Computation Graphs + Backpropagation

LING 575K Deep Learning for NLP

Shane Steinert-Threlkeld

April 11 2022

Today's Plan

- Finish neural network intro [batch computation, …]
- Computation graph abstraction
- Backpropagation
  - "Calculus on computation graphs"
- Forward/backward API

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/21-22/575k/hw1/ref/vocabulary.py vocabulary.py`

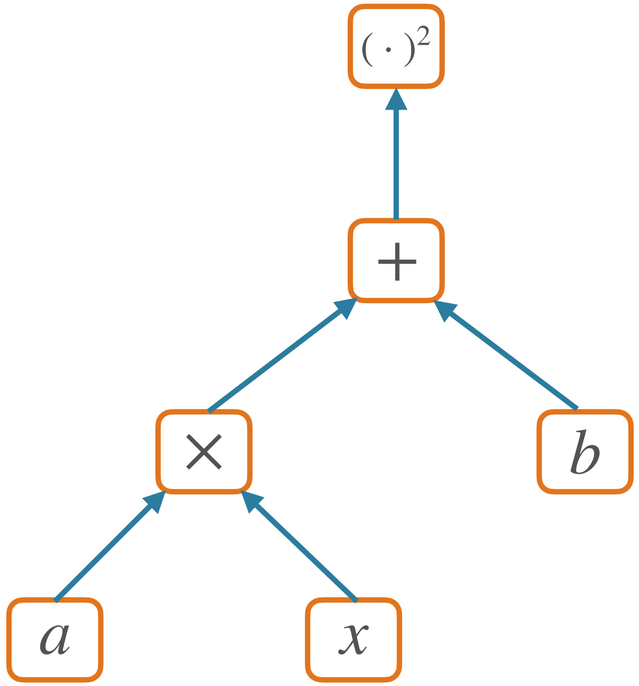
Computation Graphs

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
- Two types of computation:
  - Forward: compute outputs given inputs
  - Backward: compute gradients

Computation Graph Example

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



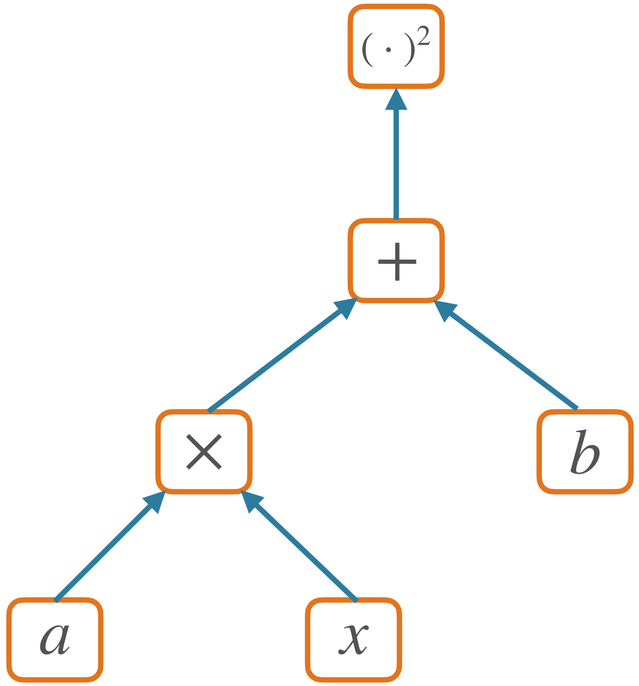
Forward Pass

- 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

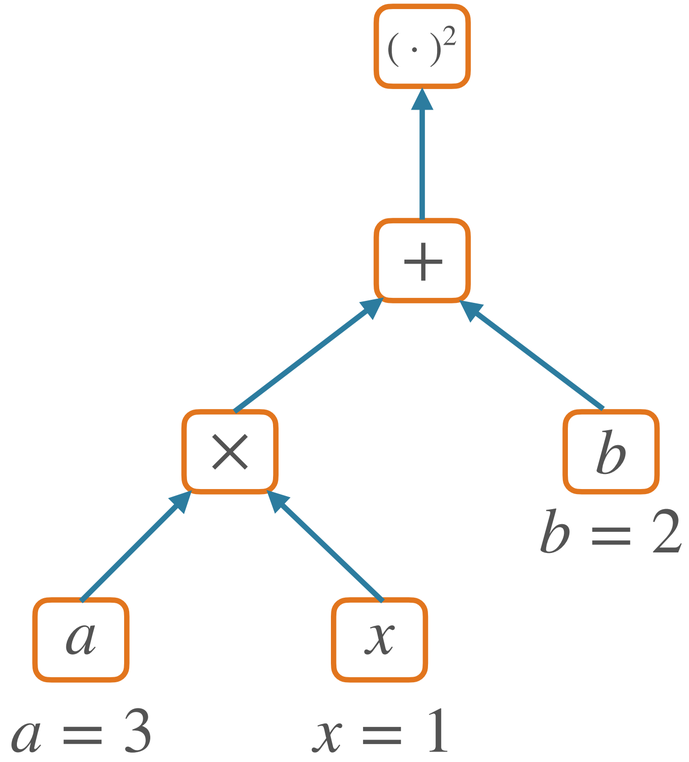
Computation Graph Example

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



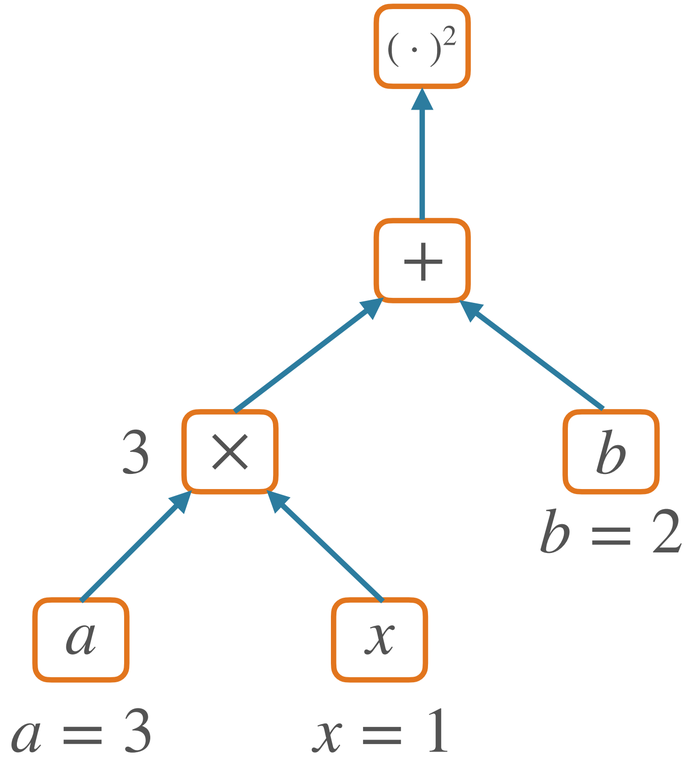
Computation Graph Example

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



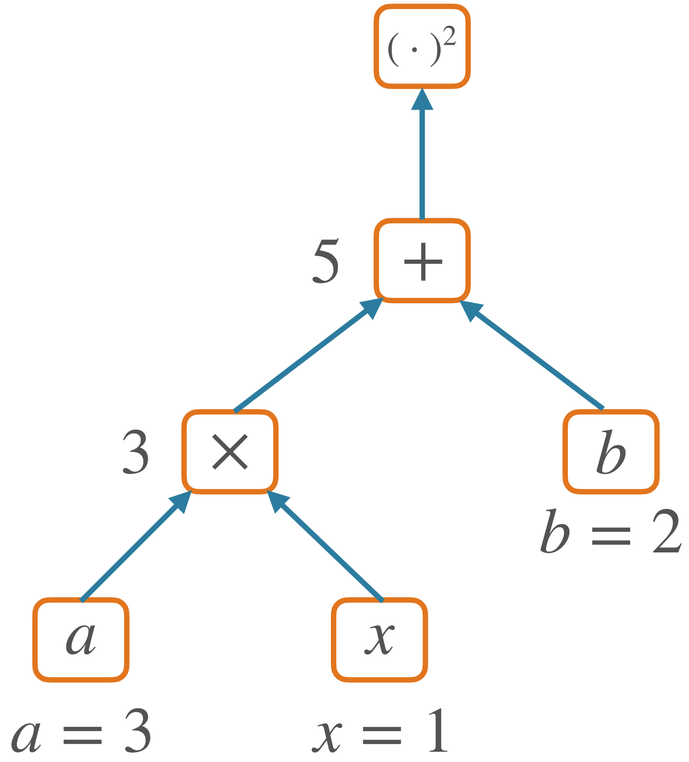
Computation Graph Example

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



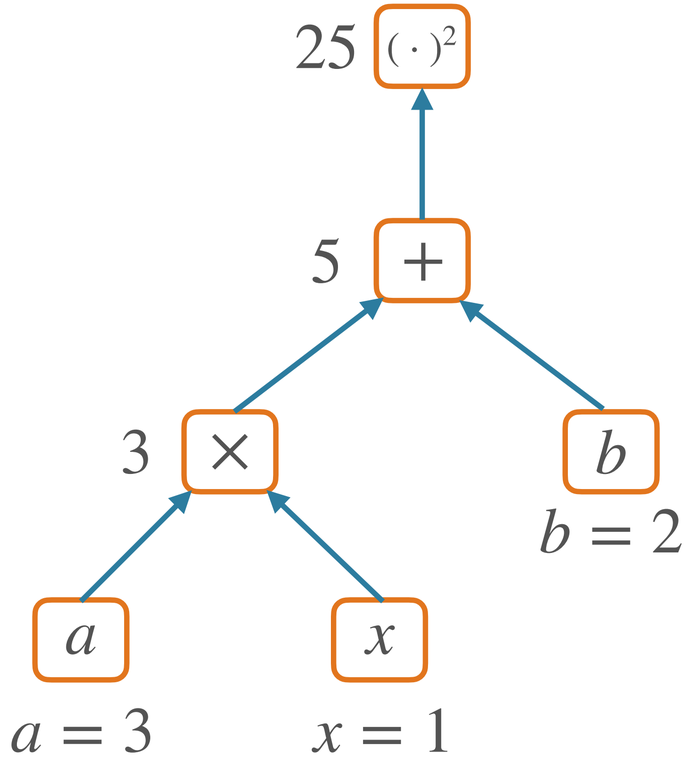
Computation Graph Example

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



Computation Graph Example

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

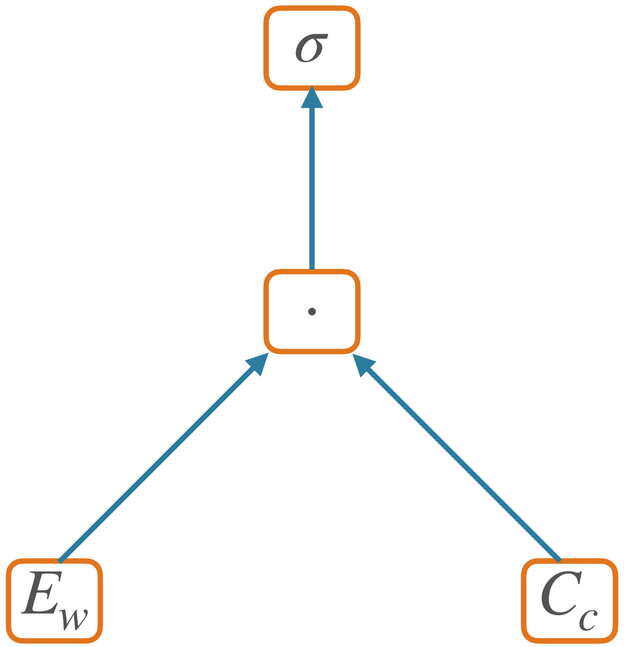


Nodes in a Graph

- Node: 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

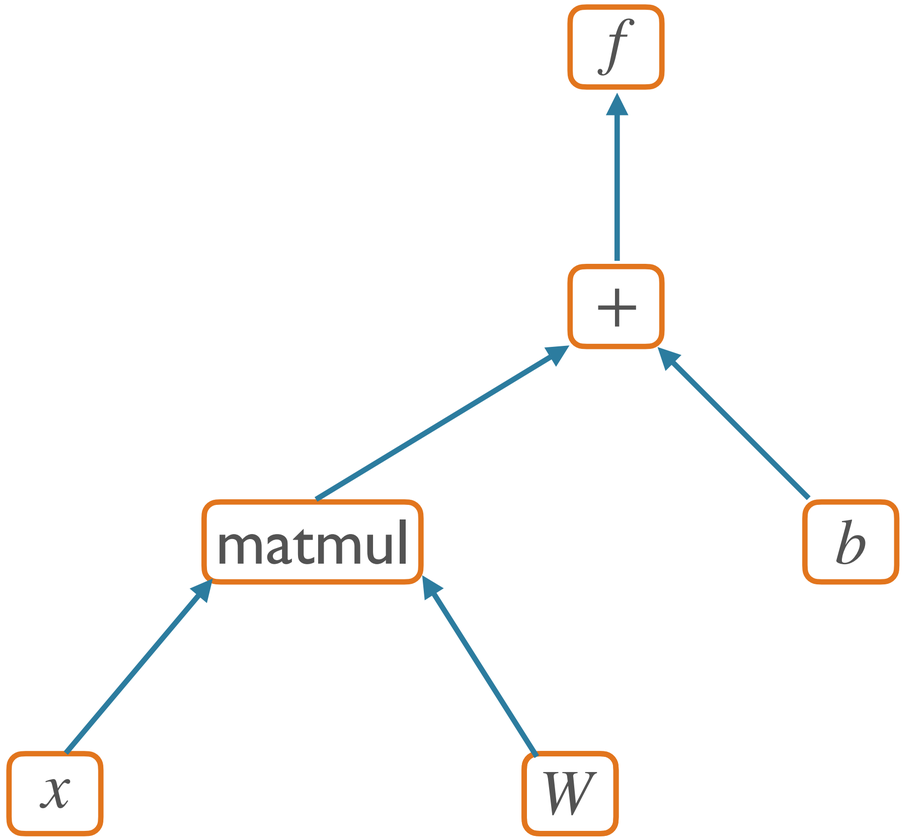
SGNS as a Graph

$$P(1 \mid w, c) = \sigma\left(E_w \cdot C_c\right)$$



Hidden Layer Graph

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



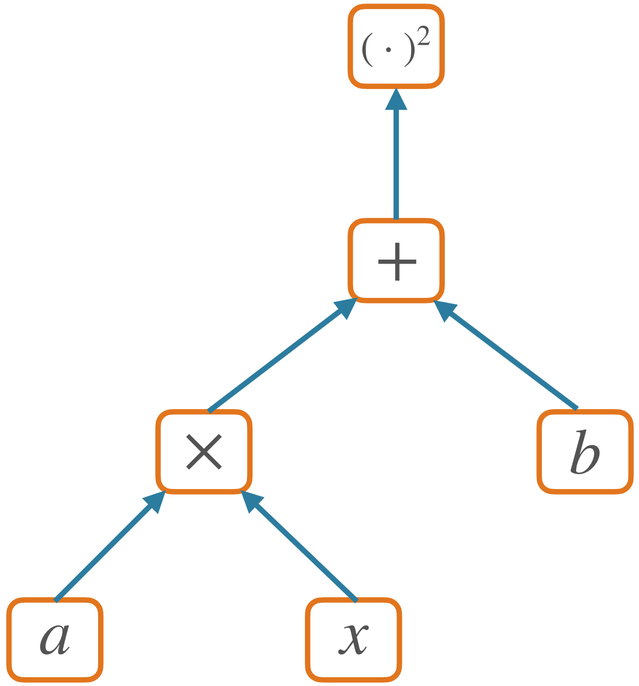
Backpropagation

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

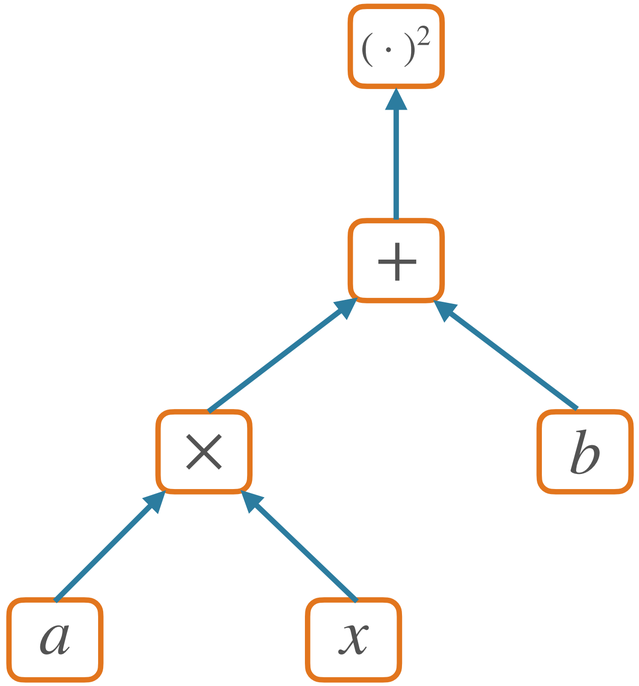
Computing Derivatives

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



Computing Derivatives

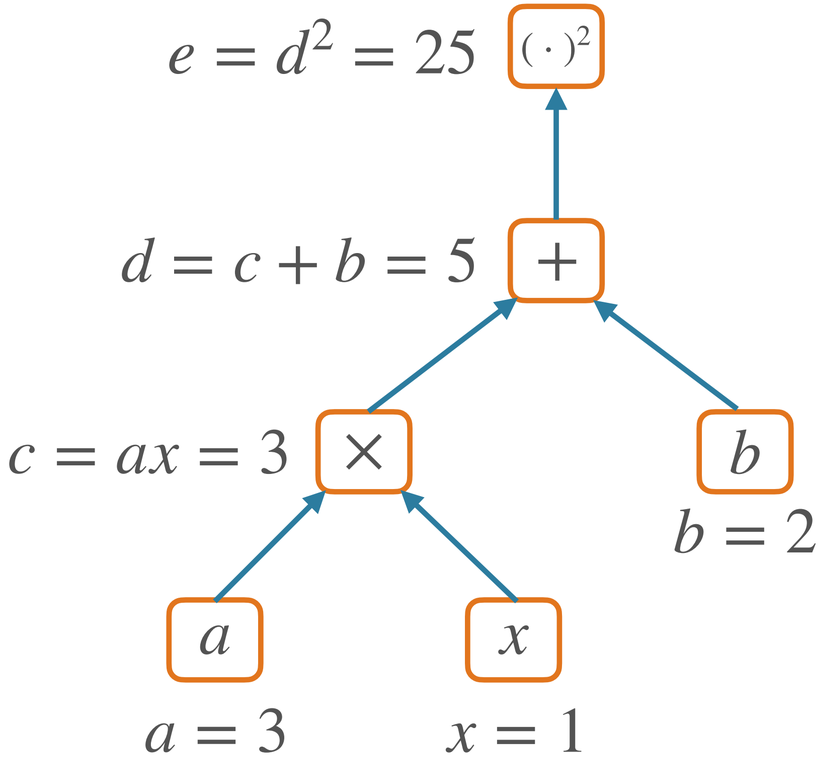
$$f(x; a, b) = (ax + b)^2$$



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

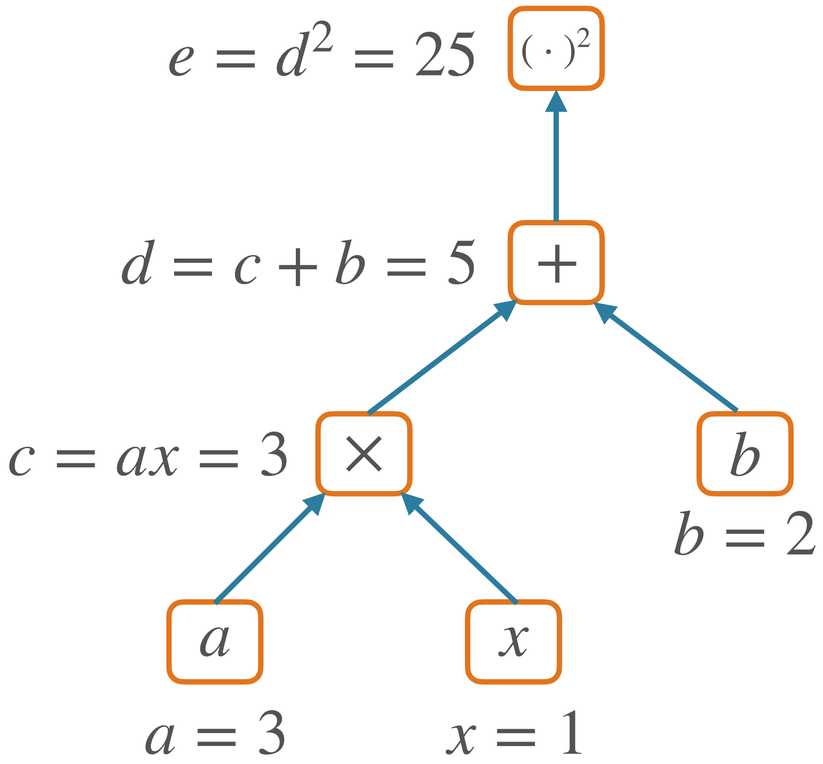
Backpropagation Example

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



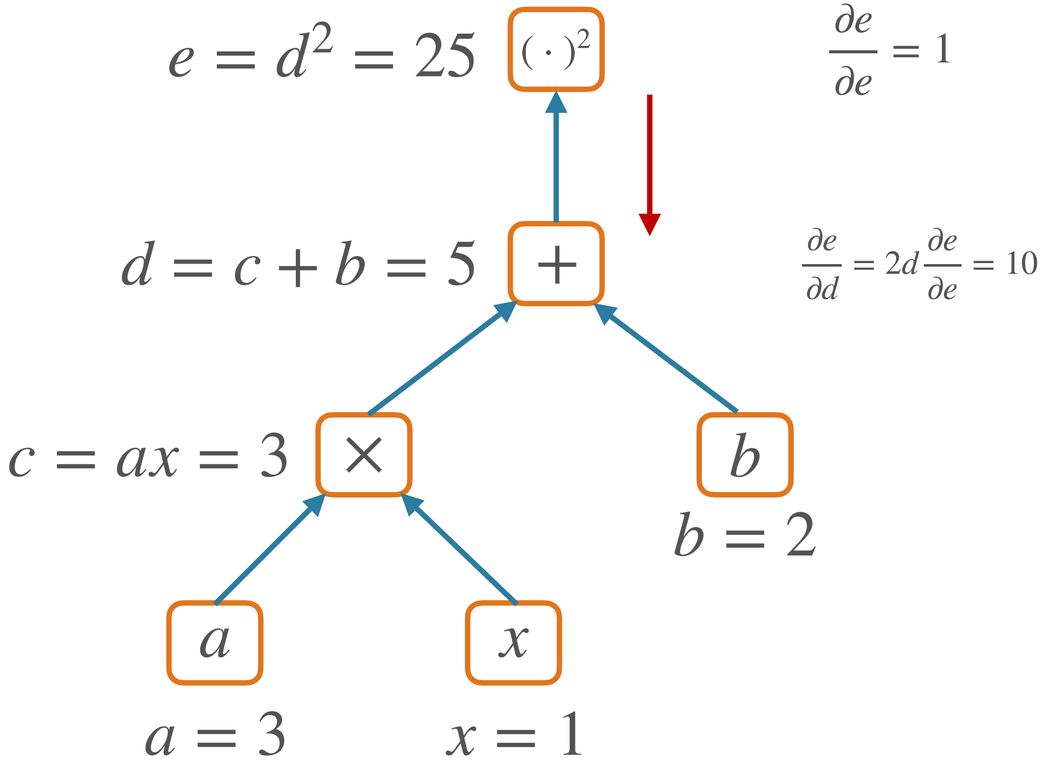
Backpropagation Example

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



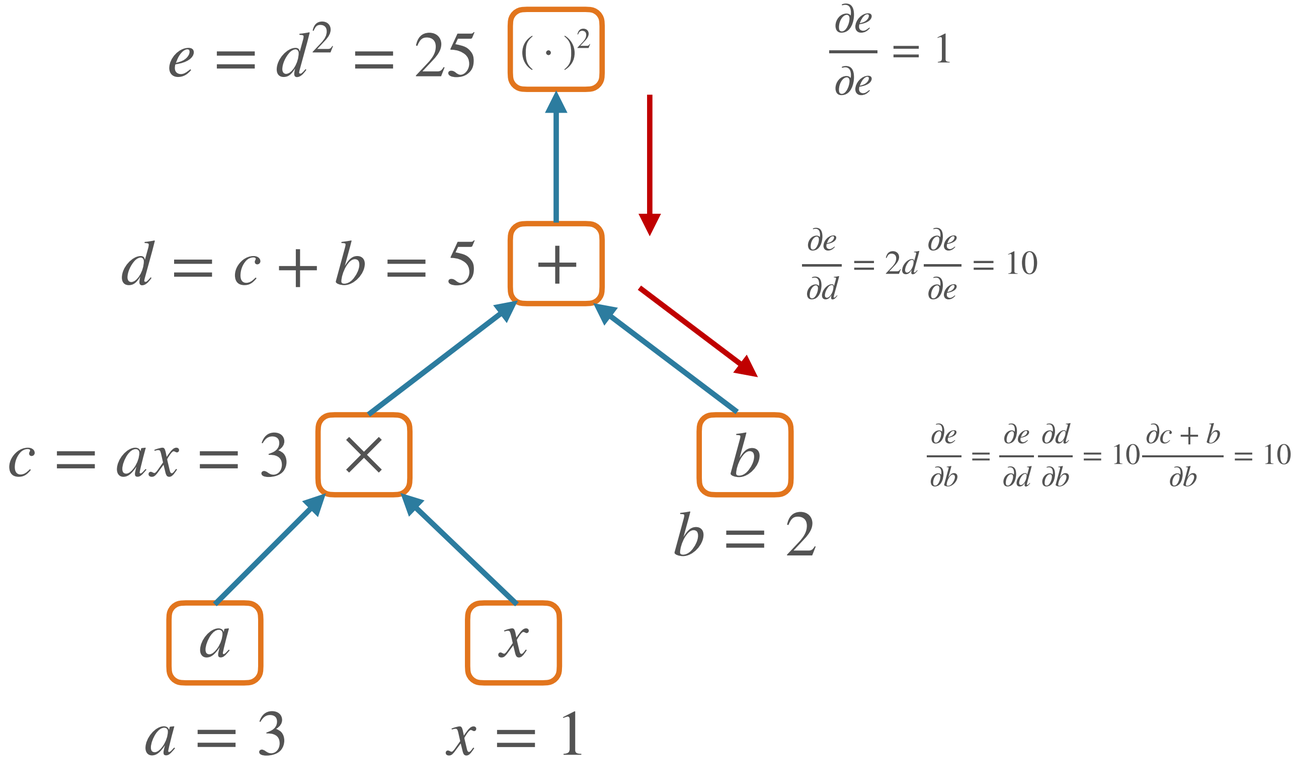
Backpropagation Example

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



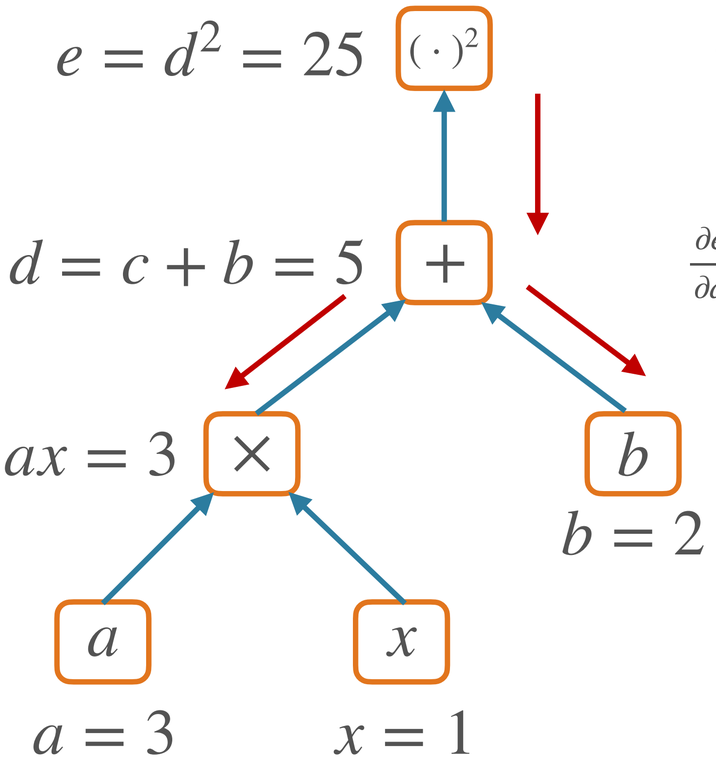
Backpropagation Example

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



Backpropagation Example

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



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

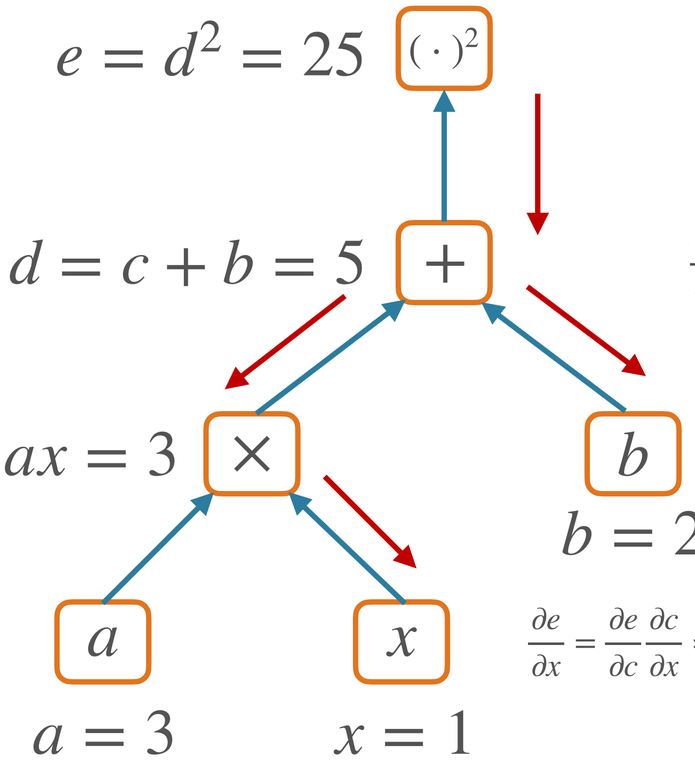
$$\frac{\partial e}{\partial d} = 2d \frac{\partial e}{\partial e} = 10$$

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

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

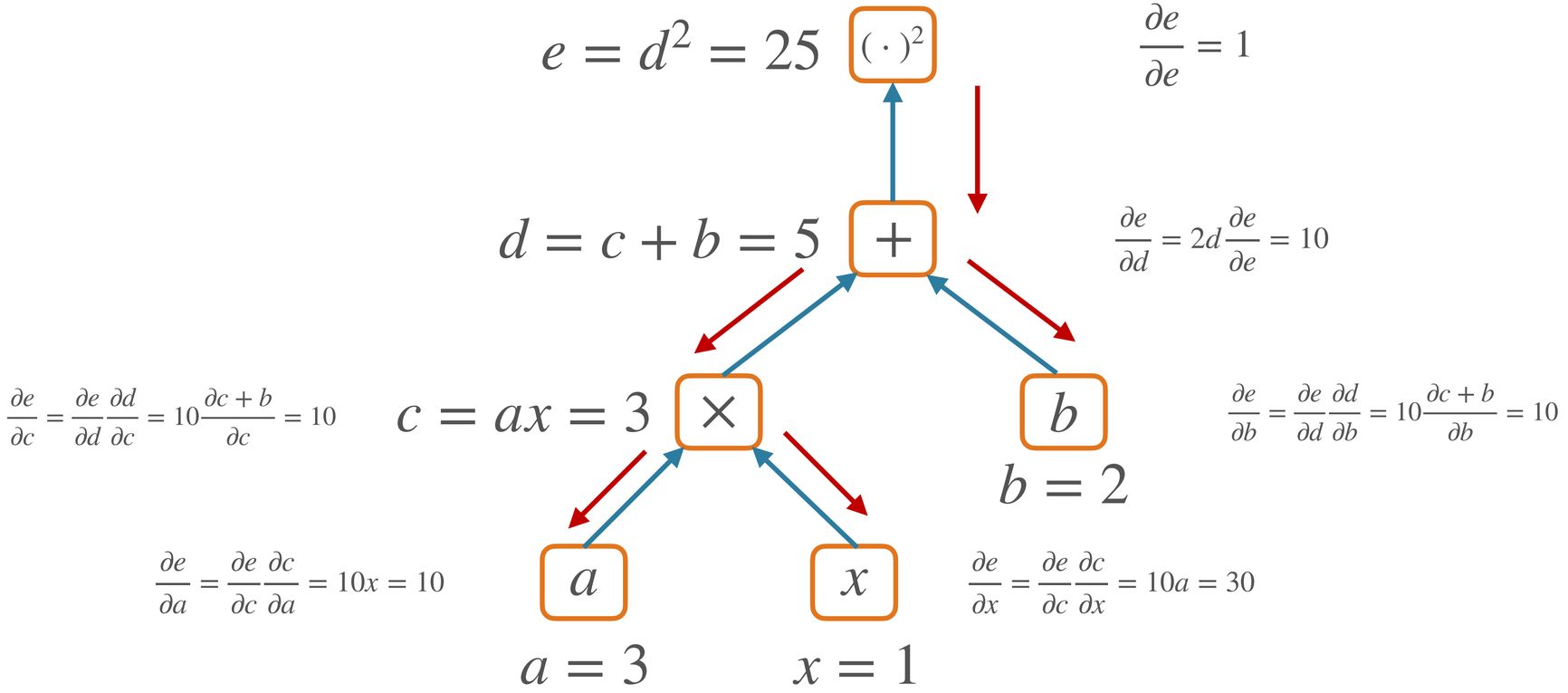
Backpropagation Example

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



Backpropagation Example

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



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

```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()
```

From Tensor class in edugrad

Backpropagation Algorithm

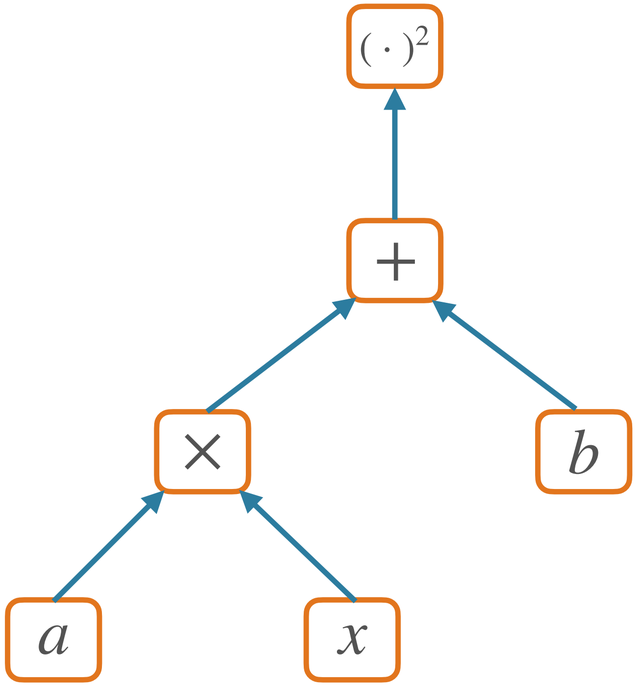
```
def backward(self) -> None:
    """Run backward pass from a scalar tensor.

    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

Local gradient + chain rule application

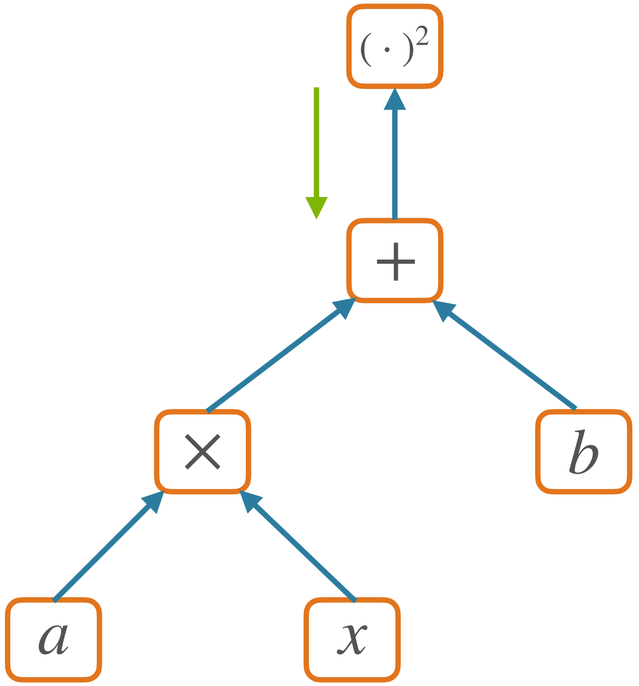
Why back-propagation?

- 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



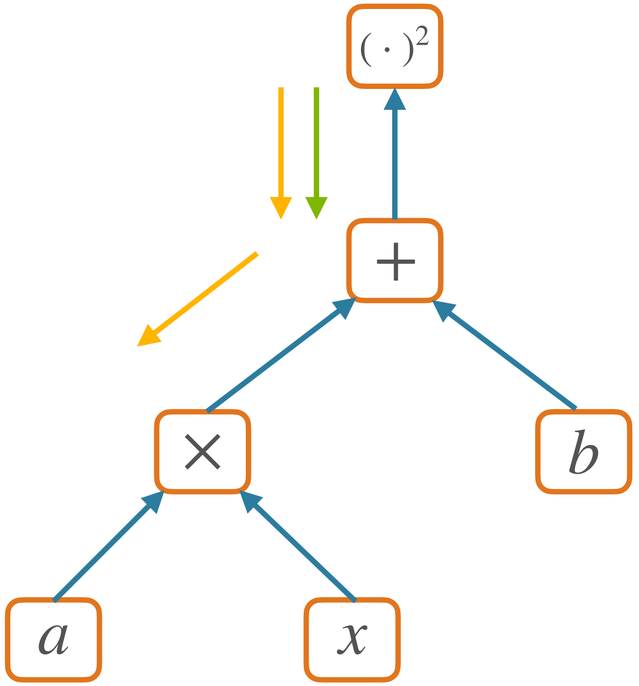
Why back-propagation?

- 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



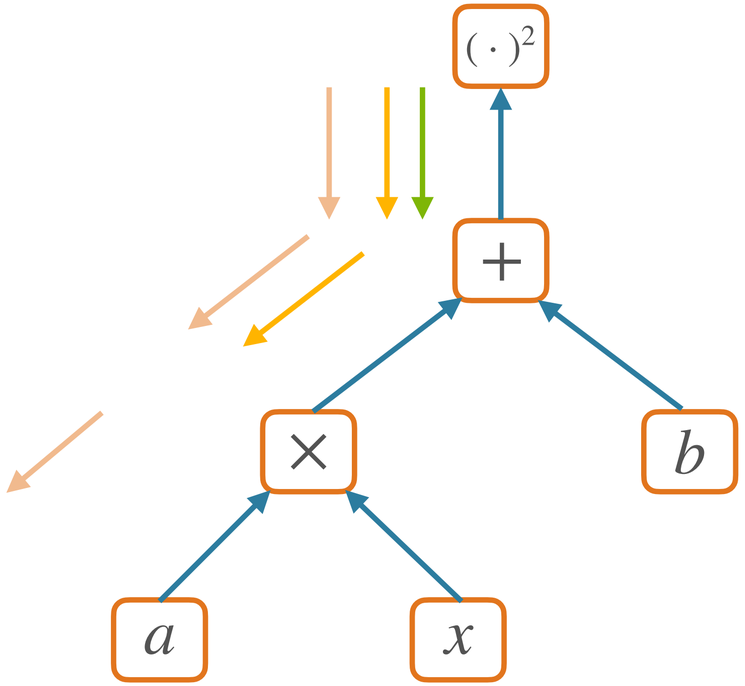
Why back-propagation?

- 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



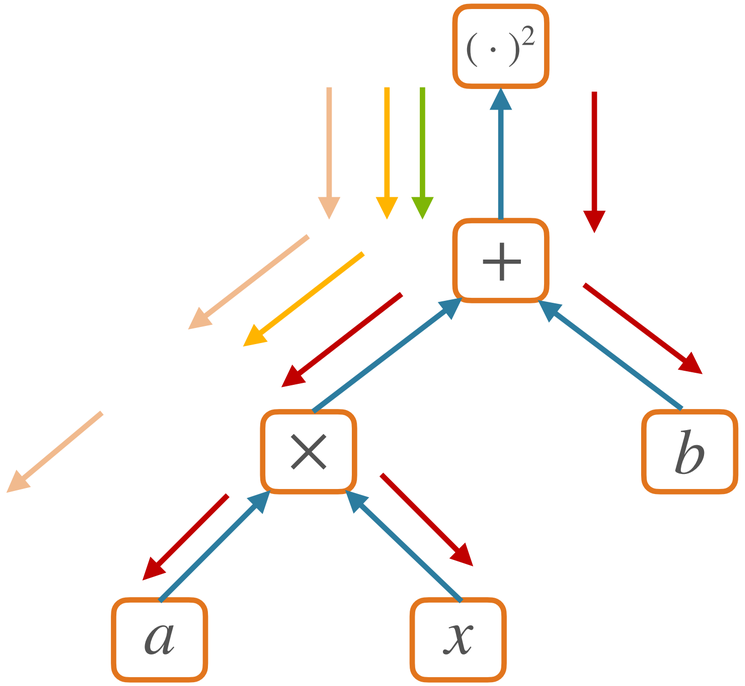
Why back-propagation?

- 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



Why back-propagation?

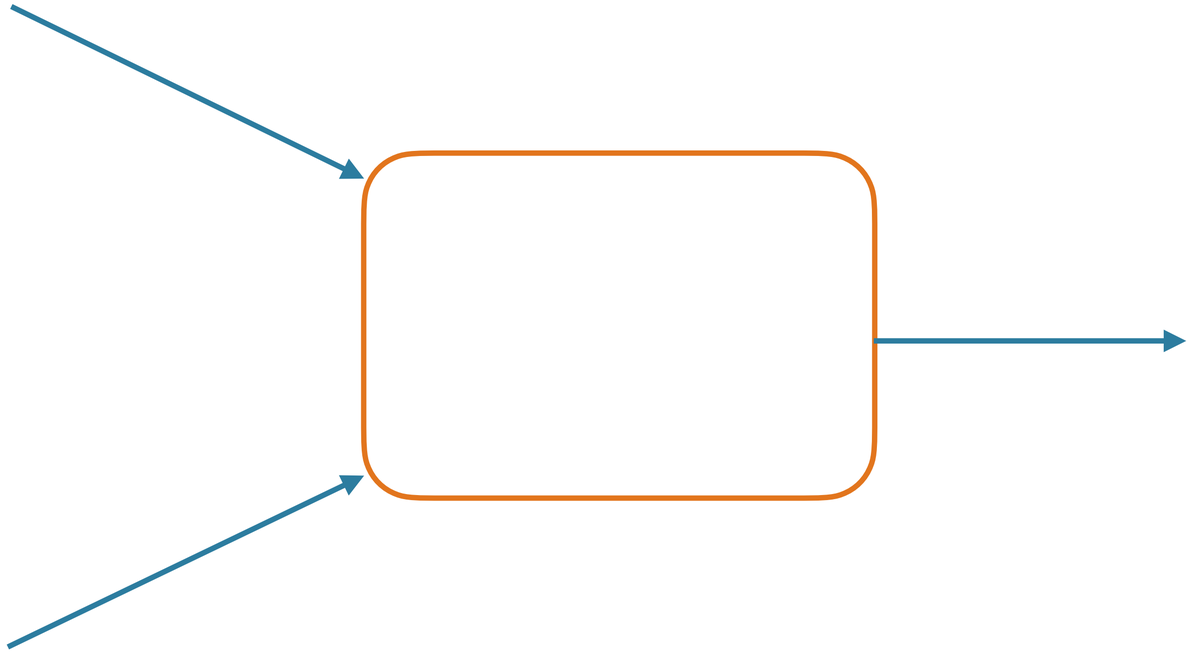
- Extremely efficient method for computing all gradients
  - Compute *once*
  - Store and re-use redundant computation
  - Whence a form of dynamic programming
- Traverse each edge once, instead of once per dependency path



Forward/backward API

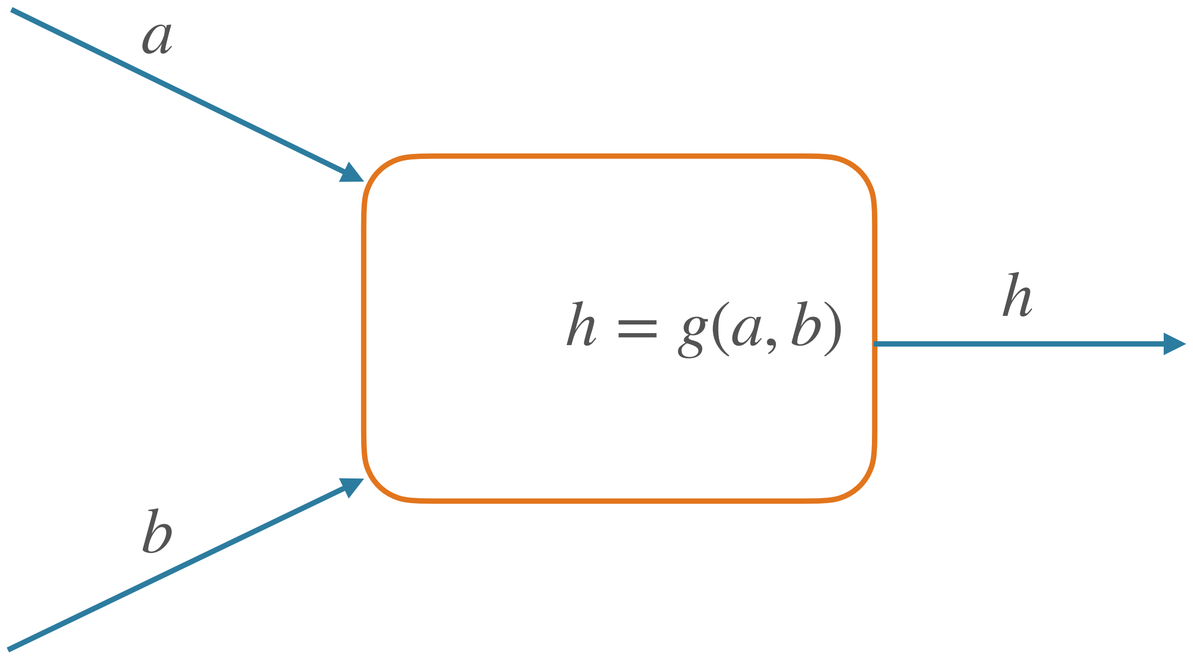
Nodes in Computational Graph

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



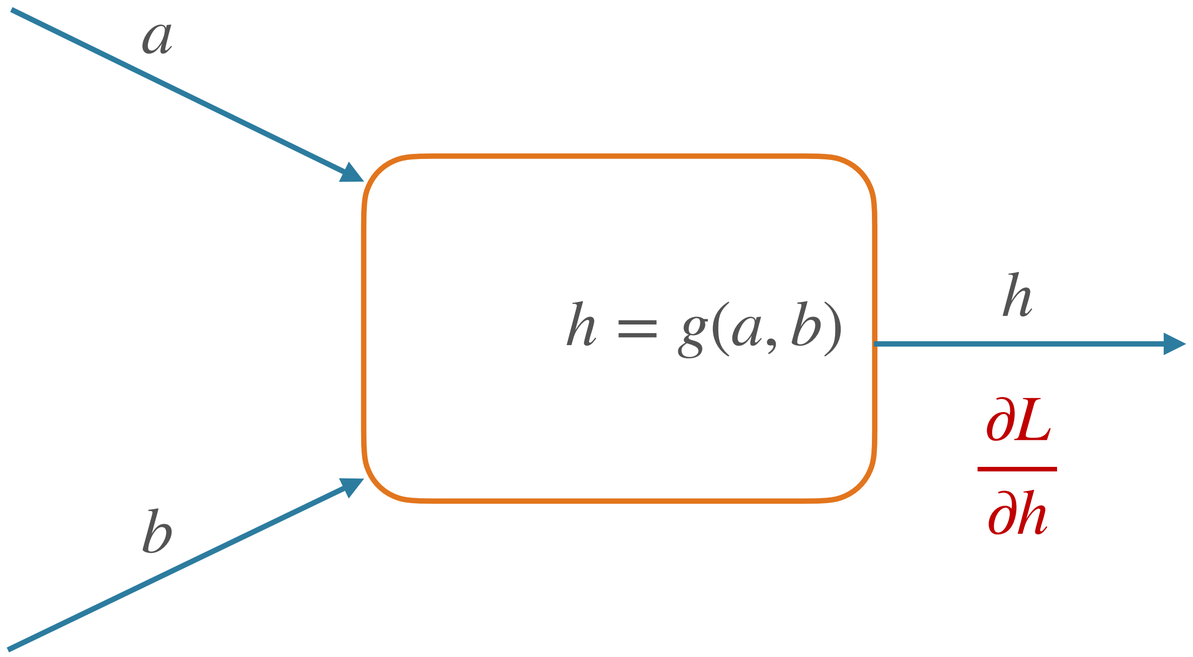
Nodes in Computational Graph

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



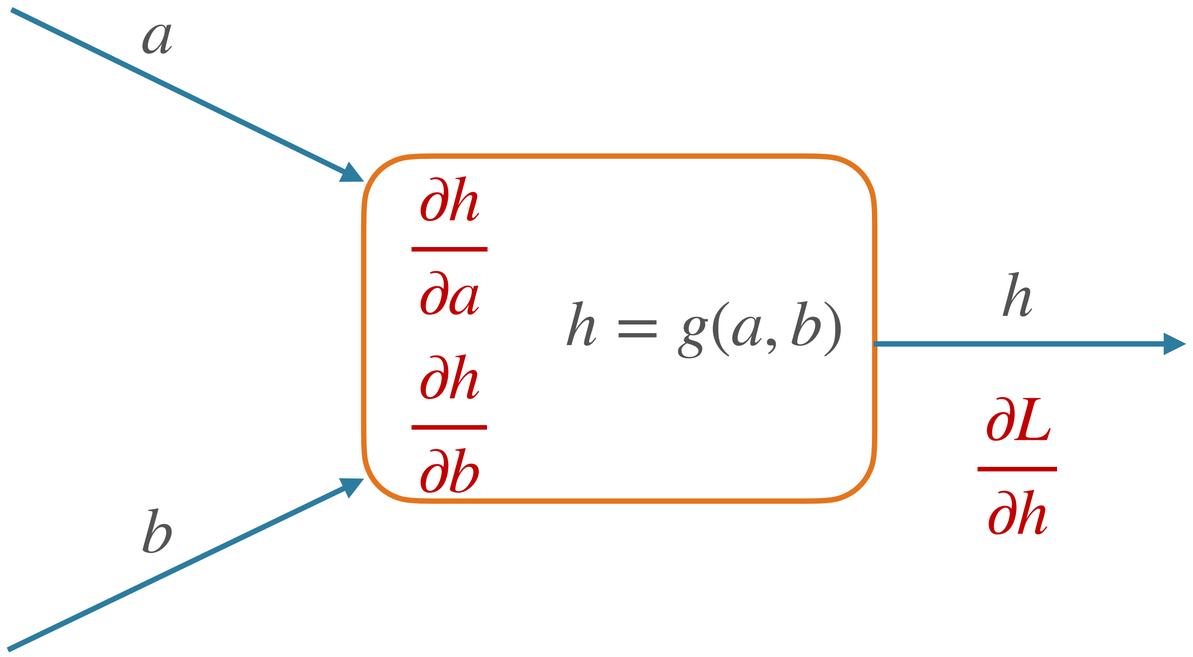
Nodes in Computational Graph

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



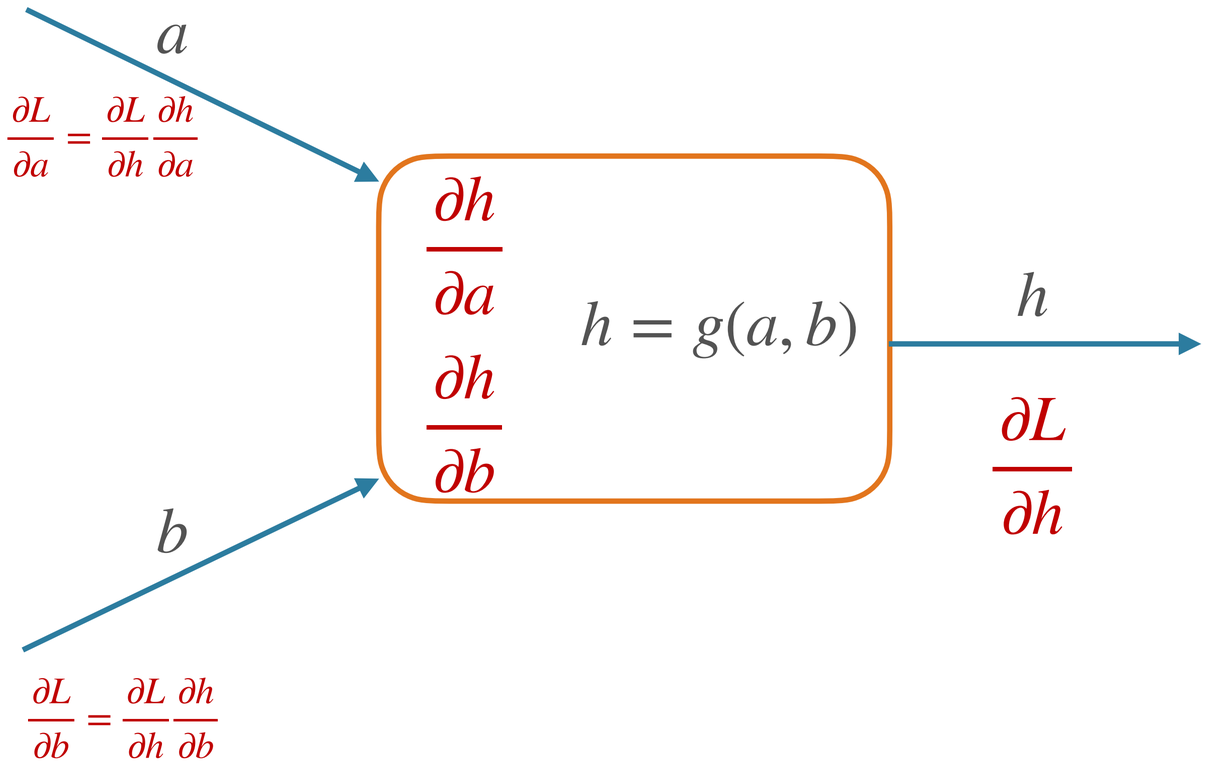
Nodes in Computational Graph

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



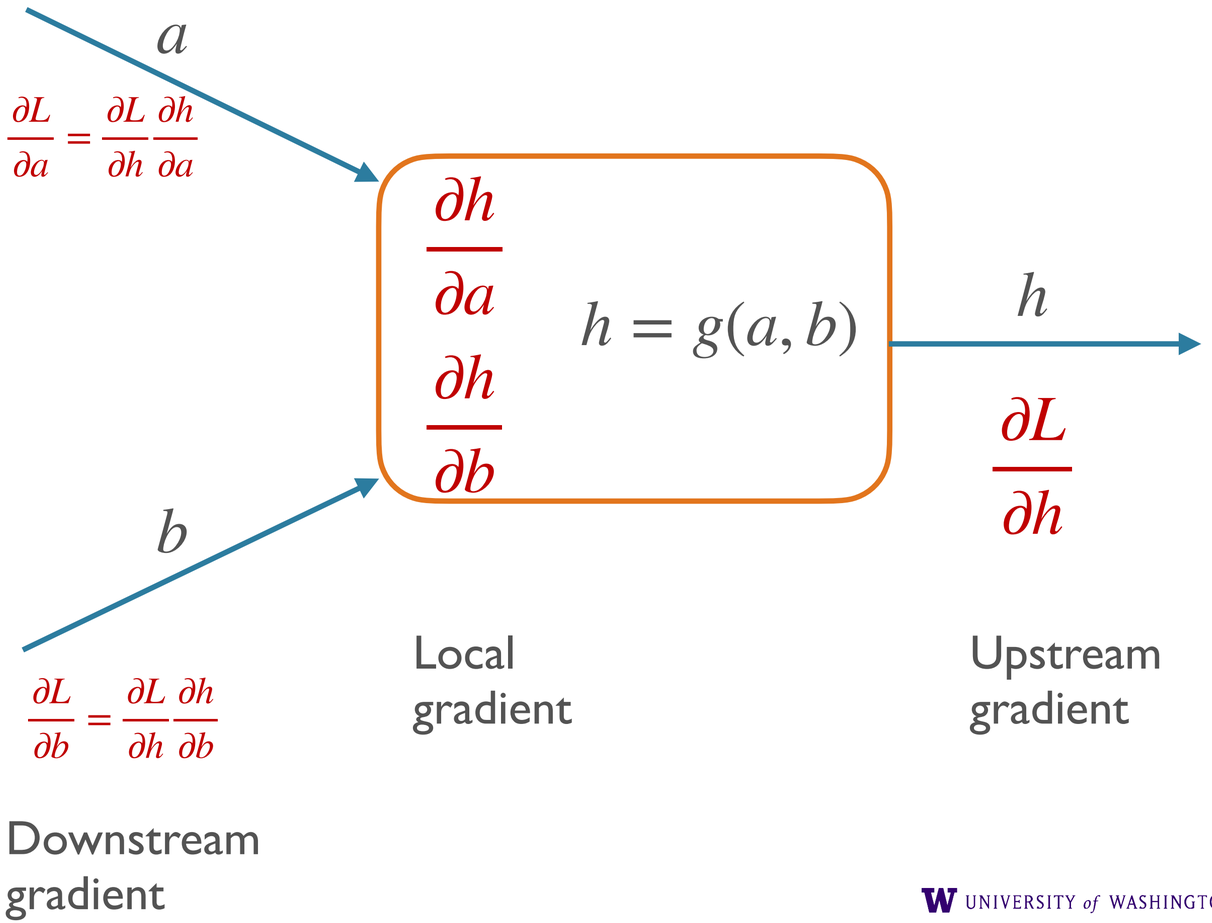
Nodes in Computational Graph

- 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



Forward/Backward API

```python
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
```

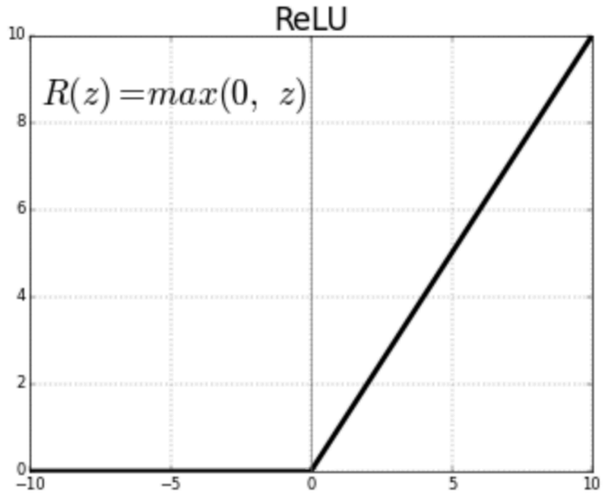
$$\frac{\partial L}{\partial a} \qquad \frac{\partial L}{\partial b}$$

Example: ReLU

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

  def backward(ctx, grad_output):
```

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

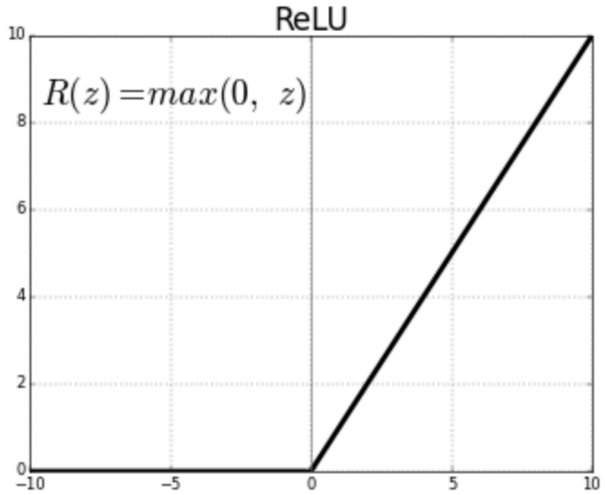
Example: ReLU



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

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

  def backward(ctx, grad_output):
```

Example: ReLU

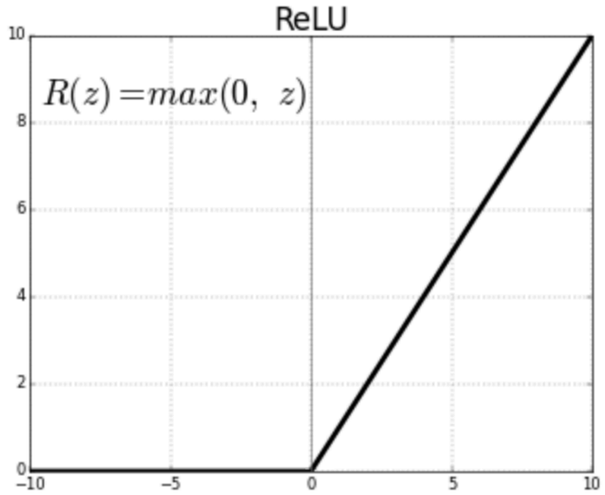


$\text{ReLU}(x) = \max(0,x)$

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

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

  def backward(ctx, grad_output):
```

Example: ReLU



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

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

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

  def backward(ctx, grad_output):
```

🤔🤔🤔 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

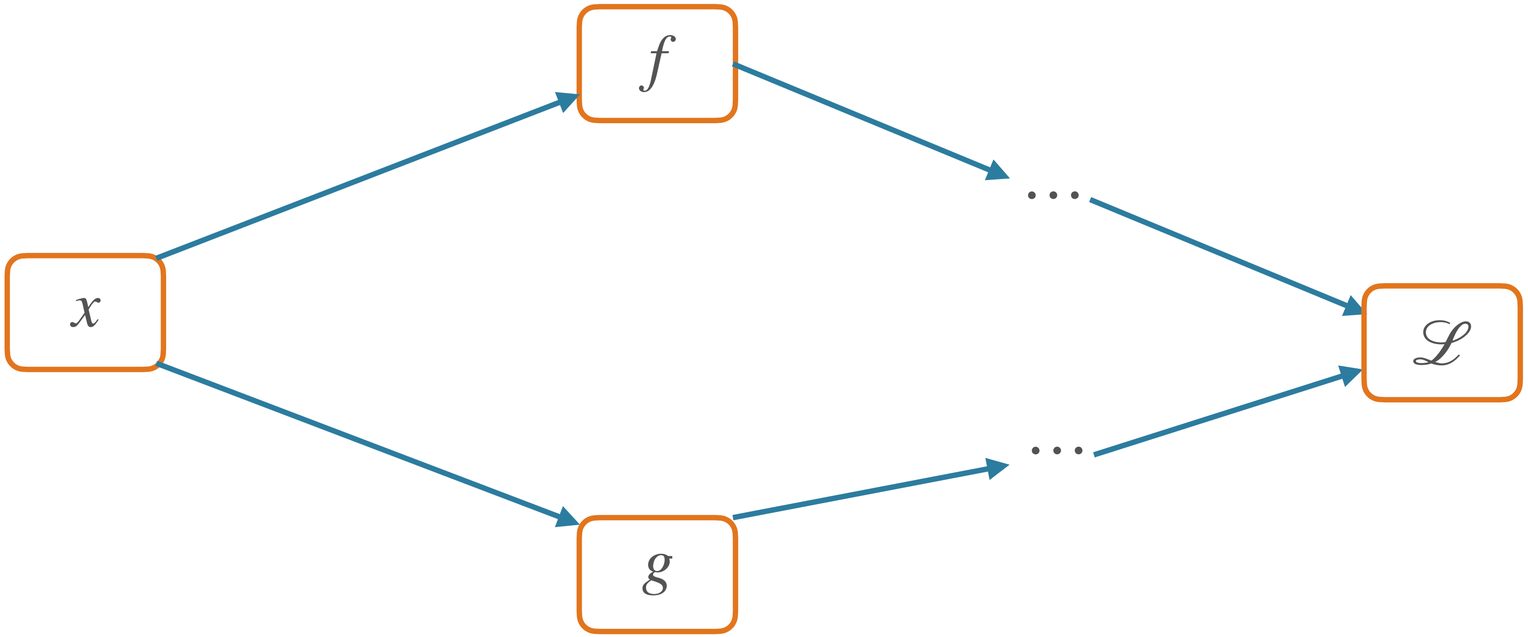
```python
@tensor_op
class relu(Operation):
    @staticmethod
    def forward(ctx, value):
        new_val = np.maximum(0, value)
        ctx.append(new_val)
        return new_val

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

Save and retrieve the input value!

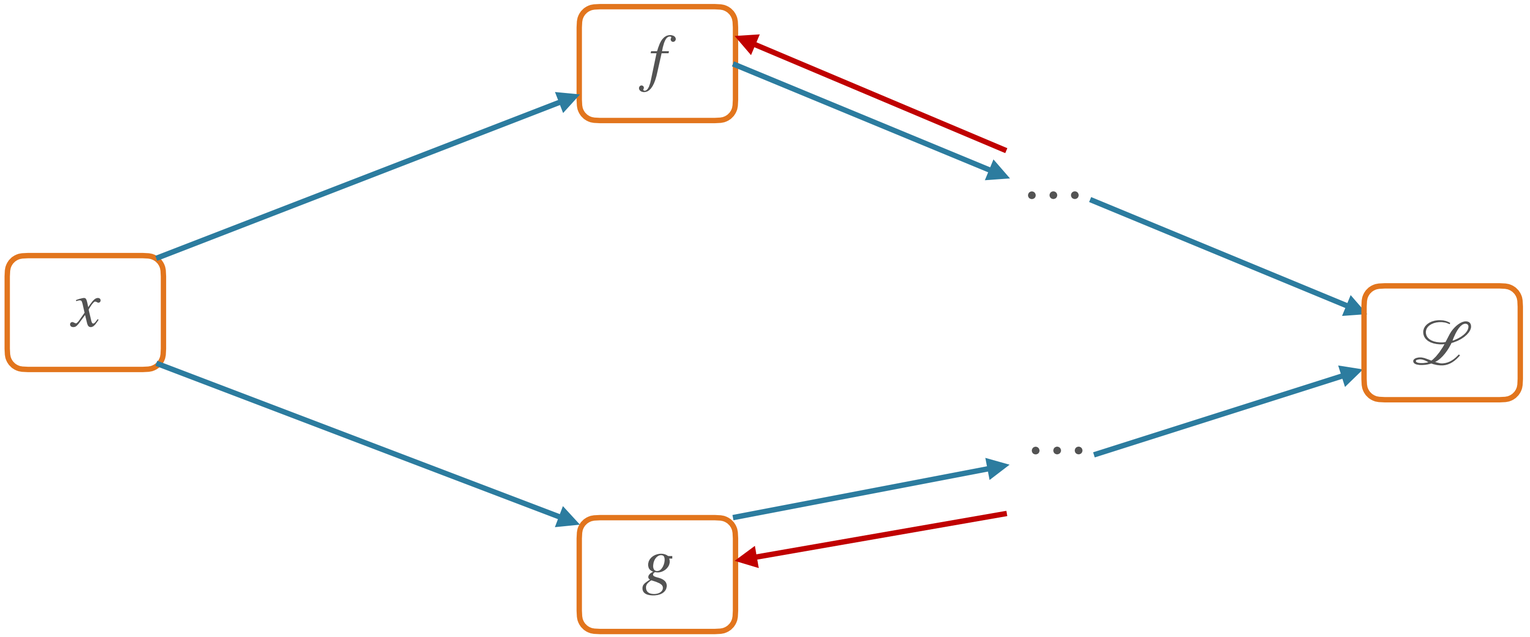
NB: list, one downstream gradient per input (in this case, one)

local gradient times upstream gradient

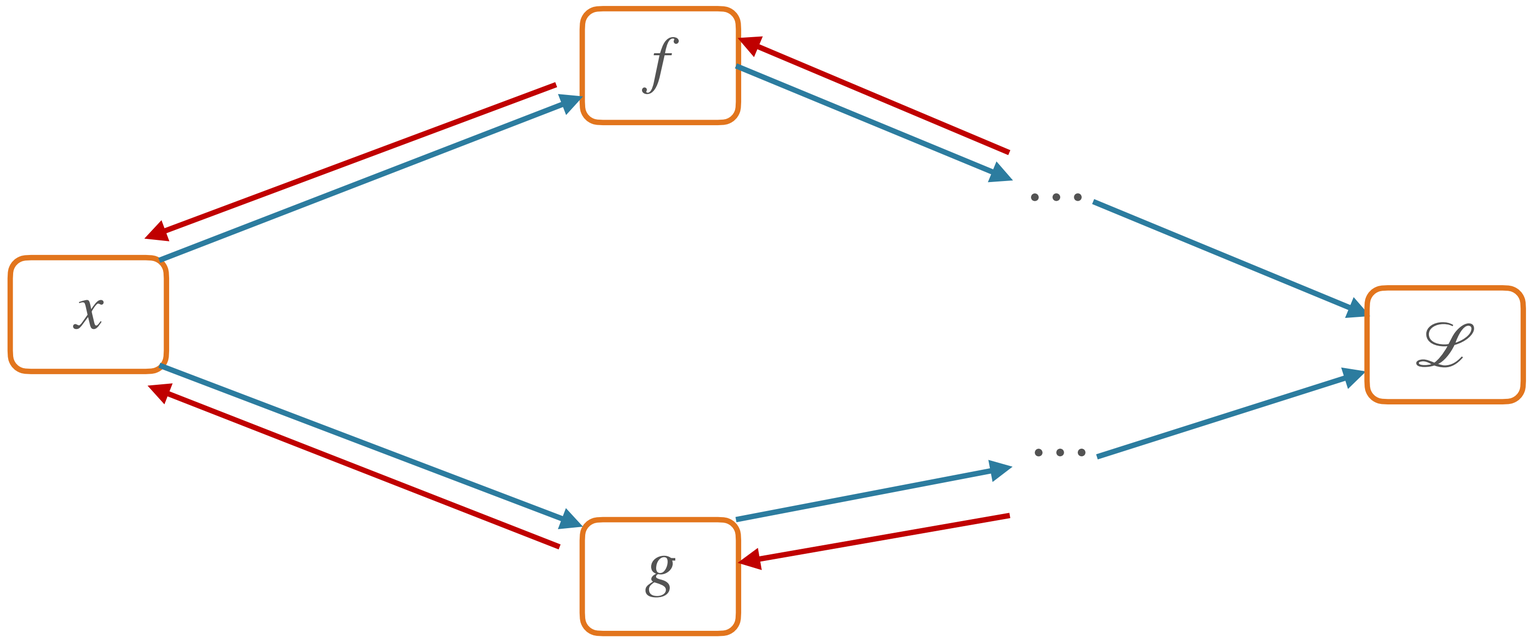
Adding Gradients with Multiple Outputs



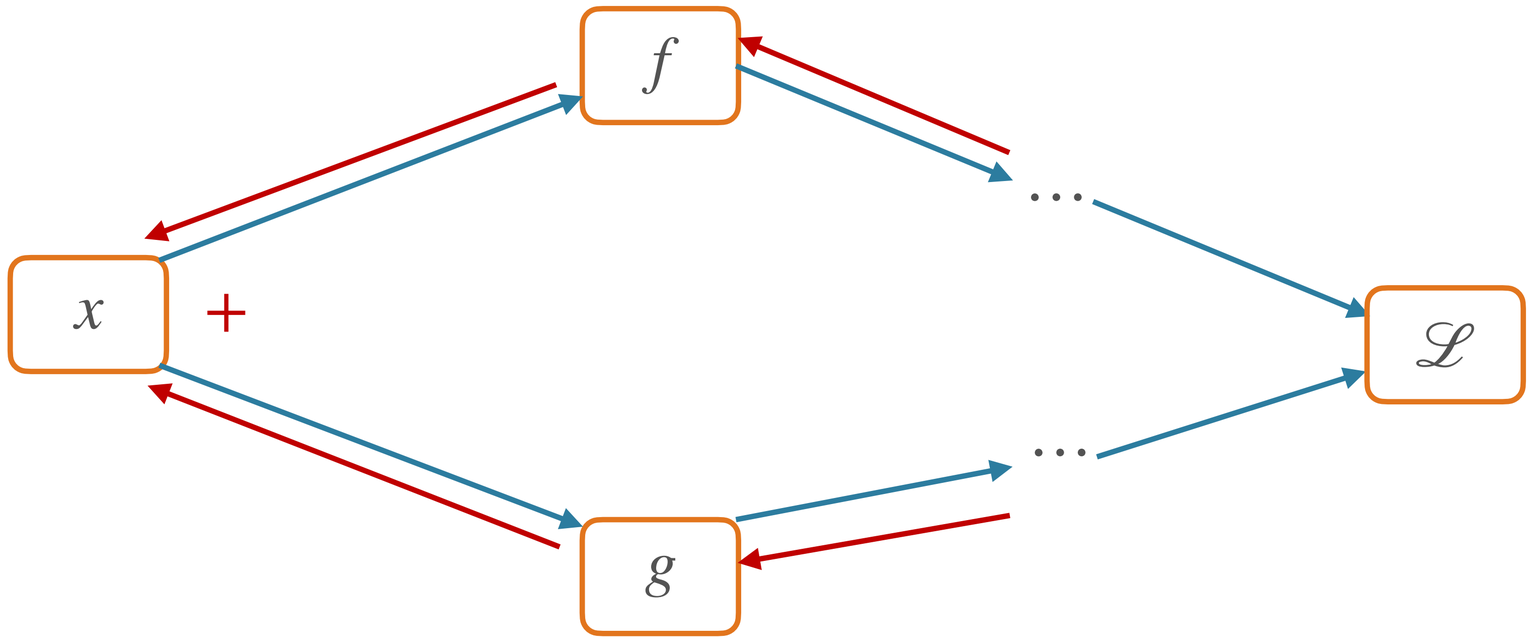
Adding Gradients with Multiple Outputs



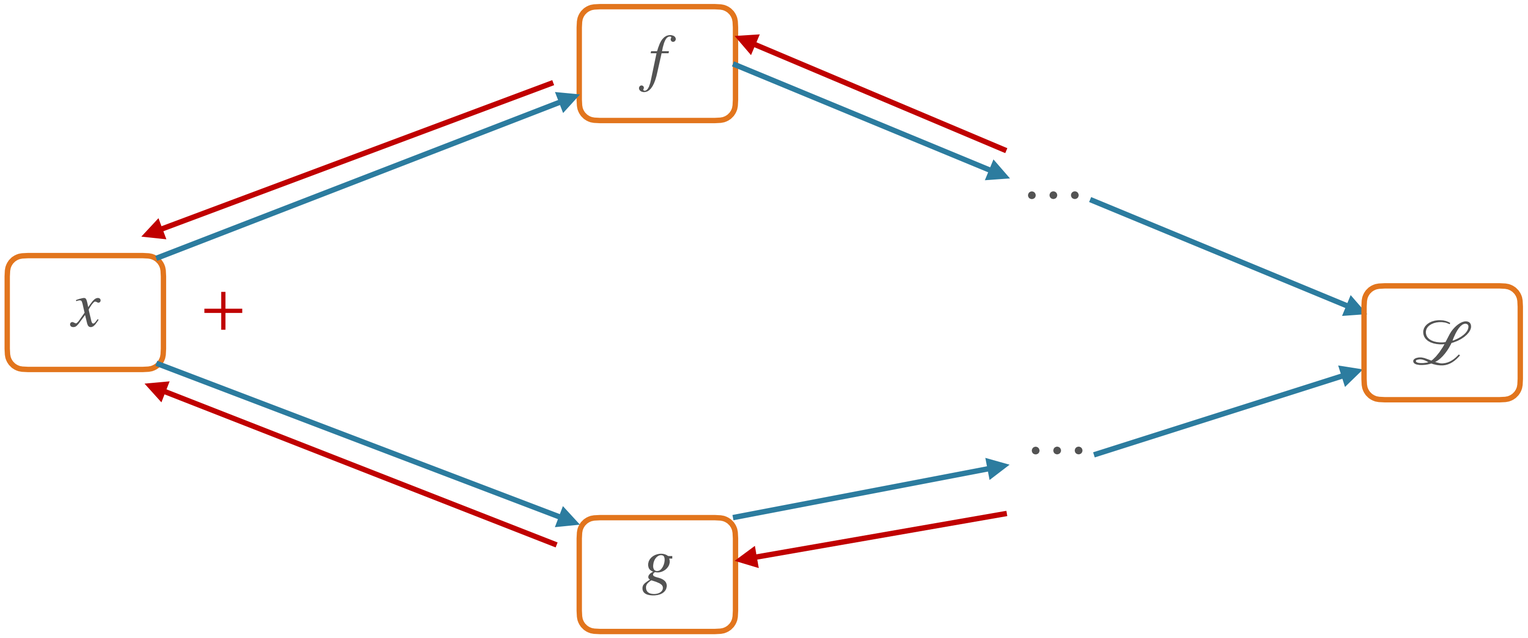
Adding Gradients with Multiple Outputs



Adding Gradients with Multiple Outputs



Adding Gradients with Multiple Outputs



Multivariable chain rule:

$$\frac{\partial \mathscr{L}}{\partial x} = \frac{\partial \mathscr{L}}{\partial f}\frac{\partial f}{\partial x} + \frac{\partial \mathscr{L}}{\partial g}\frac{\partial g}{\partial x}$$

Adding Gradients with Multiple Outputs

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

Live demo and/or exercise!

Adding Gradients with Multiple Outputs

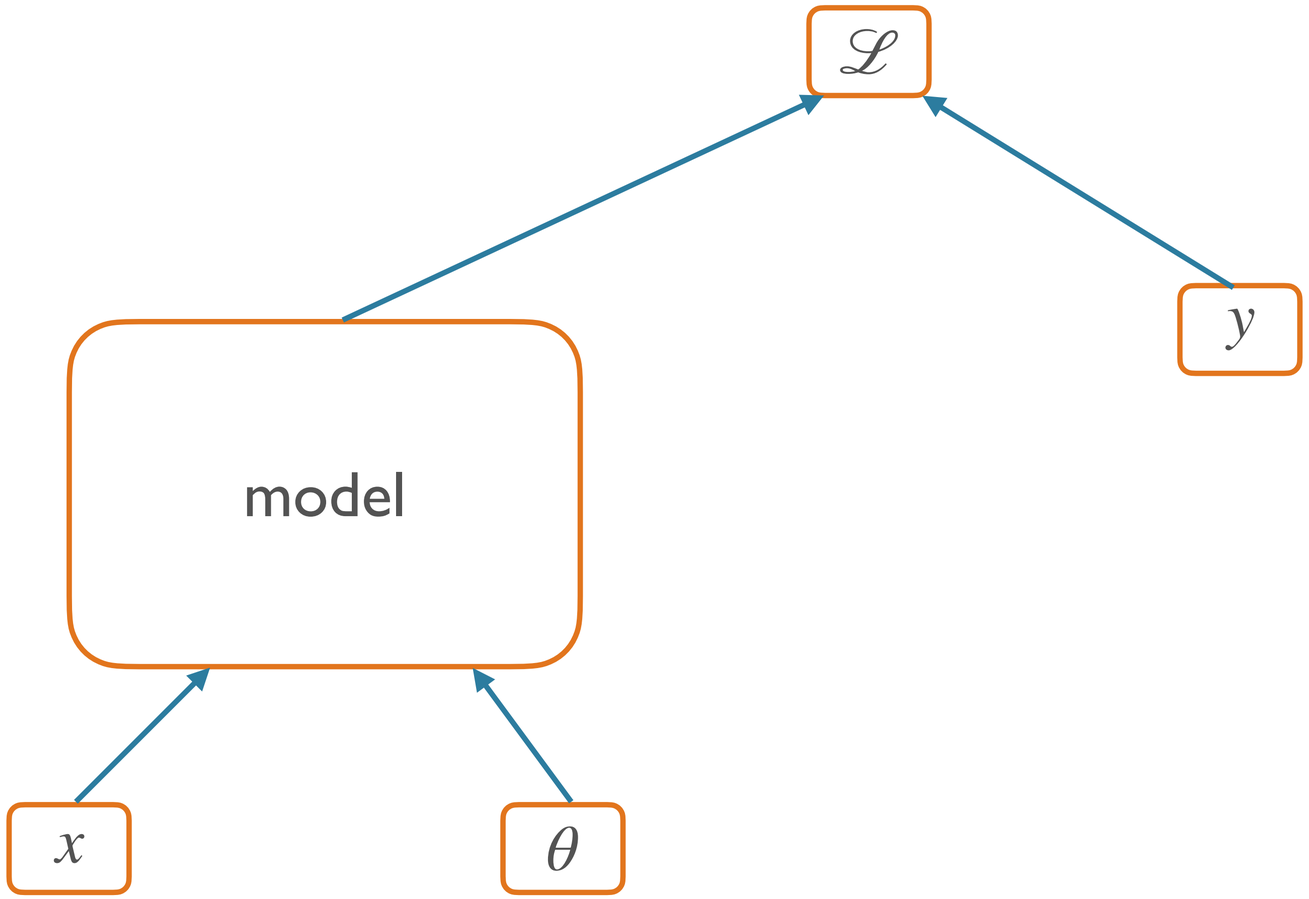
```
def _backward():
    grads = op.backward(ctx, new_tensor.grad)
    for idx in range(len(inputs)):
        inputs[idx].grad += grads[idx]
```

Adding Gradients with Multiple Outputs

```
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



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”

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”

Backprop the loss!

```
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!

Update the parameters

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

Yes, you should understand backdrop!

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
  - 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