

# 计算图与 自动微分



ZOMI



BUILDING A BETTER CONNECTED WORLD

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# 关于本内容

## 1. 内容背景

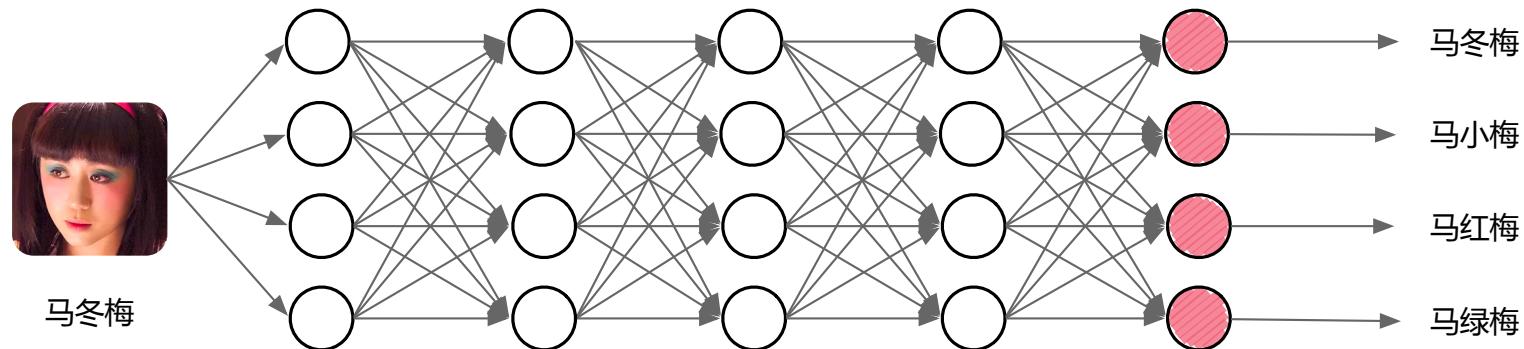
- 计算图基础介绍

## 2. 具体内容

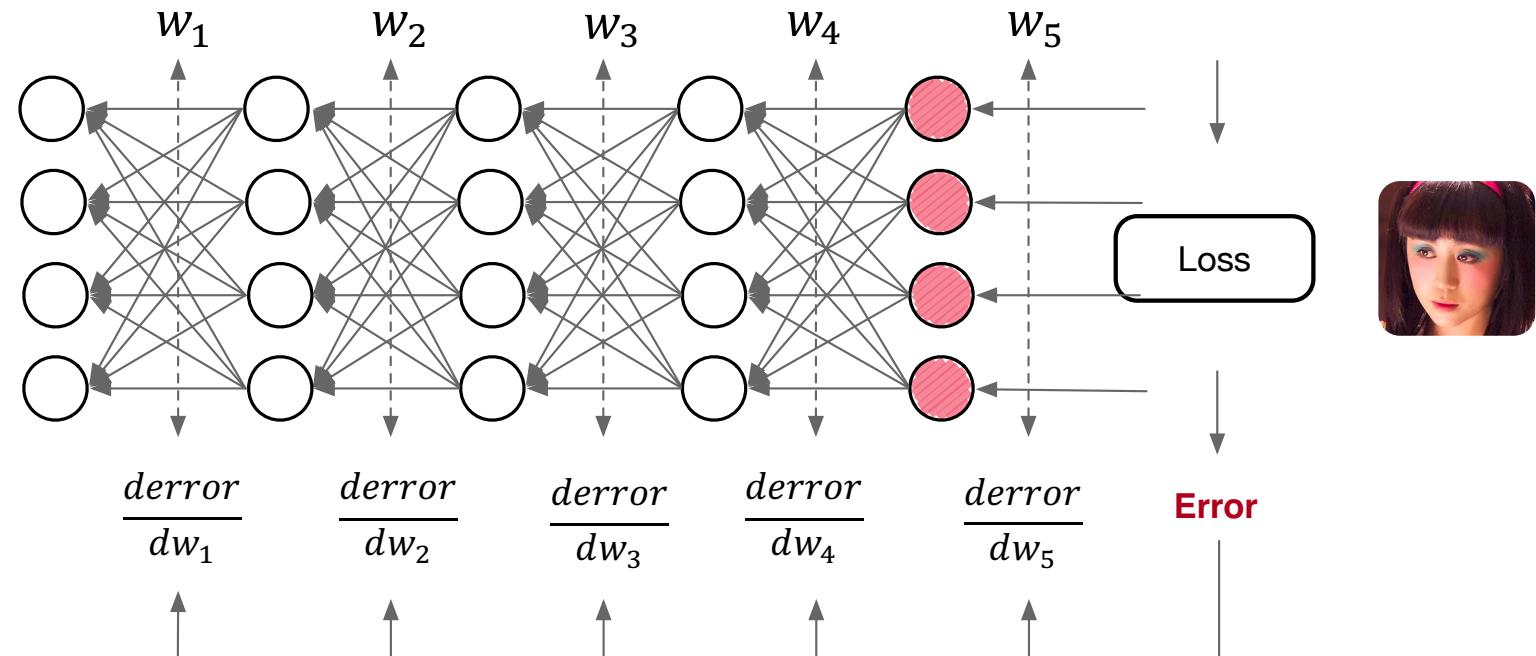
- 计算图（数据流图）：AI系统化问题 – 计算图的提出
- 计算图和自动微分：深度学习与微分 - 回顾自动微分 – 计算图表达自动微分
- 图的调度和执行：单算子调度 – 图切多设备调度 – 控制流控制
- 计算图的挑战与未来

# 深度学习训练流程：主要计算阶段

1. 前向计算：

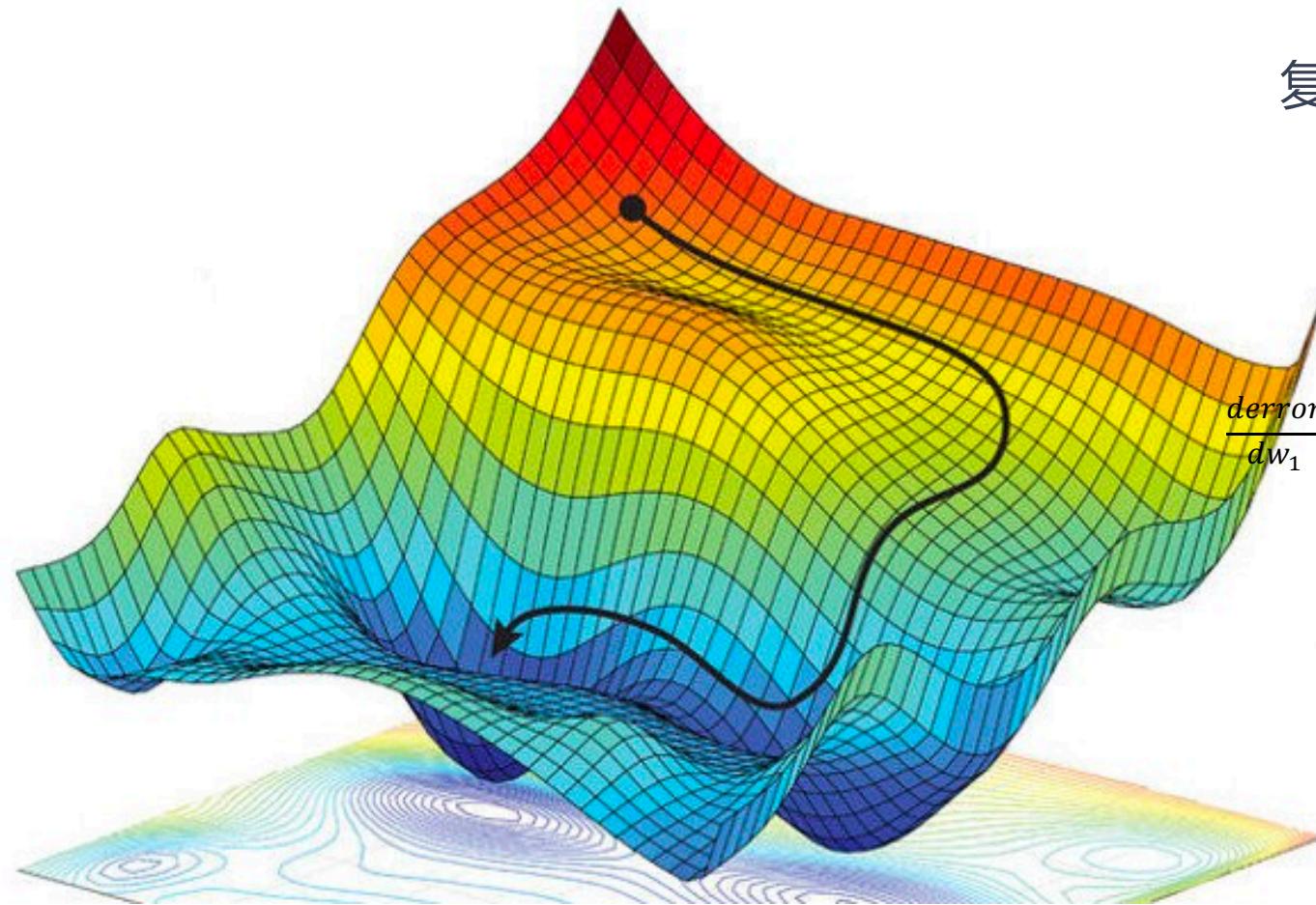


2. 反向计算：



3. 更新可学习的权重参数：

# 深度学习训练流程：数学表示



复杂的带参数的高度非凸函数

参数的一阶梯度迭代更新

$$\frac{derror}{dw_1}$$

$$\frac{derror}{dw_2}$$

$$\frac{derror}{dw_3}$$

$$\frac{derror}{dw_4}$$

$$\frac{derror}{dw_5}$$

Loss



# 训练流程核心：求导

- 求导是一个经典的问题

$$L(x) = \exp(\exp(x) + \exp(x)^2) + \sin(\exp(x) + \exp(x)^2)$$

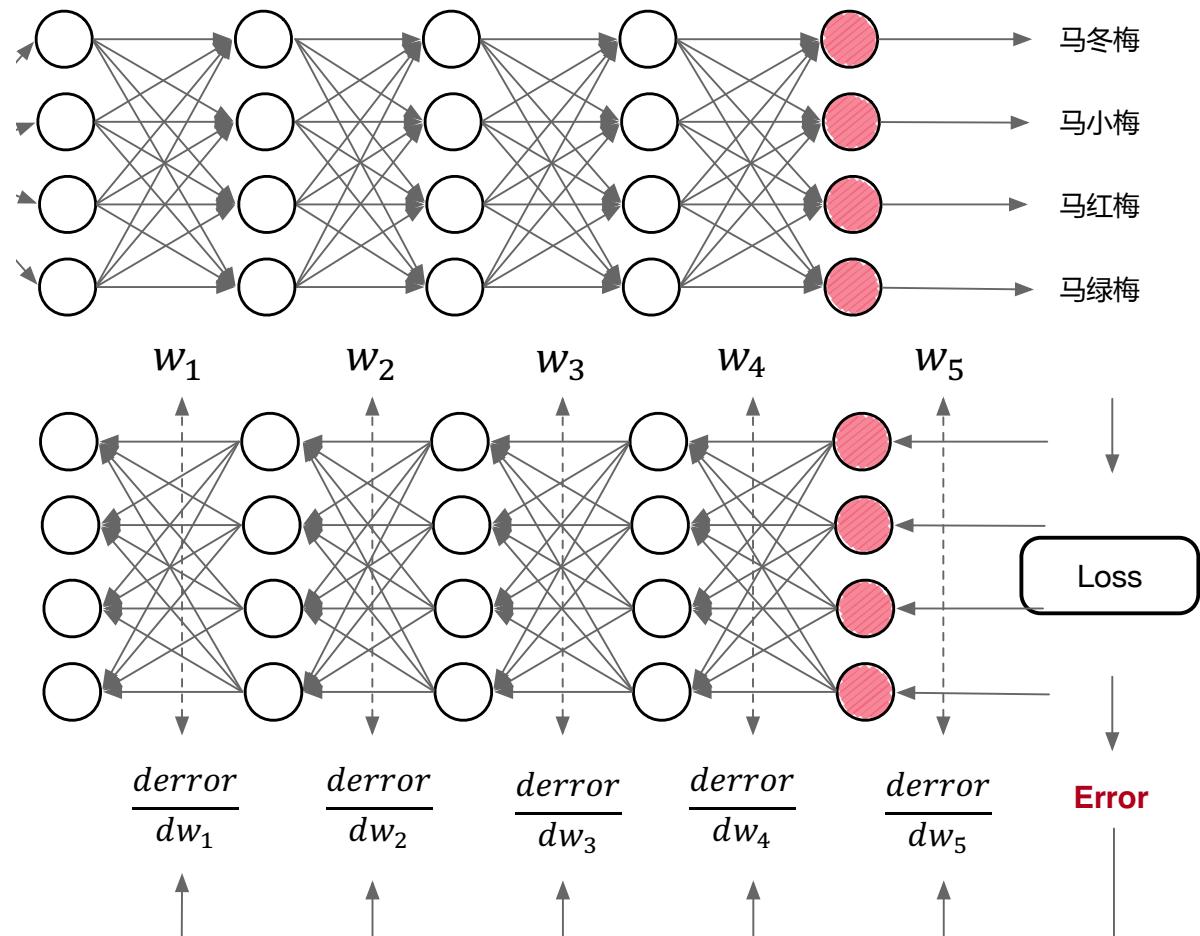
- 深度学习计算的核心：计算网络模型的参数，并更新其梯度

$$L(w) = Loss(f(w, x_i), y_i) \quad \Rightarrow \quad \frac{\partial L(w)}{\partial w}$$

- **自动微分**：原子操作构成的复杂前向计算程序，关注自动生成高效的反向计算程序

# 自动微分

```
class LeNet(nn.Module):  
  
    def __init__(self):  
        super(LeNet, self).__init__()  
        self.conv1 = nn.Conv2d(1, 6, 5, padding=2)  
        self.conv2 = nn.Conv2d(6, 16, 5)  
        self.fc1 = nn.Linear(16*5*5, 120)  
        self.fc2 = nn.Linear(120, 84)  
        self.fc3 = nn.Linear(84, 10)  
  
    def forward(self, x):  
        x = F.max_pool2d(F.relu(self.conv1(x)), (2, 2))  
        x = F.max_pool2d(F.relu(self.conv2(x)), (2, 2))  
        x = x.view(-1, self.num_flat_features(x))  
        x = F.relu(self.fc1(x))  
        x = F.relu(self.fc2(x))  
        x = self.fc3(x)  
        return x
```



# 符号微分 ( Symbolic Differentiation )

符号微分：通过求导法则和导数变换公式，精确计算函数的导数

- 将原表达式转换为导数表达式：

$$\frac{d}{\partial x}(f(x) + g(x)) \rightarrow \frac{d}{\partial x}f(x) + \frac{d}{\partial x}g(x)$$

$$\frac{d}{\partial x}(f(x) \cdot g(x)) \rightarrow \left( \frac{d}{\partial x}f(x) \right)g(x) + f(x)\left( \frac{d}{\partial x}g(x) \right)$$

**优势** • 精确数值结果

**缺点** • 表达式膨胀

## 深度学习中的应用问题

- 深度学习网络非常大 -> 待求导函数复杂 -> 难以高效的求解
- 部分算子无法求导：如 Relu, Switch 等

# 数值微分 ( Numerical Differentiation )

## 数值微分：使用有限差分进行近似导数

- 可以使用有限差分来近似：

$$\frac{\partial f(x)}{\partial x_i} \approx \frac{f(x + he_i) - f(x)}{h}, \text{ where } h > 0$$

- |           |        |           |                                       |
|-----------|--------|-----------|---------------------------------------|
| <b>优势</b> | • 容易实现 | <b>缺点</b> | • 计算结果不精确<br>• 计算复杂度高<br>• 对 $h$ 的要求高 |
|-----------|--------|-----------|---------------------------------------|

## 深度学习中的应用问题

- 数值计算中的截断和近似问题导致无法得到精确导数
- 部分算子无法求导：如 Relu, Switch 等

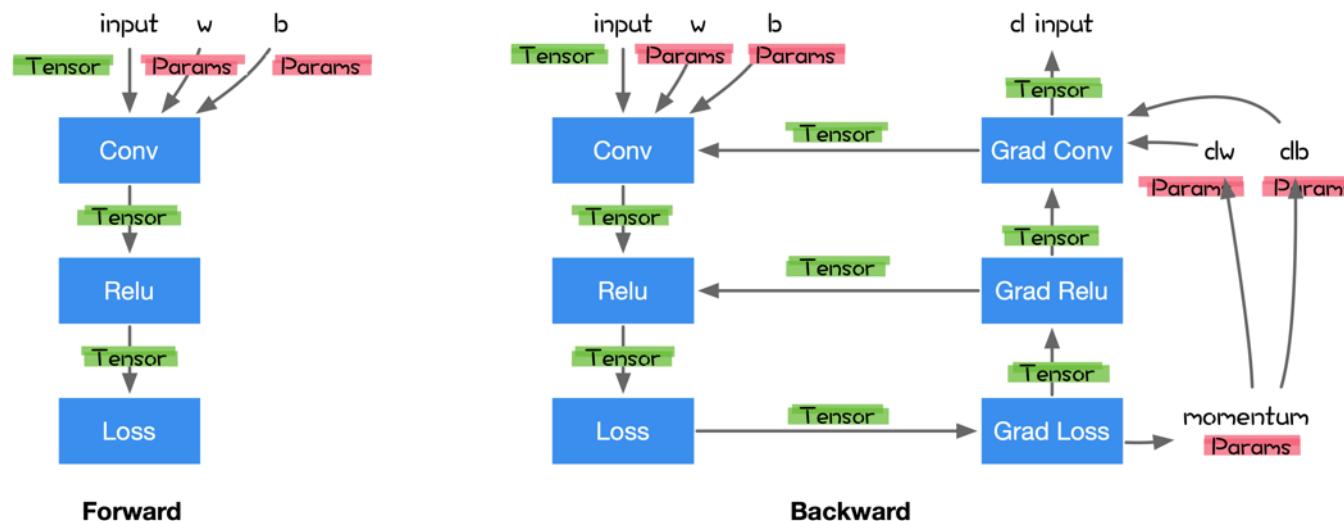
# 自动微分 ( Auto Differentiation ) I

自动微分：所有数值计算都由有限的基本运算组成

基本运算的导数表达式是已知的

通过链式法则将数值计算各部分组合成整体

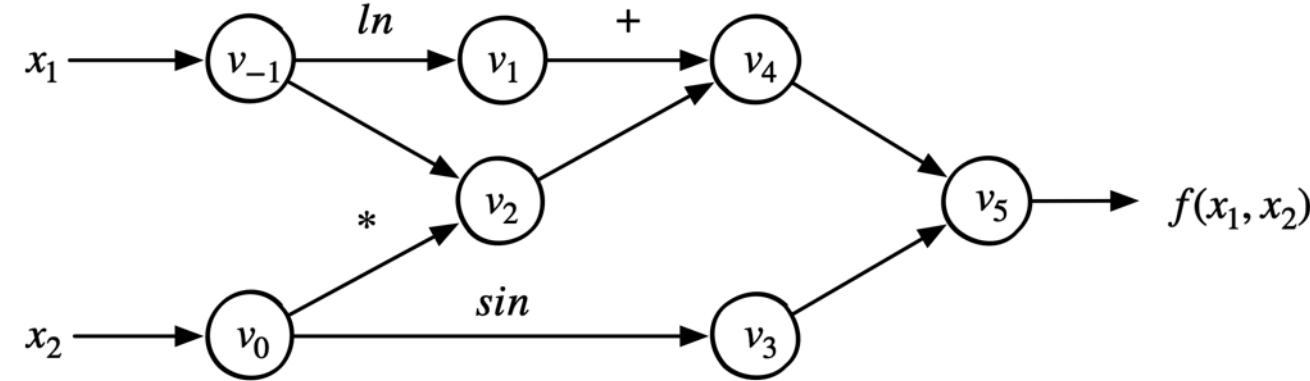
表达式追踪 ( Evaluation Trace ) : 追踪数值计算过程的中间变量



# 自动微分 ( Auto Differentiation ) II

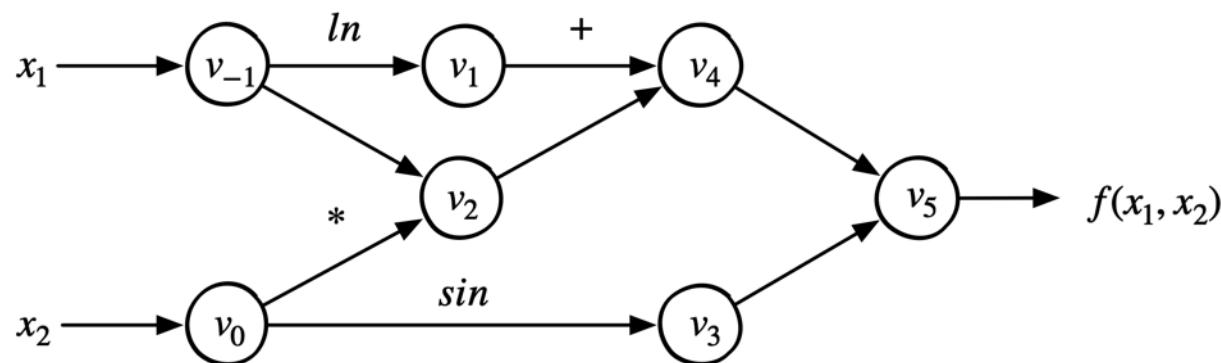
- 引入中间变量将一个复杂的函数，分解成一系列基本函数
- 将这些基本函数构成一个计算流图

$$f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$$



# 自动微分 ( Auto Differentiation ) (II)

- 引入中间变量将一个复杂的函数，分解成一系列基本函数
- 将这些基本函数构成一个计算流图

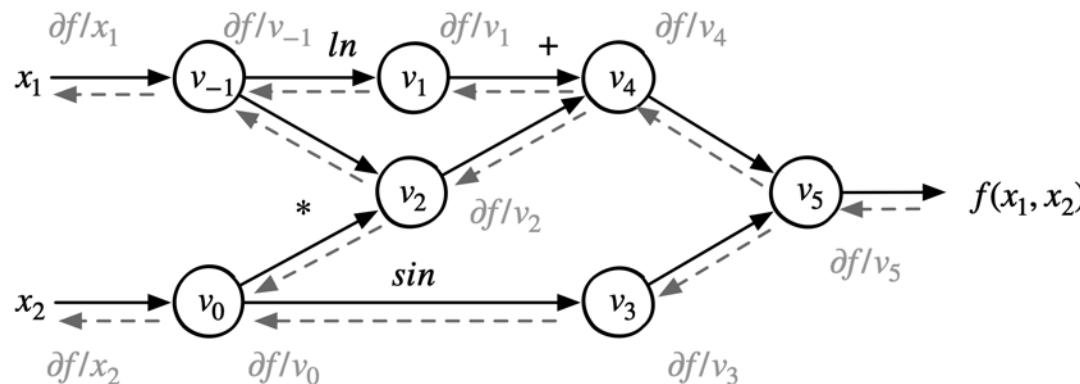


Forward Primal Trace

$v_{-1} = x_1$	$= 2$
$v_0 = x_2$	$= 5$
<hr/>	
$v_1 = \ln v_{-1}$	$= \ln 2$
$v_2 = v_{-1} \times v_0$	$= 2 \times 5$
$v_3 = \sin v_0$	$= \sin 5$
$v_4 = v_1 + v_2$	$= 0.693 + 10$
$v_5 = v_4 - v_3$	$= 10.693 + 0.959$
<hr/>	
$y = v_5$	$= 11.652$

# 自动微分 ( Auto Differentiation ) (II)

- 引入中间变量将一个复杂的函数，分解成一系列基本函数
- 将这些基本函数构成一个计算流图



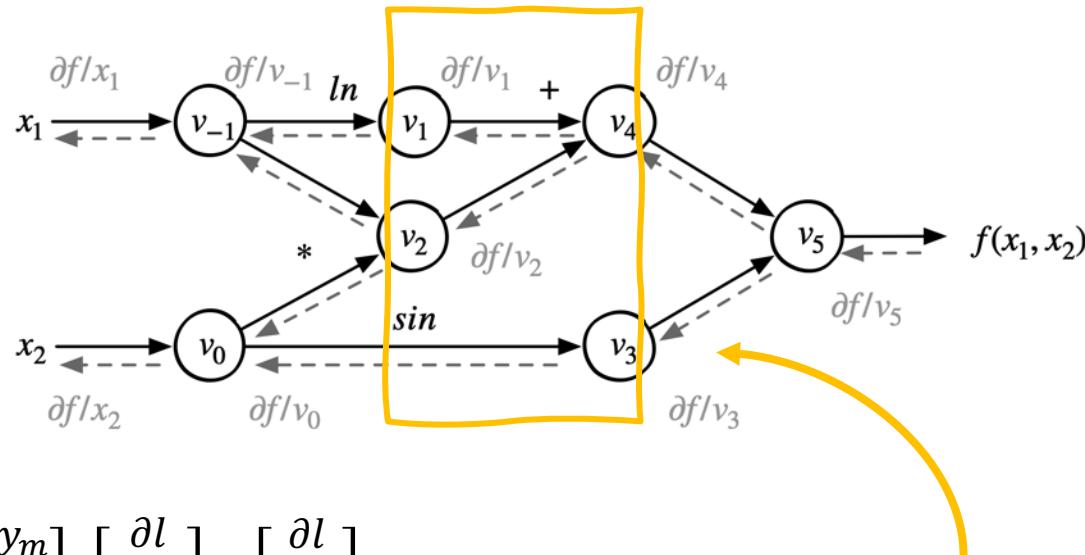
Reverse Adjoint (Derivative) Trace		
$\bar{x}_1 = \bar{v}_{-1}$	= 5.5	
$\bar{x}_2 = \bar{v}_0$	= 1.716	
$\bar{v}_{-1} = \bar{v}_{-1} + \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}} = \bar{v}_{-1} + \bar{v}_1 / v_{-1} = 5.5$		
$\bar{v}_0 = \bar{v}_0 + \bar{v}_2 \frac{\partial v_2}{\partial v_0} = \bar{v}_0 + \bar{v}_2 \times v_{-1} = 1.716$		
$\bar{v}_{-1} = \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}} = \bar{v}_2 \times v_0 = 5$		
$\bar{v}_0 = \bar{v}_3 \frac{\partial v_3}{\partial v_0} = \bar{v}_3 \times \cos v_0 = -0.284$		
$\bar{v}_2 = \bar{v}_4 \frac{\partial v_4}{\partial v_2} = \bar{v}_4 \times 1 = 1$		
$\bar{v}_1 = \bar{v}_4 \frac{\partial v_4}{\partial v_1} = \bar{v}_4 \times 1 = 1$		
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \times (-1) = -1$		
$\bar{v}_4 = \bar{v}_5 \frac{\partial v_5}{\partial v_4} = \bar{v}_5 \times 1 = 1$		
$\bar{v}_5 = \bar{y}$	= 1	

# 自动微分 ( Auto Differentiation ) (III)

$$Y = G(X) \quad \Rightarrow \quad J_f = \begin{bmatrix} \frac{\partial Y}{\partial X_1} & \dots & \frac{\partial Y}{\partial X_n} \end{bmatrix}$$

$$J_f = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \dots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \dots & \frac{\partial y_m}{\partial x_n} \end{bmatrix}$$

雅克比矩阵  $J$



$$J^T \cdot \vec{v} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \dots & \frac{\partial y_m}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial x_n} & \dots & \frac{\partial y_m}{\partial x_n} \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial l}{\partial y_1} \\ \vdots \\ \frac{\partial l}{\partial y_m} \end{bmatrix} = \begin{bmatrix} \frac{\partial l}{\partial x_1} \\ \vdots \\ \frac{\partial l}{\partial x_n} \end{bmatrix}$$



$$\vec{v} = \begin{bmatrix} \frac{\partial l}{\partial y_1} & \dots & \frac{\partial l}{\partial y_m} \end{bmatrix}^T$$

后一层损失函数对当前层输出的导数

vector-Jacobian的乘积

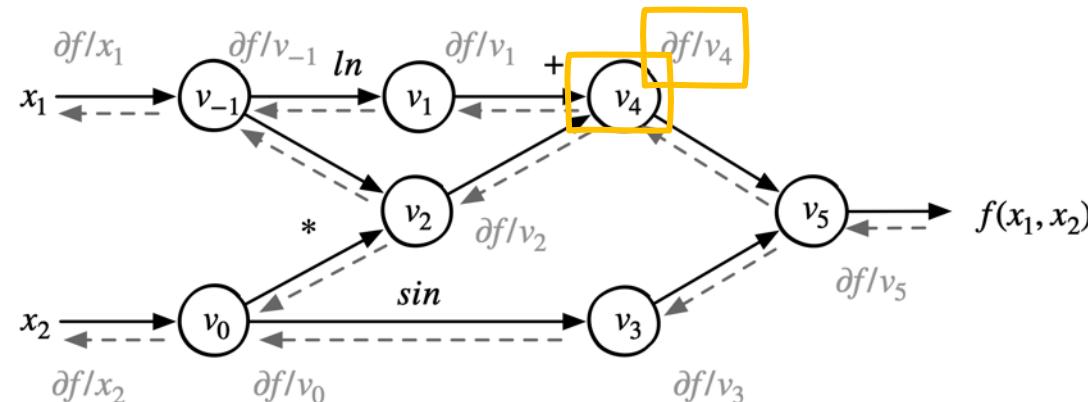
# 自动微分 ( Auto Differentiation ) (III)

注册前向计算结点和反向计算结点

前向结点接受输入计算输出

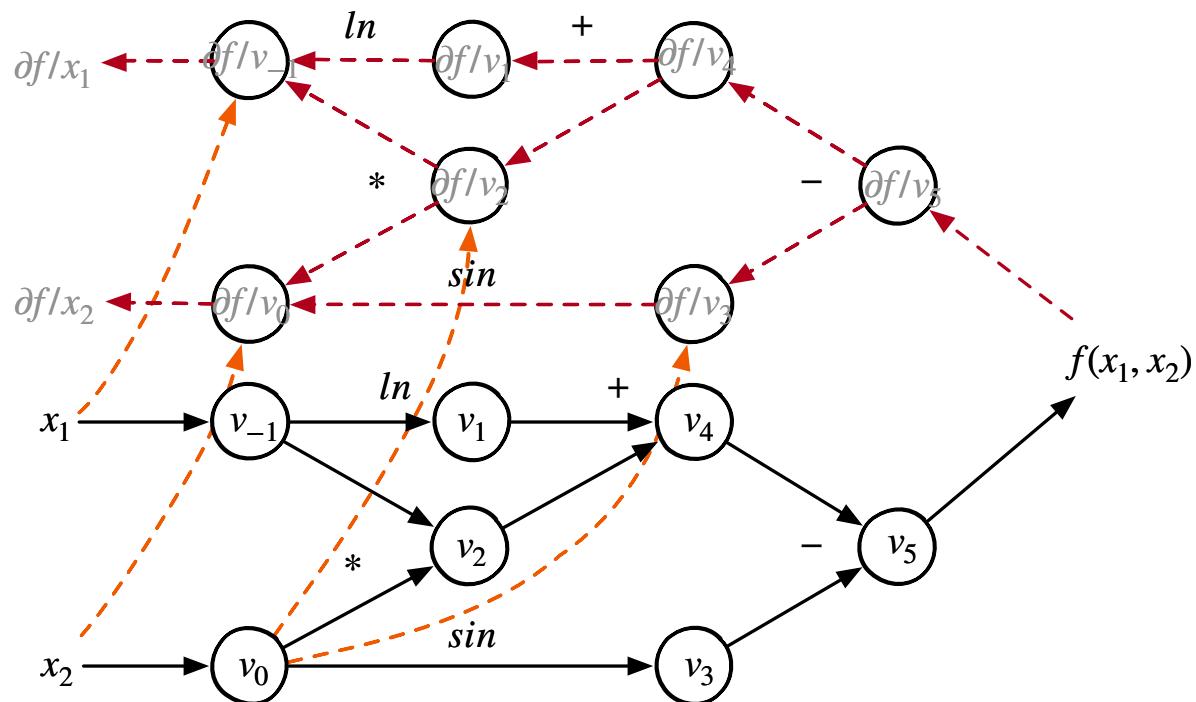
反向结点接受损失函数对当前张量操作输出的梯度  $v$

计算当前张量操作每个输入的vector-Jacobian乘积



# 自动微分 ( Auto Differentiation ) (III)

有向无环图 ( DAG, Directed Acyclic Graph )



Reverse Adjoint (Derivative) Trace		
$\bar{x}_1 = \bar{v}_{-1}$		= 5.5
$\bar{x}_2 = \bar{v}_0$		= 1.716
$\bar{v}_{-1} = \bar{v}_{-1} + \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}} = \bar{v}_{-1} + \bar{v}_1 / v_{-1} = 5.5$		
$\bar{v}_0 = \bar{v}_0 + \bar{v}_2 \frac{\partial v_2}{\partial v_0} = \bar{v}_0 + \bar{v}_2 \times v_{-1} = 1.716$		
$\bar{v}_{-1} = \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}} = \bar{v}_2 \times v_0 = 5$		
$\bar{v}_0 = \bar{v}_3 \frac{\partial v_3}{\partial v_0} = \bar{v}_3 \times \cos v_0 = -0.284$		
$\bar{v}_2 = \bar{v}_4 \frac{\partial v_4}{\partial v_2} = \bar{v}_4 \times 1 = 1$		
$\bar{v}_1 = \bar{v}_4 \frac{\partial v_4}{\partial v_1} = \bar{v}_4 \times 1 = 1$		
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \times (-1) = -1$		
$\bar{v}_4 = \bar{v}_5 \frac{\partial v_5}{\partial v_4} = \bar{v}_5 \times 1 = 1$		
$\bar{v}_5 = \bar{y}$		= 1

# 思考

- 正向模式 和 反向模式 计算量是否相等？
- AI框架或者深度学习任务中为什么大多使用反向模式？

# 在深度学习框架中实现自动微分（I）

前向计算并保留中间计算结果

根据反向模式的原理依次计算出中间导数

表达式追踪（Evaluation Trace）：追踪数值计算过程的中间变量

**主要问题：**

- 需要保存大量中间计算结果
- 方便跟踪计算过程



Forward Primal Trace		Reverse Adjoint (Derivative) Trace
$v_{-1} = x_1$	= 2	$\bar{x}_1 = \bar{v}_{-1}$ = 5.5
$v_0 = x_2$	= 5	$\bar{x}_2 = \bar{v}_0$ = 1.716
$v_1 = \ln v_{-1}$	= ln 2	$\bar{v}_{-1} = \bar{v}_{-1} + \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}}$ = $\bar{v}_{-1} + \bar{v}_1/v_{-1}$ = 5.5
$v_2 = v_{-1} \times v_0$	= $2 \times 5$	$\bar{v}_0 = \bar{v}_0 + \bar{v}_2 \frac{\partial v_2}{\partial v_0}$ = $\bar{v}_0 + \bar{v}_2 \times v_{-1}$ = 1.716
$v_3 = \sin v_0$	= sin 5	$\bar{v}_{-1} = \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}}$ = $\bar{v}_2 \times v_0$ = 5
$v_4 = v_1 + v_2$	= $0.693 + 10$	$\bar{v}_0 = \bar{v}_3 \frac{\partial v_3}{\partial v_0}$ = $\bar{v}_3 \times \cos v_0$ = -0.284
$v_5 = v_4 - v_3$	= $10.693 + 0.959$	$\bar{v}_2 = \bar{v}_4 \frac{\partial v_4}{\partial v_2}$ = $\bar{v}_4 \times 1$ = 1
$y = v_5$	= 11.652	$\bar{v}_1 = \bar{v}_4 \frac{\partial v_4}{\partial v_1}$ = $\bar{v}_4 \times 1$ = 1
		$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3}$ = $\bar{v}_5 \times (-1)$ = -1
		$\bar{v}_4 = \bar{v}_5 \frac{\partial v_5}{\partial v_4}$ = $\bar{v}_5 \times 1$ = 1
		$\bar{v}_5 = \bar{y}$ = 1

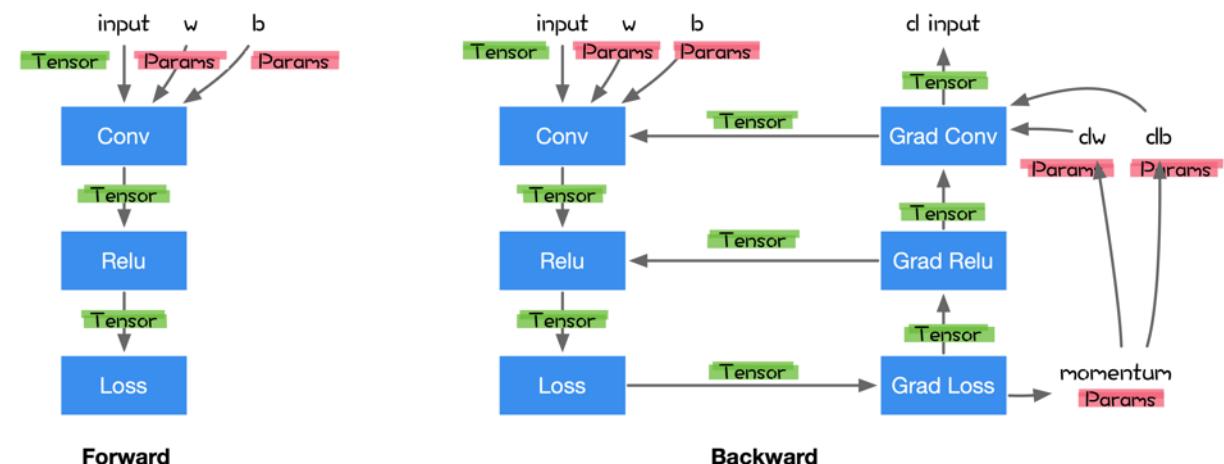
# 在深度学习框架中实现自动微分 (II)

将导数的计算也表示成计算图

通过 Graph IR 来对计算图进行统一表示

**主要特点：**

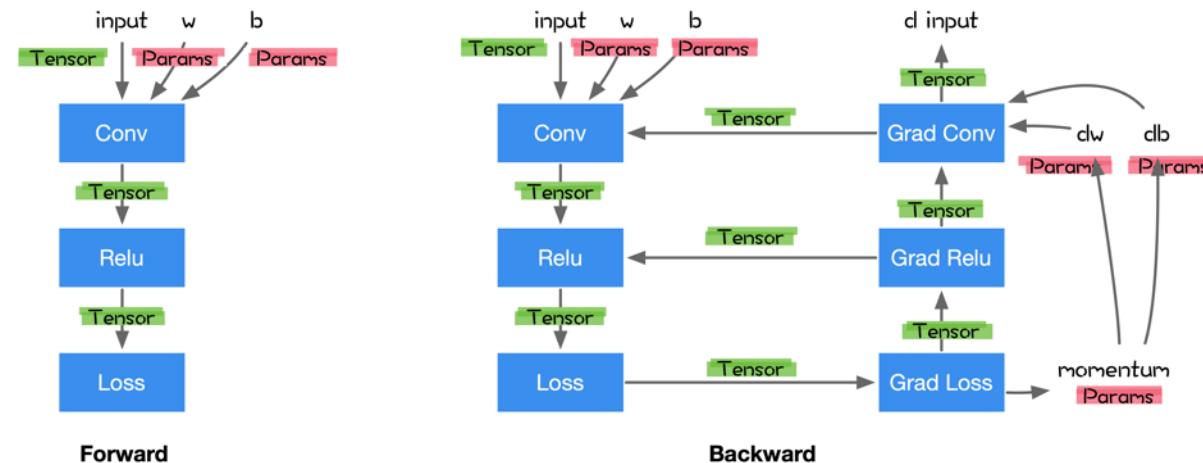
- 不便于调试跟踪计算和数学表达过程
- 方便全局图优化
- 节省内存



# 在深度学习框架中实现自动微分 ( III )

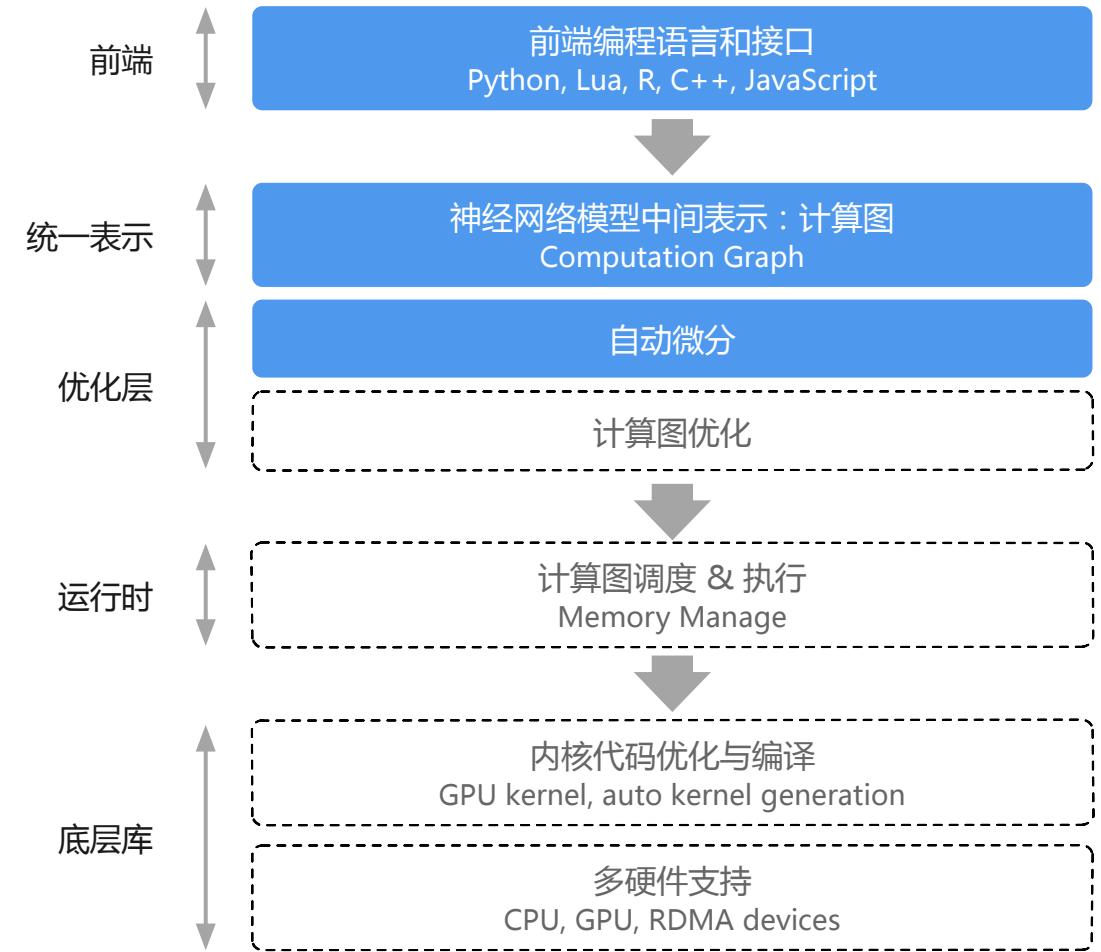
## 优化Pass :

- 给定前向数据流图
- 以损失函数为根节点广度优先遍历前向数据流图
- 按照对偶结构自动生成出求导数据流图



# Review

- **模型表示**：计算图
- **前端语言**：用来构建计算图
- **自动微分**：基于反向模式的原理，构建计算图



# Summary

1. 了解神经网络/AI系统中训练流程跟微分之间的关系
2. 回顾自动微分的正反向模式和计算图中的自动微分
3. 了解自动微分在深度学习中的一个实现表示





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