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自动微分模式



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关于本课程

1. 课程背景

- AI框架中自动微分的重要性

2. 课程内容

- 微分基本概念：数值微分 - 符号微分 - 自动微分
- 自动微分模式：前向微分 – 后向微分 – 雅克比原理
- 具体实现方式：表达式或图 – 操作符重载OO – 源码转换 AST
- MindSpore实现：基于图表示的源码转换Graph Base AST
- 自动微分的未来
- 自动微分的挑战

What is AD

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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

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

Forward Primal Trace

$$\begin{array}{lll} v_{-1} = x_1 & = 2 \\ \hline v_0 = x_2 & = 5 \\ \hline v_1 = \ln v_{-1} & = \ln 2 \\ v_2 = v_{-1} \times v_0 & = 2 \times 5 \\ v_3 = \sin v_0 & = \sin 5 \\ v_4 = v_1 + v_2 & = 0.693 + 10 \\ v_5 = v_4 - v_3 & = 10.693 + 0.959 \\ \hline y = v_5 & = 11.652 \end{array}$$



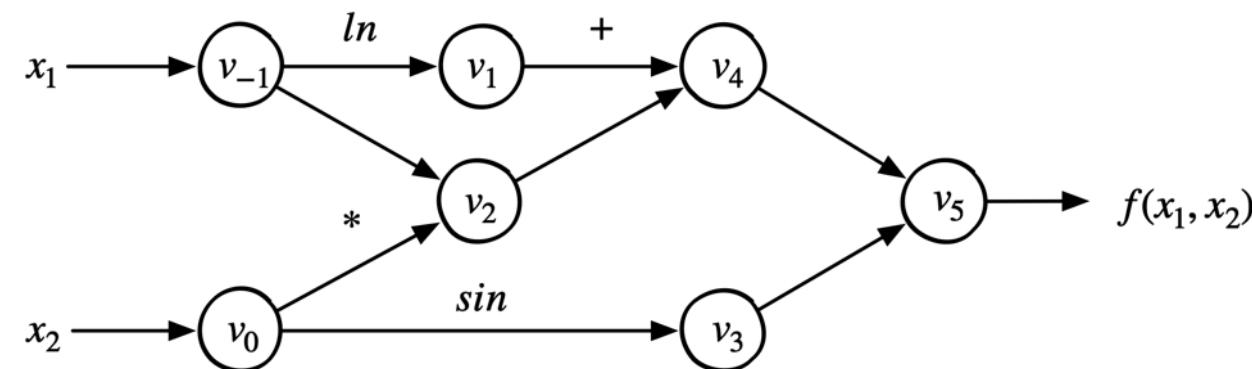
What is AD

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原函数：

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

原函数转换成DAG (有向无环图)：



根据链式求导法则展开：

$$\frac{\partial f}{\partial x_1} = \frac{\partial v_{-1}}{\partial x_1} \left(\frac{\partial v_1}{\partial v_{-1}} \frac{\partial v_4}{\partial v_1} + \frac{\partial v_2}{\partial v_{-1}} \frac{\partial v_4}{\partial v_2} \right) \frac{\partial v_5}{\partial v_4} \frac{\partial f}{\partial v_5}$$

AD Forward Mode

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

$$\dot{v}_i = \frac{\partial v_i}{\partial x_1} \quad \dot{y}_j = \frac{\partial y_j}{\partial x_i}$$

Forward Primal Trace

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



Forward Tangent (Derivative) Trace

$\dot{v}_{-1} = \dot{x}_1$	$= 1$
$\dot{v}_0 = \dot{x}_2$	$= 0$
$\dot{v}_1 = \dot{v}_{-1}/v_{-1}$	$= 1/2$
$\dot{v}_2 = \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	$= 1 \times 5 + 0 \times 2$
$\dot{v}_3 = \dot{v}_0 \times \cos v_0$	$= 0 \times \cos 5$
$\dot{v}_4 = \dot{v}_1 + \dot{v}_2$	$= 0.5 + 5$
$\dot{v}_5 = \dot{v}_4 - \dot{v}_3$	$= 5.5 - 0$
$\dot{y} = \dot{v}_5$	$= 5.5$



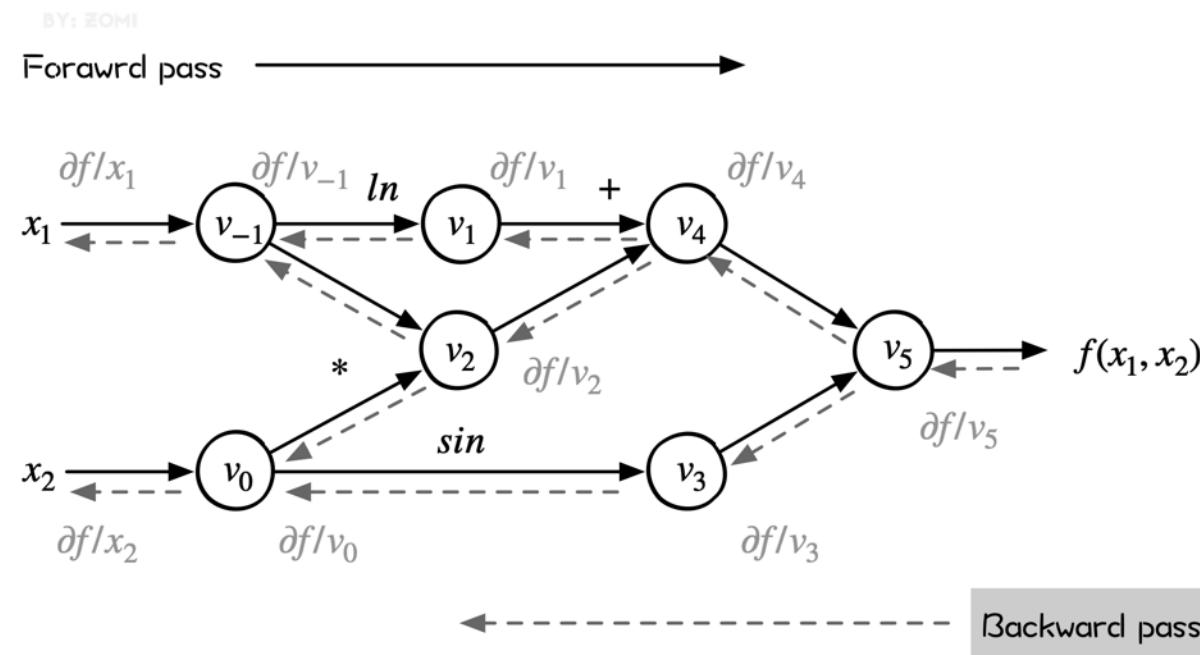
What is AD

[M]^s

原函数：

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

原函数转换成DAG：



根据链式求导法则展开：

$$\frac{\partial f}{\partial \mathbf{x}} = \sum_{k=1}^N \frac{\partial f}{\partial v_k} \frac{\partial v_k}{\partial \mathbf{x}}$$

AD Reverse Mode

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

$$\bar{v}_i = \frac{\partial y_i}{\partial v_i}$$

Forward Primal Trace

$$\begin{array}{ll} v_{-1} = x_1 & = 2 \\ v_0 = x_2 & = 5 \end{array}$$

$$v_1 = \ln v_{-1} = \ln 2$$

$$v_2 = v_{-1} \times v_0 = 2 \times 5$$

$$v_3 = \sin v_0 = \sin 5$$

$$v_4 = v_1 + v_2 = 0.693 + 10$$

$$v_5 = v_4 - v_3 = 10.693 + 0.959$$

$$y = v_5 = 11.652$$

Reverse Adjoint (Derivative) Trace

$$\begin{array}{lll} \bar{x}_1 = \bar{v}_{-1} & & = 5.5 \\ \bar{x}_2 = \bar{v}_0 & & = 1.716 \end{array}$$

$$\bar{v}_{-1} = \bar{v}_{-1} + \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}} = \bar{v}_{-1} + \bar{v}_1 / v_{-1} = 5.5$$

$$\bar{v}_0 = \bar{v}_0 + \bar{v}_2 \frac{\partial v_2}{\partial v_0} = \bar{v}_0 + \bar{v}_2 \times v_{-1} = 1.716$$

$$\bar{v}_{-1} = \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}} = \bar{v}_2 \times v_0 = 5$$

$$\bar{v}_0 = \bar{v}_3 \frac{\partial v_3}{\partial v_0} = \bar{v}_3 \times \cos v_0 = -0.284$$

$$\bar{v}_2 = \bar{v}_4 \frac{\partial v_4}{\partial v_2} = \bar{v}_4 \times 1 = 1$$

$$\bar{v}_1 = \bar{v}_4 \frac{\partial v_4}{\partial v_1} = \bar{v}_4 \times 1 = 1$$

$$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \times (-1) = -1$$

$$\bar{v}_4 = \bar{v}_5 \frac{\partial v_5}{\partial v_4} = \bar{v}_5 \times 1 = 1$$

$$\bar{v}_5 = \bar{y} = 1$$

Jacobian Matrix

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对于函数 $\vec{y} = f(\vec{x})$ ，其中 $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$ ，那么 \vec{y} 中关于 \vec{x} 的梯度可以表示为 Jacobian 矩阵：

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

AD Forward Mode: Jacobian-Vector Production

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对于函数 $\vec{y} = f(\vec{x})$ ，其中 $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$ ，那么 \vec{y} 中关于 \vec{x} 的梯度可以表示为 Jacobian 矩阵：

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

设置 \vec{v} 是关于函数 $l = g(\vec{y})$ 的梯度：

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

Jacobian - vector 积就是函数 l 中关于 x_1 的梯度：

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

AD Reverse Mode: Vector-Jacobian Production

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对于函数 $\vec{y} = f(\vec{x})$ ，其中 $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$ ，那么 \vec{y} 中关于 \vec{x} 的梯度可以表示为 Jacobian 矩阵：

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

设置 \vec{v} 是关于函数 $l = g(\vec{y})$ 的梯度：

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

vector – Jacobian 积就是函数 l 中关于 \vec{x} 的梯度：

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

Reverse Mode VS Forward Mode

对于函数 $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$ ，有 Jacobian 矩阵：

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

对于一个输出变量 y_i 进行一次反向模式，迭代计算出 Jacobian 矩阵每一行

对于一个输入变量 x_i 进行一次前向模式，迭代计算出 Jacobian 矩阵每一列

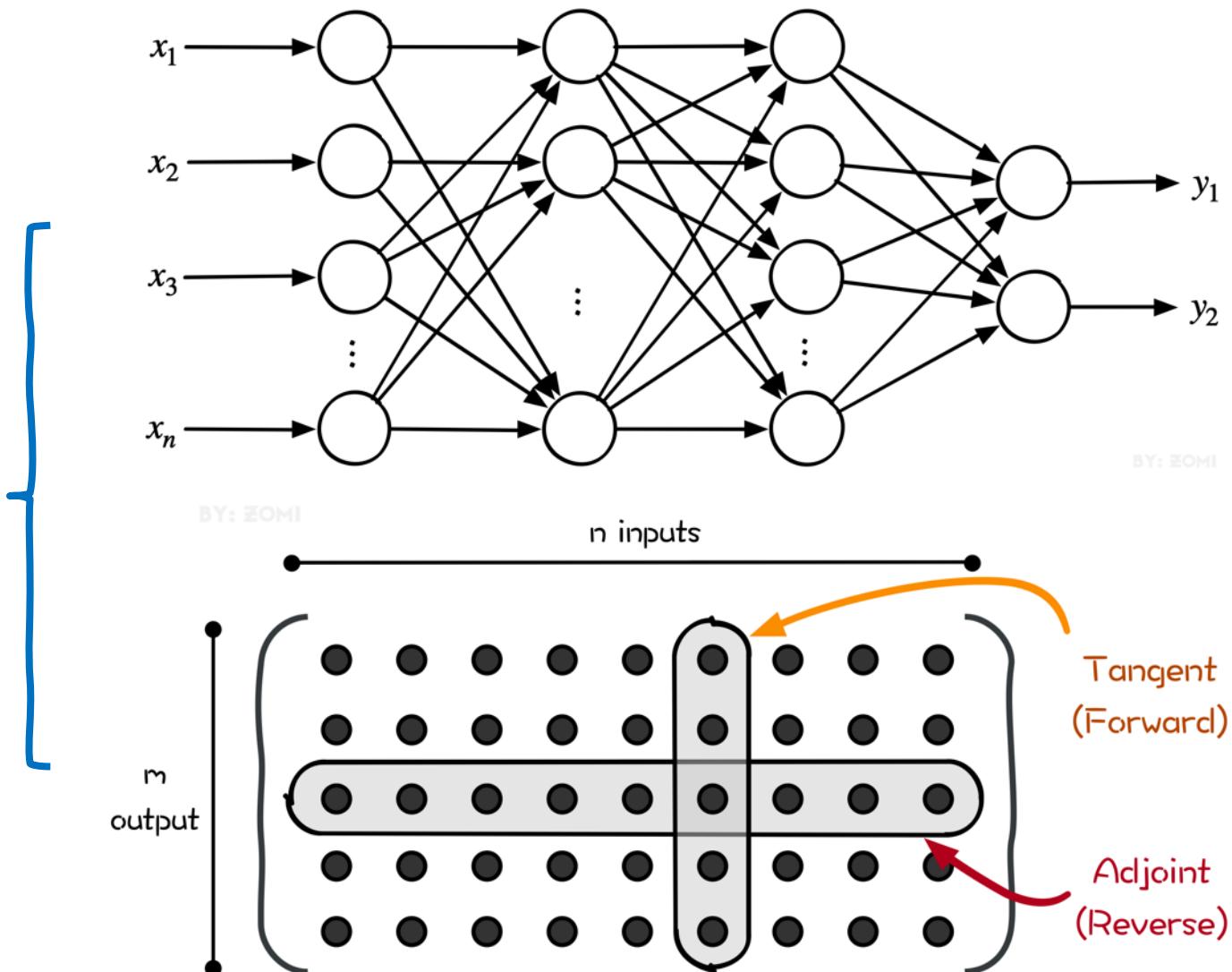
- 当 $m > n$ ，适合使用前向模式自动微分；
- 当 $n > m$ ，适合使用反向模式自动微分；

Automatic Differentiation in ML

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Jacobian 矩阵：

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



Automatic Differentiation

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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

链式法则将结果，组合得到整体程序的求导结果：

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

分为前向模式和反向模式，均为求解 Jacobian 矩阵：

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

- 优势**
- 数值精度高
 - 无表达式膨胀

- 缺点**
- 需要存储中间求导结果
 - 占用大量计算机内存

Conclusion

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1. 了解到自动微分分为前向微分和反向微分
2. 了解雅克比矩阵的基本原理和表示，前向和反向微分模式的雅克比表示
3. 了解了自动微分的优缺点和在AI框架中常用的基本模式

BUILDING A BETTER CONNECTED WORLD

THANK YOU

TEAMS

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