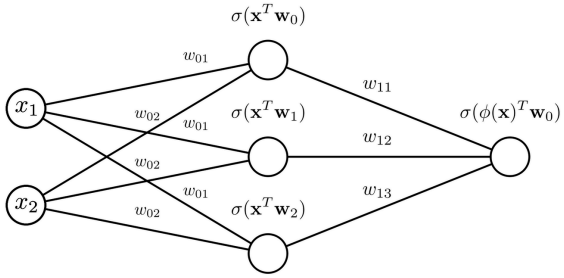
Automatic differentiation: Motivation

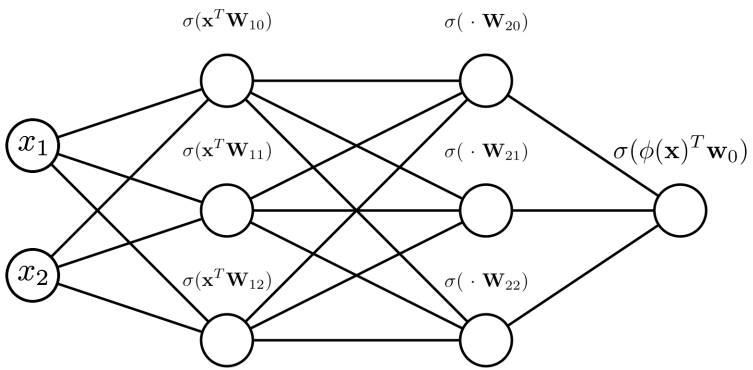


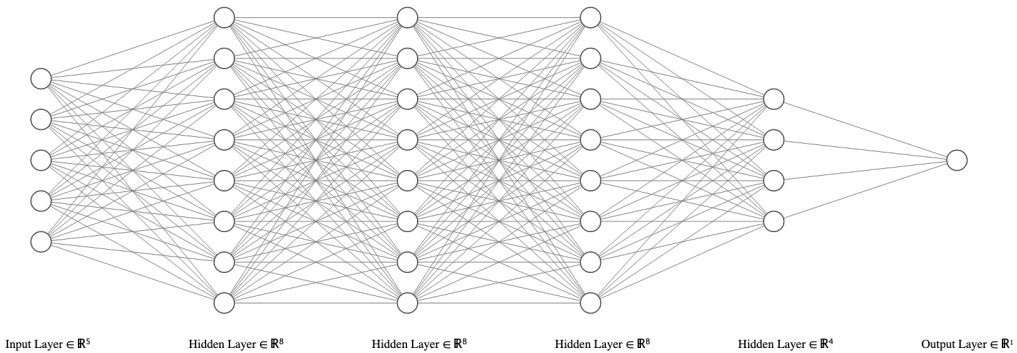
$$\mathbf{NLL}(\mathbf{w}_0, \mathbf{W}, \mathbf{X}, \mathbf{y}) = -\sum_{i=1}^{N} \log \sigma\big((2y_i - 1)\phi(\mathbf{x}_i)^T\mathbf{w}\big)$$

$$= -\sum_{i=1}^{N} \log \sigma\big((2y_i - 1)\sigma\big(w_{01} \cdot \sigma(x_1 W_{11} + x_2 W_{12}) + w_{02} \cdot \sigma(x_1 W_{21} + x_2 W_{22}) + w_{03} \cdot \sigma(x_1 W_{31} + x_2 W_{32})\big)\big)$$

Automatic differentiation: Motivation

$$\mathbf{NLL}(\mathbf{w}_0, \mathbf{W}, \mathbf{X}, \mathbf{y}) = -\sum_{i=1}^{N} \log \sigma\big((2y_i - 1)\phi(\mathbf{x}_i)^T \mathbf{w}\big)$$





Derivatives revisited

Given a function $f: \mathbb{R} \to \mathbb{R}$, a derivative is the *instantaneous rate of change*

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Derivatives revisited

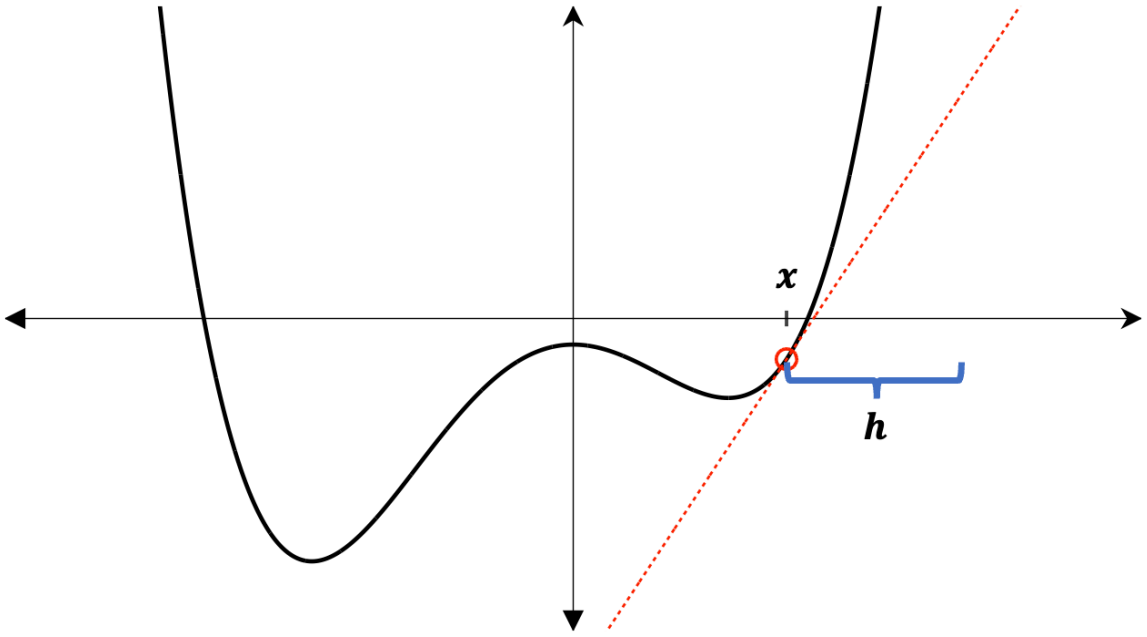
Given a function $f: \mathbb{R} \to \mathbb{R}$, a derivative is the *instantaneous rate of change*

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Equivalently, it's the slope of the *optimal linear approximation* of f near x.

Derivatives revisited

Optimal linear approximation



Consider the question:

"If I perturb x by h, how does the output change?"

The chain rule

Where does this appear?

Consider the chain rule

$$\frac{\partial}{\partial x} f\big(g(x)\big) \cdot 1 = f'\big(g(x)\big) \cdot g'(x) \cdot 1$$

If I perturb x by 1, by how much does $f\big(g(x)\big)$ change?

(under a first-order approx.)

The chain rule

Where does this appear?

Consider the chain rule

$$\frac{\partial}{\partial x} f\big(g(x)\big) \cdot 1 = f'\big(g(x)\big) \cdot \underbrace{g'(x) \cdot 1}$$

If I perturb x by 1, by how much does $g(x)$ change?

The chain rule

Where does this appear?

Consider the chain rule

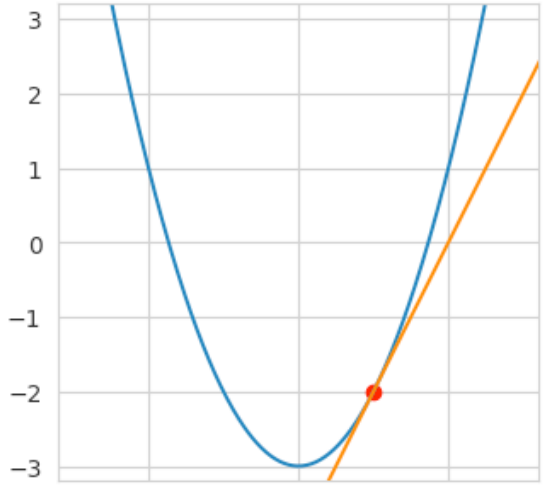
$$\frac{\partial}{\partial x} f\big(g(x)\big) \cdot 1 = f'\big(g(x)\big) \cdot h$$

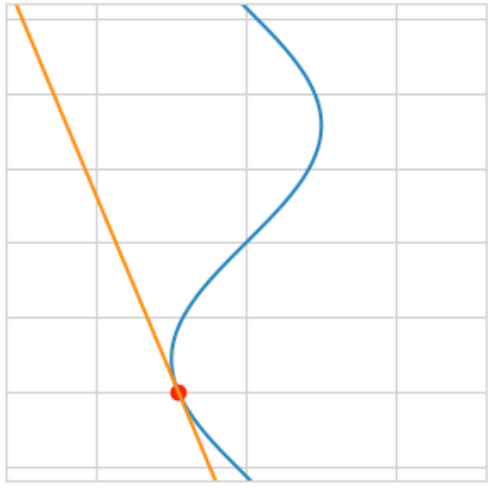
If I perturb $g(x)$ by h, by how much does $f(g(x))$ change?

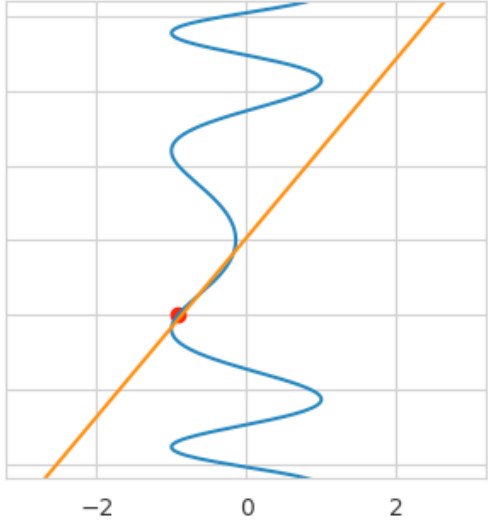
(to the first order)

To find the derivative of a complicated function, we iteratively map input perturbations to output perturbations for each sub-function

Chain rule illustrated







Useful notation

$$\frac{d}{dx} f(g(x)) = f'(g(x))g'(x)$$

$$b = g(x)$$

$$a = f(b)$$

$$\frac{da}{dx} = \frac{da}{db}\frac{db}{dx}$$

Corresponds to code

```
b = x ** 2
a = log(b)
```

Useful notation

```
b = x ** 2
a = log(b)
```

$$b = g(x)$$

$$a = f(b)$$

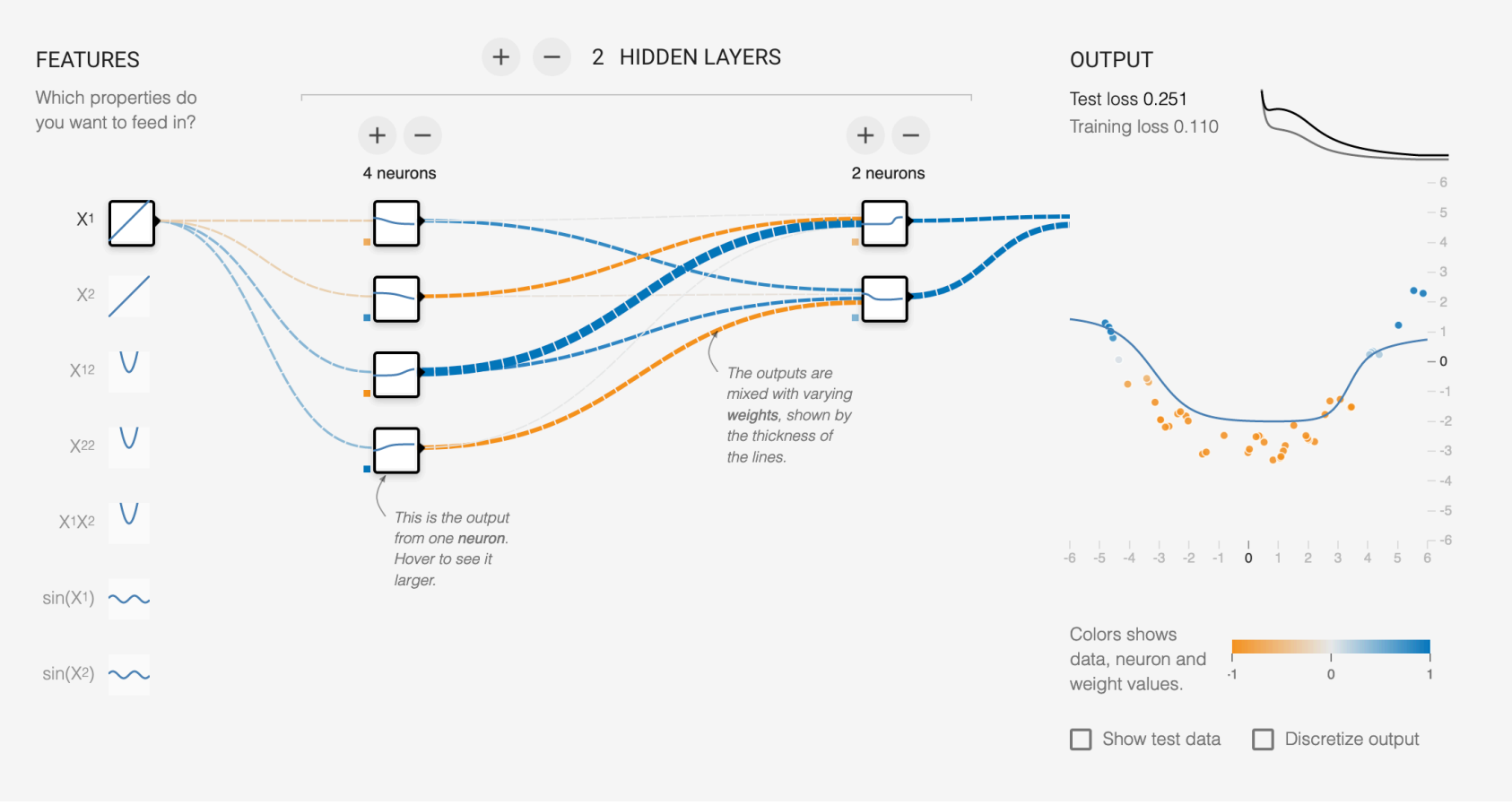
$$a = \log(b), \quad b = x^2$$

$$\frac{da}{dx} = \frac{da}{db}\frac{db}{dx}$$

$$\frac{da}{db} = \qquad \frac{db}{dx} =$$

$$\frac{da}{dx} =$$

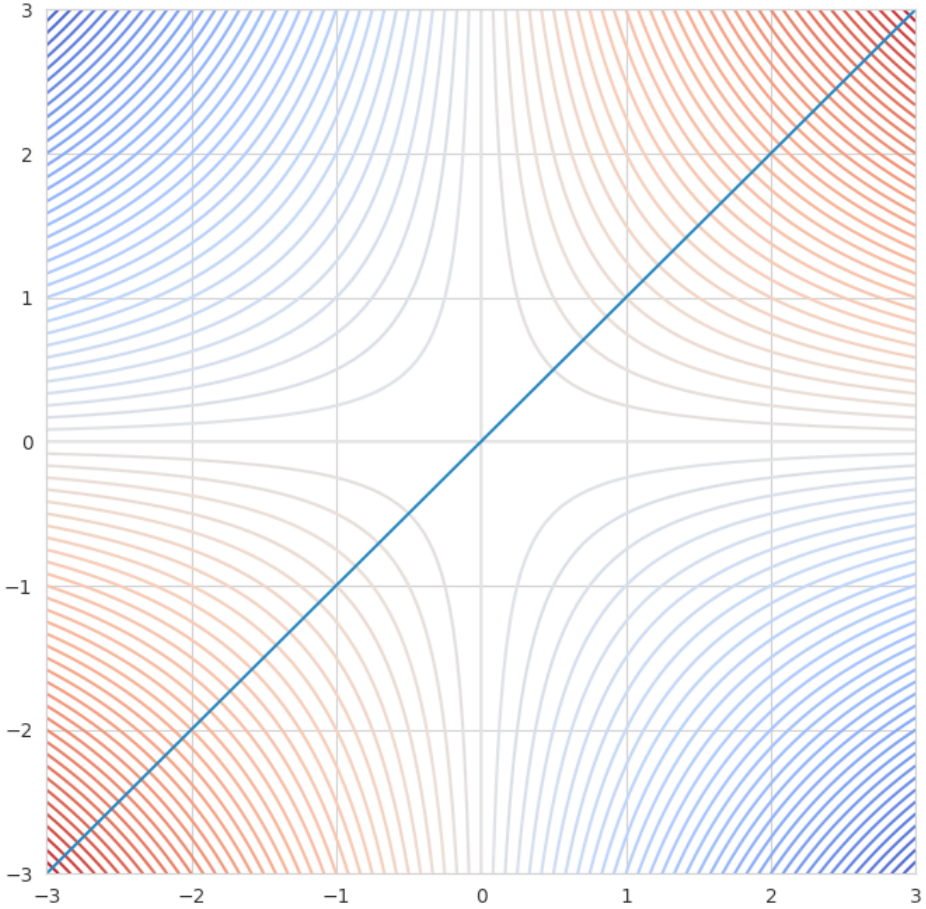
Neural networks



Total derivatives

$$\frac{df(y(x), z(x))}{dx} = \frac{df}{dy}\frac{dy}{dx} + \frac{df}{dz}\frac{dz}{dx}$$

Total derivatives



$$f(x, y) = xy$$

$$\frac{df}{dx} = y \qquad \frac{df}{dy} = x$$

$$\frac{d}{dx} f(x, x) =$$

Total derivatives

$$\frac{df(y(x), z(x))}{dx} = \frac{df}{dy}\frac{dy}{dx} + \frac{df}{dz}\frac{dz}{dx}$$

Total derivatives

$$\frac{df(y(x),x)}{dx} = \frac{df}{dy}\frac{dy}{dx} + \frac{df}{dx}$$

Partial derivatives

$$\frac{df(y(x),x)}{dx} = \frac{\partial f}{\partial y}\frac{\partial y}{\partial x} + \frac{\partial f}{\partial x}$$

Composing the chain rule

$$L = -\log \sigma\left(wx^2\right)$$

$$a = x^2$$

$$b = wa$$

$$c = \sigma(b)$$

$$g = \log c$$

$$L = -g$$

Composing the chain rule

$$L = -\log \sigma\left(wx^2\right)$$

$$a = x^2$$

$$b = wa$$

$$c = \sigma(b)$$

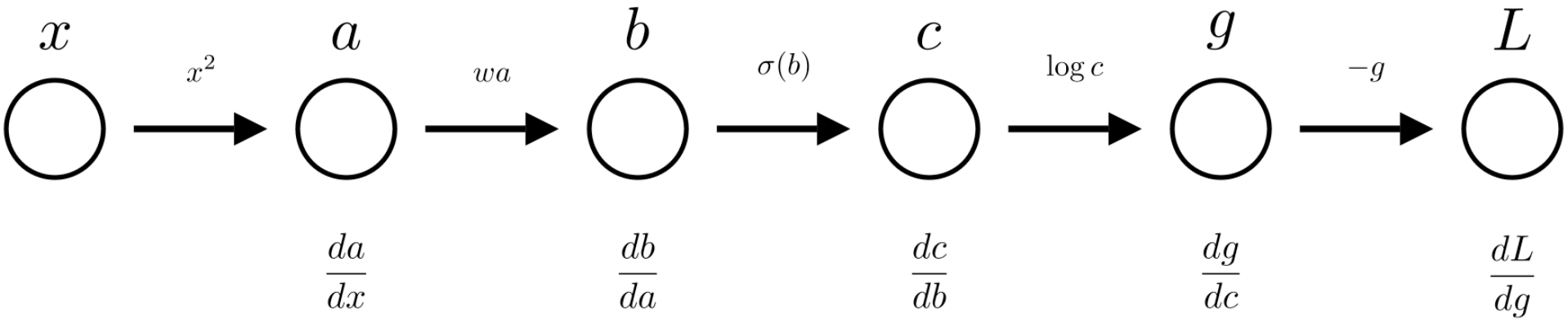
$$g = \log c$$

$$L = -g$$

$$\frac{dL}{dx} = \frac{dL}{dg}\frac{dg}{dc}\frac{dc}{db}\frac{db}{da}\frac{da}{dx}$$

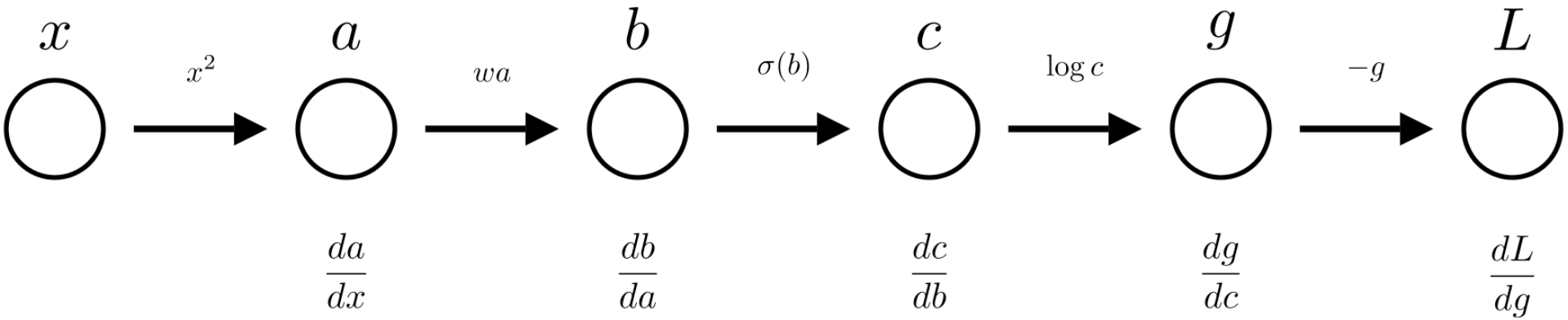
Computational graphs

$$L = -\log \sigma\left(wx^2\right)$$



Forward-mode automatic differentiation

$$L = -\log \sigma\left(wx^2\right)$$



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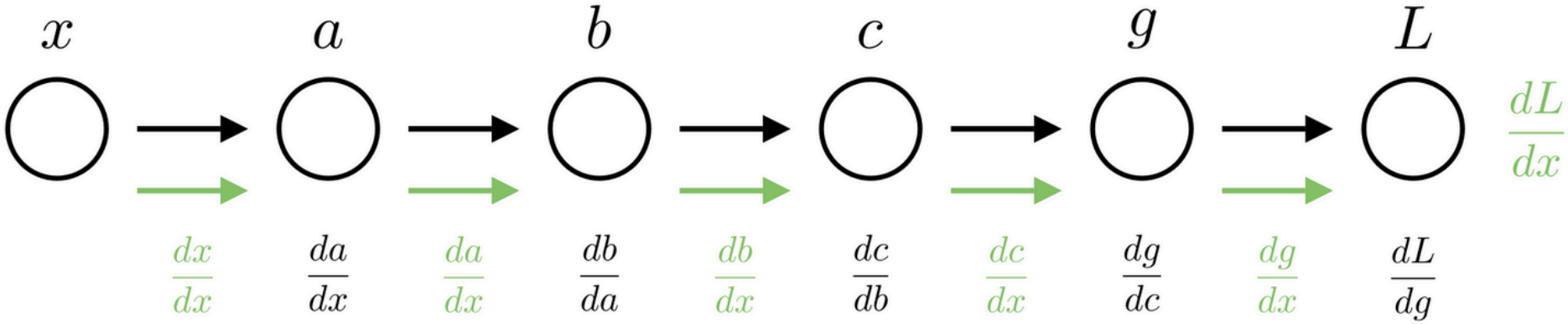

Automatic differentiation with multiple inputs

$$-\log \sigma(w_1 x_1 + w_2 x_2 + w_3 x_3)$$

$$\frac{dL}{d\mathbf{x}} = \begin{bmatrix} \frac{dL}{dx_1} \\ \frac{dL}{dx_2} \\ \frac{dL}{dx_3} \end{bmatrix}$$

Automatic differentiation with multiple inputs

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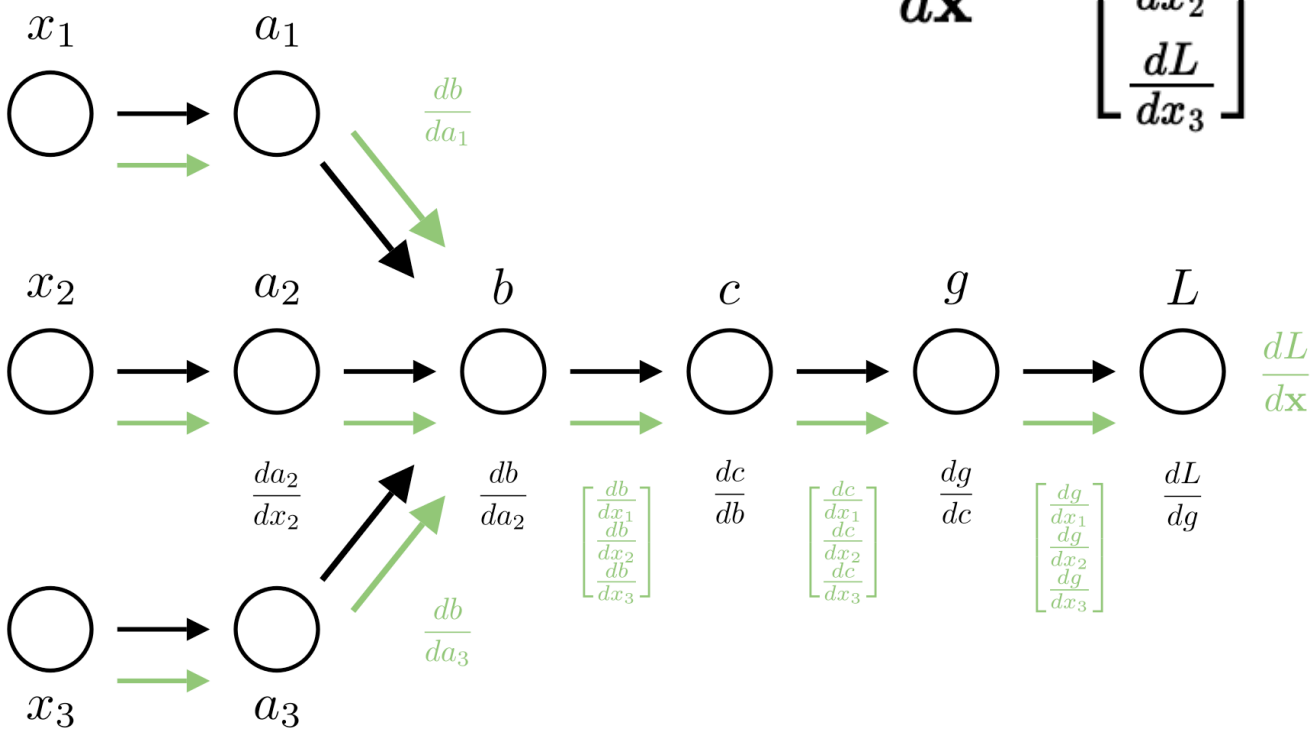

Reusing values

```
def loss(x):
    a = x ** 2
    b = 5 * a
    c = log(a)
    g = b * c
    L = -g
    return L
```

$$a = x^2$$

$$b = 5a$$

$$c = \log a$$

$$g = bc$$

$$L = -b$$

Reusing values

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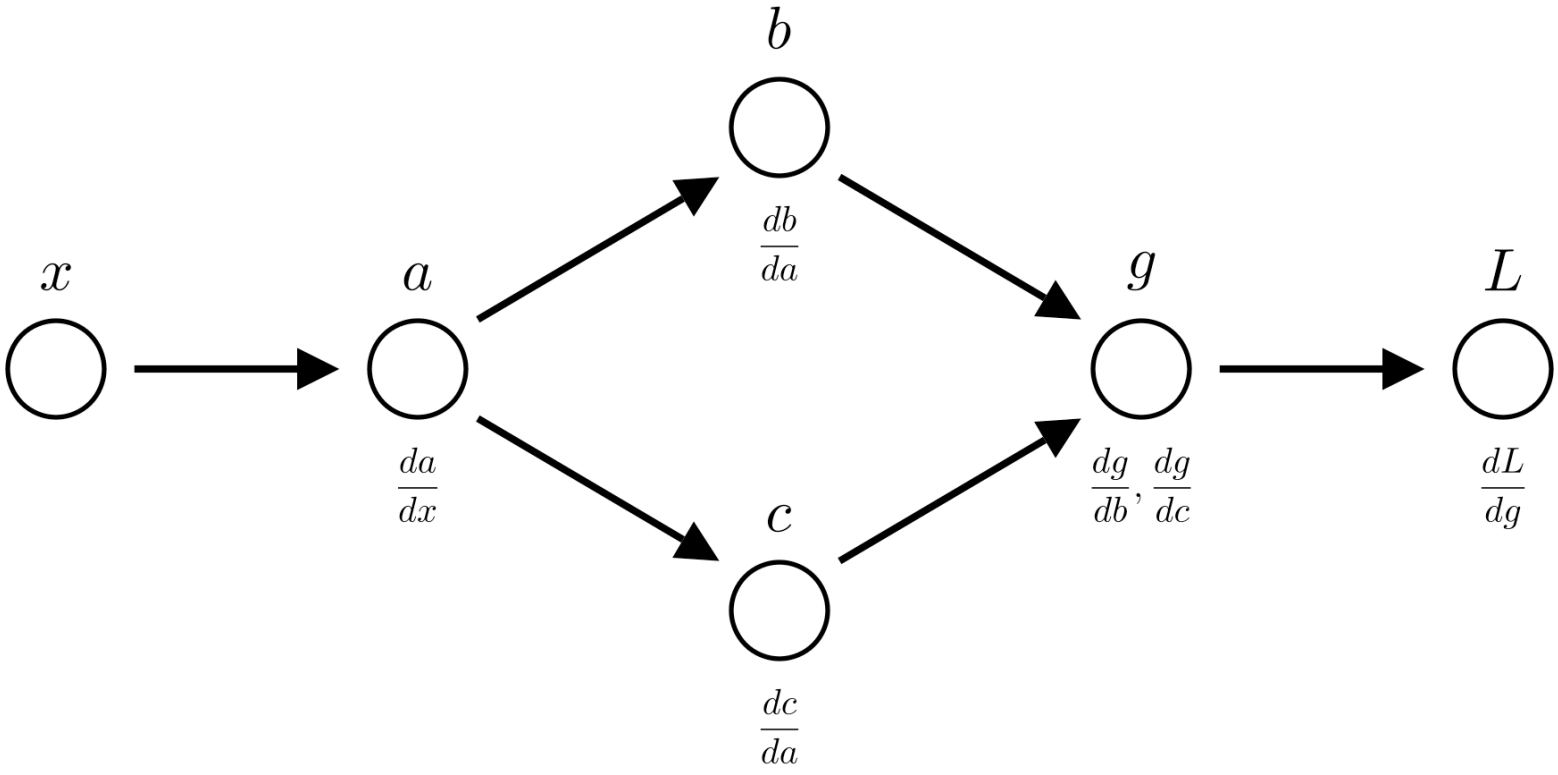


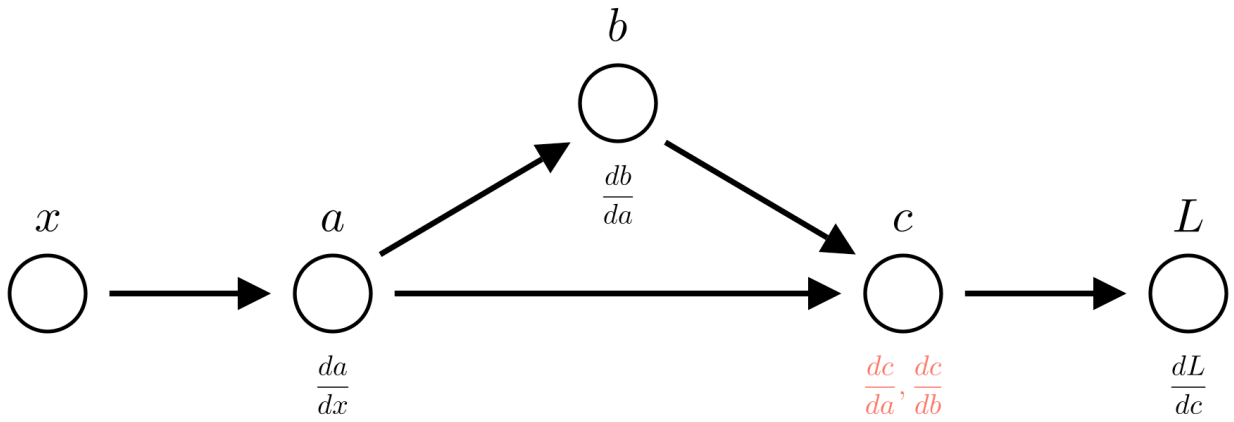
Partial derivatives revisited

$$a = x^2$$

$$b = 5a$$

$$c = ab$$

$$L = -c$$



$$\frac{dc}{da} =$$

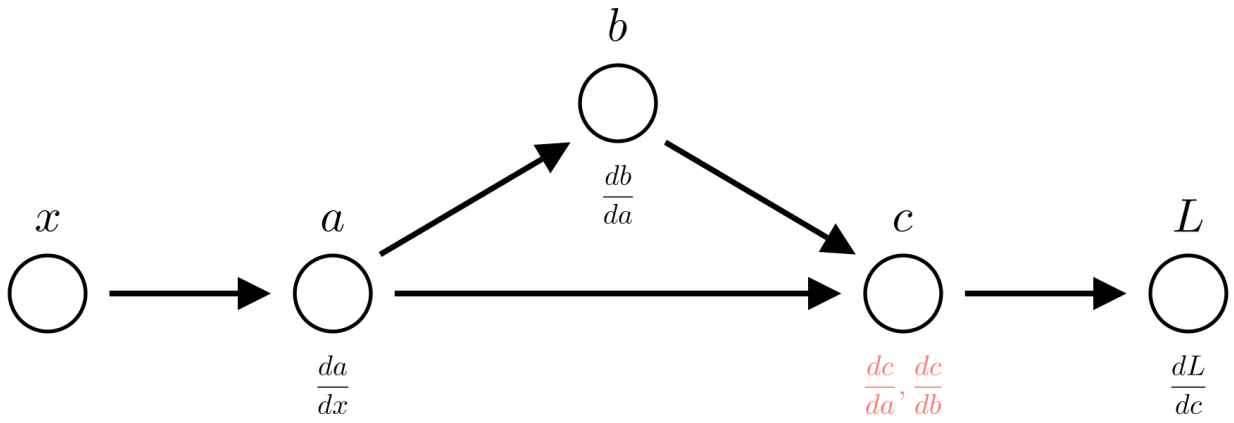
Partial derivatives revisited

$$a = x^2$$

$$b = 5a$$

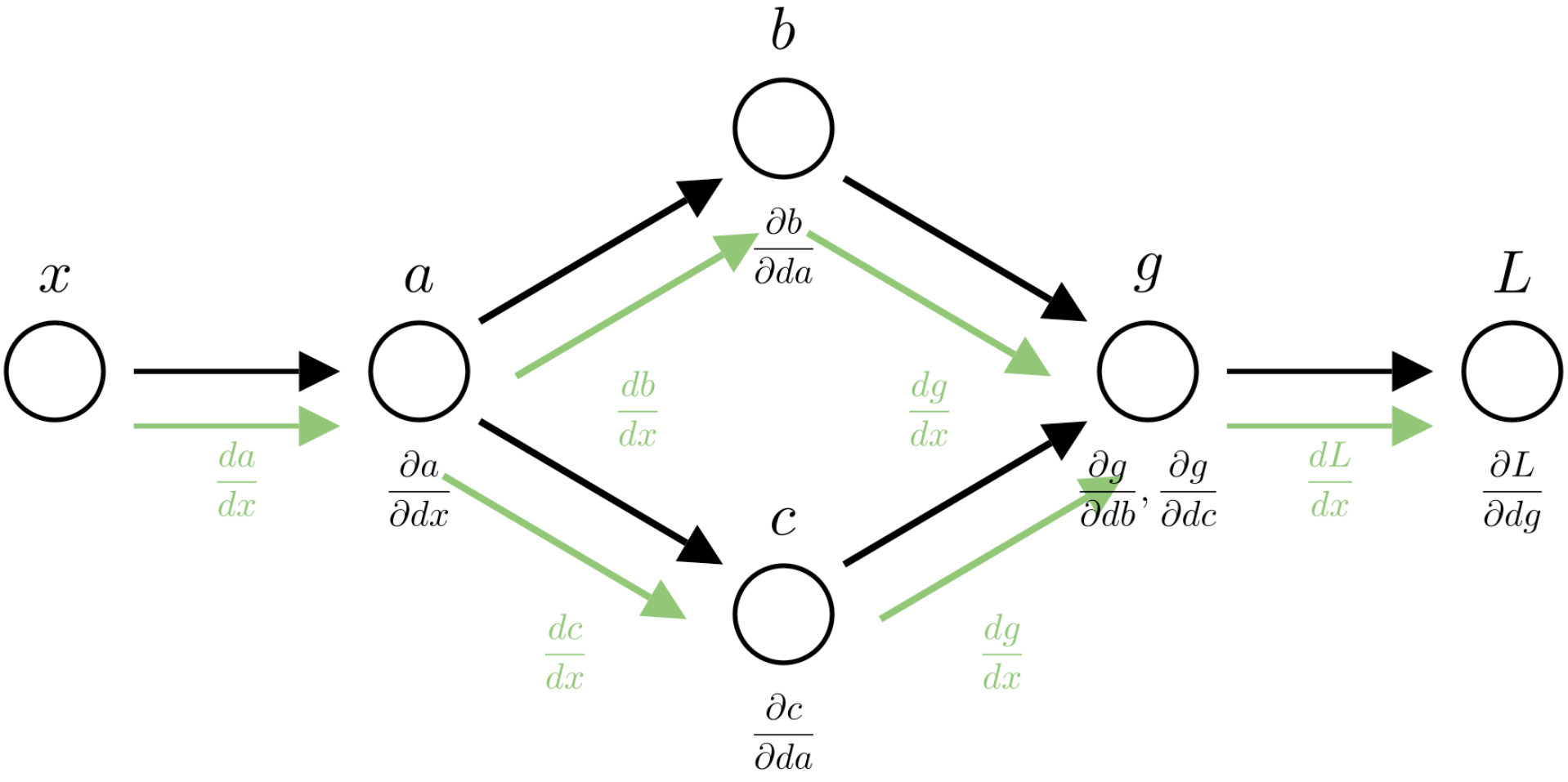
$$c = ab$$

$$L = -c$$

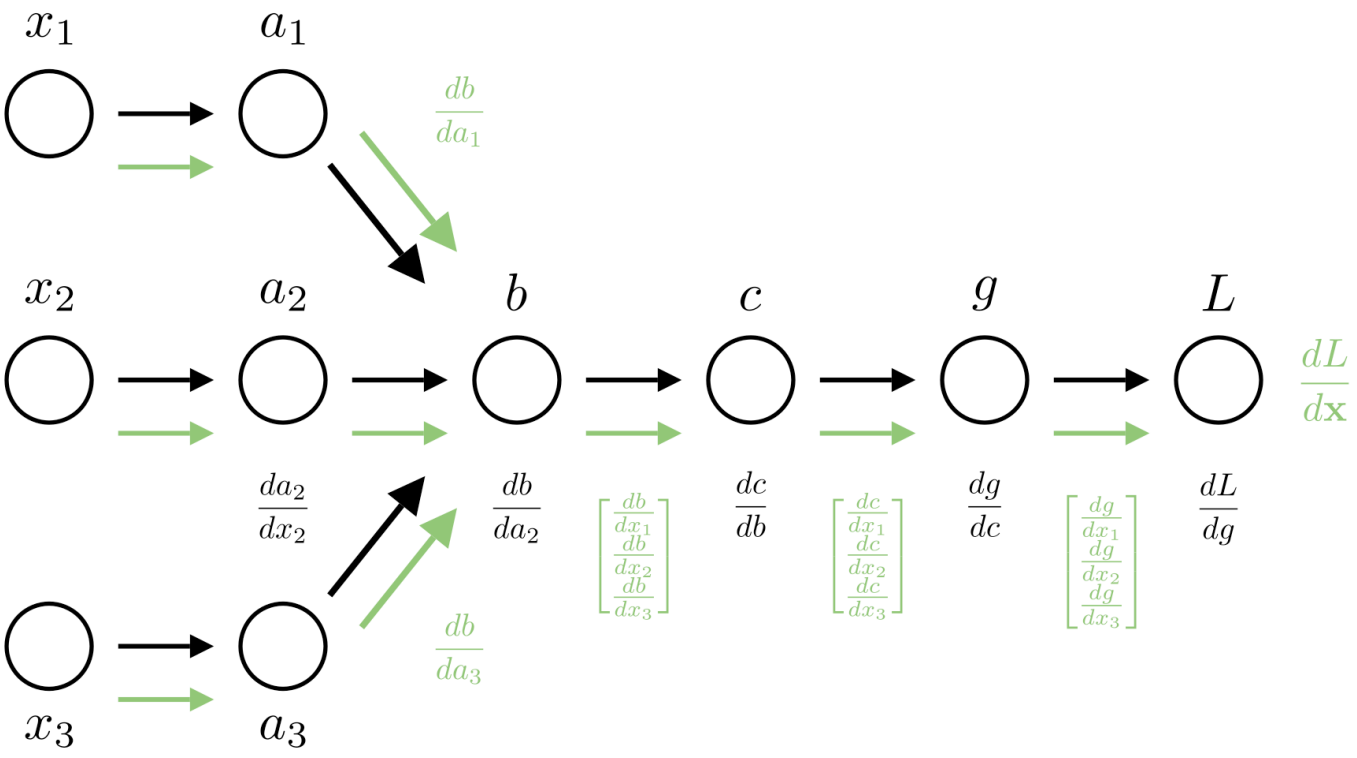


$$\frac{dc}{da} = \frac{\partial c}{\partial a} + \frac{\partial c}{\partial b}\frac{\partial b}{\partial a} = 5a + 5a = 10a$$

Partial derivatives revisited

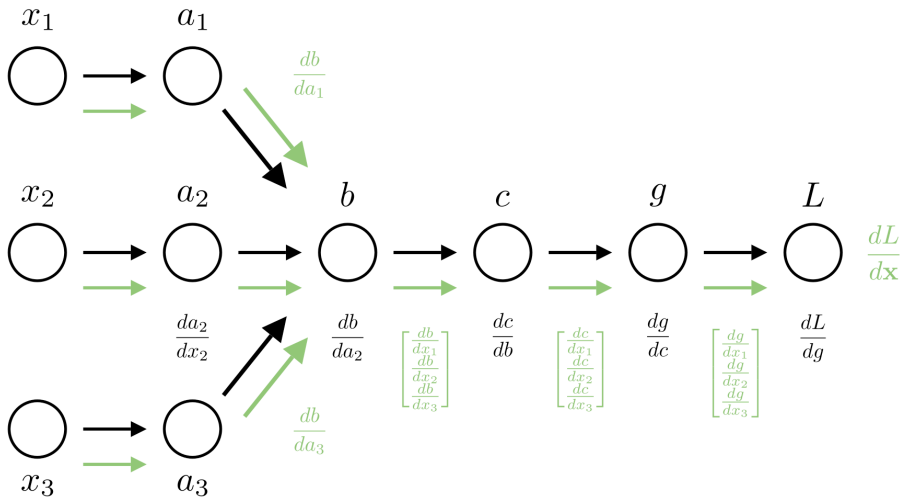


Implementing automatic differentiation



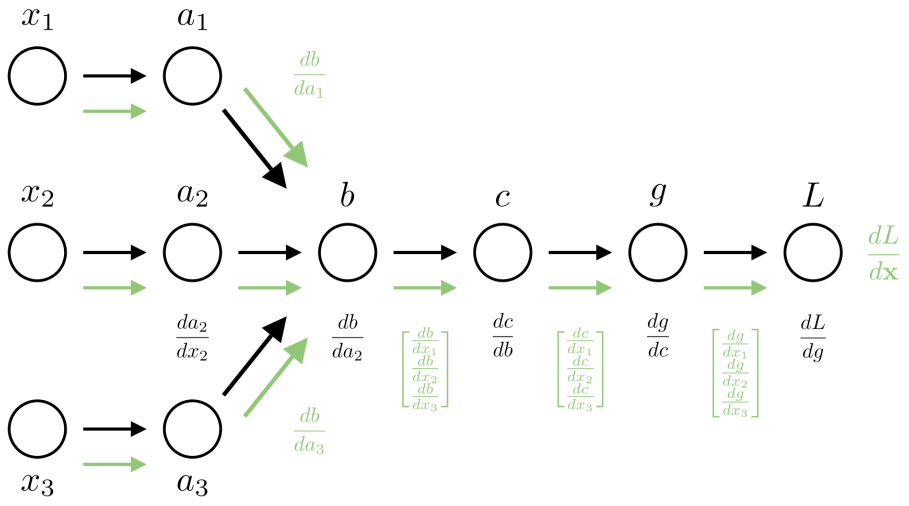
Implementing automatic differentiation

```python
class ForwardValue:
    '''
    Base class for automatic differentiation operations. Represents variable delcaration.
    Subclasses will overwrite func and grads to define new operations.

    Properties:
        parent_values    (list): A list of raw values of each input (as floats)
        value   (float): The value of the result of this operation
        forward_grads (dict): A dictionary mapping inputs to gradients
    '''

    def __init__(self, *args):
        self.parent_values = [arg.value if isinstance(arg, ForwardValue) else arg for arg in args]
        self.value = self.forward_pass(args)

        if len(self.forward_grads.keys()) == 0:
            self.forward_grads = {self: 1}


    def func(self, input):
        '''
        Compute the value of the operation given the inputs.
        For declaring a variable, this is just the identity function (return the input).

        Args:
            input (float): The input to the operation
        Returns:
            value (float): The result of the operation
        '''
        return input

    def grads(self, *args):
        '''
        Compute the derivative of the operation with respect to each input.
        In the base case the derivative of the identity function is just 1. (da/da = 1).

        Args:
            input (float): The input to the operation
        Returns:
            grads (tuple): The derivative of the operation with respect to each input
                           Here there is only a single input, so we return a length-1 tuple.
        '''
        return (1,)

    def forward_pass(self, args):
        # Calls func to compute the value of this operation
        self.forward_grads = {}
        return self.func(*self.parent_values)
```



Implementing automatic differentiation

```python
class _add(ForwardValue):
    # Addition operator (a + b)
    def func(self, a, b):
        return a + b

    def grads(self, a, b):
        return 1., 1.

class _neg(ForwardValue):
    # Negation operator (-a)
    def func(self, a):
        return -a

    def grads(self, a):
        return (-1.,)

class _sub(ForwardValue):
    # Subtraction operator (a - b)
    def func(self, a, b):
        # Your code here

    def grads(self, a, b):
        # Your code here
```



Calculus for vectors (Jacobian)

Now let's consider a vector-valued function $f: \mathbb{R}^n \to \mathbb{R}^m$

e.g. $f(x_1, x_2, \ldots, x_n) = (y_1, y_2, \ldots, y_m)$

We define the instantaneous rate of change via the **Jacobian matrix**, whose entries are **partial derivatives**

$$\frac{\partial f}{\partial x} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \frac{\partial y_m}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix}$$

The Jacobian is also called the **derivative** of f. It is a $m \times n$ matrix

Each partial derivative fixes the other inputs and treats f as scalar-input scalar-output

Calculus for vectors (Jacobian)

$d \times d$ matrix

$$\mathbf{y} = \mathbf{A}\mathbf{x}$$

$\mathbf{y}$: output, $\mathbf{x}$: inputs

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = A$$

A: Jacobian

$$\frac{\partial y_i}{\partial x_j} = \frac{\partial}{\partial x_j} \sum_{k=1}^{d} A_{ik} x_k$$

0 if $k \neq j$

$$\frac{\partial y_i}{\partial x_j} = A_{ij}$$

Calculus for vectors (Jacobian)

d-length vector

d-length vector

$$\mathbf{y} = \mathbf{x}^2$$

$$\frac{\partial y_1}{\partial x_1} = 2x_1$$

d

$$Y = \begin{bmatrix} x_1^2 \\ x_2^2 \\ x_3^2 \\ \vdots \end{bmatrix}$$

$$\frac{\partial y_i}{\partial x_j} = 0 \quad \text{if } i \neq j$$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = d \begin{bmatrix} 2x_1 & 0 & 0 & 0 & 0 \\ 0 & 2x_2 & 0 & 0 & 0 \\ 0 & 0 & 2x_3 & 0 & \checkmark \\ 0 & 0 & & & \end{bmatrix}$$

0

Jacobians and gradients

Scalar output: $f(\vec{x}) \rightarrow \mathbb{R}$, $\vec{x} \in \mathbb{R}^d$

$f: \mathbb{R}^n \rightarrow \mathbb{R}^m$

When $m = 1$, (scalar-valued output) the Jacobian is called the **gradient**

$$\frac{\partial f}{\partial x} = \left[\frac{\partial y}{\partial x_1} \quad \frac{\partial y}{\partial x_2} \quad \dots \quad \frac{\partial y}{\partial x_n}\right] = \nabla_{\vec{x}} f$$

Notes:

- The Jacobian of a scalar-valued function is a row vector.
- The gradient is often described as a column vector

Chain rule for Jacobians

$f \circ g : \mathbb{R}^n \to \mathbb{R}^m$

$x \in \mathbb{R}^n \xrightarrow{g} g(x) \in \mathbb{R}^k \xrightarrow{f} f(g(x)) \in \mathbb{R}^m$

An easy extension of the chain rule exists:

Given $f: \mathbb{R}^k \to \mathbb{R}^m$ and $g: \mathbb{R}^n \to \mathbb{R}^k$

$f(g(x))$

$$\underbrace{\frac{\partial f(g(x))}{\partial x}}_{m \times n} = \underbrace{\frac{\partial f(y)}{\partial y}}_{m \times k} \cdot \underbrace{\frac{\partial g(x)}{\partial x}}_{k \times n}$$

Where $y = g(x)$.

$f(g(x))' = f'(g(x))\, g'(x)$

$\frac{df}{dy} \cdot \frac{dg}{dx}$

Forward-mode with vectors

MSE for linear regression

X: $N \times d$ matrix, y: N vector

w: d vector

Want: $\frac{\partial L}{\partial w} = ?$

$$\mathbf{a} = \mathbf{X}\mathbf{w} \qquad \frac{\partial a}{\partial w} = X$$

$$\mathbf{b} = \mathbf{y} - \mathbf{a} \qquad \frac{\partial b}{\partial a} = -1$$

$b = (y - Xw)$

$$\mathbf{c} = \mathbf{b}^2 \qquad \frac{\partial c}{\partial b} = 2b$$

$$g = \sum_{i=1}^{N} c_i \qquad \frac{\partial g}{\partial c} = 1$$

$$L = \frac{1}{N} g \qquad \frac{\partial L}{\partial g} = \frac{1}{N}$$

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial g} \cdot \frac{\partial g}{\partial c} \cdot \frac{\partial c}{\partial b} \cdot \frac{\partial b}{\partial a} \cdot \frac{\partial a}{\partial w}$$

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$\begin{bmatrix} 2b_1 & 0 & 0 \\ 0 & 2b_2 & 0 \\ 0 & 0 & 2b_3 \end{bmatrix}$$

$$\frac{\partial L}{\partial c_1}$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}$$

X: N×d
w: d
y: N

Forward-mode with vectors

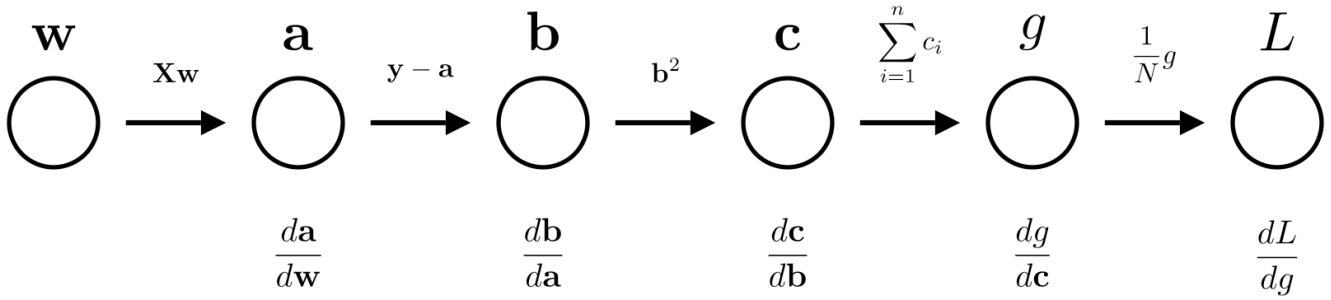
$$\mathbf{a} = \mathbf{X}\mathbf{w}$$

$$\mathbf{b} = \mathbf{y} - \mathbf{a}$$

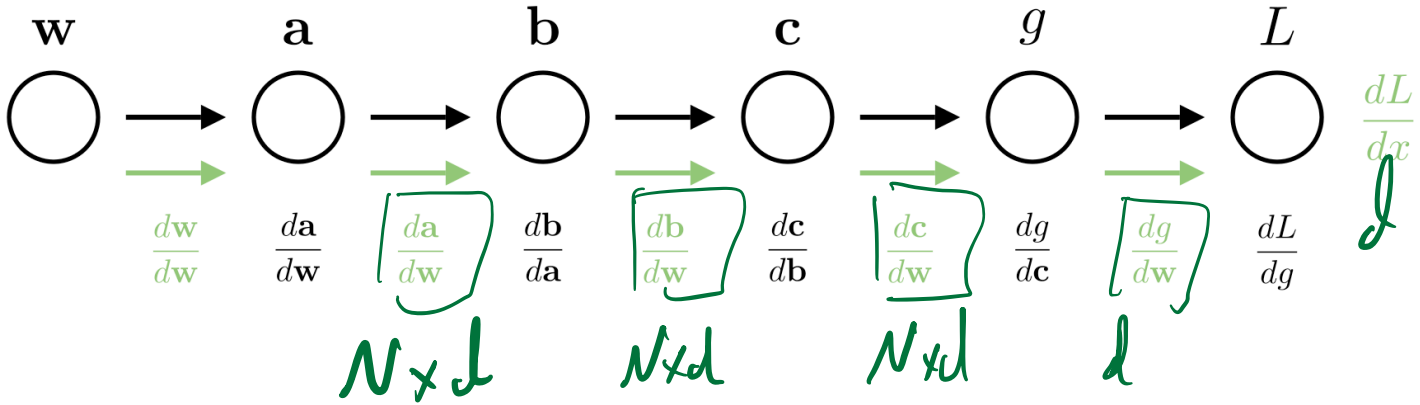
$$\mathbf{c} = \mathbf{b}^2$$

$$g = \sum_{i=1}^{N} c_i$$

$$L = \frac{1}{N} g$$



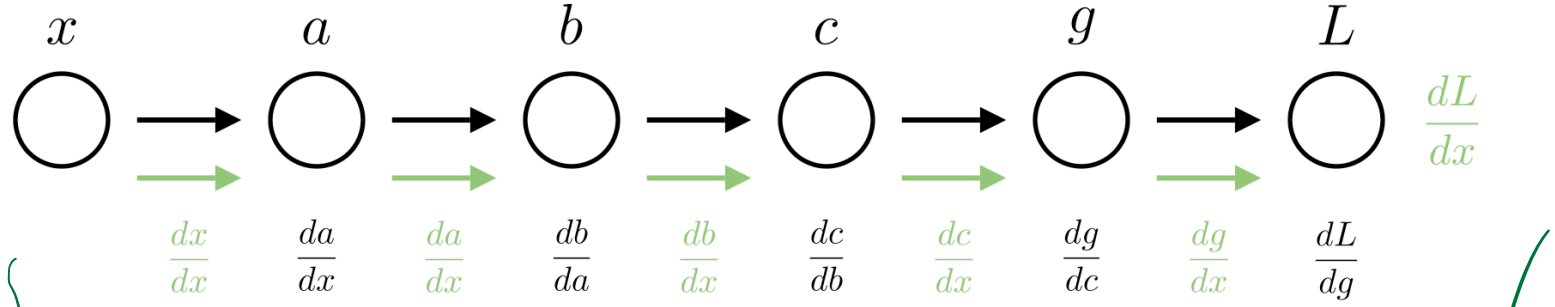
Forward mode



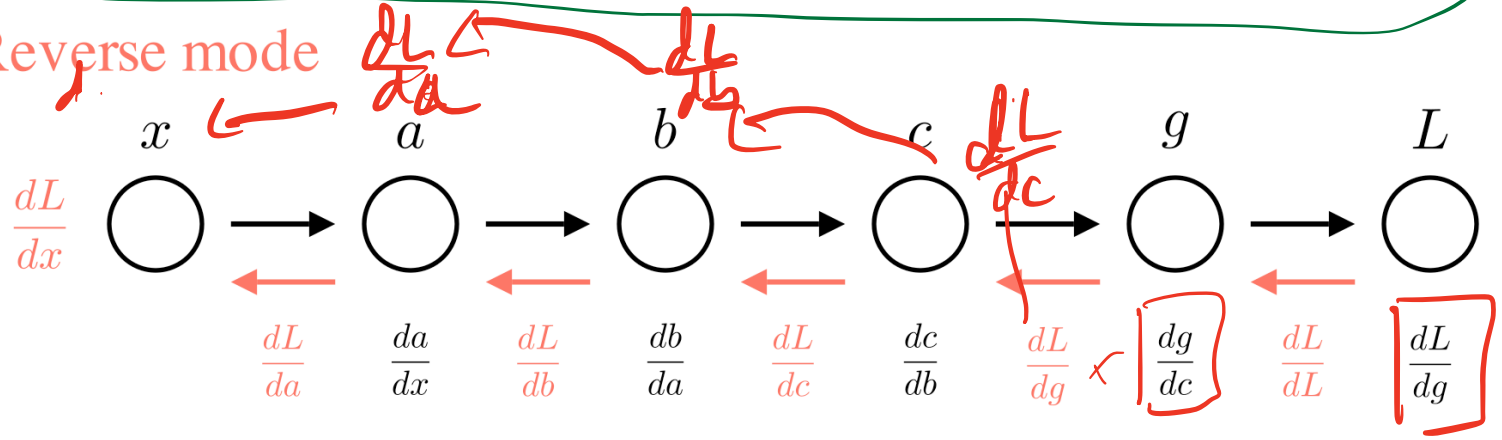
Reverse-mode AD

$$\frac{dL}{dx} = \frac{da}{dx}\cdot\frac{db}{da}\cdot\frac{dc}{db}\cdot\frac{dg}{dc}\cdot\frac{dL}{dg}$$

Forward mode

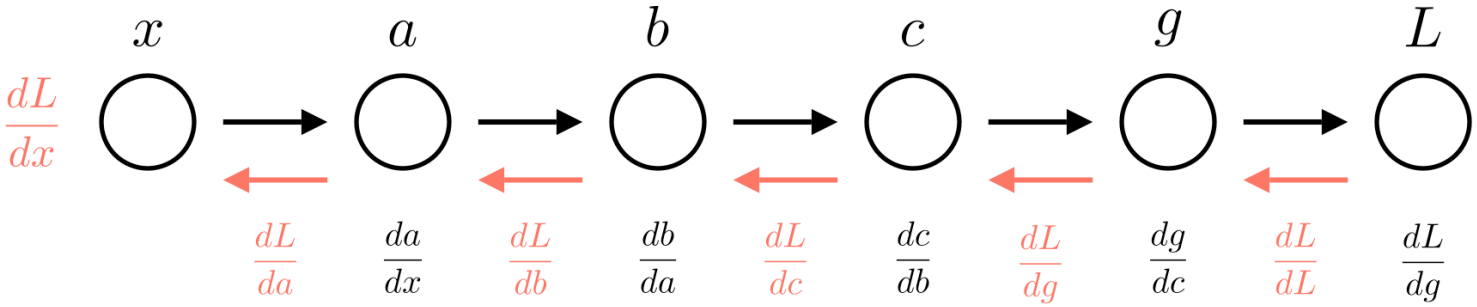


Reverse mode



Reverse mode

Reverse-mode AD



Define inputs

```
a = AutogradValue(5)
b = AutogradValue(2)
```

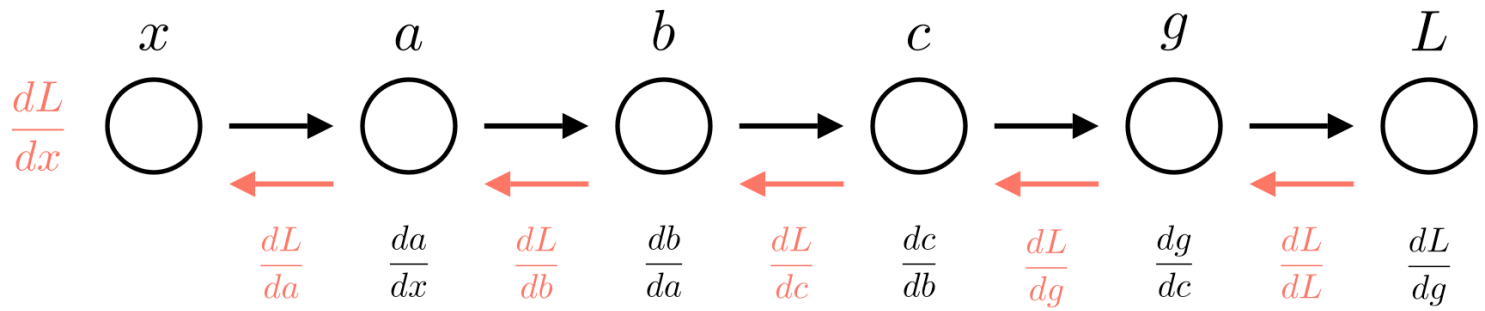
Compute operations

```
c = a + b
L = log(c)
```

Get derivatives

```
L.backward()
dL_da = a.grad
```

Reverse-mode AD



Define inputs

```
a = AutogradValue(5)
b = AutogradValue(2)
```

Compute operations

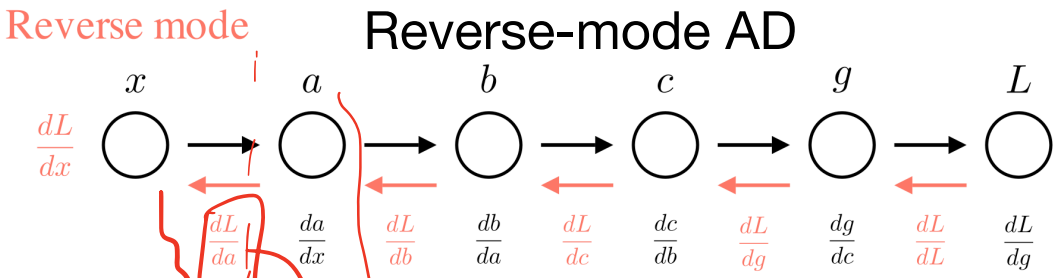
```
c = a + b
L = log(c)
```

Get derivatives

```
L.backward()
dL_da = a.grad
```

Operations with non-Autograd values

```
s = 4
L = s * a
dL_da = a.grad # Will work because a is an AutogradValue
dL_ds = s.grad # Will give an error because s is not an AutogradValue
```



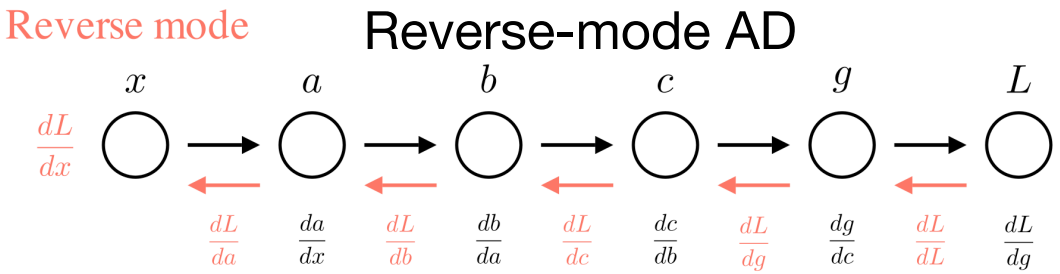

```python
class AutogradValue:
    '''
    Base class for automatic differentiation operations.
    Represents variable delcaration. Subclasses will overwrite
    func and grads to define new operations.

    Properties:
        parents (list):  A list of the inputs to the operation,
                         may be AutogradValue or float
        args    (list):  A list of raw values of each
                         input (as floats)
        grad    (float): The derivative of the final loss with
                         respect to this value (dL/da)
        value   (float): The value of the result of this operation
    '''

    def __init__(self, *args):
        self.parents = list(args)
        self.args = [arg.value if isinstance(arg, AutogradValue)
                     else arg
                     for arg in self.parents]
        self.grad = 0.
        self.value = self.forward_pass()

    def forward_pass(self):
        # Calls func to compute the value of this operation
        return self.func(*self.args)
```

$c = a + b$

a b

c

$\frac{dc}{da}$ $\frac{dc}{dg}$




```
class AutogradValue:
    '''
    Base class for automatic differentiation operations.
    Represents variable delcaration. Subclasses will overwrite
    func and grads to define new operations.

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                         may be AutogradValue or float
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                         input (as floats)
        grad    (float): The derivative of the final loss with
                         respect to this value (dL/da)
        value   (float): The value of the result of this operation
    '''

    def __init__(self, *args):
        self.parents = list(args)
        self.args = [arg.value if isinstance(arg, AutogradValue)
                     else arg
                     for arg in self.parents]
        self.grad = 0.
        self.value = self.forward_pass()

    def forward_pass(self):
        # Calls func to compute the value of this operation
        return self.func(*self.args)
```

Base class (input)

```
class AutogradValue:
    def func(self, input):
        '''
        Compute the value of the operation given the inputs.
        For declaring a variable, this is just the identity
        function (return the input).

        Args:
            input (float): The input to the operation
        Returns:
            value (float): The result of the operation
        '''
        return input
```

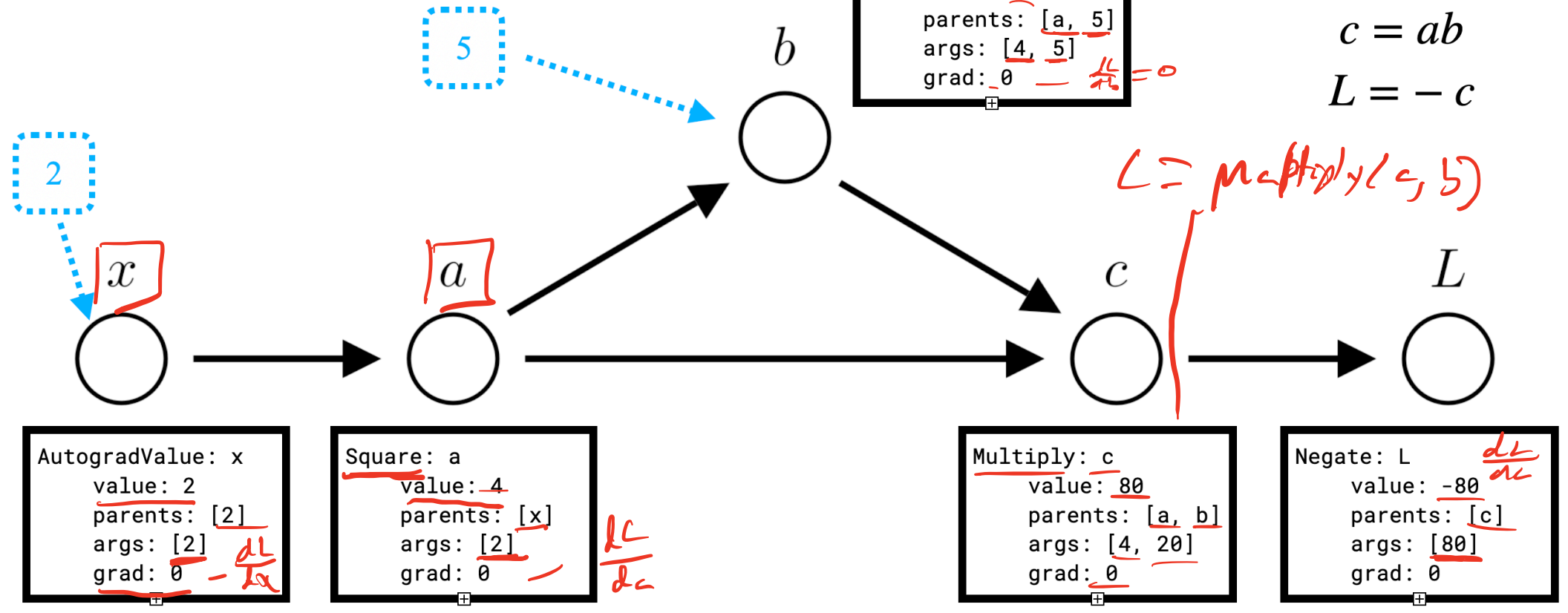
Sub-class (operation)

```
class _square(AutogradValue):
    # Square operator (a ** 2)
    def func(self, a):
        return a ** 2
```

```
x = AutogradValue(2)
a = x ** 2
b = 5 * a
c = b * a
L = -c
```

Forward pass

$$x = 2$$
$$a = x^2$$
$$b = 5a$$
$$c = ab$$
$$L = -c$$

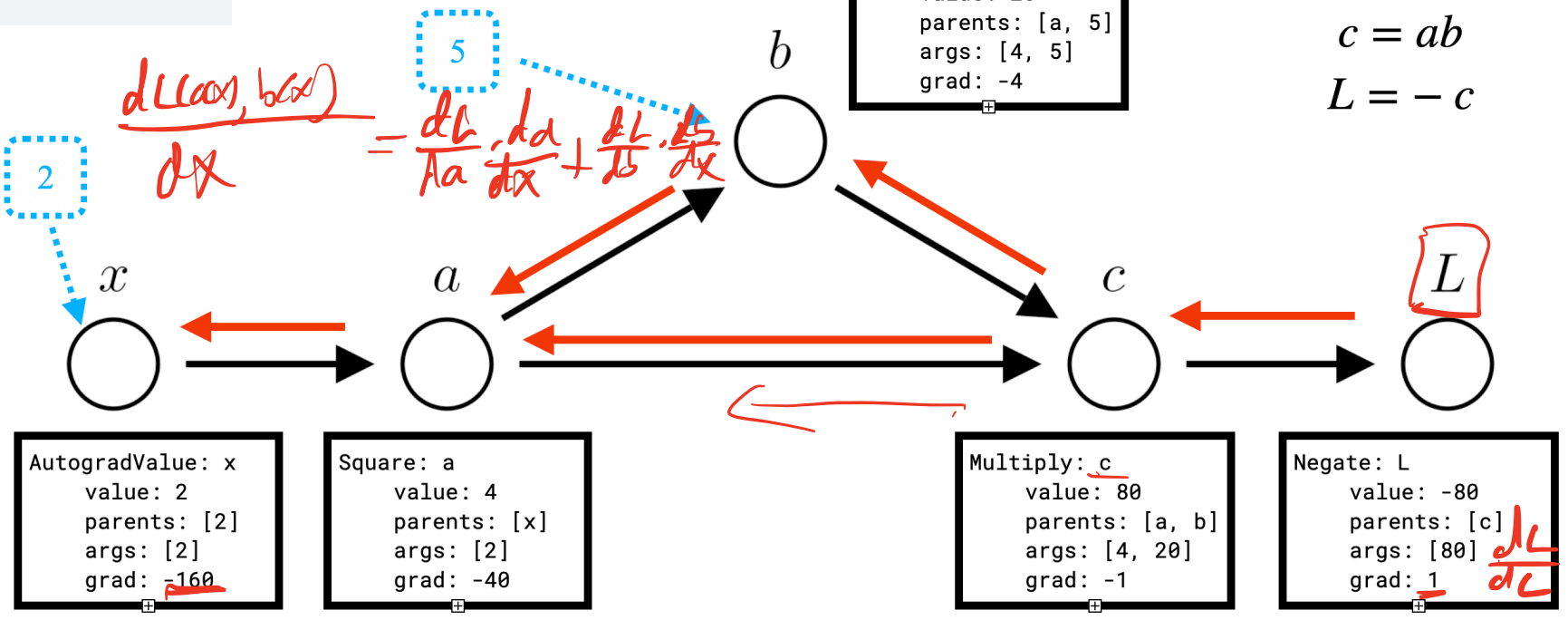


```
x = AutogradValue(2)
a = x ** 2
b = 5 * a
c = b * a
L = -c
```

```
L.backward()
print('dL_dx', x.grad)
```

Backward pass

$$x = 2$$
$$a = x^2$$
$$b = 5a$$
$$c = ab$$
$$L = -c$$



$\frac{dL}{dx} = -160$

5: $\frac{dL}{dx} = \frac{dL}{da}\frac{da}{dx} = -40 \cdot 4$

4: $\frac{dL}{da} = \frac{dL}{dc}\frac{dc}{da} + \frac{dL}{db}\frac{db}{da} = -1 \cdot 20 + -4 \cdot 5 = -40$

2: $\frac{dL}{dc} = -1$

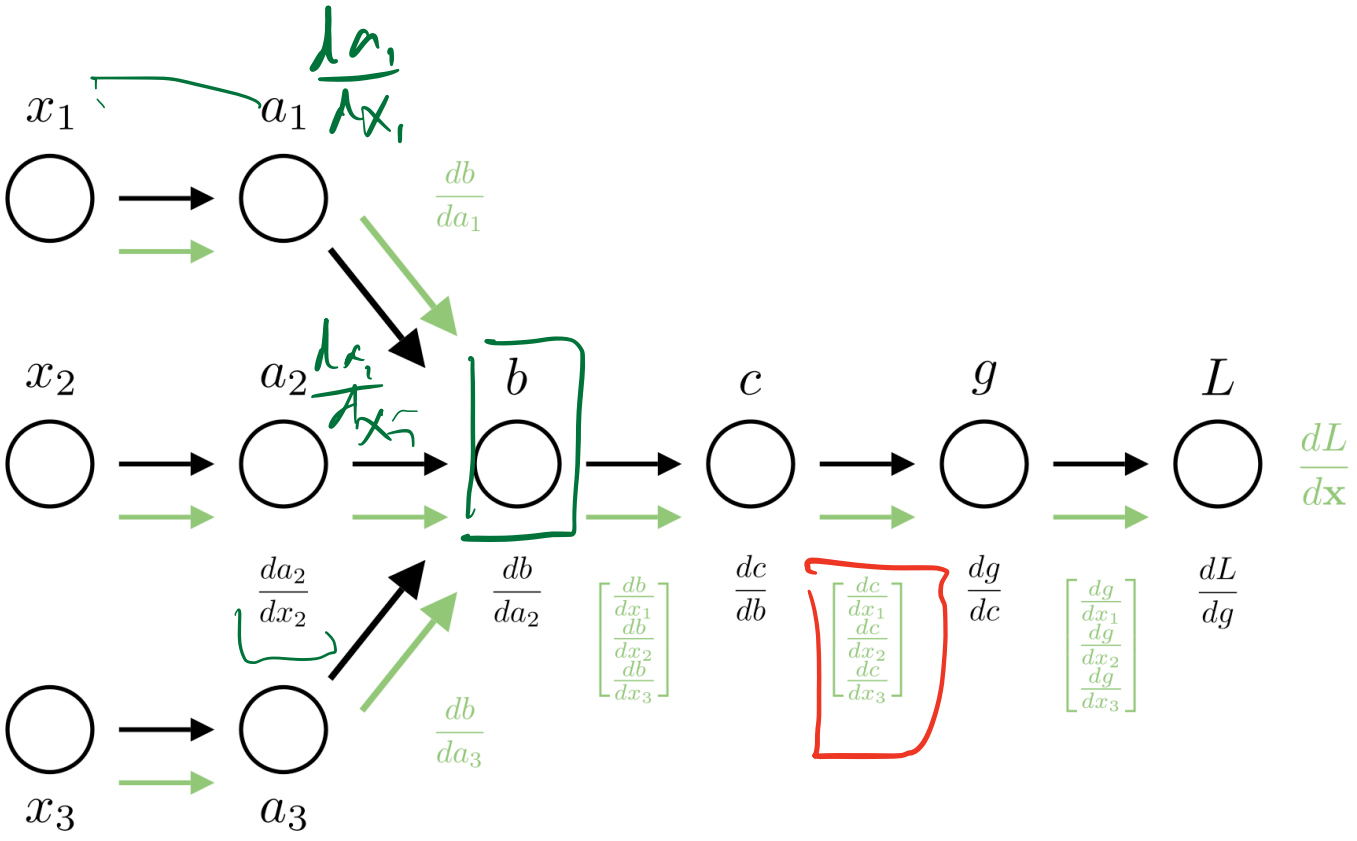
3: $\frac{dL}{db} = \frac{dL}{dc}\frac{dc}{db} = -1 \cdot 4$

1: $\frac{dL}{dL} = 1$

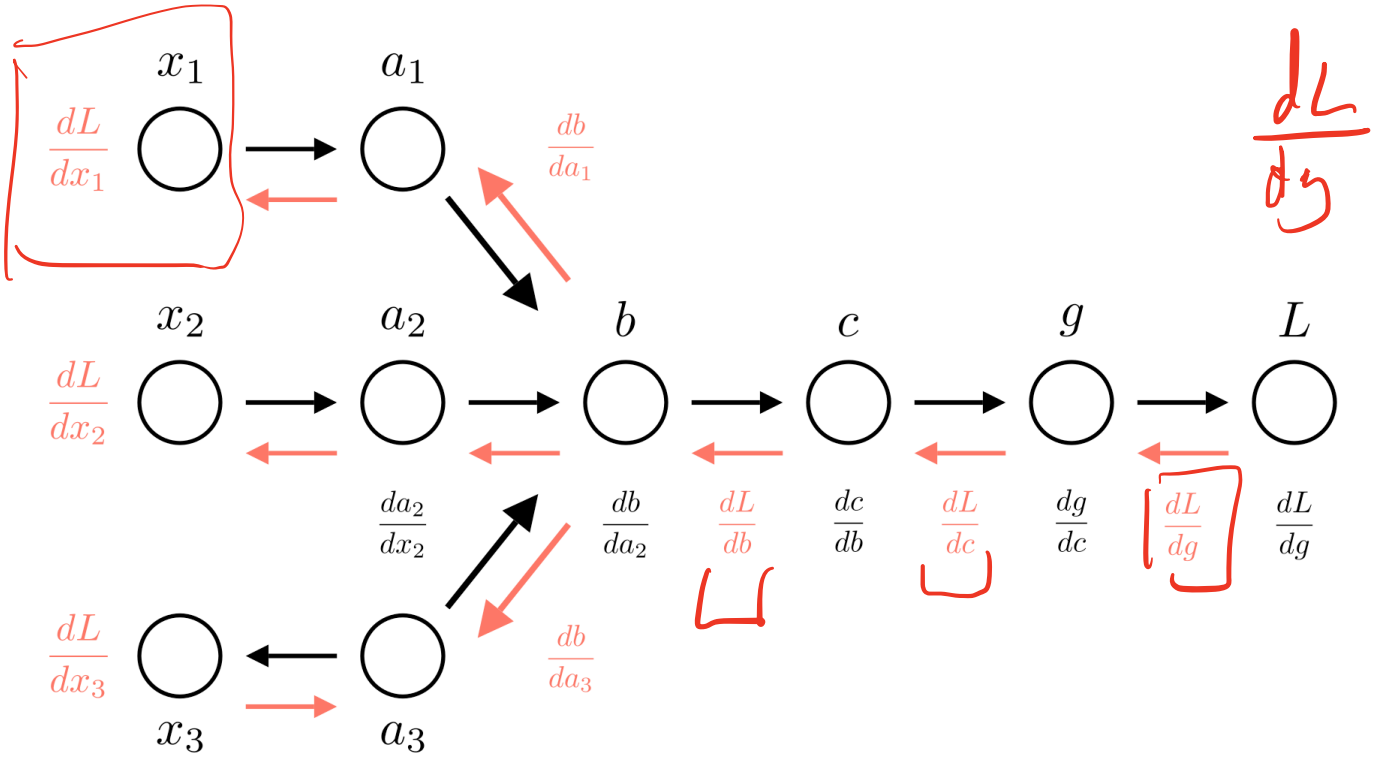
Backward pass

```
class AutogradValue:
        def grads(self, *args):
        '''
        Compute the derivative of the operation with respect to each input.
        In the base case the derivative of the identity function is just 1. (da/da = 1).

        Args:
            input (float): The input to the operation
        Returns:
            grads (tuple): The derivative of the operation with respect to each input
                           Here there is only a single input, so we return a length-1 t
        '''
        return (1,)

class _square(AutogradValue):
    # Square operator (a ** 2)
    def grads(self, a):
        return (2 * a,)
```

Why reverse mode?



Why reverse mode?



Reverse-mode with vectors

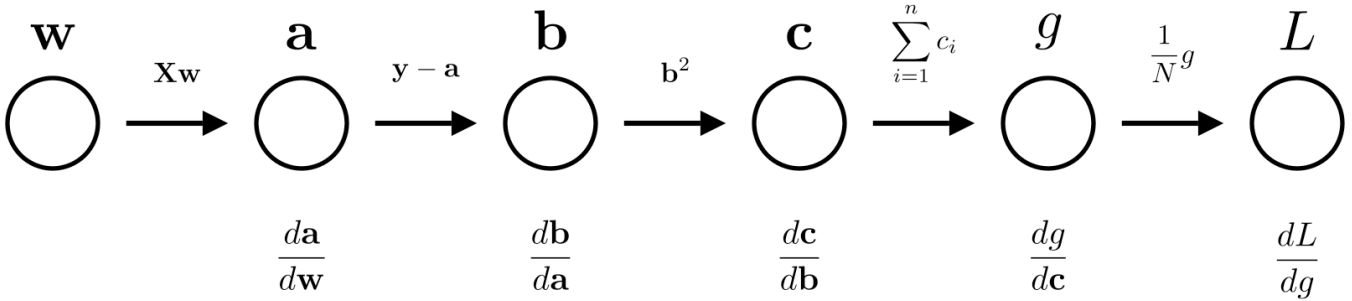
$$\mathbf{a} = \mathbf{X}\mathbf{w}$$

$$\mathbf{b} = \mathbf{y} - \mathbf{a}$$

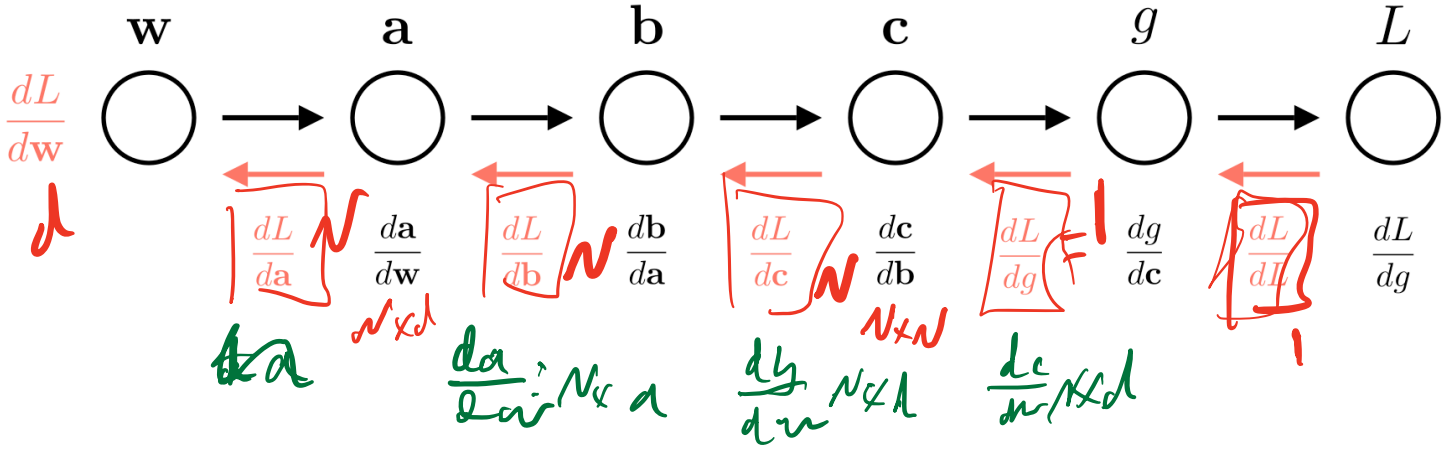
$$\mathbf{c} = \mathbf{b}^2$$

$$g = \sum_{i=1}^{N} c_i$$

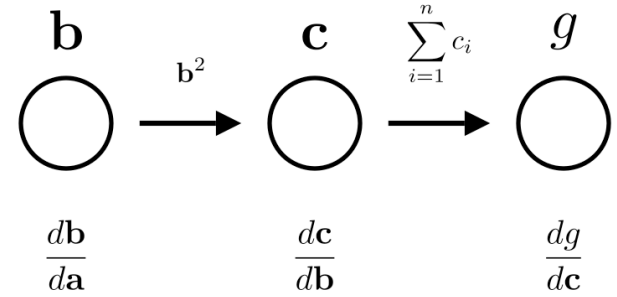
$$L = \frac{1}{N} g$$



Reverse mode

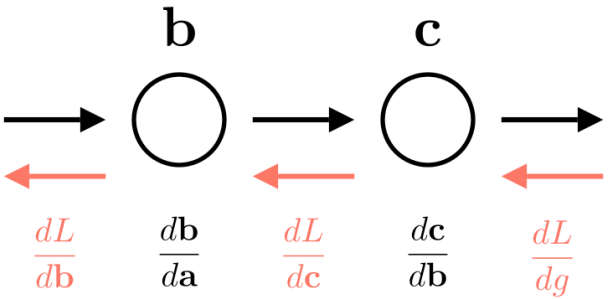


Jacobian computation



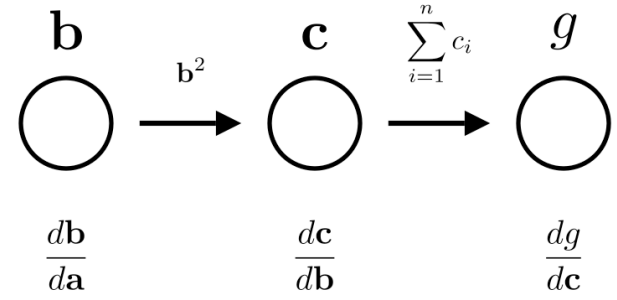
$$\mathbf{c} = \mathbf{b}^2, \quad \mathbb{R}^n \to \mathbb{R}^n$$

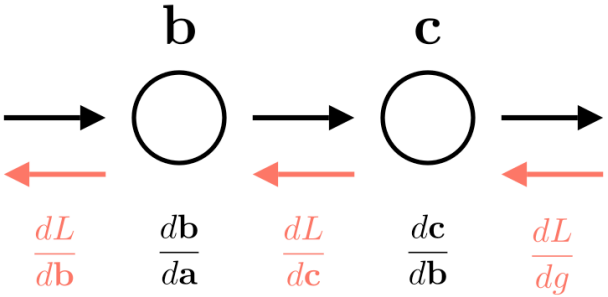
$$\frac{d\mathbf{c}}{d\mathbf{b}} =$$



$$\frac{dL}{d\mathbf{b}} = \frac{dL}{d\mathbf{c}}\frac{d\mathbf{c}}{d\mathbf{b}} =$$

Jacobian computation



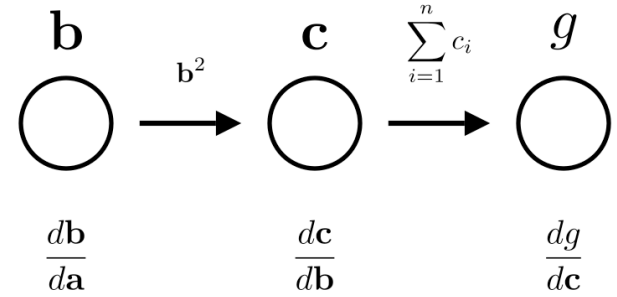


$$\mathbf{c} = \mathbf{b}^2, \quad \mathbb{R}^n \to \mathbb{R}^n$$

$$\frac{d\mathbf{c}}{d\mathbf{b}} = \begin{bmatrix} \frac{\partial c_1}{\partial b_1} & 0 & \dots & 0 \\ 0 & \frac{\partial c_2}{\partial b_2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \frac{\partial c_N}{\partial b_d} \end{bmatrix}$$

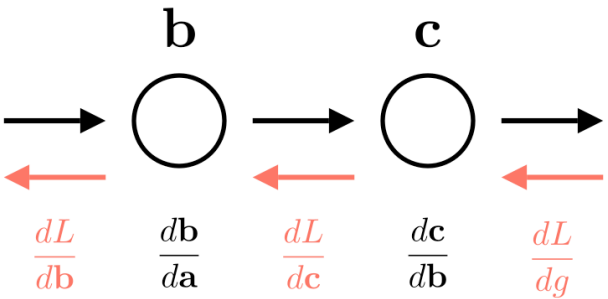
$$\frac{dL}{d\mathbf{b}} = \frac{dL}{d\mathbf{c}} \frac{d\mathbf{c}}{d\mathbf{b}} =$$

Vector-Jacobian Product



$$\mathbf{c} = \mathbf{b}^2, \quad \mathbb{R}^n \to \mathbb{R}^n$$

$$\frac{d\mathbf{c}}{d\mathbf{b}} = \begin{bmatrix} \frac{\partial c_1}{\partial b_1} & 0 & \dots & 0 \\ 0 & \frac{\partial c_2}{\partial b_2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \frac{\partial c_N}{\partial b_d} \end{bmatrix}$$



$$\frac{dL}{d\mathbf{b}} = \frac{dL}{d\mathbf{c}}\frac{d\mathbf{c}}{d\mathbf{b}} = \begin{bmatrix} \frac{dL}{dc_1}\frac{dc_1}{db_1} \\ \frac{dL}{dc_2}\frac{dc_2}{db_2} \\ \vdots \\ \frac{dL}{dc_N}\frac{dc_N}{db_N} \end{bmatrix}$$

Jacobian computation

$$\mathbf{a} = \mathbf{X}\mathbf{w}, \qquad \frac{d\mathbf{a}}{d\mathbf{X}}$$

$$\frac{dL}{d\mathbf{X}} = \frac{dL}{d\mathbf{a}}^{T} \frac{d\mathbf{a}}{d\mathbf{X}}$$

$$\frac{dL}{dX_{jk}} = \sum_{i=1}^{N} \frac{\partial L}{\partial a_i} \frac{\partial a_i}{\partial X_{jk}}$$

Jacobian computation

$$\mathbf{a} = \mathbf{X}\mathbf{w}, \qquad \frac{d\mathbf{a}}{d\mathbf{X}}$$

$$\frac{dL}{d\mathbf{X}} = \frac{dL}{d\mathbf{a}}^{T} \frac{d\mathbf{a}}{d\mathbf{X}}$$

$$\frac{dL}{dX_{jk}} = \sum_{i=1}^{N} \frac{\partial L}{\partial a_i} \frac{\partial a_i}{\partial X_{jk}}$$

```
dL_da, da_dx  # The computed gradients/jacobians
da_dx = da_dx.reshape((da_dx.shape[0], -1))
dL_dx = np.dot(dL_da, da_dx)
dL_dx = dL_dx.reshape(x.shape)
```

Jacobian computation

$$\mathbf{a} = \mathbf{X}\mathbf{w}, \quad \frac{d\mathbf{a}}{d\mathbf{X}}$$

$$\frac{dL}{d\mathbf{X}} = \frac{dL}{d\mathbf{a}}^T \frac{d\mathbf{a}}{d\mathbf{X}}$$

$$\frac{dL}{dX_{jk}} = \sum_{i=1}^{N} \frac{\partial L}{\partial a_i} \frac{\partial a_i}{\partial X_{jk}}$$

$$\mathbf{a} = \mathbf{X}\mathbf{w}, \quad \frac{d\mathbf{a}}{d\mathbf{X}}$$

$$a_i = \sum_{k=1}^{d} X_{ik} w_k$$

$$\frac{\partial a_i}{\partial X_{jk}} = \frac{\partial}{\partial X_{jk}} \sum_{k=1}^{d} X_{ik} w_k = \mathbb{I}(i=j) w_k$$

$$\frac{\partial L}{\partial X_{ik}} = \frac{\partial L}{\partial a_i} \frac{\partial a_i}{\partial X_{ik}} = \frac{\partial L}{\partial a_i} w_k$$

Jacobian computation

```
w_mat = w.reshape((1, -1)) # reshape w to 1 x d
dL_da_mat = dL_da.reshape((-1, 1)) # reshape dL_da to N x 1
dL_dx = w_mat * dL_da_mat # dL_dx becomes N x d, entry ik = dL_da_i * w_k
```

```
dL_da, da_dx  # The computed gradients/jacobians
da_dx = da_dx.reshape((da_dx.shape[0], -1))
dL_dx = np.dot(dL_da, da_dx)
dL_dx = dL_dx.reshape(x.shape)
```

$$\mathbf{a} = \mathbf{X}\mathbf{w}, \qquad \frac{d\mathbf{a}}{d\mathbf{X}}$$

$$a_i = \sum_{k=1}^{d} X_{ik} w_k$$

$$\frac{\partial a_i}{\partial X_{jk}} = \frac{\partial}{\partial X_{jk}} \sum_{k=1}^{d} X_{ik} w_k = \mathbb{I}(i=j) w_k$$

$$\frac{\partial L}{\partial X_{ik}} = \frac{\partial L}{\partial a_i} \frac{\partial a_i}{\partial X_{ik}} = \frac{\partial L}{\partial a_i} w_k$$

Vector-Jacobian products

$$f(\mathbf{x}) = \mathbf{x} + \mathbf{a}$$

$$\mathbf{v}^T \frac{d\mathbf{f}}{d\mathbf{x}} =$$

$$f(\mathbf{x}) = \log \mathbf{x}$$

$$\mathbf{v}^T \frac{d\mathbf{f}}{d\mathbf{x}} =$$