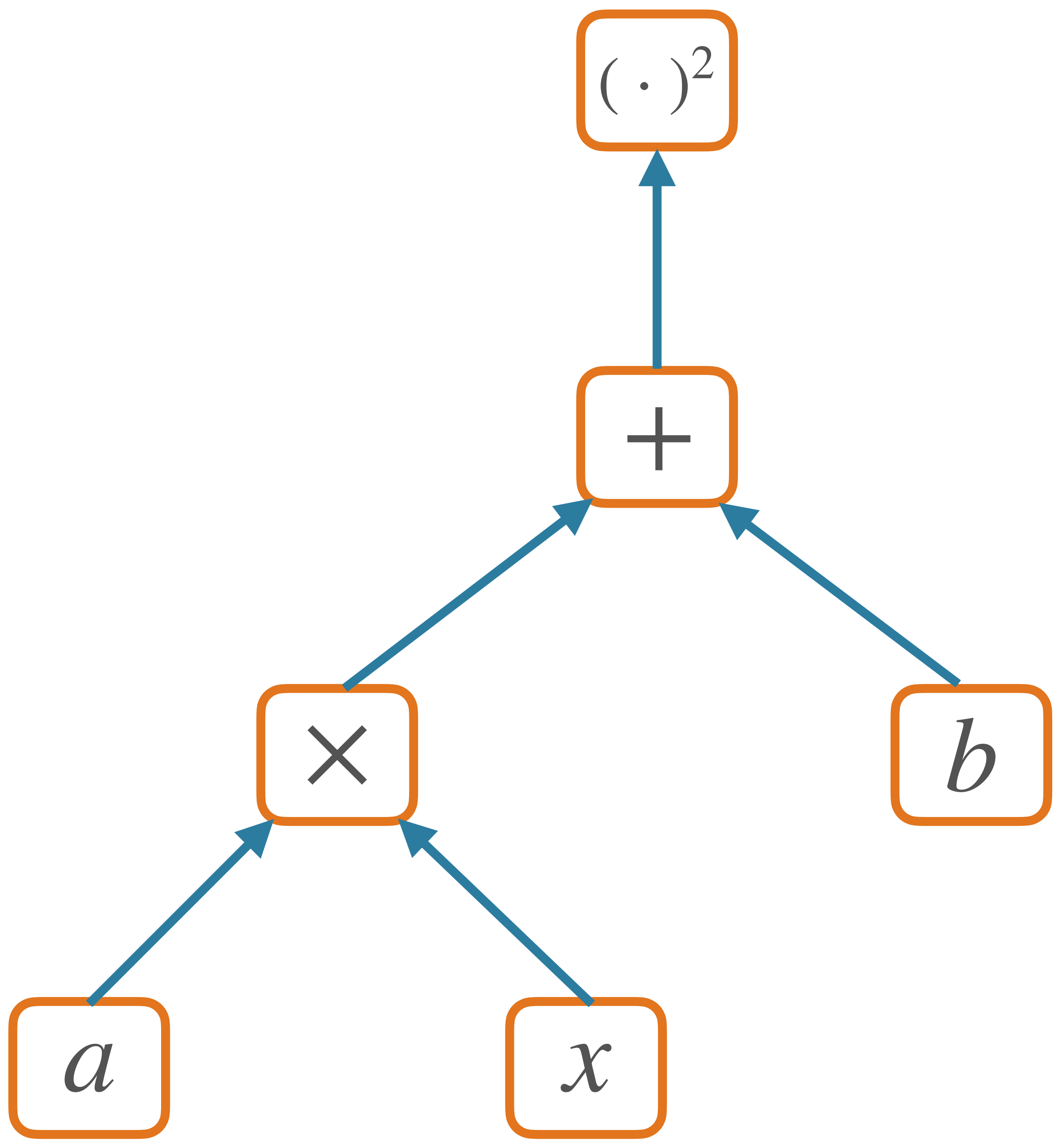

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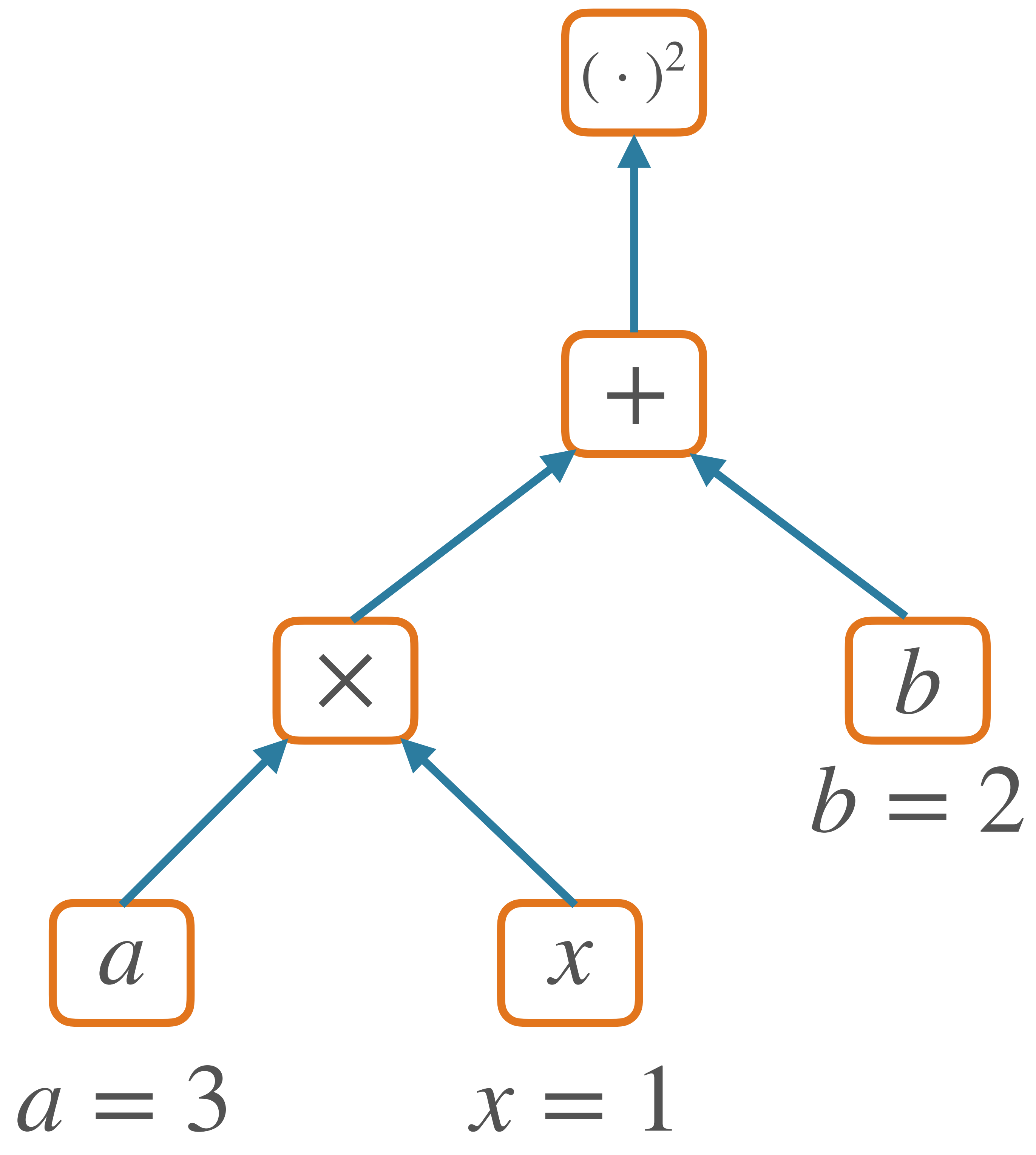

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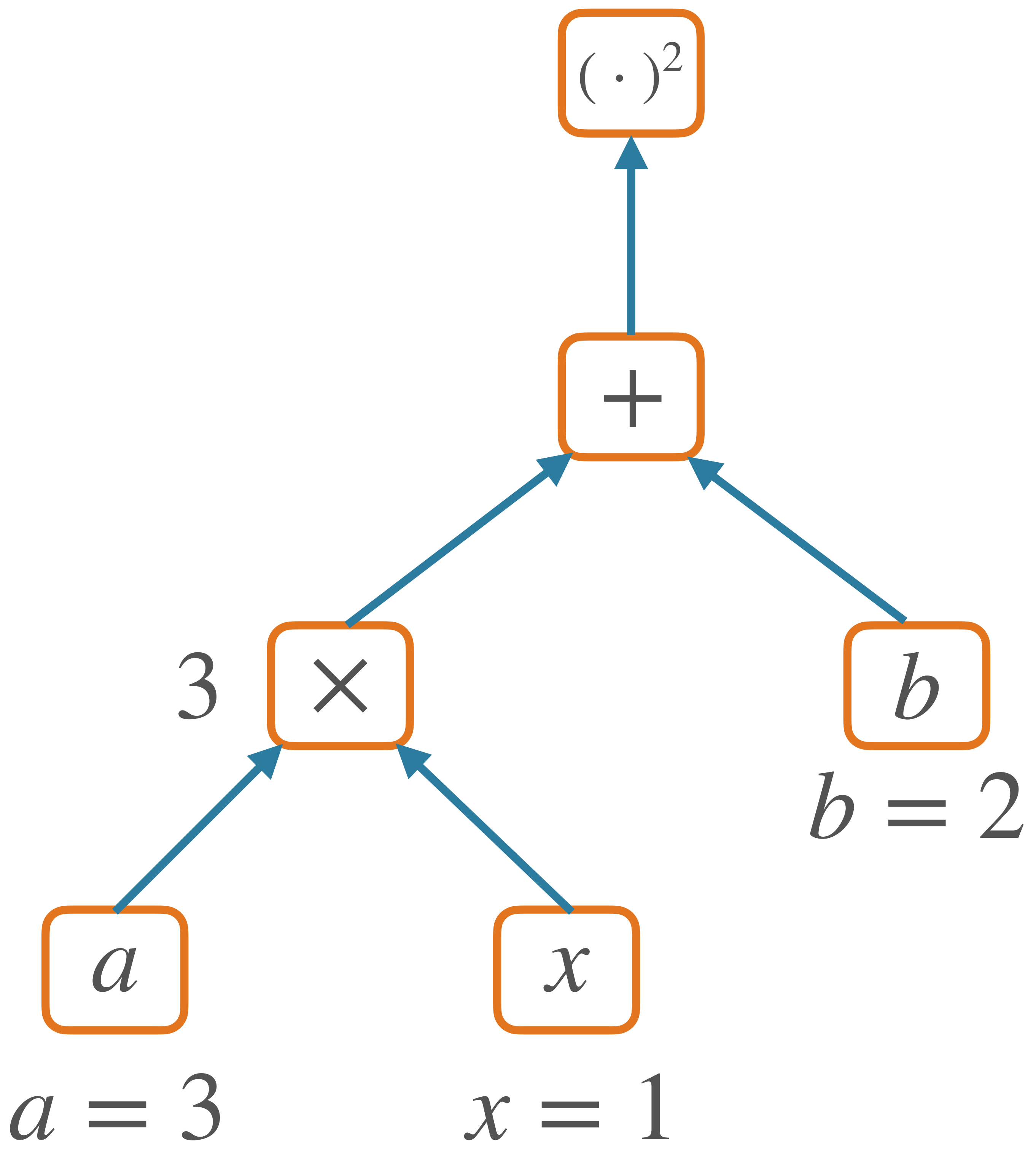

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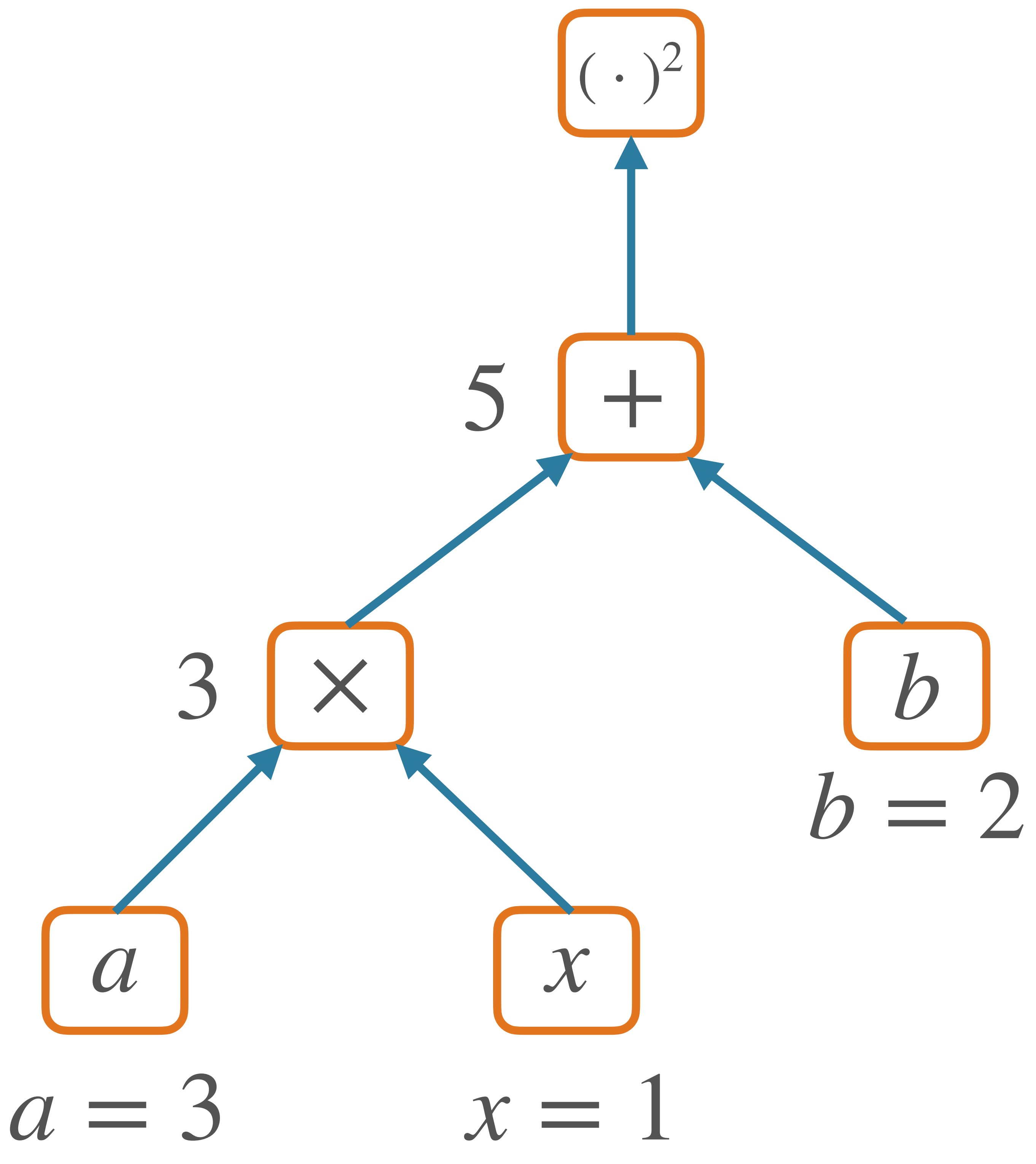

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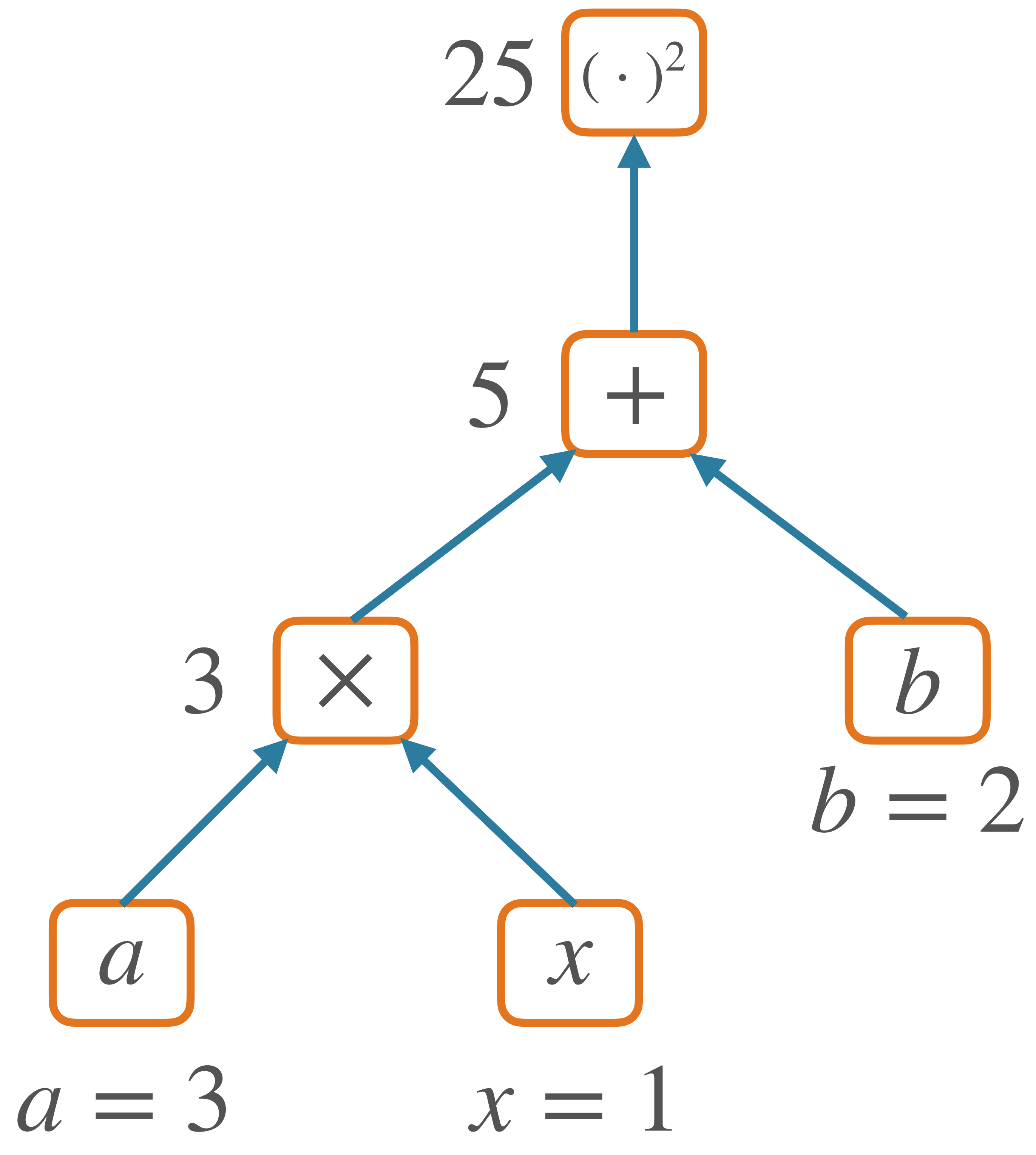
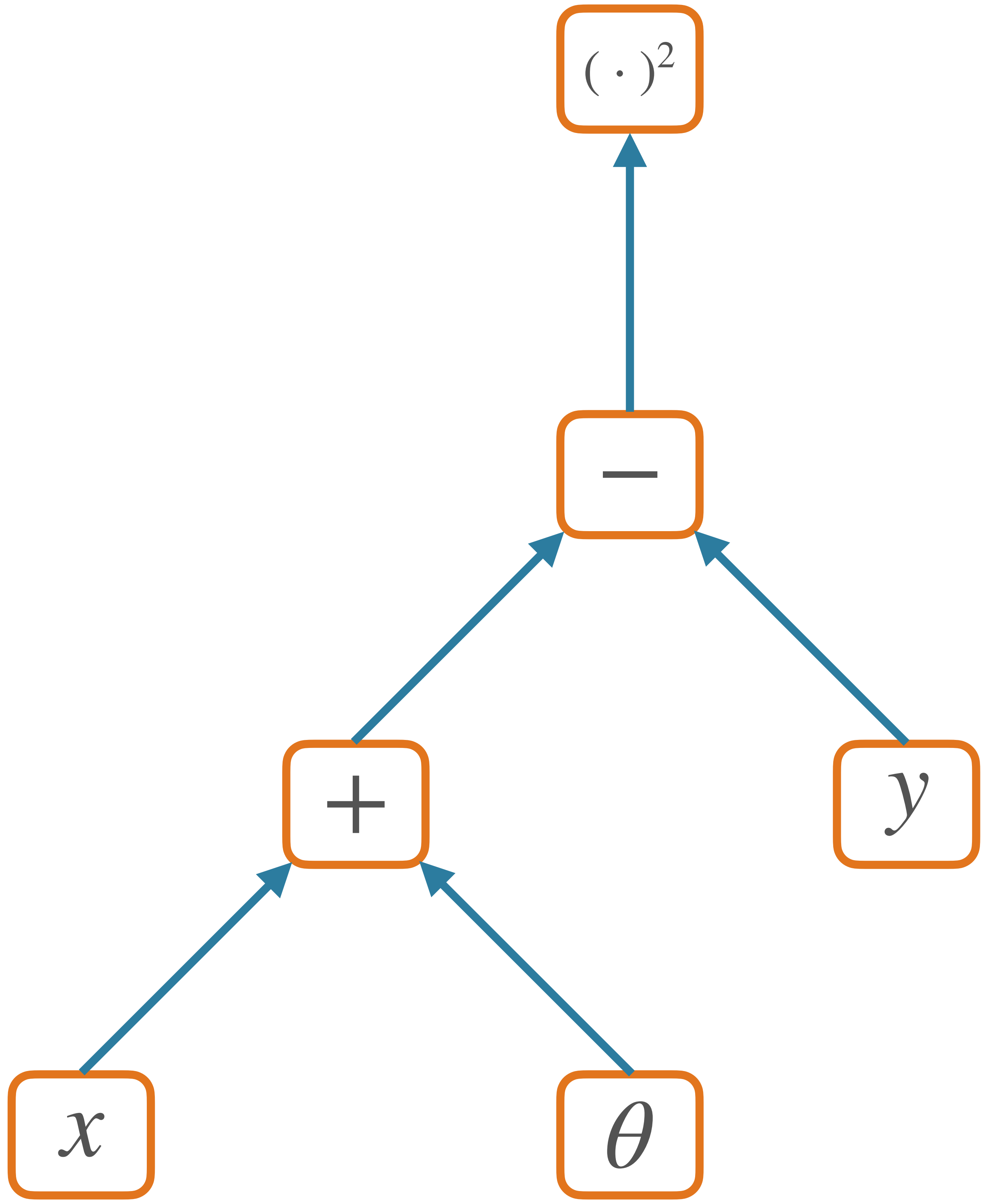


Nodes in a Graph

- 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**

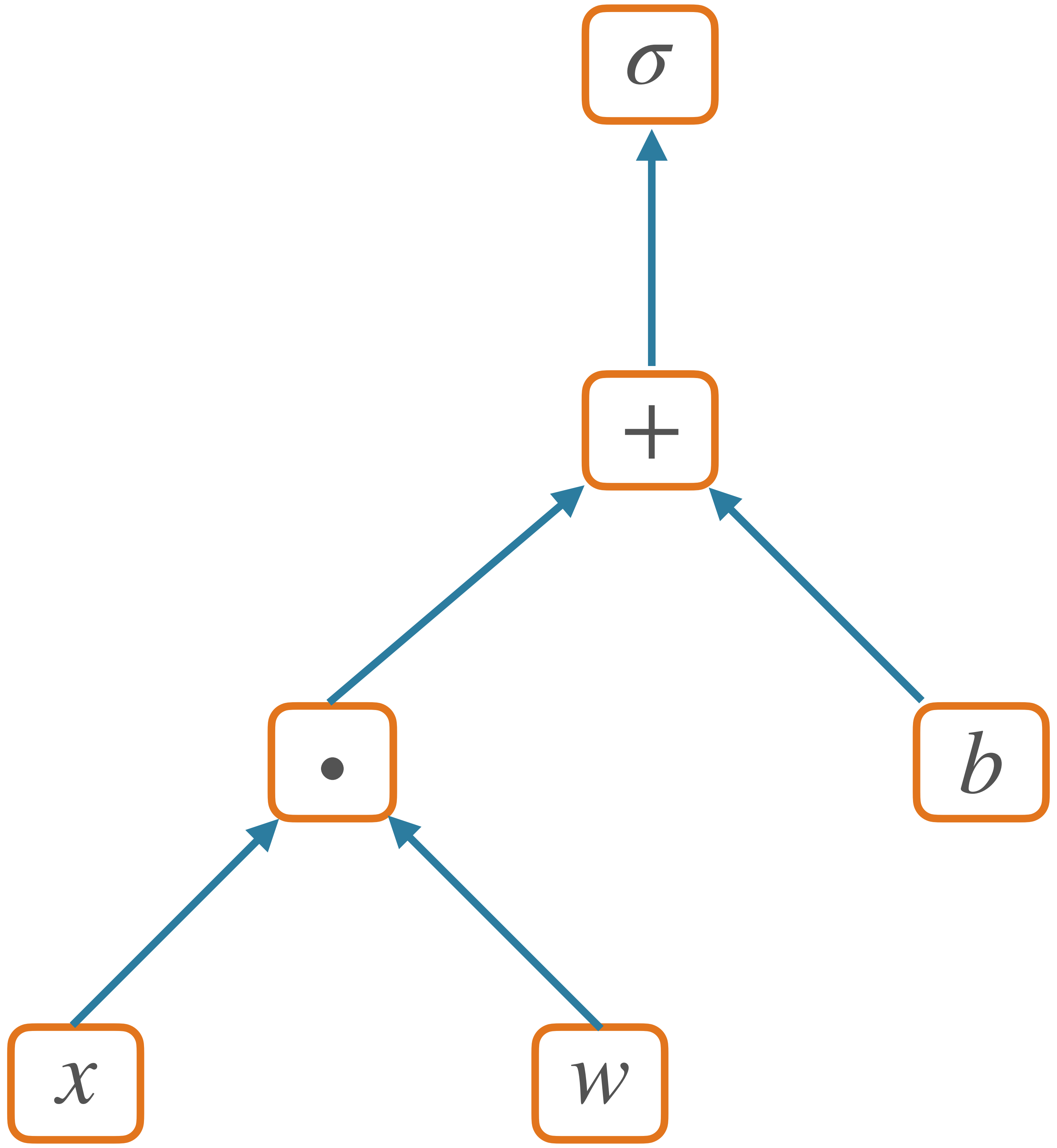
Secret Number Game Graph (Loss)

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



Perceptron Graph

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



Backpropagation

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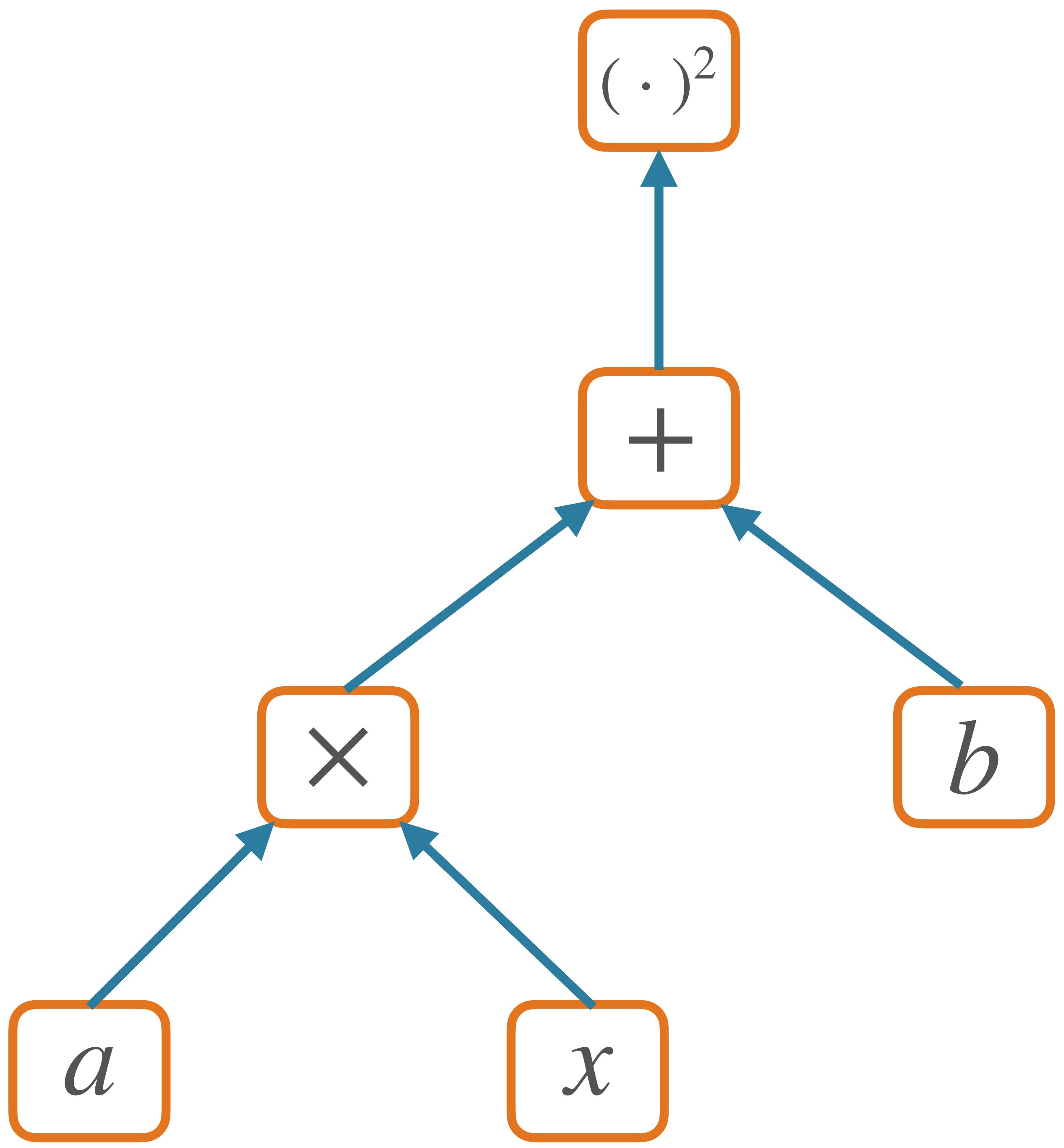
- The real victory of the graph abstraction comes in **computing gradients**
- Backpropagation
  - A **dynamic programming** algorithm on computation graphs
  - **Gradient** of an output to be computed **with respect to *every node*** in the graph

Chain Rule (of Calculus)

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

Computing Derivatives

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



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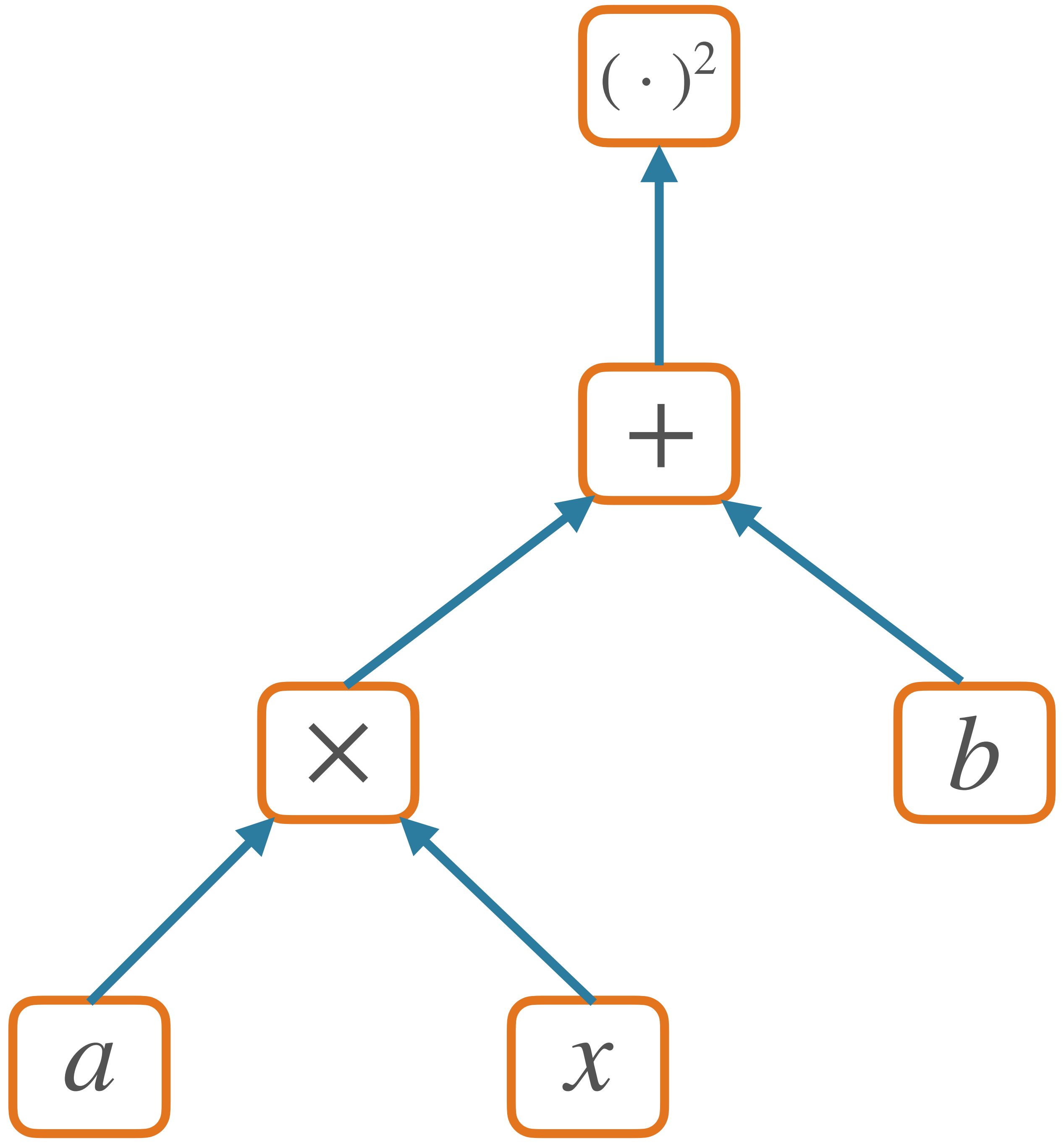

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial (ax+b)} \frac{\partial (ax+b)}{\partial x}$$
$$= 2(ax+b)a$$
$$\frac{\partial f}{\partial a} = 2(ax+b)x$$
$$\frac{\partial f}{\partial b} = 2(ax+b)$$

Nodes in Computational Graph

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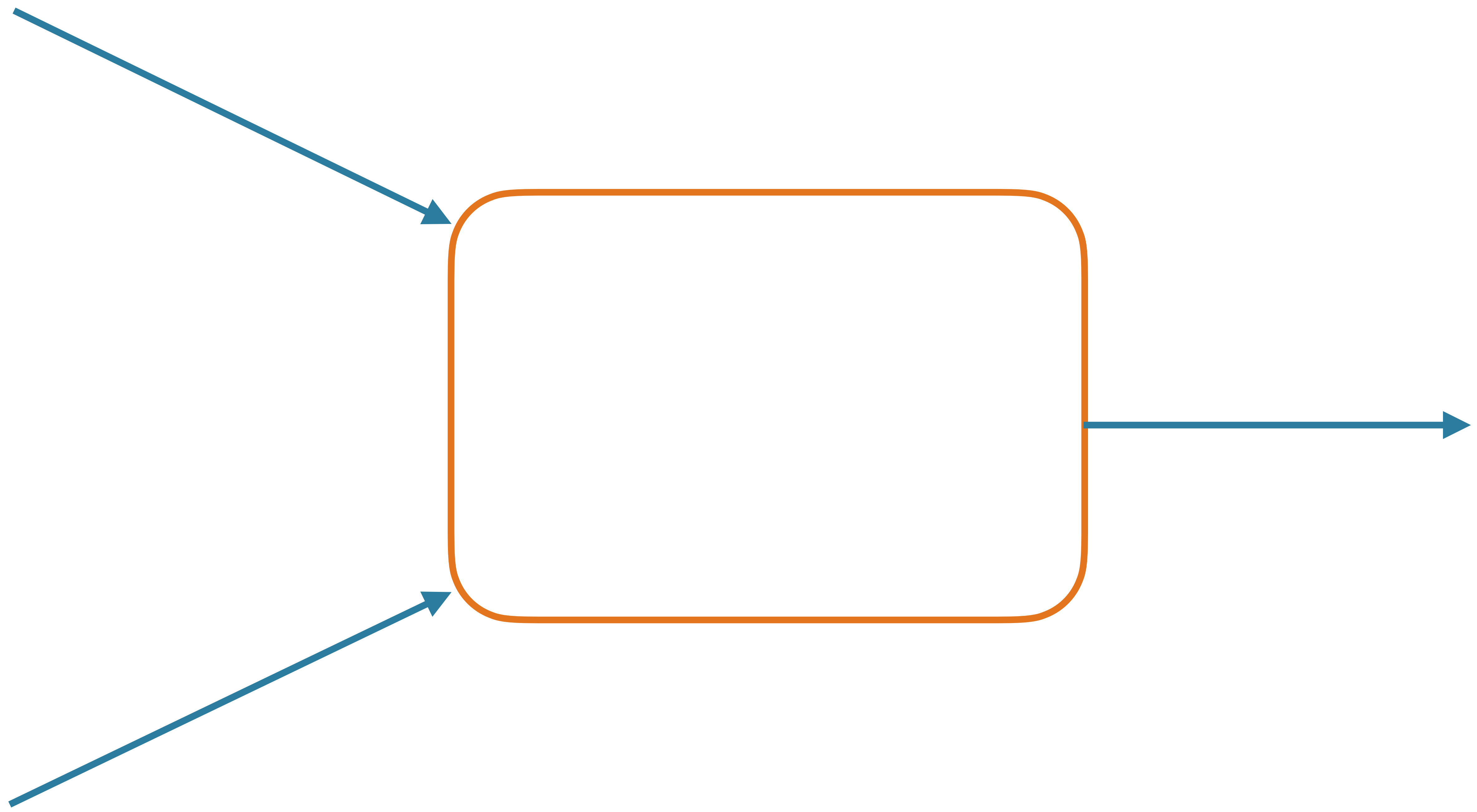

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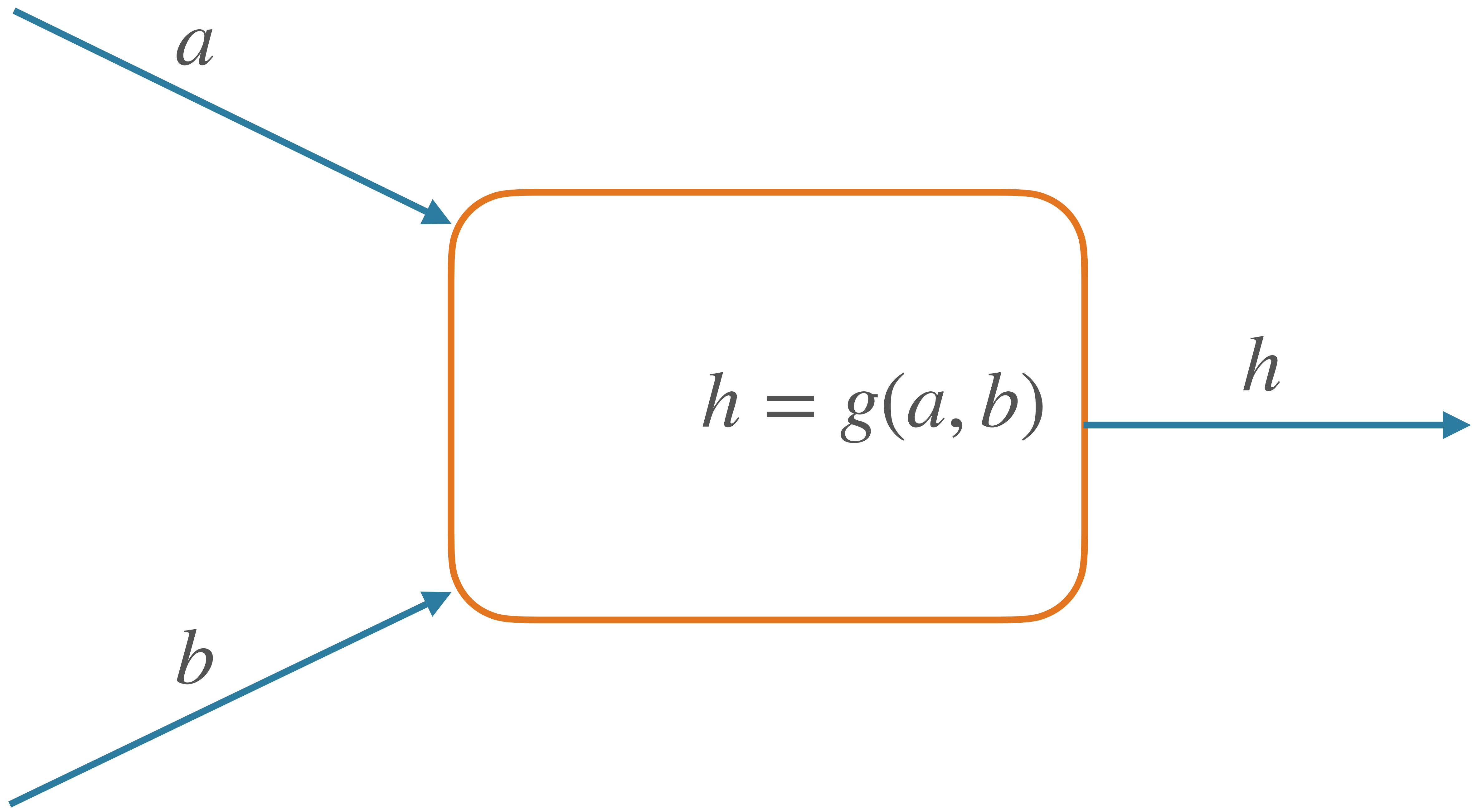

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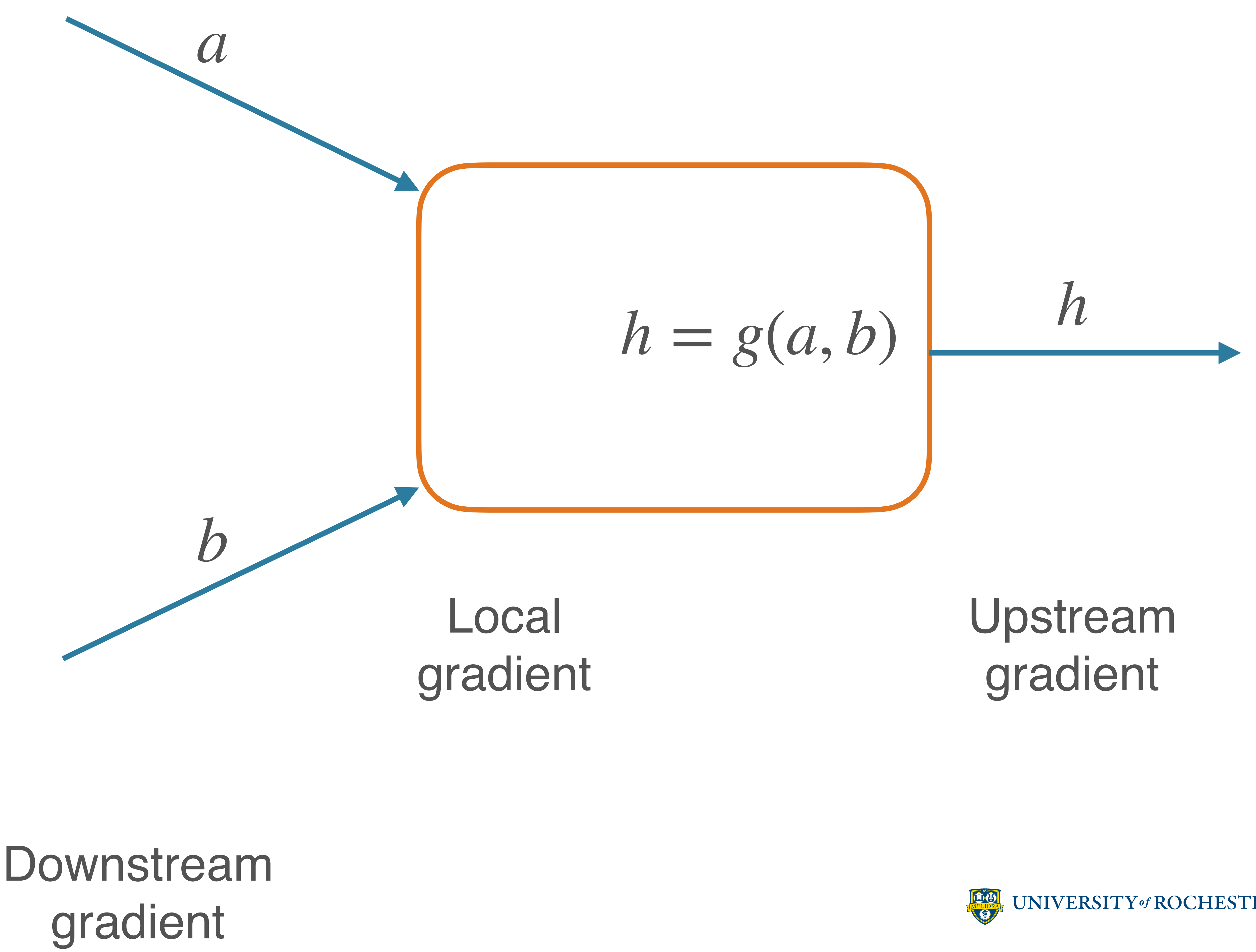

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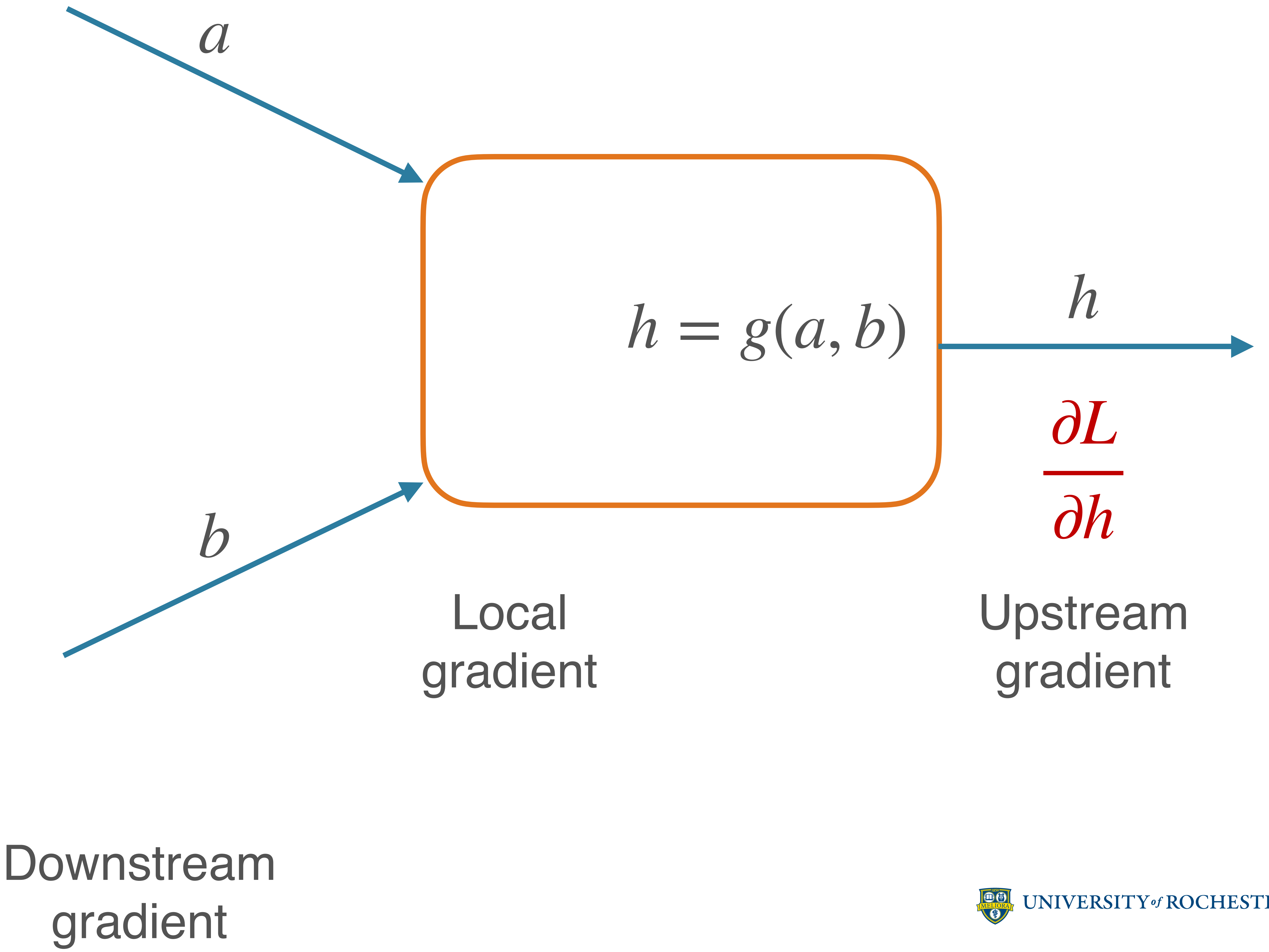

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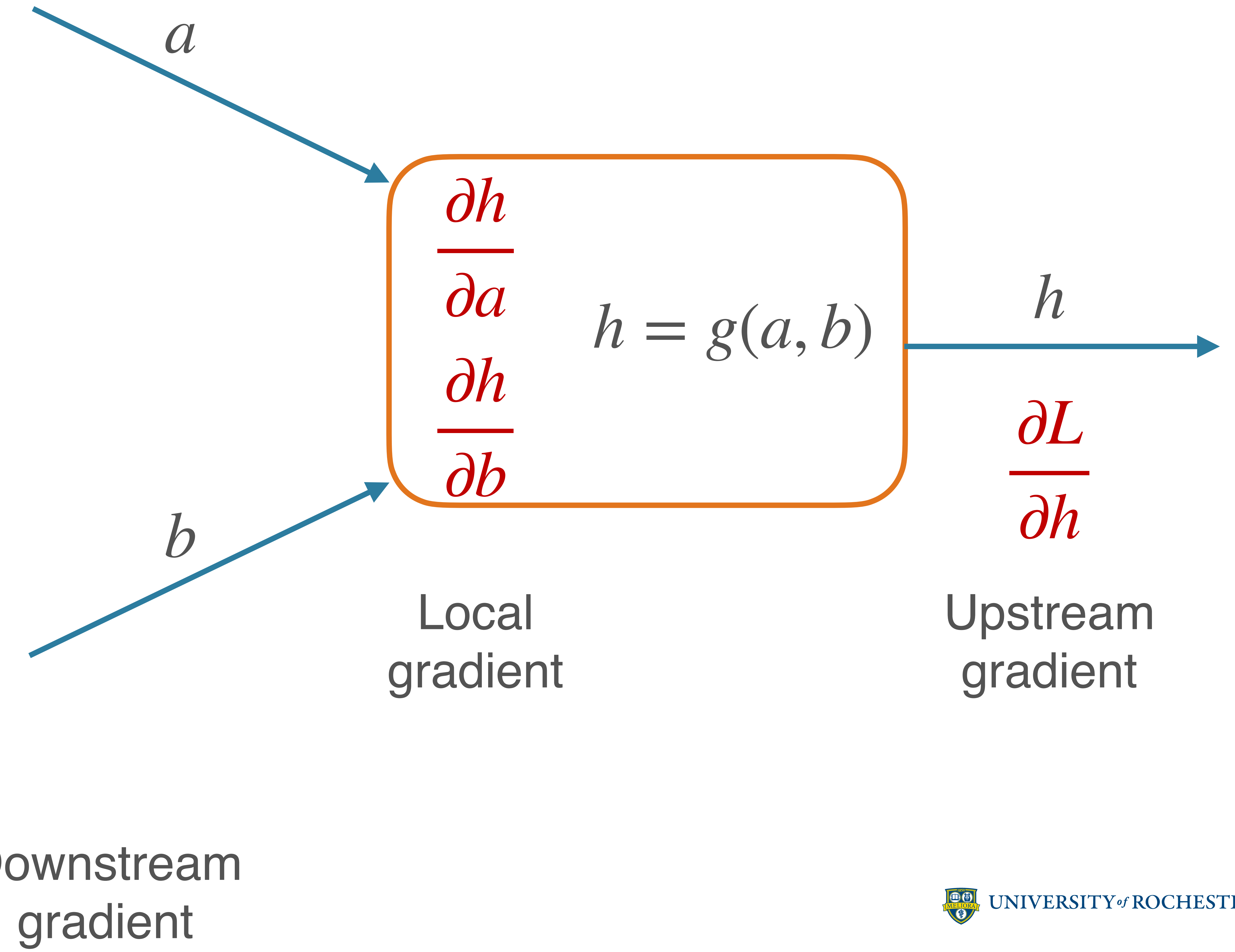

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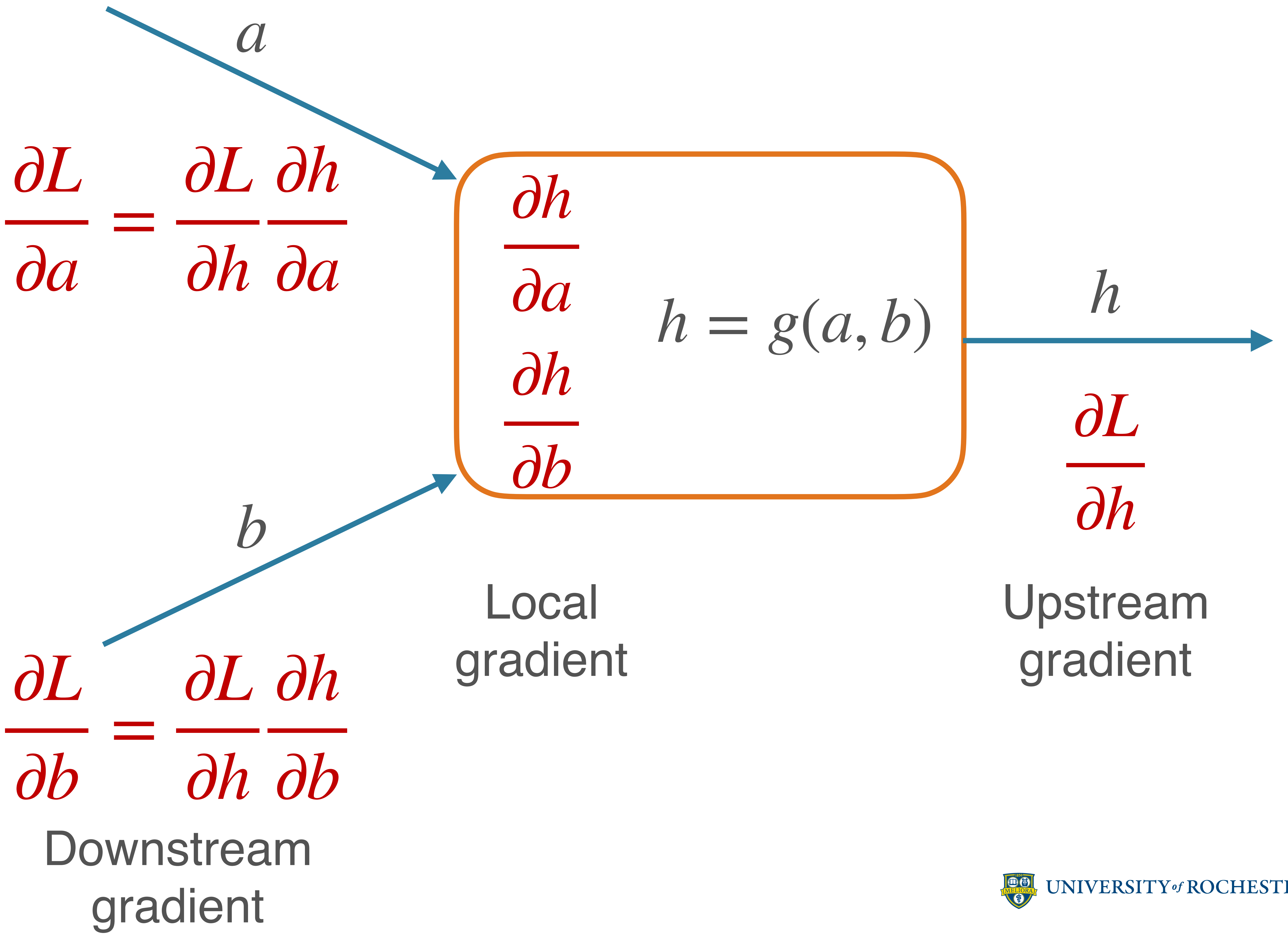

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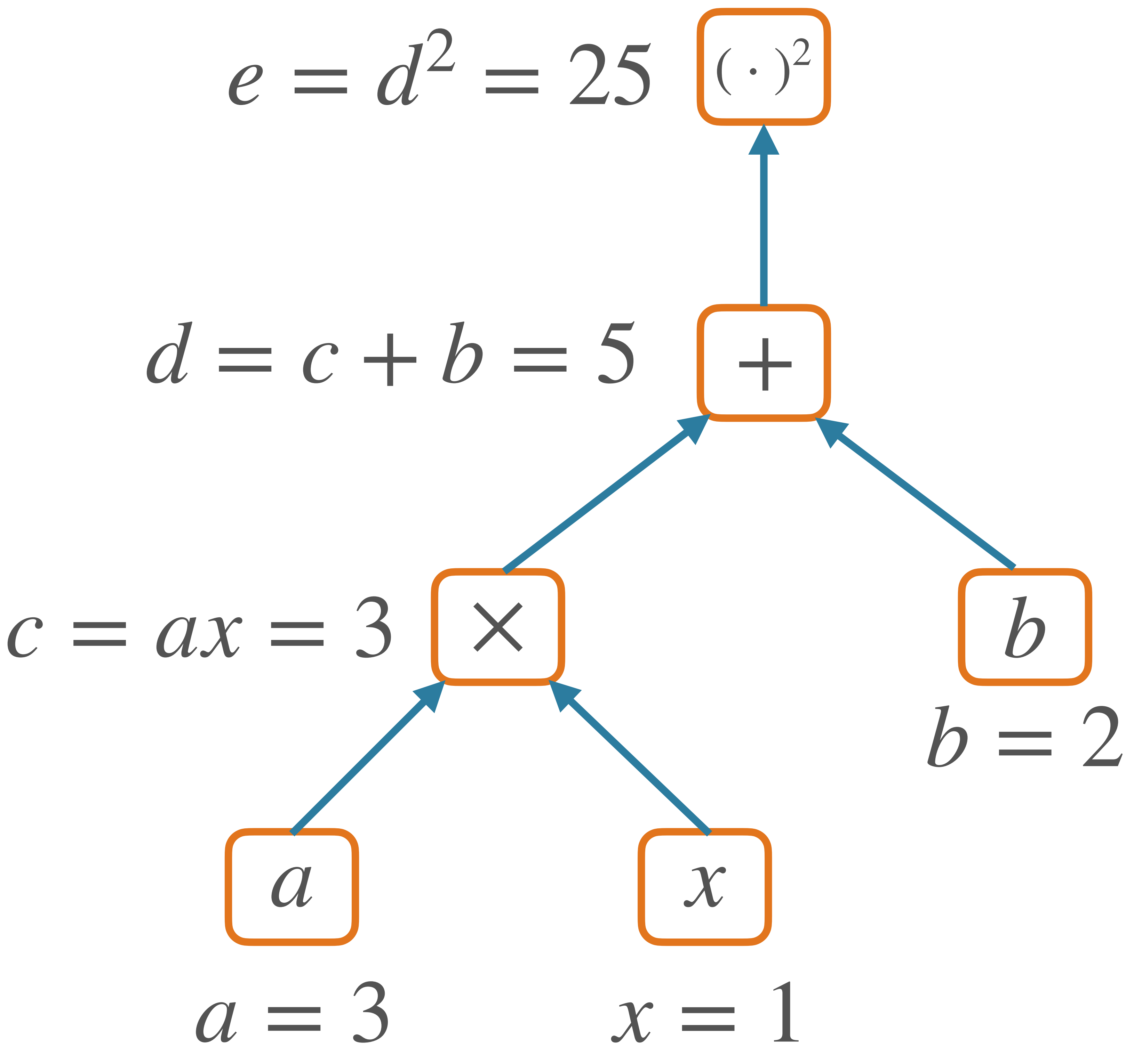

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$$\frac{\partial e}{\partial e} = 1$$

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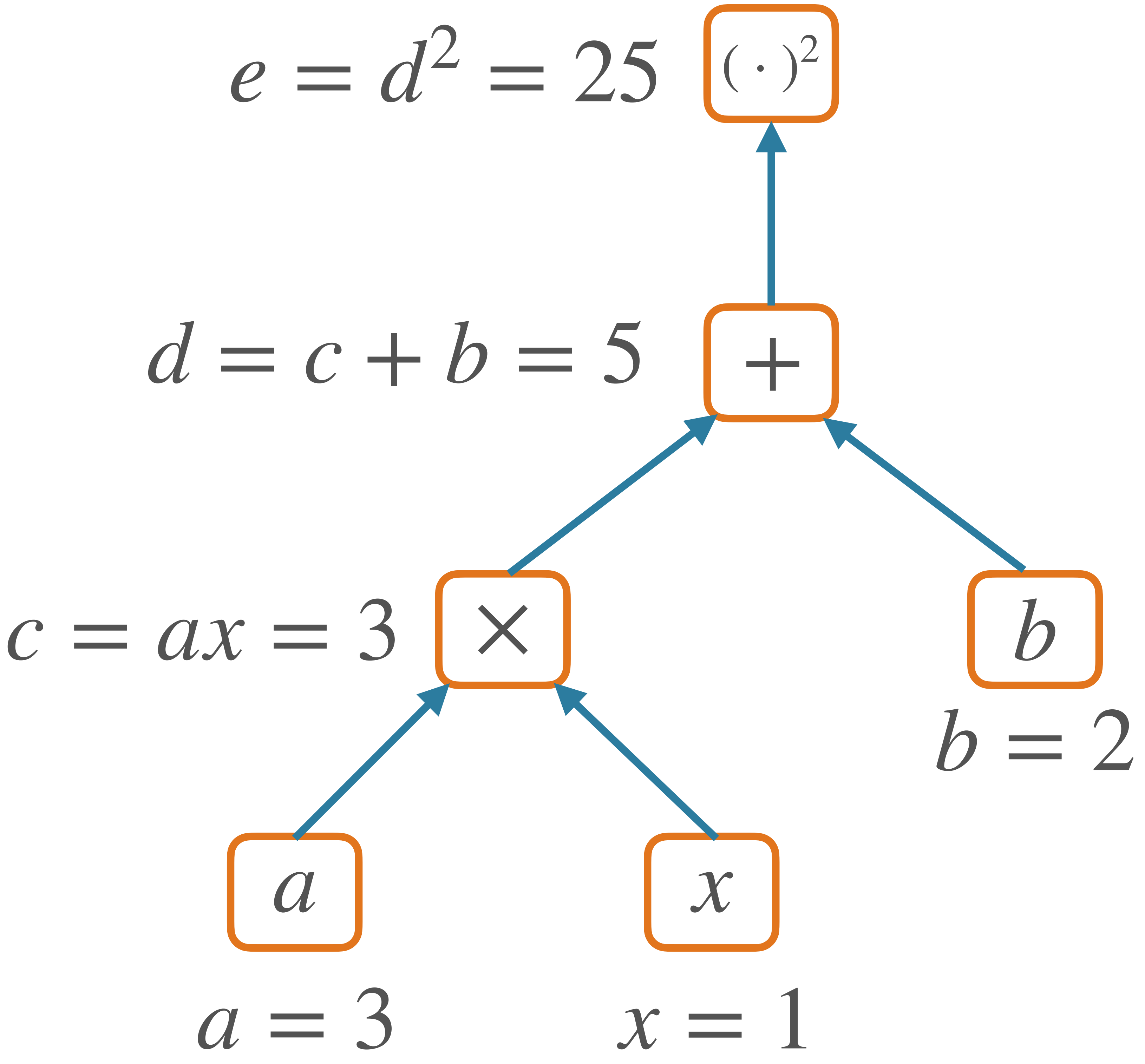

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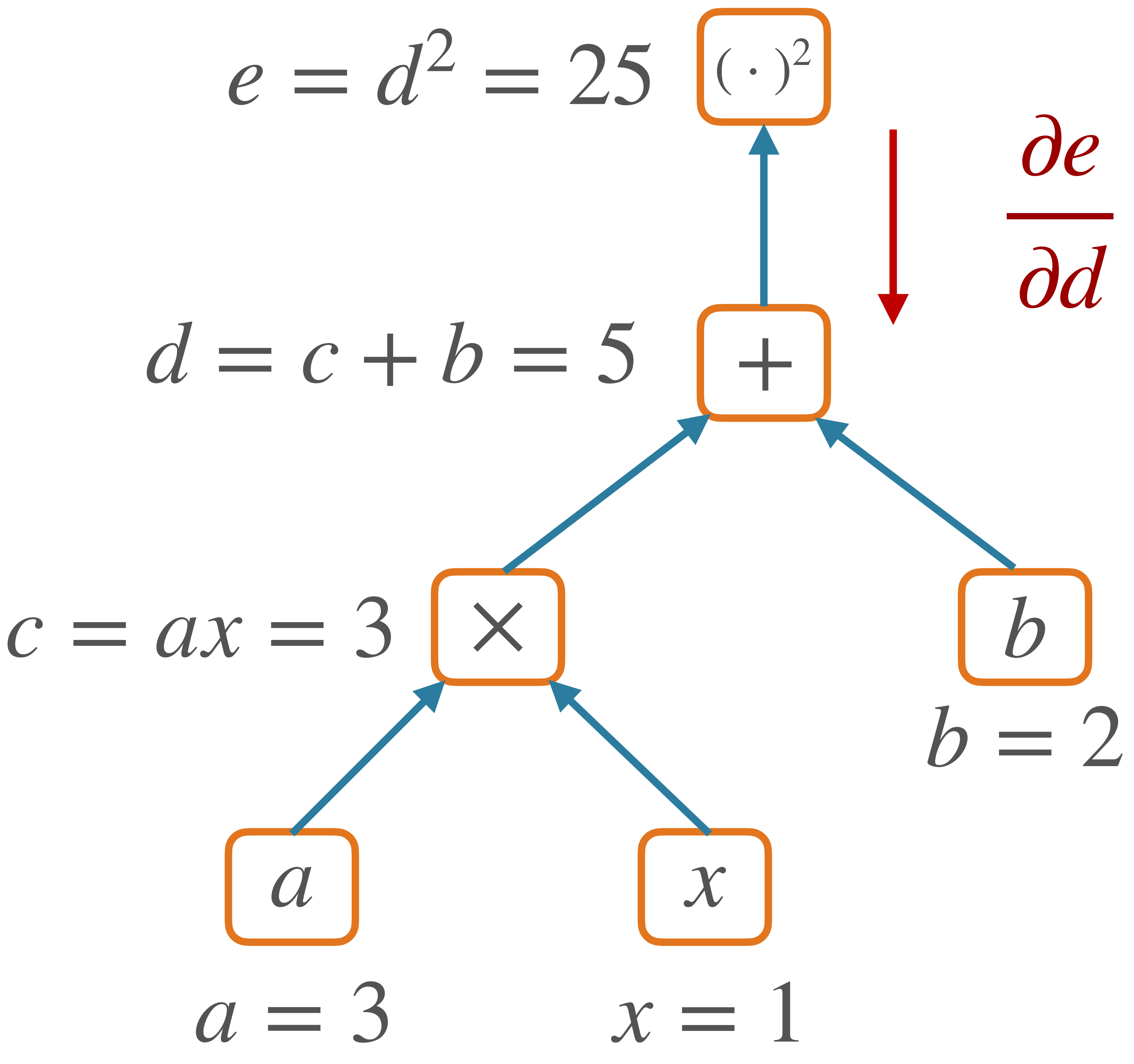

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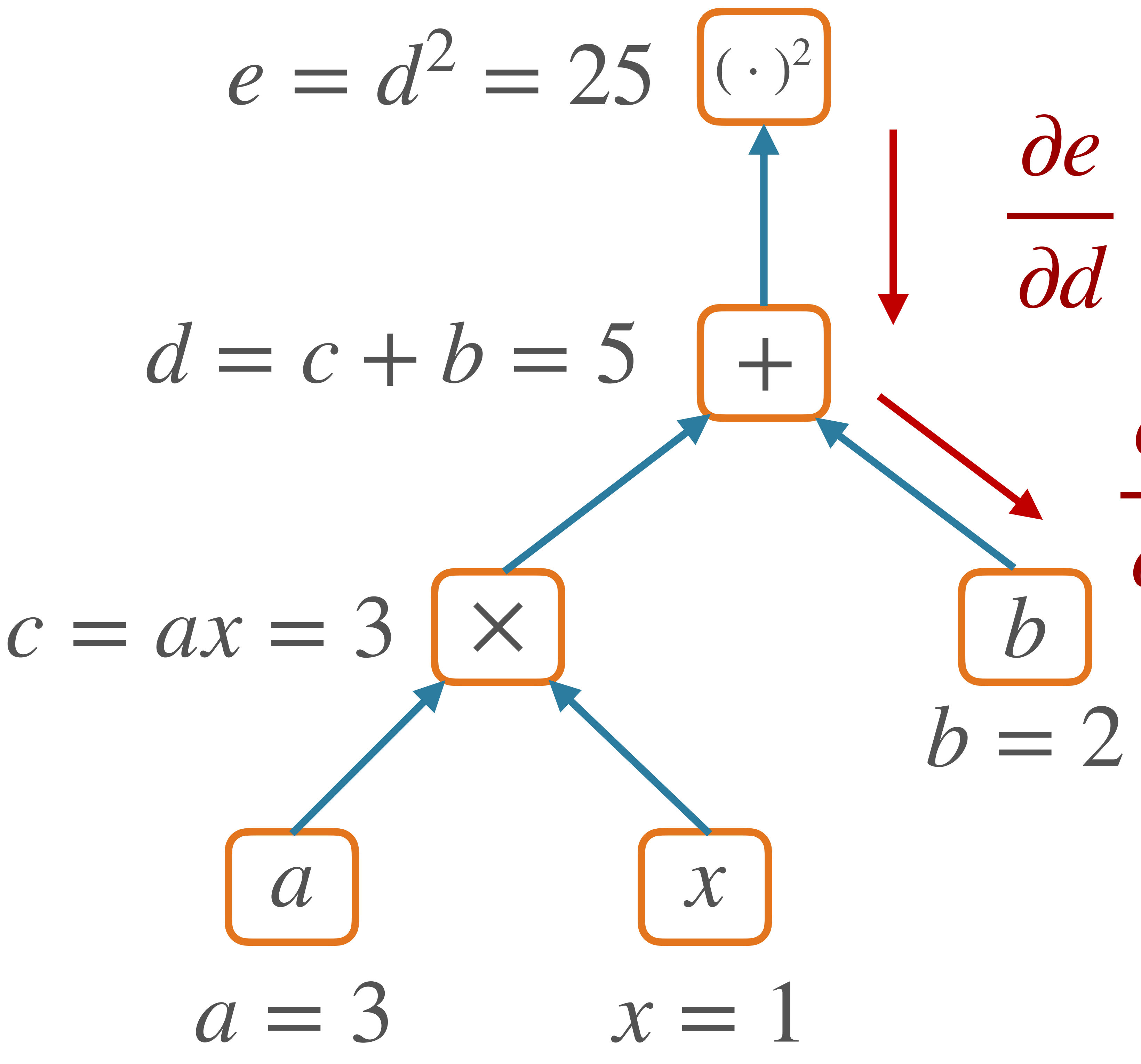

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Backpropagation Example

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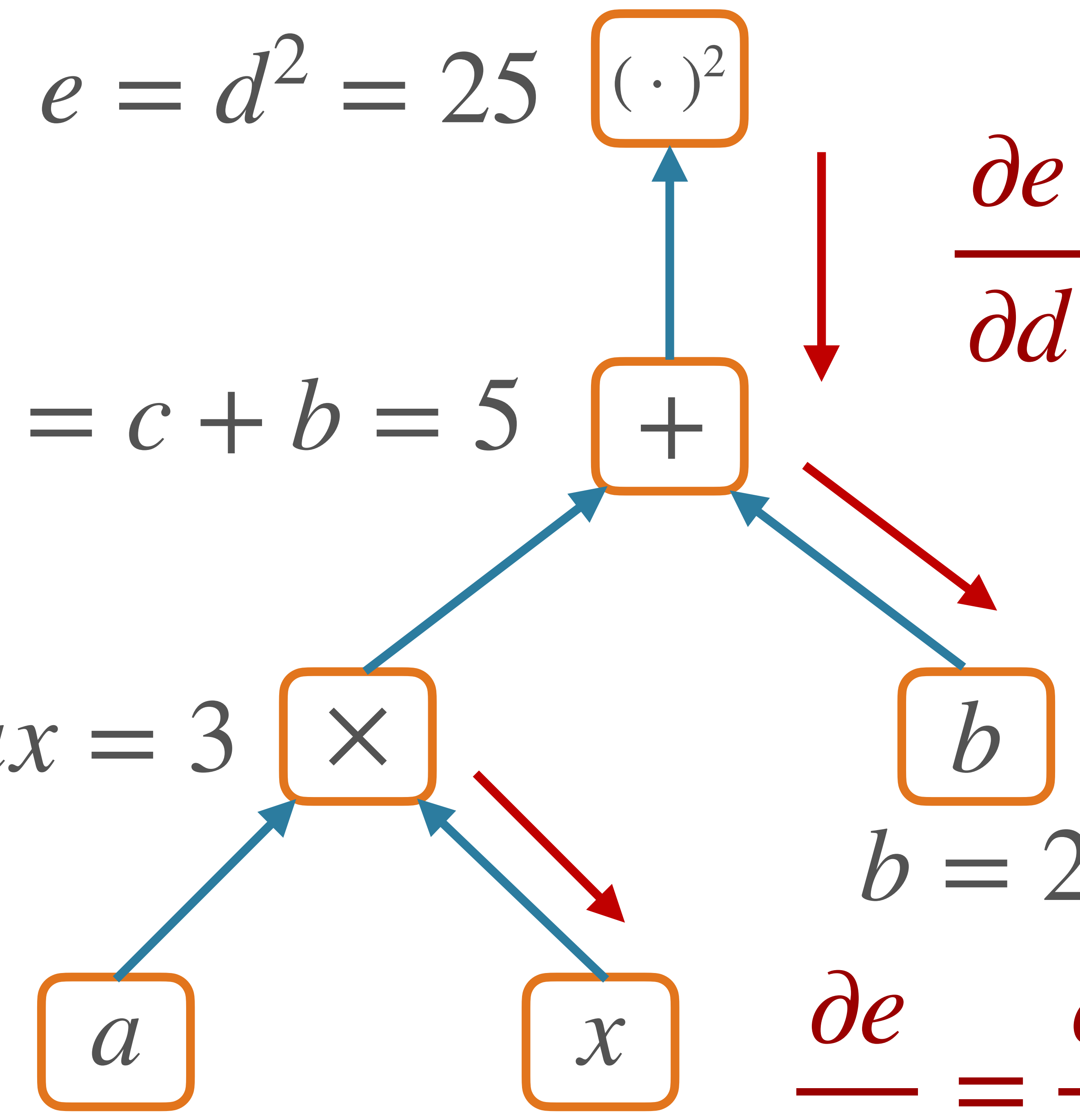
$$f(x; a, b) = (ax + b)^2$$

$$e = d^2 = 25$$

$$d = c + b = 5$$

$$c = ax = 3$$



$$b = 2$$

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

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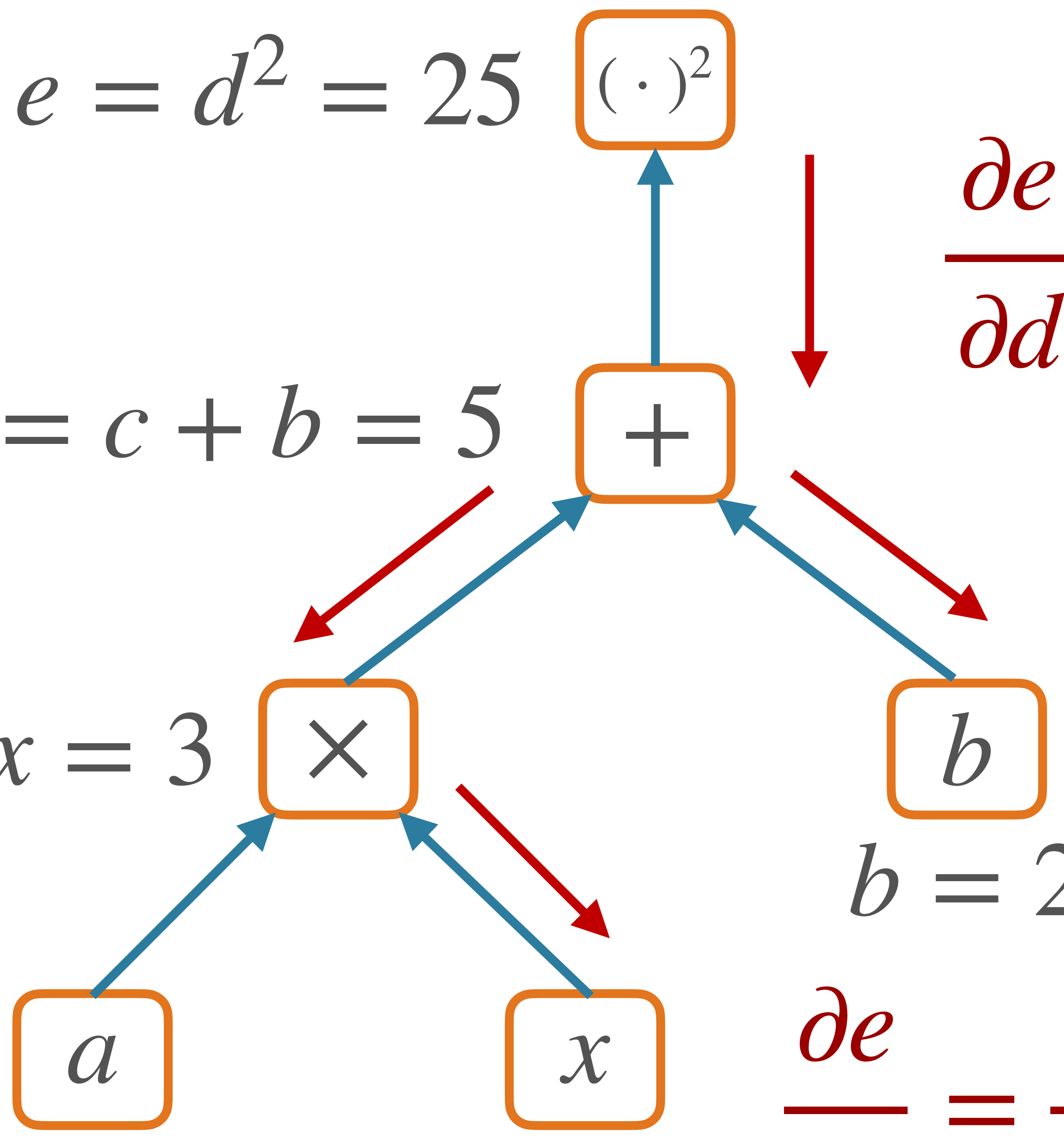

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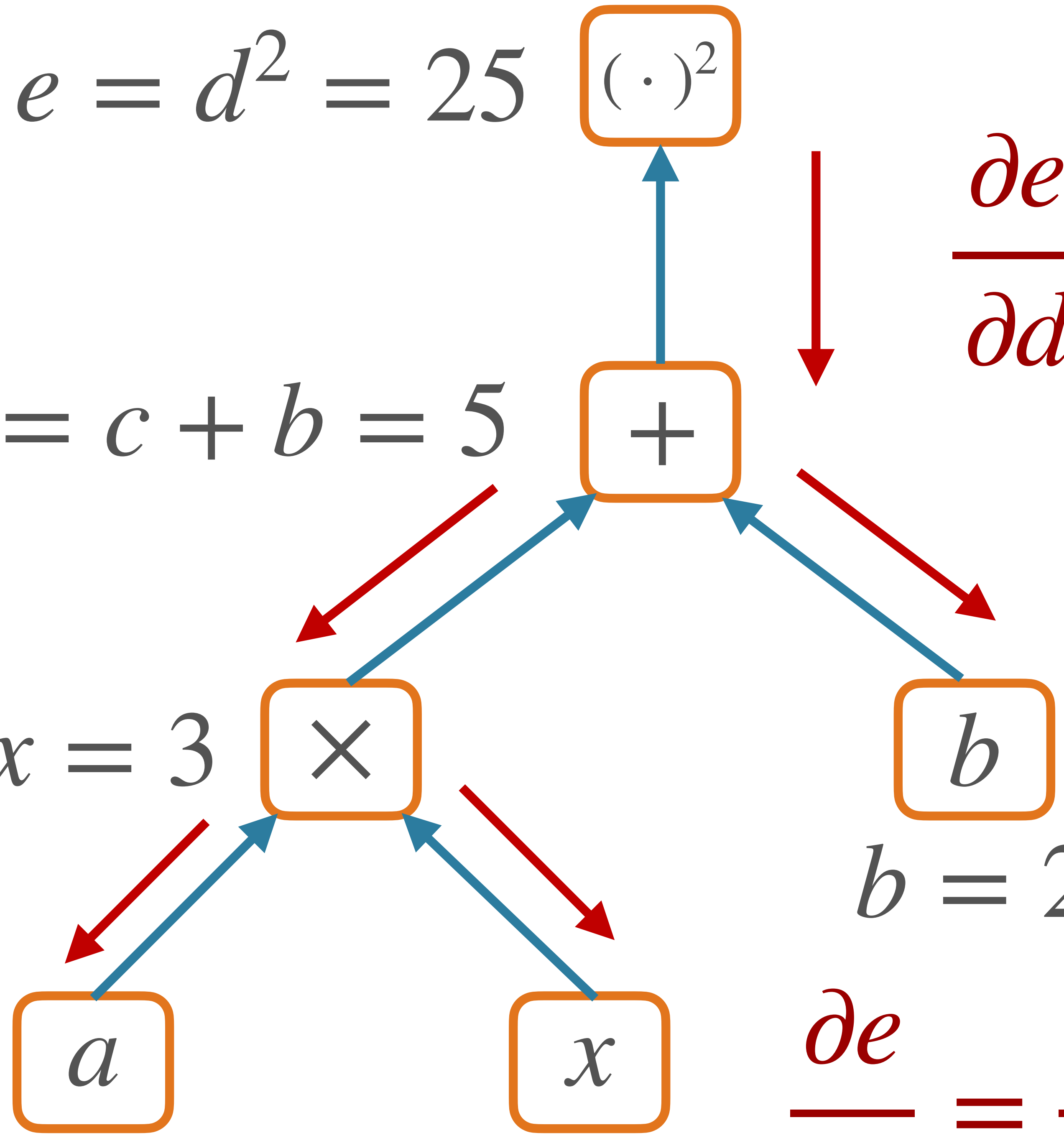

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$$a = 3 \qquad x = 1$$

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()
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From Tensor class in [edugrad]

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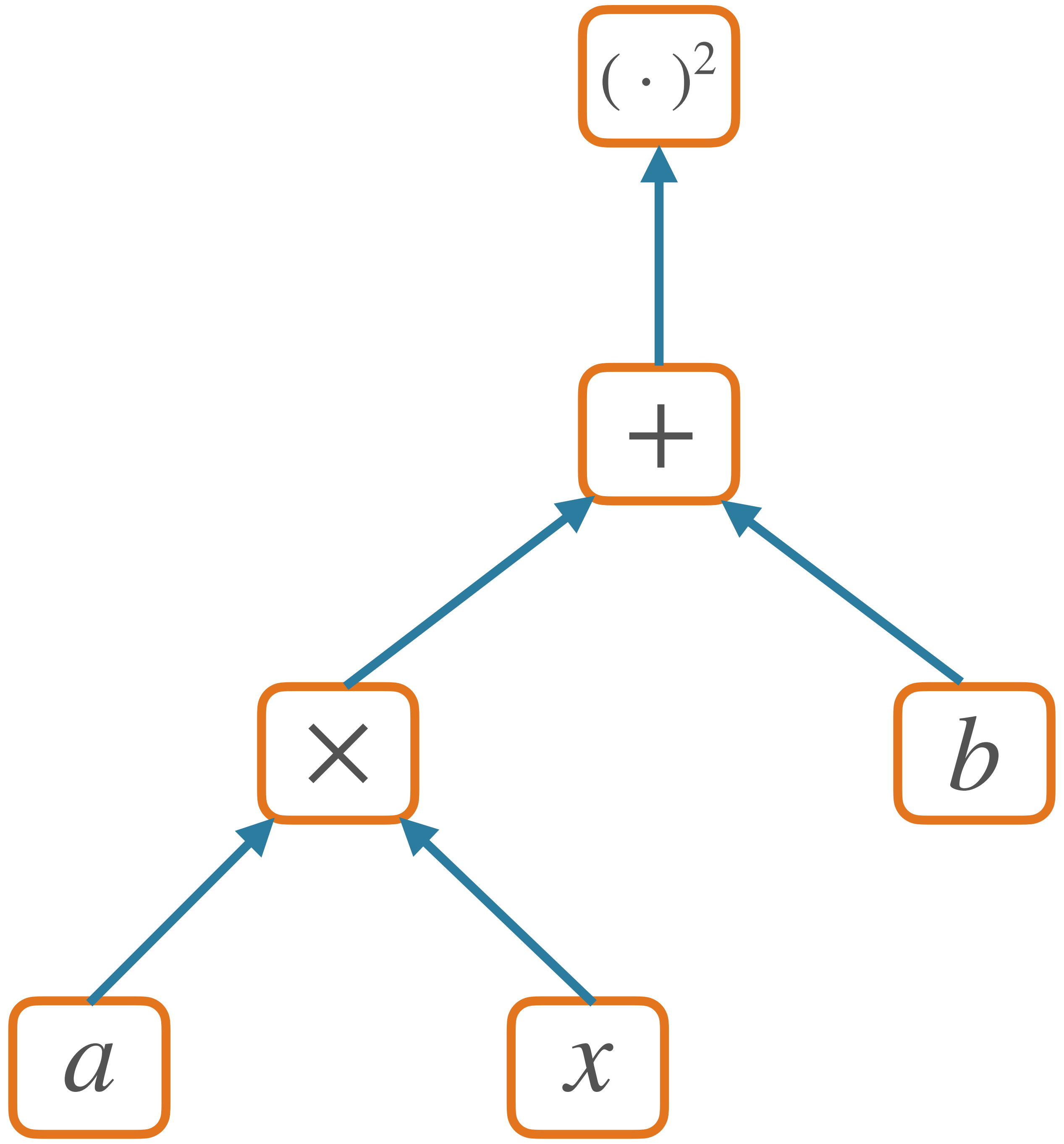
Local gradient + chain rule application

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



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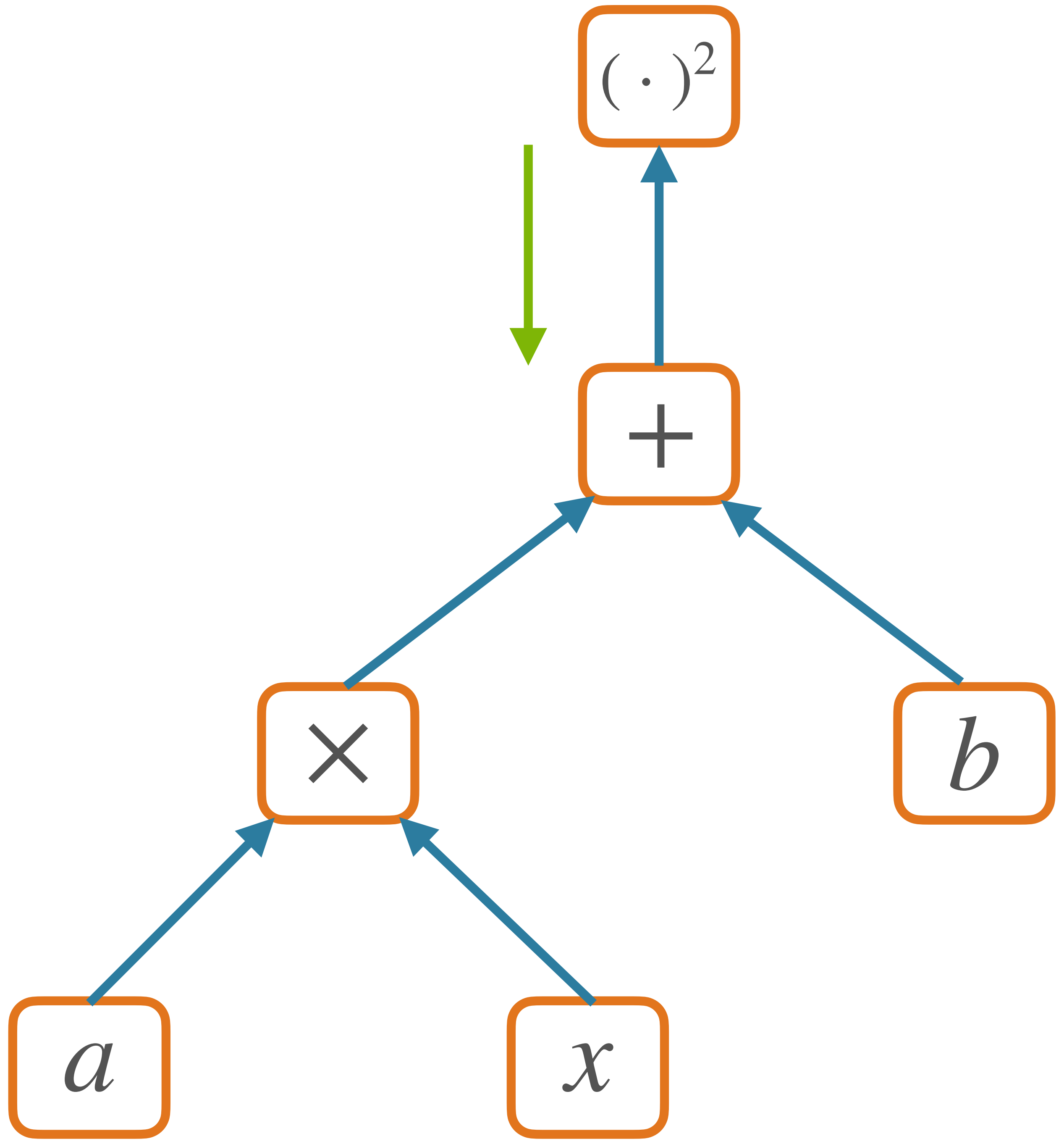

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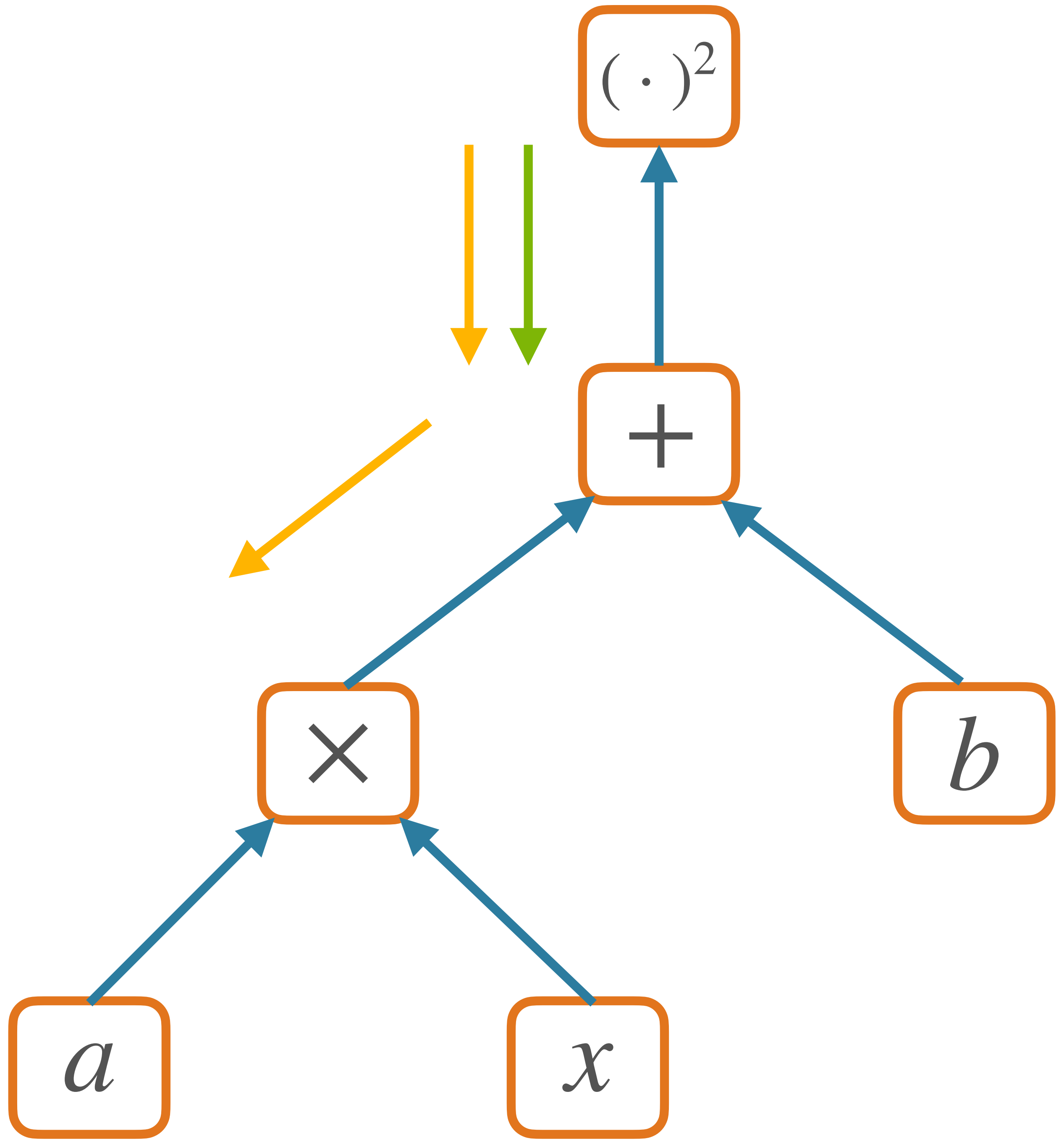

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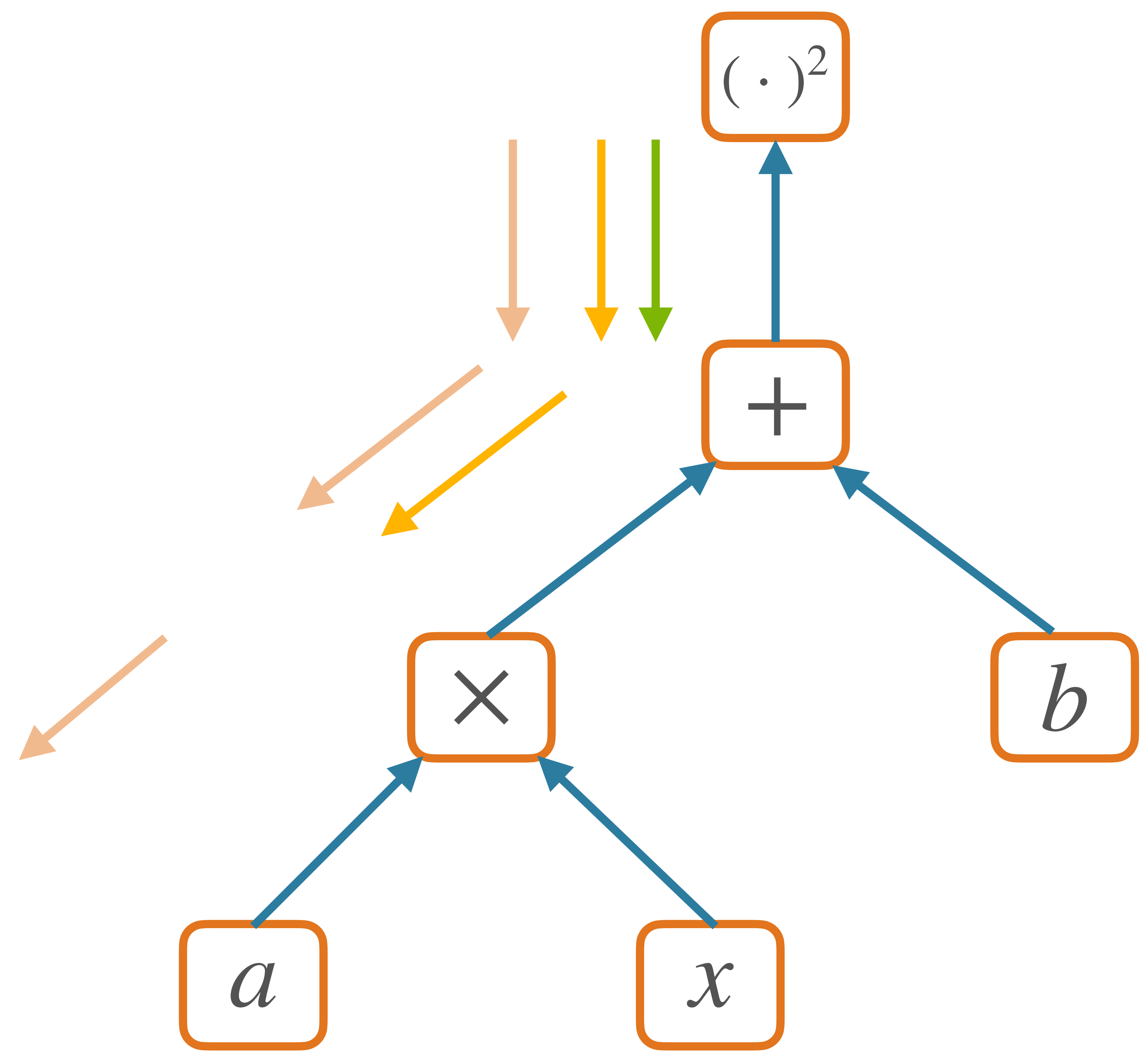

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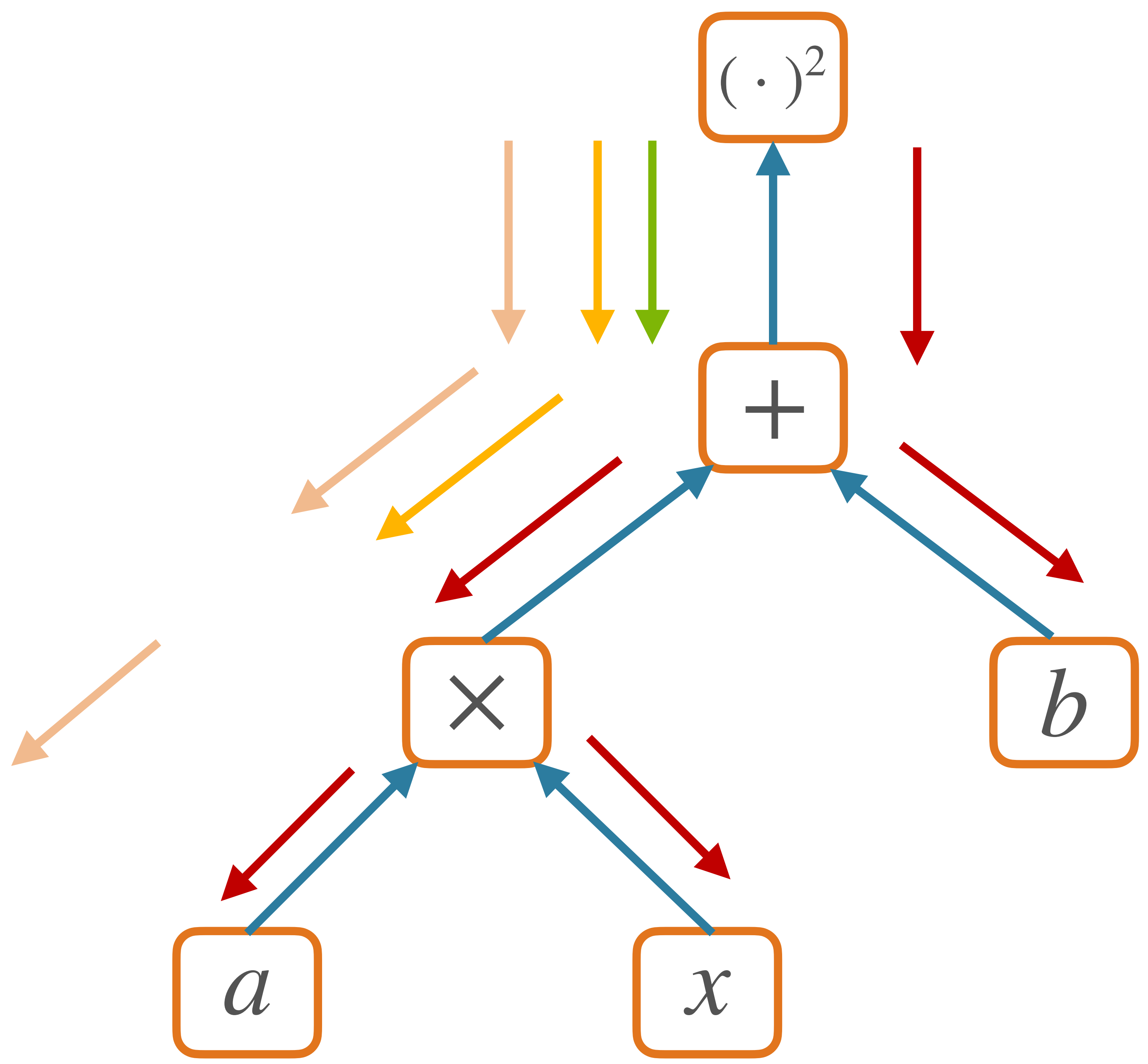

Forward/backward API

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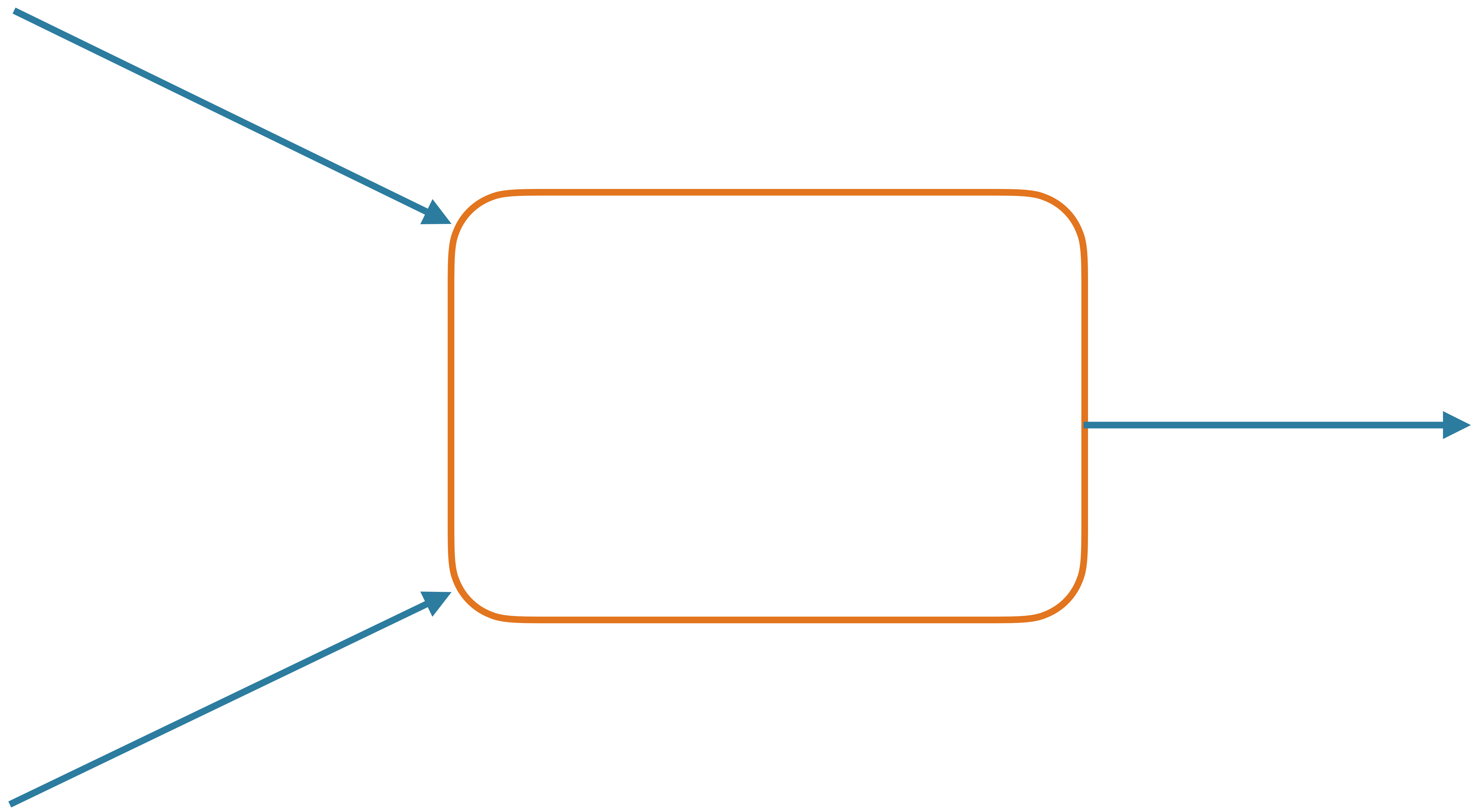

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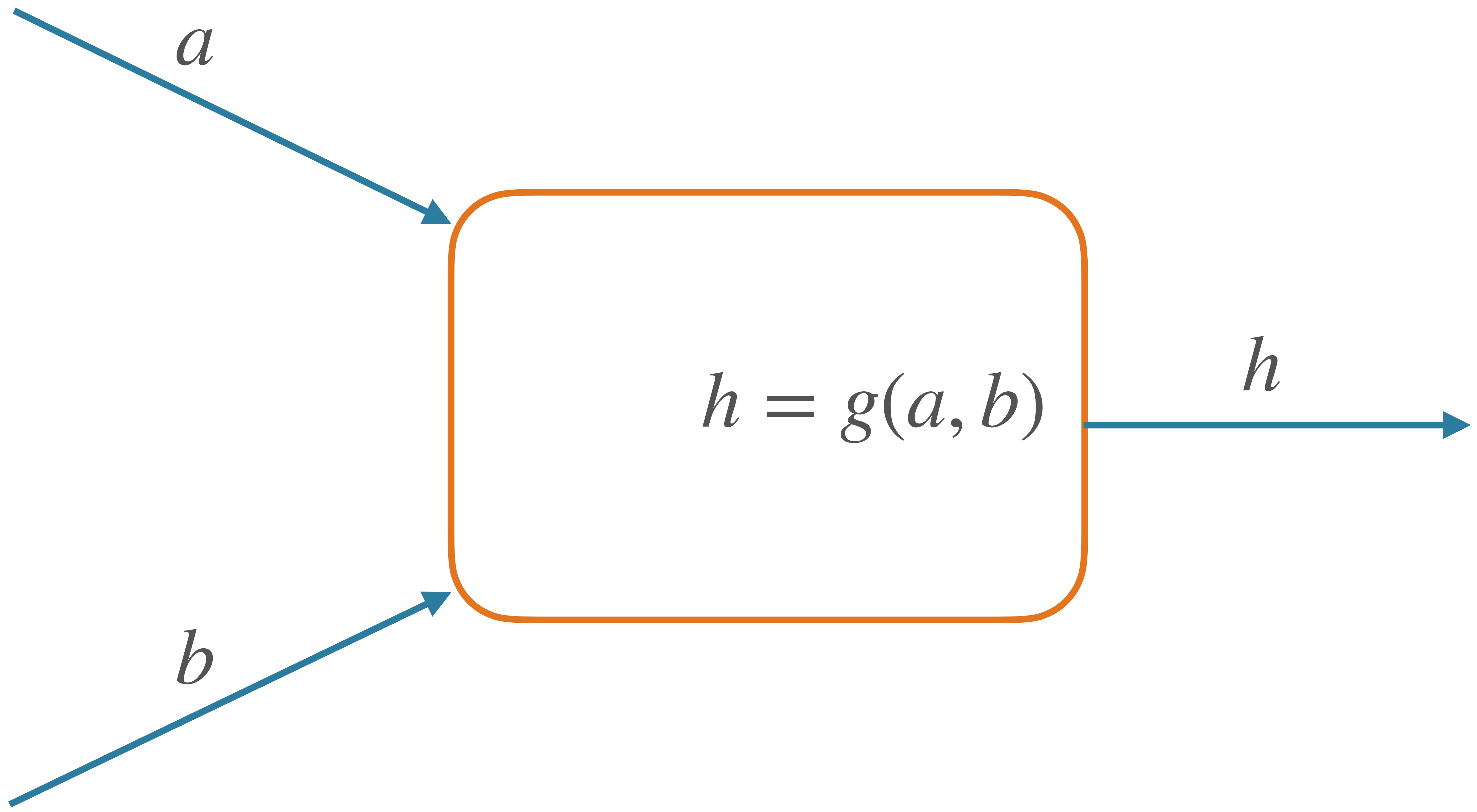

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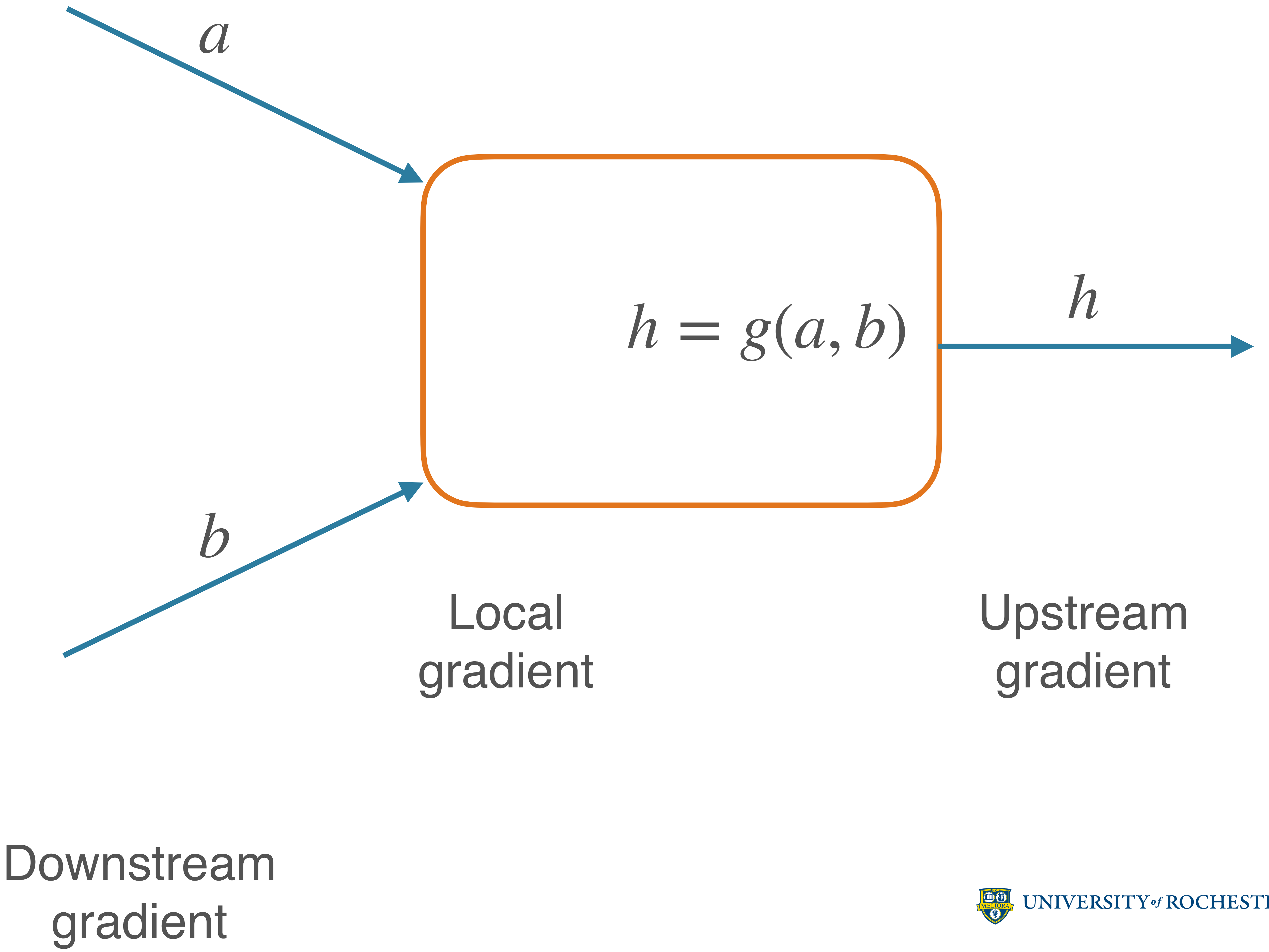

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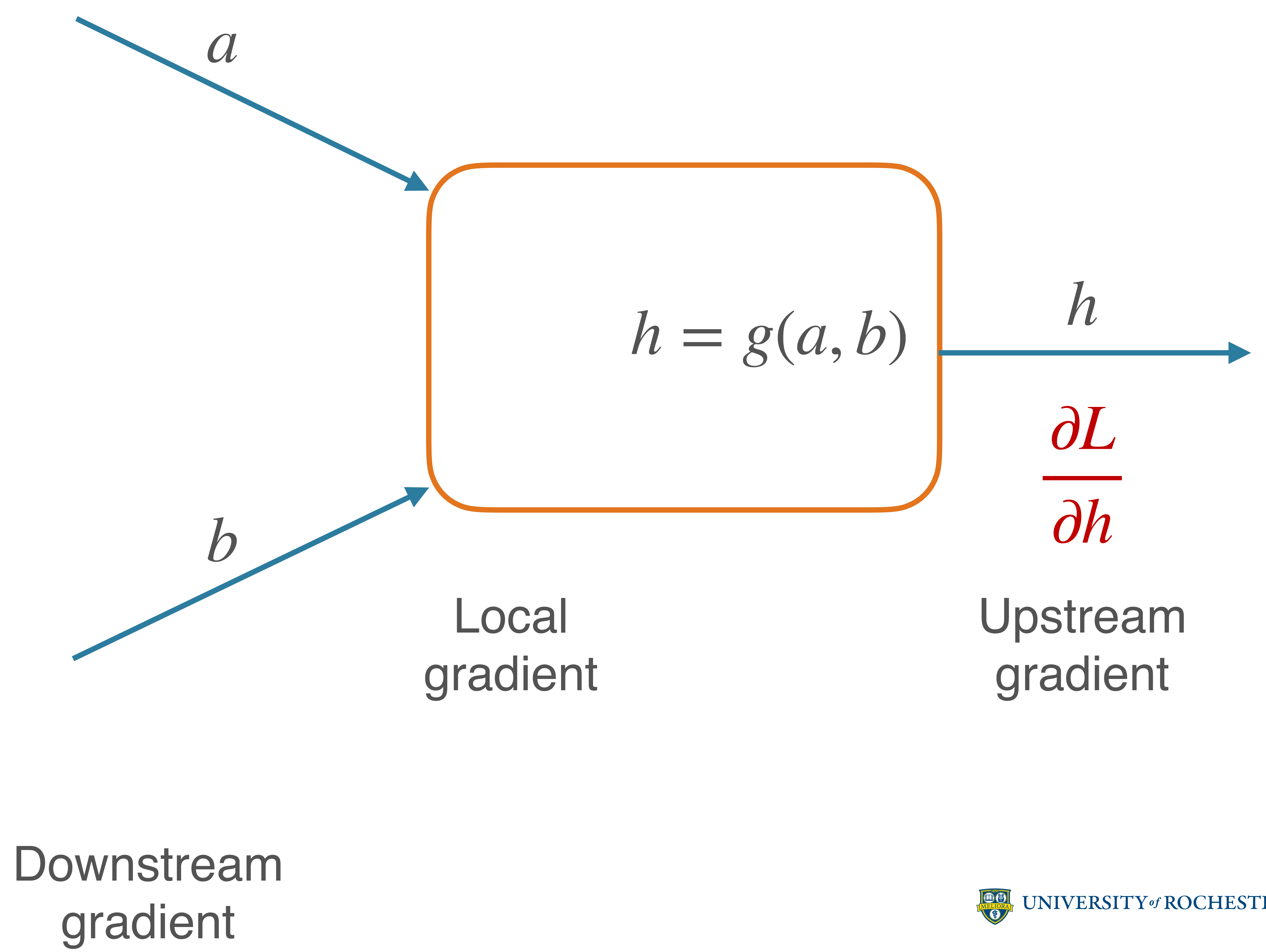

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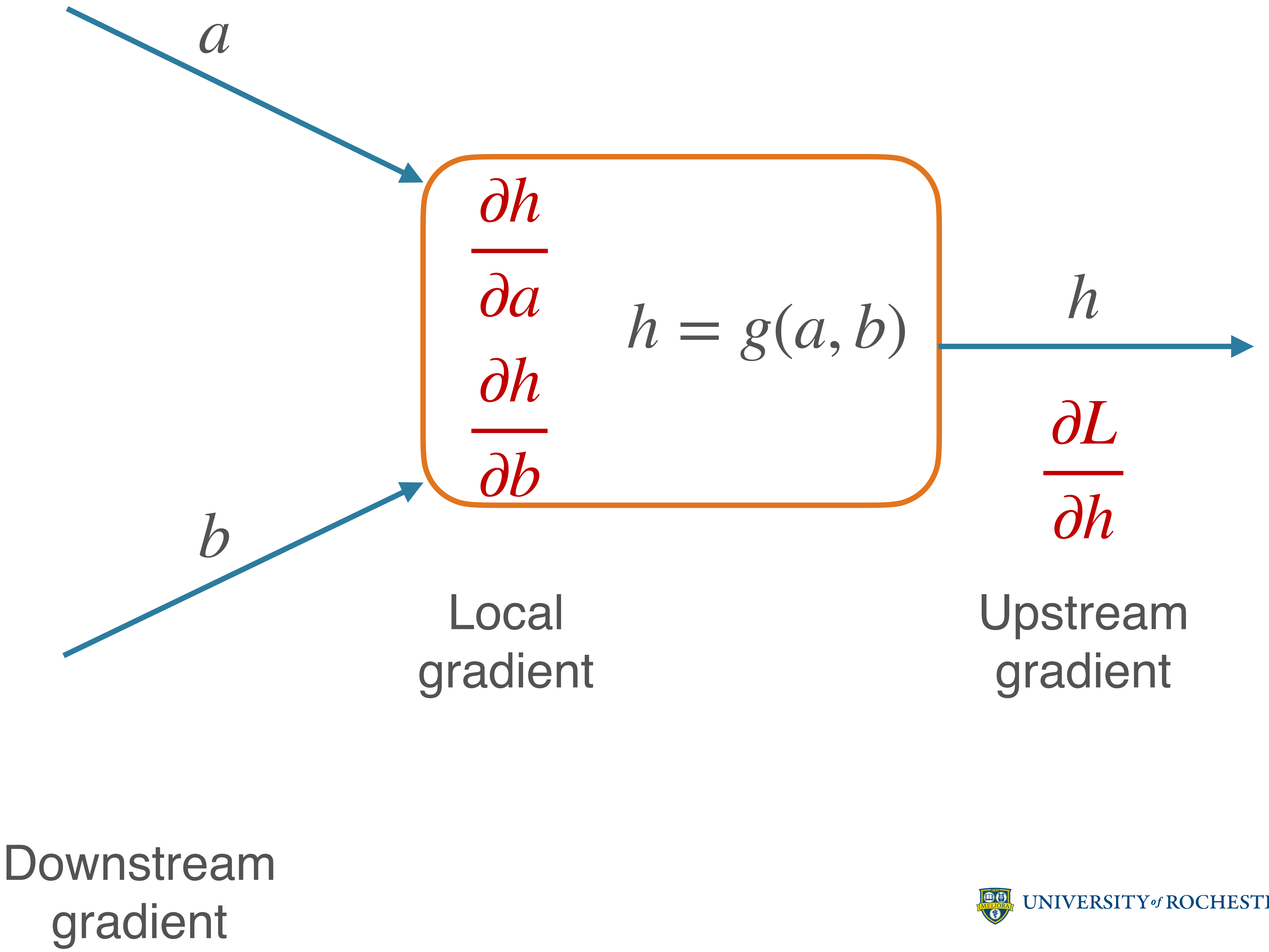

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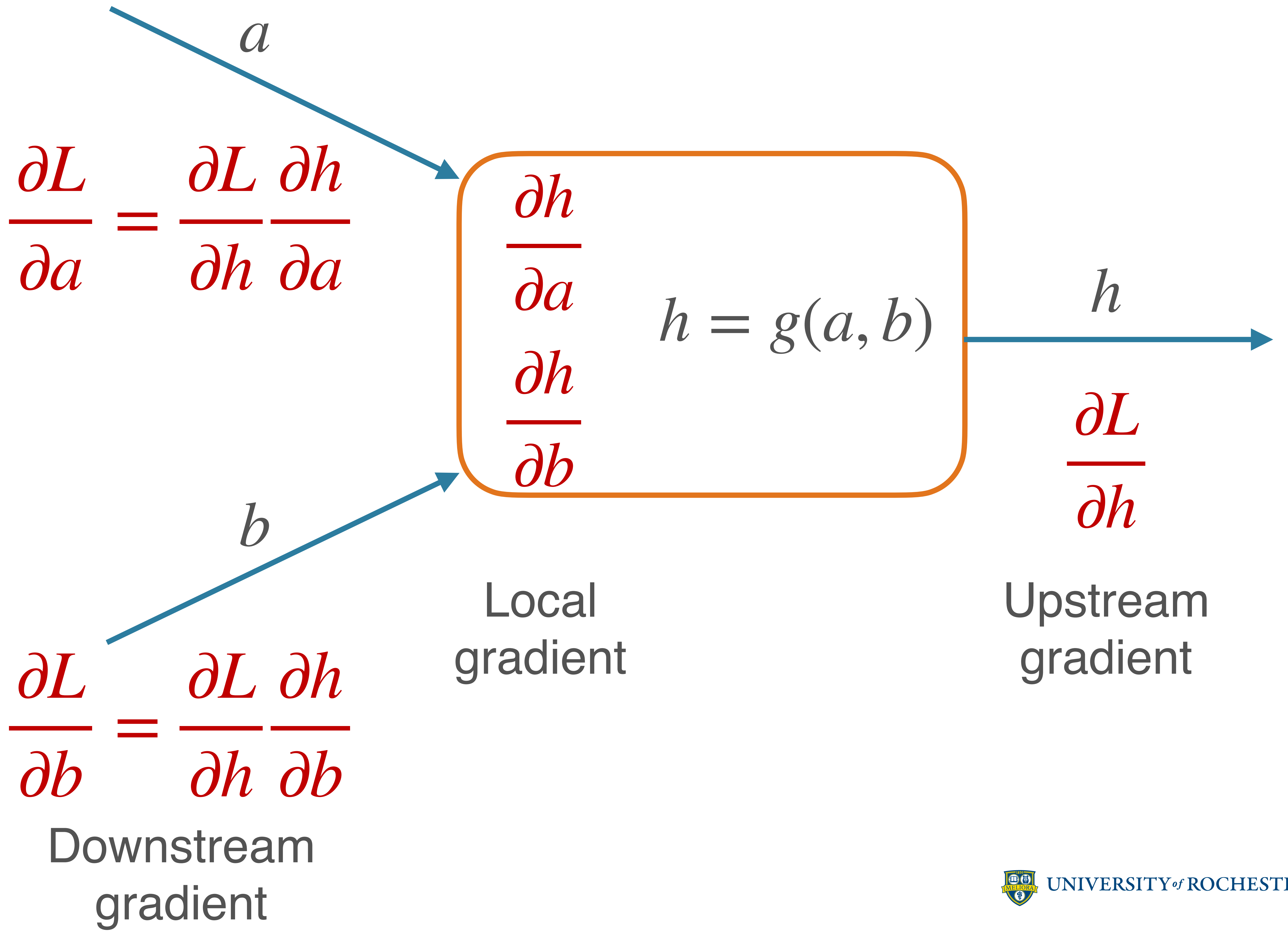


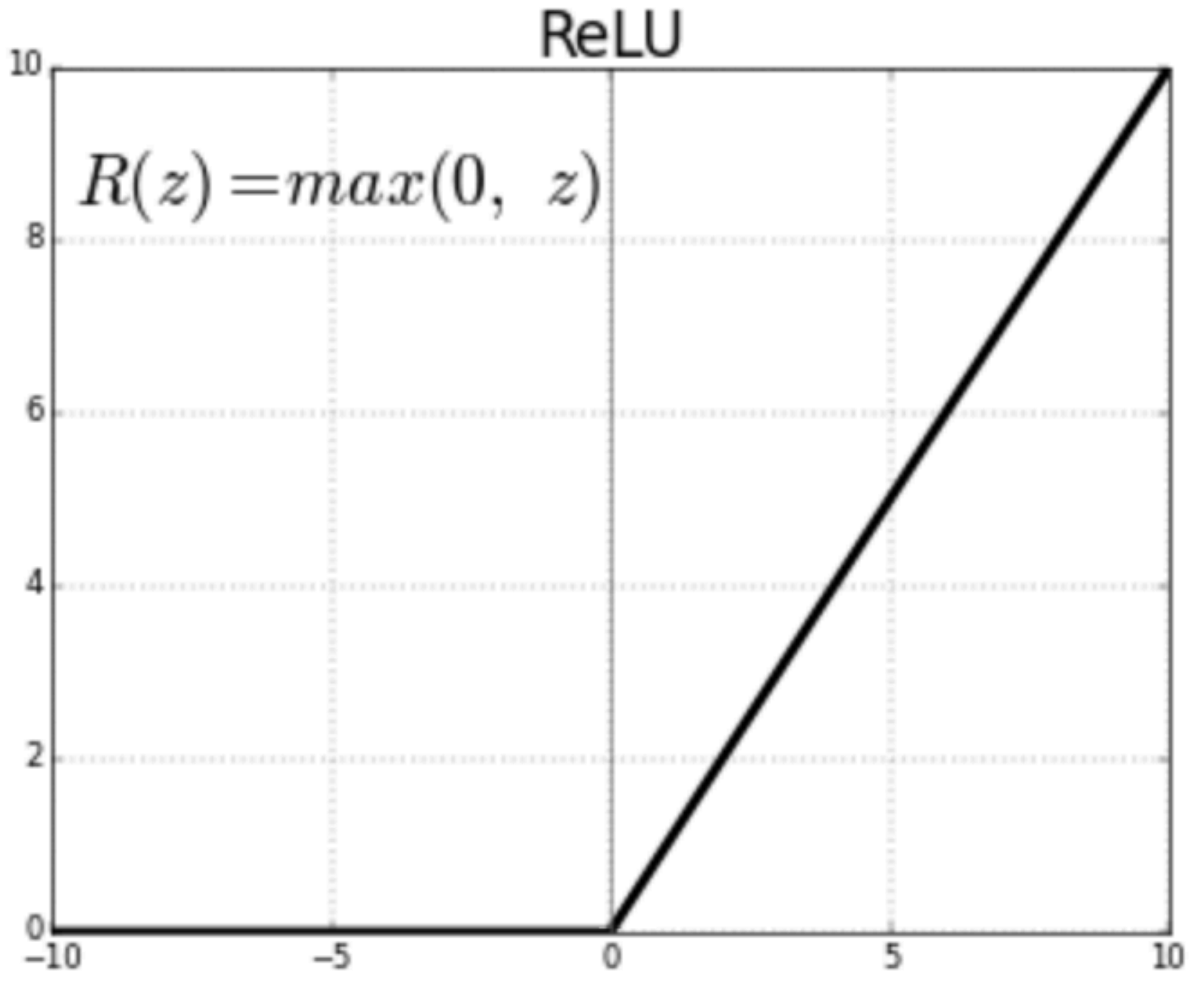
Example: Addition

```python
@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

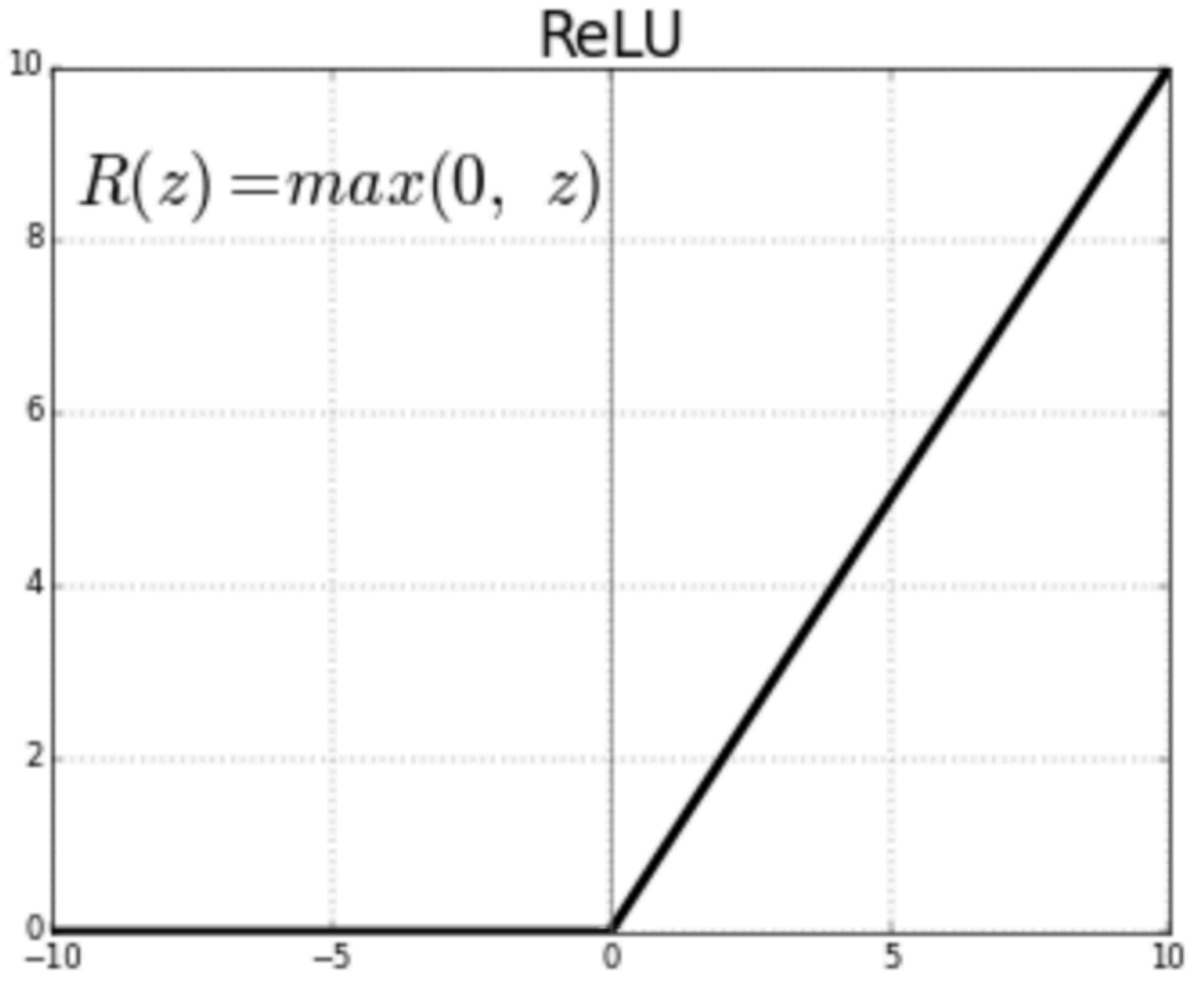


$\text{ReLU}(x) = \max(0, x)$

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

  def backward(ctx, grad_output):
```

Example: ReLU



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

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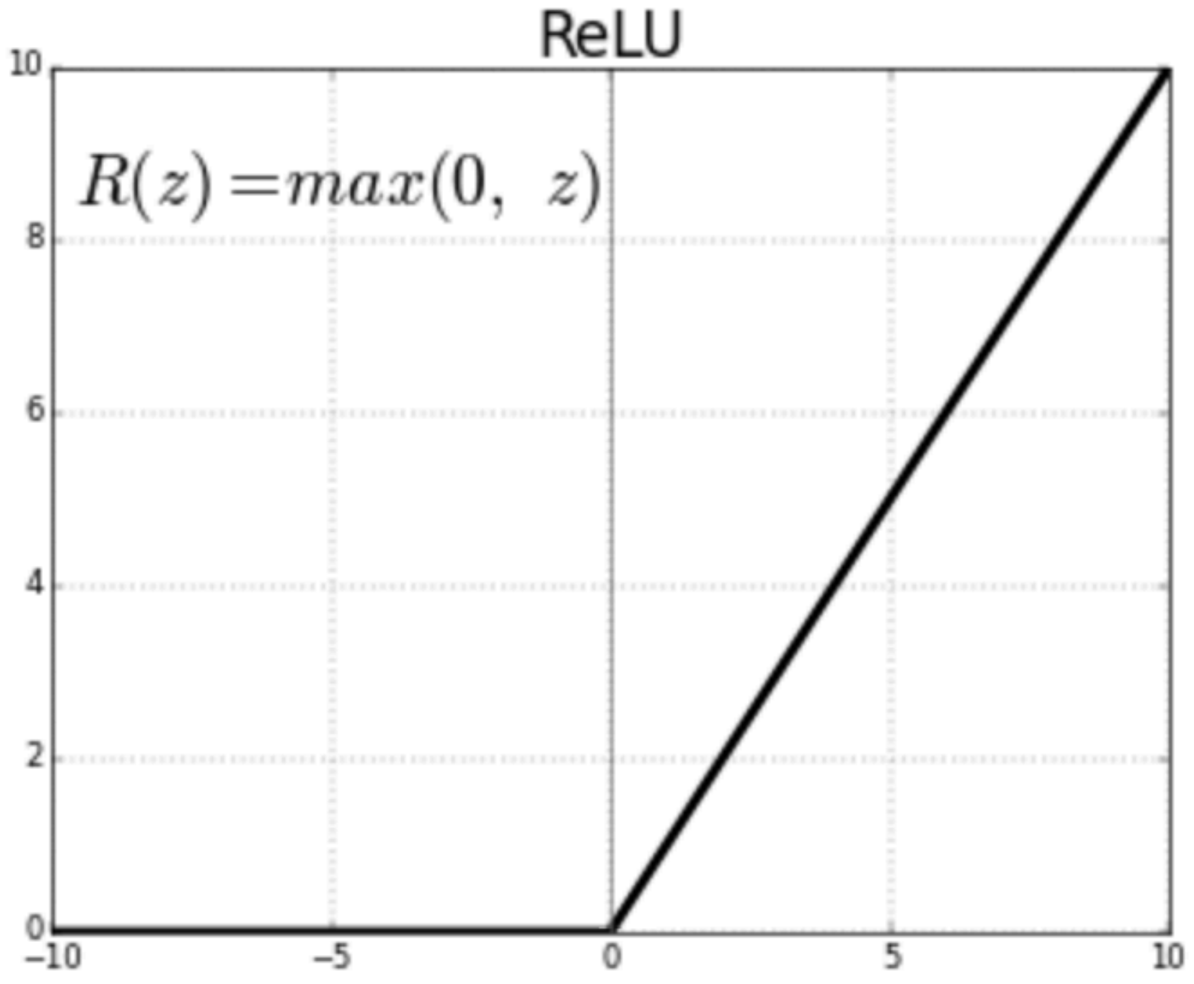

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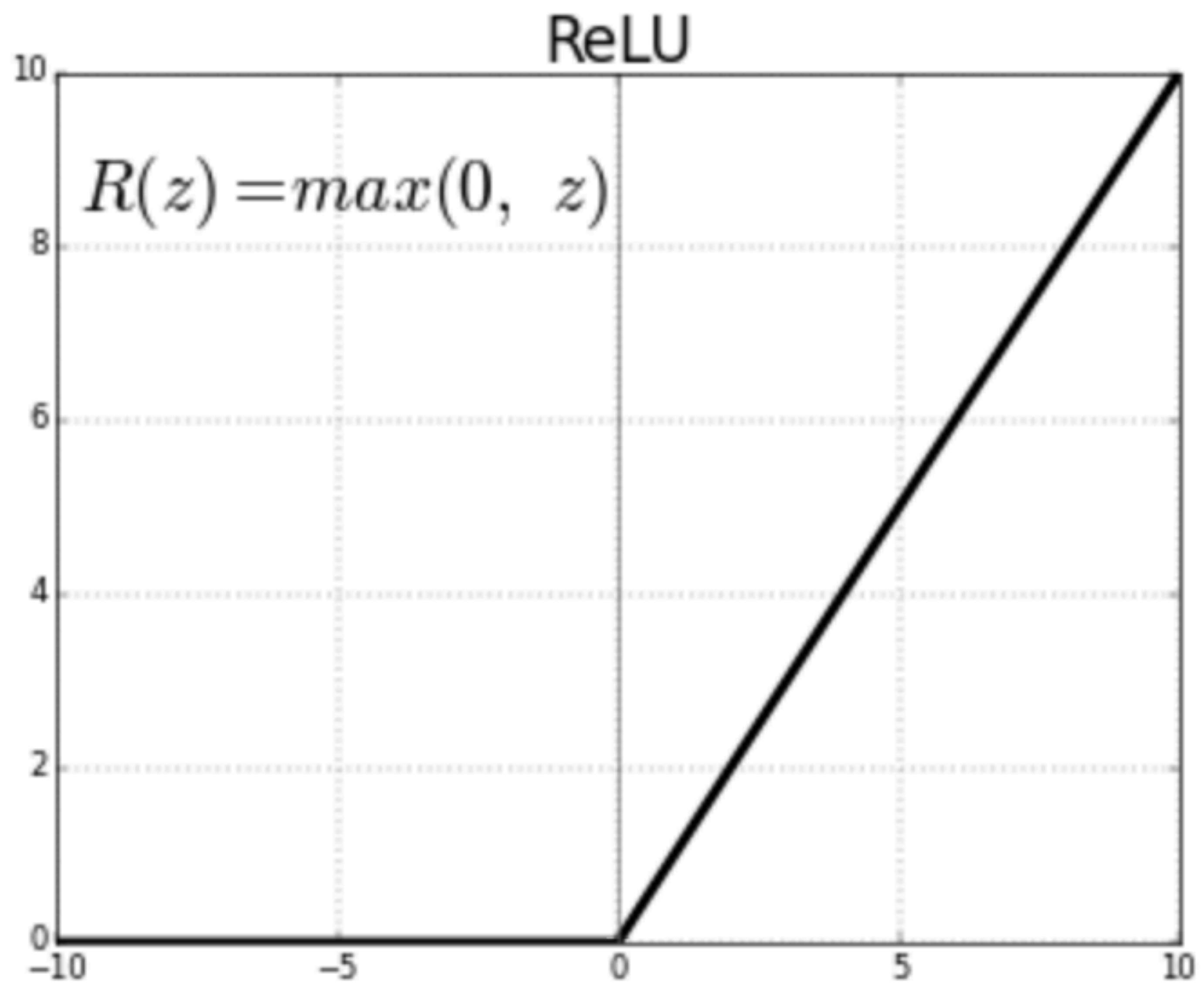
🤔🤔🤔 where's x???

Example: ReLU

```python
@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]
```



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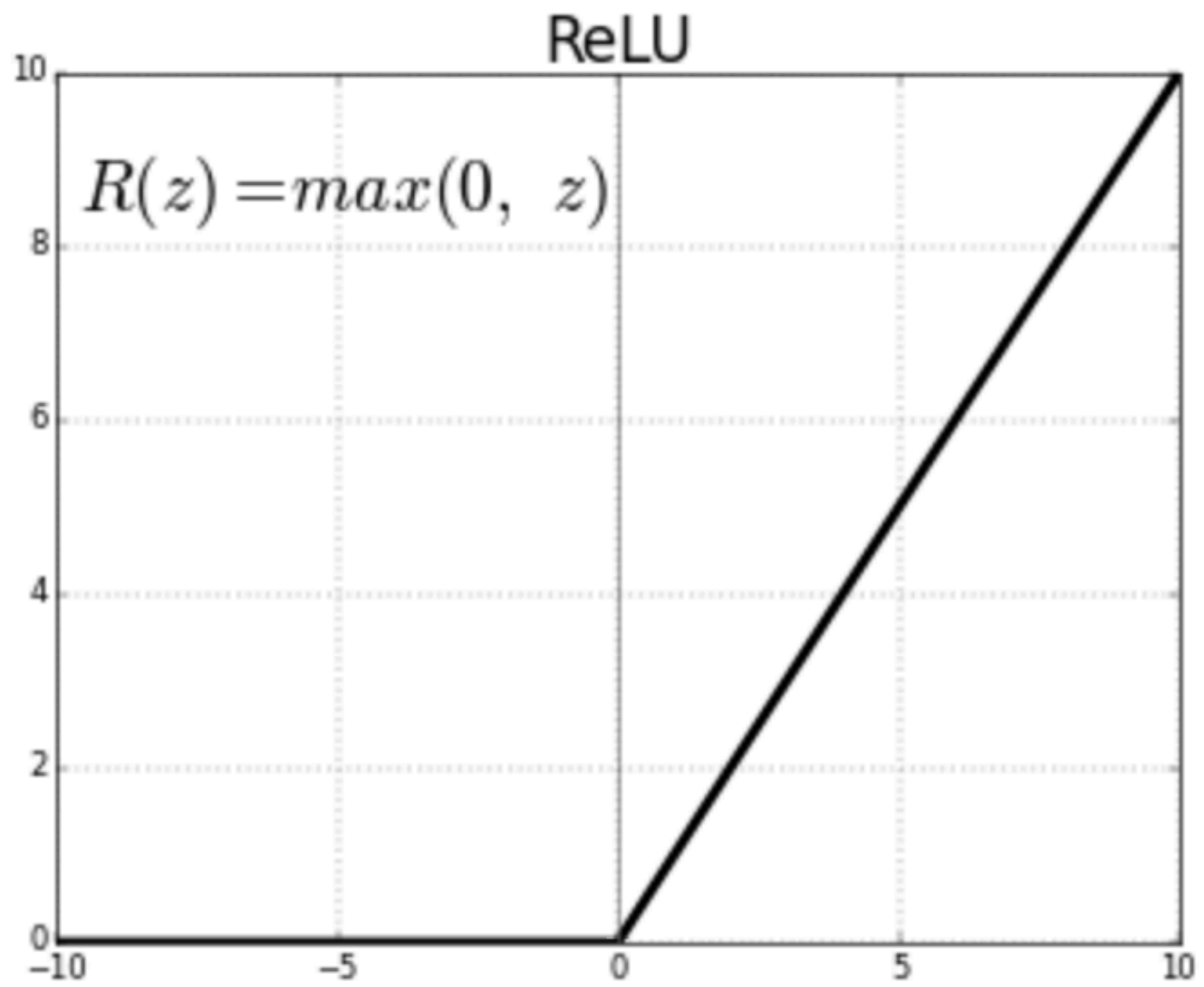

Save and retrieve the input value!

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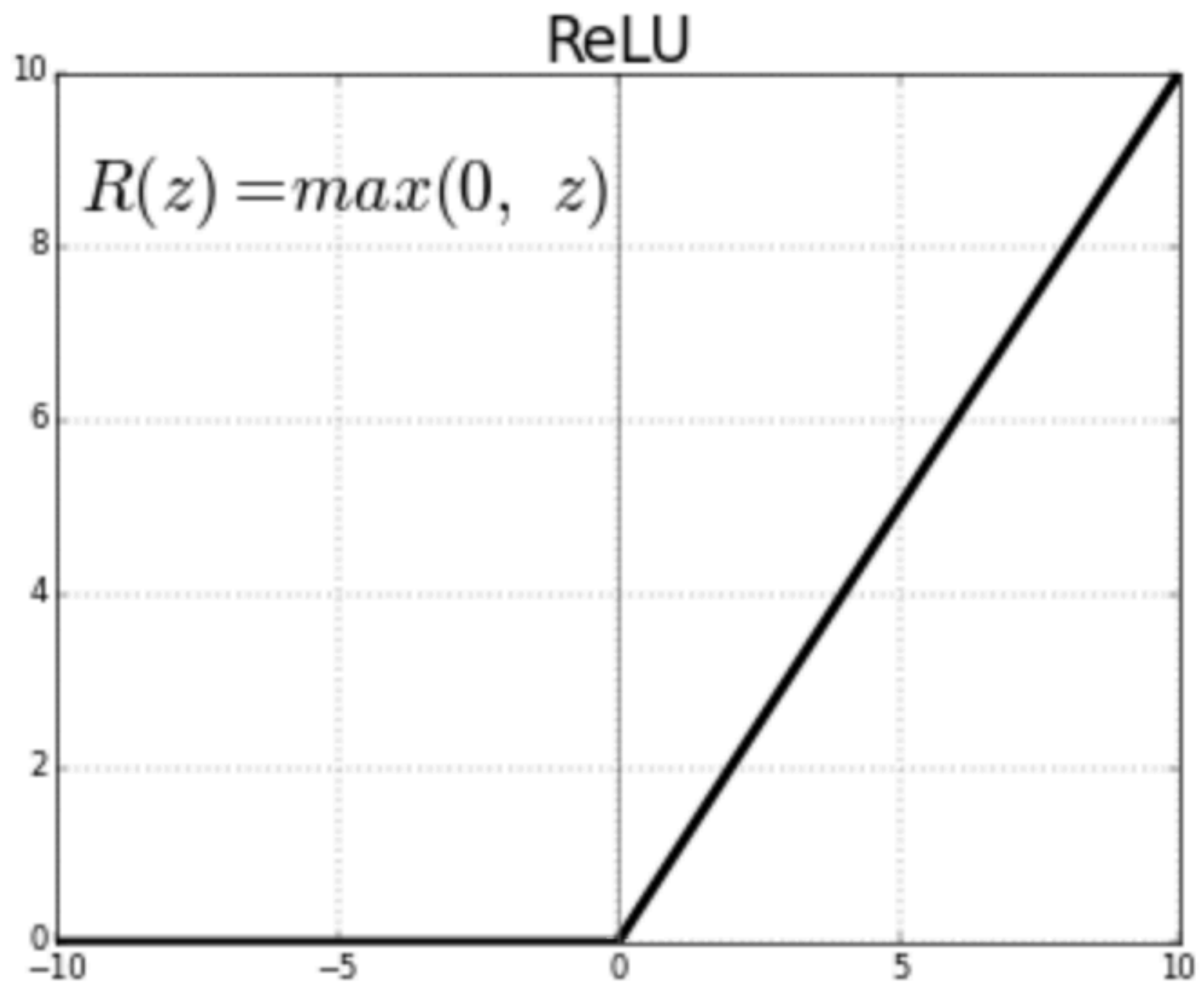
class relu(Operation):
    @staticmethod
    def forward(ctx, value):
        new_val = np.maximum(0, value)
        ctx.append(new_val)
        return new_val

    @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

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@tensor_op
class relu(Operation):
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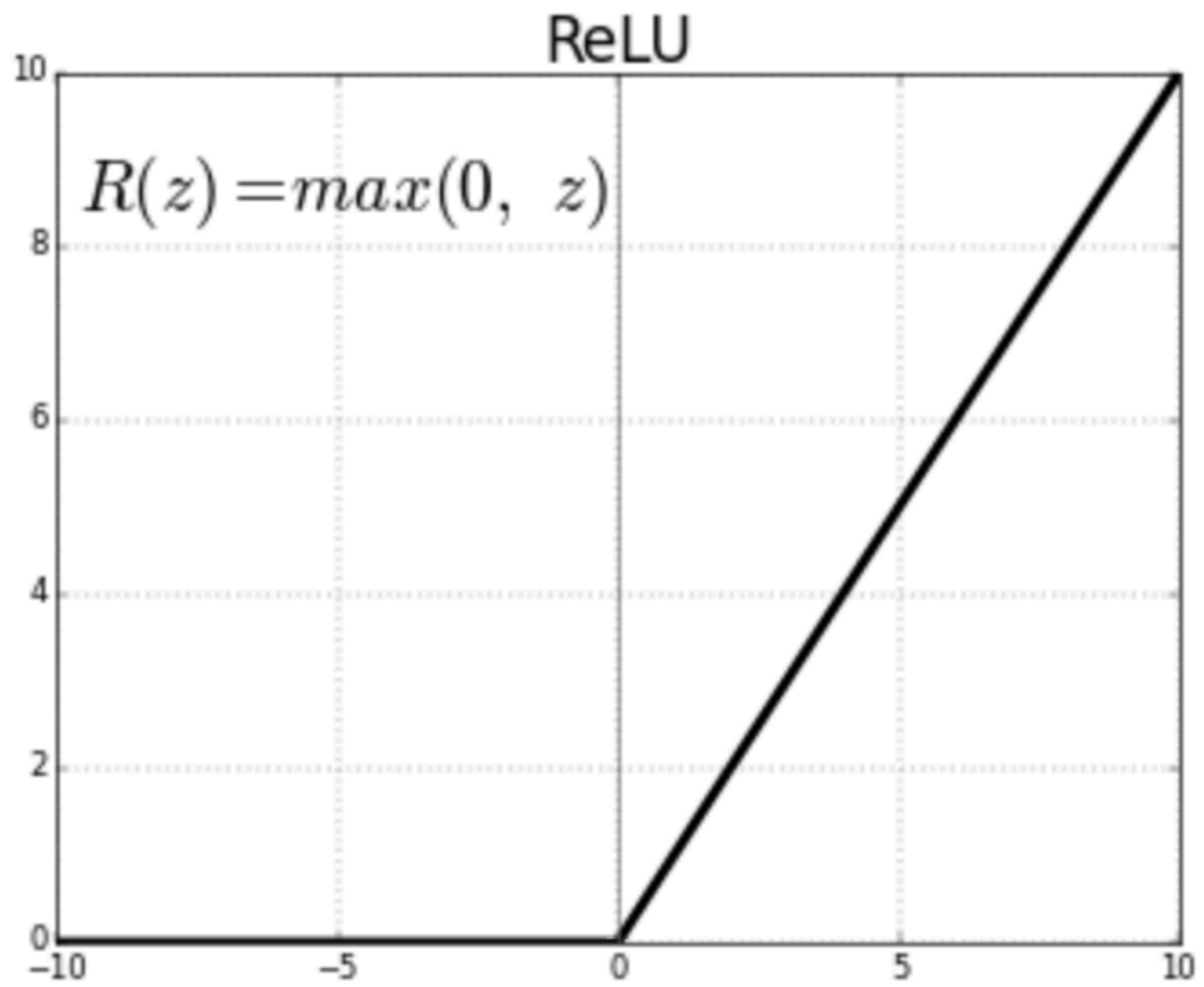
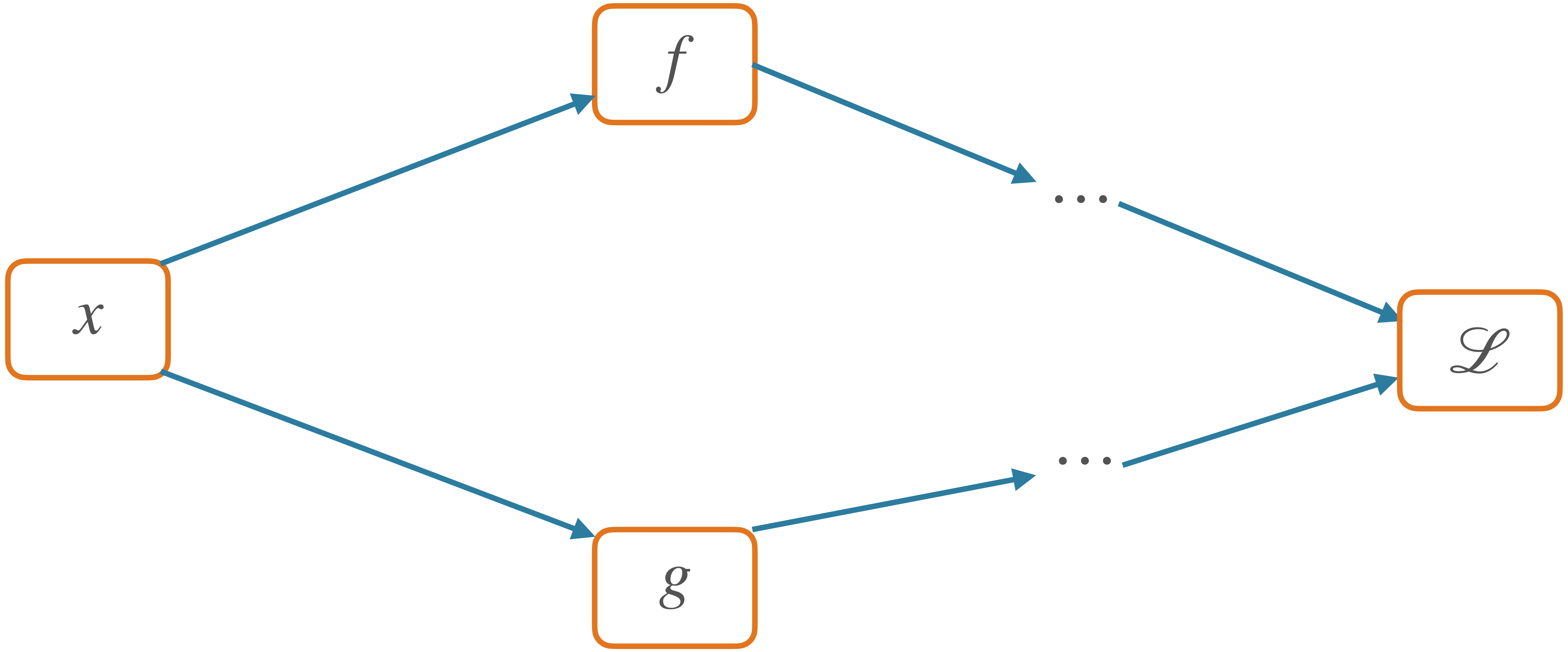


Save and retrieve the input value!

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

local gradient times upstream gradient

Adding Gradients with Multiple Outputs



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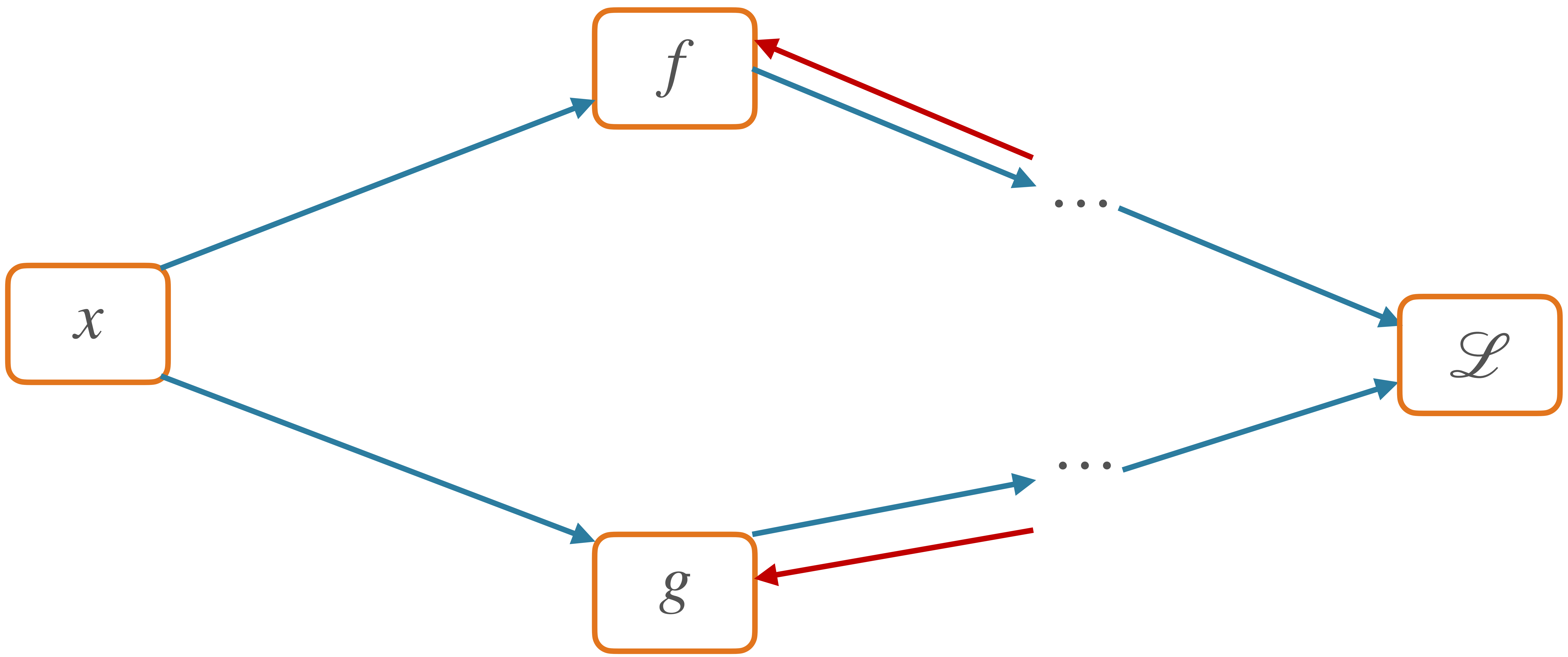

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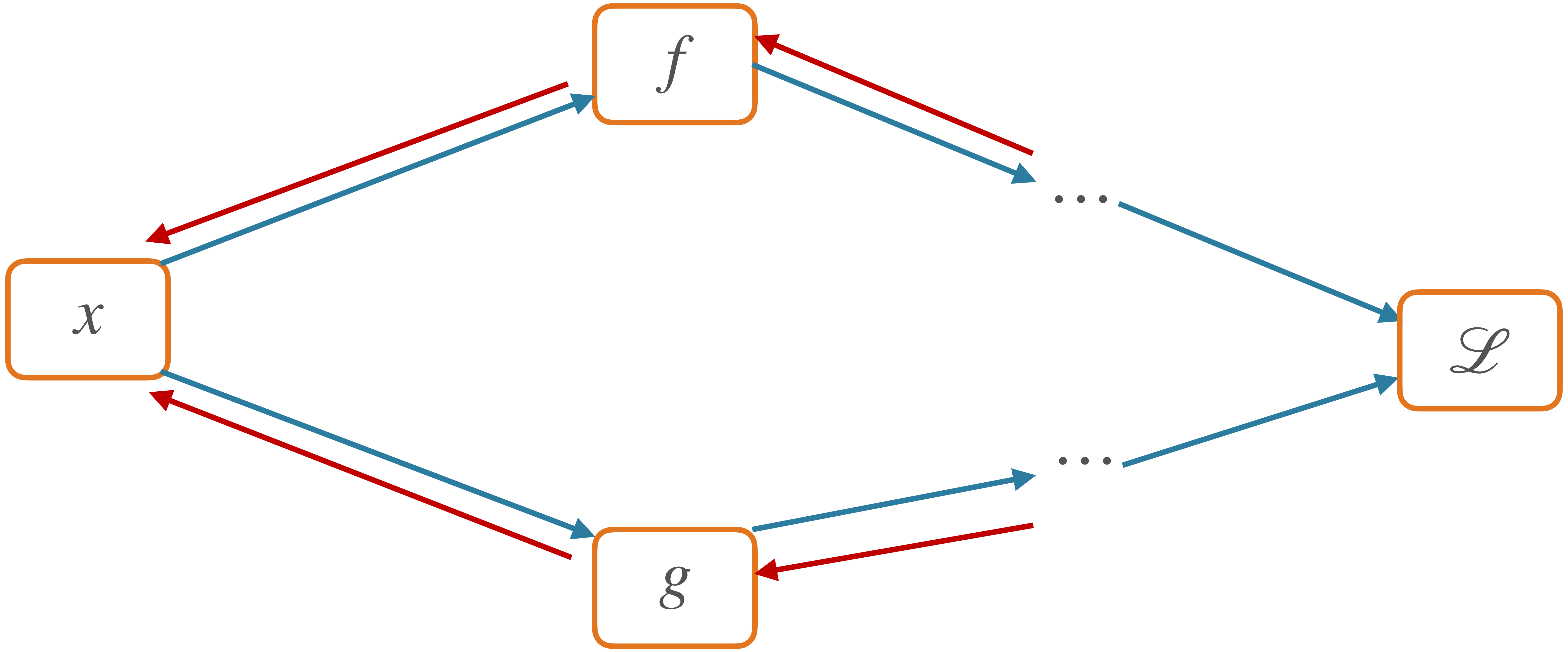

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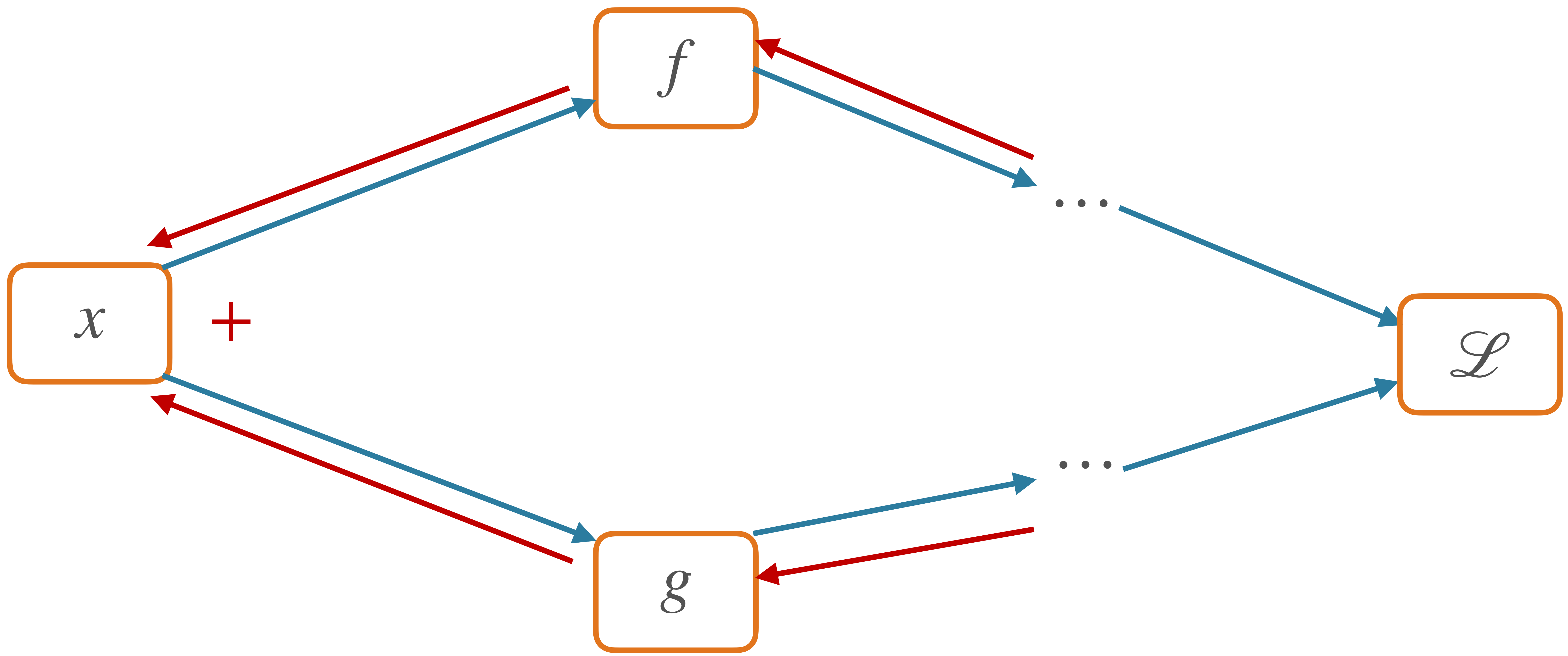

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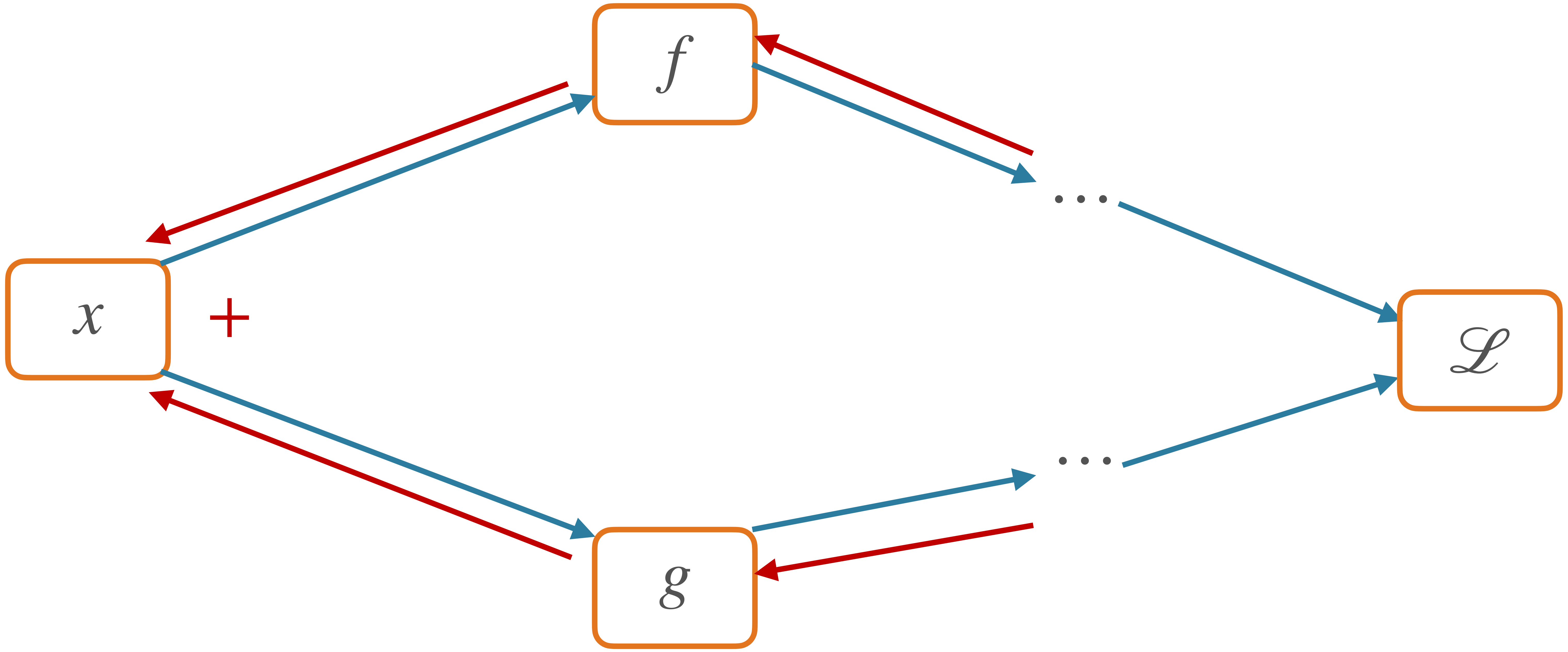


Multivariable chain rule: $\dfrac{\partial L}{\partial x} = \dfrac{\partial L}{\partial f}\dfrac{\partial f}{\partial x} + \dfrac{\partial L}{\partial g}\dfrac{\partial g}{\partial x}$

Adding Gradients with Multiple Outputs

Live demo and/or exercise!

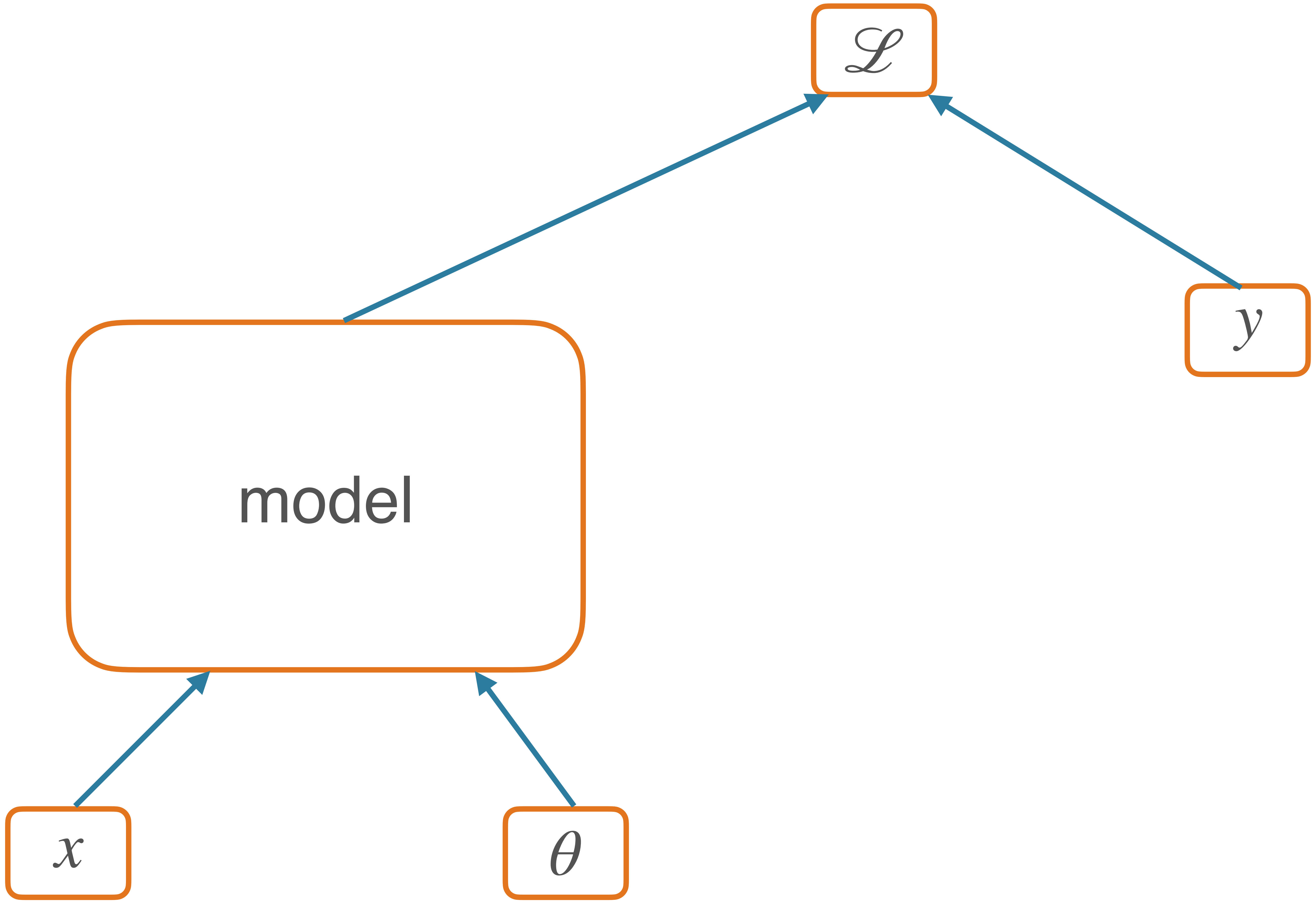
$$f(x) = x^2 \times 3x$$

Adding Gradients with Multiple Outputs

```python
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()
```

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Backprop the loss

Update the parameters