Neural Networks II: Backpropagation

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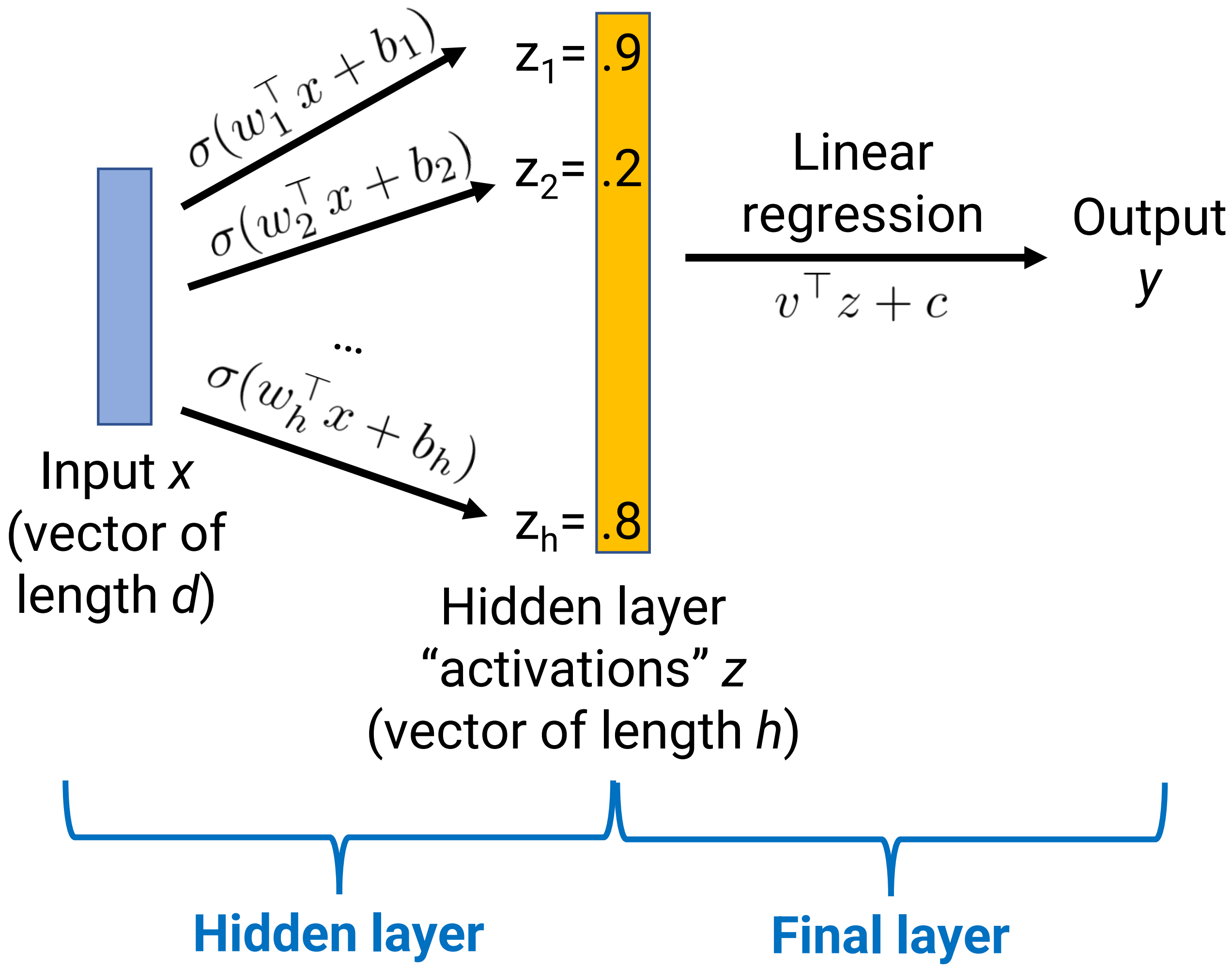
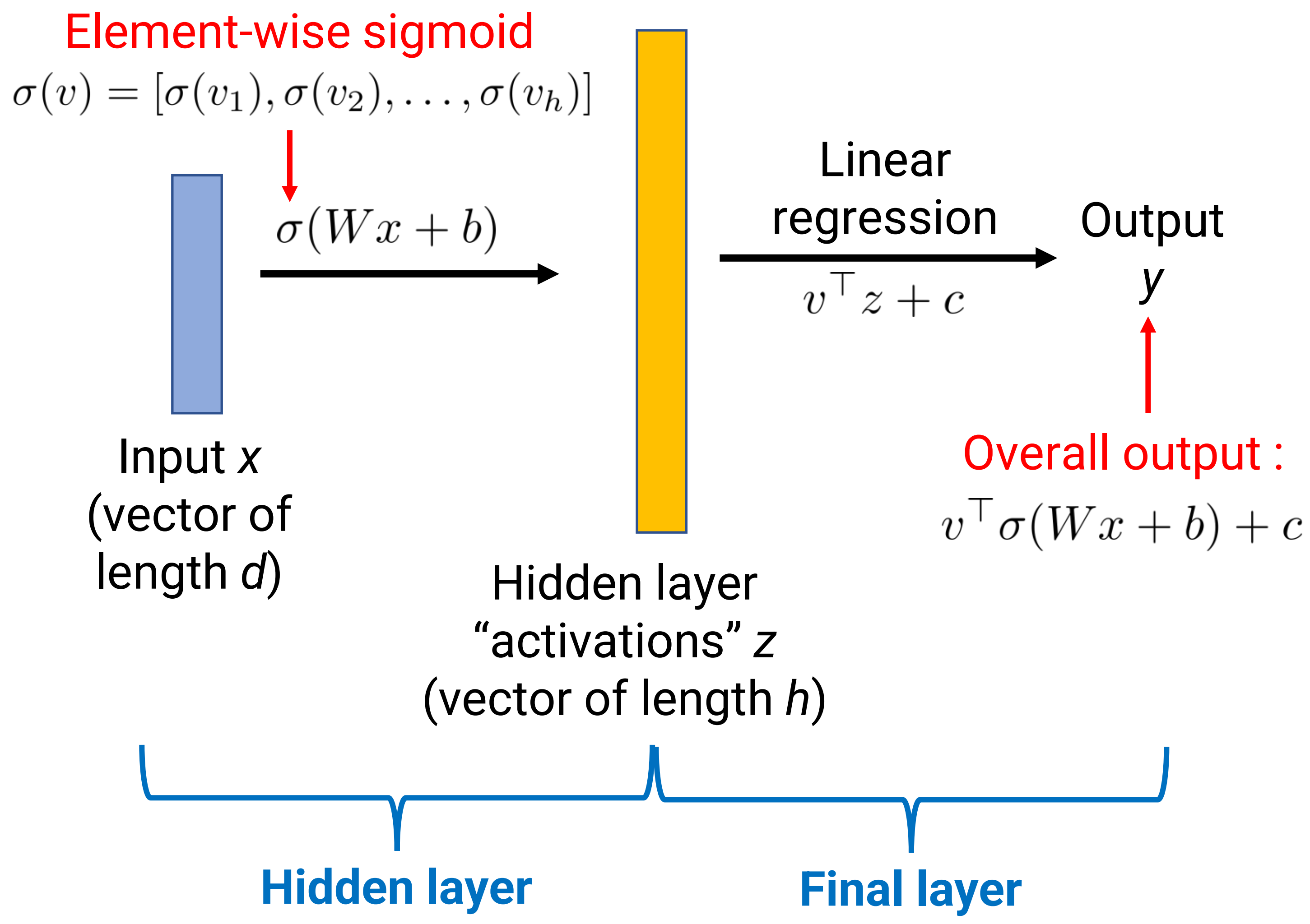
USC CSCI 467, Spring 2024
February 13, 2024

Review: Neural Networks (2-layer MLP)



- Hidden layer = A bunch of logistic regression classifiers
  - Parameters: $\boldsymbol{w_j}$ and $\boldsymbol{b_j}$ for each classifier, for each $j=1, \ldots, h$
  - h = number of neurons in hidden layer ("hidden nodes")
  - Produces "activations"= learned feature vector
- Final layer = linear model
  - For regression: linear model with weight vector $\boldsymbol{v}$ and bias $\boldsymbol{c}$

Review: Neural Networks (2-layer MLP)

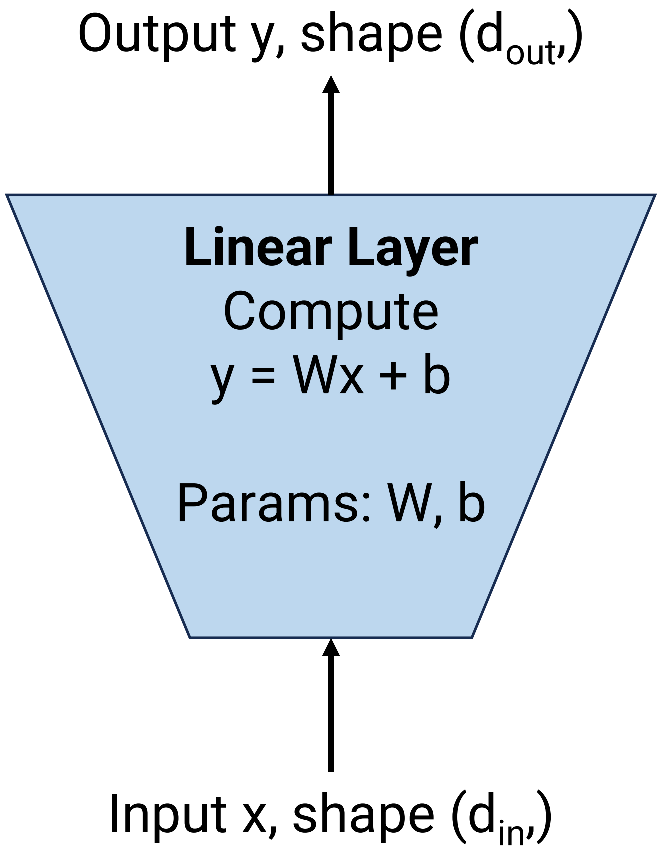


- Hidden layer = A bunch of logistic regression classifiers
  - Parameters: $\boldsymbol{w}_j$ and $\boldsymbol{b}_j$ for each classifier, for each $j=1, \ldots, h$
  - Equivalently: matrix $\boldsymbol{W}$ (h x d) and vector $\boldsymbol{b}$ (length h)
  - h = number of neurons in hidden layer ("hidden nodes")
  - Produces "activations"= learned feature vector
- Final layer = linear model
  - For regression: linear model with weight vector $\boldsymbol{v}$ and bias $\boldsymbol{c}$
- **Parameters of model are** $\boldsymbol{\theta = (W, b, v, c)}$

Review: Neural Network Building Blocks

(1) Linear Layer

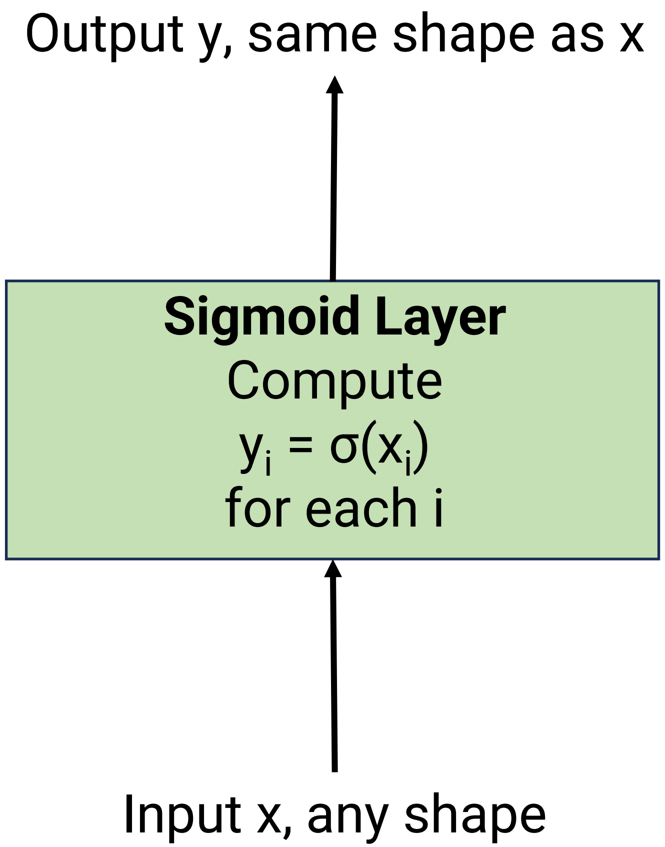
- Input x: Vector of dimension d_{in}
- Output y: Vector of dimension d_{out}
- Formula: $y = Wx + b$
- Parameters
  - W: d_{out} x d_{in} matrix
  - b: d_{out} vector
- In pytorch: nn.Linear()



Review: Neural Network Building Blocks

(2) Non-linearity Layer

- Input x: Any number/vector/matrix
- Output y: Number/vector/matrix of same shape
- Possible formulas:
  - Sigmoid: y = σ(x), elementwise
  - Tanh: y = tanh(x), elementwise
  - Relu: y = max(x, 0), elementwise
- Parameters: None
- In pytorch: torch.sigmoid(), nn.functional.relu(), etc.



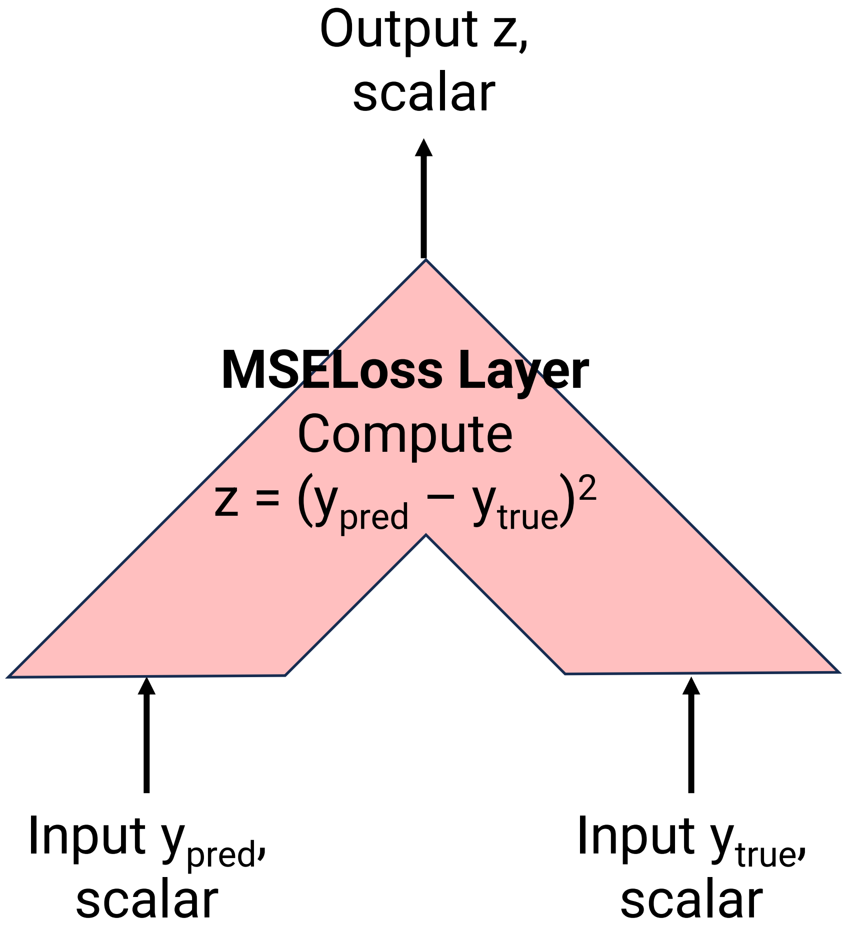
Review: Neural Network Building Blocks

(3) Loss Layer

- Inputs:
  - y_{pred}: shape depends on task
  - y_{true}: scalar (e.g., correct regression value or class index)
- Output z: scalar
- Possible formulas:
  - Squared loss: y_{pred} is scalar, $z = (y_{pred} - y_{true})^2$
  - Softmax regression loss: y_{pred} is vector of length C,

$$z = -\left(y_{\text{pred}}[y_{\text{true}}] - \log \sum_{i=1}^{C} \exp(y_{\text{pred}}[i]) \right)$$

- Parameters: None
- In pytorch: nn.MSELoss(), nn.CrossEntropyLoss(), etc.



Review: Training Neural Networks

Linear Regression

- Model's output is

$$g(x) = w^\top x + b$$

- (Unregularized) loss function is

$$\frac{1}{n}\sum_{i=1}^{n}(g(x^{(i)}) - y^{(i)})^2$$

Regression w/ Neural Networks

- Model's output is

$$g(x) = v^\top \sigma(Wx + b) + c$$

- **Use same loss function**, in terms of g!

$$\frac{1}{n}\sum_{i=1}^{n}(g(x^{(i)}) - y^{(i)})^2$$

Training objective for both types of models:

$$\frac{1}{n}\sum_{i=1}^{n}\ell\left(y^{(i)}, g(x^{(i)})\right), \text{ where } \ell(y,u) = (y-u)^2$$

Also applies for logistic regression, softmax regression, etc.

Review: Training Neural Networks

General loss function: $\frac{1}{n}\sum_{i=1}^{n}\ell\left(y^{(i)}, g(x^{(i)})\right)$

Model's output, depends on all model parameters θ (includes all layers)

- How to minimize? Gradient Descent!

$$\theta \leftarrow \theta - \eta \cdot \underbrace{\frac{1}{n}\sum_{i=1}^{n}\nabla_\theta \ell\left(y^{(i)}, g(x^{(i)})\right)}_{\text{Average of per-example gradients}}$$

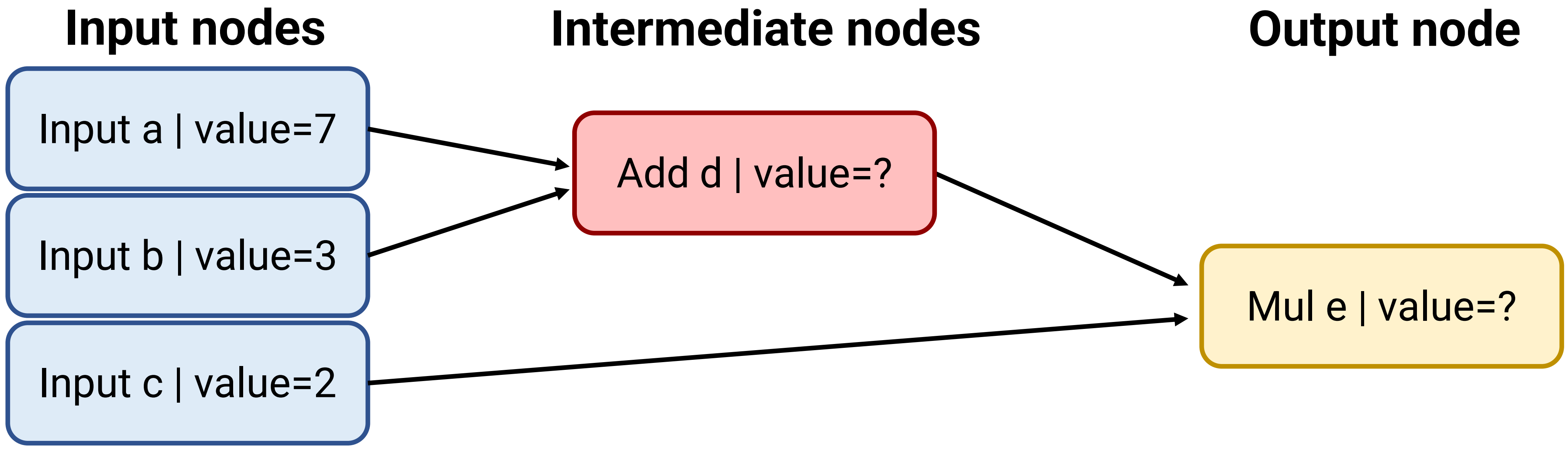
- **Today: How to compute gradient of loss w.r.t. parameters for any neural network**
  - So many different ways to assemble building blocks
  - Don't want to re-do gradient calculations by hand each time
  - **Can we write an algorithm to do it?**

Today's Plan

- The computation graph
- Backpropagation on trees
- Backpropagation on DAGs

Computation Graph

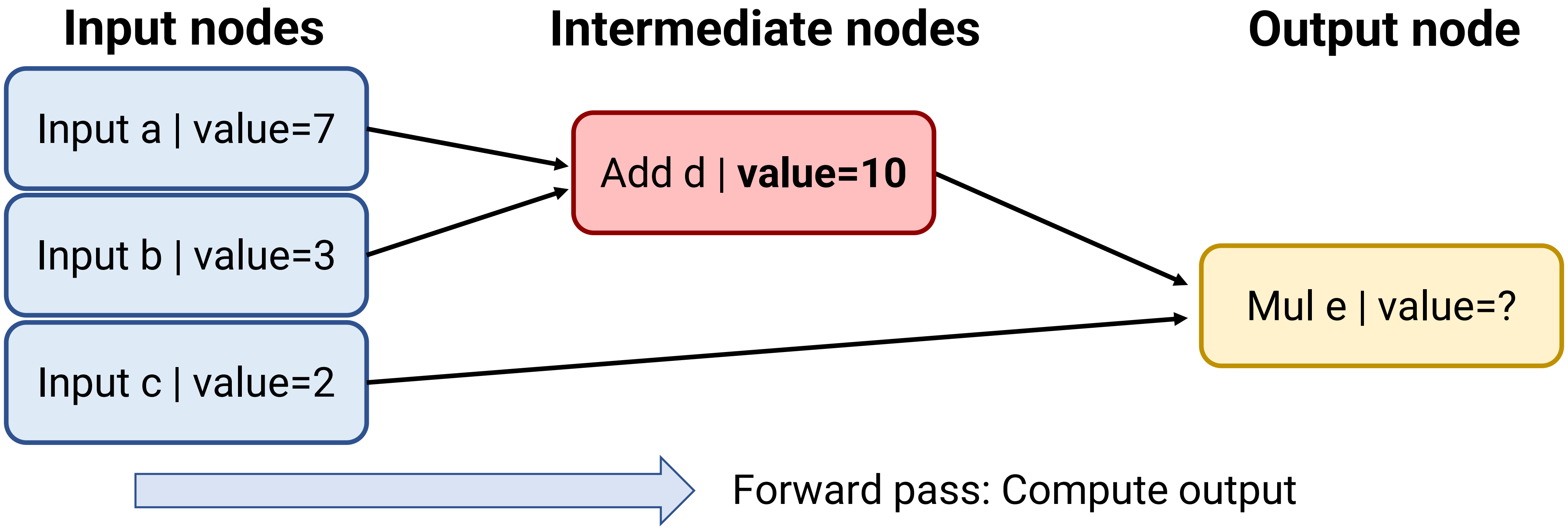
<u>Computation graph for ***(a + b) * c*** when *a=7, b=3, c=2*</u>



Different way of drawing the “building blocks” of neural networks

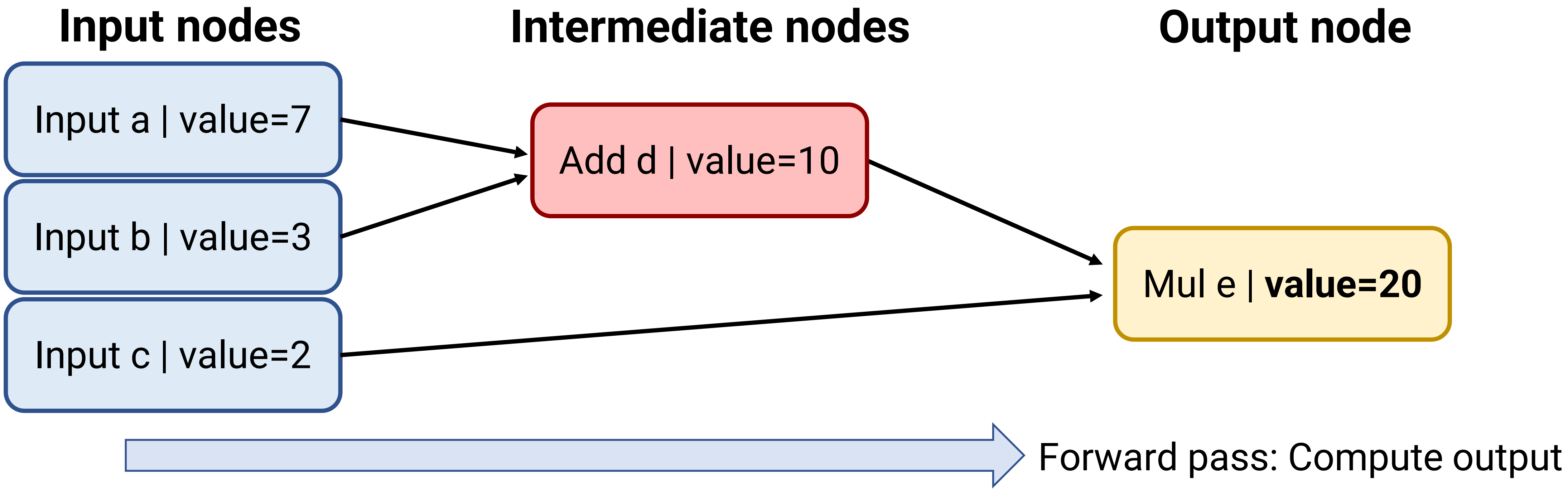
Computation Graph

Computation graph for ***(a + b) * c*** when *a=7, b=3, c=2*



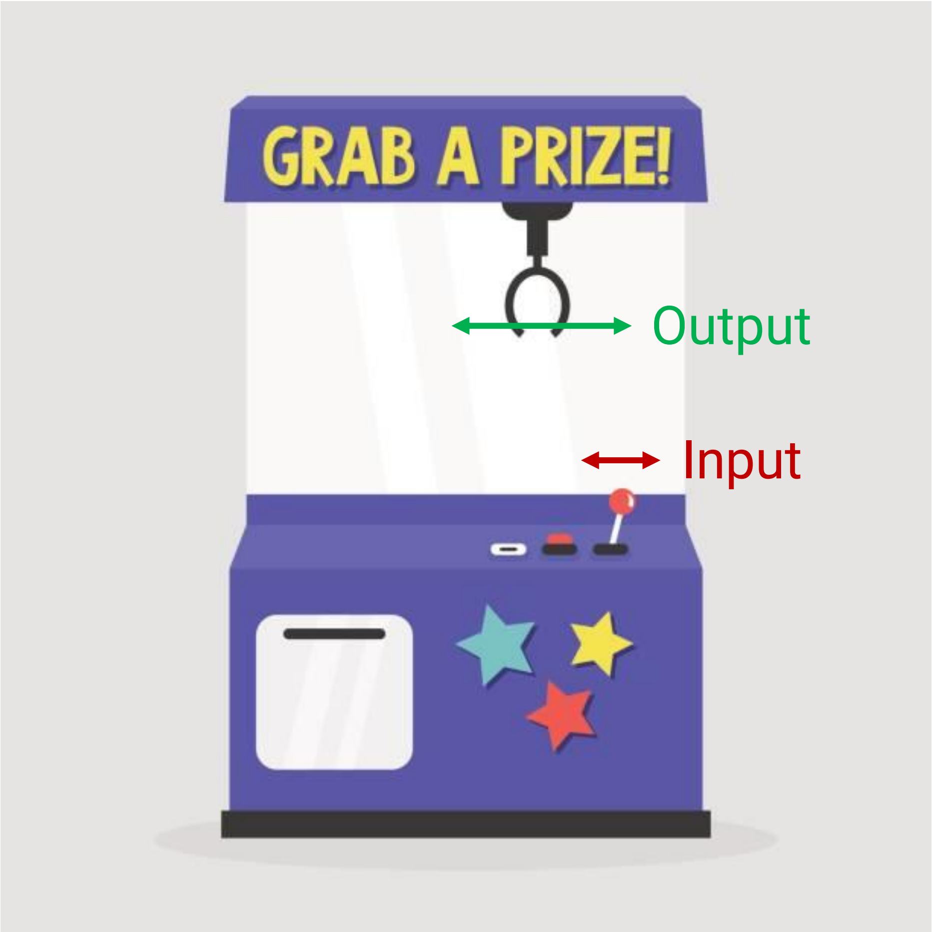
Computation Graph

<u>Computation graph for ***(a + b) * c*** when *a=7, b=3, c=2*</u>



Gradient checking

- **Numerical gradients**: A simpler but less efficient way to compute gradients
- What does $\partial y/\partial x$ mean?
  - If I change *x* by epsilon, by what proportion of epsilon does *y* change?
- We can just compute this for every input node!
- Pro: Easy to implement, useful to check correctness
- Con: Slow—requires O(#inputs) function evaluations



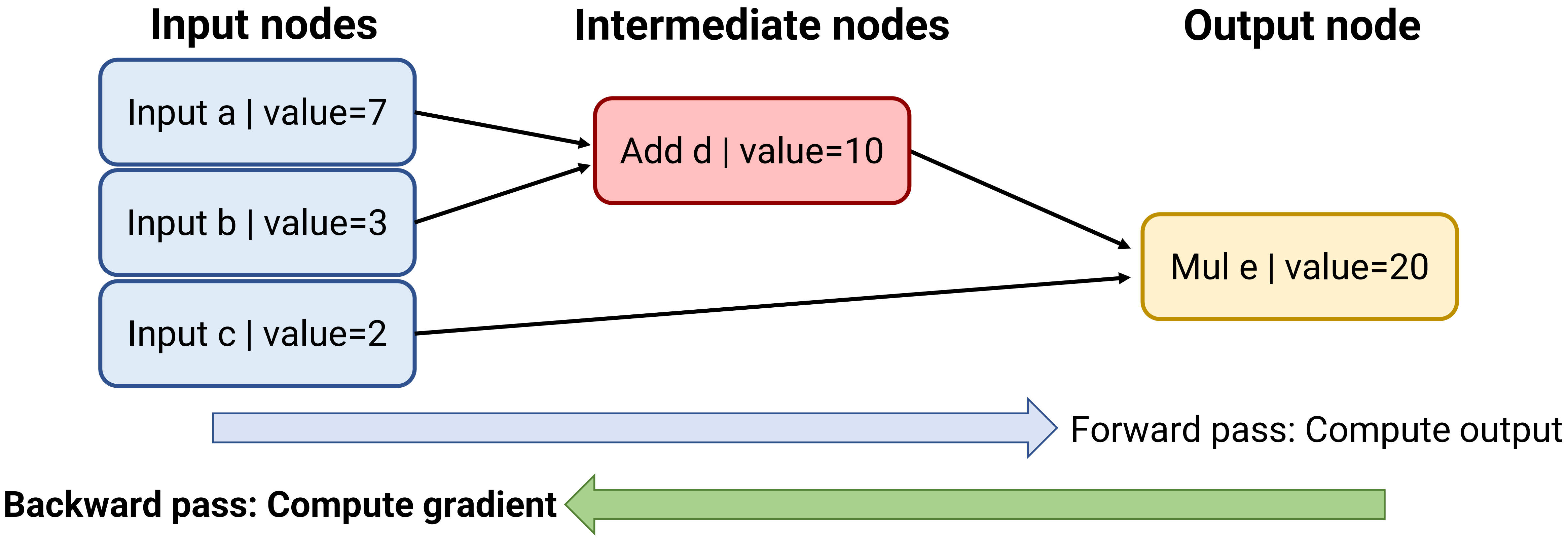
Let's implement!

Today’s Plan

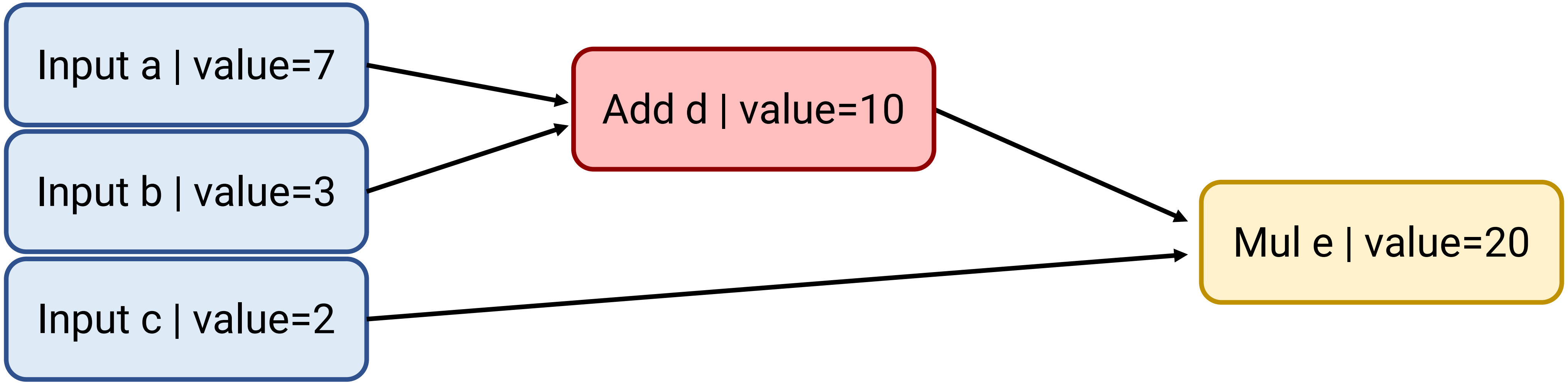
- The computation graph
- Backpropagation on trees
- Backpropagation on DAGs

Computation Graph

<u>Computation graph for ***(a + b) * c*** when *a=7, b=3, c=2*</u>

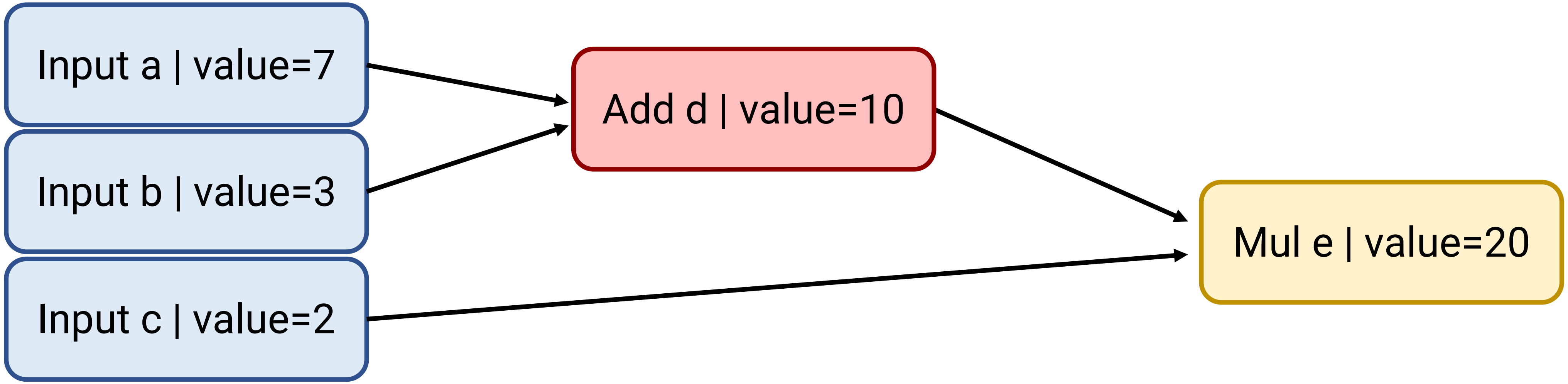


Backpropagation on trees



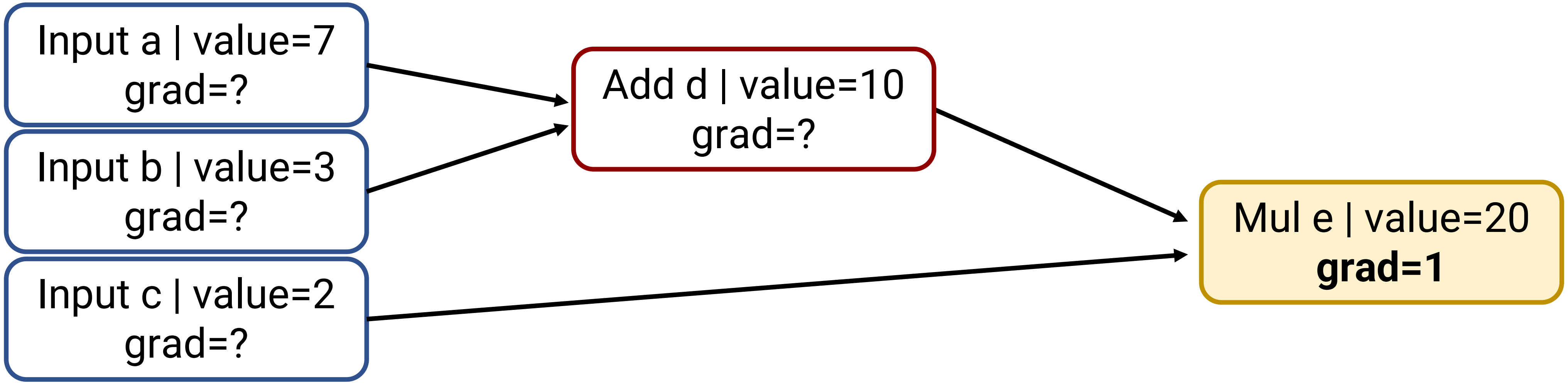
- For now: assume that the computation graph is a tree
  - Each node is only used in a single computation
  - Root of tree is output
  - Leaves of tree are inputs
- Idea: Recursively compute ***∂(output)/∂(node)*** **for each node**, starting at output

Backpropagation on trees



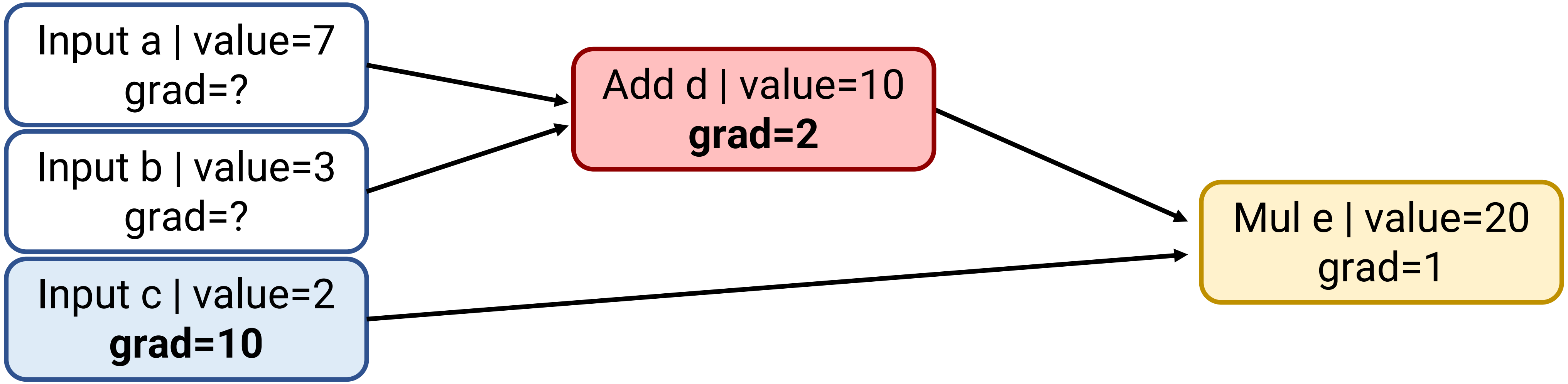
- Goal: Compute gradient *[∂e/∂a, ∂e/∂b, ∂e/∂c]*

Backpropagation on trees



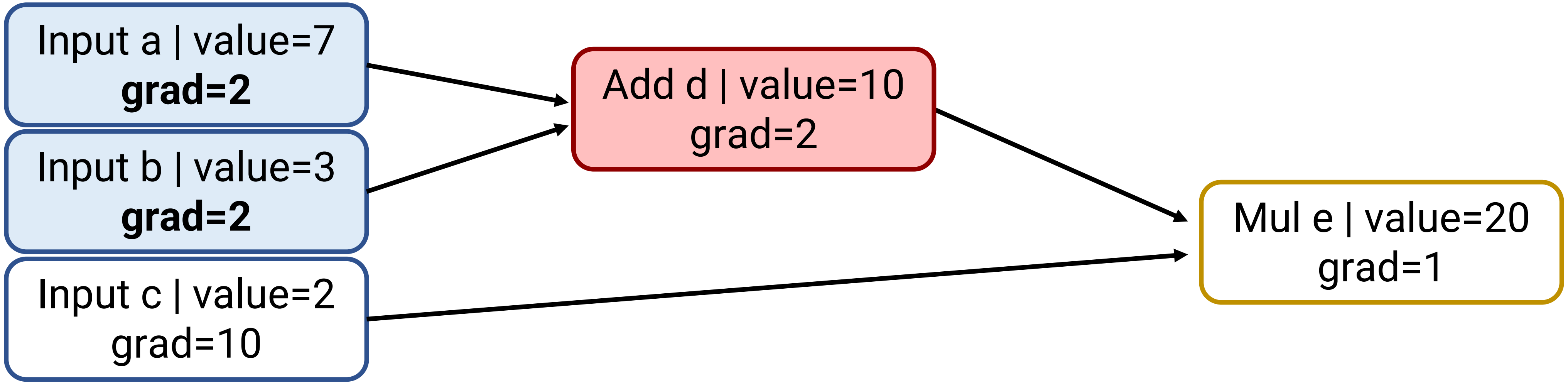
- Goal: Compute gradient *[∂e/∂a, ∂e/∂b, ∂e/∂c]*
- Step 1: Base case: $\partial e/\partial e = 1$

Backpropagation on trees



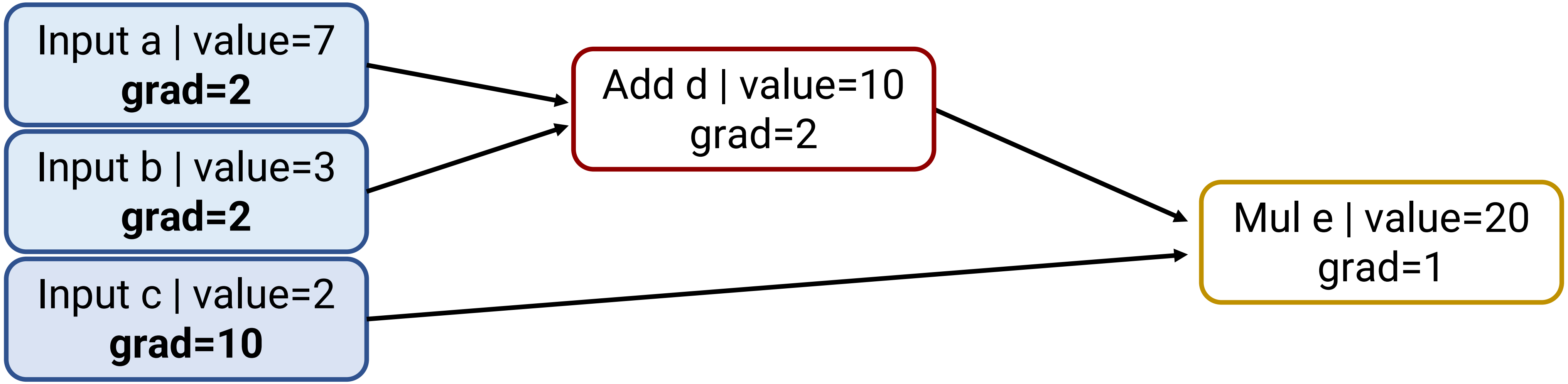
- Goal: Compute gradient *[∂e/∂a, ∂e/∂b, ∂e/∂c]*
- Step 2: How does **Mul** (node e) "distribute" gradient to its children?
  - *∂(x*y)/∂x = y*
  - Chain Rule: *∂(out)/∂x* = *∂(out)/ ∂(x*y)* * *∂(x*y)/∂x* = *∂(out)/ ∂(x*y)* * *y*
  - General rule: Child gets parent's gradient * value of other child

Backpropagation on trees



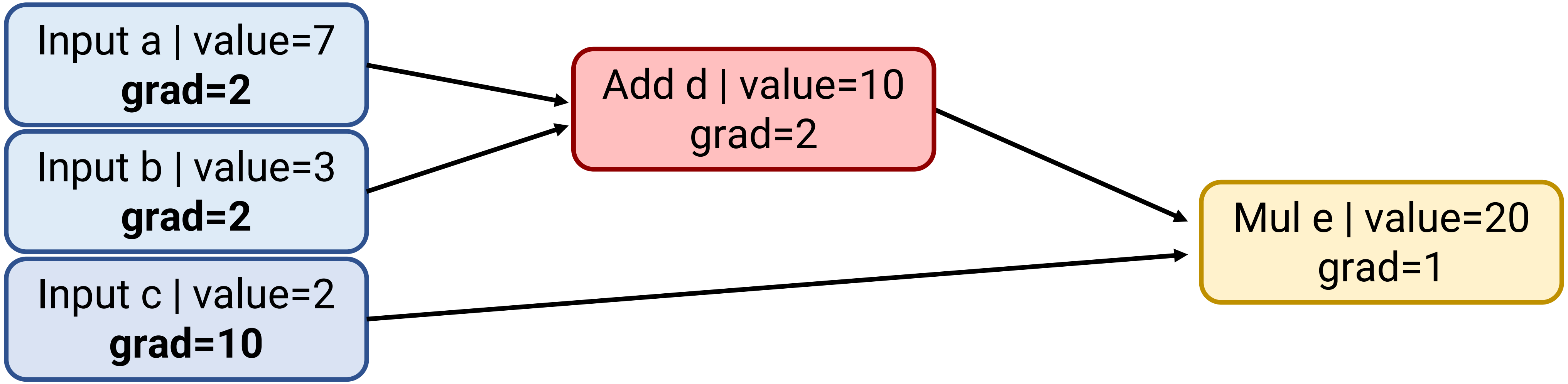
- Goal: Compute gradient *[∂e/∂a, ∂e/∂b, ∂e/∂c]*
- Step 3: How does **Add** (node d) "distribute" gradient to its children?
  - *∂(x+y)/∂x = 1*
  - Chain Rule: *∂(out)/∂x* = *∂(out)/ ∂(x+y)* * *∂(x+y)/∂x* = *∂(out)/ ∂(x+y)* * *1*
  - General rule: Child gets parent's gradient * 1

Backpropagation on trees



- Goal: Compute gradient *[∂e/∂a, ∂e/∂b, ∂e/∂c]*
- Step 4: Leaf nodes
  - Don’t need to do anything

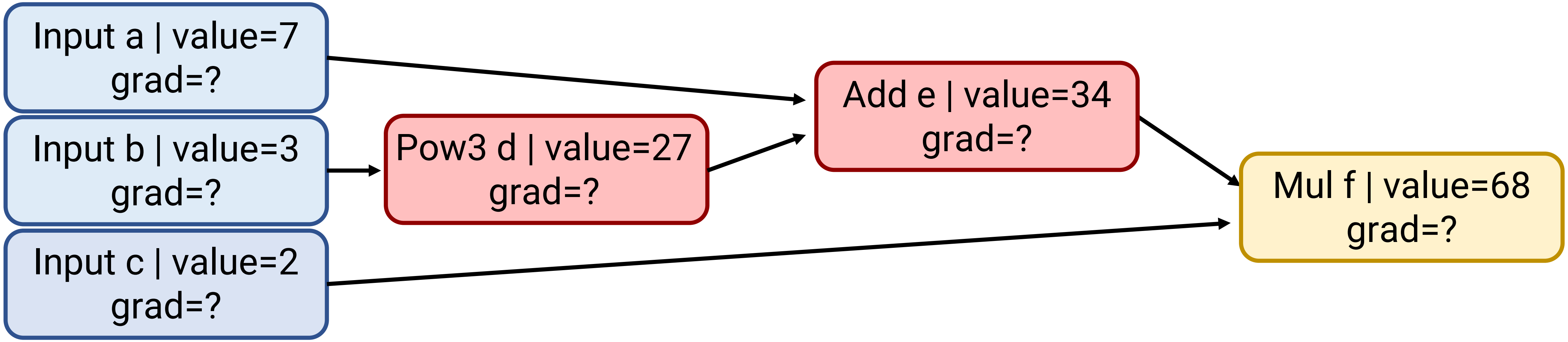
Backpropagation on trees



- Goal: Compute gradient *[∂e/∂a, ∂e/∂b, ∂e/∂c]*
- Overall Recipe
  - Do forward pass
  - Start at root and recurse over children
  - Each node knows how to take gradient of itself with respect to each child
  - By Chain Rule, child.grad = parent.grad * *∂(parent)/∂(child)*

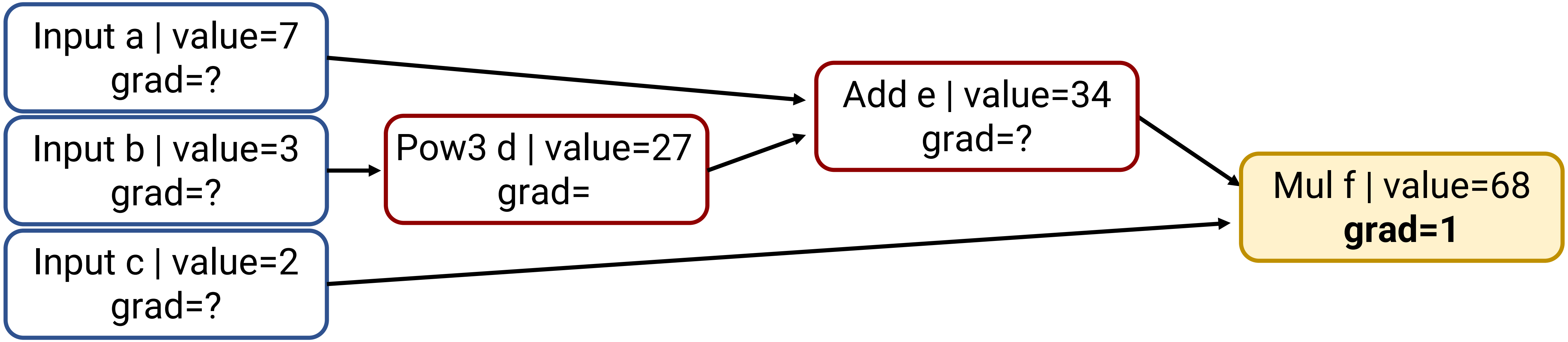
Let’s implement!

PowerNode



New function: $(a + b^3) * c$ where $a=7, b=3, c=2$

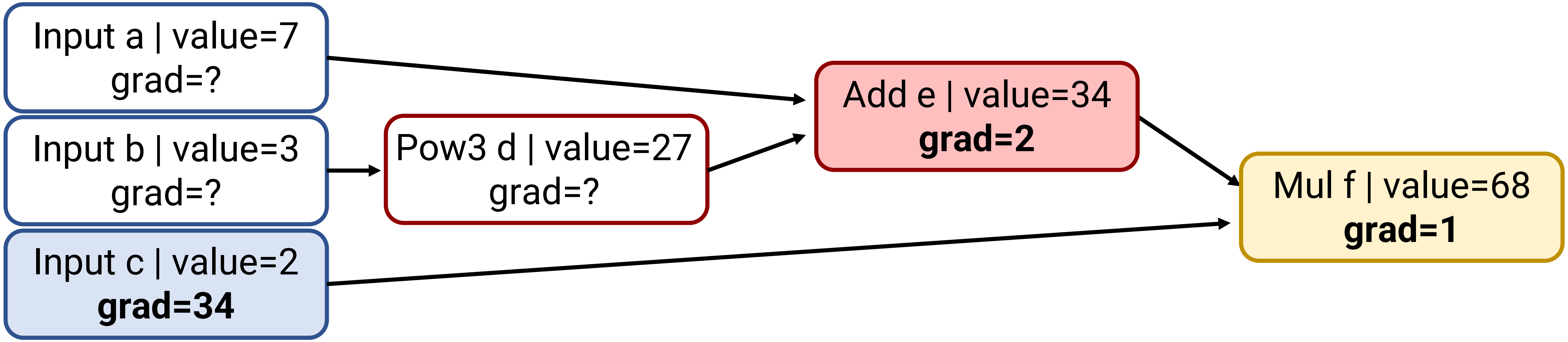
PowerNode



<u>New function: $(a + b^3) * c$ where $a=7, b=3, c=2$</u>

- Goal: Compute gradient *[∂f/∂a, ∂f/∂b, ∂f/∂c]*
- Step 1: Base case: $\partial f/\partial f = 1$

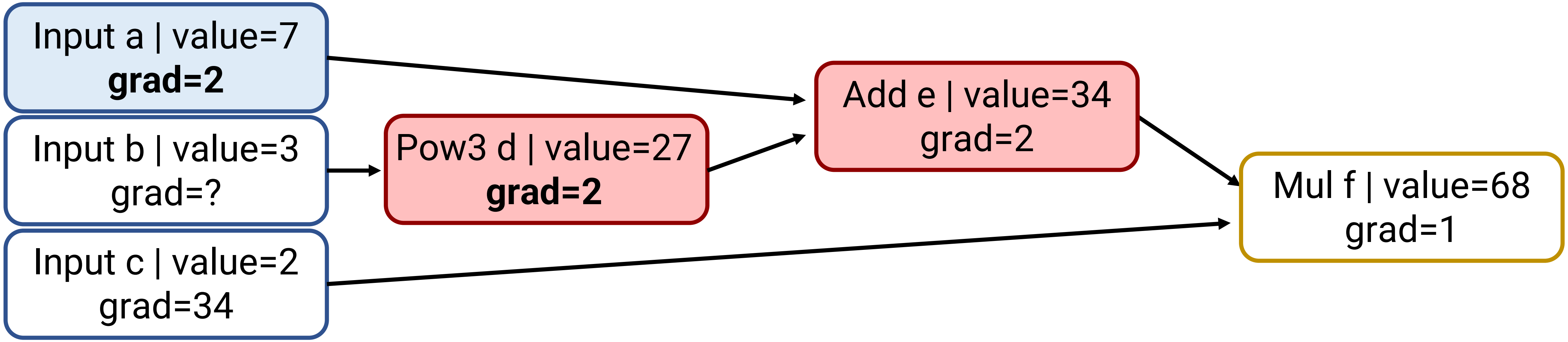
PowerNode



New function: *(a + b^3) * c* where *a=7, b=3, c=2*

- Goal: Compute gradient *[∂f/∂a, ∂f/∂b, ∂f/∂c]*
- Step 2: Distribute **Mul** (node f) gradient to children

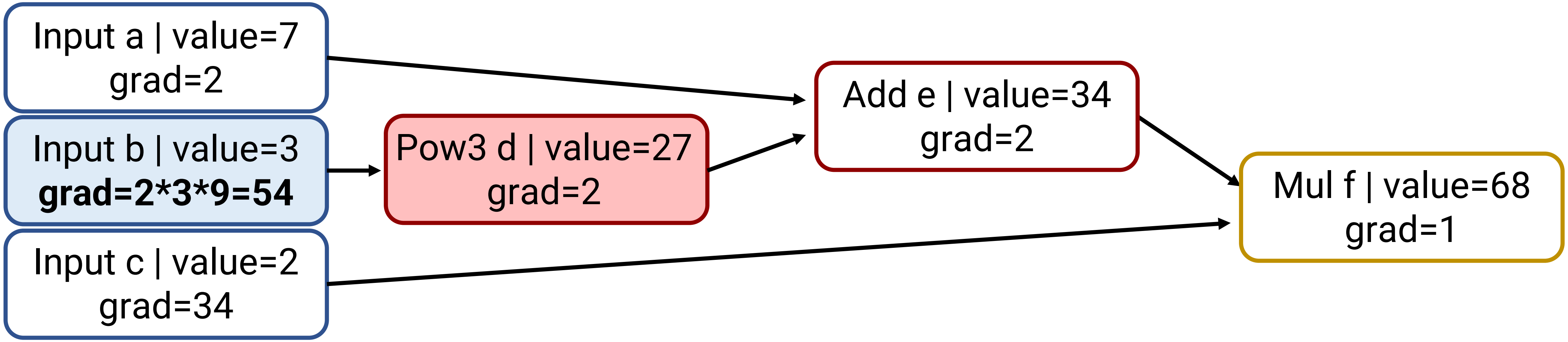
PowerNode



New function: *(a + b*^{3}*) * c* where *a=7, b=3, c=2*

- Goal: Compute gradient *[∂f/∂a, ∂f/∂b, ∂f/∂c]*
- Step 3: Distribute **Add** (node e) gradient to children

PowerNode

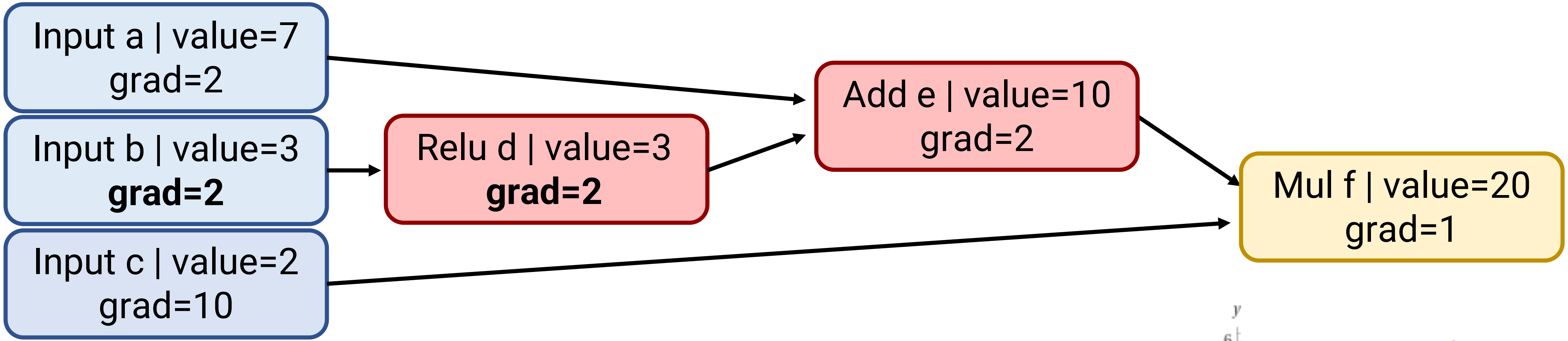


New function: $(a + b^3) * c$ where $a=7, b=3, c=2$

- Goal: Compute gradient $[\partial f/\partial a, \partial f/\partial b, \partial f/\partial c]$
- Step 4: Distribute **Pow3** (node d) gradient to children
  - $\partial(x^p)/\partial x = p * x^{p-1}$
  - By Chain Rule: Child gets parent's gradient * $p * child^{p-1}$

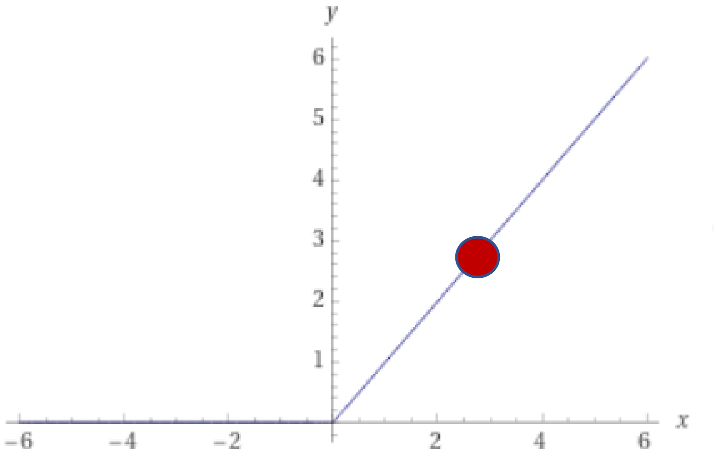
Let’s implement!

ReluNode



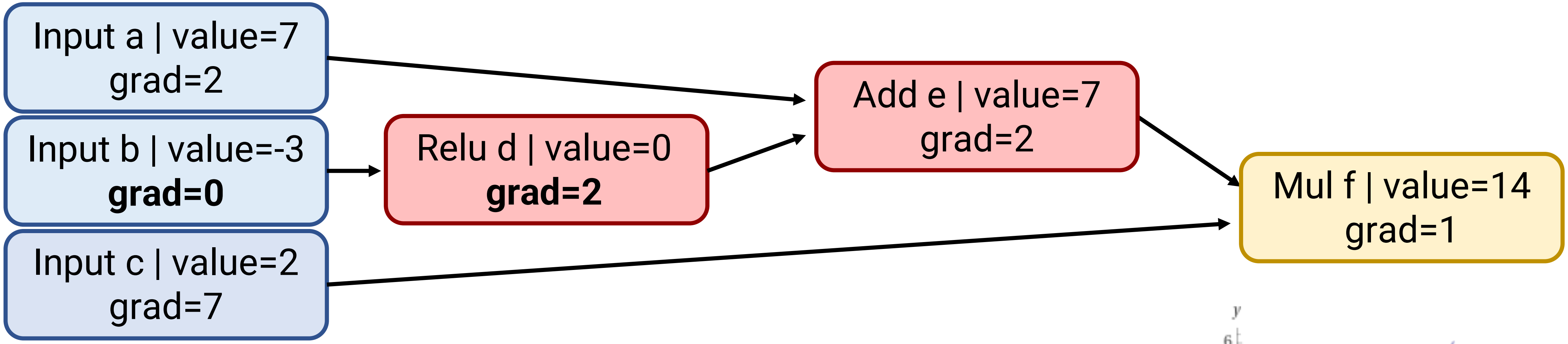
<u>New function: *(a + Relu(b)) * c* where *a=7, b=3, c=2*</u>

- Steps 1-3 are the same
- Step 4: Relu
  - *∂(Relu(x))/∂x = 1 if x > 0, 0 if x ≤ 0*
  - **If child > 0, child.grad = parent.grad * 1**
  - If child ≤ 0, child.grad = 0



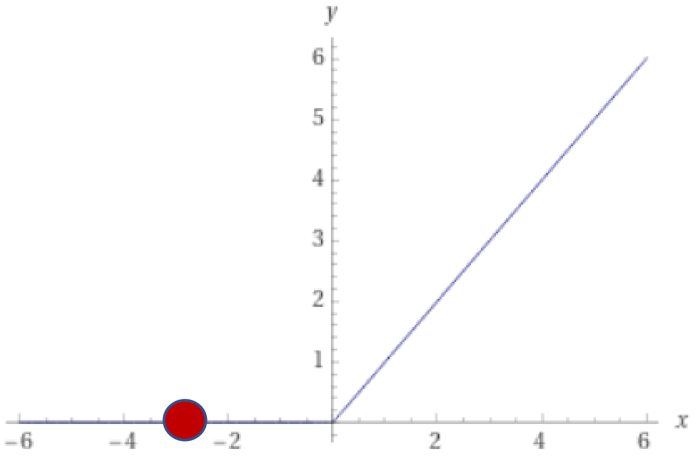
$$\mathrm{ReLU}(z) = \max(z, 0)$$

ReluNode



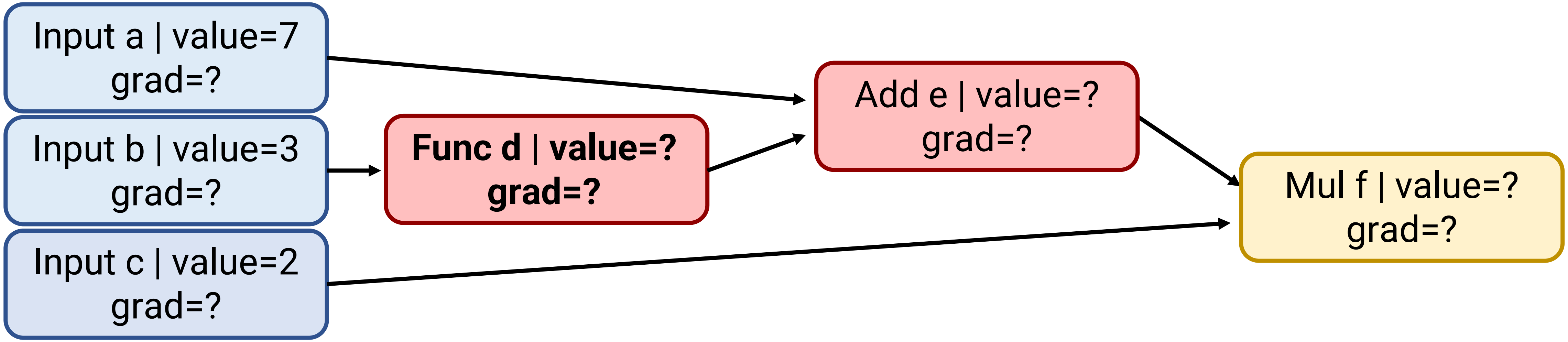
<u>New function: *(a + Relu(b)) * c* where *a=7*, ***b=-3***, *c=2*</u>

- Steps 1-3 are the same
- Step 4: Relu
  - *∂(Relu(x))/∂x = 1 if x > 0, 0 if x ≤ 0*
  - If child > 0, child.grad = parent.grad * 1
  - **If child ≤ 0, child.grad = 0**



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

Generic Unary Function



<u>New function: *(a + Func(b)) * c* where *a=7, b=3, c=2*</u>

- Steps 1-3 are the same
- Step 4: Func (generic function)
  - child.grad = parent.grad * *∂(Func(child))/∂child*

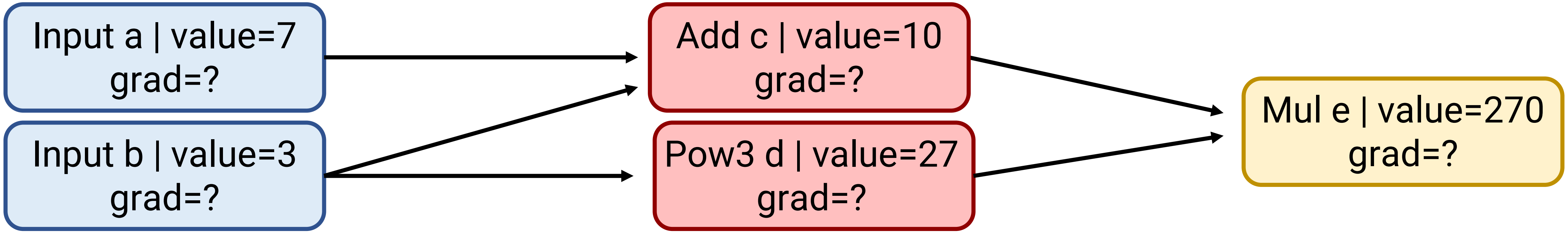
Announcements

- Project proposals due today @ 11:59pm
  - Submit as a group on Gradescope, list all teammates
  - One submission per group
- HW2 released, due Thursday, February 29
- Midterm exam Tuesday, March 7
  - In-class, 80 minutes in SLH 100
  - Allowed one double-sided 8.5x11 sheet of notes
  - I highly recommend writing this yourself (good for memory)
- Section Friday: Pytorch (library that does backpropagation)

Today's Plan

- The computation graph
- Backpropagation on trees
- Backpropagation on DAGs

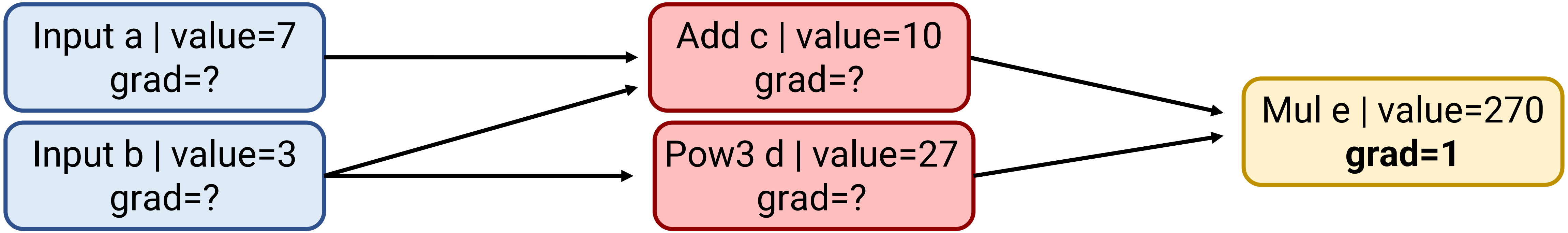
DAG Computation Graphs



<u>New function: *(a +* ***b****)* * ***b***^{3} where *a=7, b=3*</u>

- This is no longer a tree!
- Still a directed acyclic graph
- Let’s see why our previous algorithm fails

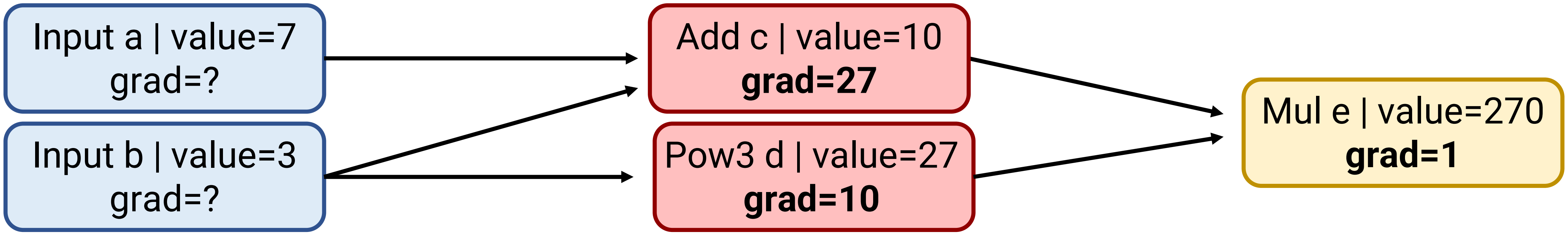
DAG Computation Graphs



<u>New function: *(a +* ***b****)* * $\boldsymbol{b}^3$ where *a=7, b=3*</u>

- Goal: Compute gradient *[∂e/∂a, ∂e/∂b]*
- Step 1: Base case: *∂e/∂e = 1*

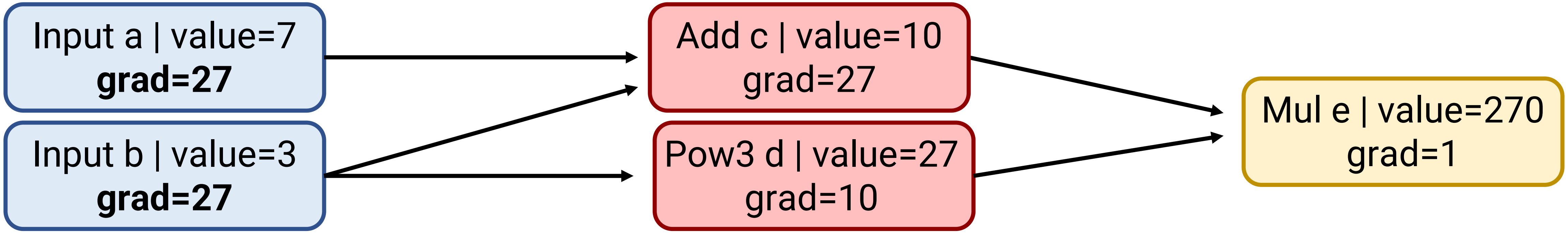
DAG Computation Graphs



New function: $(a + \mathbf{b}) * \mathbf{b}^3$ where $a=7, b=3$

- Goal: Compute gradient *[∂f/∂a, ∂f/∂b]*
- Step 2: Distribute **Mul** (node e) gradient to children

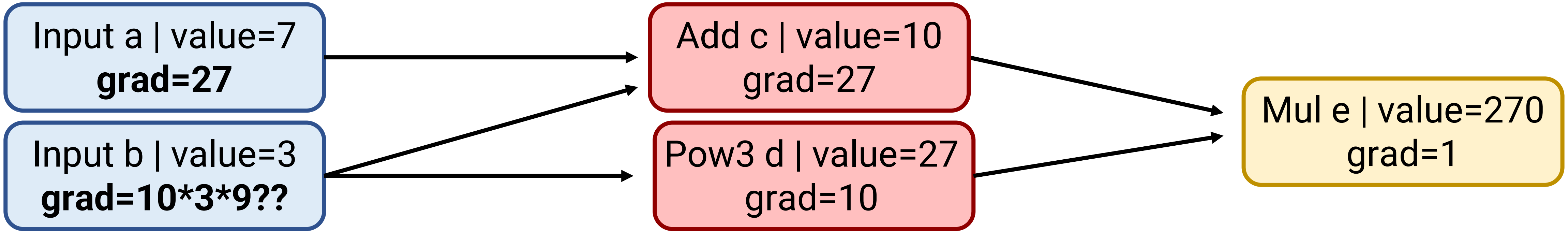
DAG Computation Graphs



<u>New function: *(a + **b**) * **b**³* where *a=7, b=3*</u>

- Goal: Compute gradient *[∂e/∂a, ∂e/∂b]*
- Step 3: Distribute **Add** (node c) gradient to children

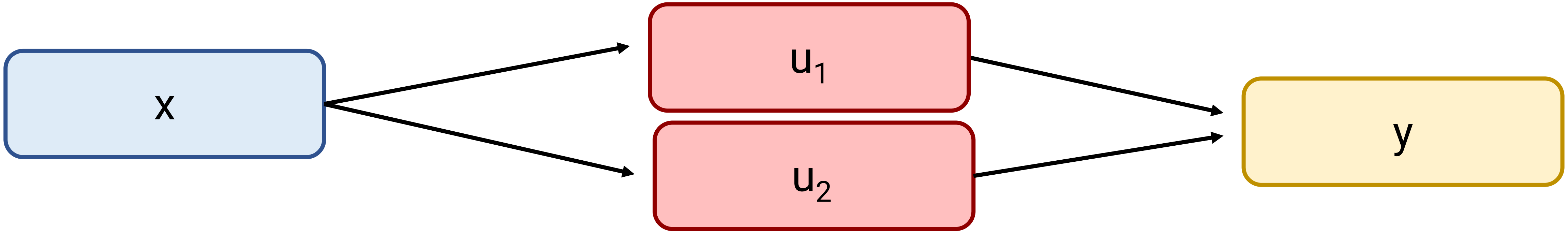
DAG Computation Graphs



New function: $(a + \mathbf{b}) * \mathbf{b}^3$ where $a=7, b=3$

- Goal: Compute gradient $[\partial e/\partial a, \partial e/\partial b]$
- Step 4: Distribute **Pow3** (node d) gradient to child
  - By Chain Rule: Child gets parent's gradient * $p * child^{p-1}$
- Problem: We have overwritten the gradient from b to Add (node c)!

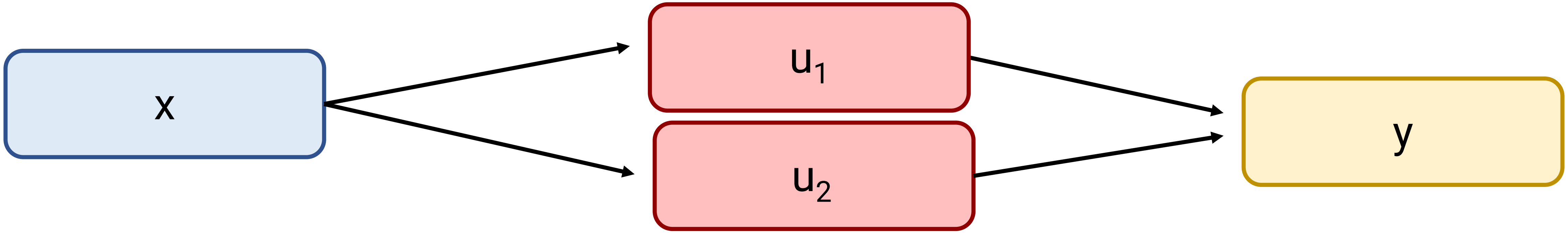
Multivariate chain rule



- Minimal example
  - u_1 and u_2 depend on variable x (i.e., x has two parents)
  - y depends on both u_1 and u_2
- By Multivariate Chain Rule: $\partial y/\partial x = \boxed{\partial y/\partial u_1 * \partial u_1/\partial x + \partial y/\partial u_2 * \partial u_2/\partial x}$
  - Changing x by epsilon changes each parent a bit; Effects add for small epsilon
  - Generalization of multiplying derivatives is matrix multiplication of Jacobians

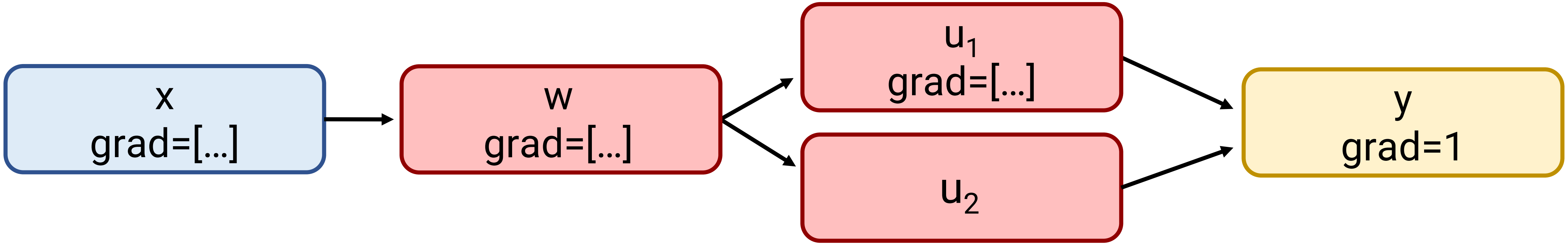
Dot product of
$[\partial y/\partial u_1, \partial y/\partial u_2]$ &
$[\partial u_1/\partial x, \partial u_2/\partial x]$

Multivariate chain rule



- Minimal example
  - u_1 and u_2 depend on variable x (i.e., x has two parents)
  - y depends on both u_1 and u_2
- By Multivariate Chain Rule: $\partial y/\partial x = \partial y/\partial u_1 * \partial u_1/\partial x + \partial y/\partial u_2 * \partial u_2/\partial x$
- node.grad = **sum over parents** of parent.grad * *∂(parent)/∂(child)*
- At each parent node, run child.grad **+=** parent.grad * *∂(parent)/∂(child)*

What order of traversal?

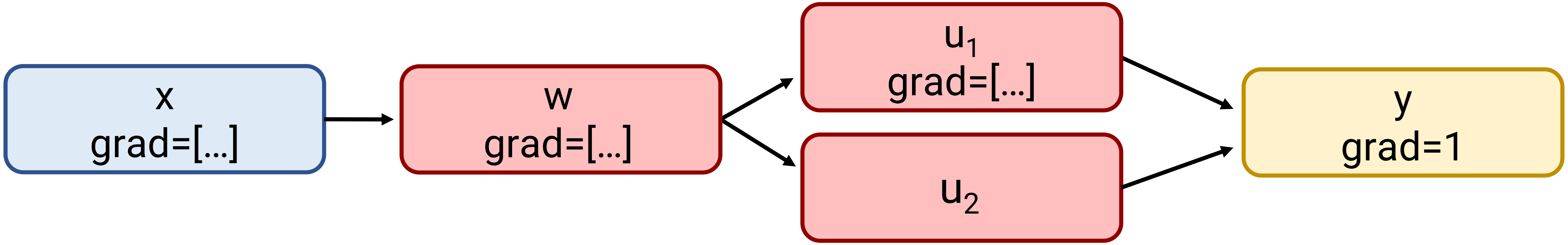


Current code:

- y.backward()
    - u1.backward()
        - **w.backward()**
            - **x.backward()**
    - u2.backward()
        - **w.backward()**
            - **x.backward()**

- Going recursively double-counts
    - First call to w.backward() makes final x.grad too large
- Solution: **Topological sort the nodes**
    - Iterate in reverse order, starting from output
    - Ensures that we process each node after all of its parents

What order of traversal?

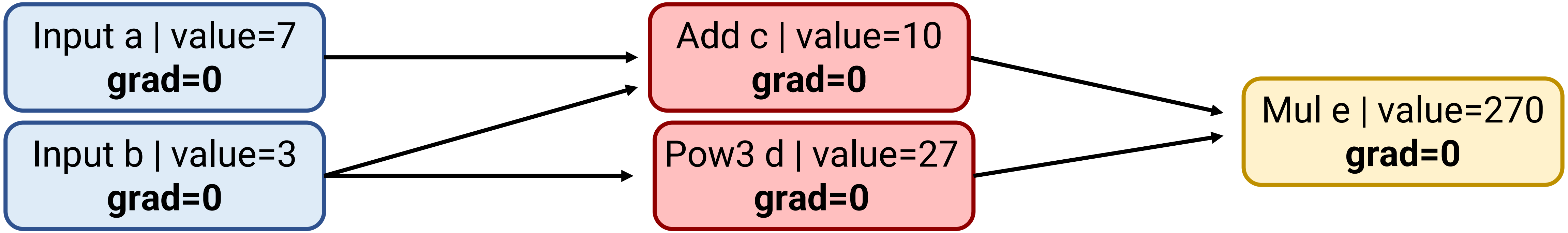


Better code:

- topo_order = [x, w, u_1, u_2, y]
- Iterate in reverse order:
  - y.backward()
  - u2.backward()
  - u1.backward()
  - w.backward()
  - x.backward()

- Going recursively double-counts
  - First call to w.backward() makes final x.grad too large
- Solution: **Topological sort the nodes**
  - Iterate in reverse order, starting from output
  - Ensures that we process each node after all of its parents

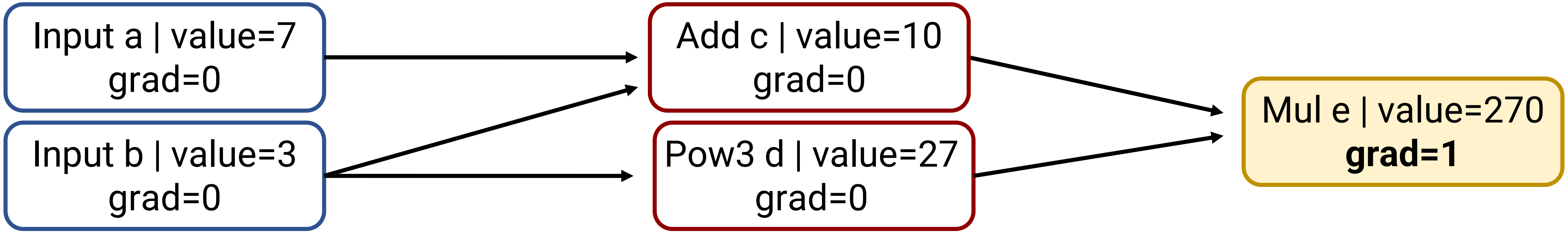
Backpropagation on DAGs



New function: $(a + \mathbf{b}) * \mathbf{b}^3$ where $a=7, b=3$

- Goal: Compute gradient $[\partial e/\partial a, \partial e/\partial b]$
- Topological sort: [a, b, c, d, e]
- Step 0: Initialize all gradients to 0

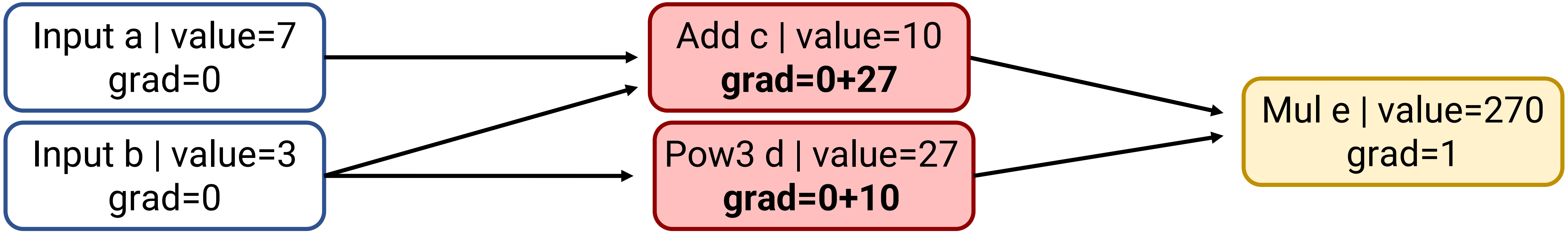
Backpropagation on DAGs



New function: $(a + \mathbf{b}) * \mathbf{b}^3$ where $a=7, b=3$

- Goal: Compute gradient $[\partial e/\partial a, \partial e/\partial b]$
- Topological sort: [a, b, c, d, e]
- Step 1: Base case: $\partial e/\partial e = 1$

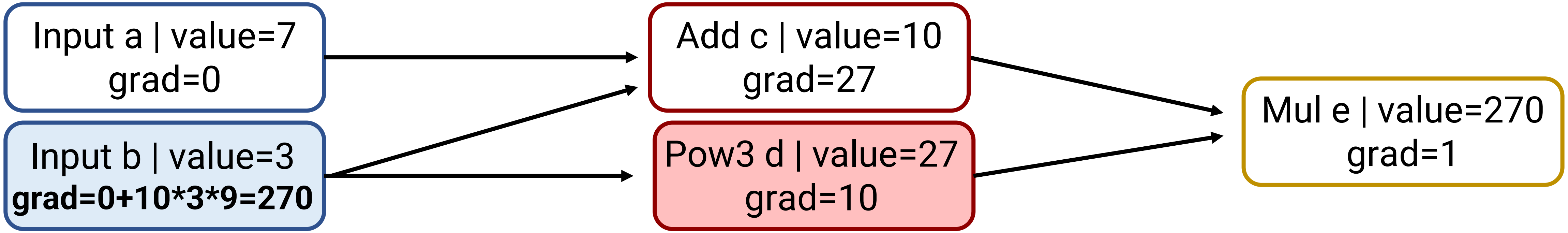
Backpropagation on DAGs



<u>New function: *(a + **b**) * **b**³* where *a=7, b=3*</u>

- Goal: Compute gradient *[∂e/∂a, ∂e/∂b]*
- Topological sort, reversed: [e, d, c, b, a]
- Step 2: Propagate **Mul** node e to children

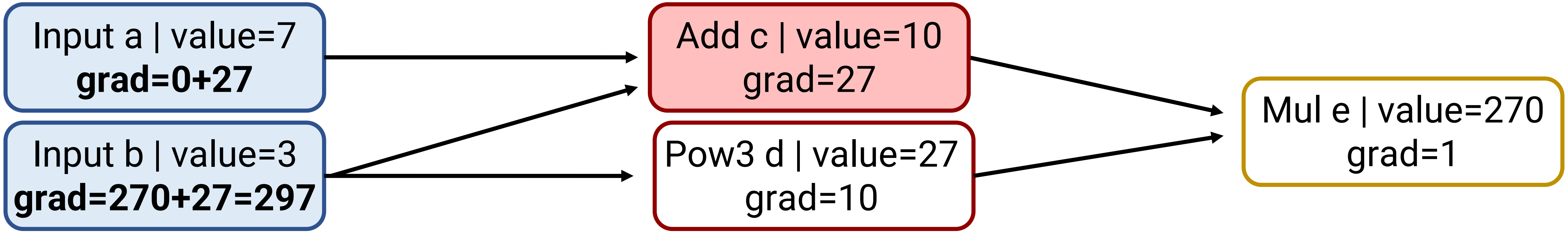
Backpropagation on DAGs



New function: *(a +* ***b****)* *** b*** ^{3} where *a=7, b=3*

- Goal: Compute gradient *[∂e/∂a, ∂e/∂b]*
- Topological sort, reversed: [e, d, c, b, a]
- Step 3: Propagate **Pow3** node d to child

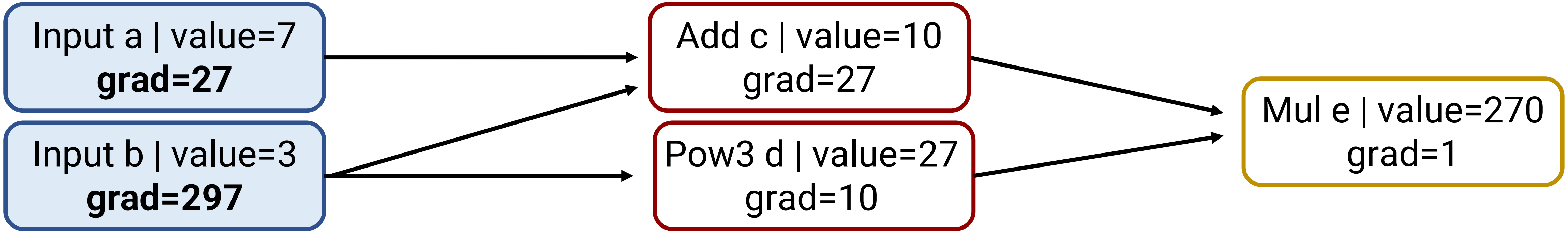
Backpropagation on DAGs



<u>New function: *(a + **b**) * **b**^{3}* where *a=7, b=3*</u>

- Goal: Compute gradient *[∂e/∂a, ∂e/∂b]*
- Topological sort, reversed: [e, d, c, b, a]
- Step 4: Propagate **Add** node c to children

Backpropagation on DAGs

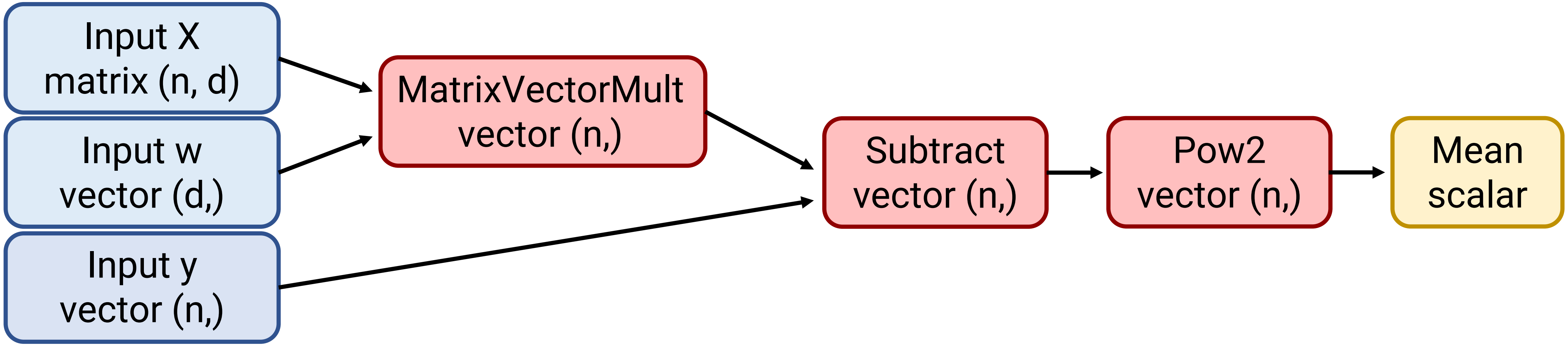


New function: $(a + \boldsymbol{b}) * \boldsymbol{b}^3$ where $a=7, b=3$

- Goal: Compute gradient $[\partial e/\partial a, \partial e/\partial b]$
- Topological sort, reversed: [e, d, c, b, a]
- Step 5, 6: a.backward(), b.backward() do nothing

Let’s implement!

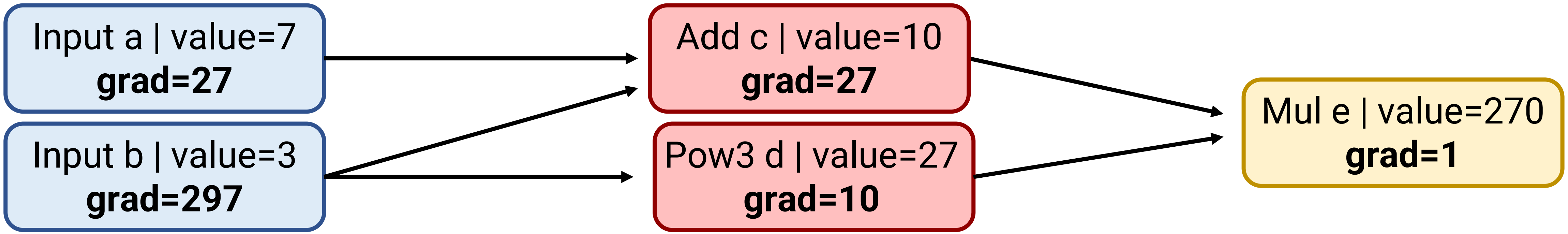
Backpropagation for vectors and matrices



<u>Computation graph for mean((Xw – y)²), i.e. Linear Regression</u>

- Basically the same, but each node can be a vector or matrix!
  - Each node.grad stores ∇_{node}output
  - Parents know how to update ∇_{child}output based on ∇_{parent}output

Conclusion



- Backpropagation computes gradient of output with respect to all nodes in computation graph
  - Forward pass: Compute values of all nodes
  - Backward pass: Iterate through nodes in reverse order,
    At each parent node, run child.grad **+=** parent.grad * *∂(parent)/∂(child)*
- Big picture: Makes it easy to run gradient descent on arbitrary computation graphs
  - Easy to try new architectures for neural networks