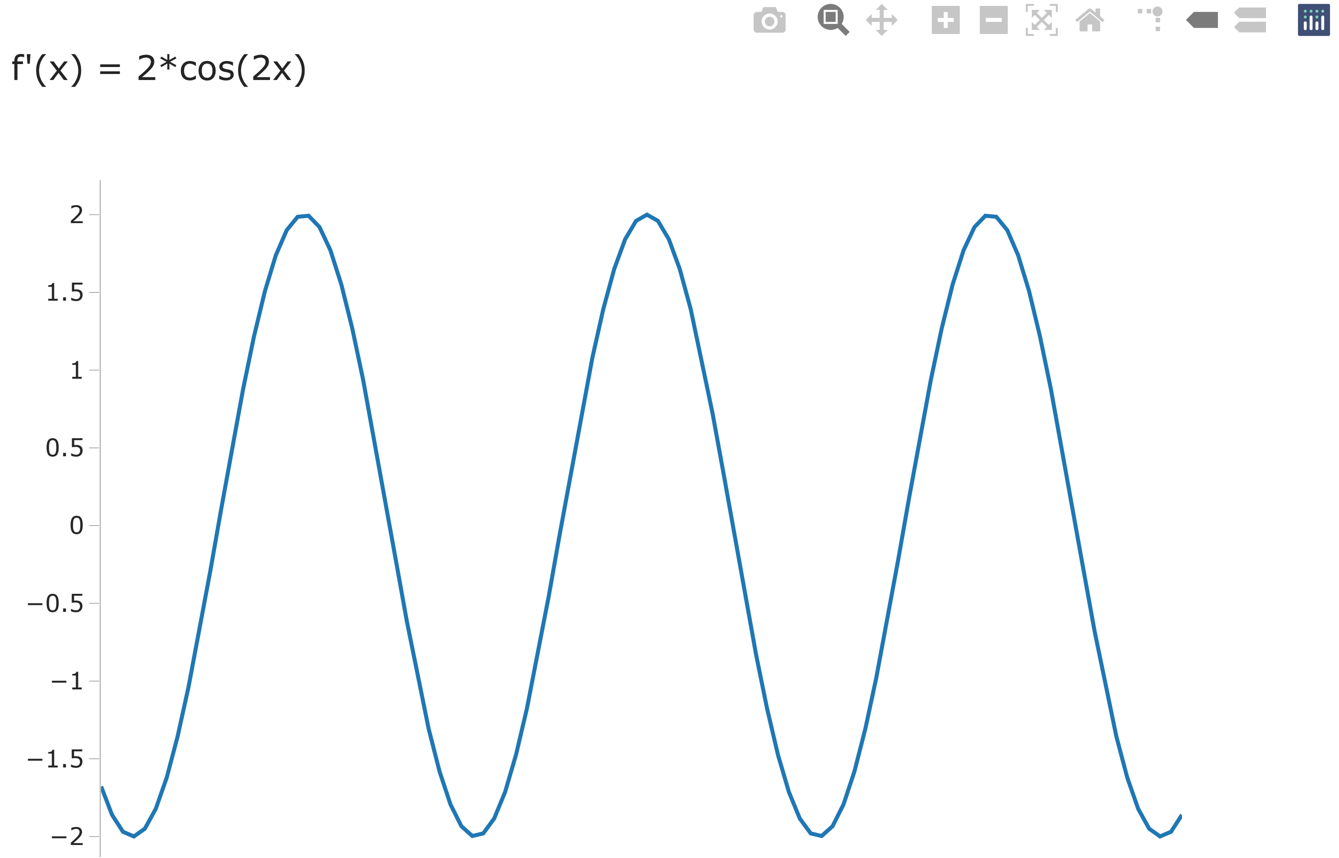
Module 1.2 - Autodifferentiation

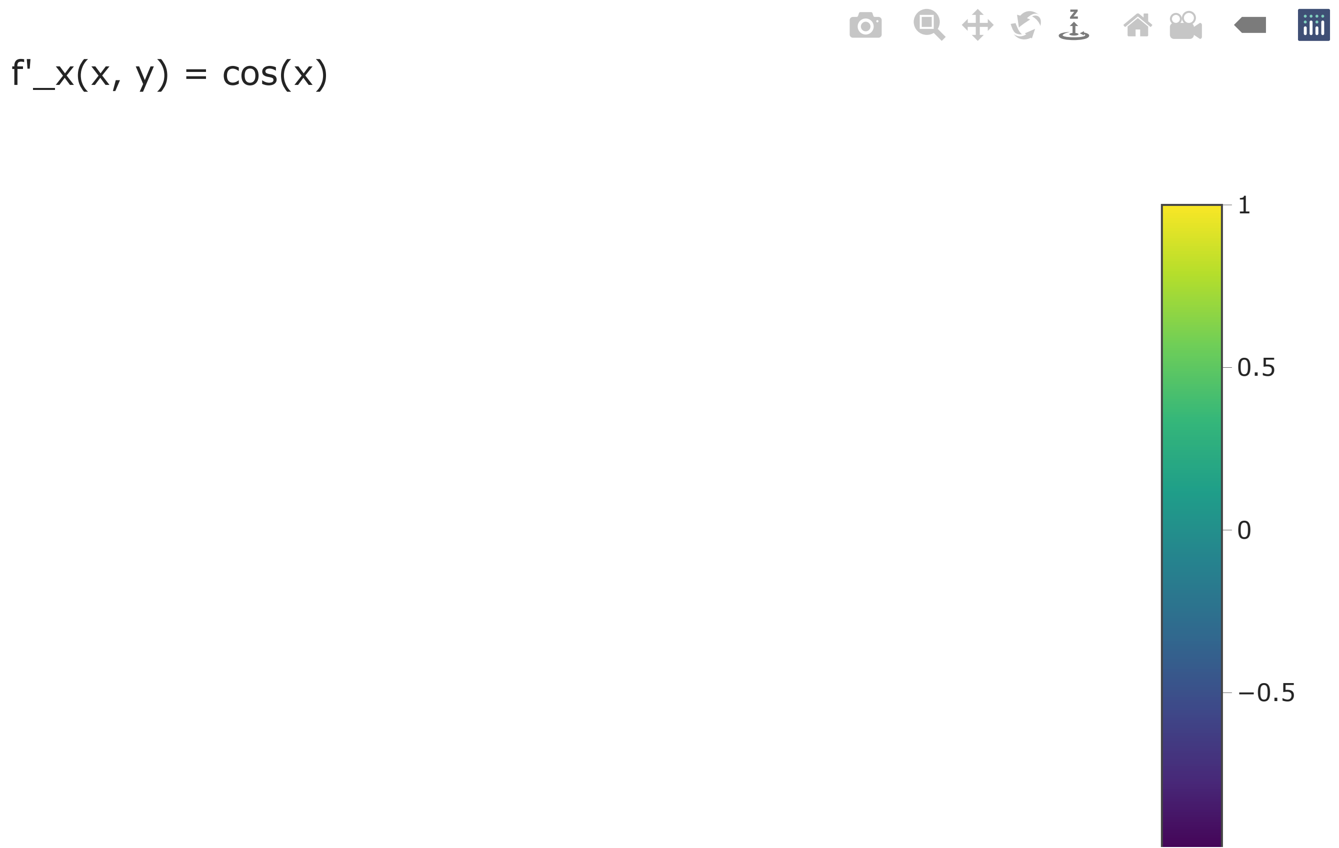
Symbolic Derivative

$$f(x) = \sin(2x) \Rightarrow f'(x) = 2\cos(2x)$$



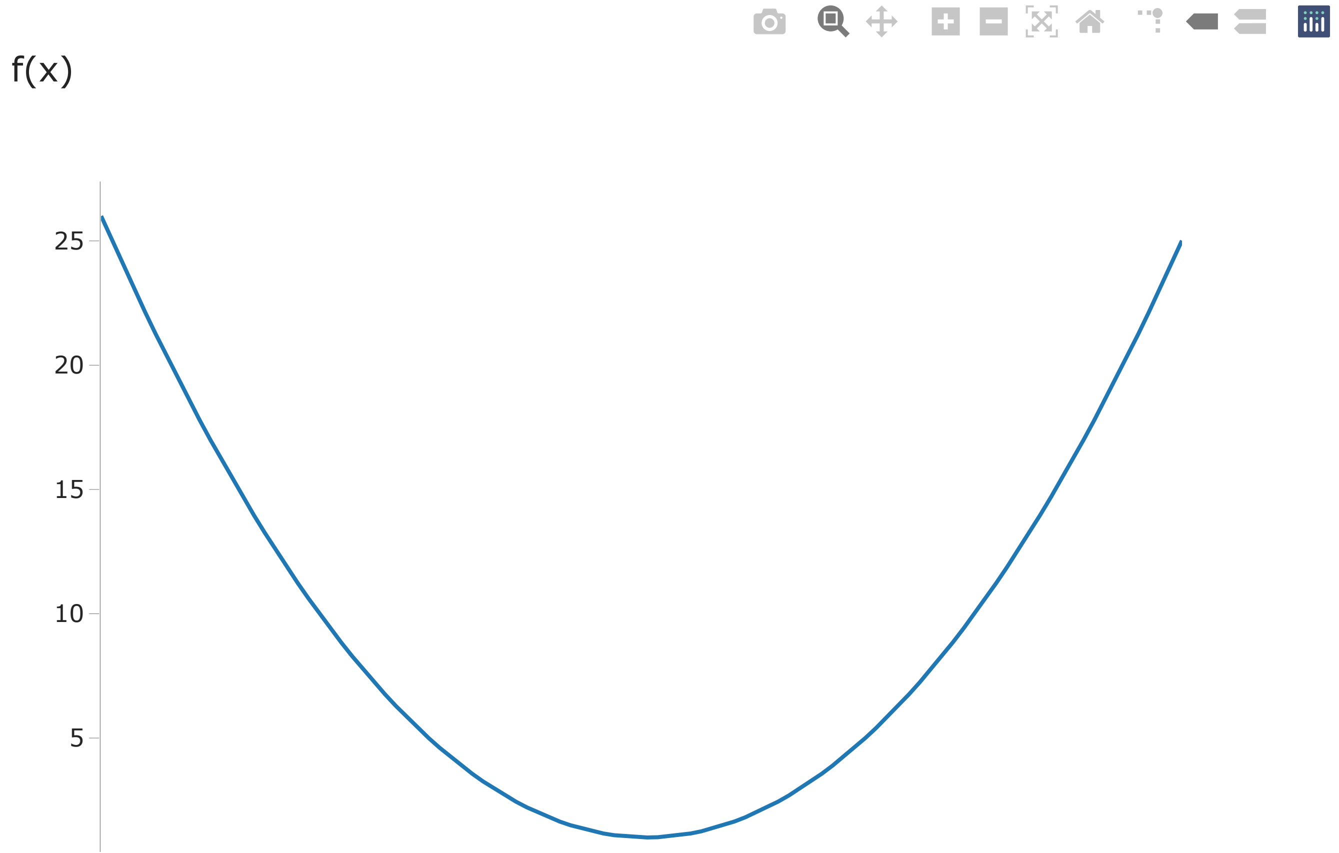
Derivatives with Multiple Arguments

$$f'_x(x, y) = \cos(x) \quad f'_y(x, y) = -2\sin(y)$$



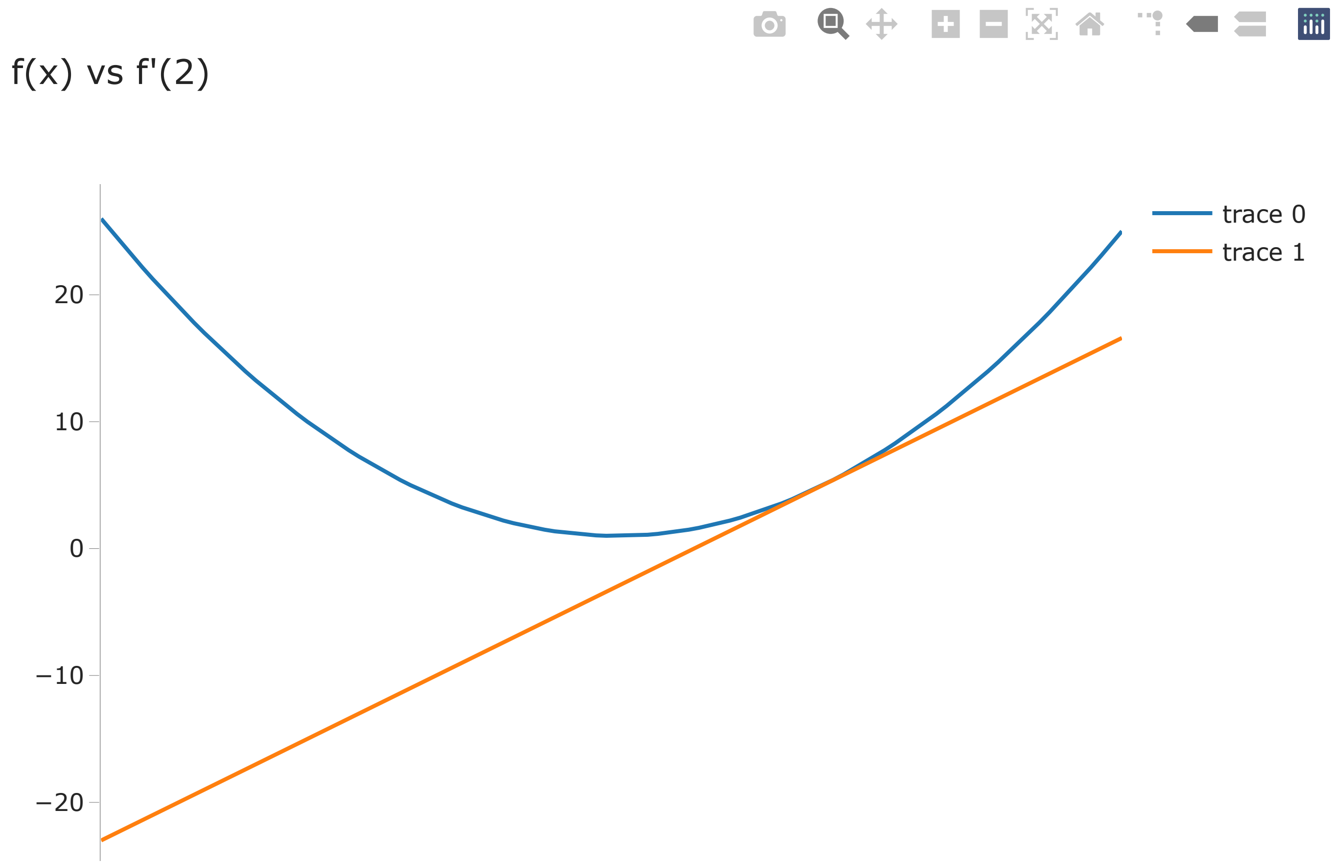
Review: Derivative

$$f(x) = x^2 + 1$$



Review: Derivative

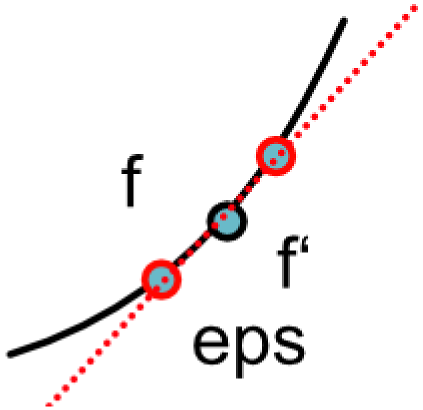
$$f'(x) = 2x$$



Numerical Derivative: Central Difference

Approximate derivatative

$$f'(x) \approx \frac{f(x+\epsilon) - f(x-\epsilon)}{2\epsilon}$$



Derivative as higher-order function

$$f(x) = \ldots$$

$$f'(x) = \ldots$$

```
def derivative(f: Callable[[float], float]) -> Callable[[float], float]:
    def f_prime(x: float) -> float:
        ...

    return f_prime
```

Quiz

Outline

- Autodifferentiation
- Computational Graph
- Backward
- Chain Rule

Autodifferentiation

Goal

- Write down arbitrary code
- Transform to compute deriviative
- Use this to fit models

How does this differ?

- Are these symbolic derivatives?
  - No, don't get out mathematical form
- Are these numerical derivatives?
  - No, don't use local evaluation.

Overview: Autodifferentiation

- *Forward* Pass - Trace arbitrary function
- *Backward* Pass - Compute derivatives of function

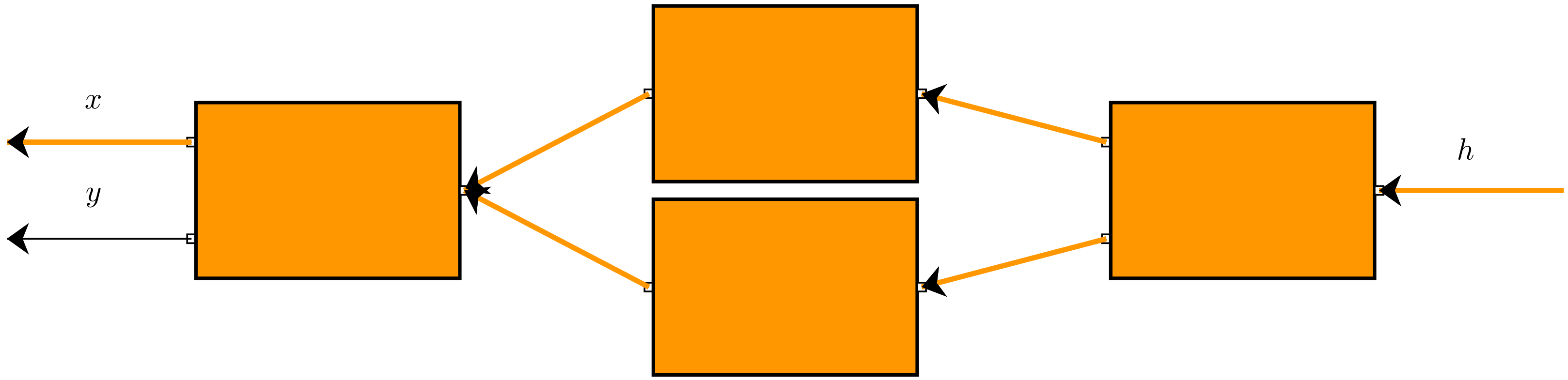
Forward Pass

- User writes mathematical code
- Collect results and computation graph

Backward Pass

- Minitorch uses graph to compute derivative 1, 2,

```
[['$x$', '$y$'], ['', ''], ['', ''], ['$h$']] 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 : Linear Model

- Our forward computes

$$\mathcal{L}(w, b) = -\log \sigma(x; w, b)$$

  where

$$m(x; w, b) = x_1 \times w_1 + x_2 \times w_2 + b$$

- Our backward computes

$$\mathcal{L}'_w(w, b) \;\; \mathcal{L}'_b(w, b)$$

Derivative Checks

- Property: All three of these should roughly match

Strategy

1. Replace generic numbers.

2. Replace mathematical functions.

3. Track with functions have been applied.

Computation Graph

Strategy

- Act like a numerical value to user
- Trace the operations that are applied
- Hide access to internal storage

Box Diagrams

$$f(x) = \mathrm{ReLU}(x)$$

```
[['$x_1$'], ['$f(x_1)$']] 0 0
[['$x_2$'], ['$f(x_2)$']] 0 0
```

Box Diagrams

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

```
[['$x$', '$y$'], ['$f(x, y)$']] 0 0
[['$x$', '$y$'], ['$f(x, y)$']] 0 1
```

Code Demo

How does this work

- Arrows are intermediate values
- Boxes are function application

$$f(x) = \mathrm{ReLU}(x)$$

$$g(x) = \log(x)$$

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

Implementation

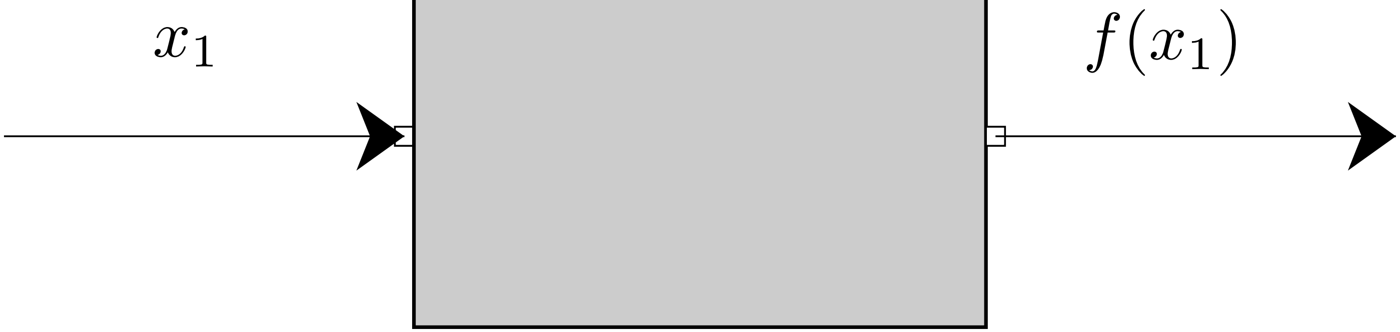
Functions

- Functions are implemented as static classes
- We implement hidden `forward` and `backward` methods
- User calls `apply` which handles wrapping / unwrapping

Functions

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

[['x_1'], ['$f(x_1)$']] 0 0




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

Multi-arg Functions

```
[['$x$', '$y$'], ['$f(x, y)$']] 0 0
[['$x$', '$y$'], ['$f(x, y)$']] 0 1
```


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

Variables

- *Wrap* a numerical value

```
x_1 = Scalar(10.0)
x_2 = Scalar(0.0)
```

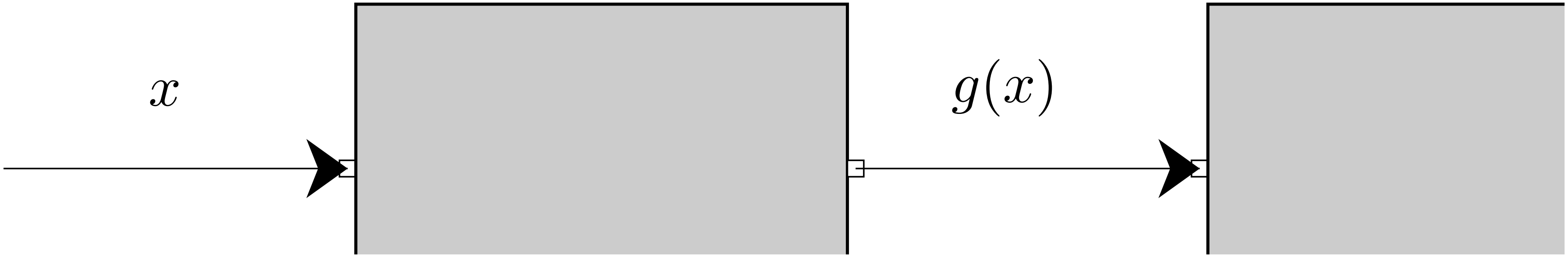
Using scalar variables.

```
x = Scalar(10.0)
z = TimesFive.apply(x)


def apply(cls, val: Scalar) -> Scalar:
    ...
    unwrapped = val.data
    new = cls.forward(unwapped)
    return Scalar(new)
    ...
```

Multiple Steps

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




```
x = Scalar(10.0)
y = Scalar(5.0)
z = TimesFive.apply(x)
out = TimesFive.apply(z)
```

Tricks

- Use operator overloading to ensure that functions are called

```
out2 = x * y


def __mul__(self, b: Scalar) -> Scalar:
    return Mul.apply(self, b)
```

- Many functions e.g. `sub` can be implemented with other calls.

Notes

- Since each operation creates a new variable, there are no loops.
- Cannot modify a variable. Graph only gets larger.

Backwards

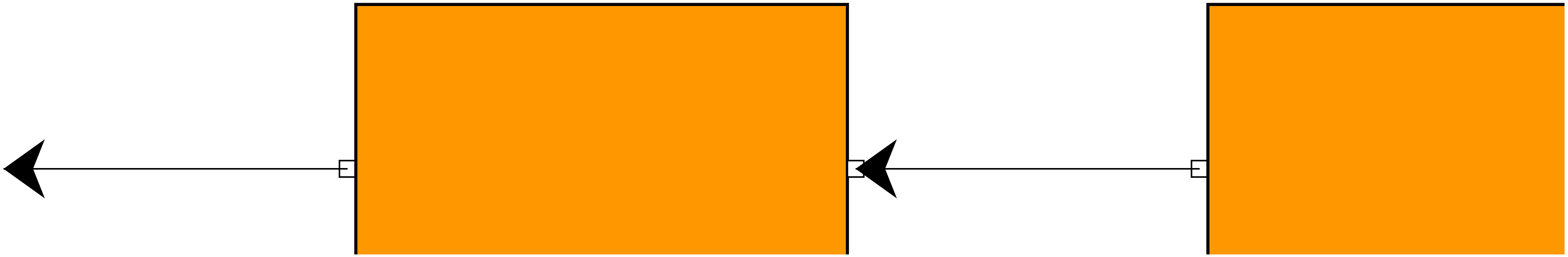
How do we get derivatives?

- Base case: compute derivatives for single functions
- Inductive case: define how to propagate a derivative

Base Case: Coding Derivatives

- For each f we need to also provide f'
- This part can be done through manual symbolic differentiation

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



Code

- Backward use f'
- Returns $f'(x) \times d$

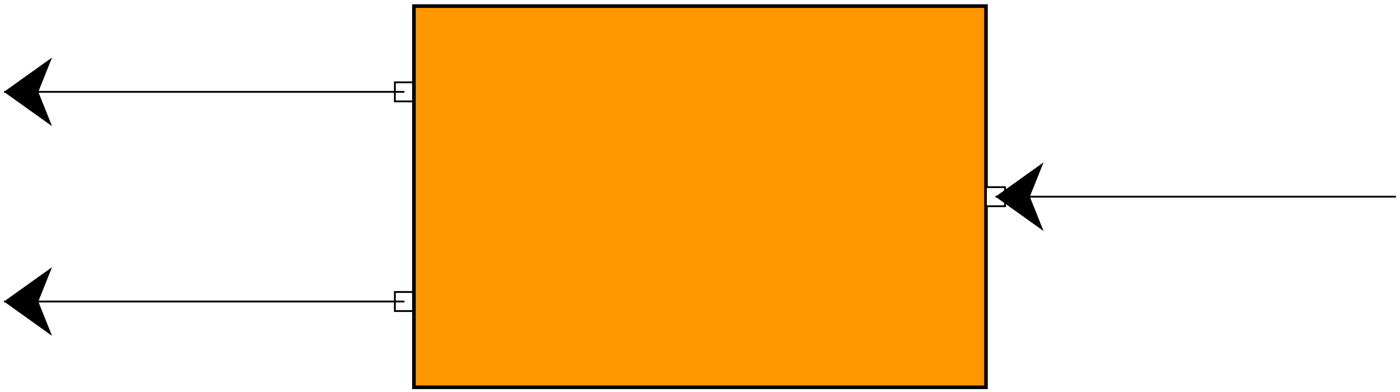
```python
class TimesFive(ScalarFunction):
    @staticmethod
    def forward(ctx, x: float) -> float:
        return x * 5

    @staticmethod
    def backward(ctx, d: float) -> float:
        f_prime = 5
        return f_prime * d
```

Two Arg

- What about $f(x, y)$
- Returns $f'_x(x, y) \times d$ and $f'_y(x, y) \times d$

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



Code

```
class AddTimes2(ScalarFunction):
    @staticmethod
    def forward(ctx, x: float, y: float) -> float:
        return x + 2 * y

    @staticmethod
    def backward(ctx, d) -> Tuple[float, float]:
        return d, 2 * d
```

What is Context?

- Context on `forward` is given to `backward`
- May be called at different times.

Context

Consider a function `Square`

- $g(x) = x^2$ that squares x
- Derivative function uses variable $g'(x) = 2 \times x$
- However backward doesn't take args

```
def backward(ctx, d_out):
    ...
```

Context

Arguments to backward must be saved in context. ::

```
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_out: float) -> Tuple[float, float]:
        x = ctx.saved_values
        f_prime = 2 * x
        return f_prime * d_out
```

Context Internals

Run `Square`

```
x = minitorch.Scalar(10)
x_2 = Square.apply(x)
x_2.history
```

```
ScalarHistory(last_fn=<class '__main__.Square'>, ctx=Context(no_grad=Fals
e, saved_values=(10.0,)), inputs=[Scalar(10.000000)])
```