Module 1.3 - Backprop

Functions

- Function $f(x) = x \times 5$

```
class TimesFive(ScalarFunction):
    @staticmethod
    def forward(ctx, x: float) -> float:
        return x * 5
```

```
[[''], ['']] 0 0
```

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Multi-arg Functions

- Function $f(x, y) = x \times y$

```python
class Mul(ScalarFunction):
    @staticmethod
    def forward(ctx, x: float, y: float) -> float:
        return x * y
```

```
[['', ''], ['']] 0 0
[['', ''], ['']] 0 1
```

Context

$$f(x) = x \times x$$

$$f'(x) = 2 \times x$$

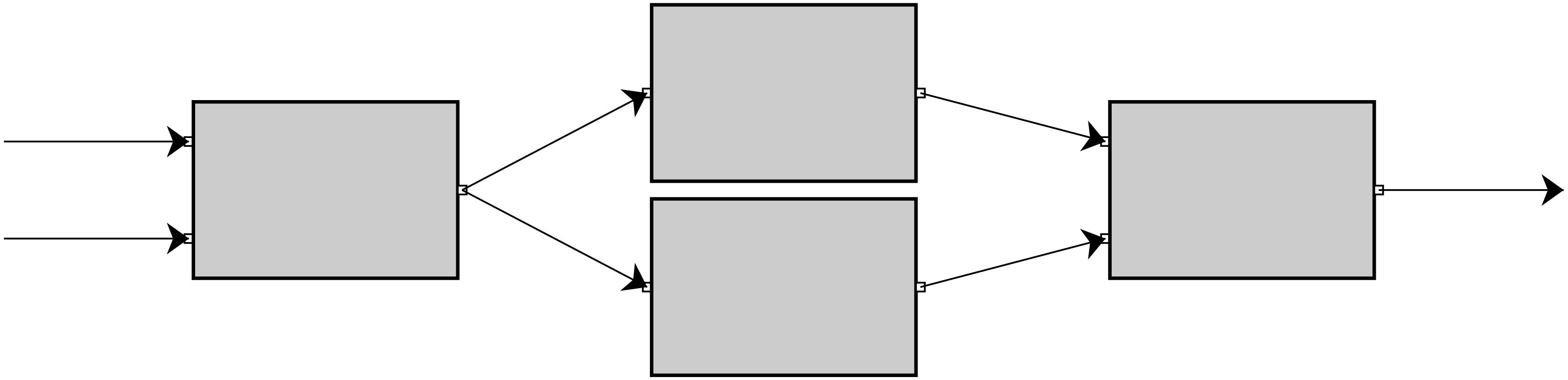
```
class Square(ScalarFunction):
    @staticmethod
    def forward(ctx: Context, x: float) -> float:
        ctx.save_for_backward(x)
        return x * x

    @staticmethod
    def backward(ctx: Context, d: float) -> Tuple[float, float]:
        (x,) = ctx.saved_values
        f_prime = 2 * x
        return f_prime * d
```

[[''], ['']] 0 0

Computational Graph

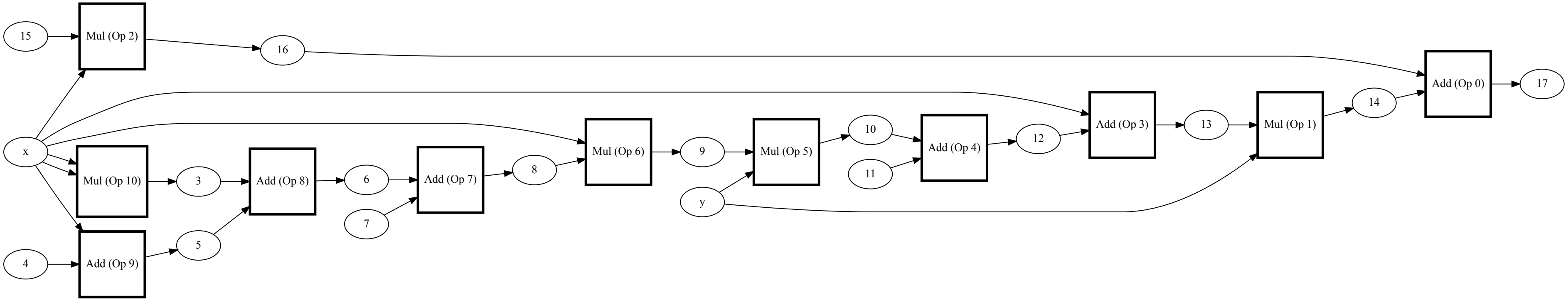
```
[['', ''], [''], ['', ''], ['']] 0 0
[['', ''], [''], ['', ''], ['']] 0 1
[['', ''], [''], ['', ''], ['']] 1 0
[['', ''], [''], ['', ''], ['']] 1 0
[['', ''], [''], ['', ''], ['']] 2 0
[['', ''], [''], ['', ''], ['']] 2 1
```



Forward Graph

```
def expression():
    x = Scalar(1.0, name="x")
    y = Scalar(1.0, name="y")
    if True:
        z = (sum([1, x, x * x, 65]) * x * y + 6 + x) * y + 10.0 * x

    return z
```



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Lecture Quiz

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Outline

- Chain Rule
- Backpropagation

Chain Rule

Graph Structure

```python
x = Scalar(2.0)
x_2 = Square.apply(x)
print(x_2.history)
print(x_2.history.inputs[0].history)
```

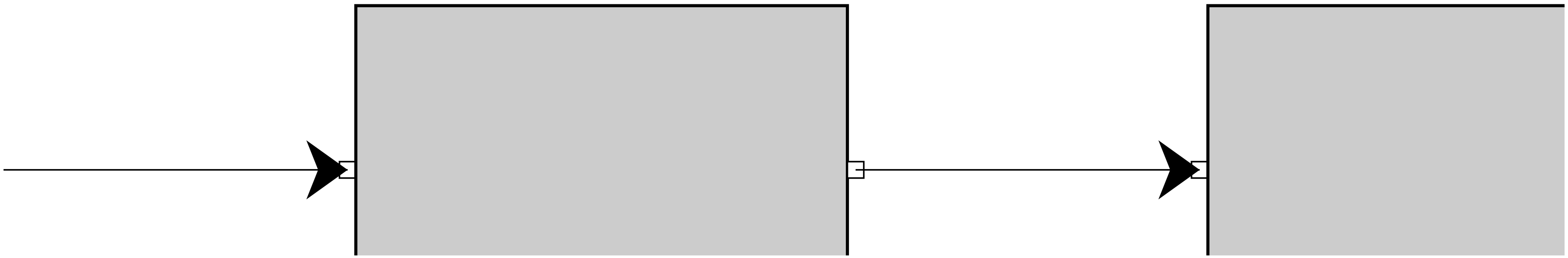
```
ScalarHistory(last_fn=<class '__main__.Square'>, ctx=Context(no_grad=Fals
e, saved_values=(2.0,)), inputs=[Scalar(2.000000)])
ScalarHistory(last_fn=None, ctx=None, inputs=())
```

Derivative

```
x = Scalar(2.0)
x_2 = Square.apply(x)
x_3 = Square.apply(x_2)
x_3.backward()
print(x.derivative)
```

```
32.0
```

```
[[''], [''], ['']] 0 0
[[''], [''], ['']] 1 0
```



Chain Rule

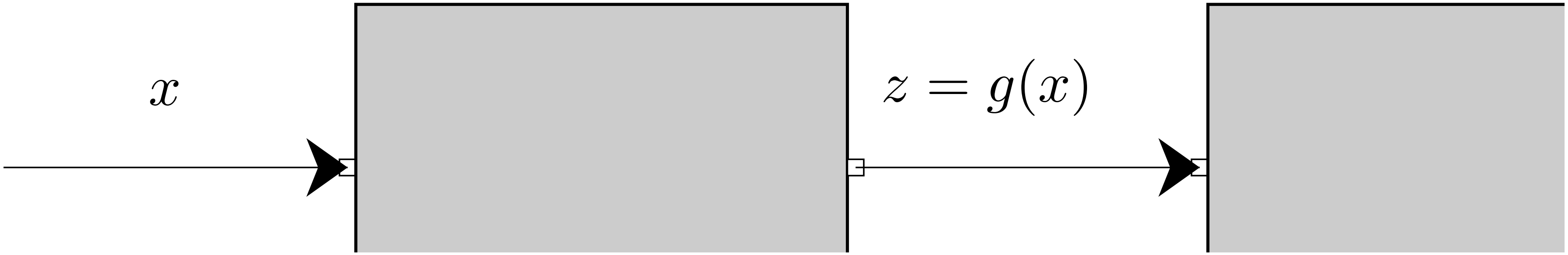
Compute derivative from chain

$$f'_x(g(x)) = g'(x) \times f'_{g(x)}(g(x))$$

Chain Rule

$$z = g(x)$$
$$d = f'(z)$$
$$f'_x(g(x)) = g'(x) \times d$$

```
[['$x$'], ['$z = g(x)$'], ['$f(g(x))$']] 0 0
[['$x$'], ['$z = g(x)$'], ['$f(g(x))$']] 1 0
```




```
[["$d\\cdot g'(x)$"], ["$f'(z)$"], ['$1$']] 0 0
[["$d\\cdot g'(x)$"], ["$f'(z)$"], ['$1$']] 1 0
```

Example: Chain Rule

$$log(x)^2$$

$$\begin{aligned} f(z) &= z^2 \\ g(x) &= \log(x) \end{aligned}$$

Example: Chain Rule

$$
\begin{aligned}
f'(z) &= 2z \times 1 \\
g'(x) \quad &= 1/x
\end{aligned}
$$

What is the combination?

$$f'_x(g(x))$$

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Example: Chain Rule

$$((x)^2)^2$$

$$\begin{aligned} f(z) &= z^2 \\ g(x) &= x^2 \end{aligned}$$

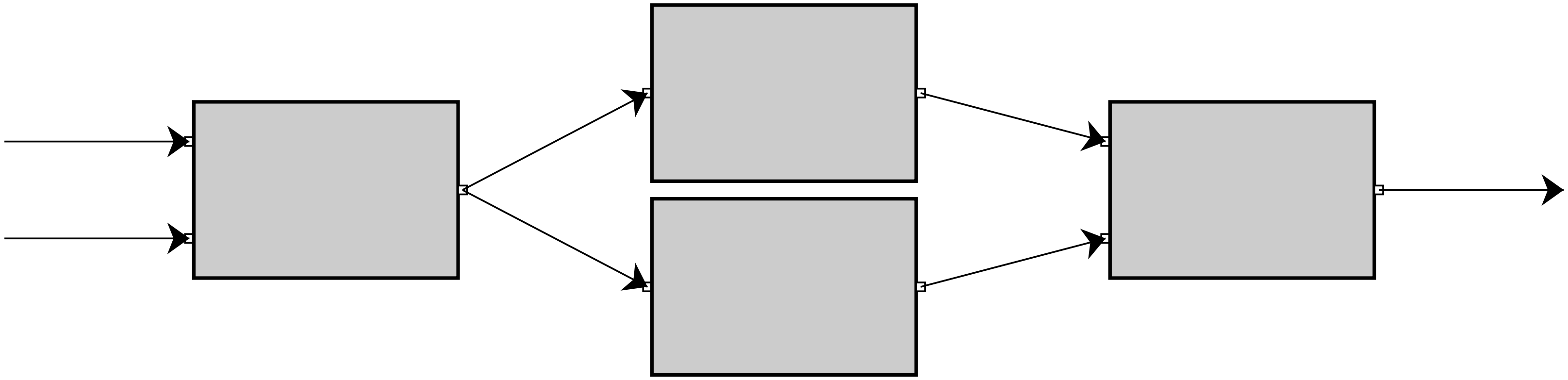
$$\begin{aligned} f'(z) &= \mathbf{2} \times z \\ g'(x) &= \mathbf{2} \times x \end{aligned}$$

$$f'_x(g(x)) = \mathbf{2} \times x \times \mathbf{2} \times x^2 = 4x^3$$

Two Arguments: Chain

$$f(g(x,y))$$

```
[['', ''], [''], ['', ''], ['']] 0 0
[['', ''], [''], ['', ''], ['']] 0 1
[['', ''], [''], ['', ''], ['']] 1 0
[['', ''], [''], ['', ''], ['']] 1 0
[['', ''], [''], ['', ''], ['']] 2 0
[['', ''], [''], ['', ''], ['']] 2 1
```



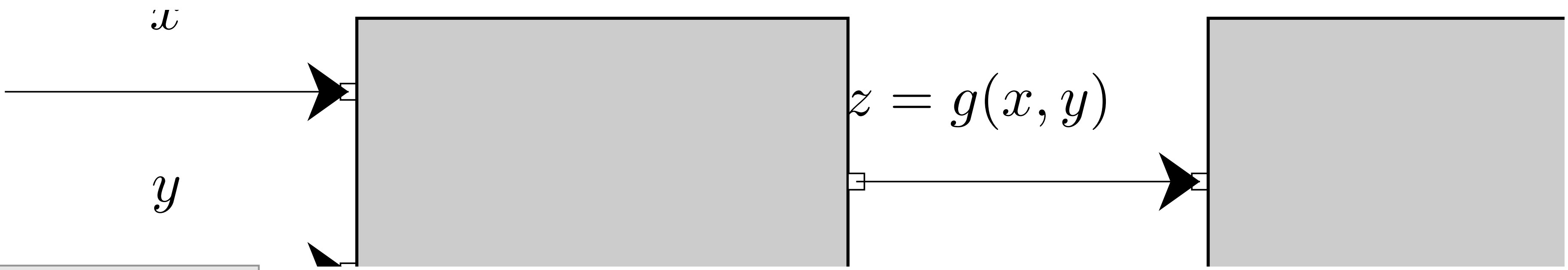
Two Arguments: Chain

$$f'_x(g(x,y)) = g'_x(x,y) \times f'_{g(x,y)}(g(x,y))$$
$$f'_y(g(x,y)) = g'_y(x,y) \times f'_{g(x,y)}(g(x,y))$$

Two Arguments: Chain

$$z = g(x, y)$$
$$d = f'(z)$$
$$f'_x(g(x, y)) = g'_x(x, y) \times d_{out}$$
$$f'_y(g(x, y)) = g'_y(x, y) \times d_{out}$$

```
[['$x$', '$y$'], ['$z = g(x, y)$'], ['$h(x,y))$']] 0 0
[['$x$', '$y$'], ['$z = g(x, y)$'], ['$h(x,y))$']] 0 1
[['$x$', '$y$'], ['$z = g(x, y)$'], ['$h(x,y))$']] 1 0
```



Example: Chain Rule

$$(x \times y)^2$$

$$\begin{aligned} f(z) \quad &= z^2 \\ g(x, y) &= (x \times y) \end{aligned}$$

Example: Chain Rule

$$f'(z) = 2z \times 1$$
$$g'_x(x, y) = y$$
$$g'_y(x, y) = x$$

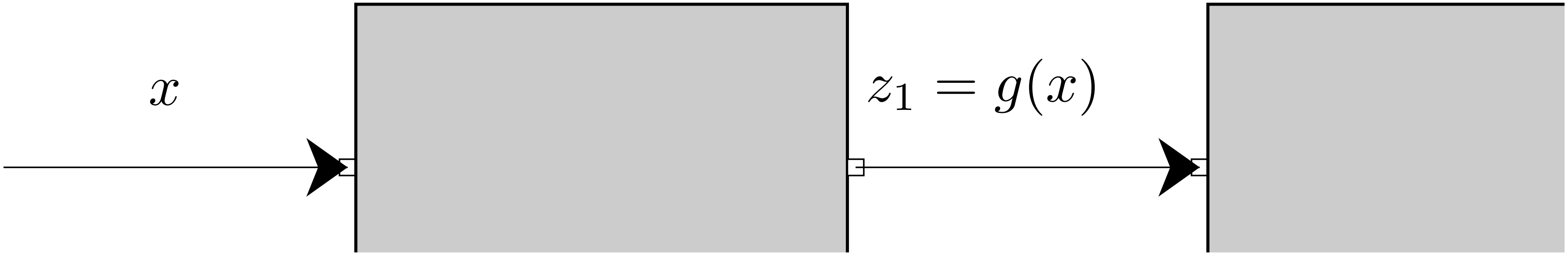
What is the combination?

$$f'_x(g(x, y)) = 2zy$$
$$f'_y(g(x, y)) = 2zx$$

Multivariable Chain

$$f(g(x), h(x))$$

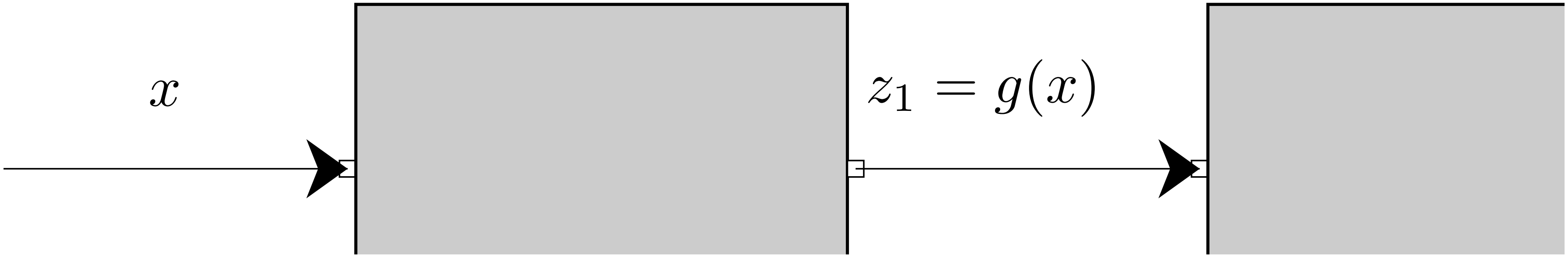
```
[['$x$'], ['$z_1 = g(x)$', '$z_2 = g(x)$'], ['$h(x))$']] 0 0
[['$x$'], ['$z_1 = g(x)$', '$z_2 = g(x)$'], ['$h(x))$']] 1 0
```



Multivariable Chain

$$d = 1 \cdot f'_{z_1}(z_1, z_2) + 1 \cdot f'_{z_2}(z_1, z_2)$$
$$h'_x(x) = d \cdot g'_x(x)$$

[['x'], ['$z_1 = g(x)$', '$z_2 = g(x)$'], ['$h(x))$']] 0 0
[['x'], ['$z_1 = g(x)$', '$z_2 = g(x)$'], ['$h(x))$']] 1 0

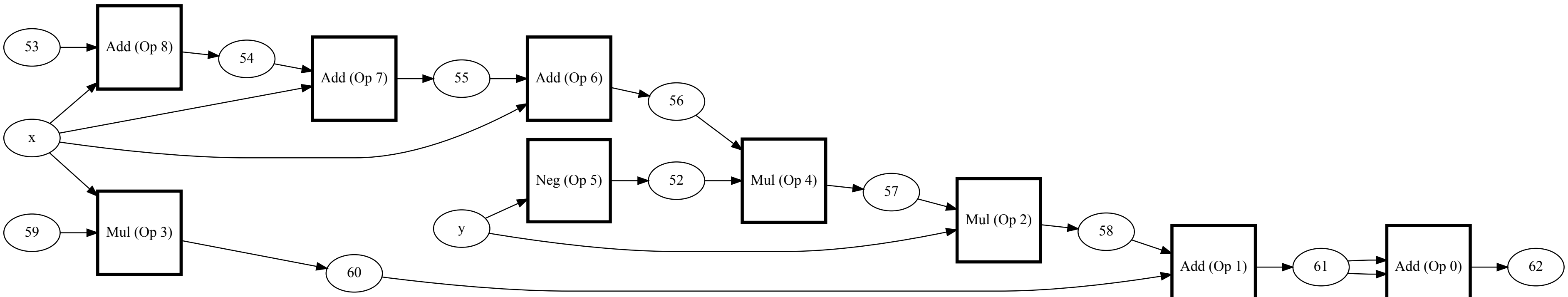


[["$d \\cdot g'_x(x)$"], ["$f'_{z_1}(z_1, z_2)$", "$f'_{z_2}(z_1, z_2)
$"], ['$h1$']] 0 0
[["$d \\cdot g'_x(x)$"], ["$f'_{z_1}(z_1, z_2)$", "$f'_{z_2}(z_1, z_2)
$"], ['$h1$']] 1 0

Backpropagation

Complex Graphs

```
def expression():
    x = Scalar(1.0, name="x")
    y = Scalar(1.0, name="y")
    z = -y * sum([x, x, x]) * y + 10.0 * x
    return z + z
```



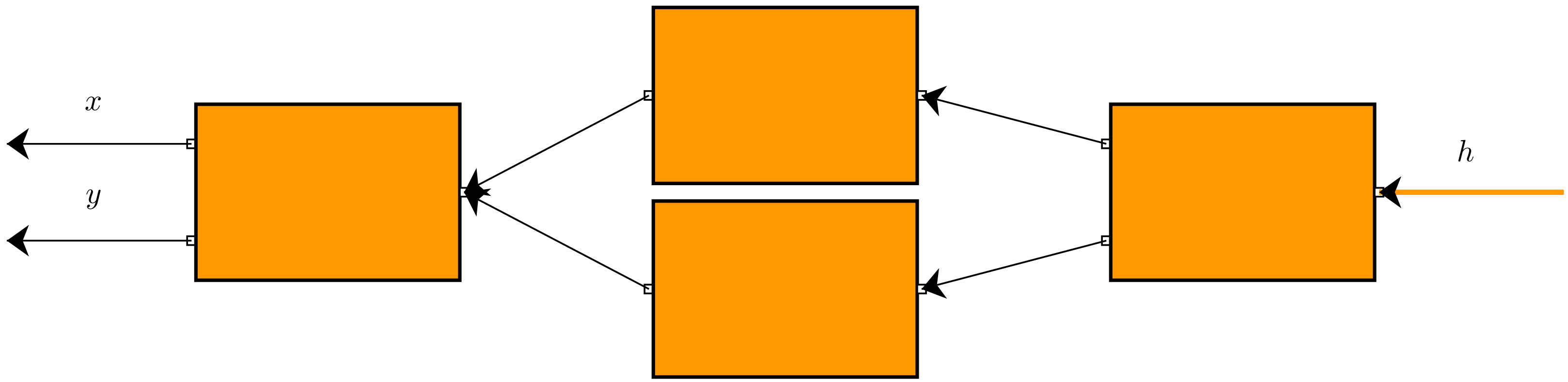
Goal

- Efficient implementation of chain-rule
- Assume access to the graph.
- Goal: Call backward once per variable

Full Graph

$$z = x \times y$$
$$h(x, y) = \log(z) + \exp(z)$$

```
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 1
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 1
```



Tool

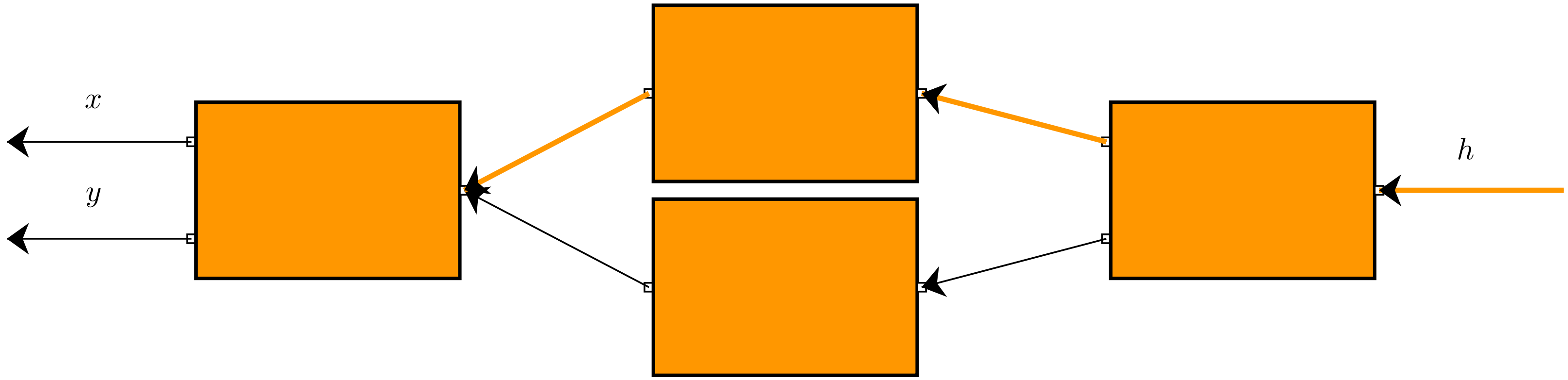
If we have:

- the derivative with respect to a scalar
- the function last called on the scalar

We can apply the chain rule through that function.

Step

```
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 1
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 1
```




```
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 1
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 1
```

Issue

Order matters!

- If we proceed without finishing a variable, we may need to apply chain rule multiple times

Desired property: all derivatives for a variable before backward.

Ordering Step

- Do not process any Variable until all downstream Variables are done.

- Collect a list of the Variables first.

Topological Sorting

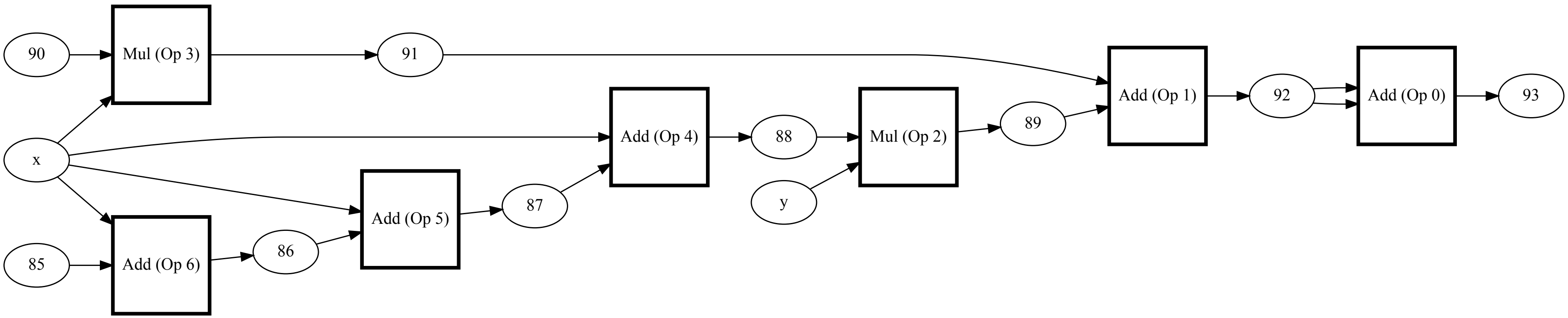
- Topological Sorting
- High-level -> Run depth first search and mark nodes.

Topological Sorting

```
visit(last)

function visit(node n)
  if n has a mark then return

  for each node m with an edge from n to m do
      visit(m)

  mark n with a permanent mark
  add n to list
```

Topological Sorting

```python
def expression():
    x = Scalar(1.0, name="x")
    y = Scalar(1.0, name="y")
    z = sum([x, x, x]) * y + 10.0 * x
    return z + z
```



Backpropagation

- Graph propagation
- Ensure flow to original Variables.

Terminology

- Leaf: Variable created from scratch
- Non-Leaf: Variable created with a Function
- Constant: Term passed in that is not a variable

Algorithm: Outer Loop

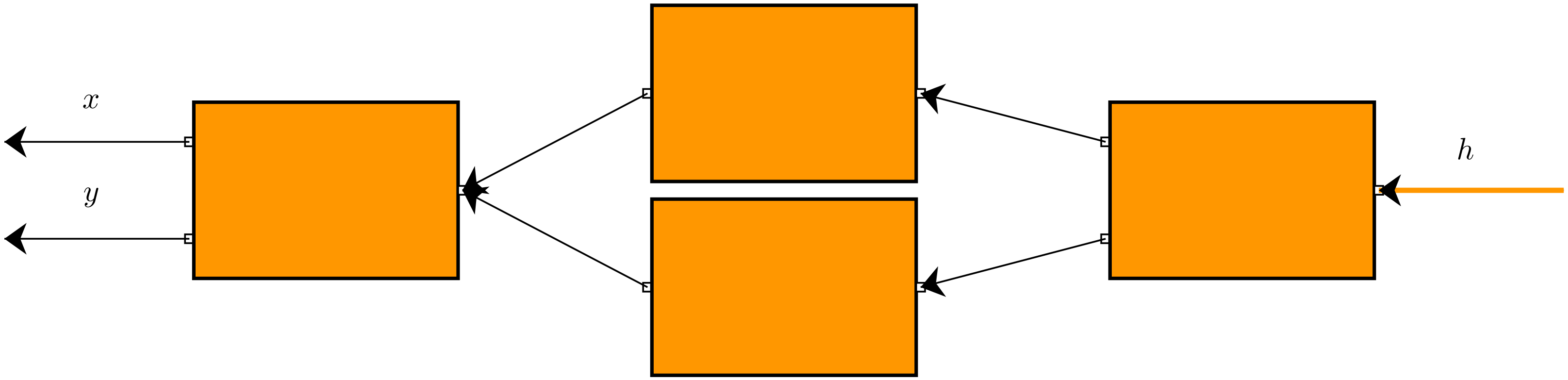
1. Call topological sort
2. Create dict of Variables and derivatives
3. For each node in backward order:

Algorithm: Inner Loop

1. if Variable is leaf, add its final derivative
2. if the Variable is not a leaf, 1) call backward with d 2) loop through all the Variables+derivative 3) accumulate derivatives for the Variable

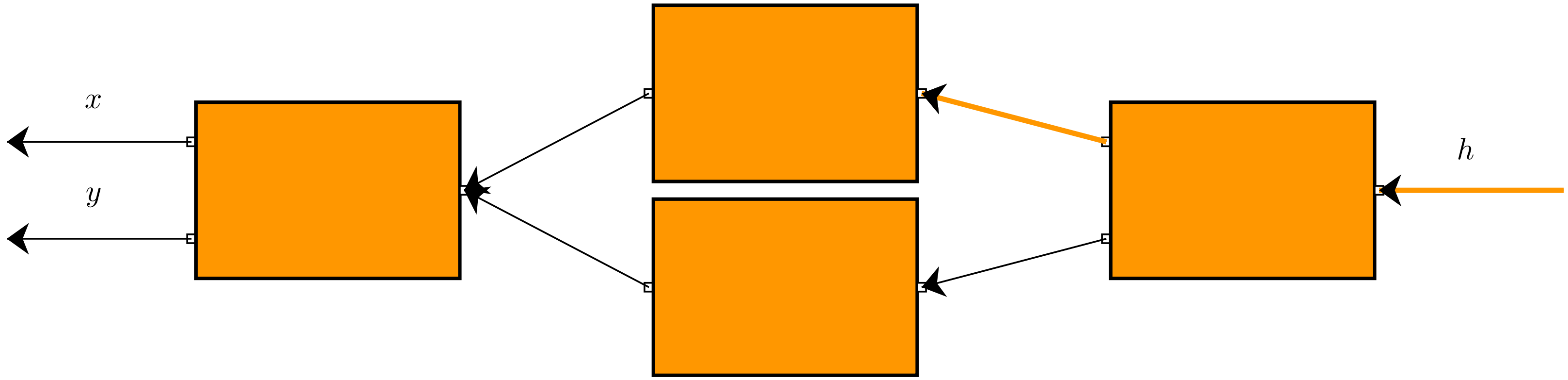
Example

```
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 1
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 1
```



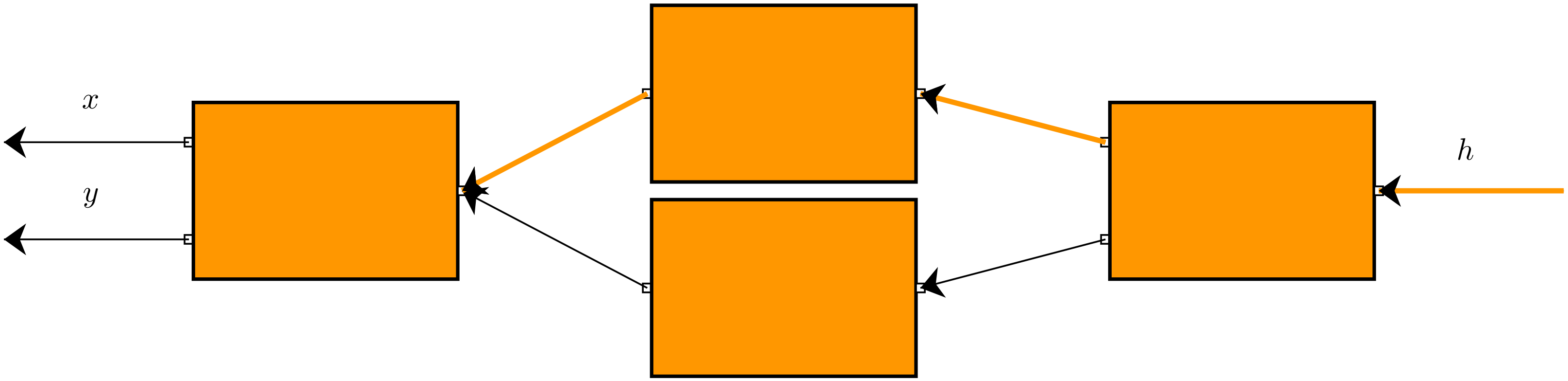
Example

```
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 1
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 1
```



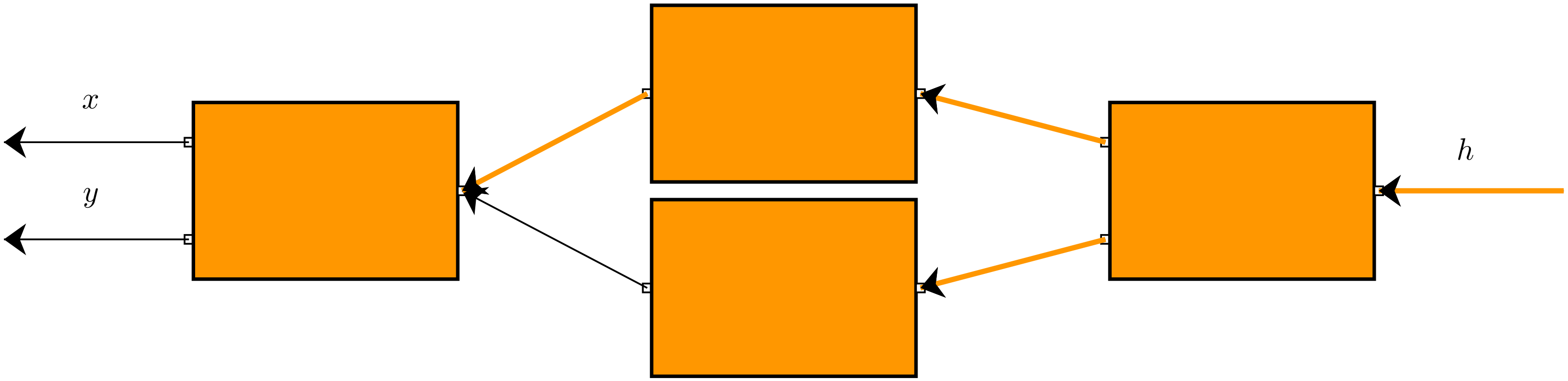
Example

```
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 1
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 1
```



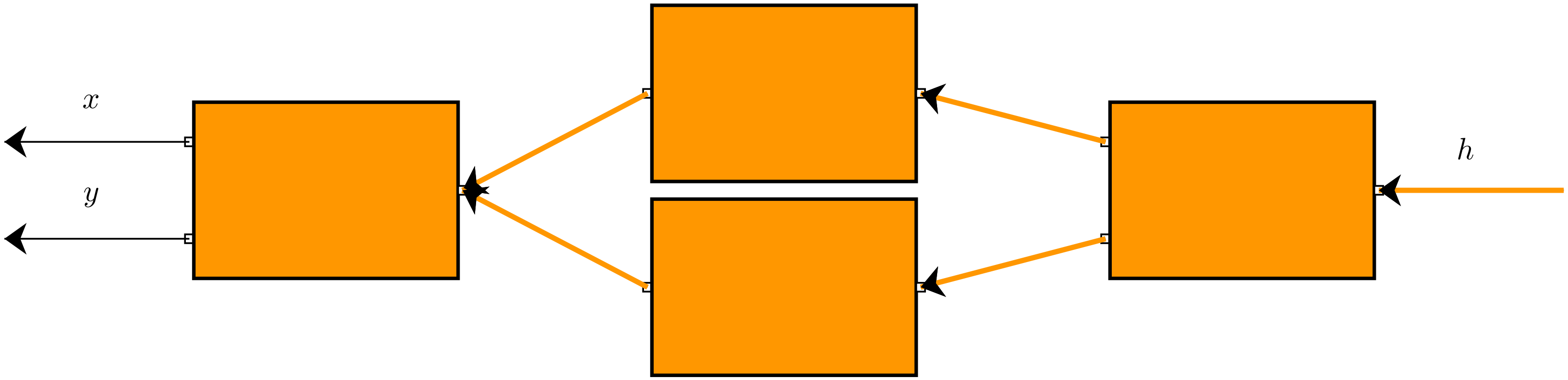
Example

```
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 1
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 1
```



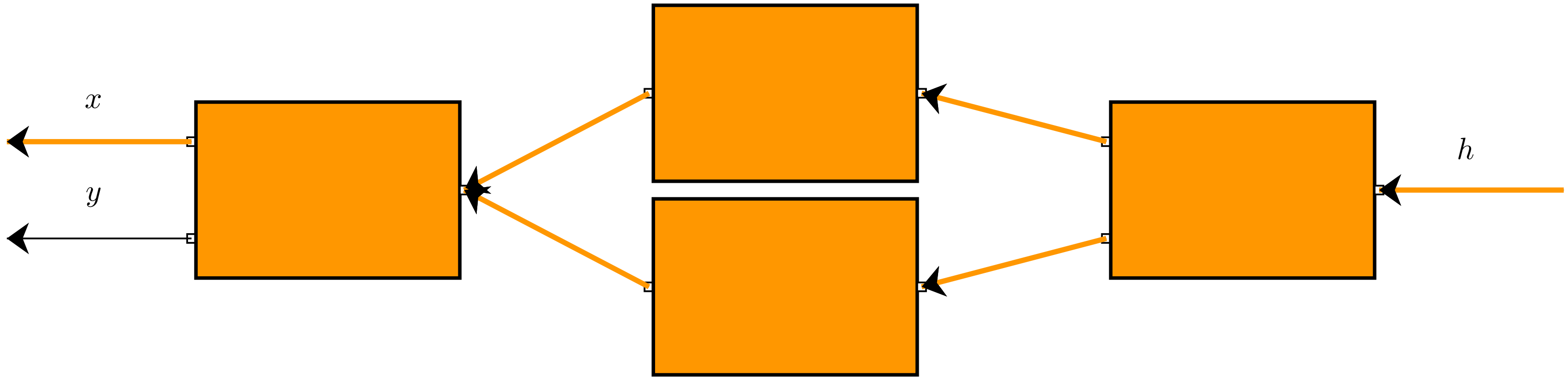
Example

```
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 1
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 1
```



Example

```
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 1
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 1
```



Example

```
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 0 1
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 1 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 0
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 2 1
```