



# 向量链式法则

- 标量链式法则

$$y = f(u), u = g(x) \quad \frac{\partial y}{\partial x} = \frac{\partial y}{\partial u} \frac{\partial u}{\partial x}$$

- 拓展到向量

$$\begin{array}{ccc} \frac{\partial y}{\partial \mathbf{x}} = \frac{\partial y}{\partial u} \frac{\partial u}{\partial \mathbf{x}} & \frac{\partial y}{\partial \mathbf{x}} = \frac{\partial y}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}} & \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial \mathbf{y}}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}} \\ (1, n) \quad (1,) \quad (1, n) & (1, n) \quad (1, k) \quad (k, n) & (m, n) \quad (m, k) \quad (k, n) \end{array}$$

# 例子 1

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

假设  $\mathbf{x}, \mathbf{w} \in \mathbb{R}^n, \quad y \in \mathbb{R}$

$$z = (\langle \mathbf{x}, \mathbf{w} \rangle - y)^2$$

计算

$$\begin{aligned} \frac{\partial z}{\partial \mathbf{w}} &= \frac{\partial z}{\partial b} \frac{\partial b}{\partial a} \frac{\partial a}{\partial \mathbf{w}} \\ &= \frac{\partial b^2}{\partial b} \frac{\partial a - y}{\partial a} \frac{\partial \langle \mathbf{x}, \mathbf{w} \rangle}{\partial \mathbf{w}} \end{aligned}$$

$$a = \langle \mathbf{x}, \mathbf{w} \rangle$$



$$= 2b \cdot 1 \cdot \mathbf{x}^T$$

分解

$$b = a - y$$

$$z = b^2$$

$$= 2 (\langle \mathbf{x}, \mathbf{w} \rangle - y) \mathbf{x}^T$$

## 例子 2

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

假设

$$\mathbf{X} \in \mathbb{R}^{m \times n}, \quad \mathbf{w} \in \mathbb{R}^n, \quad \mathbf{y} \in \mathbb{R}^m$$

$$z = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

计算

$$\frac{\partial z}{\partial \mathbf{w}}$$

$$\begin{aligned} \frac{\partial z}{\partial \mathbf{w}} &= \frac{\partial z}{\partial \mathbf{b}} \frac{\partial \mathbf{b}}{\partial \mathbf{a}} \frac{\partial \mathbf{a}}{\partial \mathbf{w}} \\ &= \frac{\partial \|\mathbf{b}\|^2}{\partial \mathbf{b}} \frac{\partial \mathbf{a} - \mathbf{y}}{\partial \mathbf{a}} \frac{\partial \mathbf{X}\mathbf{w}}{\partial \mathbf{w}} \end{aligned}$$

分解

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

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

$$z = \|\mathbf{b}\|^2$$



$$= 2\mathbf{b}^T \times \mathbf{I} \times \mathbf{X}$$

$$= 2(\mathbf{X}\mathbf{w} - \mathbf{y})^T \mathbf{X}$$



# 自动求导

- 自动求导计算一个函数在指定值上的导数
- 它有别于
  - 符号求导

```
In[1]:= D[4 x^3 + x^2 + 3, x]
```

```
Out[1]= 2 x + 12 x^2
```

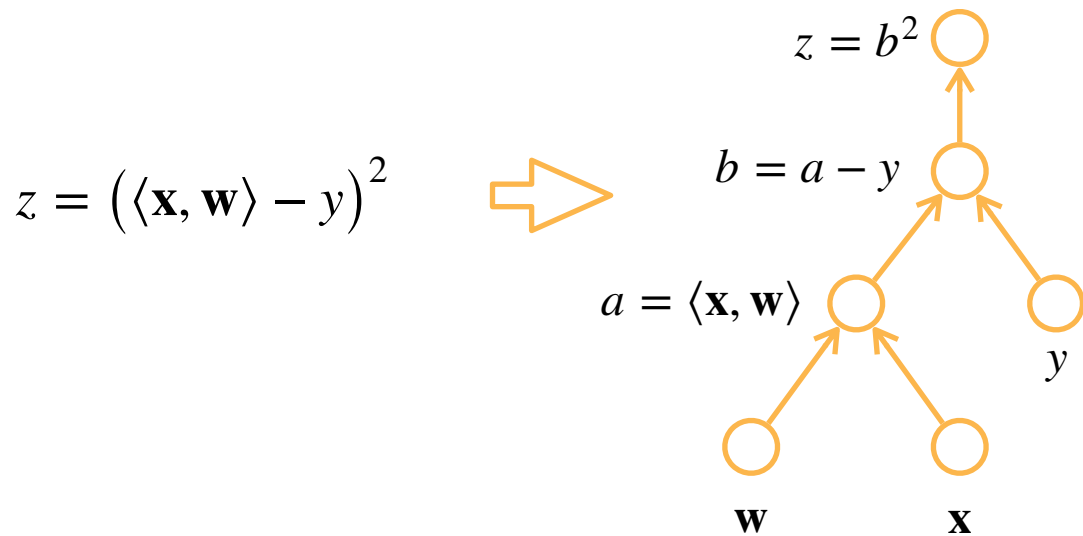
- 数值求导

$$\frac{\partial f(x)}{\partial x} = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$$

# 计算图



- 将代码分解成操作子
- 将计算表示成一个无环图





# 计算图

- 将代码分解成操作子
- 将计算表示成一个无环图
- 显示构造

```
from mxnet import sym
```

```
a = sym.var()
```

```
b = sym.var()
```

```
c = 2 * a + b
```

```
# bind data into a and b later
```



# 计算图

- 将代码分解成操作子
- 将计算表示成一个无环图
- 显式构造
  - Tensorflow/Theano/MXNet
- 隐式构造
  - PyTorch/MXNet

```
from mxnet import autograd, nd
```

```
with autograd.record():  
    a = nd.ones((2,1))  
    b = nd.ones((2,1))  
    c = 2 * a + b
```



# 自动求导的两种模式

- 链式法则:  $\frac{\partial y}{\partial x} = \frac{\partial y}{\partial u_n} \frac{\partial u_n}{\partial u_{n-1}} \cdots \frac{\partial u_2}{\partial u_1} \frac{\partial u_1}{\partial x}$
- 正向累积  $\frac{\partial y}{\partial x} = \frac{\partial y}{\partial u_n} \left( \frac{\partial u_n}{\partial u_{n-1}} \left( \cdots \left( \frac{\partial u_2}{\partial u_1} \frac{\partial u_1}{\partial x} \right) \right) \right)$
- 反向累积、又称反向传递

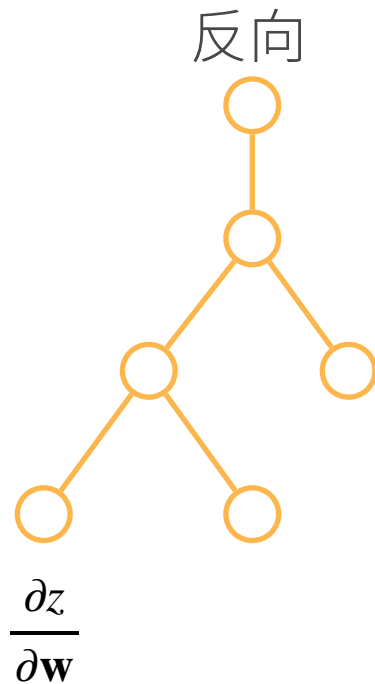
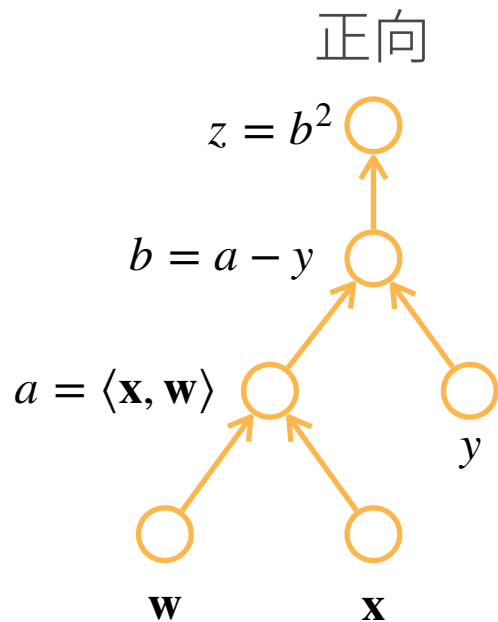
$$\frac{\partial y}{\partial x} = \left( \left( \left( \frac{\partial y}{\partial u_n} \frac{\partial u_n}{\partial u_{n-1}} \right) \cdots \right) \frac{\partial u_2}{\partial u_1} \right) \frac{\partial u_1}{\partial x}$$



# 反向累积



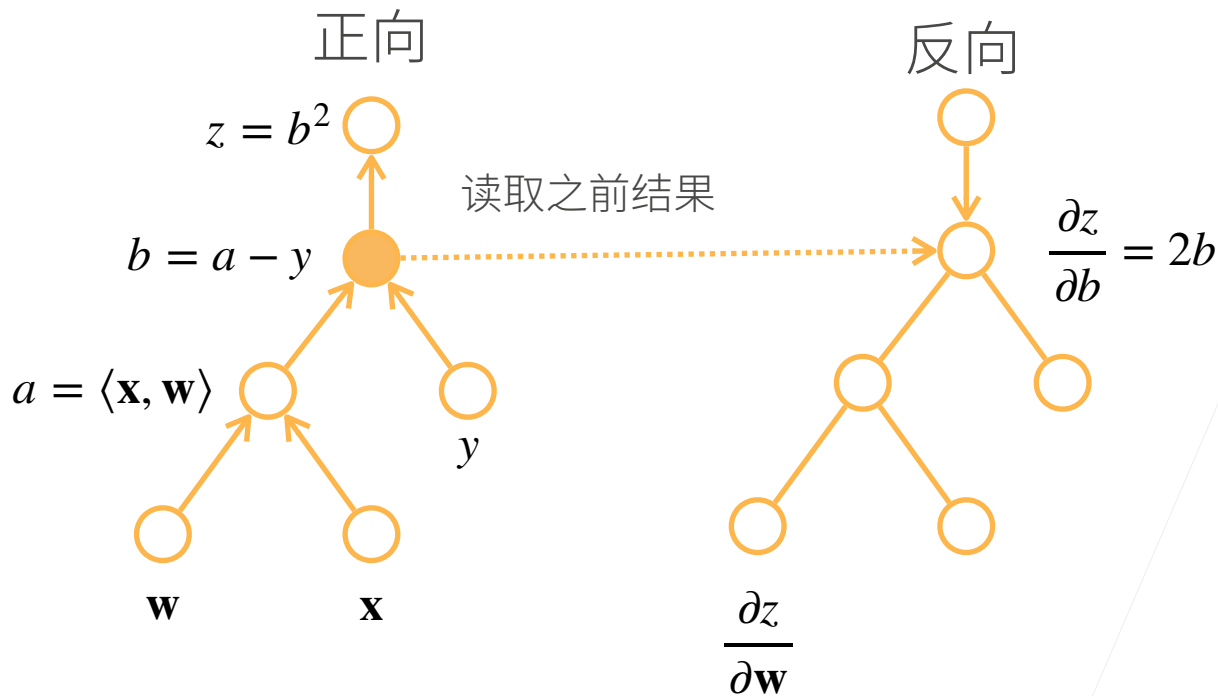
$$z = (\langle \mathbf{x}, \mathbf{w} \rangle - y)^2$$



# 反向累积



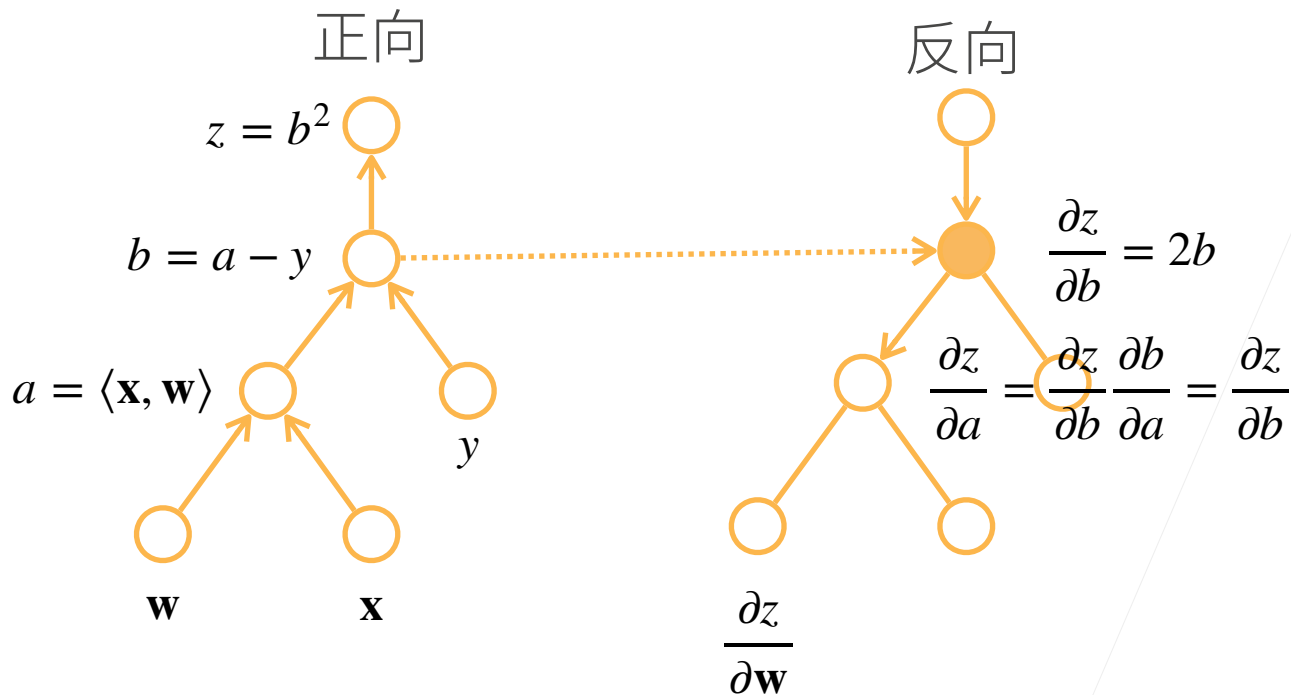
$$z = (\langle \mathbf{x}, \mathbf{w} \rangle - y)^2$$



# 反向累积



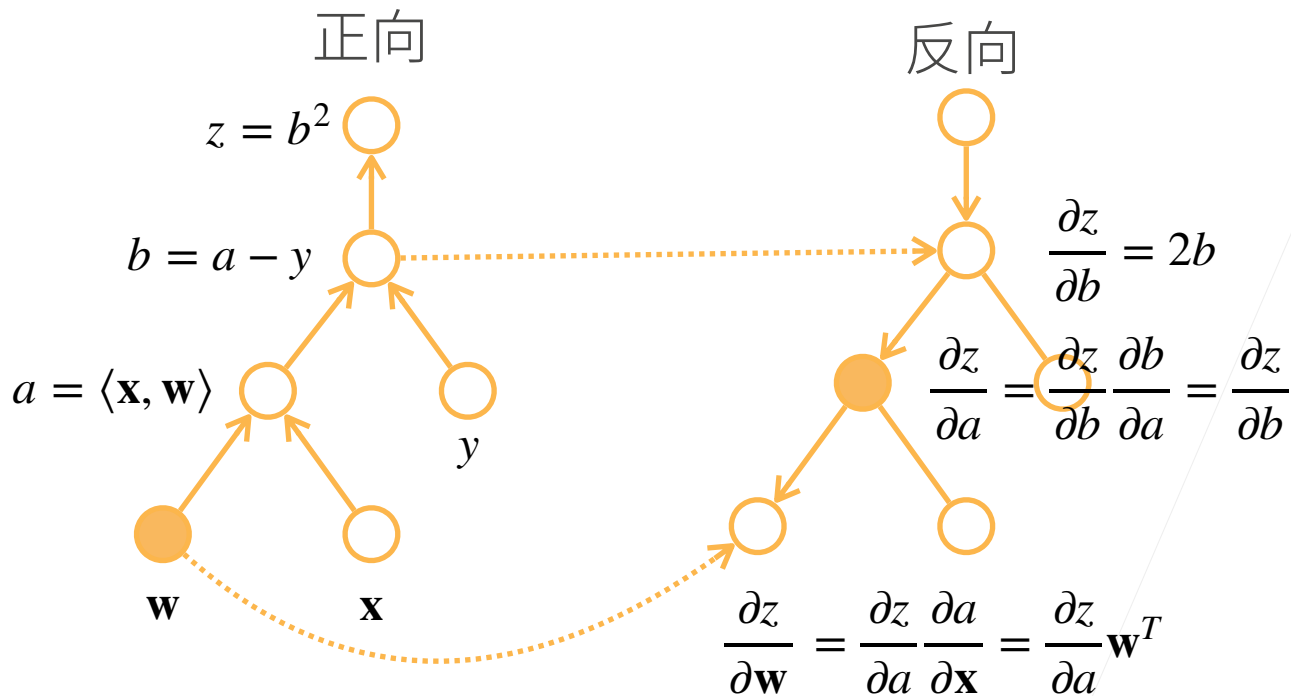
$$z = (\langle \mathbf{x}, \mathbf{w} \rangle - y)^2$$



# 反向累积



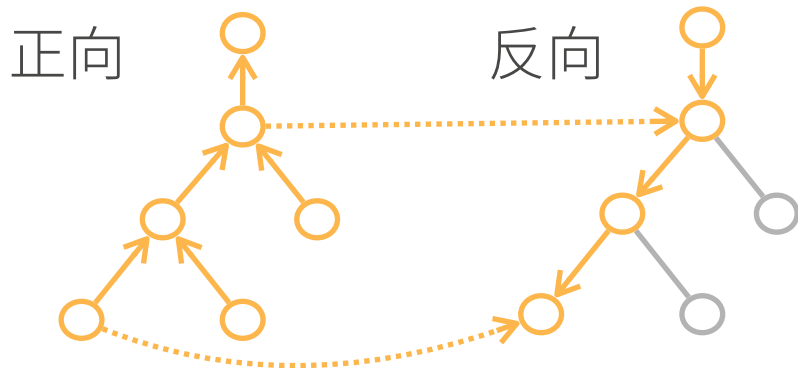
$$z = (\langle \mathbf{x}, \mathbf{w} \rangle - y)^2$$





# 反向累积总结

- 构造计算图
- 前向：执行图，存储中间结果
- 反向：从相反方向执行图
  - 去除不需要的枝





# 复杂度

- 计算复杂度:  $O(n)$ ,  $n$  是操作子个数
  - 通常正向和方向的代价类似
- 内存复杂度:  $O(n)$ , 因为需要存储正向的所有中间结果
- 跟正向累积对比:
  - $O(n)$  计算复杂度用来计算一个变量的梯度
  - $O(1)$  内存复杂度



# 线性回归

