

Computation Graphs + Backpropagation

LING 574 Deep Learning for NLP

Shane Steinert-Threlkeld

Announcements

- HW1 reference code made available in hw1/ref in our dropbox
- HW2's vocabulary.py is a symlink to vocabulary.py in hw1/ref
 - You can symbolic link to it from your directory to use:
 - `ln -s /dropbox/23-24/574/hw1/ref/vocabulary.py vocabulary.py`
- Some old file path issues: should be fixed now, but let us know!

Today's Plan

- Finish neural network intro [activation functions, batch computation, ...]
- Computation graph abstraction
- Backpropagation
 - “Calculus on computation graphs”
- Forward/backward API

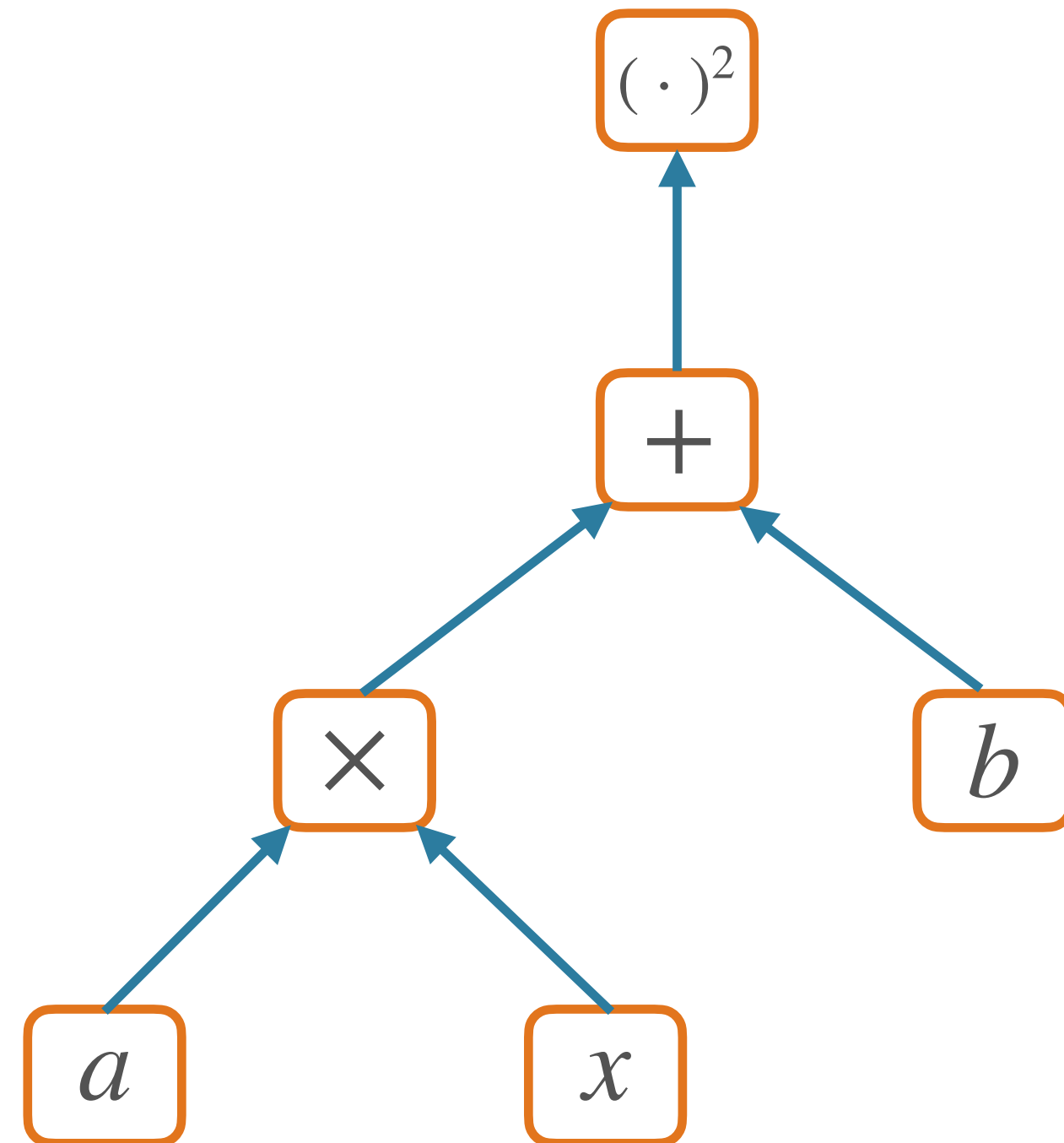
Computation Graphs

What is a computation graph?

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

Computation Graph Example

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

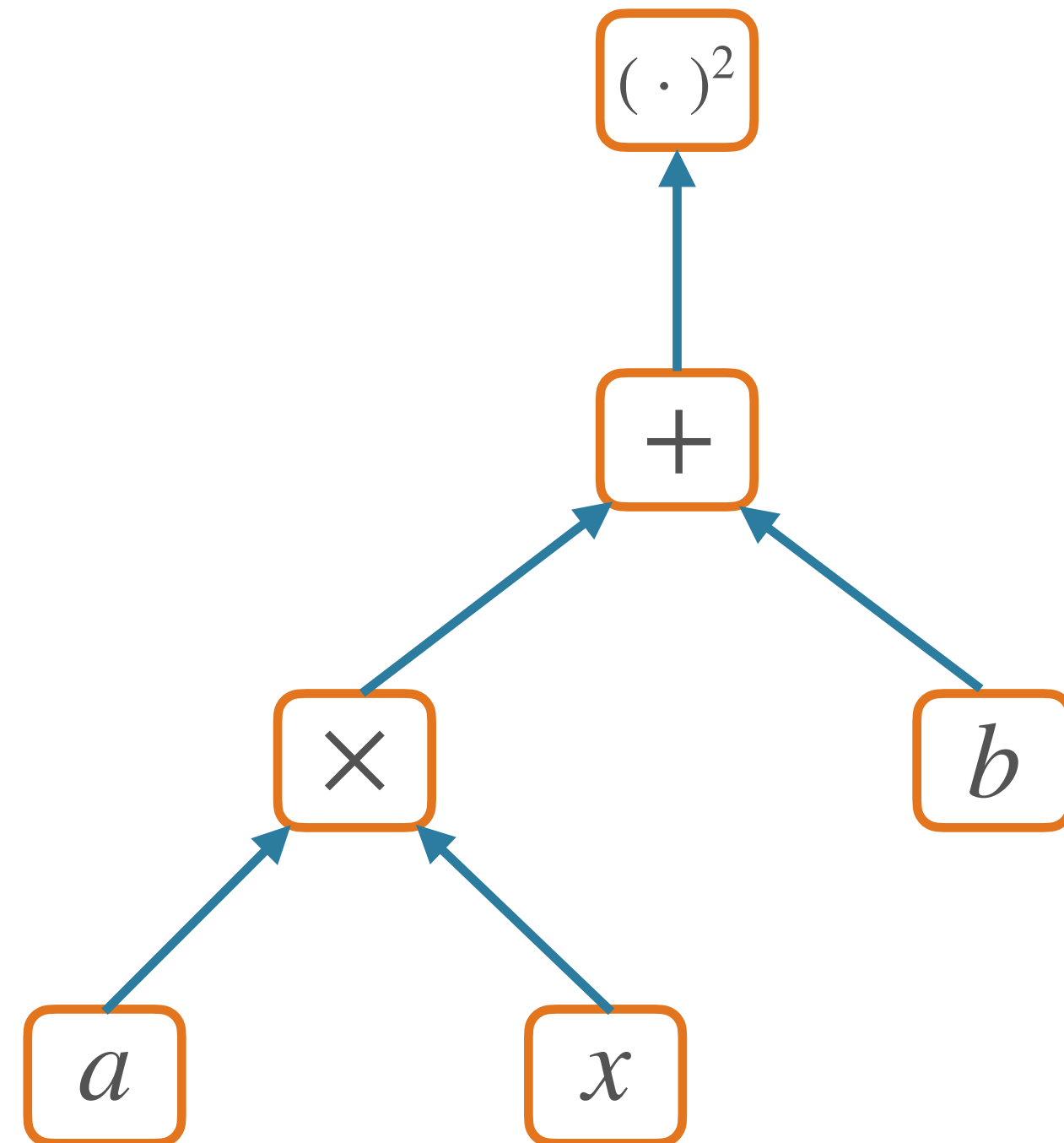


Forward Pass

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

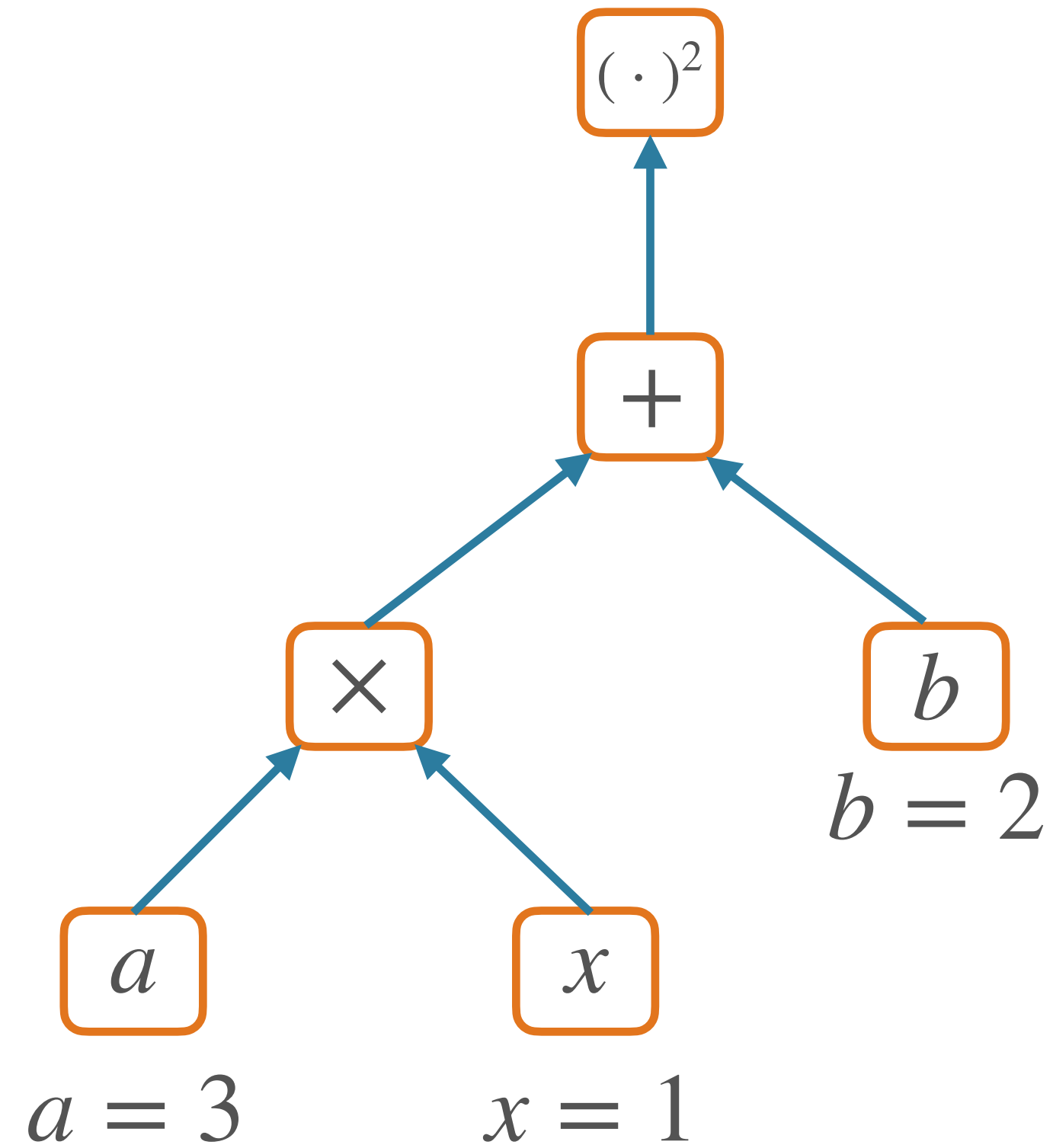
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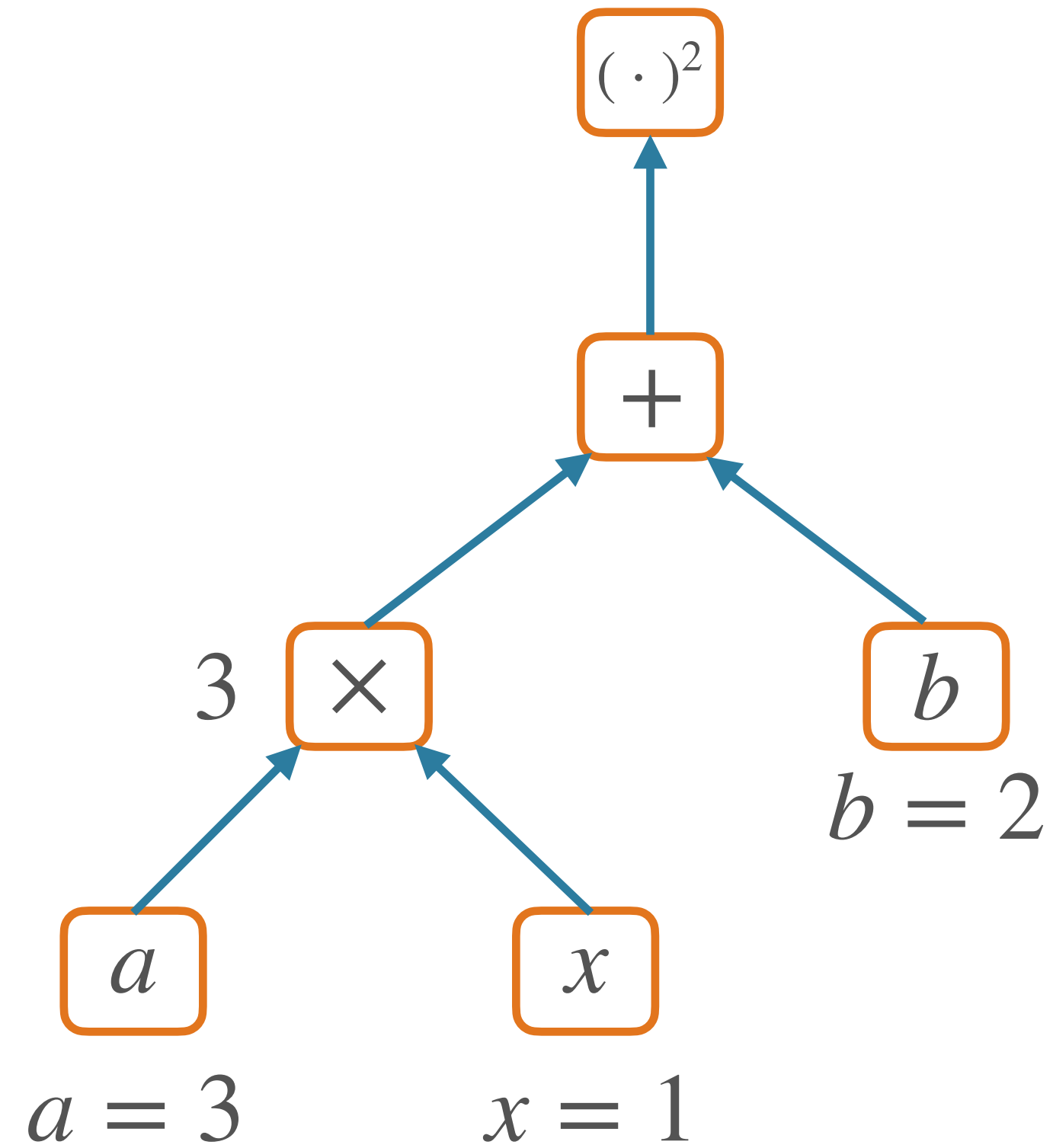
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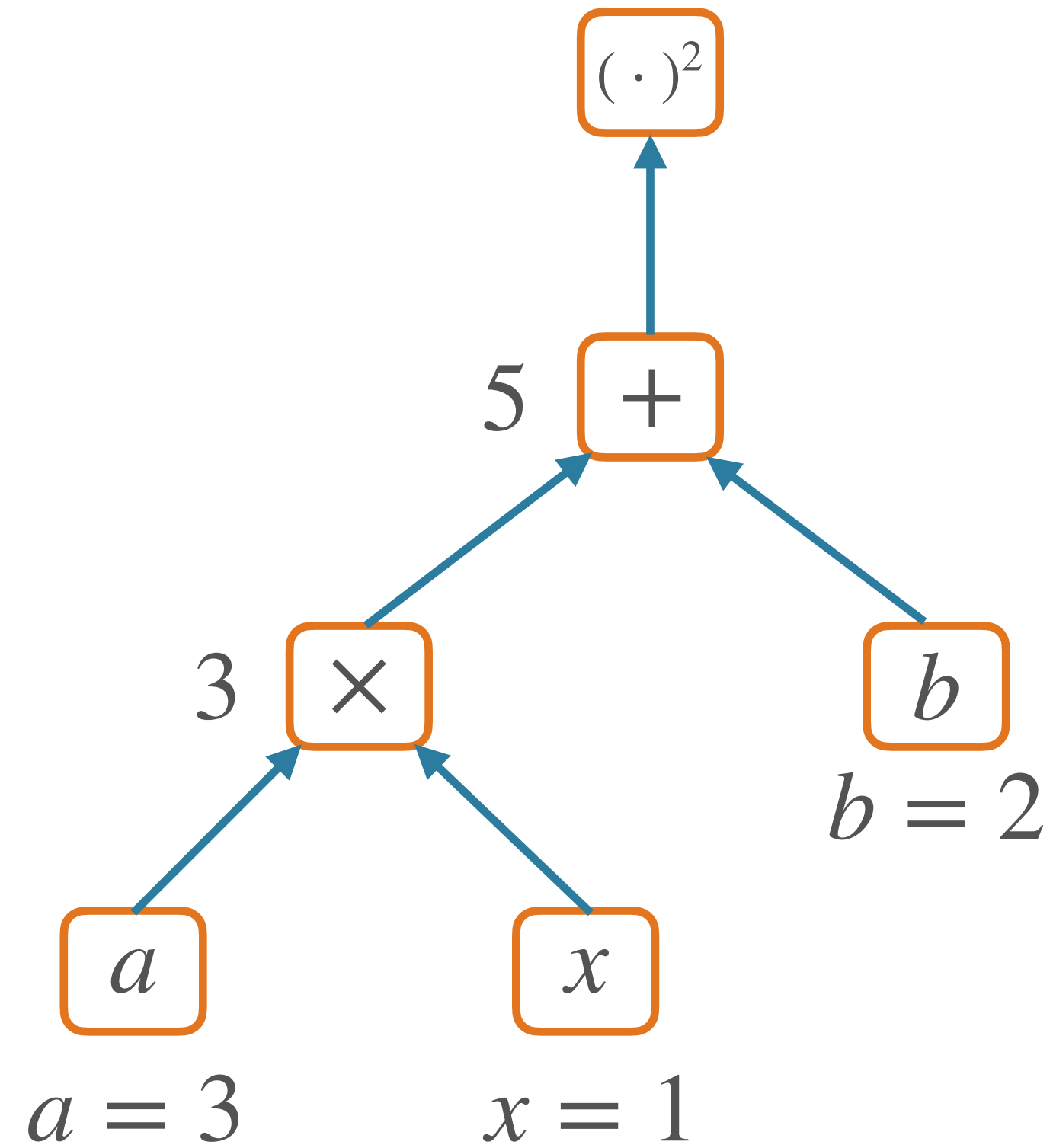
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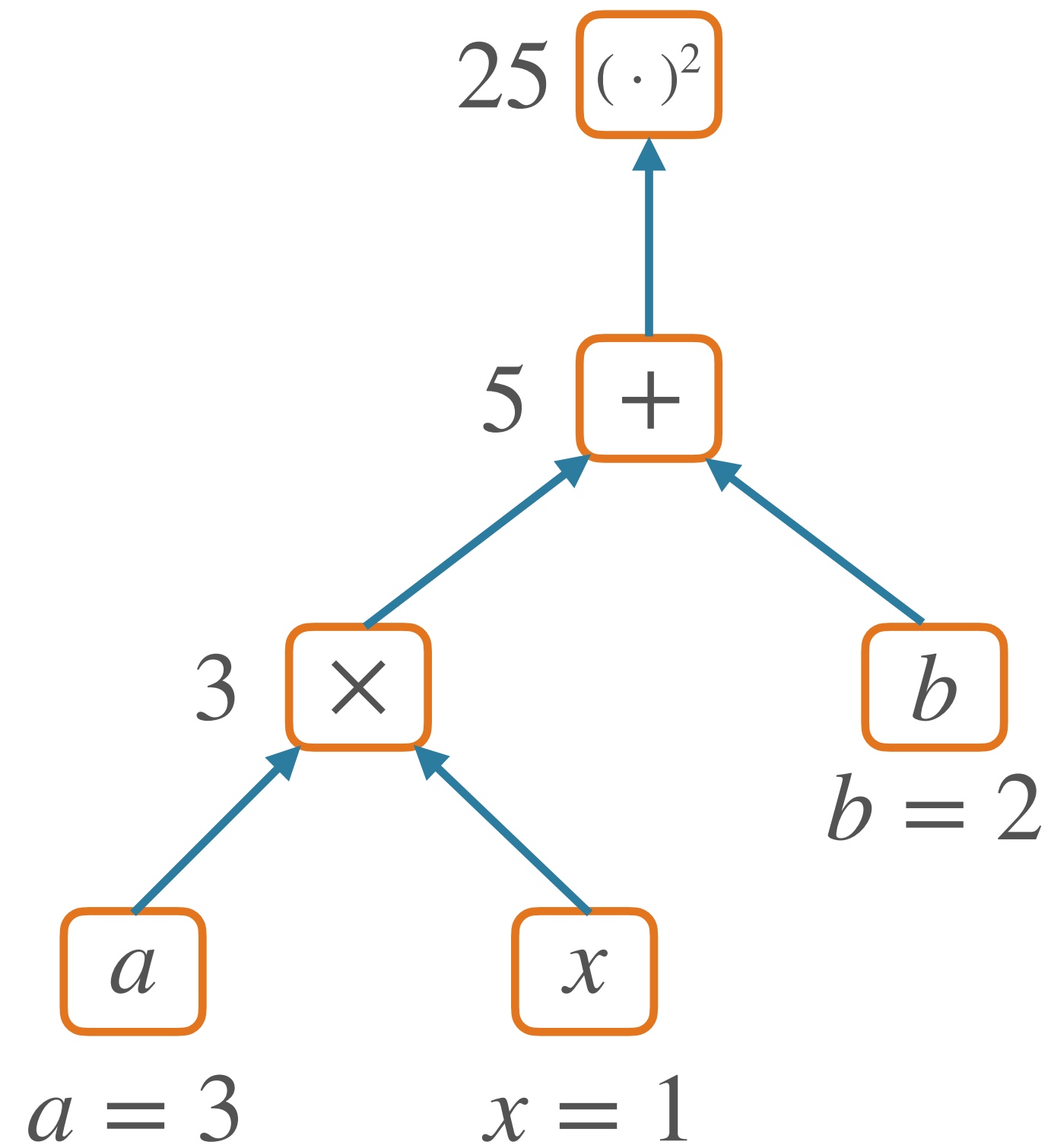
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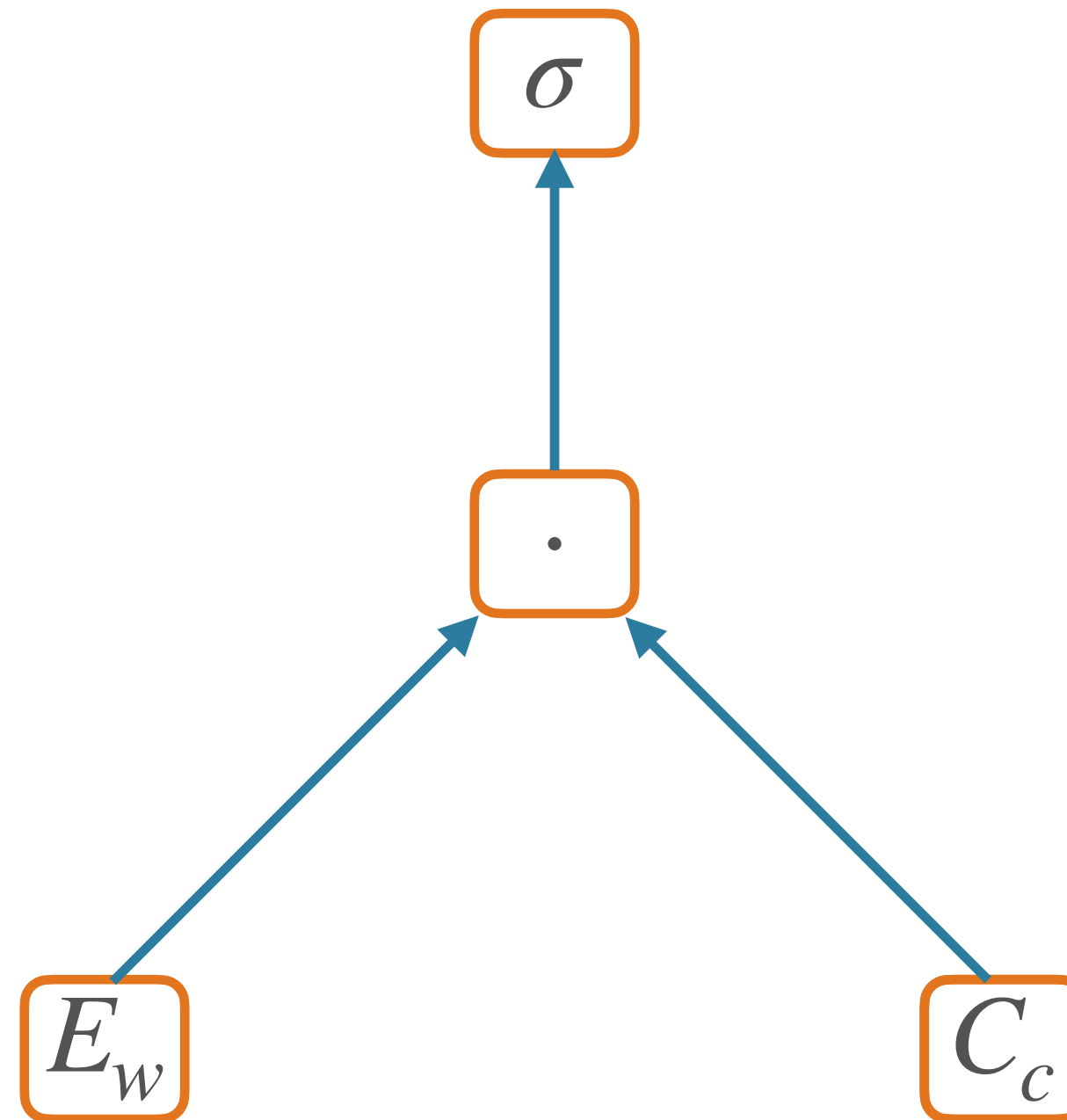


Nodes in a Graph

- Node: a Tensor value
 - e.g. numpy ndarray; n-dimensional array of values
 - Scalar, vector, matrix, ...
- Edge: function argument
 - The value of a node is a function of the values of its parents
- For **forward**: node computes its value based on its parents' values

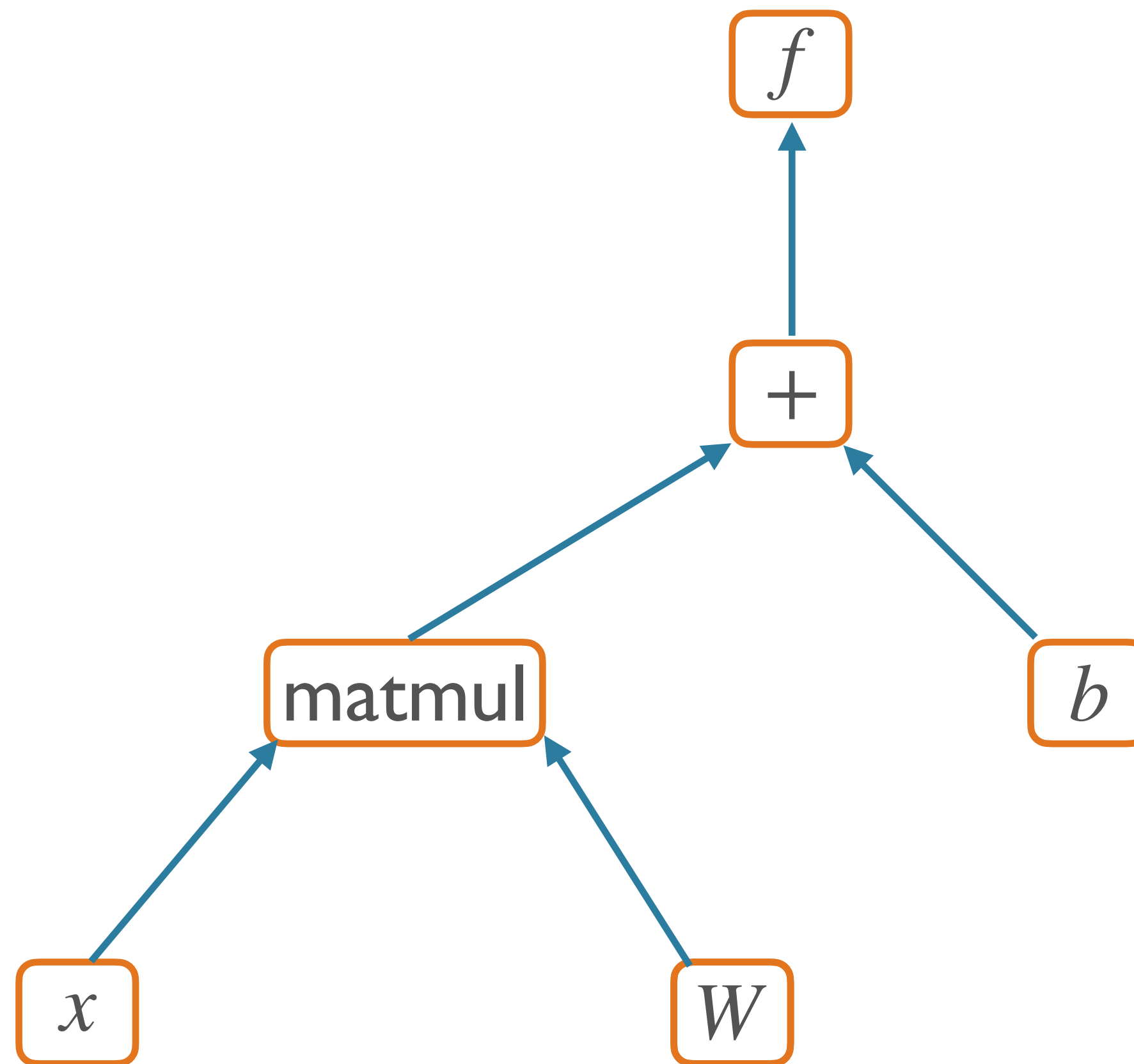
SGNS as a Graph

$$P(1 | w, c) = \sigma (E_w \cdot C_c)$$



Hidden Layer Graph

$$\hat{y} = f(xW + b)$$



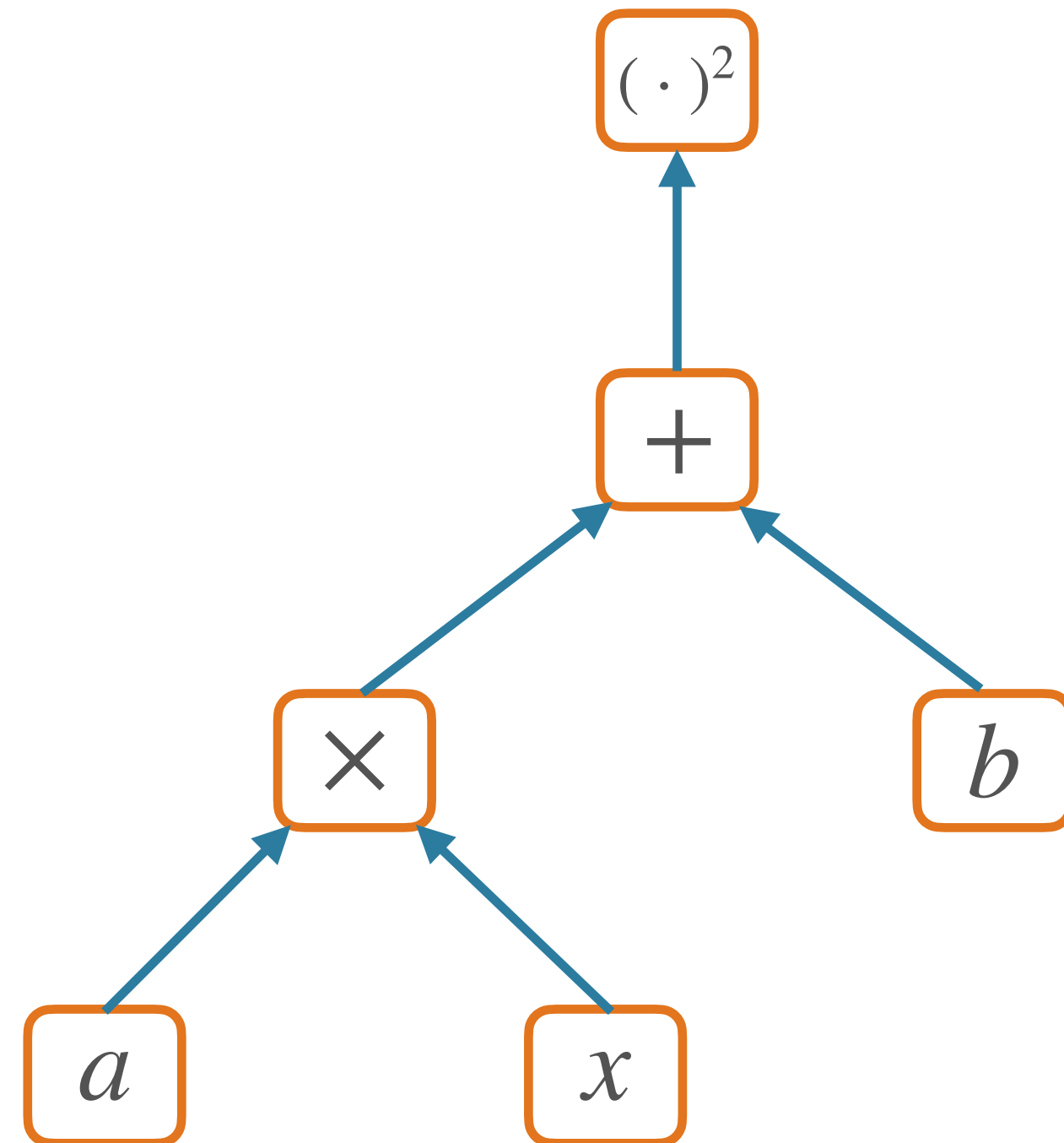
Backpropagation

So what?

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

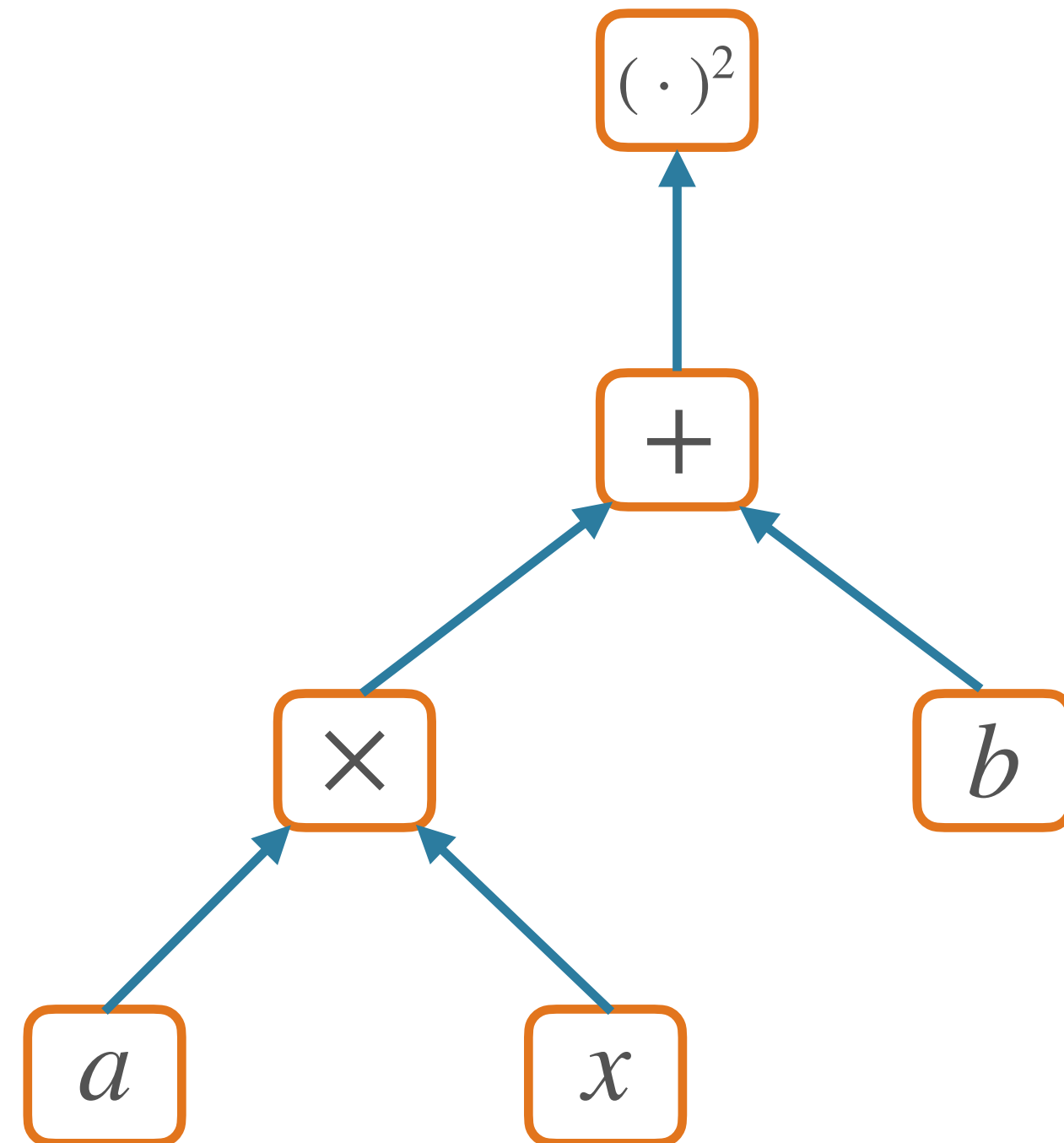
Computing Derivatives

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



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

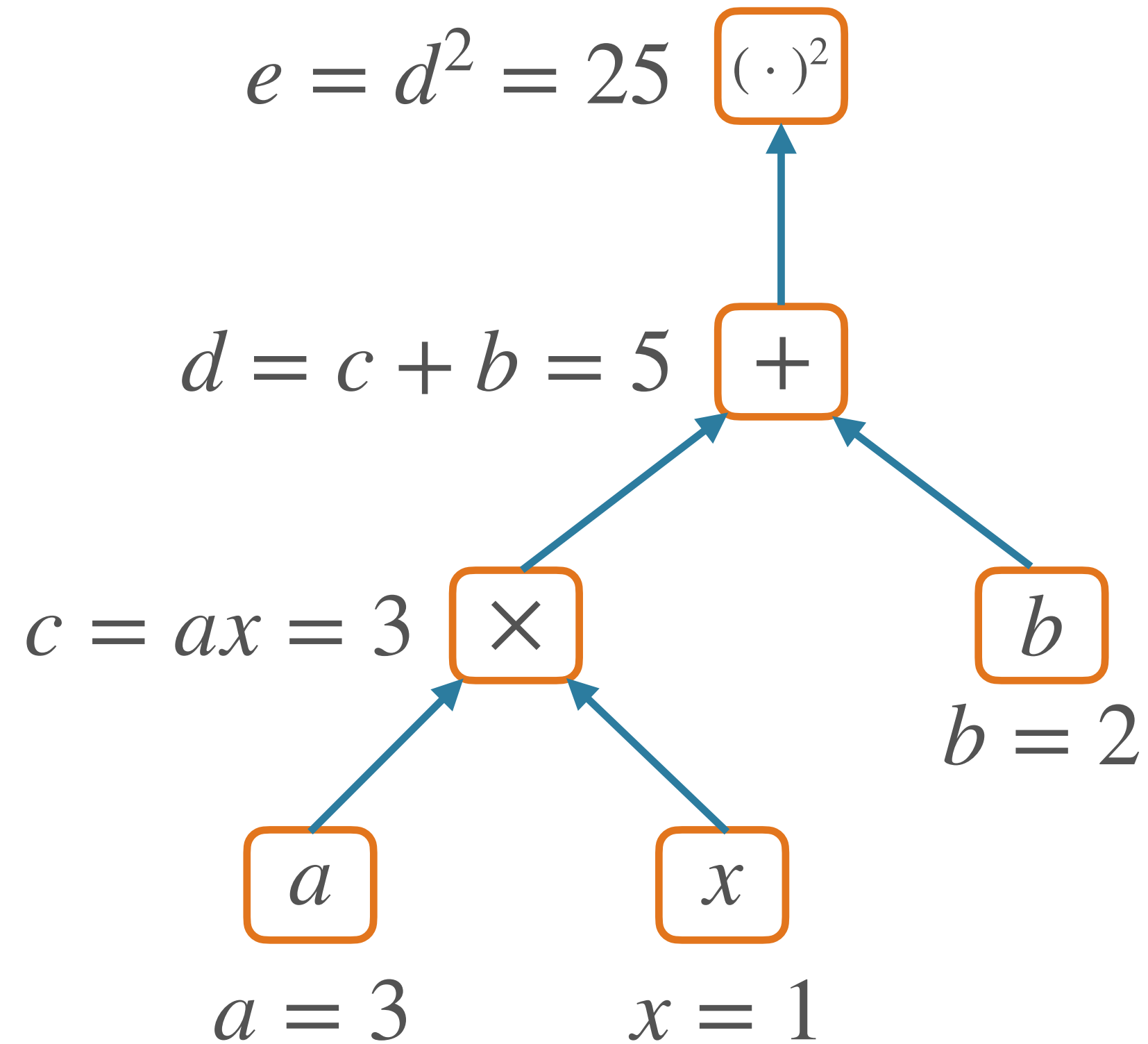
$$= 2(ax + b)a$$

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

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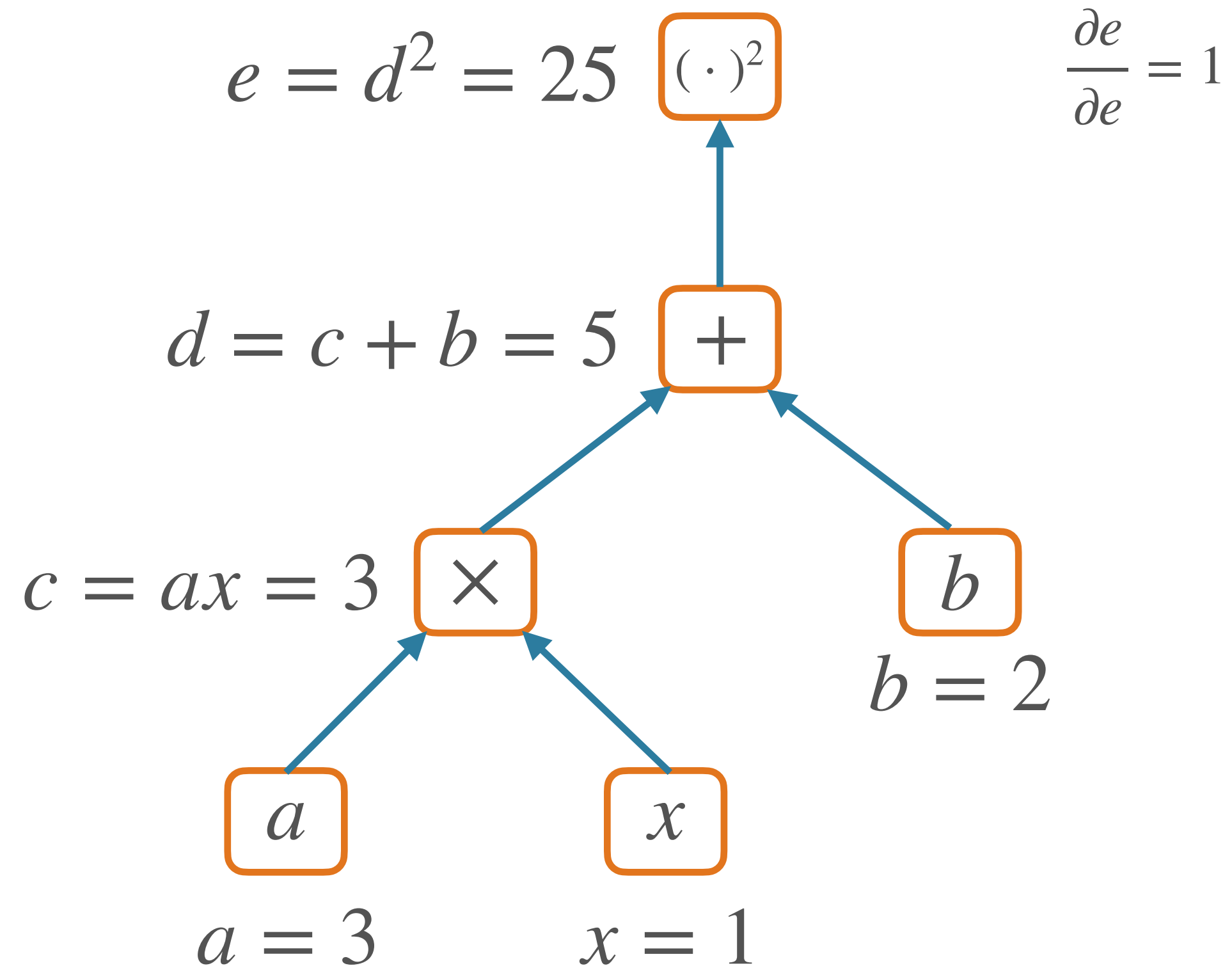
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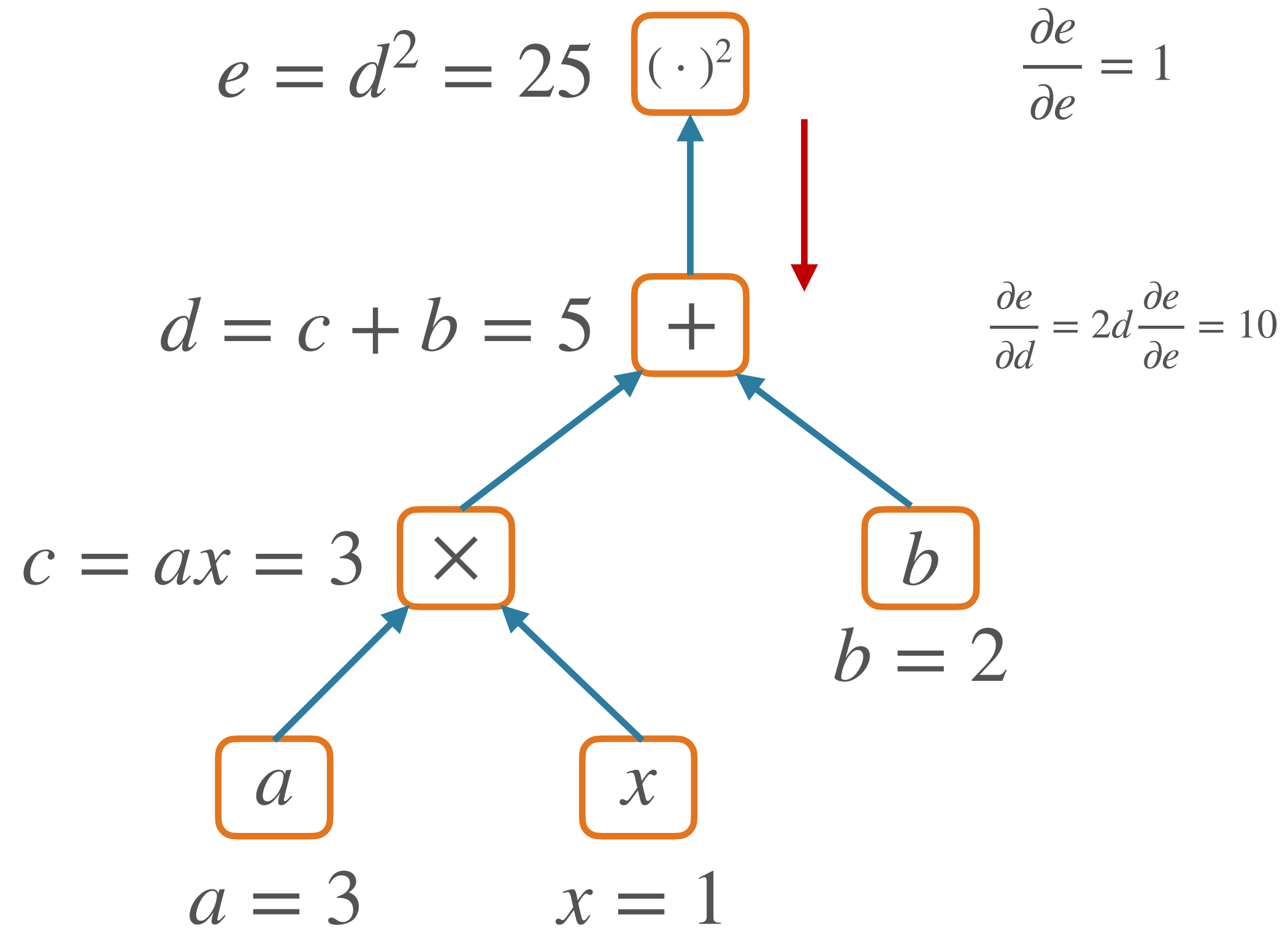
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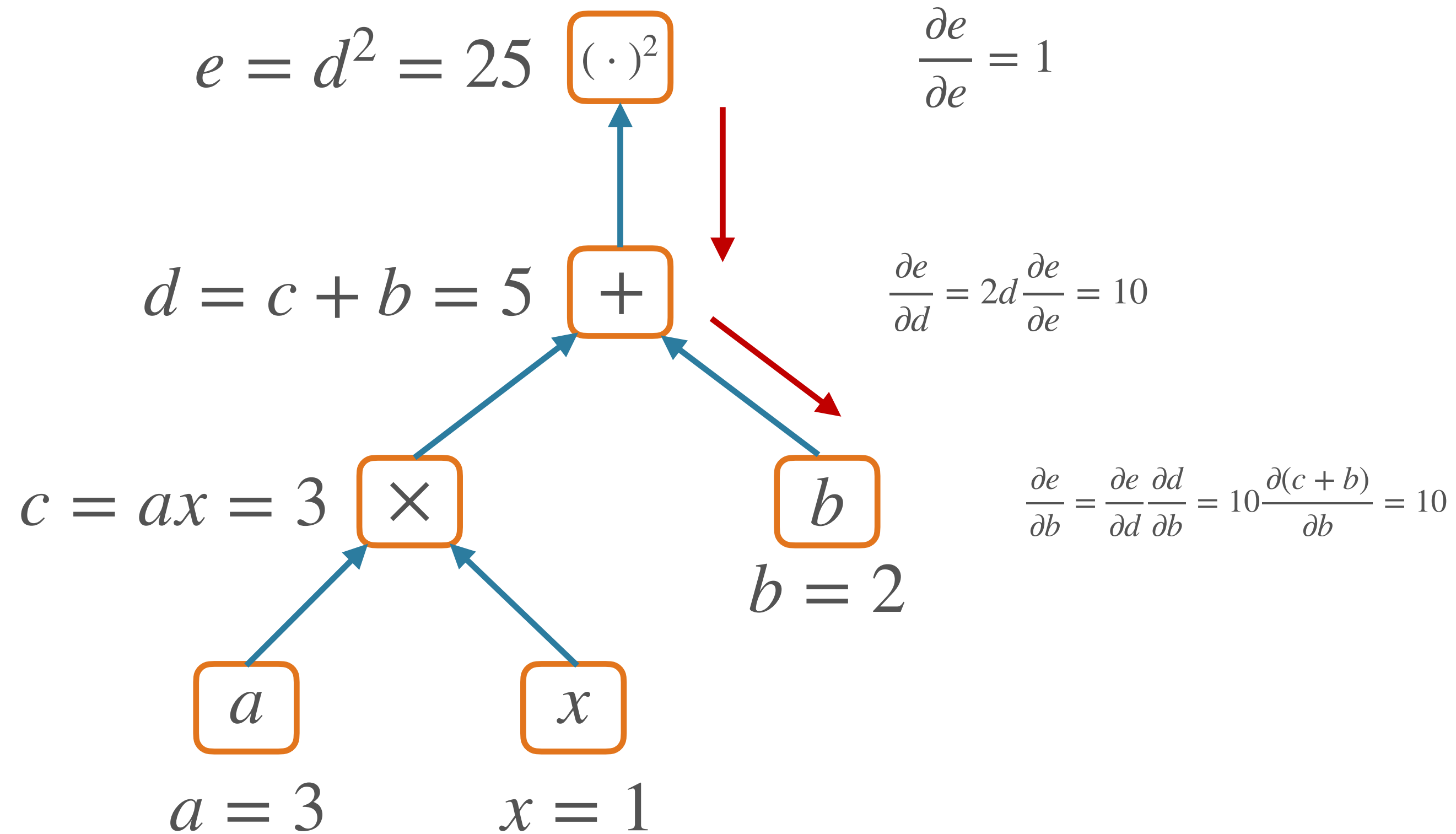
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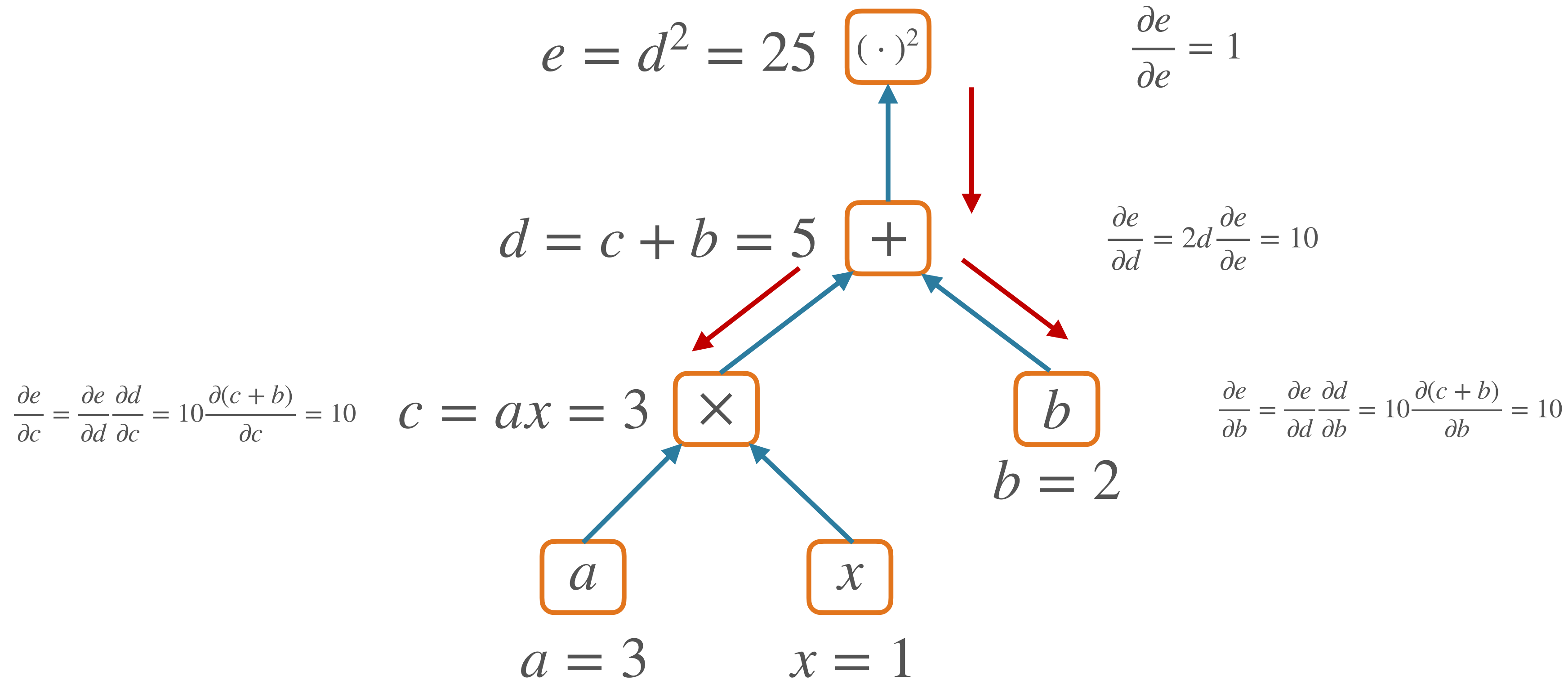
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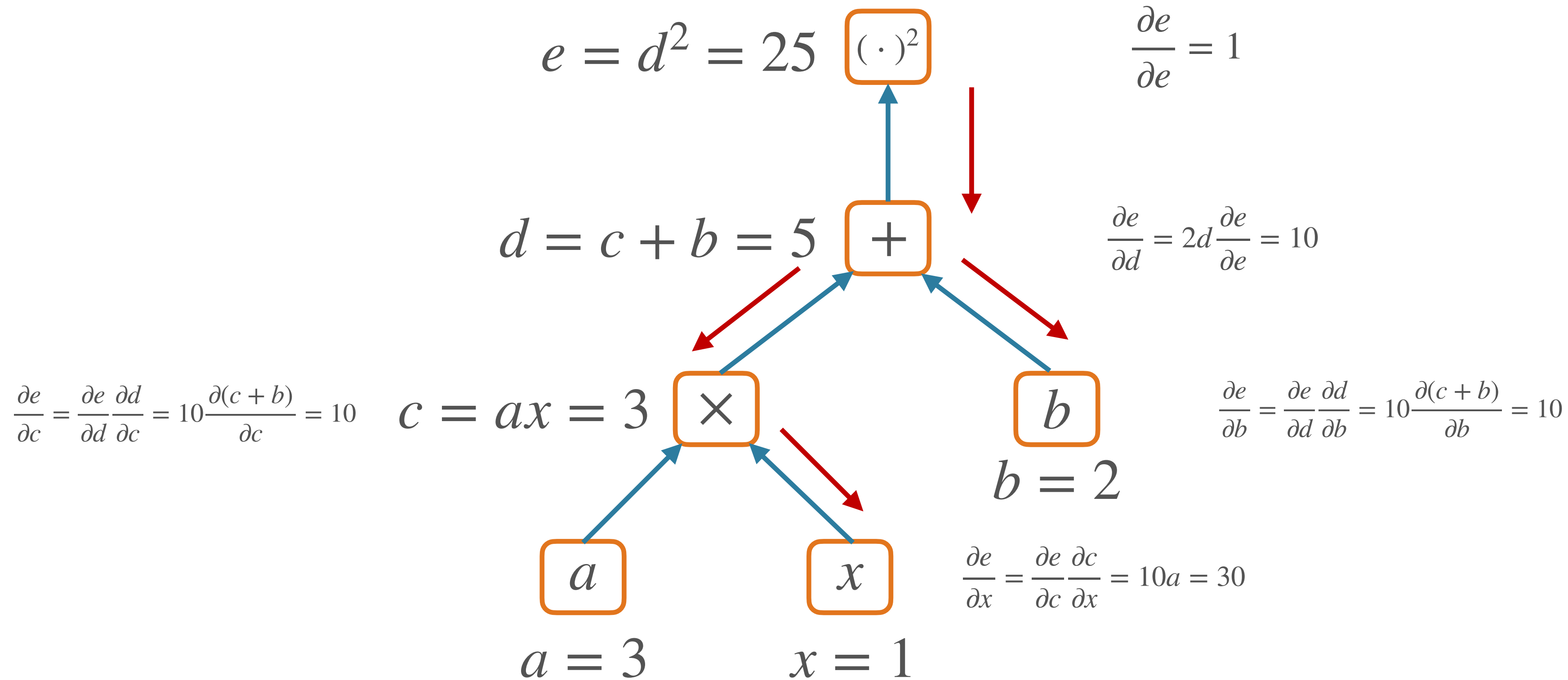
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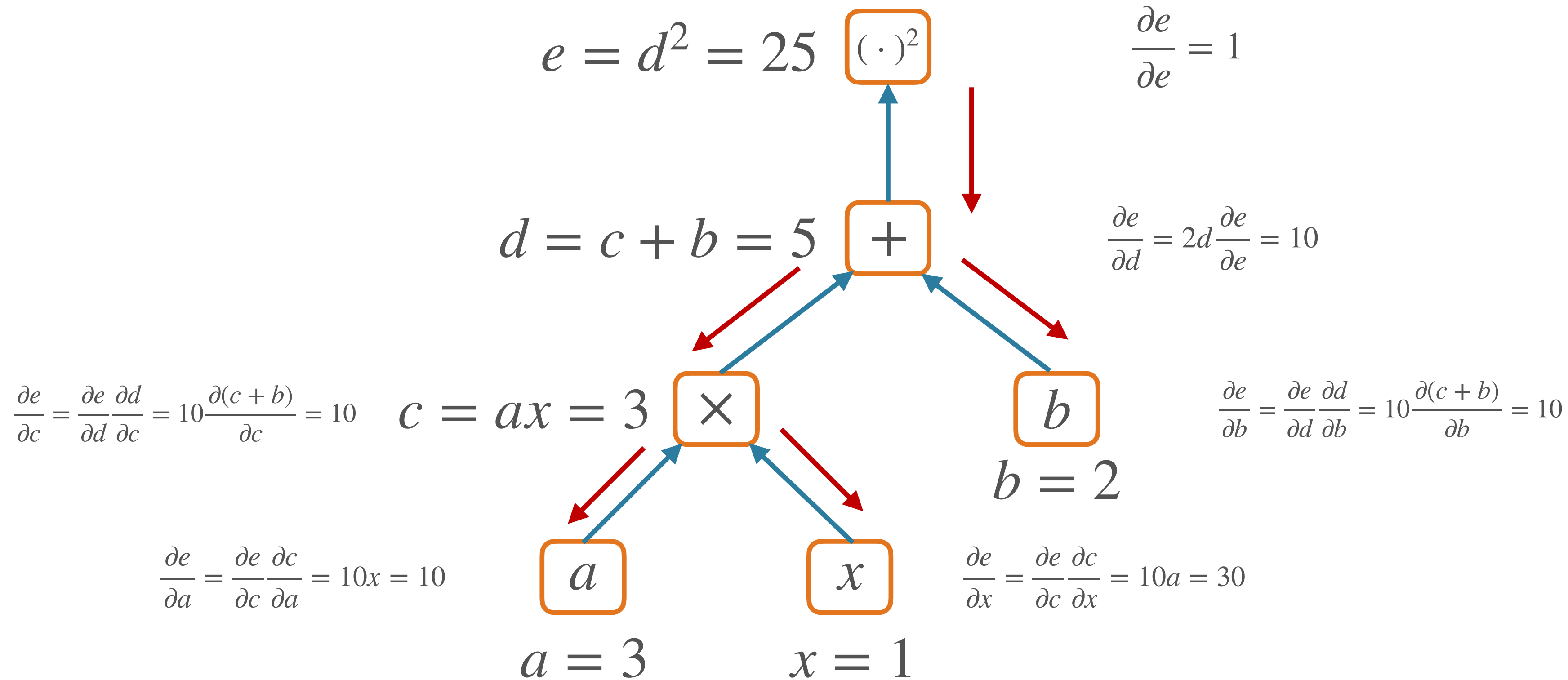
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Backpropagation

- Initialize gradient to 1 for given output node f
 - [NB: assuming that this output node is a *scalar*]
- Loop over nodes in graph in *reversed 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
 - [i.e. apply the chain rule!]

Backpropagation Algorithm

```
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()
```

From Tensor class in [edugrad](#)

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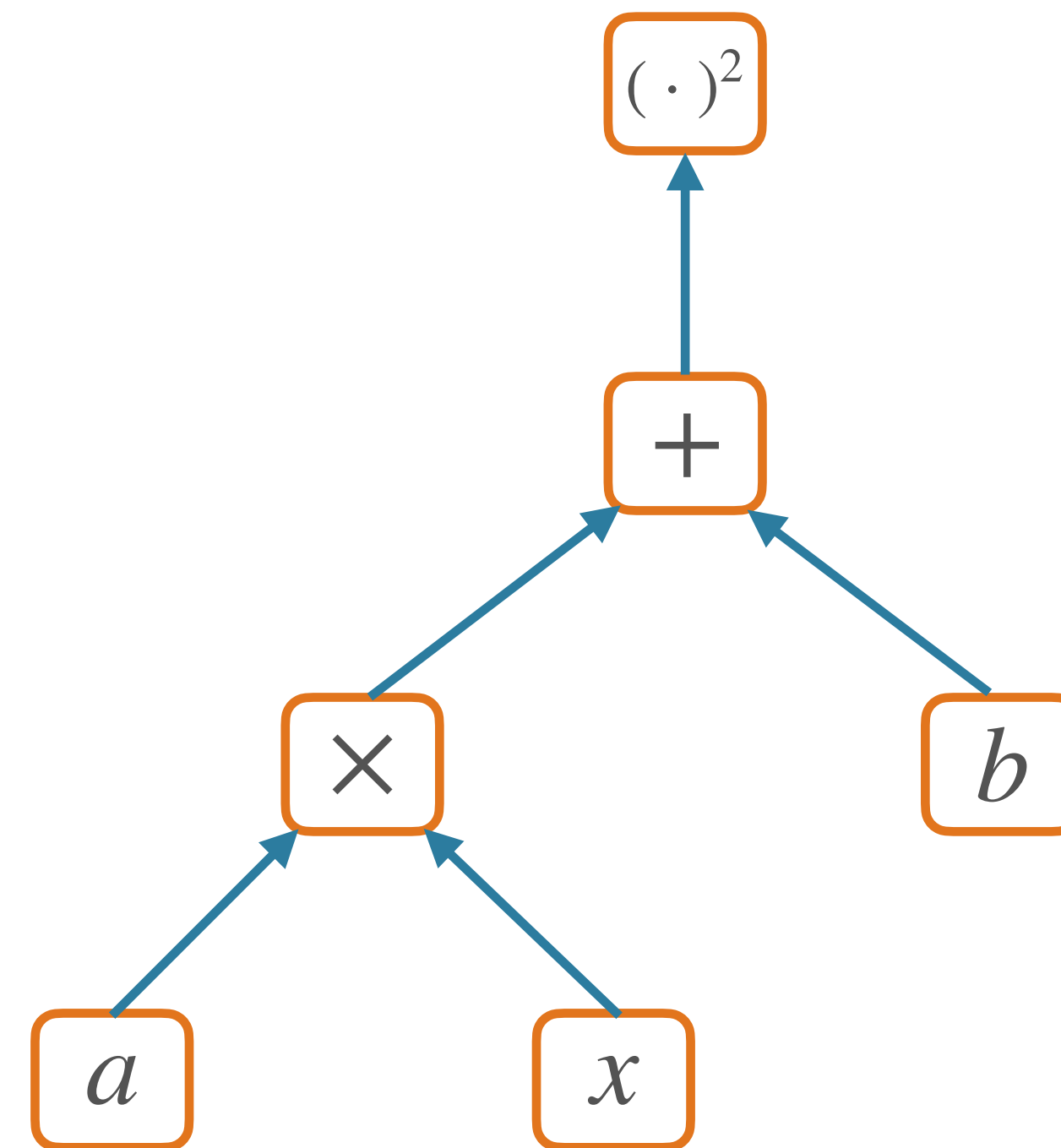
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Local gradient + chain rule application

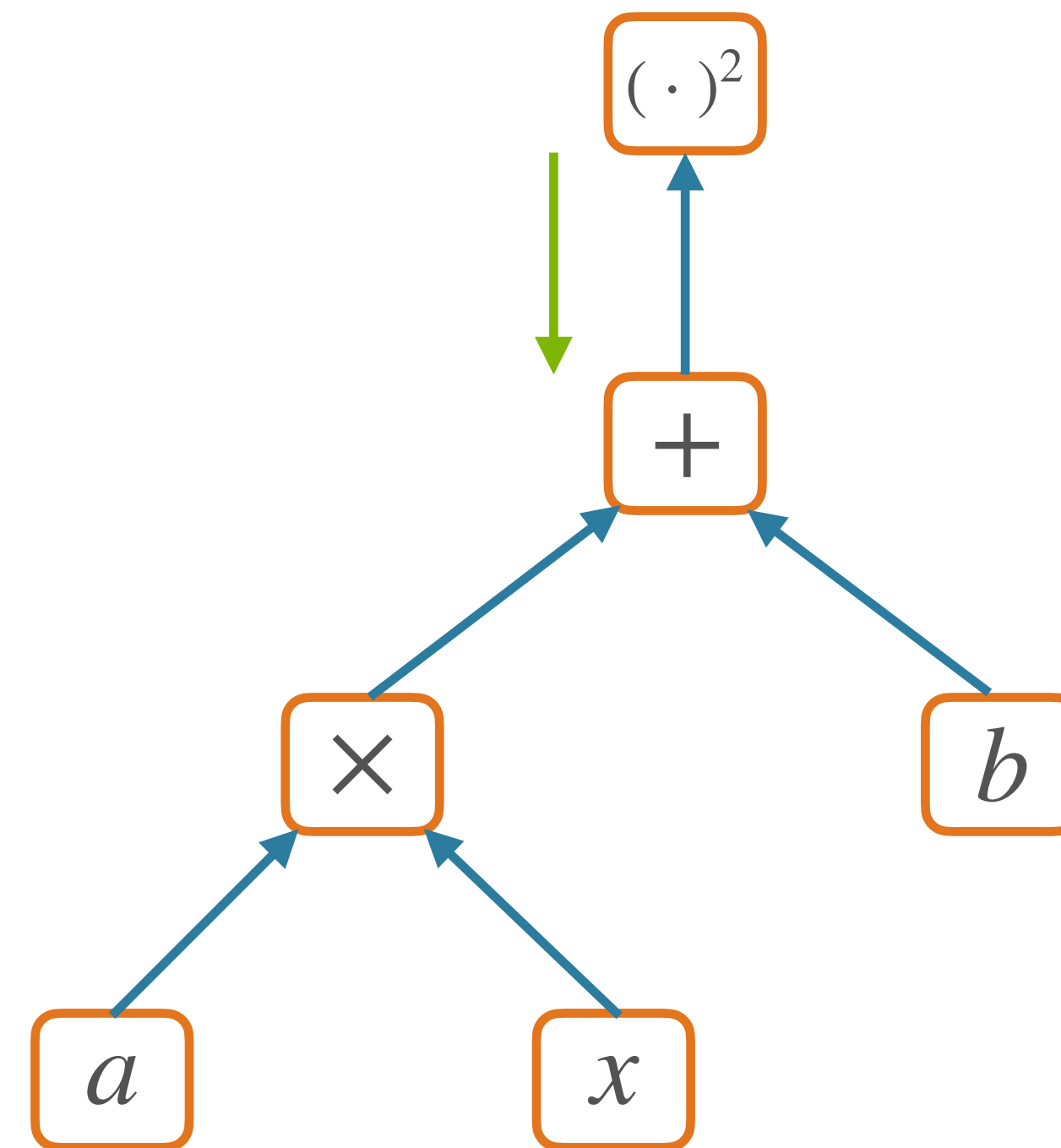
Why back-propagation?

- Extremely efficient method for computing all gradients
- Compute *once*
- Store and re-use redundant computation
- Whence a form of dynamic programming
- Traverse each edge once, instead of once per dependency path



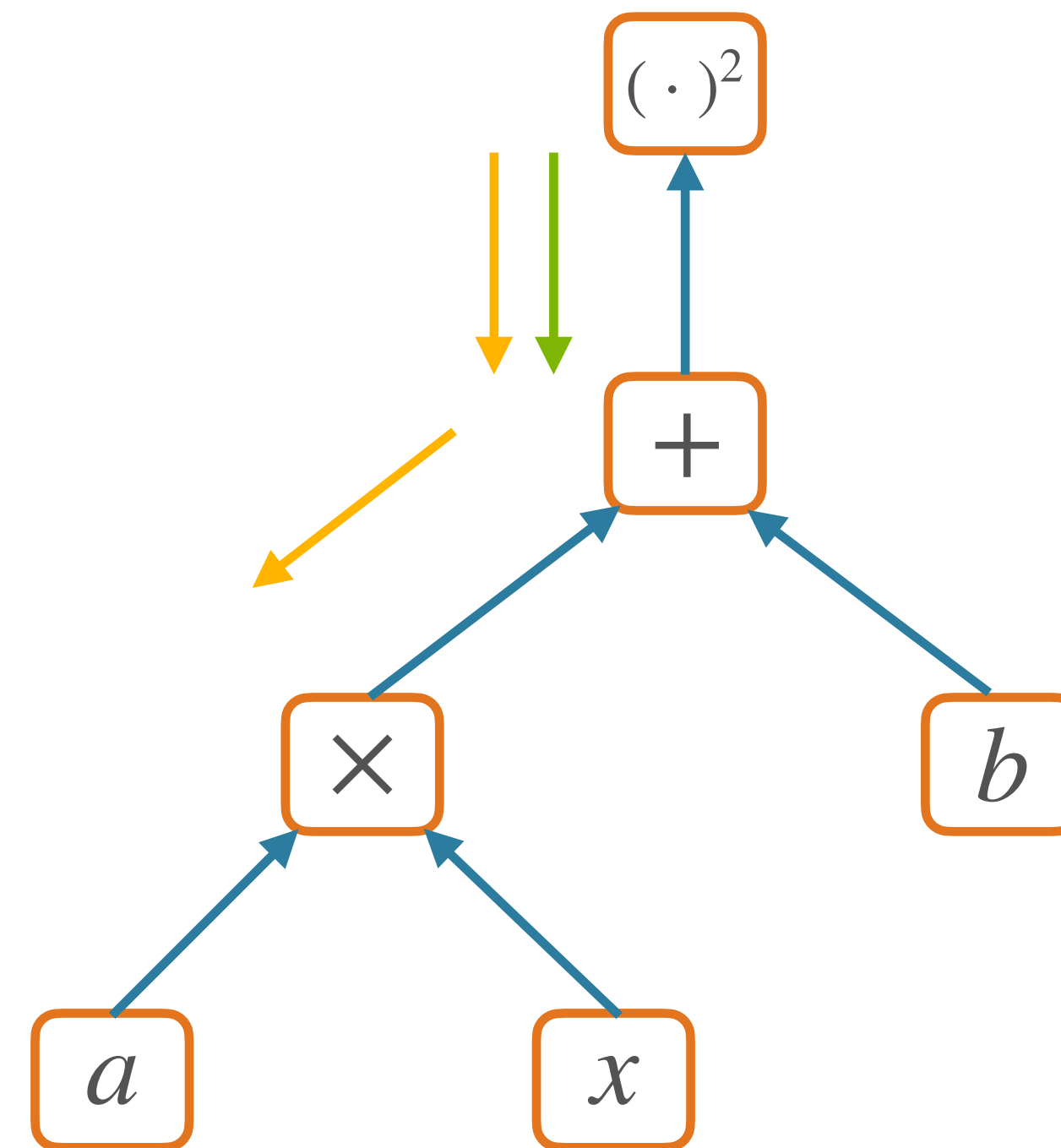
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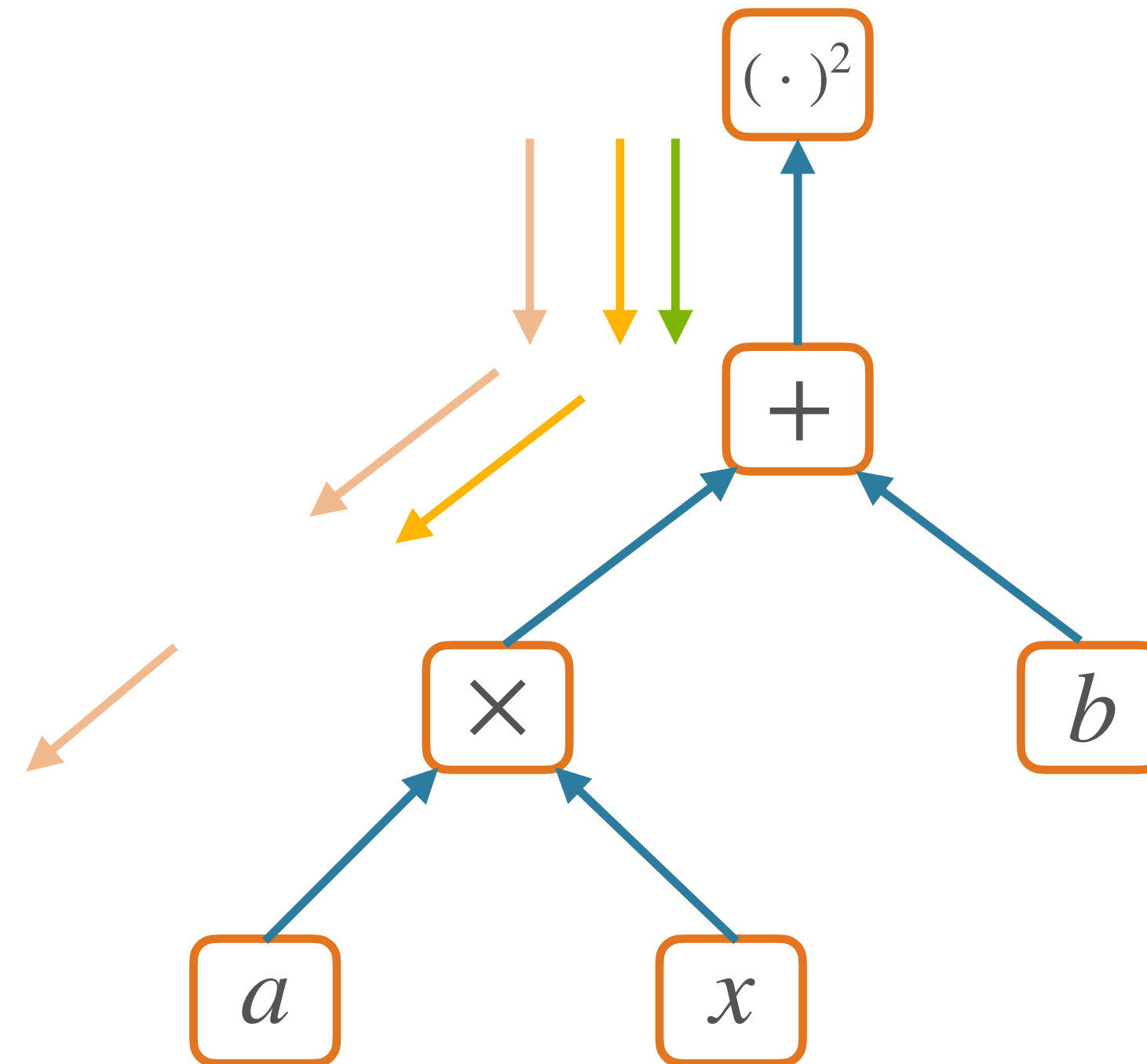
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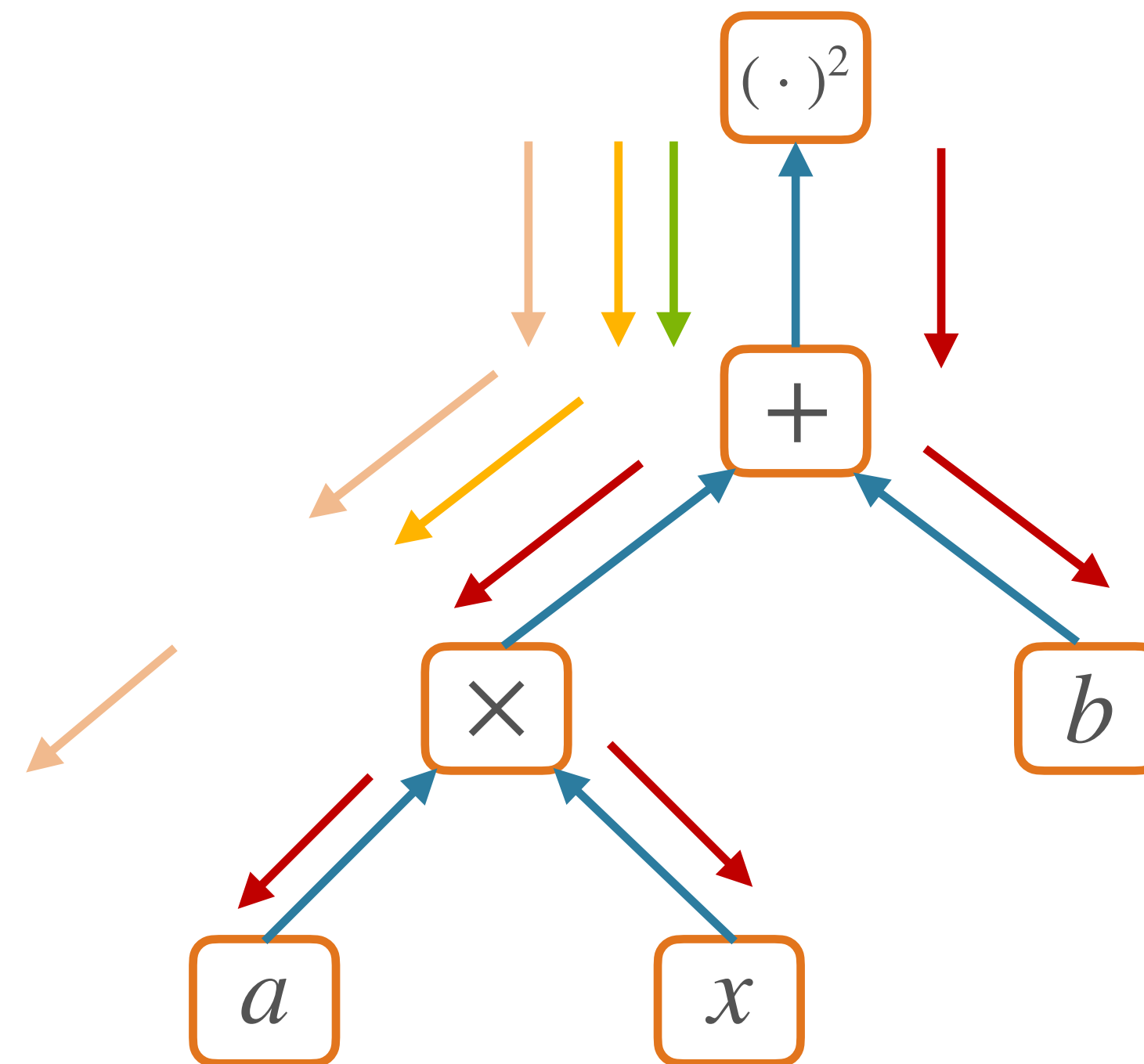
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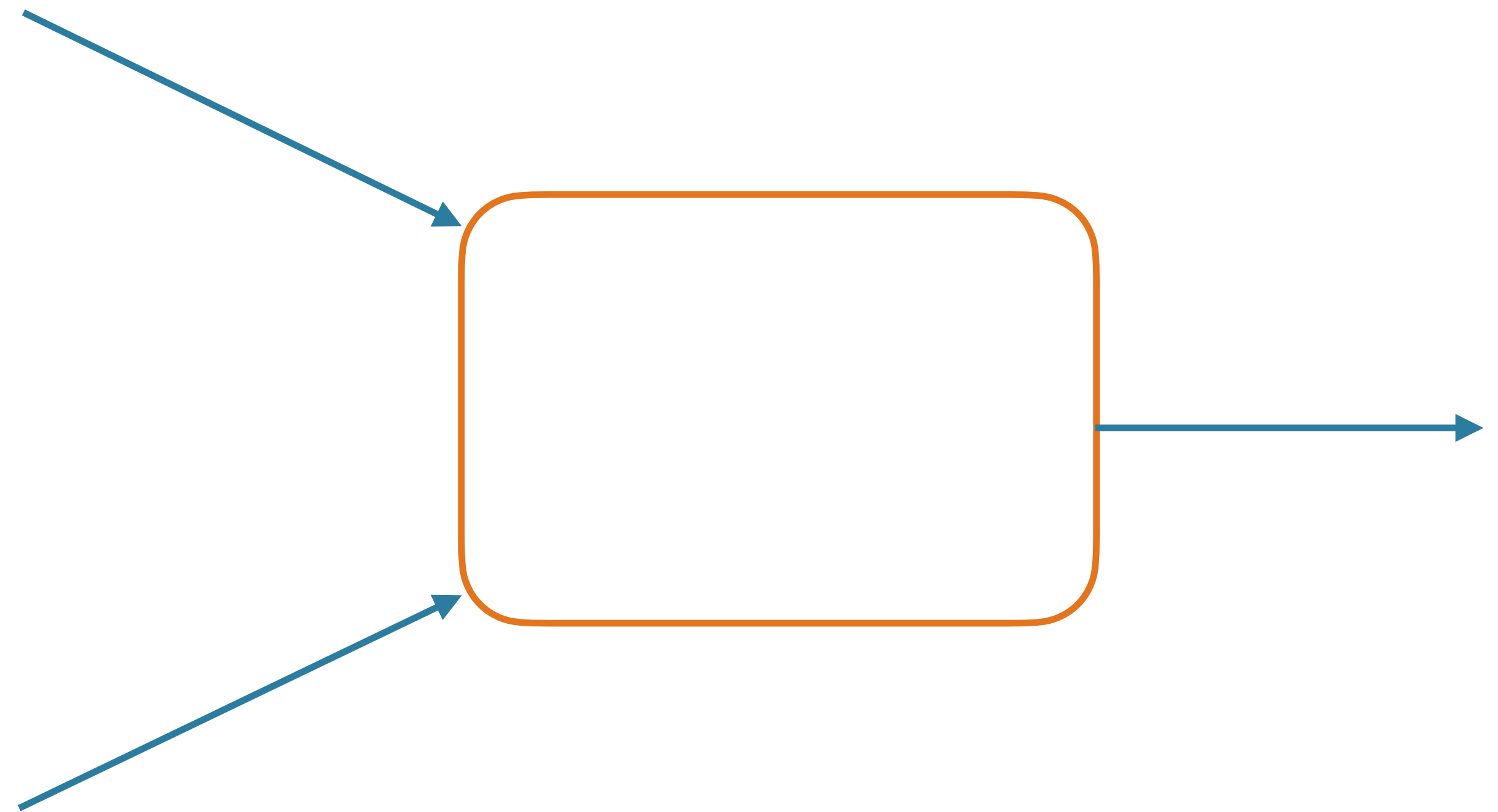
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Forward/backward API

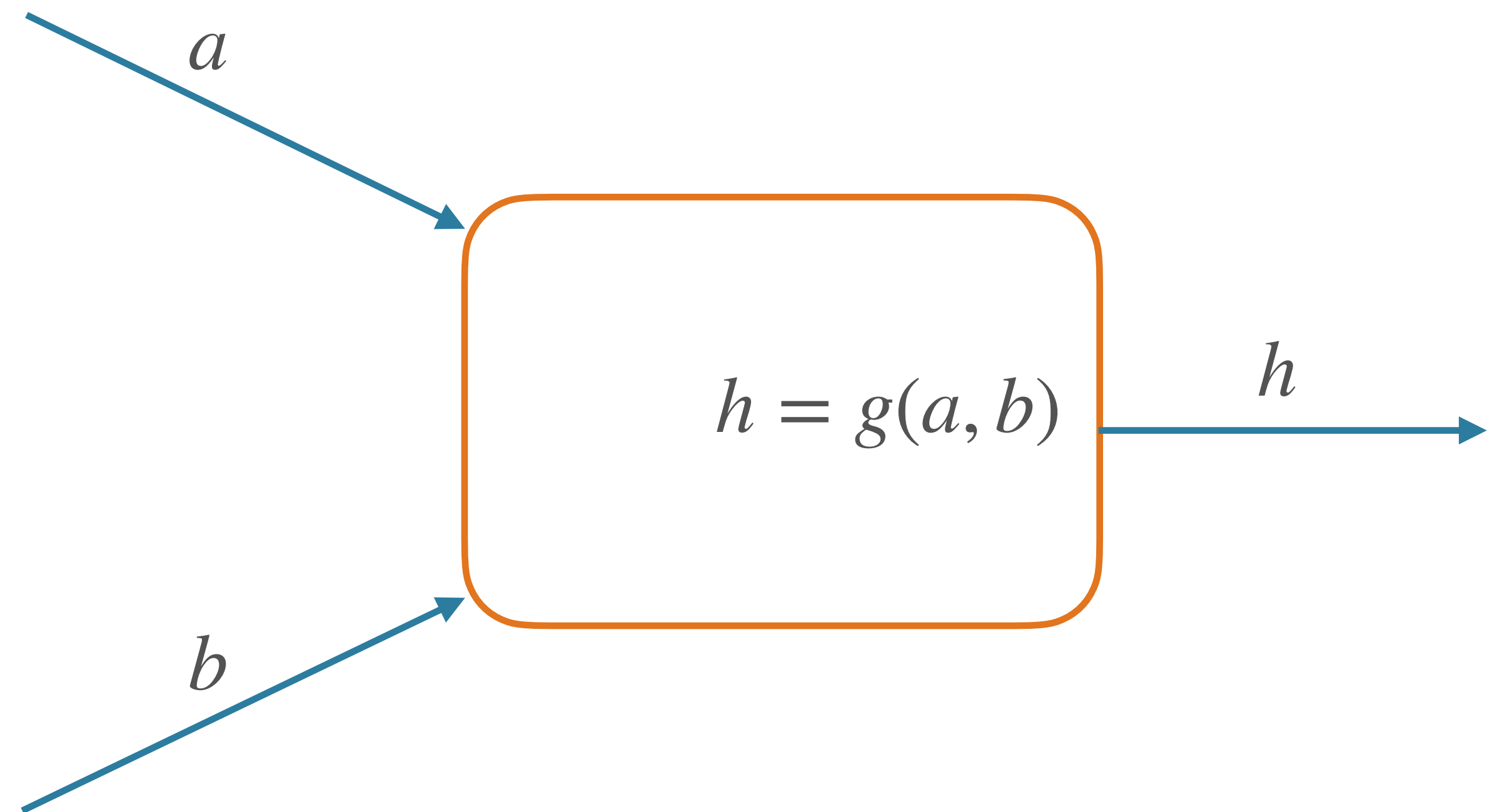
Nodes in Computational Graph

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



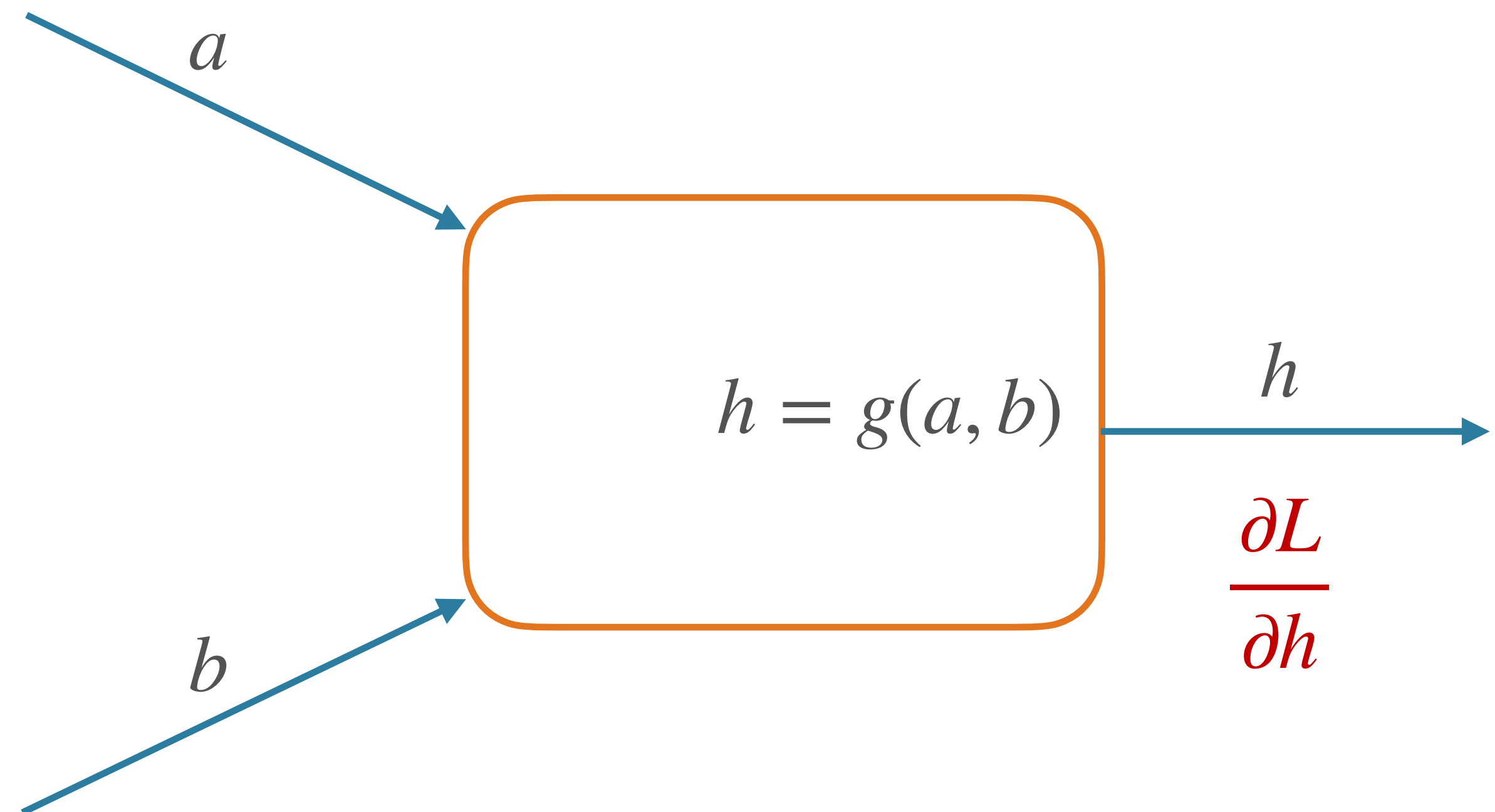
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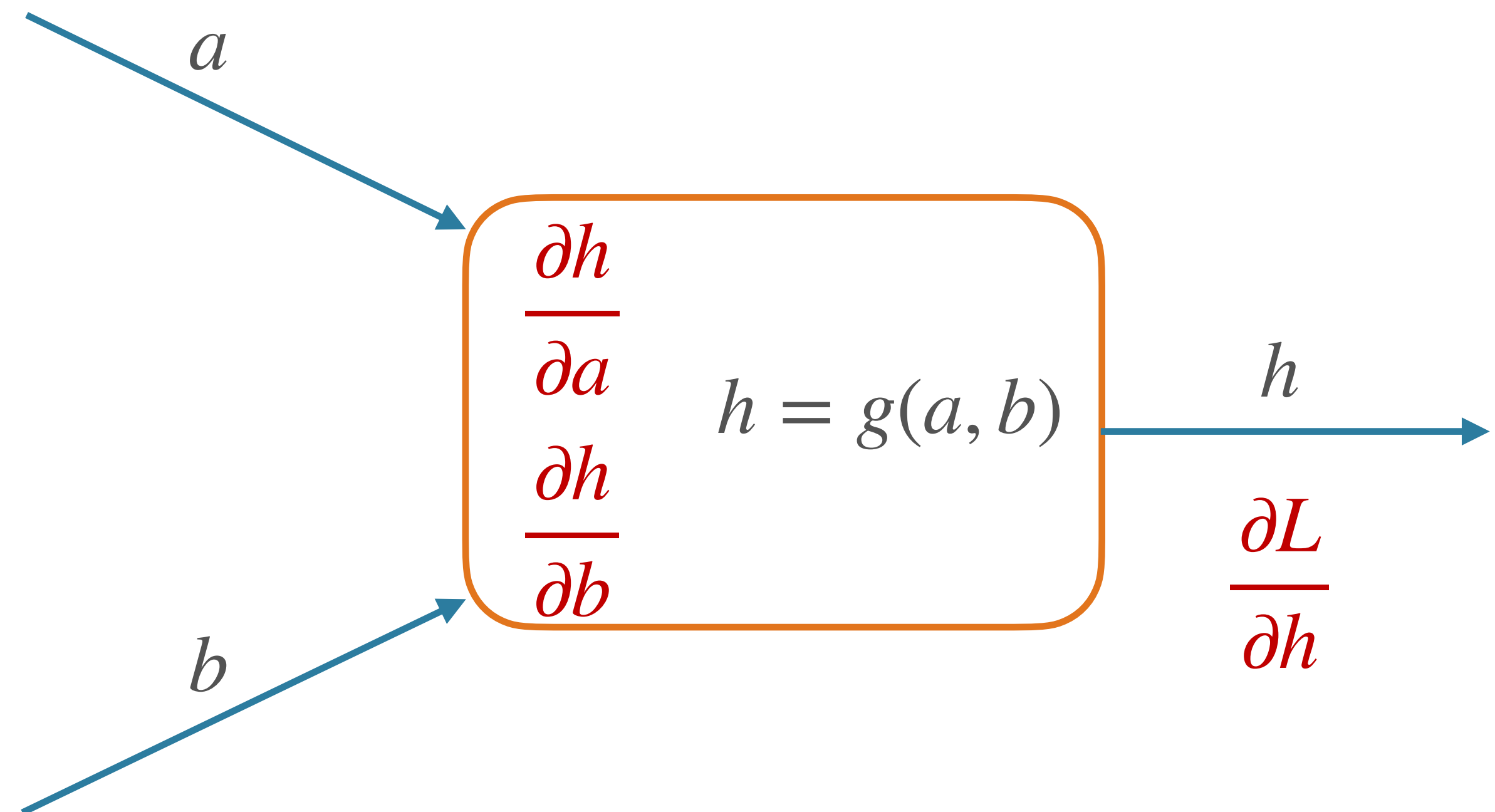
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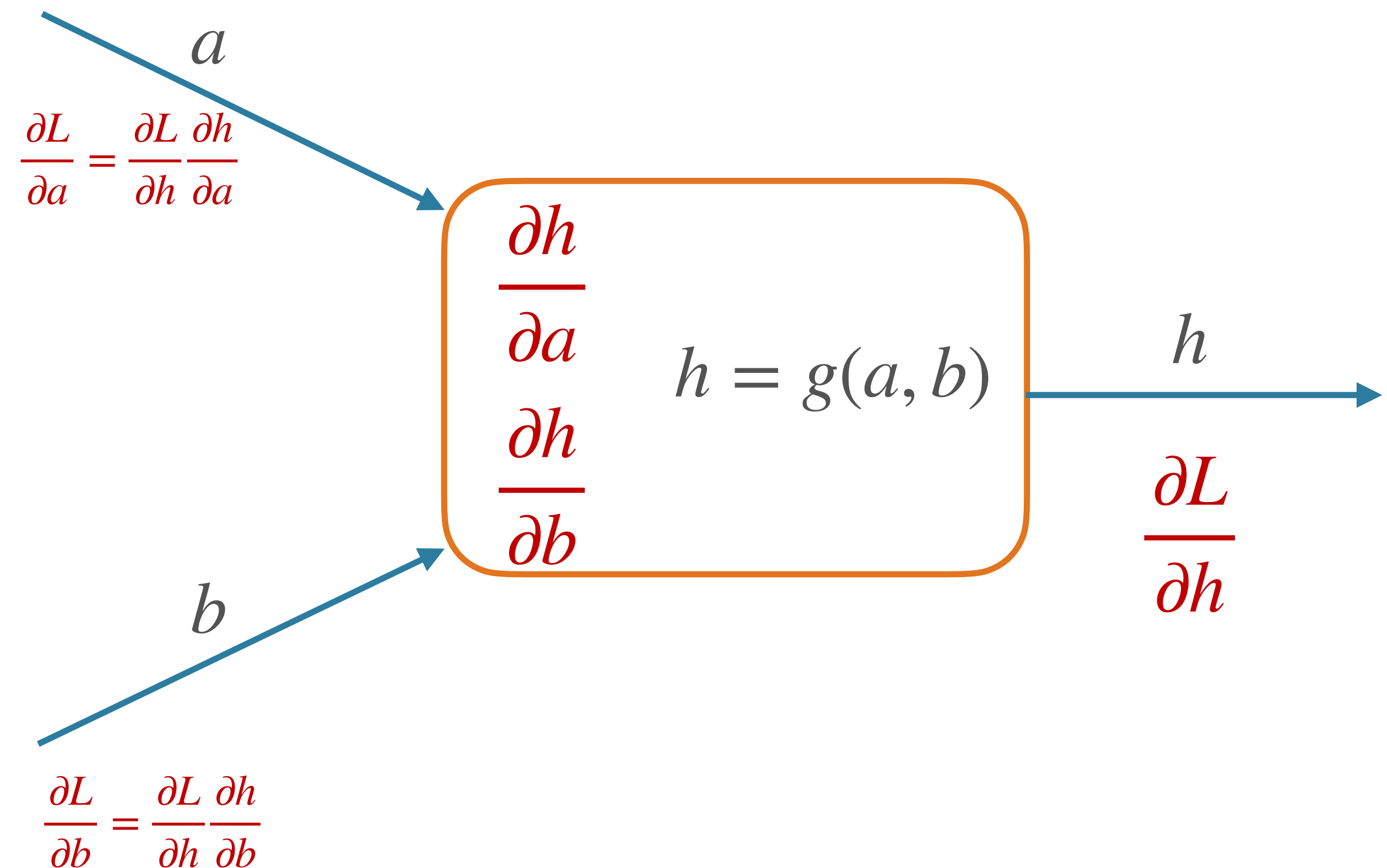
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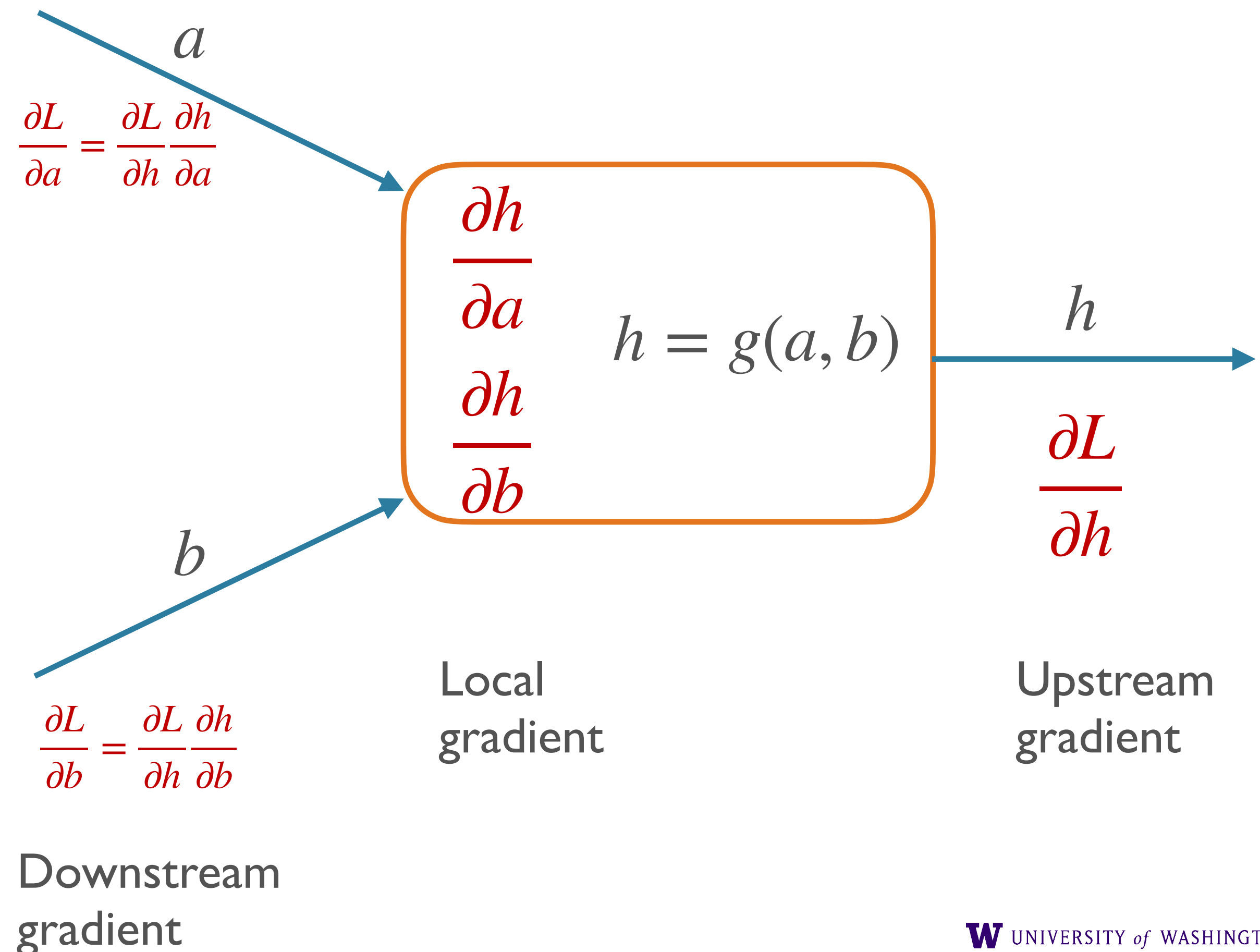
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Forward/Backward API

```
class Operation:
    @staticmethod
    def forward(
        ctx: List[np.ndarray], *inputs: List[np.ndarray], **kwargs
    ) -> np.ndarray:
        """Forward pass of an operation.

        Args:
            ctx: empty list of arrays; can be used to store values for backward pass
            inputs: arguments to this operation

        Returns:
            output of the operation, assumed to be one numpy array
        """
        raise NotImplementedError

    @staticmethod
    def backward(ctx: List[np.ndarray], grad_output: np.ndarray) -> List[np.ndarray]:
        """Backward pass of an op, returns dL / dx for each x in parents of this op.

        Args:
            ctx: stored values from the forward pass
            grad_output: dL/dv, where v is output of this node

        Returns:
            a _list_ of arrays, dL/dx, for each x that was input to this op
        """
        raise NotImplementedError
```

From my [edugrad](#) mini-library, which you will use :)

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
```

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

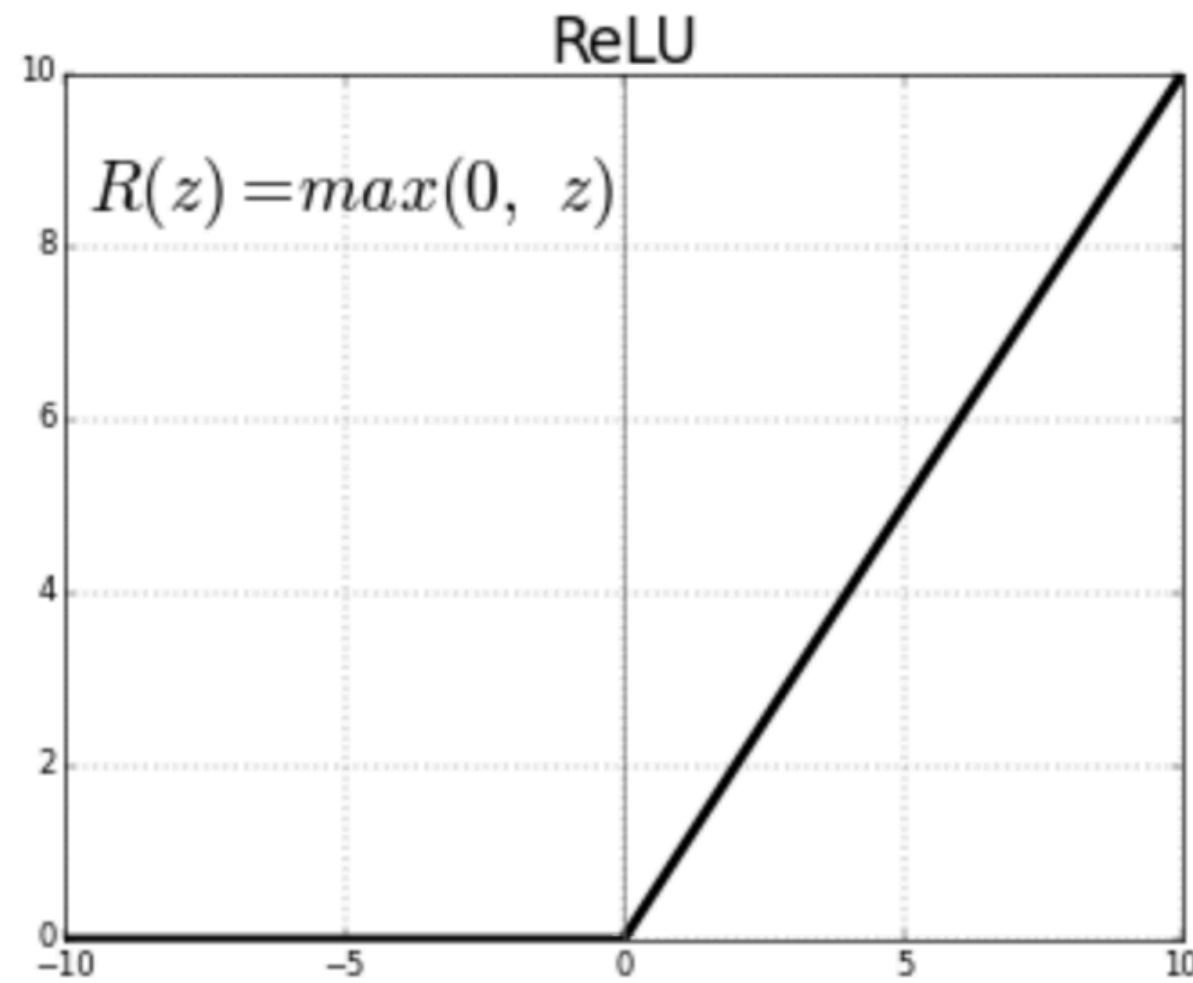
$$\frac{\partial L}{\partial b}$$

Example: ReLU

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

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

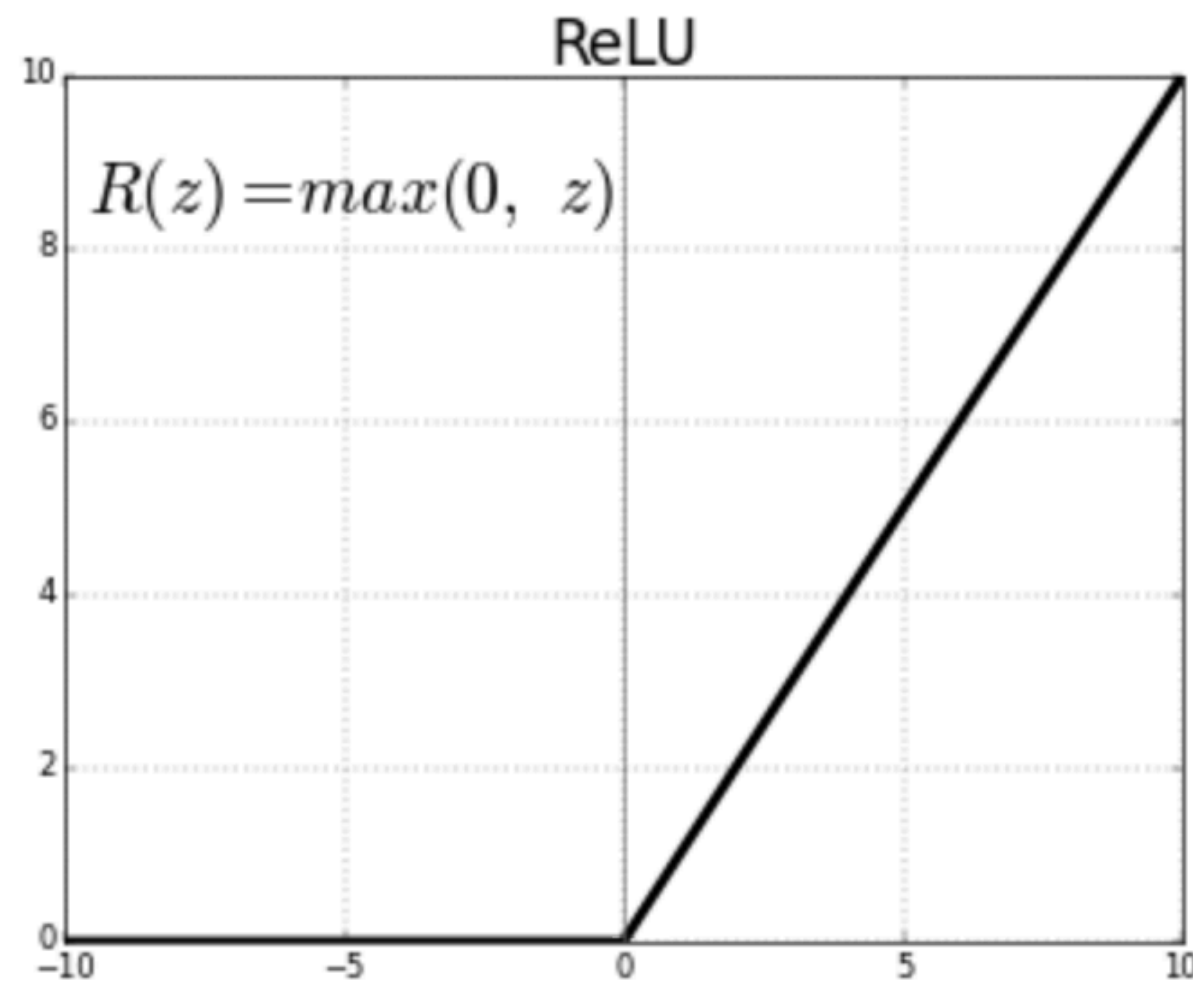
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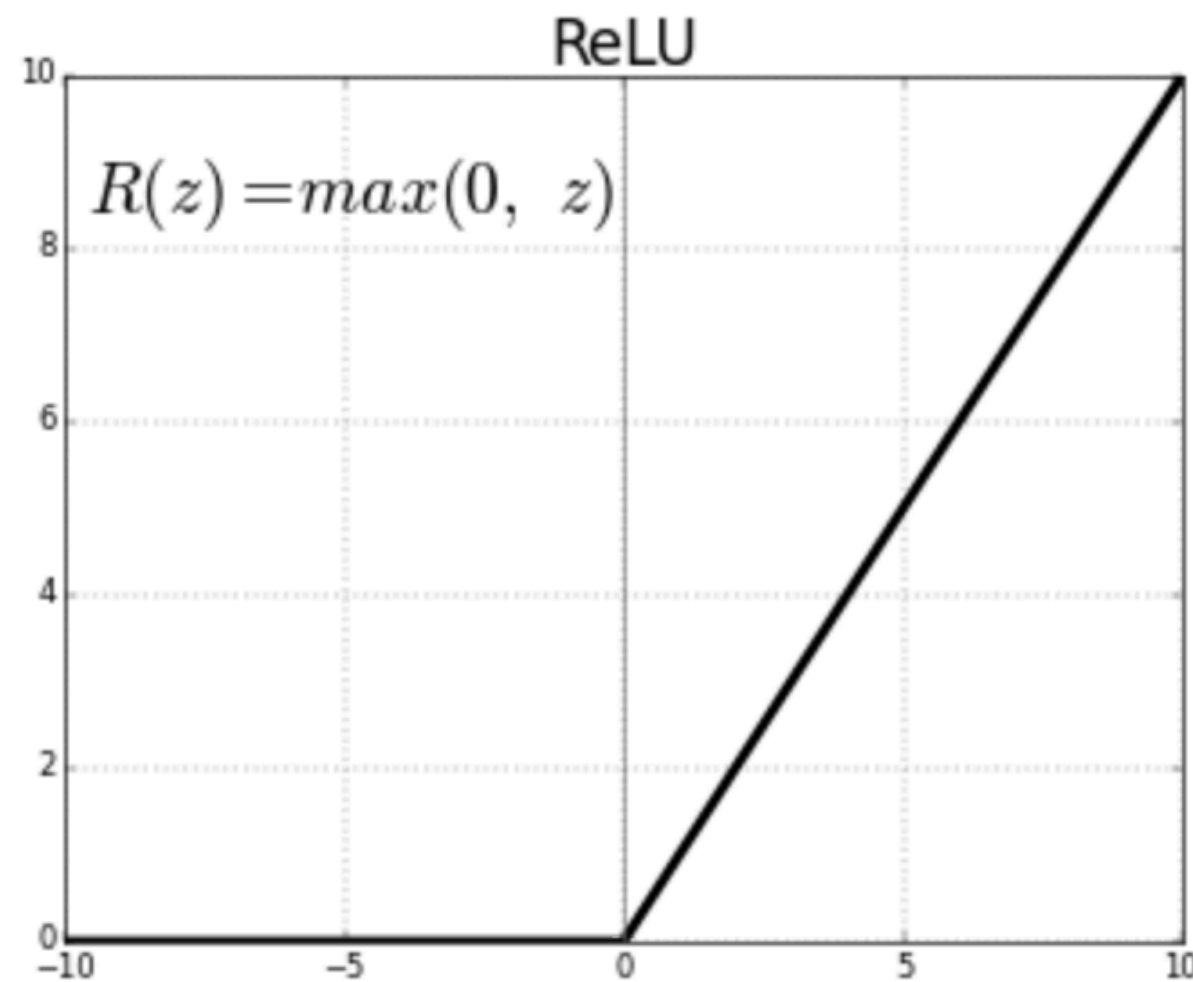


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$$\frac{\partial R}{\partial x} = \begin{cases} 1 & x > 0 \\ 0 & \text{otherwise} \end{cases}$$

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🤔🤔🤔 where's x???

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

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]
```


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Save and retrieve the input value!

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local gradient

times upstream
gradient

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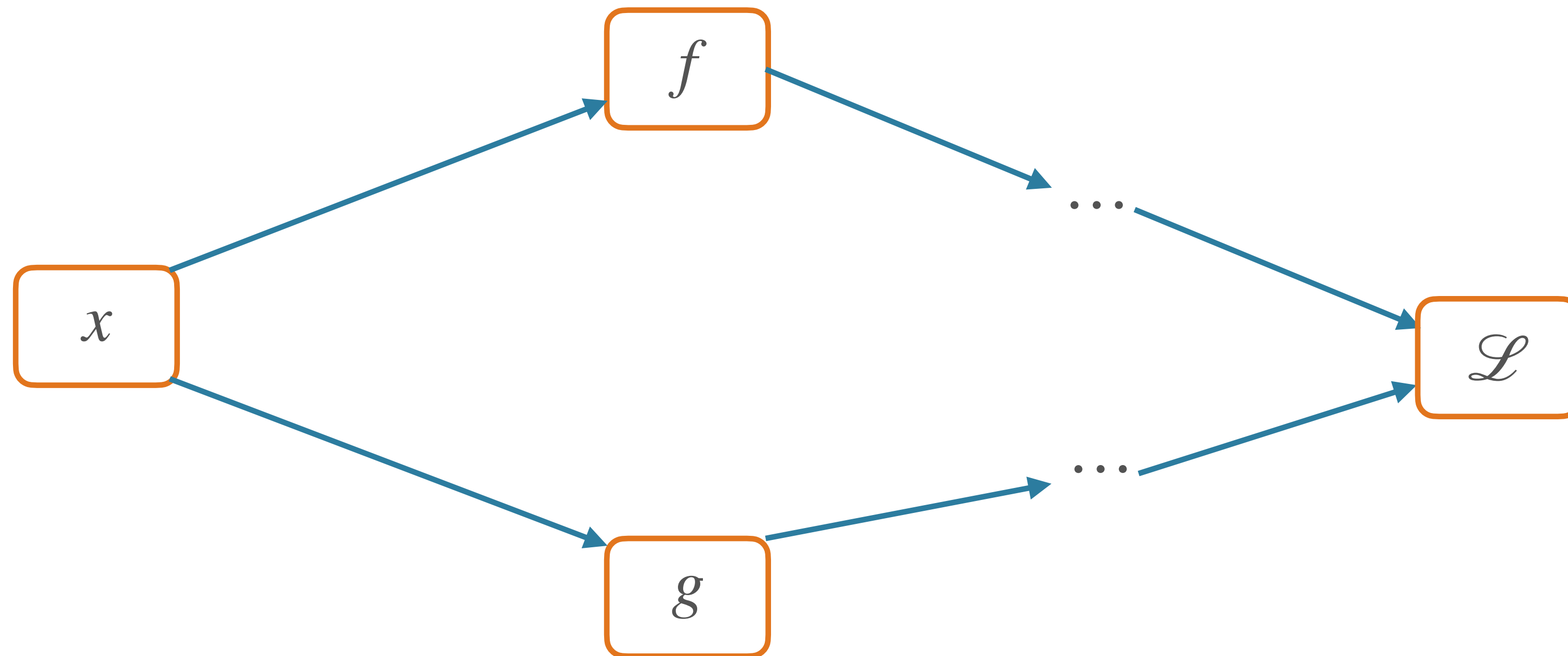
Save and retrieve the input value!

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

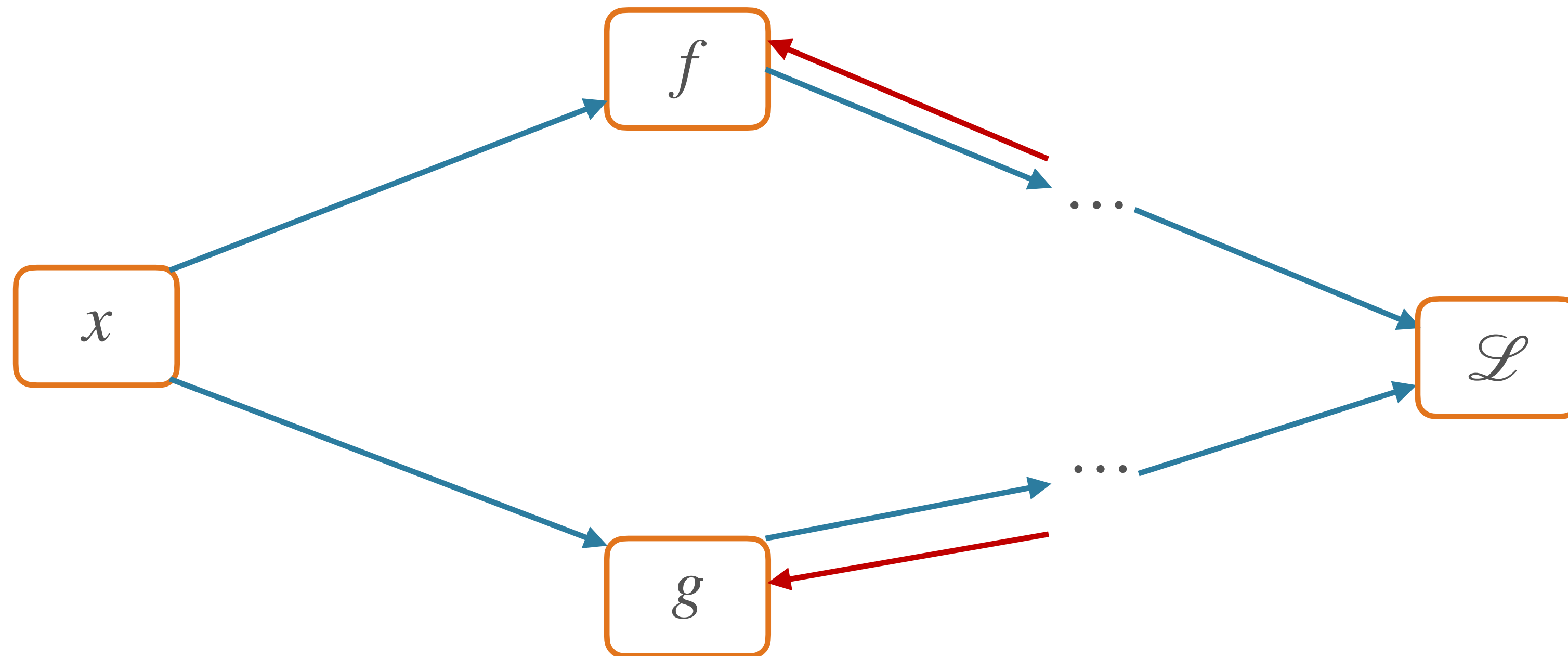
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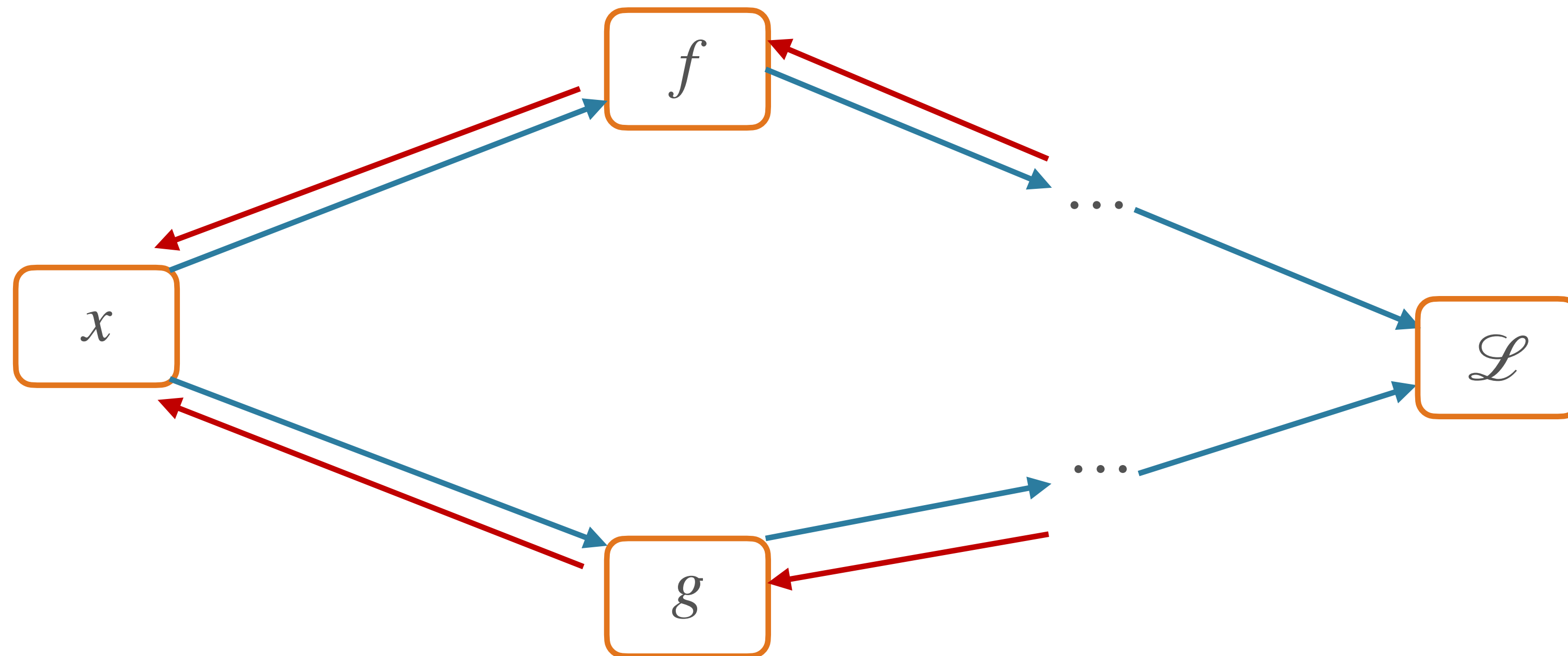
Adding Gradients with Multiple Outputs



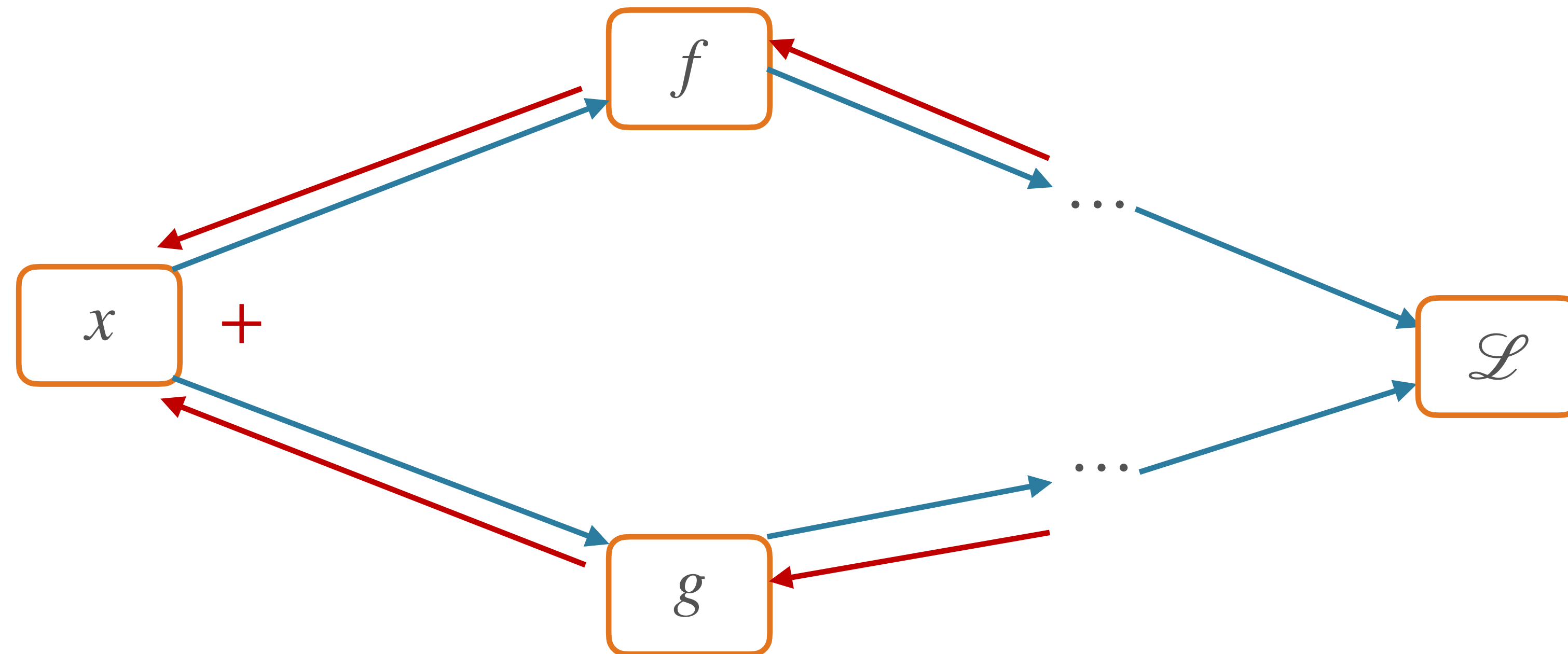
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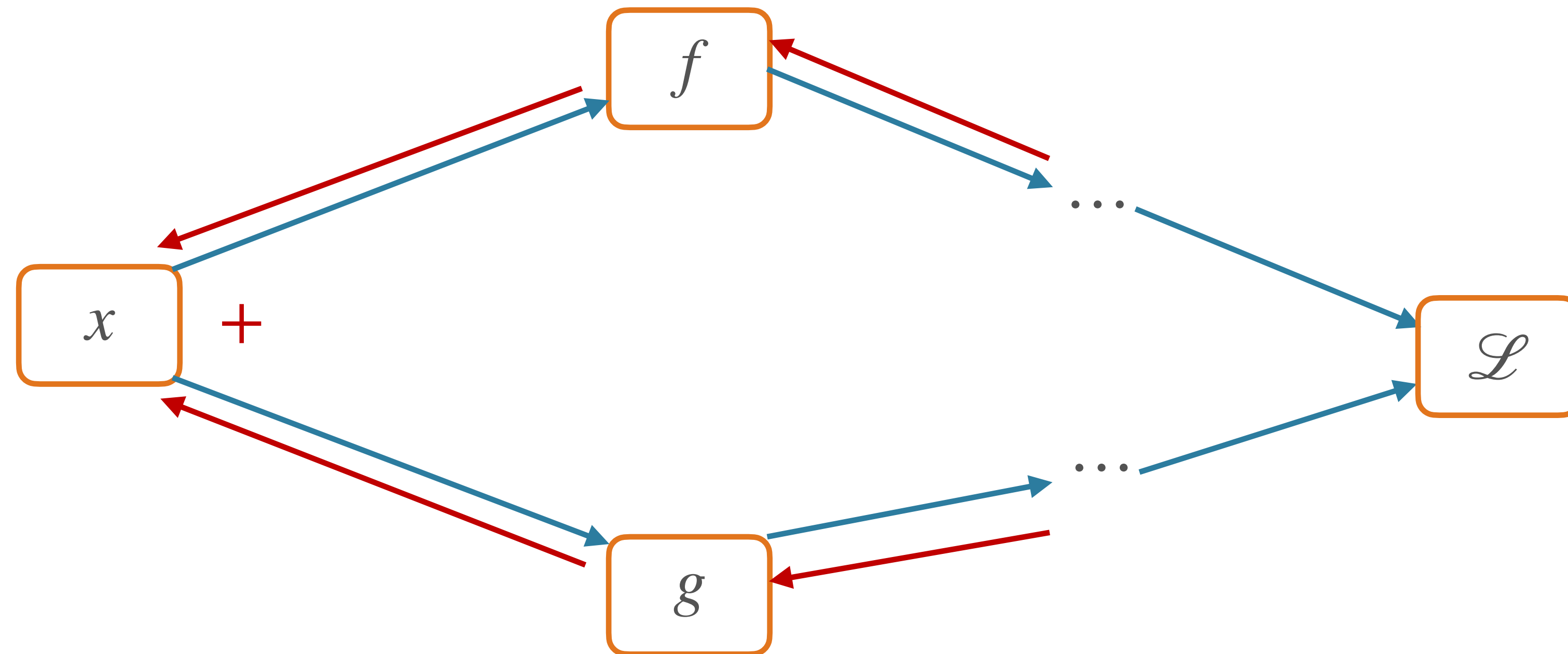
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Adding Gradients with Multiple Outputs



Adding Gradients with Multiple Outputs



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

Adding Gradients with Multiple Outputs

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

Live demo and/or exercise!

Adding Gradients with Multiple Outputs

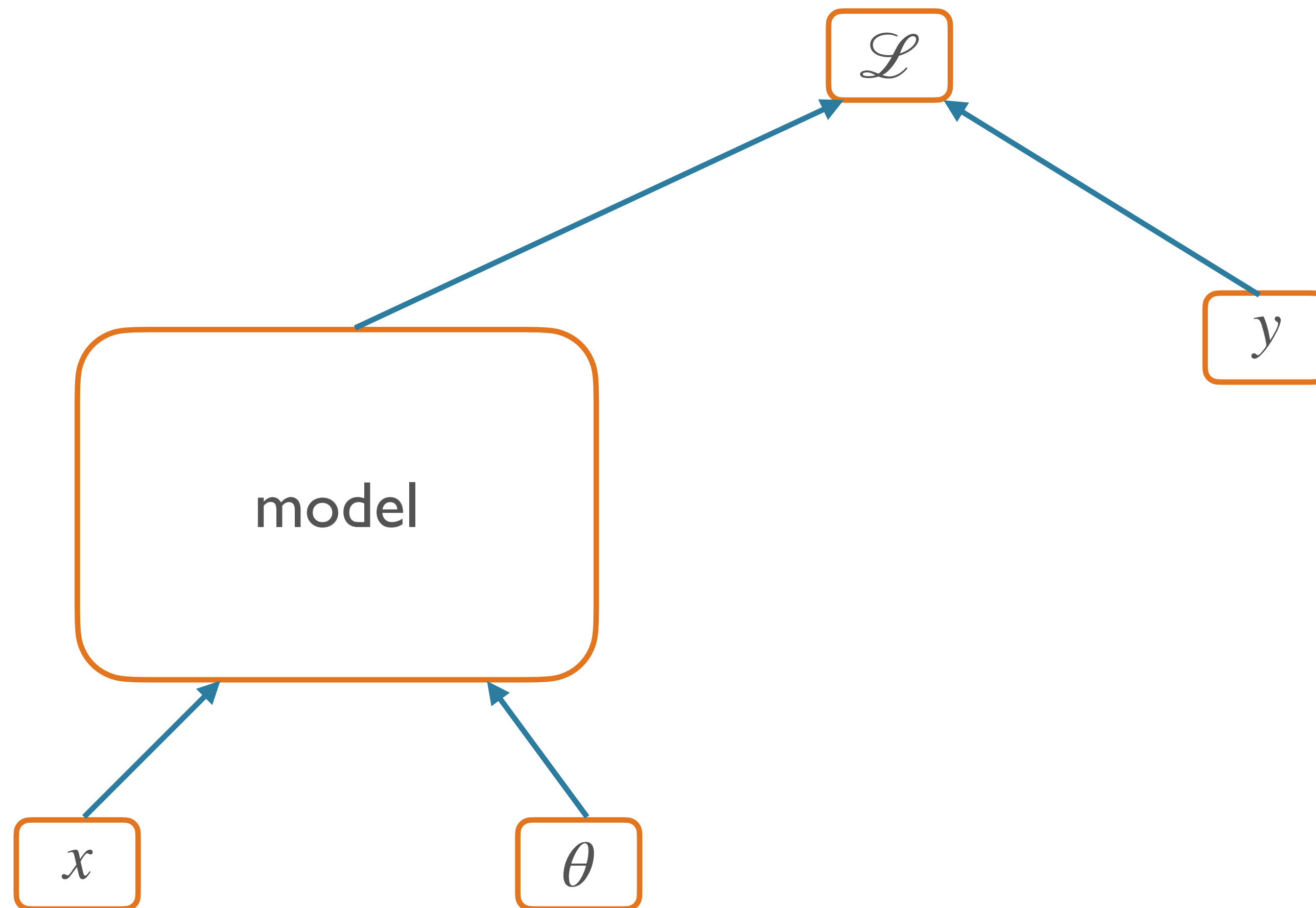
```
def _backward():  
    grads = op.backward(ctx, new_tensor.grad)  
    for idx in range(len(inputs)):  
        inputs[idx].grad += grads[idx]
```

Adding Gradients with Multiple Outputs

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

Schematic of Graph for Training



Two Modes of Graph Construction

- Static (e.g. TensorFlow <2.x)
 - First: define entire graph structure
 - Then: pass in inputs, execute nodes
 - [session.run, feed_dicts, oh my!]
- Dynamic (e.g. PyTorch, TensorFlow 2.x)
 - The graph is defined *dynamically* in the forward pass
 - E.g. operators on Tensors store the links to their input Tensors, thus building a graph

Training Loop

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

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```
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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Update the parameters



Yes, you should understand backprop!

More Resources

- Debugging:
 - Symbolic gradient computation; $f(x + h) - f(x - h)/2h$
 - Shapes! Gradients should be same shape as values [b/c scalar outputs]
- Computing vector/matrix derivatives
 - Work with small toy examples, compute for a single element, generalize
 - <https://web.archive.org/web/20240324092041/http://cs231n.stanford.edu/vecDerivs.pdf>
 - <http://web.stanford.edu/class/cs224n/readings/gradient-notes.pdf>

Next Time

- Feed-forward models for:
 - Classification: Deep Averaging Network
 - Language Modeling
- Training tips and tricks