

CS 4803 / 7643: Deep Learning

Topics:

- Automatic Differentiation
- (Finish) Forward mode vs Reverse mode AD
- Patterns in backprop

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Administrativa

- HW1 Reminder
 - Due: 09/09, 11:59pm

- HW2 out on 9/10
 - Schedule https://www.cc.gatech.edu/classes/AY2021/cs7643_fall/

- Project discussion next class

Recap from last time

How do we compute gradients?

- Analytic or “Manual” Differentiation
- ~~•~~ Symbolic Differentiation
- ✓ • Numerical Differentiation
- Automatic Differentiation
 - Forward mode AD
 - Reverse mode AD
 - aka “backprop”

Vector/Matrix Derivatives [Notation]

	S	V	M
S	$\frac{\partial y}{\partial x}$	$\frac{\partial \vec{y}}{\partial x}$	$\frac{\partial y}{\partial x}$
V	$\frac{\partial \vec{y}}{\partial x}$	$\frac{\partial \vec{y}}{\partial x}$	tensors
M	$\frac{\partial Y}{\partial x}$		

$$x, y \in \mathbb{R}$$

$$\vec{x} \in \mathbb{R}^d \quad y \in \mathbb{R}^c$$

$$X, Y \in \mathbb{R}^{m \times n}$$

$$\frac{\partial \vec{y}}{\partial x} = \begin{bmatrix} \frac{\partial y_1}{\partial x} \\ \vdots \\ \frac{\partial y_c}{\partial x} \end{bmatrix}_{c \times 1} \quad \text{num} = \frac{\text{dim } 1}{\text{rows}}$$

$$\frac{\partial L}{\partial \vec{w}} = \begin{bmatrix} \frac{\partial L}{\partial w_1} & \dots & \frac{\partial L}{\partial w_n} \end{bmatrix}_{1 \times n} \quad \text{den} = \frac{\text{dim } 2}{\text{col}}$$

Vector/Matrix Derivatives Notation

$$\frac{\partial \vec{y}}{\partial \vec{x}} =$$

$$\begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \dots & \frac{\partial y_1}{\partial x_3} & \dots & \frac{\partial y_1}{\partial x_d} \\ \dots & \dots & \frac{\partial y_c}{\partial x_3} & \dots & \dots \end{bmatrix}_{c \times d}$$

Jacobian

Vector Derivative Example

$$\frac{\partial (\vec{w}^T A \vec{w})}{\partial \vec{w}} = \underline{2 \vec{w}^T [A]}$$

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

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

$$i \cdot \left[\frac{\partial y_i}{\partial x_j} \right] = \left[a_{ij} \right]$$

$$y_i = \sum_j a_{ij} x_j$$

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

Extension to Tensors

$$\underline{X} \in \underline{\mathbb{R}}^{d_1 \times \dots \times d_n}$$

$$\underline{Y} \in \underline{\mathbb{R}}^{c_1 \times \dots \times c_n}$$



$$\begin{aligned} \rightarrow y\text{-vec} &= \boxed{Y(:)} \\ \rightarrow x\text{-vec} &= \boxed{X(:)} \end{aligned}$$

$$\frac{\partial \overrightarrow{y\text{-vec}}}{\partial \overrightarrow{x\text{-vec}}} =$$

$$\begin{bmatrix} \\ \\ \\ \end{bmatrix} \begin{matrix} c_1 \\ | \\ c_1 \end{matrix}$$

$$\frac{\partial Y[i_1, \dots, i_n]}{\partial X[j_1, \dots, j_n]}$$

Jacobian Matrix

Chain Rule: Composite Functions

$$f(g(x)) = (f \circ g)(x)$$

layers in NN

$$h(\vec{w}) \circlearrowleft f(x) = g_n(g_{n-1} \dots g_1(x))$$

$$= (g_n \circ g_{n-1} \circ \dots \circ g_1)(x)$$

Chain Rule: Scalar Case

$$\underline{x} \in \mathbb{R}^1 \xrightarrow{g_1(\cdot)} \underline{z} \in \mathbb{R}^1 \xrightarrow{g_2(\cdot)} \underline{y} \in \mathbb{R}^1$$
$$y = g_2(g_1(x))$$

$$\underline{\frac{\partial y}{\partial x}} = \left(\underline{\frac{\partial y}{\partial z}} \cdot \underline{\frac{\partial z}{\partial x}} \right)$$

Scalar mult.

Chain Rule: Vector Case

$$\vec{x} \in \mathbb{R}^d \xrightarrow[\substack{g_1(\cdot) \\ : \mathbb{R}^d \rightarrow \mathbb{R}^m}]{\quad} \vec{z} \in \mathbb{R}^m \xrightarrow[\substack{g_2(\cdot) \\ : \mathbb{R}^m \rightarrow \mathbb{R}^c}]{\quad} \vec{y} \in \mathbb{R}^c$$

$$\underbrace{\left[\frac{\partial \vec{y}}{\partial \vec{x}} \right]}_{\boxed{J_{g_2 \circ g_1}}} = \underbrace{\left[\frac{\partial \vec{y}}{\partial \vec{z}} \right]}_{J_{g_2}} \odot \underbrace{\left[\frac{\partial \vec{z}}{\partial \vec{x}} \right]}_{J_{g_1}}$$

Matrix Mult

Chain Rule: Jacobian view

Diagram illustrating the chain rule in Jacobian form:

The first matrix is the Jacobian of y_i with respect to x_j , denoted as $\frac{\partial y_i}{\partial x_j}$.

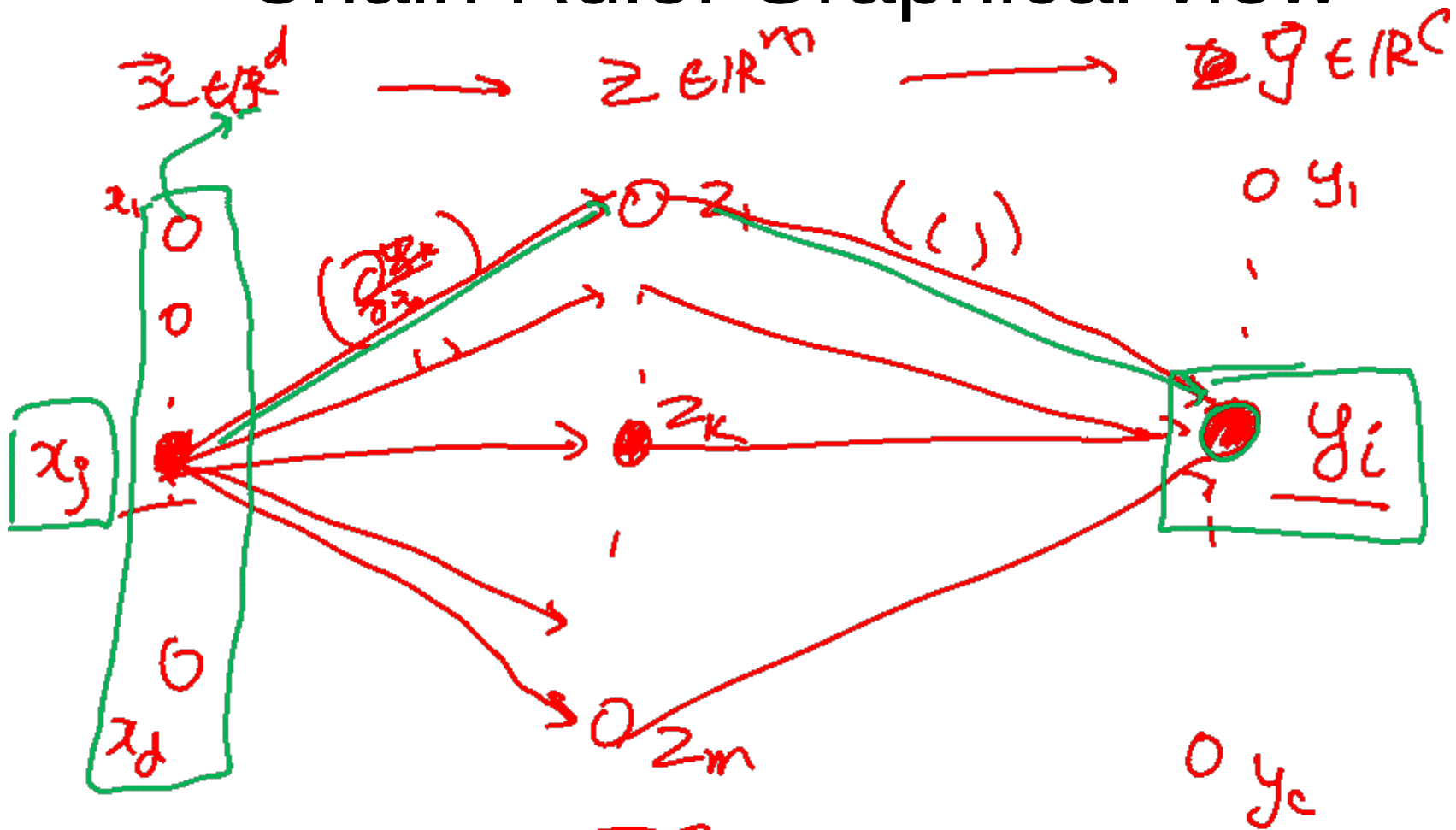
The second matrix is the row vector of partial derivatives of z with respect to z_k , denoted as $\frac{\partial z}{\partial z_k}$.

The third matrix is the column vector of partial derivatives of z_k with respect to x_j , denoted as $\frac{\partial z_k}{\partial x_j}$.

The chain rule is expressed as:

$$\frac{\partial y_i}{\partial x_j} = \sum_k \frac{\partial y_i}{\partial z_k} \frac{\partial z_k}{\partial x_j}$$

Chain Rule: Graphical view



$$\frac{\partial y_i}{\partial x_j} = \sum_{k \text{ on path}} \frac{\partial y_i}{\partial z_k} \frac{\partial z_k}{\partial x_j}$$

Chain Rule: Cascaded

$$\vec{x} = \vec{h}^0 \xrightarrow{g_1} \vec{h}^1 \in \mathbb{R}^d \xrightarrow{g_2} \vec{h}^2 \in \mathbb{R}^d \dots \xrightarrow{g_{\ell}} \vec{h}^{\ell} \rightarrow L$$

$$\begin{bmatrix} 0 \\ \vdots \\ 0 \\ 0 \\ 0 \end{bmatrix} \xrightarrow{g_1} \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix} \dots \dots \begin{bmatrix} \cdot \\ \vdots \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \xrightarrow{g_{\ell}} \begin{bmatrix} \cdot \\ \vdots \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \rightarrow L$$

$$\frac{\partial L}{\partial \vec{h}^0} = \begin{bmatrix} \frac{\partial L}{\partial \vec{h}^0} & \frac{\partial \vec{h}^{\ell}}{\partial \vec{h}^0} \\ \frac{\partial L}{\partial \vec{h}^1} & \frac{\partial \vec{h}^{\ell}}{\partial \vec{h}^1} \\ \vdots & \vdots \\ \frac{\partial L}{\partial \vec{h}^{\ell-1}} & \frac{\partial \vec{h}^{\ell}}{\partial \vec{h}^{\ell-1}} \end{bmatrix} = \begin{bmatrix} \frac{\partial L}{\partial \vec{h}^0} & \frac{\partial \vec{h}^{\ell}}{\partial \vec{h}^0} \\ \frac{\partial L}{\partial \vec{h}^1} & \frac{\partial \vec{h}^{\ell}}{\partial \vec{h}^1} \\ \vdots & \vdots \\ \frac{\partial L}{\partial \vec{h}^{\ell-1}} & \frac{\partial \vec{h}^{\ell}}{\partial \vec{h}^{\ell-1}} \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial \vec{h}^{\ell-1}}{\partial \vec{h}^{\ell-2}} \\ \vdots \\ \frac{\partial \vec{h}^2}{\partial \vec{h}^1} \end{bmatrix}$$

$$\frac{\partial L}{\partial \vec{h}^0} = \begin{bmatrix} \cdot \\ \vdots \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \xrightarrow{dxd} \begin{bmatrix} \cdot \\ \vdots \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \xrightarrow{dxd} \begin{bmatrix} \cdot \\ \vdots \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \xrightarrow{dxd} \begin{bmatrix} \cdot \\ \vdots \\ \cdot \\ \cdot \\ \cdot \end{bmatrix}$$

$\underbrace{\quad}_{O(d^2)} \quad \underbrace{\quad}_{O(d^3)}$

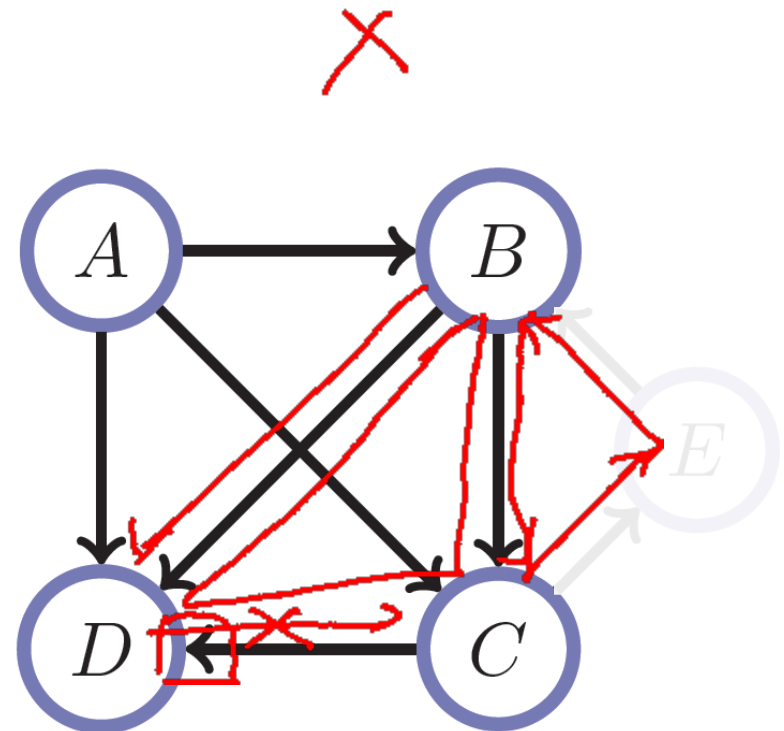
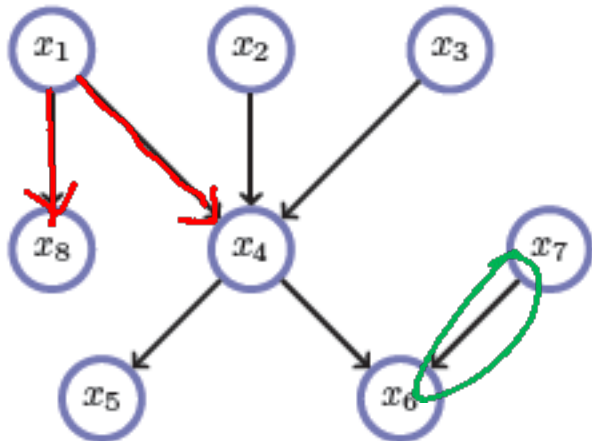
Deep Learning = Differentiable Programming

- Computation = Graph
 - Input = Data + Parameters ~
 - Output = Loss
 - Scheduling = Topological ordering
- Auto-Diff
 - A family of algorithms for implementing chain-rule on computation graphs

Directed Acyclic Graphs (DAGs)

- Exactly what the name suggests
 - Directed edges
 - No (directed) cycles
 - Underlying undirected cycles okay

DAG ✓



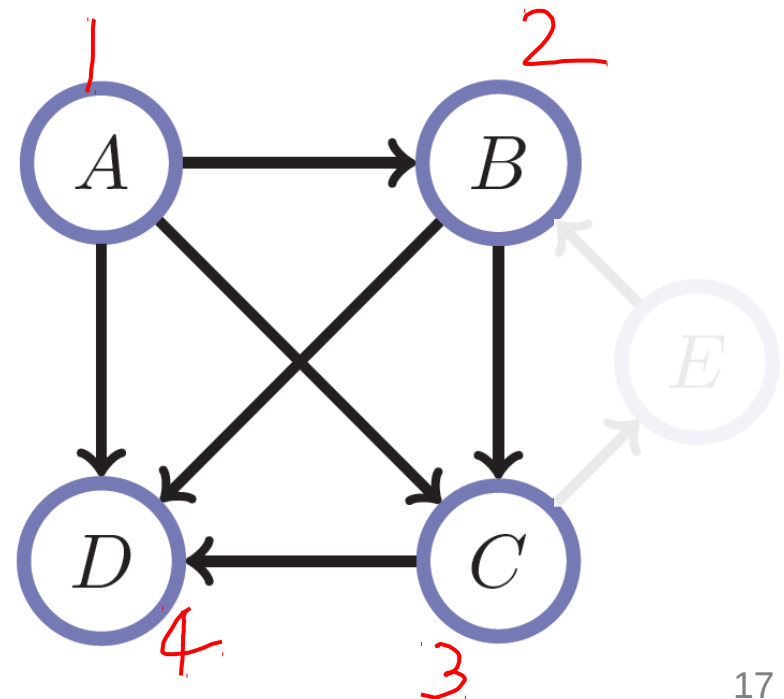
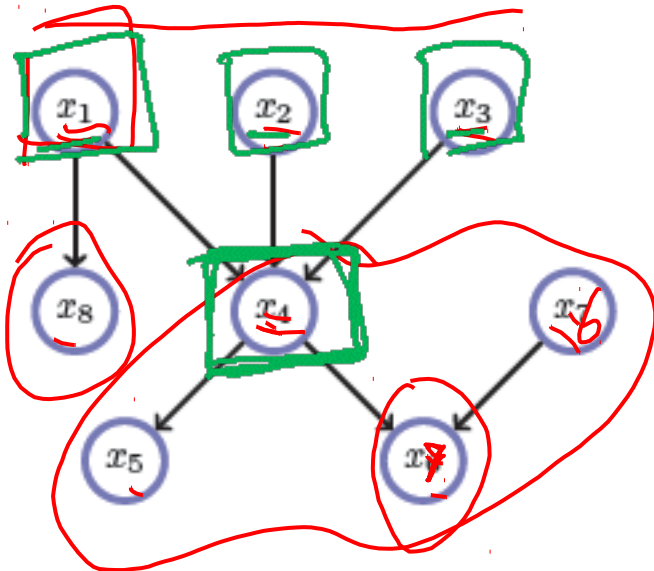
Directed Acyclic Graphs (DAGs)

- Concept
 - Topological Ordering

\exists bijection $\sigma: V \rightarrow \{1, \dots, n\}$

s.t. $\forall (v_i, v_j) \in E$

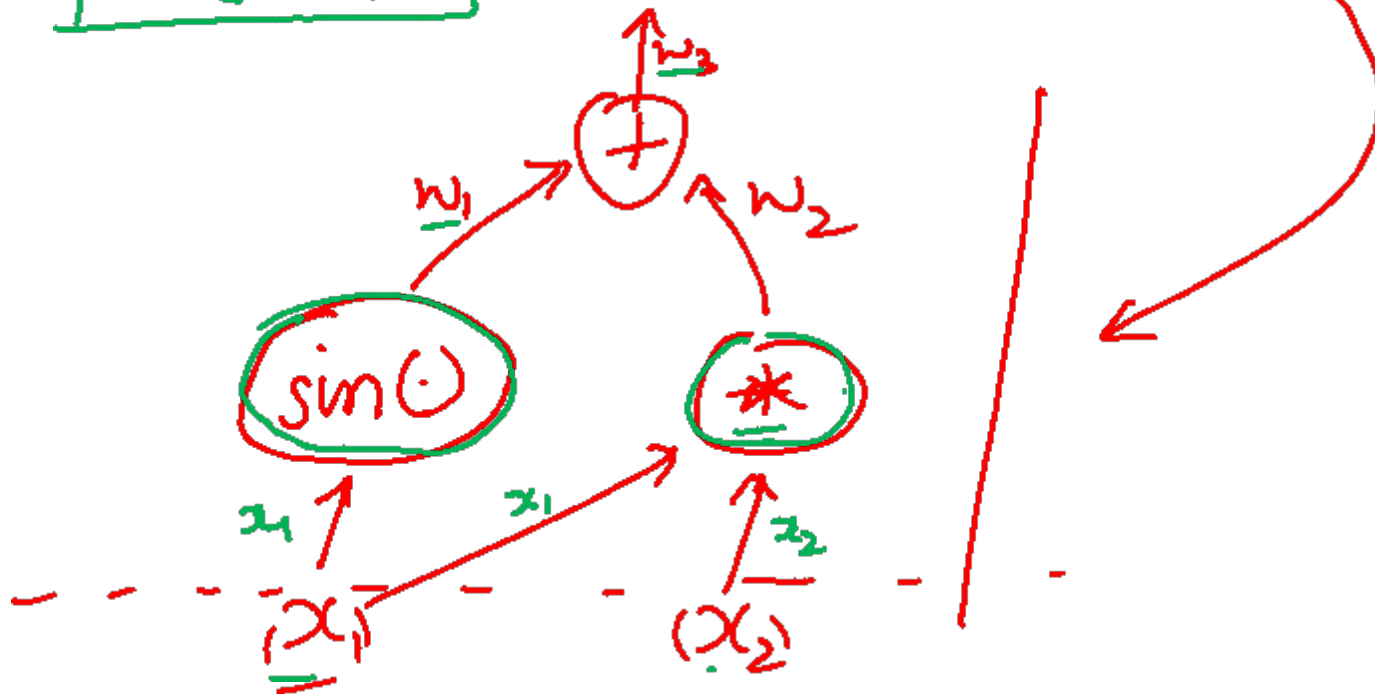
$\sigma(v_i) < \sigma(v_j)$



Computational Graphs ← DAG

- Notation

$$f(\underline{x}_1, \underline{x}_2) = \underline{x}_1 \underline{x}_2 + \sin(\underline{x}_1)$$



Deep Learning = Differentiable Programming

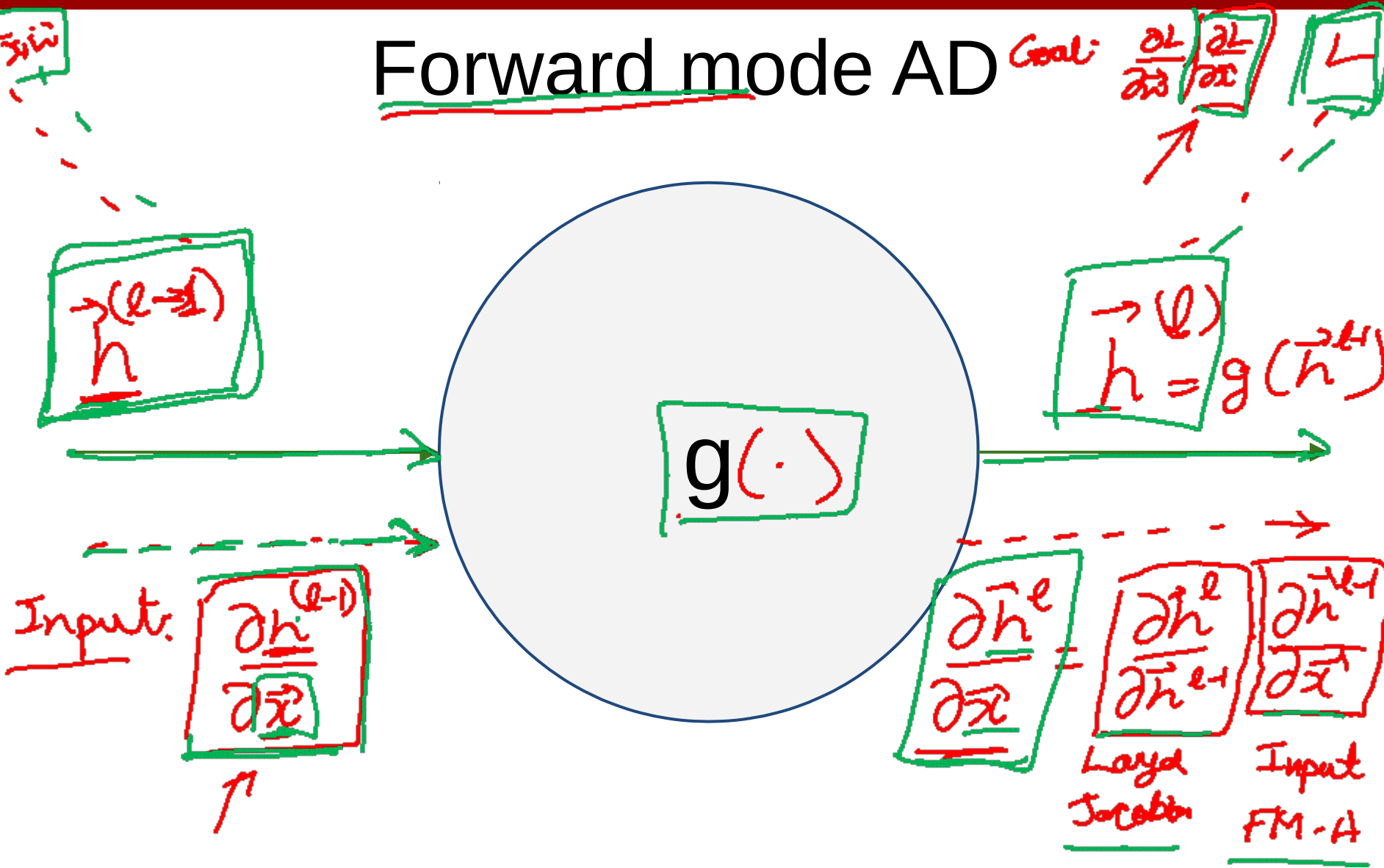
- Computation = Graph

- Input = Data + Parameters
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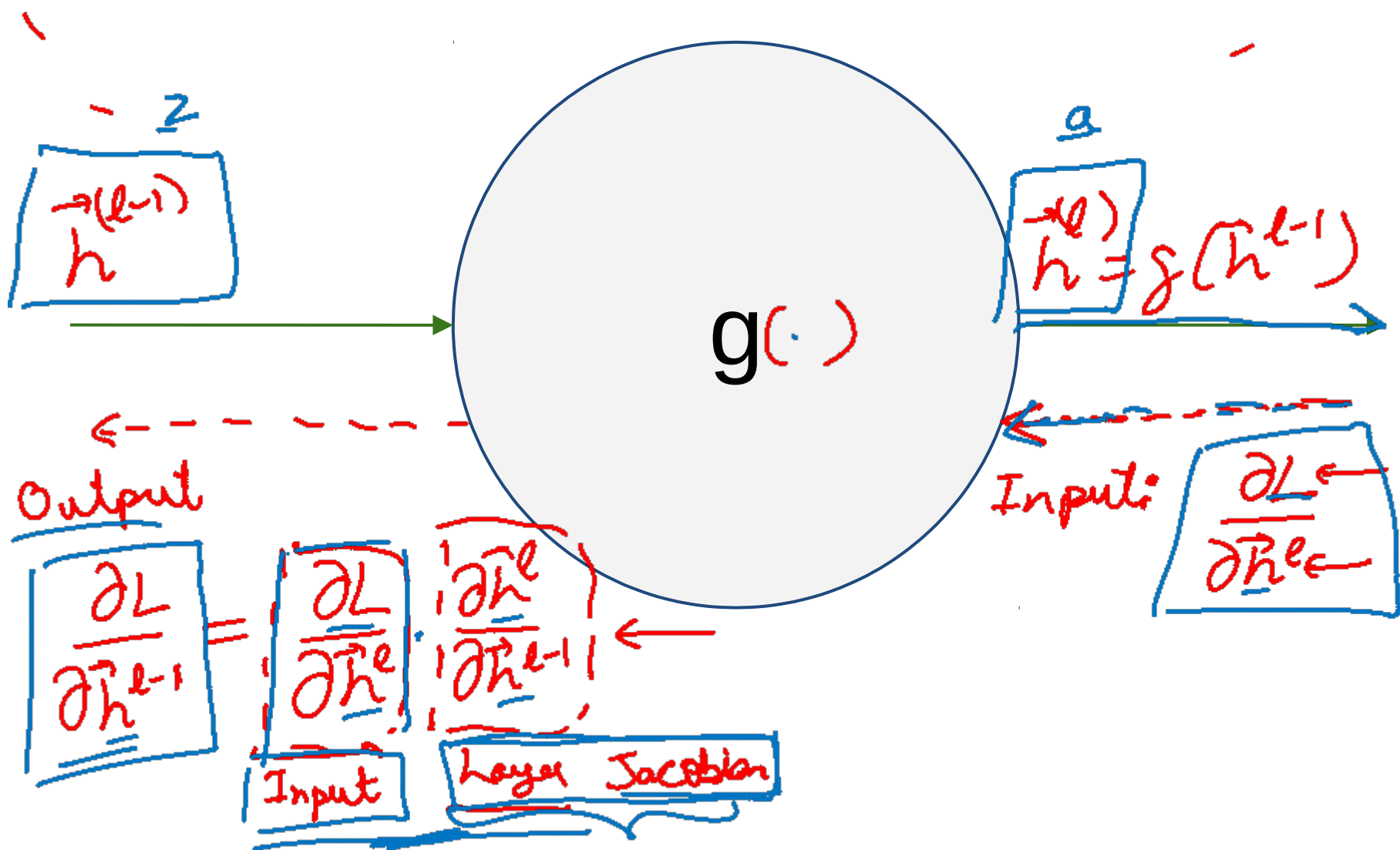
- Auto-Diff

- A family of algorithms for
implementing chain-rule on computation graphs

Forward mode AD



Reverse mode AD Goal: $\frac{\partial L}{\partial \mathbf{x}}$



Plan for Today

- Automatic Differentiation
 - (Finish) Forward mode vs Reverse mode AD
 - Backprop
 - Patterns in backprop

Example: Forward mode AD

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

$\frac{\partial f}{\partial \mathbf{x}} = \left[\frac{\partial f}{\partial x_1} \quad \frac{\partial f}{\partial x_2} \right]$

$\frac{\partial f}{\partial \mathbf{x}}$
 $= \cos(x_1) + x_2$

$w_1 = \sin(x_1)$

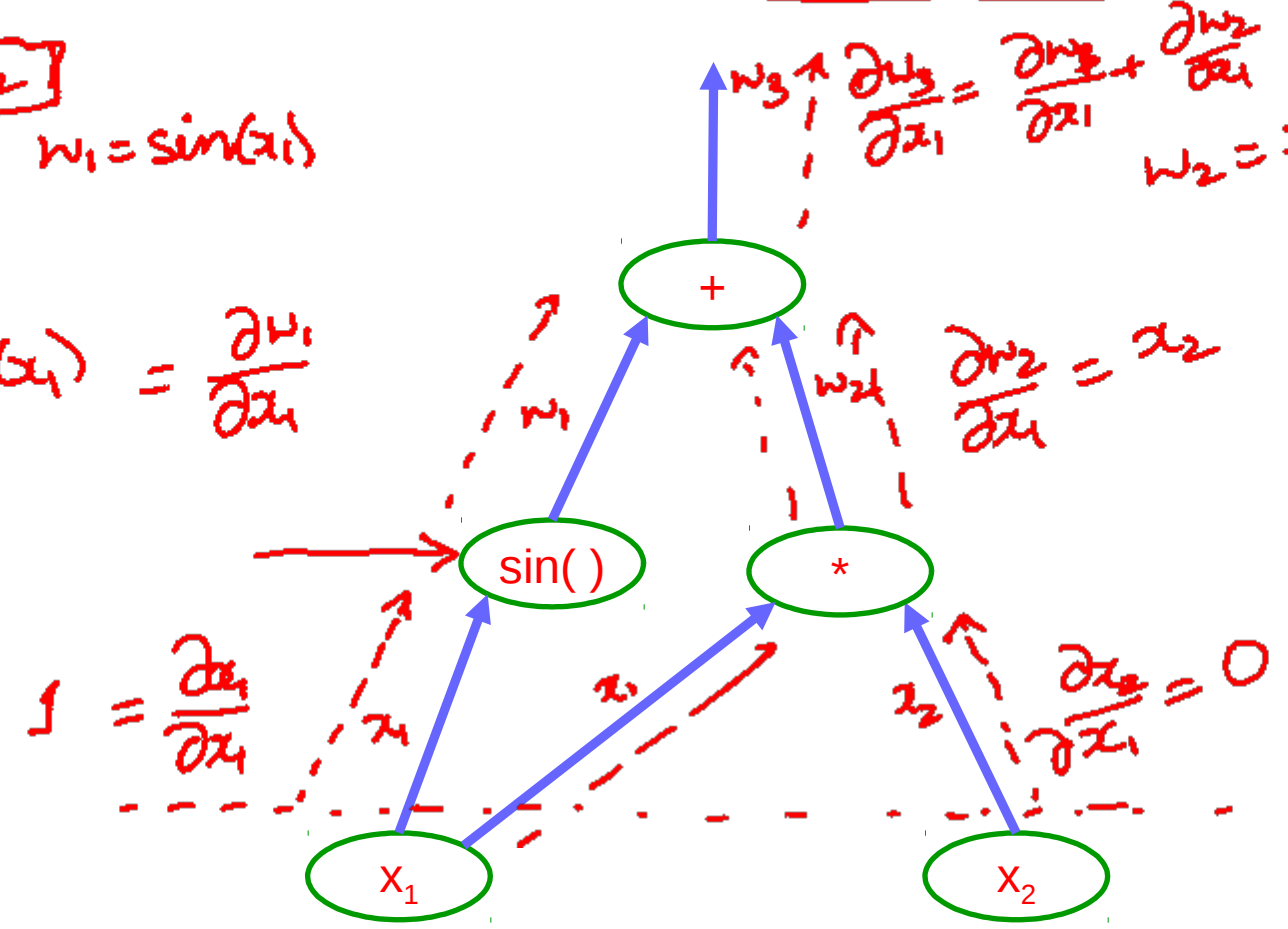
$\frac{\partial w_3}{\partial x_1} = \frac{\partial w_1}{\partial x_1} + \frac{\partial w_2}{\partial x_1}$

$w_2 = x_1 x_2$

$\cos(x_1) = \frac{\partial w_1}{\partial x_1}$

$1 = \frac{\partial x_1}{\partial x_1}$

$\frac{\partial x_2}{\partial x_1} = 0$

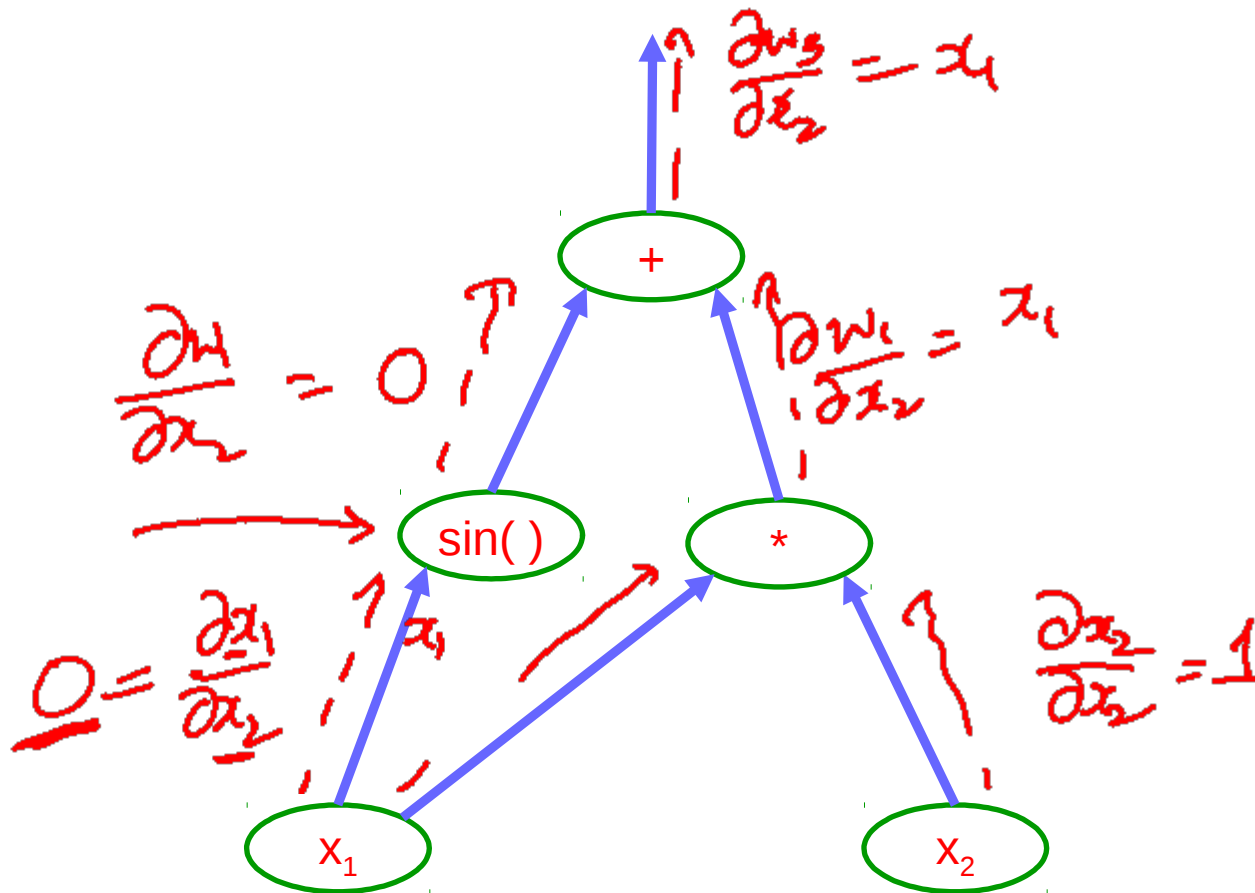


Example: Forward mode AD

$$\frac{\partial f}{\partial x_2}$$

$$= x_1$$

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



Example: Forward mode AD

$$\frac{df}{dx} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} f(x_1, x_2) = \sin(x_1) + x_1 x_2$$

for a index, x_i
compute/evaluate

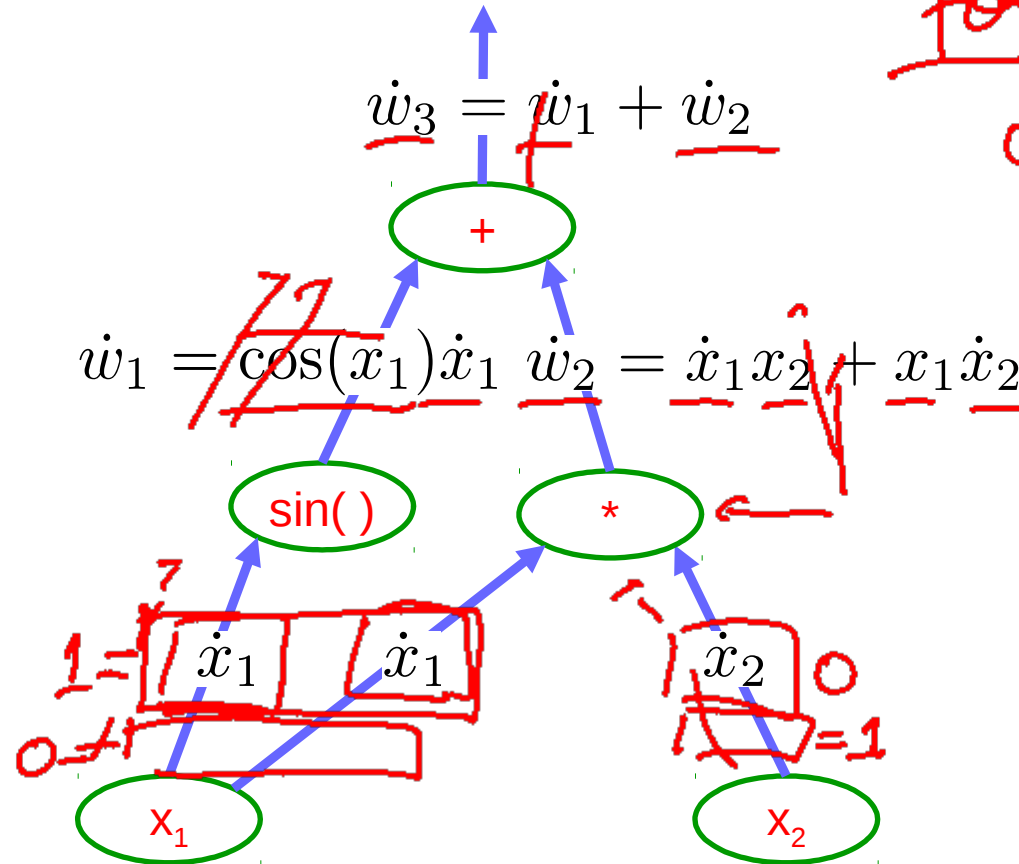
$$\dot{w}_3 = \frac{\partial w_3}{\partial a}$$

$$\dot{w}_2 = \frac{\partial w_2}{\partial a}$$

$$\dot{w}_1 = \frac{\partial w_1}{\partial a}$$

$$\dot{x}_1 = \frac{\partial x_1}{\partial a}$$

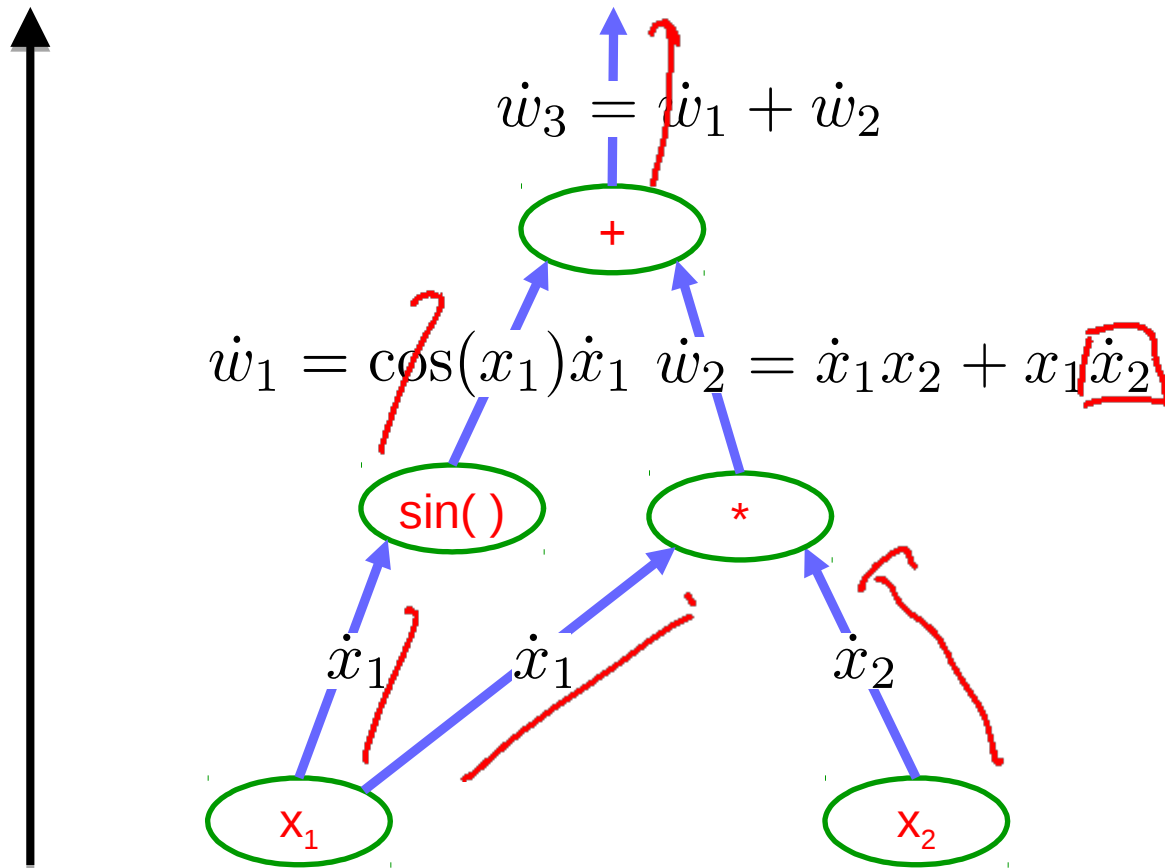
$$\dot{x}_2 = \frac{\partial x_2}{\partial a}$$



Example: Forward mode AD

$$\underline{f(x_1, x_2)} = \underline{\sin(x_1)} + x_1 x_2$$

$$\frac{\partial f}{\partial \underline{x}}$$

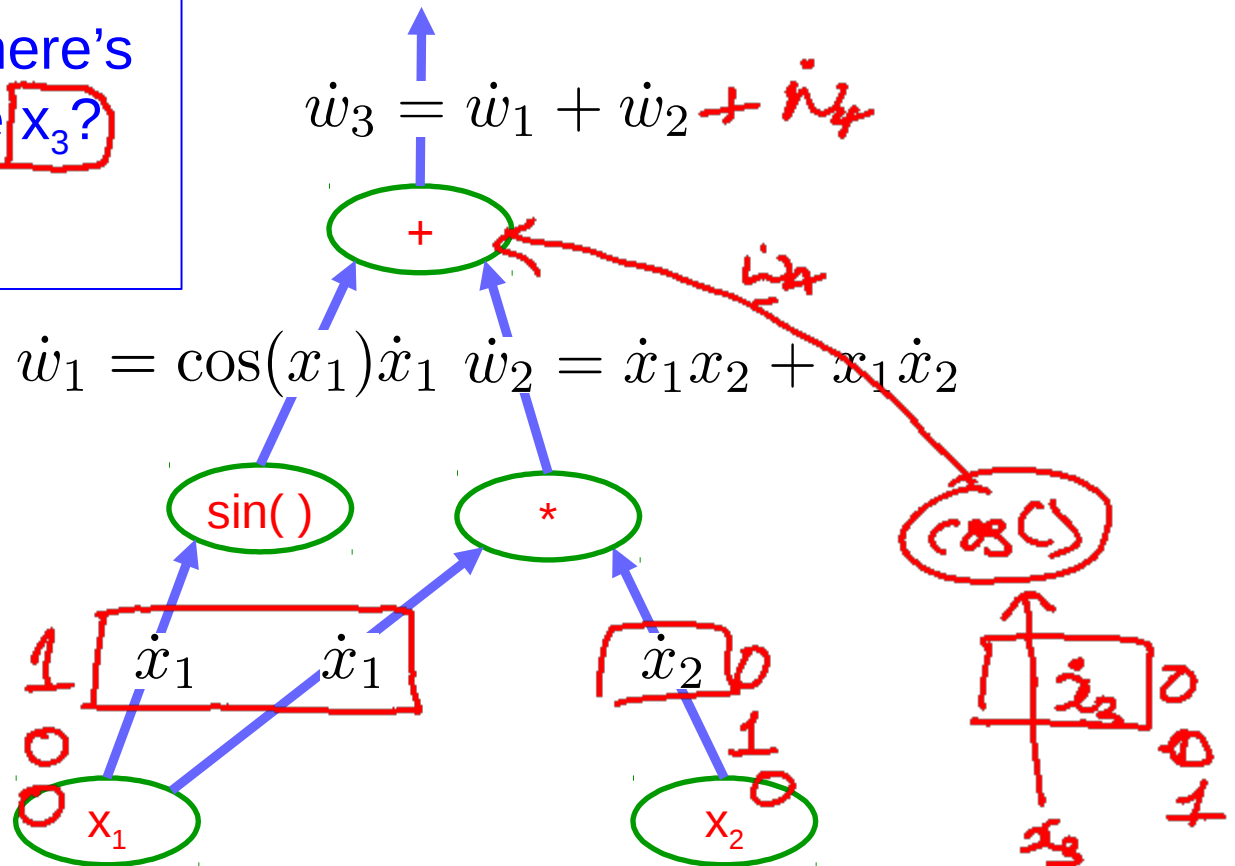


Example: Forward mode AD

$$f(x_1, x_2) = \sin(x_1) + x_1x_2 + \cos(x_3)$$

Q: What happens if there's another input variable x_3 ?

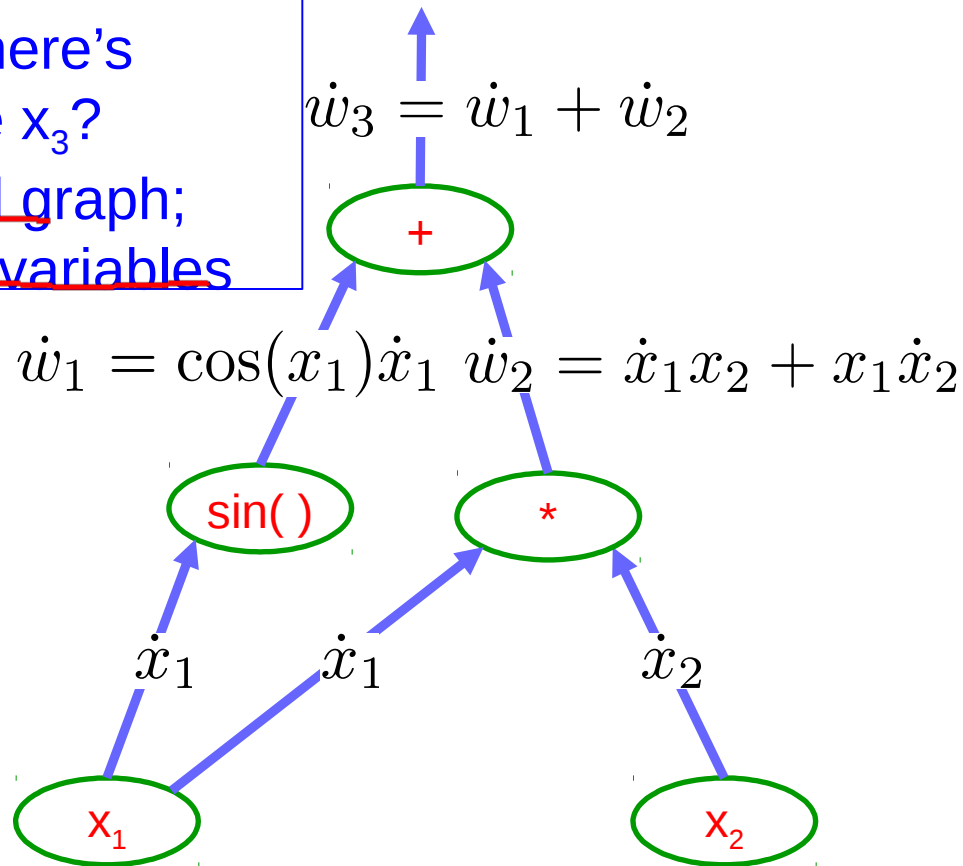
for a in {x1, x2, x3}



Example: Forward mode AD

$$f(x_1, x_2) = \sin(x_1) + x_1x_2$$

Q: What happens if there's another input variable x_3 ?
A: more sophisticated graph;
 $d+1$ "passes" for $d+1$ variables



$\frac{\partial f}{\partial x}$

Example: Forward mode AD

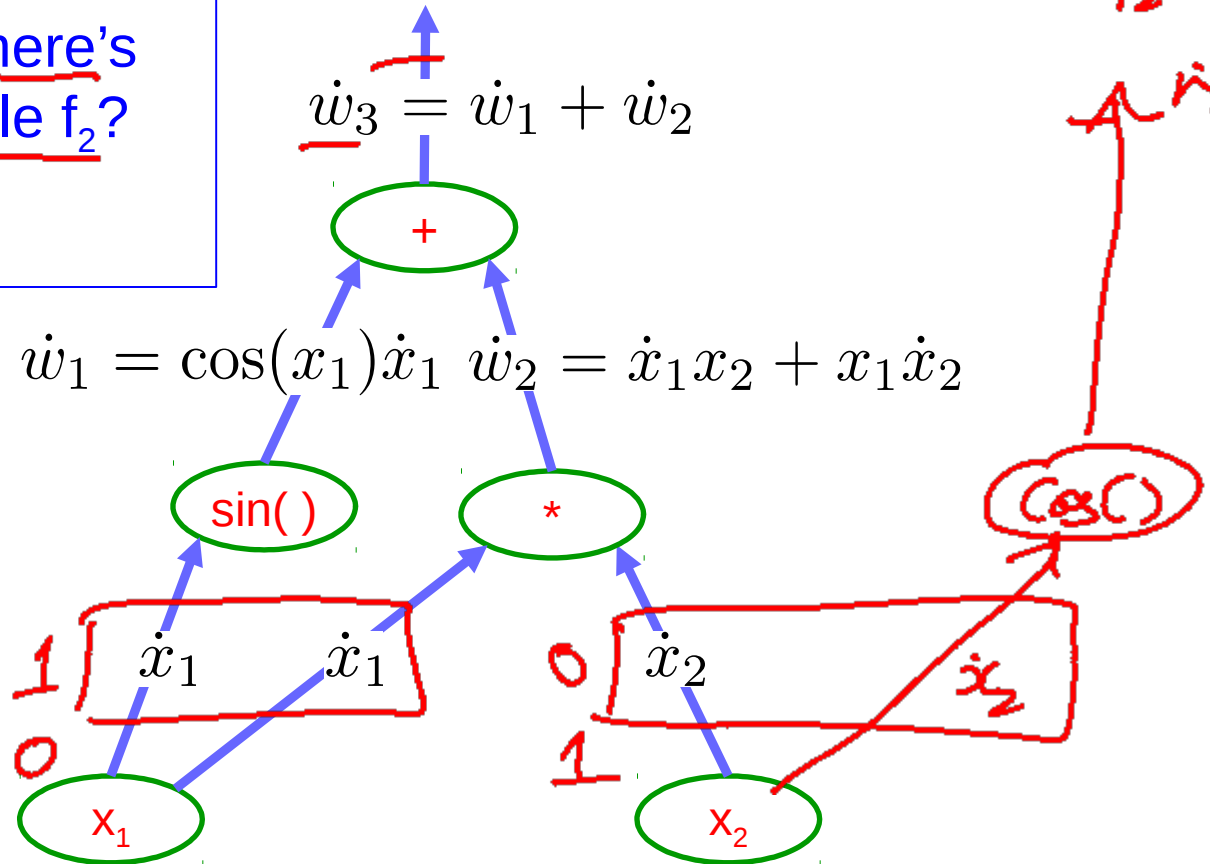
$$f_1(x_1, x_2) = \sin(x_1) + x_1x_2$$

$f_2 = \cos(x_2)$

$f_2 = \sin(x_2)$

$f_2 = \sin(x_2)$

Q: What happens if there's another output variable f_2 ?



for a in $\{x_1, x_2\}$

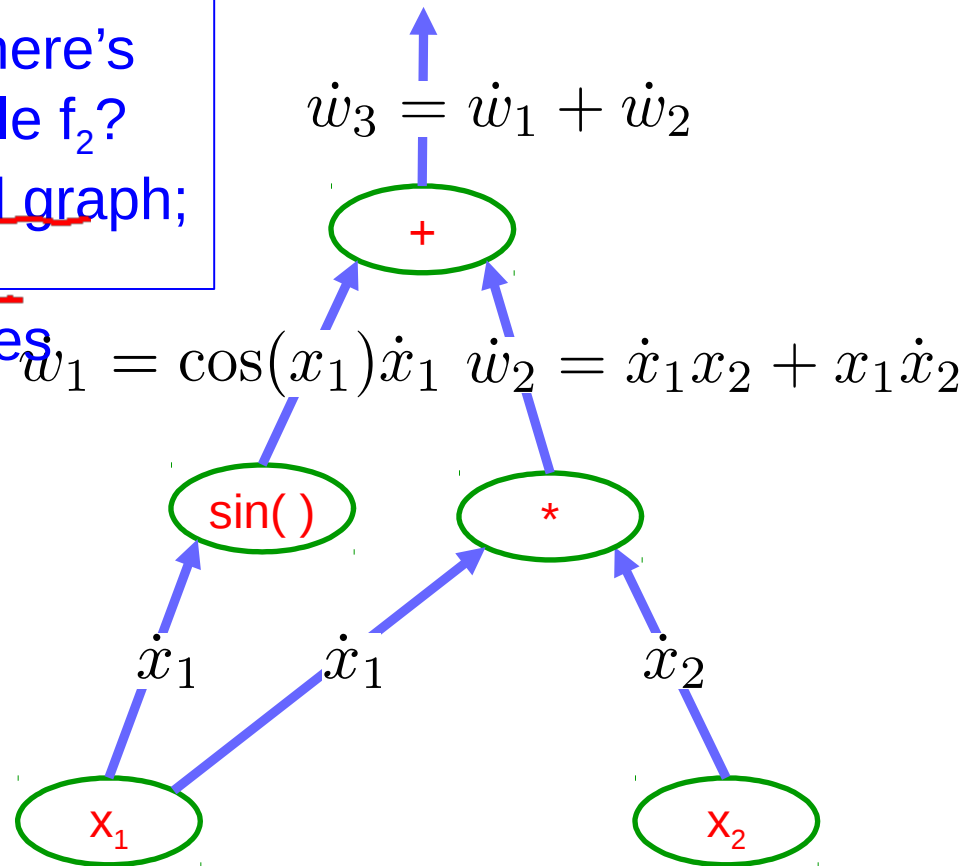
Example: Forward mode AD

$$f(x_1, x_2) = \sin(x_1) + x_1x_2$$

Q: What happens if there's another output variable f_2 ?

A: ~~more sophisticated graph;~~

~~and "passes" for variables~~



Goal: Example: Reverse mode AD

$$\frac{\partial f}{\partial \vec{x}} = \left[\frac{\partial f}{\partial x_1} \quad \frac{\partial f}{\partial x_2} \right] f(x_1, x_2) = \sin(x_1) + x_1 x_2$$

$$w_3 = w_1 + w_2$$

$$\frac{\partial w_3}{\partial w_1} = 1$$

$$\bar{w}_3 = \frac{\partial f}{\partial w_3} = \frac{\partial w_3}{\partial w_3} = 1$$

$$\bar{w}_1 = \frac{\partial f}{\partial w_1} = \frac{\partial f}{\partial w_3} \frac{\partial w_3}{\partial w_1}$$

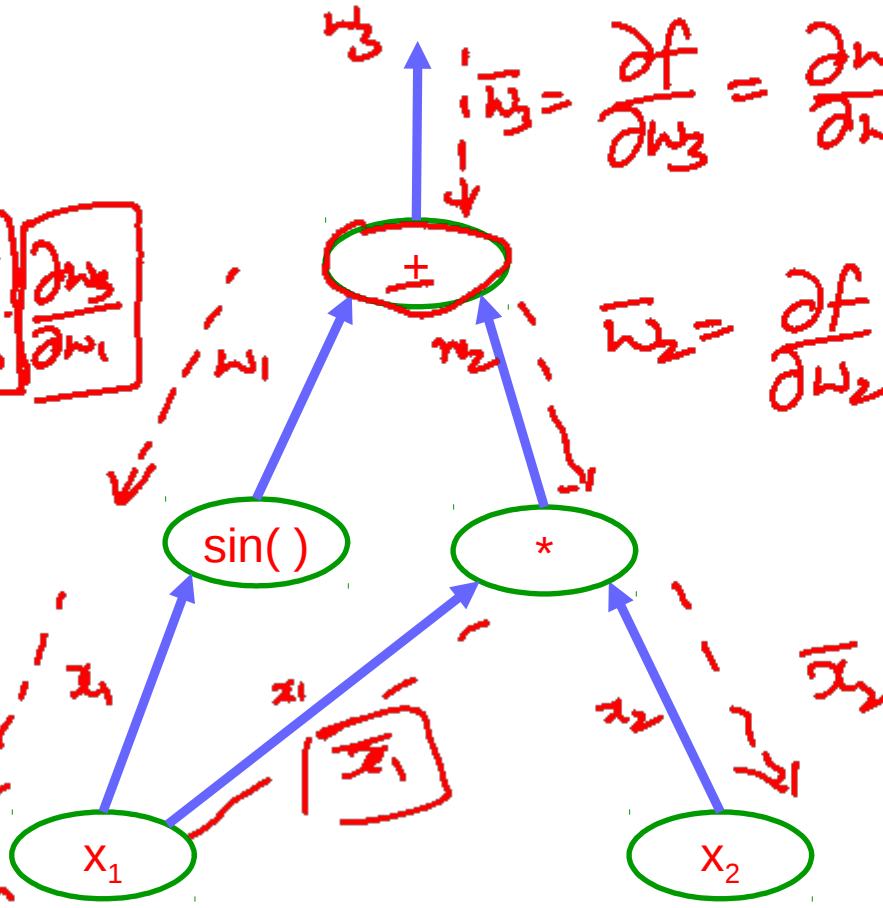
$$\bar{w}_2 = \frac{\partial f}{\partial w_2} = \frac{\partial f}{\partial w_3}$$

bug def.

$$\bar{x}_2 = \frac{\partial f}{\partial x_2}$$

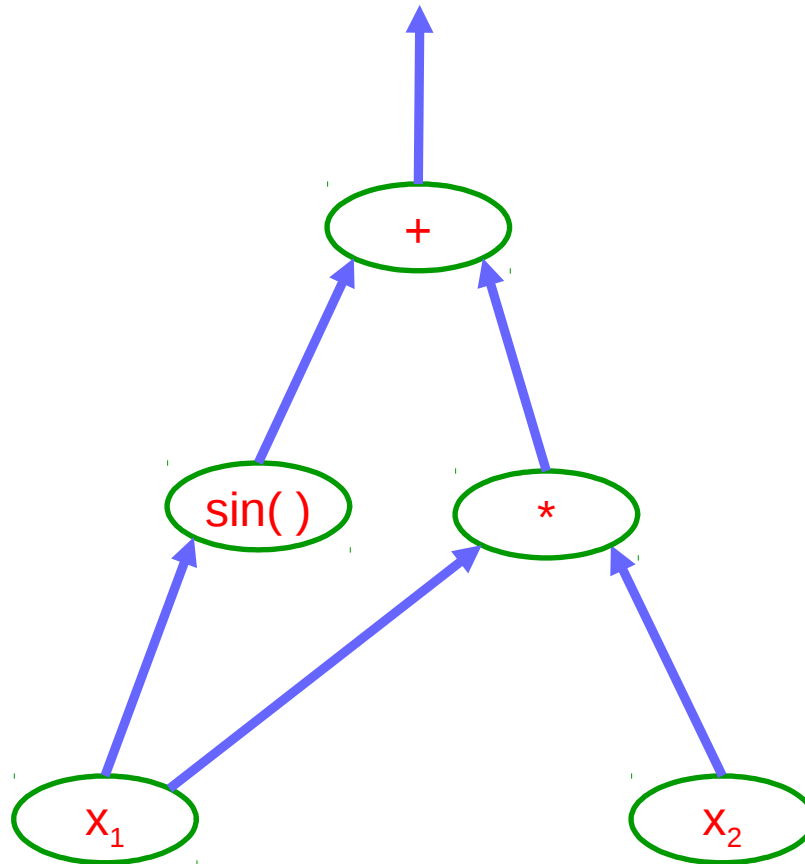
$$\bar{x}_1 = \frac{\partial f}{\partial x_1} = \frac{\partial f}{\partial w_1} \frac{\partial w_1}{\partial x_1}$$

input \bar{w}_1 to function (operator)

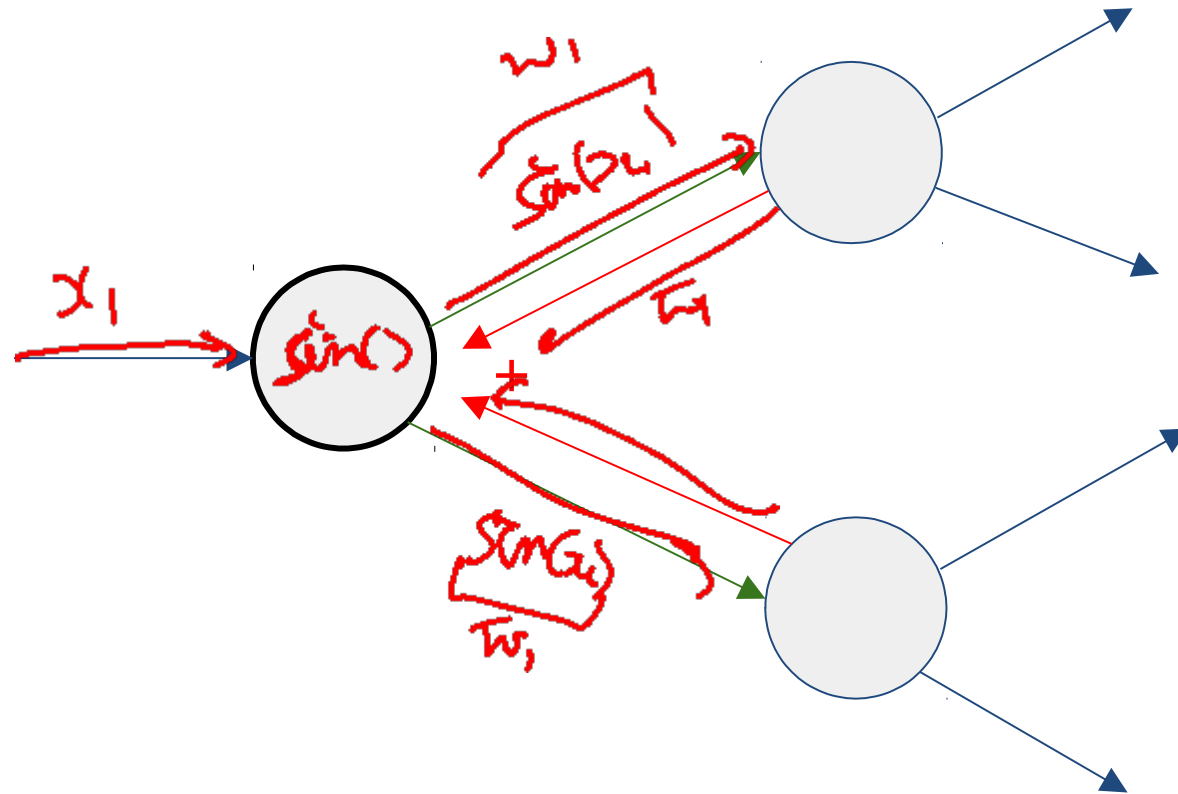


Example: Reverse mode AD

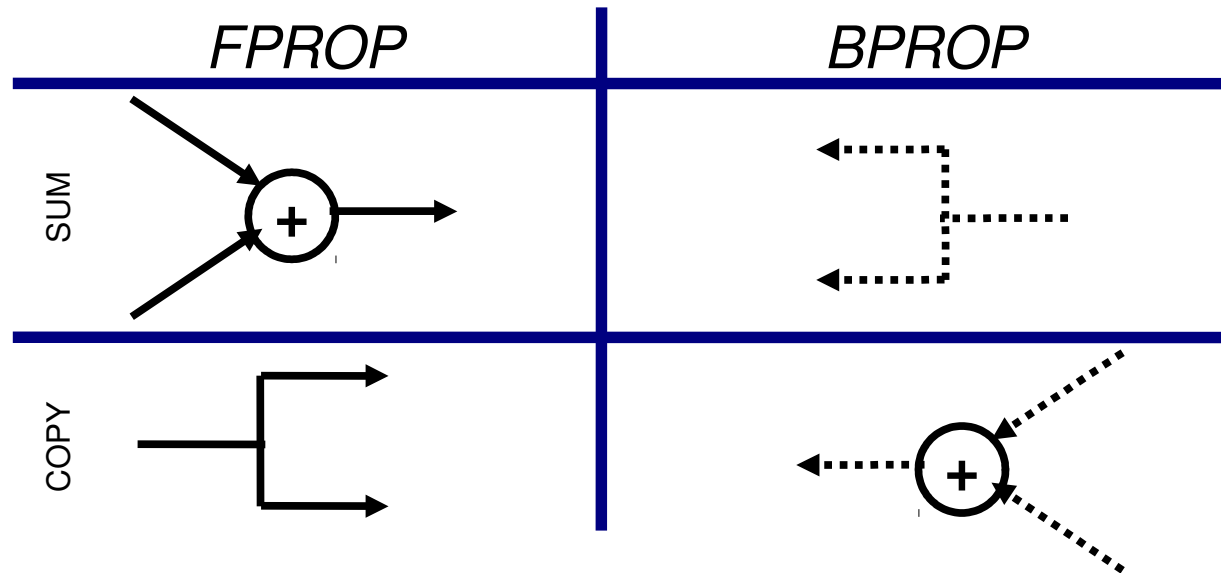
$$f(x_1, x_2) = \sin(x_1) + x_1x_2$$



Gradients add at branches



Duality in Fprop and Bprop

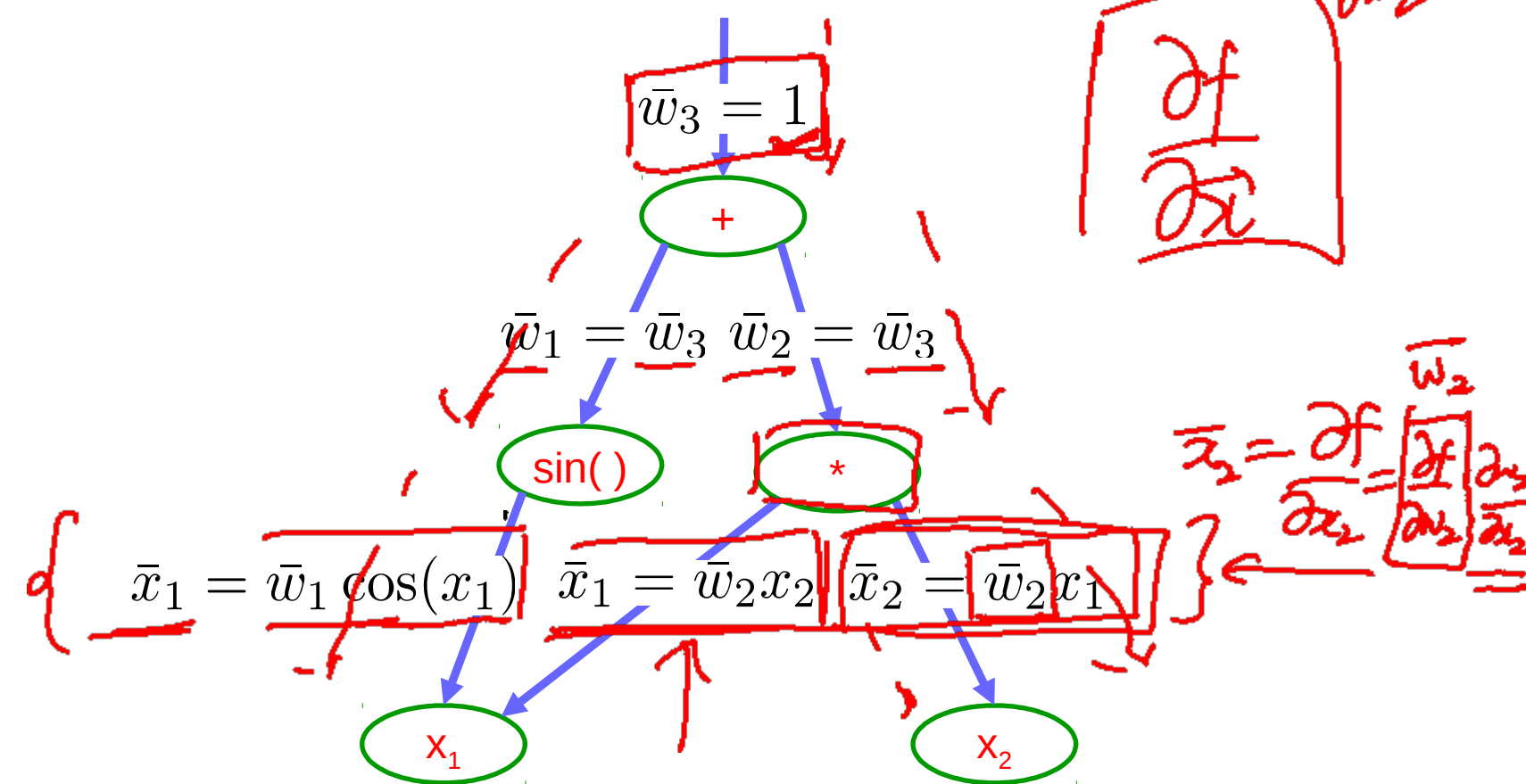


Example: Reverse mode AD

$$f(x_1, x_2) = \sin(x_1) + x_1x_2$$

Handwritten: $w_2 = x_1, x_2$
 $\frac{\partial w_2}{\partial x_2} = x_1$

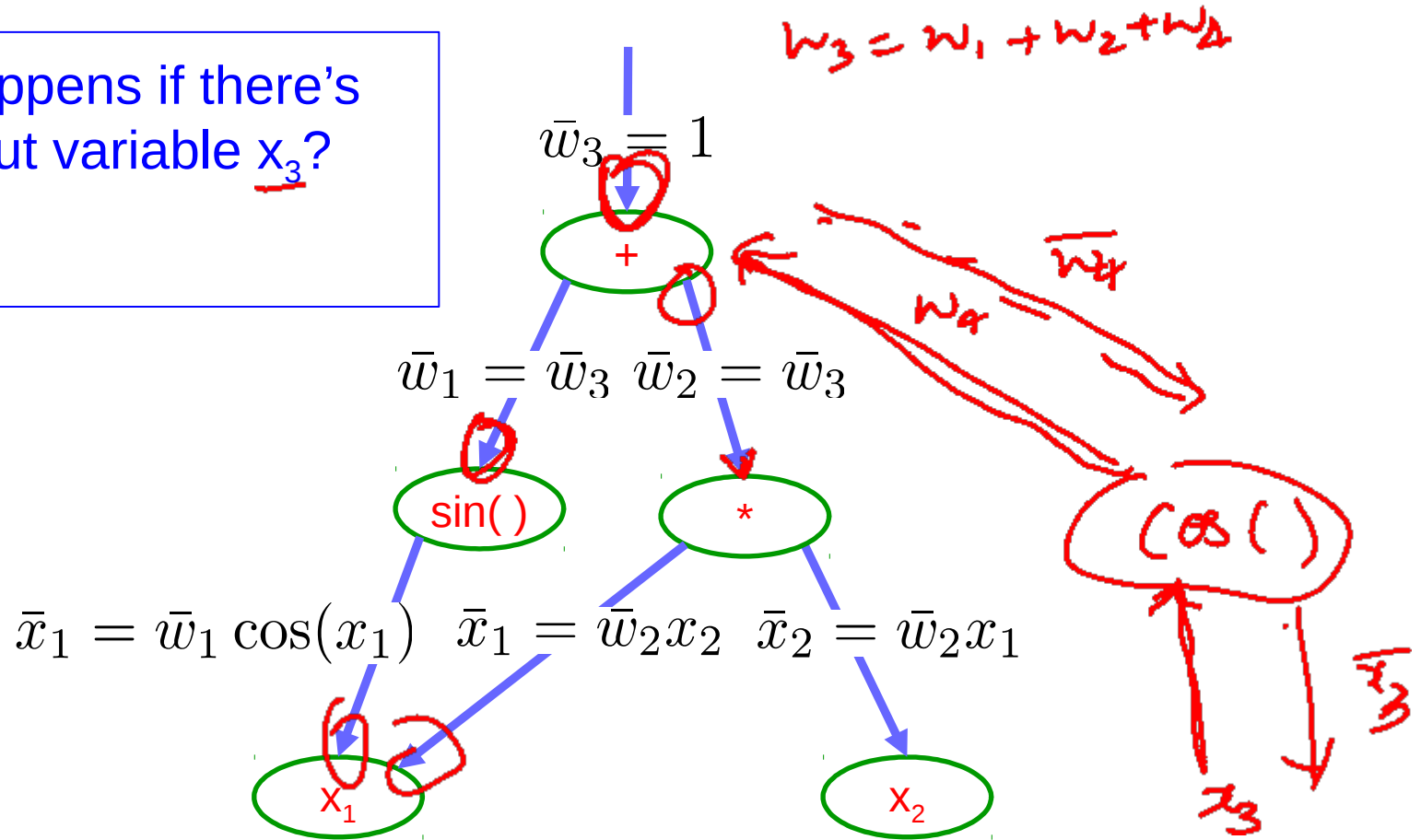
Handwritten: $\frac{\partial f}{\partial \vec{x}}$



Example: Reverse mode AD

$$f(x_1, x_2) = \sin(x_1) + x_1x_2 + \cos(x_3)$$

Q: What happens if there's another input variable x_3 ?



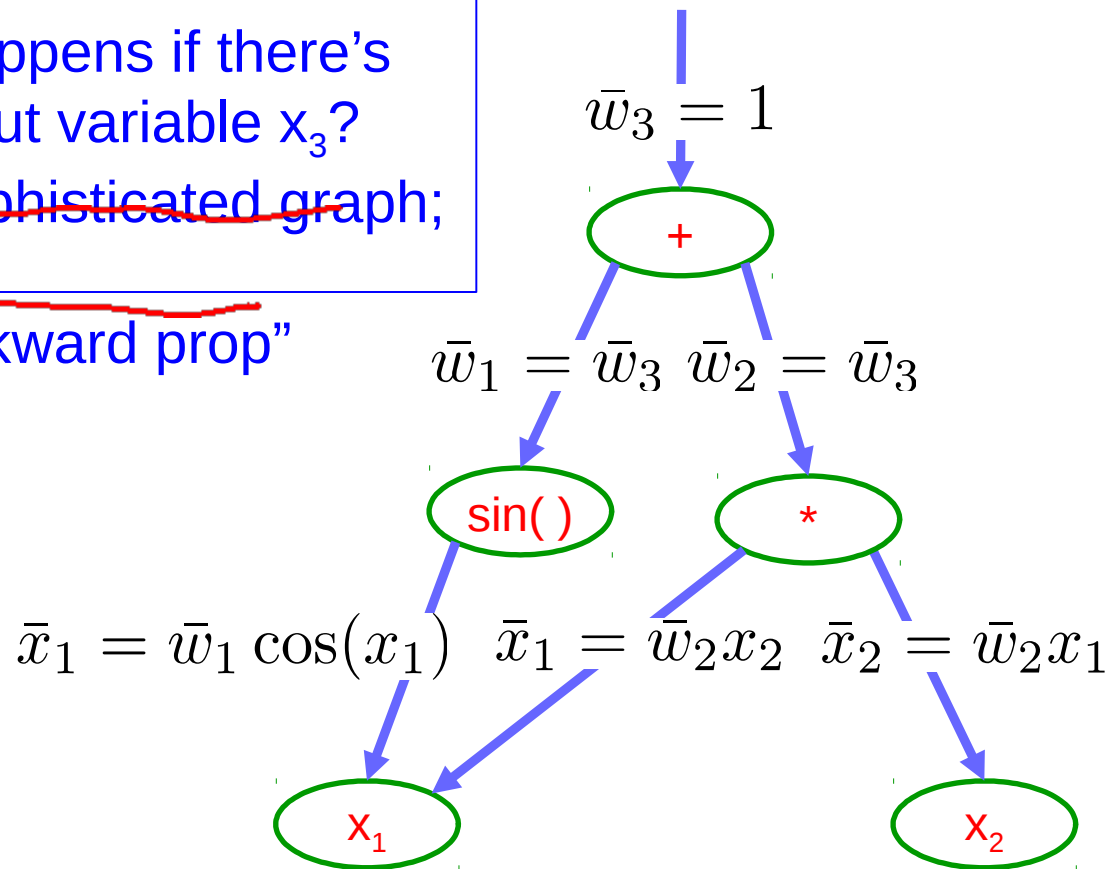
Example: Reverse mode AD

$$f(x_1, x_2) = \sin(x_1) + x_1x_2$$

Q: What happens if there's another input variable x_3 ?

A: ~~more sophisticated graph;~~

single "backward prop"



Example: Reverse mode AD

$$f_1(x_1, x_2) = \sin(x_1) + x_1 x_2 \quad f_2 = \cos(x_2)$$

Q: What happens if there's another output variable f_2 ?

for a in $\{f_1, f_2\}$

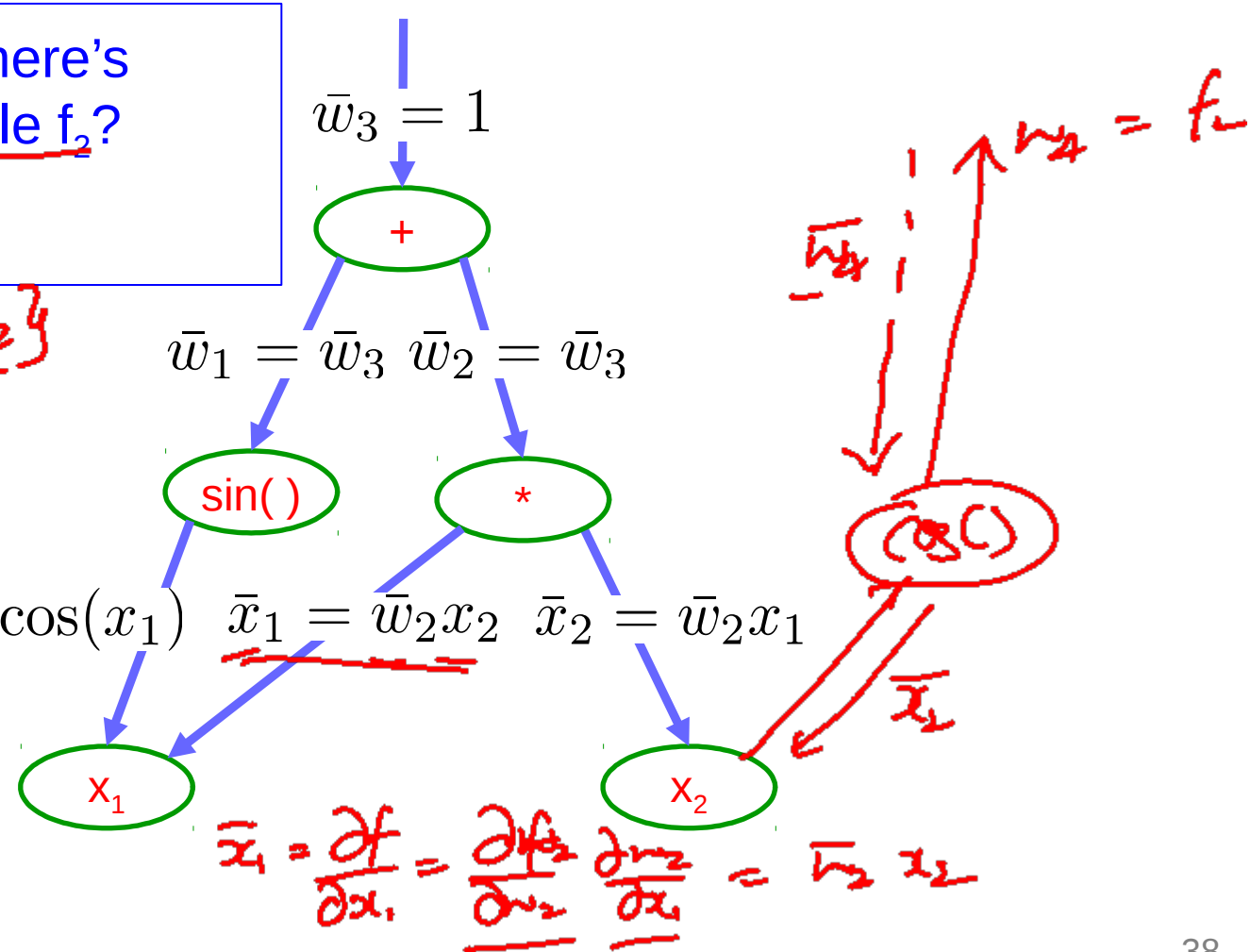
$$\bar{w}_4 = \frac{\partial a}{\partial w_4}$$

$$\bar{w}_3 = \frac{\partial a}{\partial w_3}$$

$$\bar{x}_1 = \bar{w}_1 \cos(x_1)$$

$$\bar{x}_1 = \bar{w}_2 x_2$$

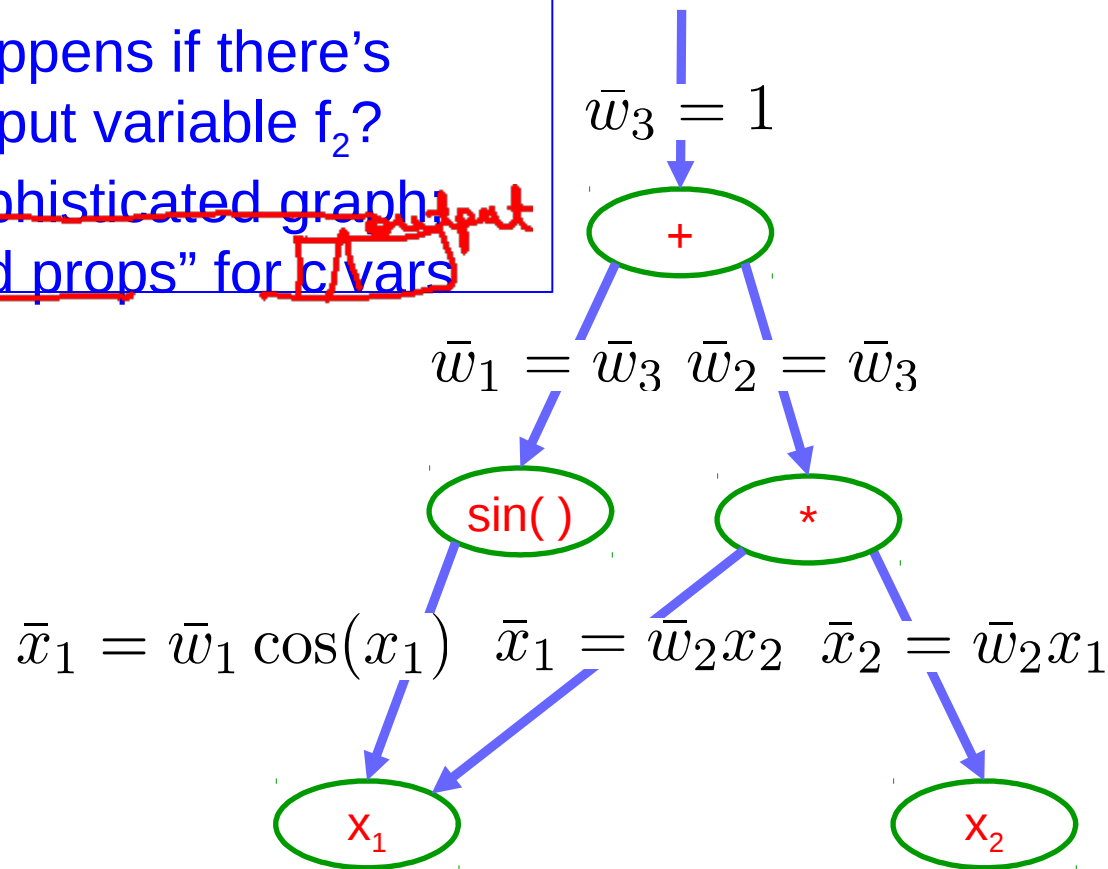
$$\bar{x}_2 = \bar{w}_2 x_1$$



Example: Reverse mode AD

$$f(x_1, x_2) = \sin(x_1) + x_1x_2$$

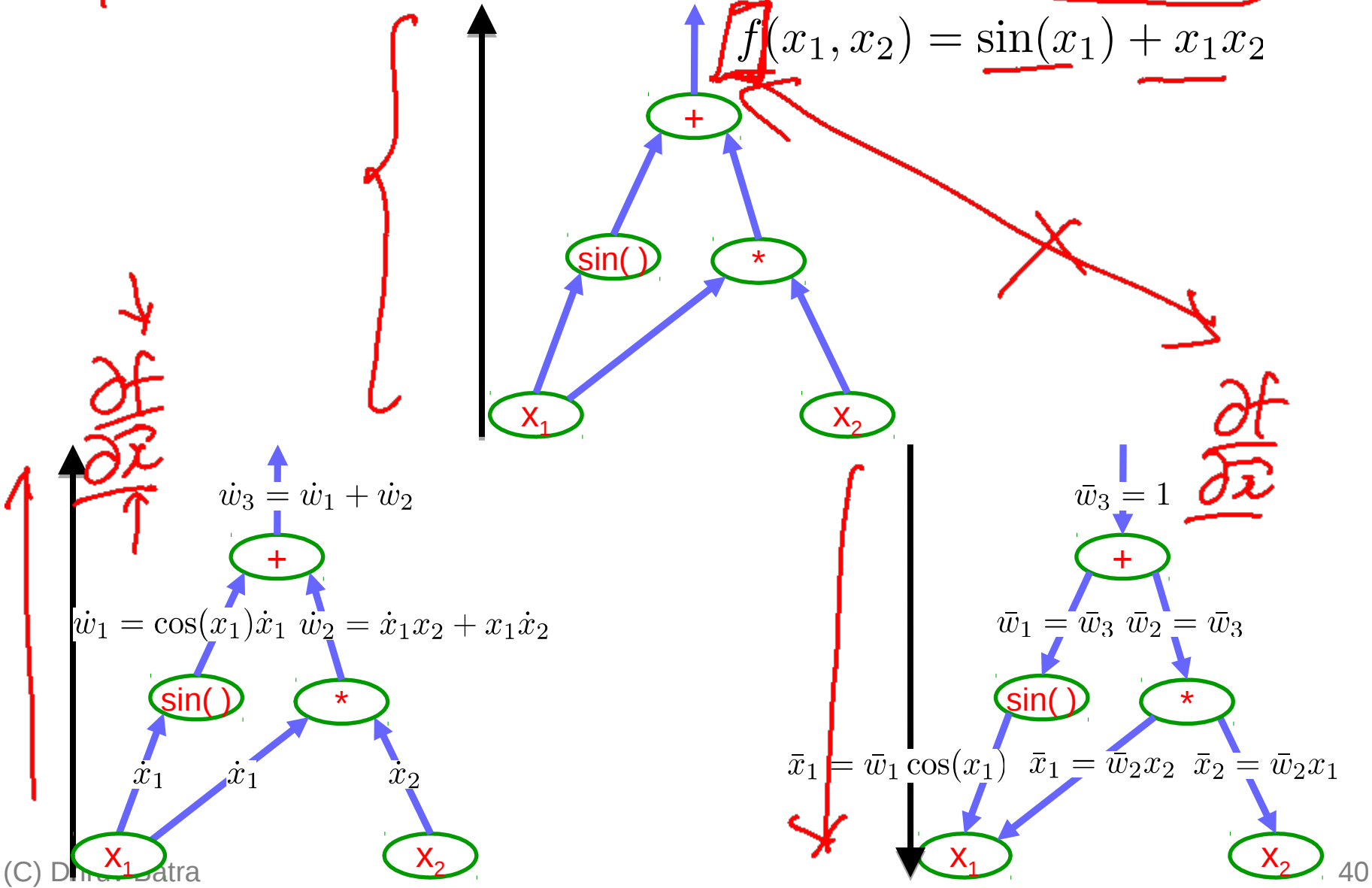
Q: What happens if there's another output variable f_2 ?
A: more sophisticated graph c "backward props" for c/vars



Forward Pass vs

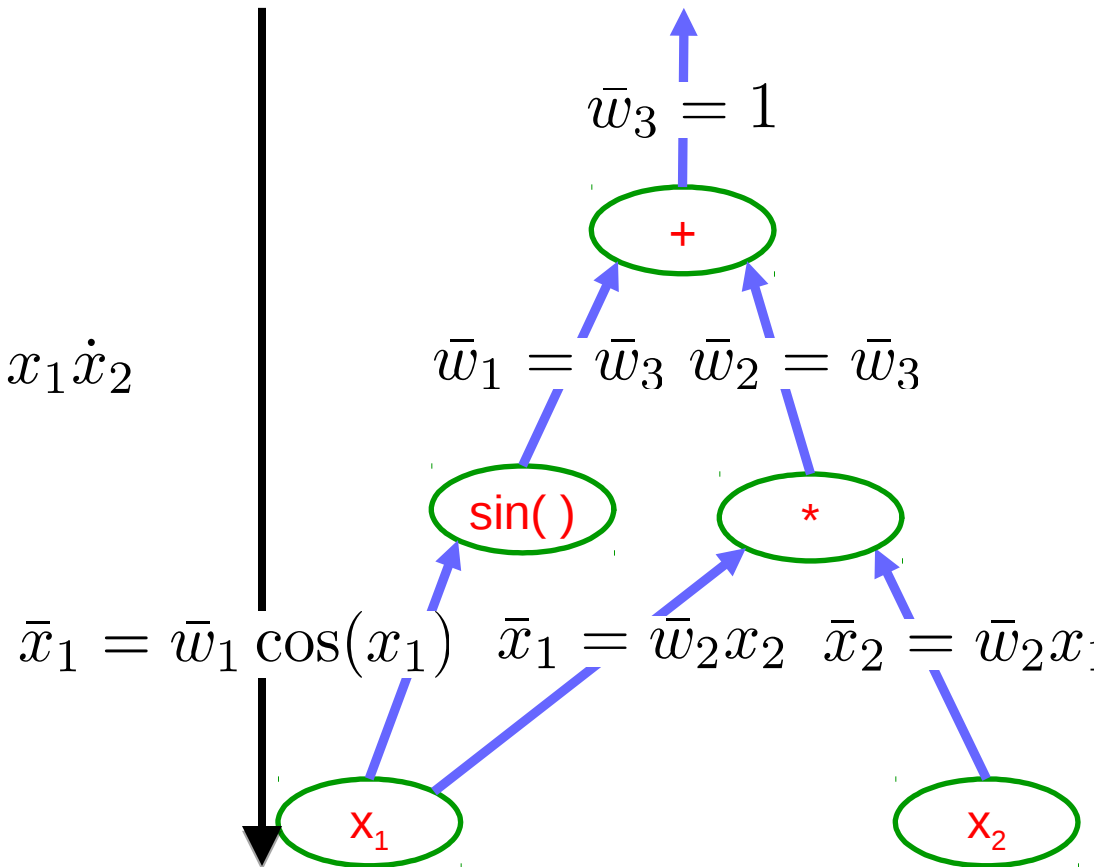
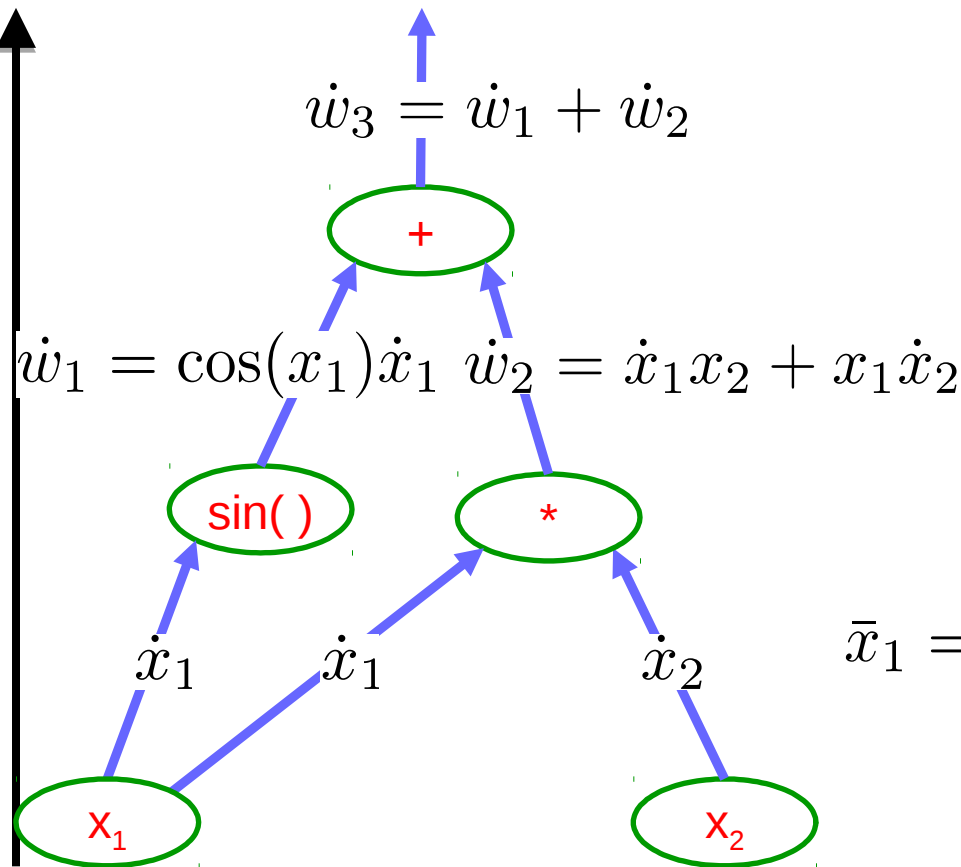
Forward mode AD vs Reverse Mode AD

$$f(x_1, x_2) = \sin(x_1) + x_1x_2$$



Forward mode vs Reverse Mode

- What are the differences?



Forward mode vs Reverse Mode

- What are the differences?



- Which one is faster to compute?

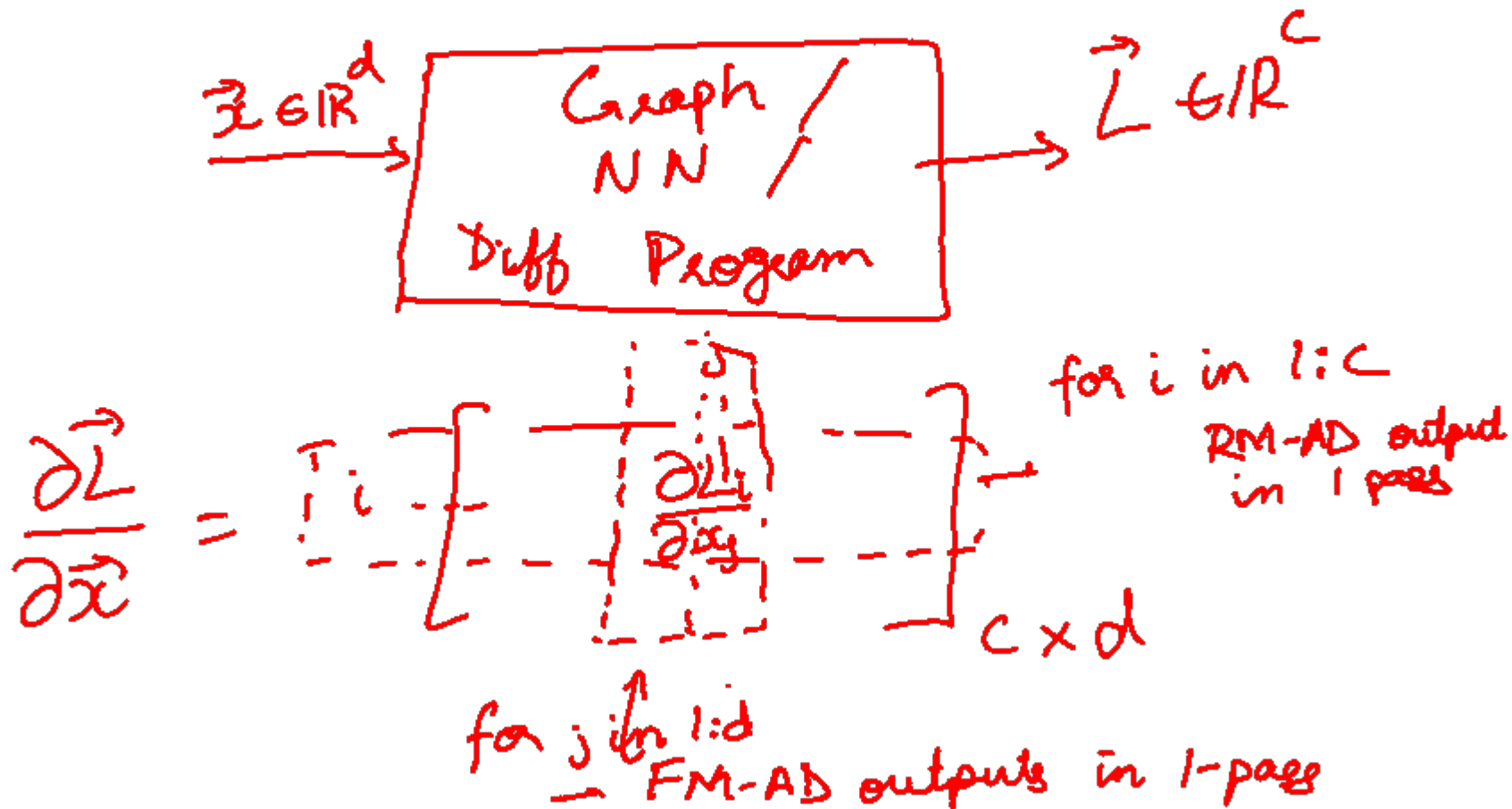
- Forward or backward?

Depends

Is $c > d$ or $d > c$?

Forward mode vs Reverse Mode

- x \rightarrow Graph \rightarrow L
- Intuition of Jacobian

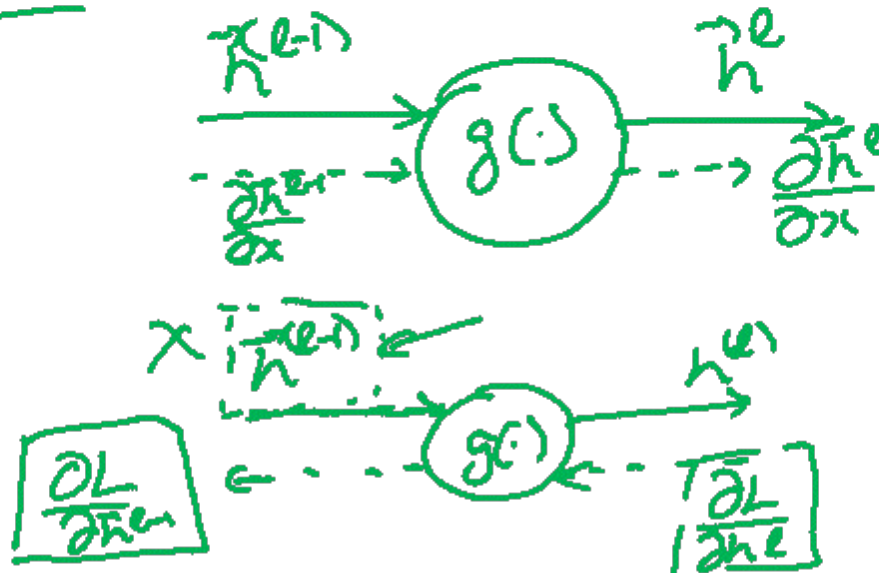


Forward mode vs Reverse Mode

- What are the differences?

- Which one is faster to compute?
 - Forward or backward?

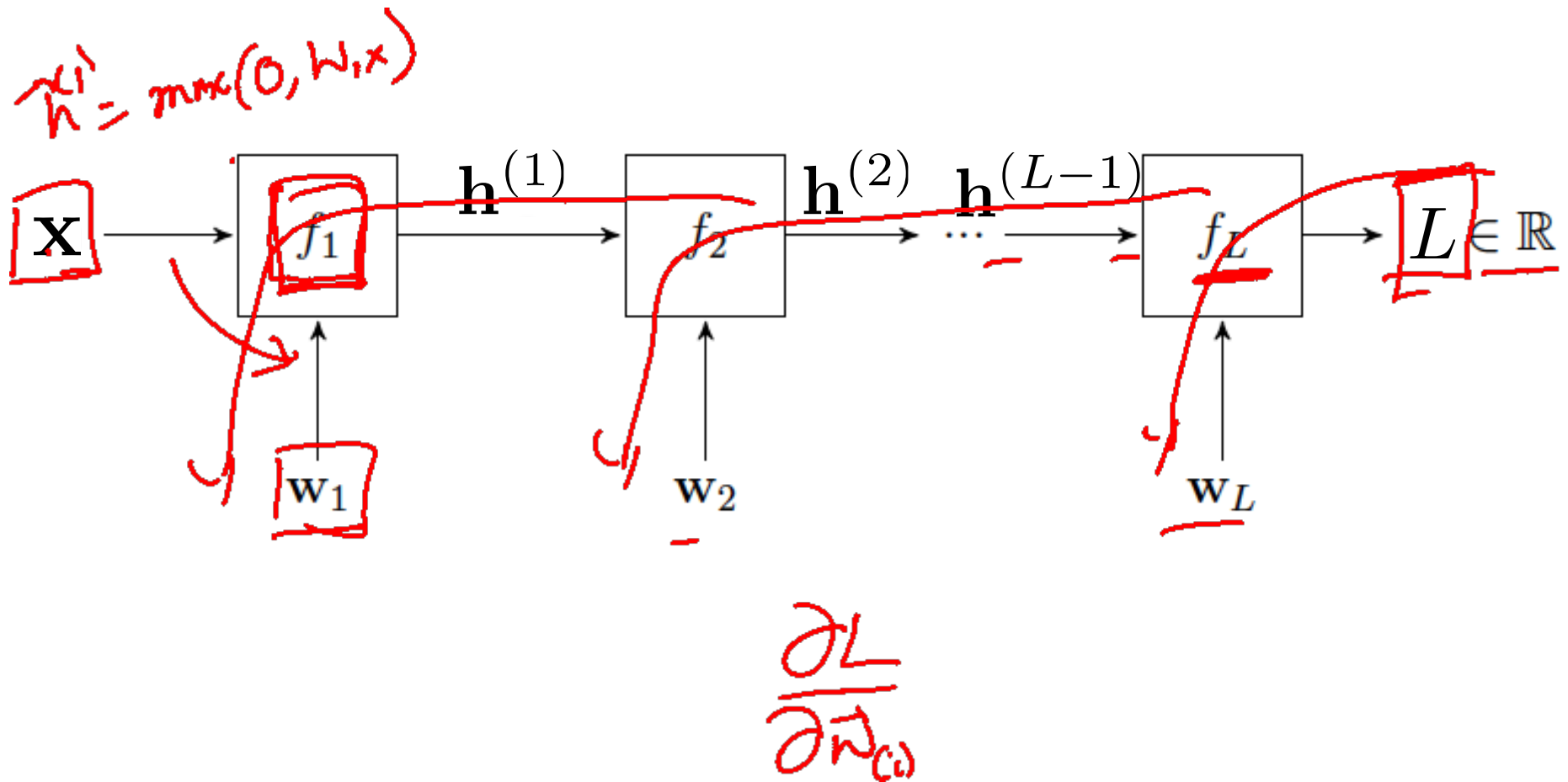
- Which one is more memory efficient (less storage)?
 - Forward or backward?



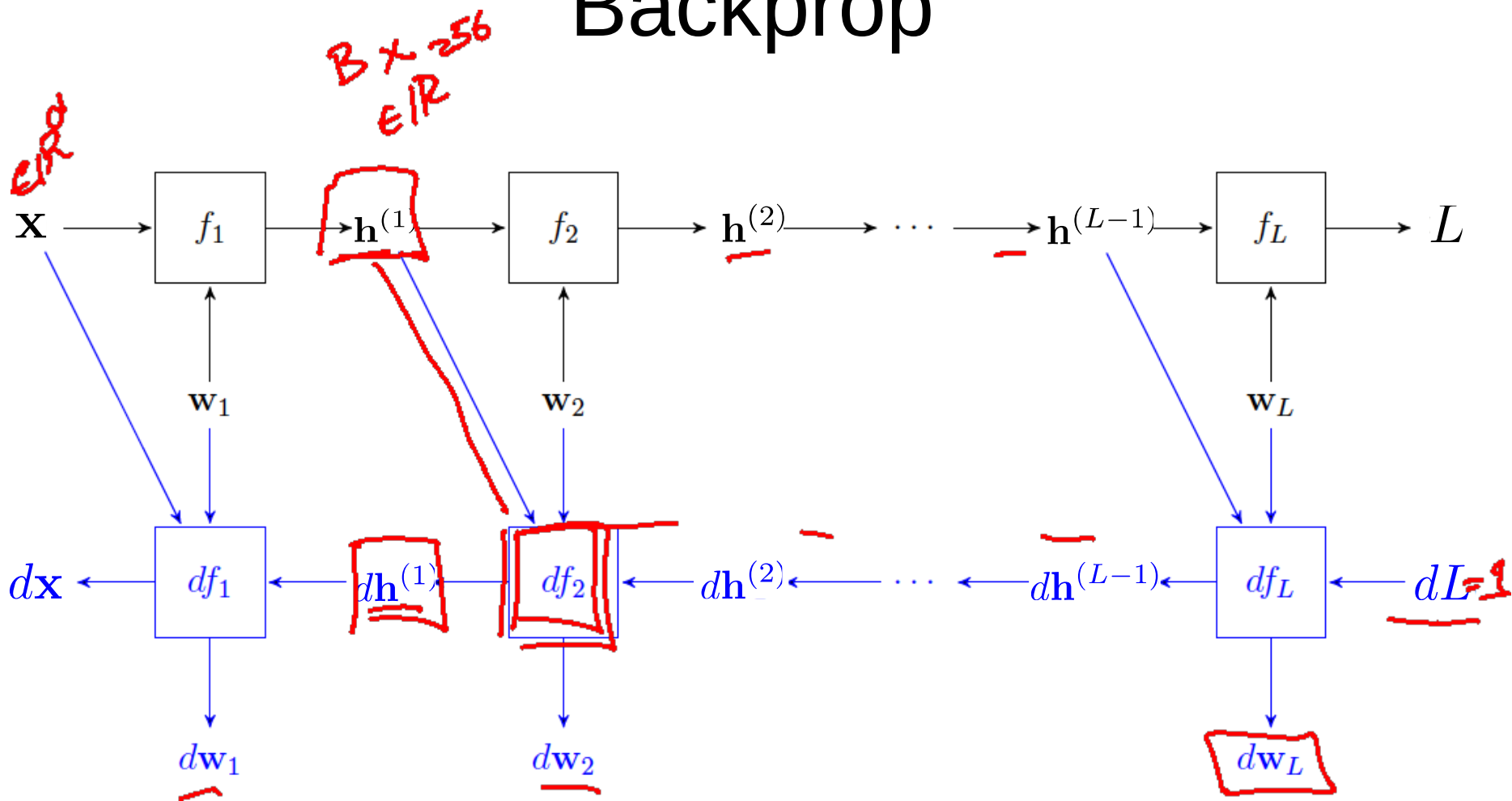
Plan for Today

- Automatic Differentiation
 - (Finish) Forward mode vs Reverse mode AD
 - Backprop
 - Patterns in backprop

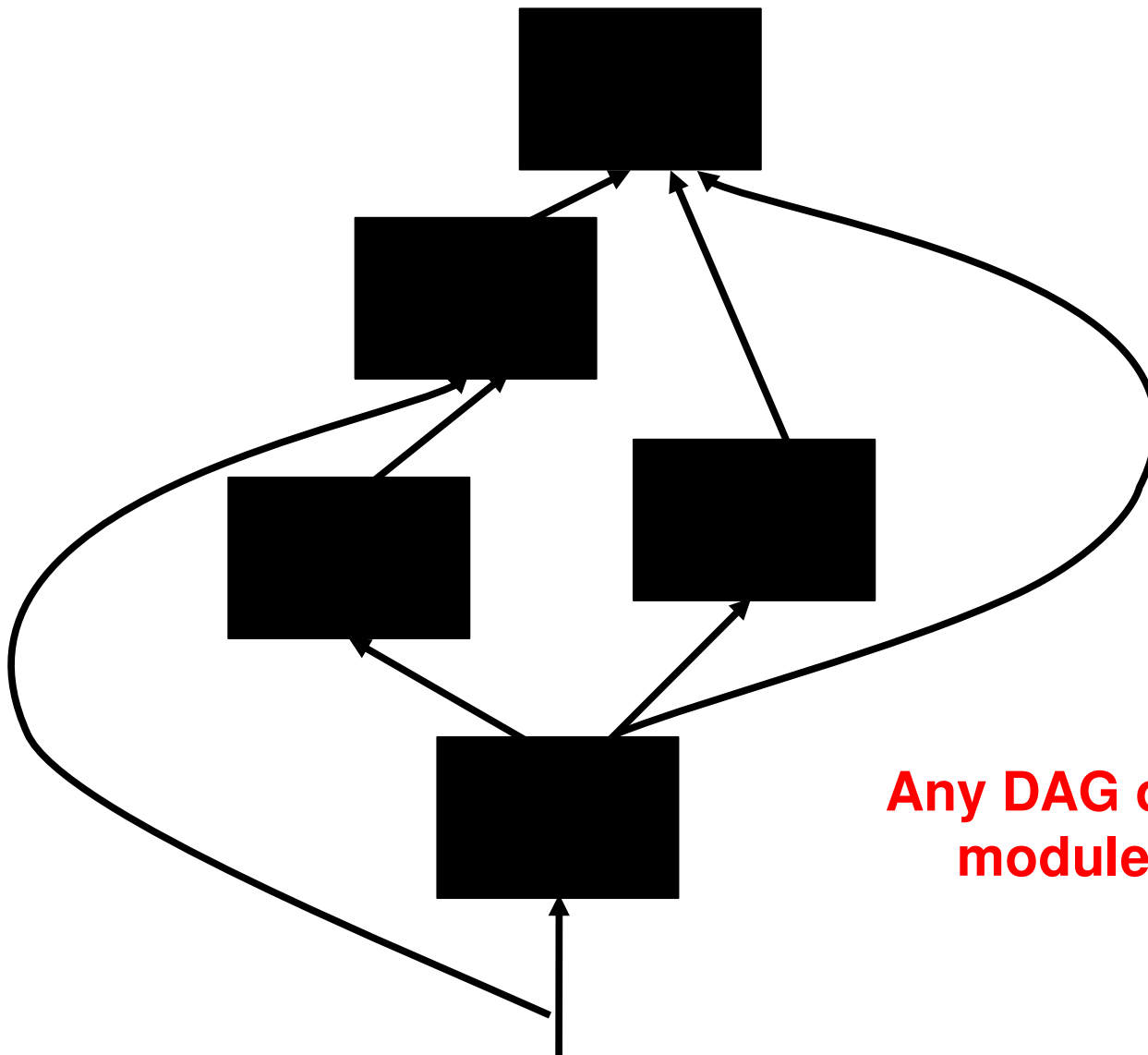
Neural Network Computation Graph



Backprop

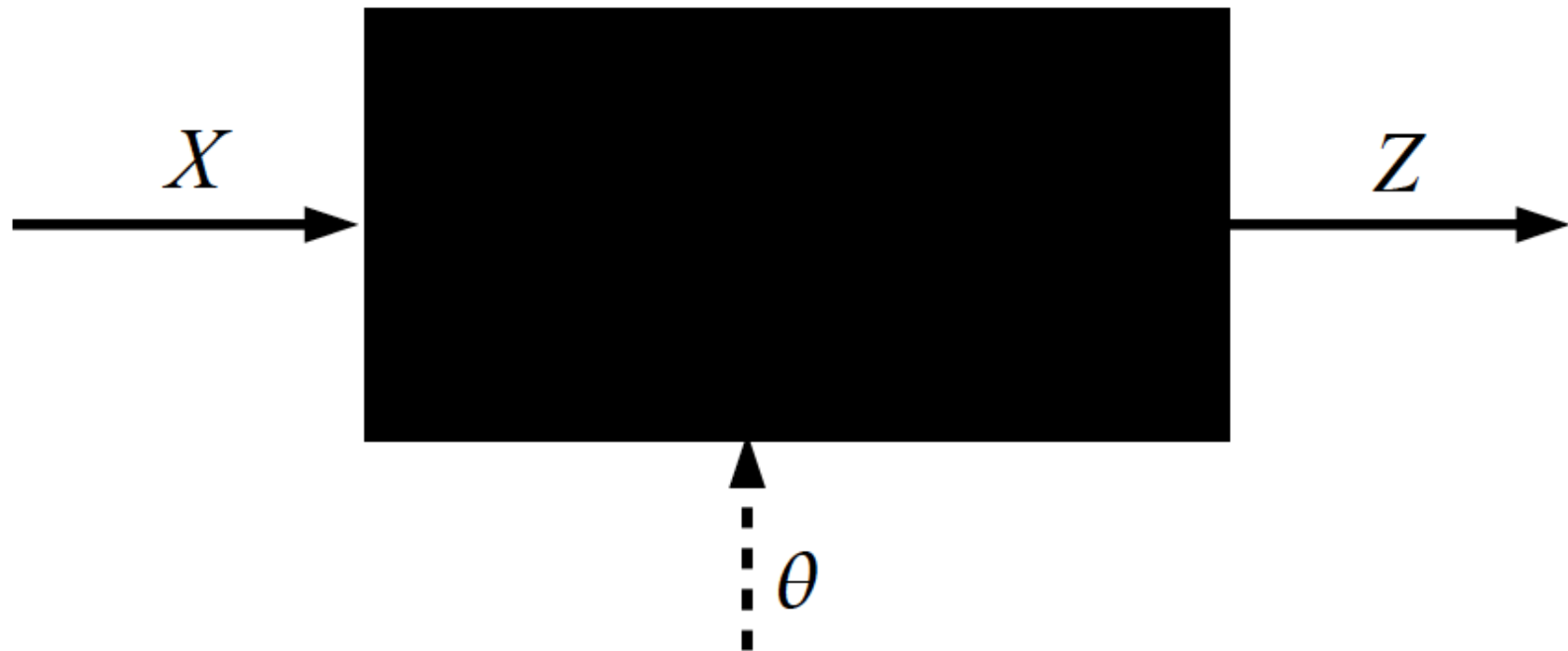


Computational Graph

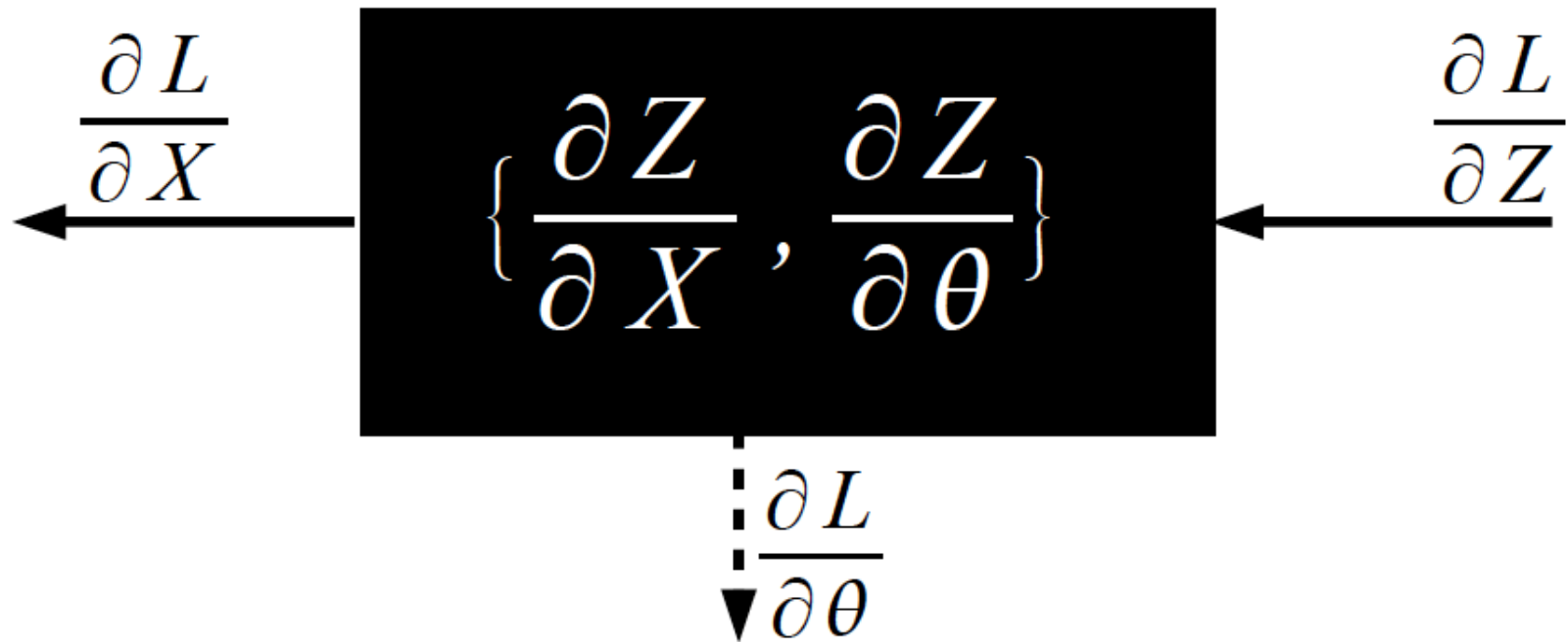


Any DAG of differentiable modules is allowed!

Key Computation: Forward-Prop

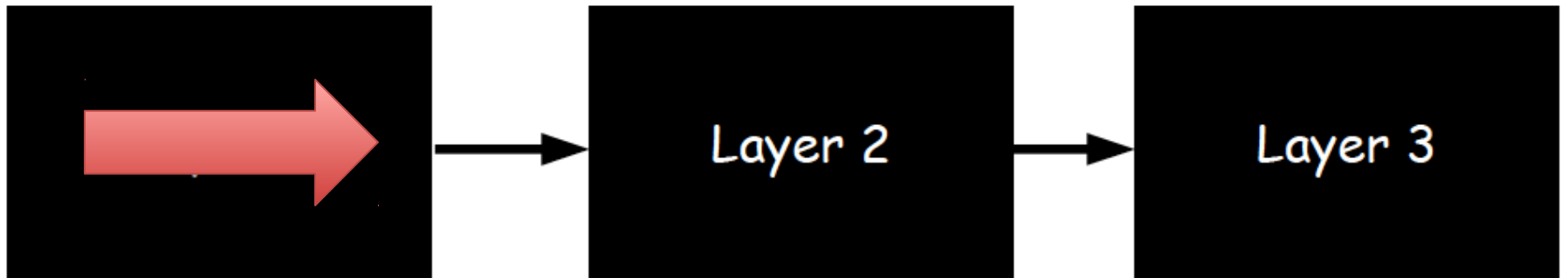


Key Computation: Back-Prop



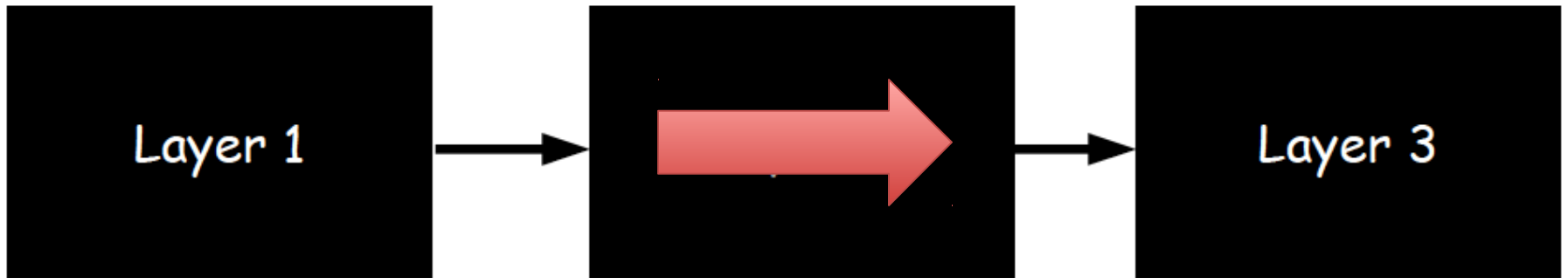
Neural Network Training

- Step 1: Compute Loss on mini-batch [F-Pass]



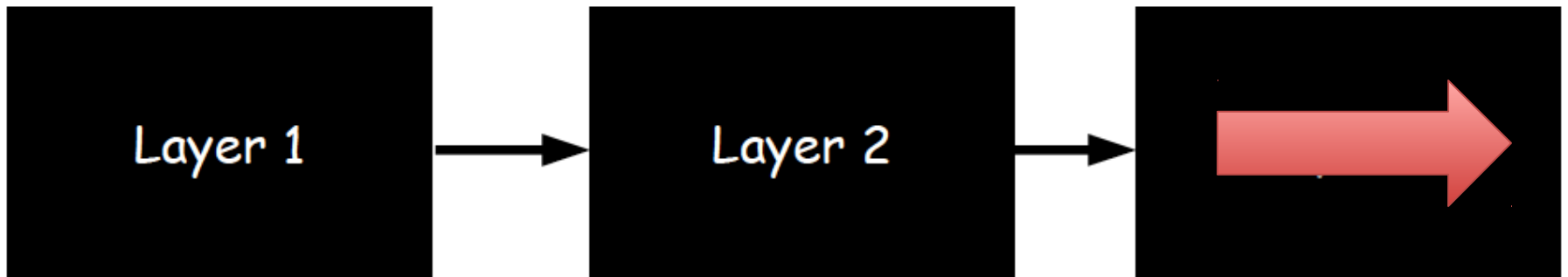
Neural Network Training

- Step 1: Compute Loss on mini-batch [F-Pass]



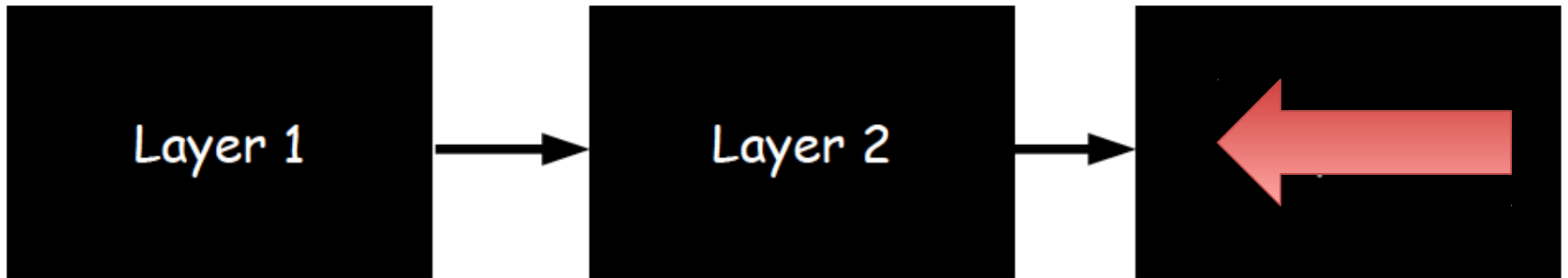
Neural Network Training

- Step 1: Compute Loss on mini-batch [F-Pass]



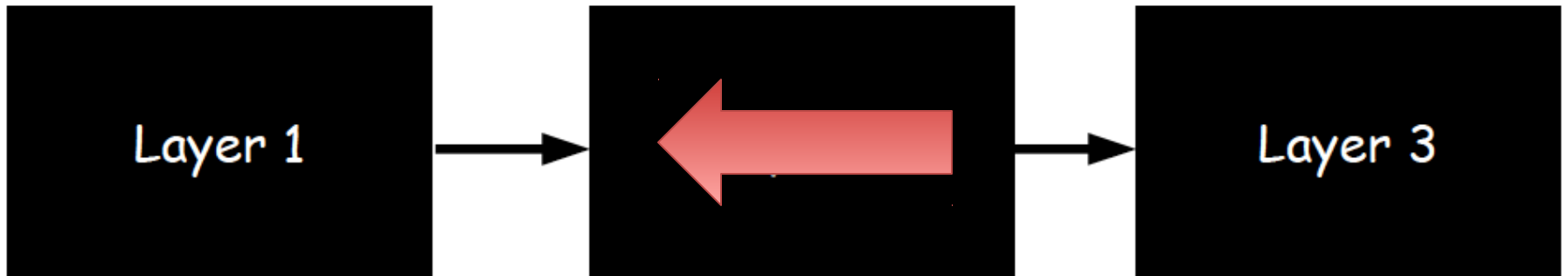
Neural Network Training

- Step 1: Compute Loss on mini-batch [F-Pass]
- Step 2: Compute gradients wrt parameters [B-Pass]



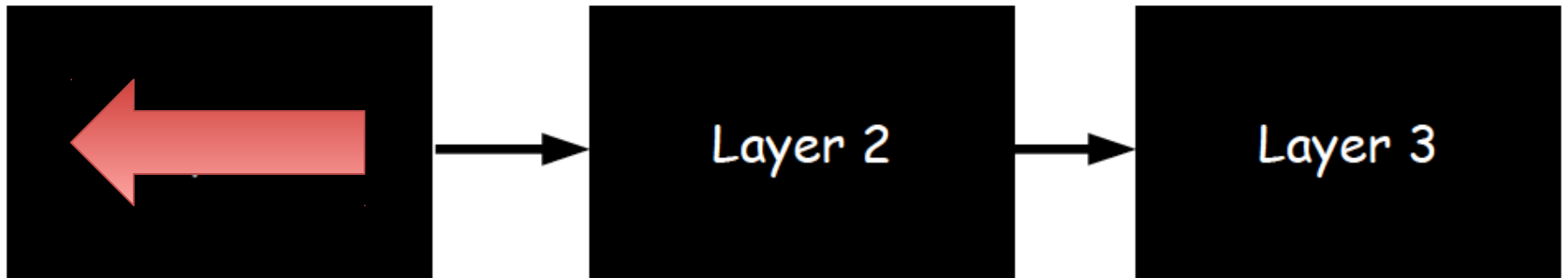
Neural Network Training

- Step 1: Compute Loss on mini-batch [F-Pass]
- Step 2: Compute gradients wrt parameters [B-Pass]



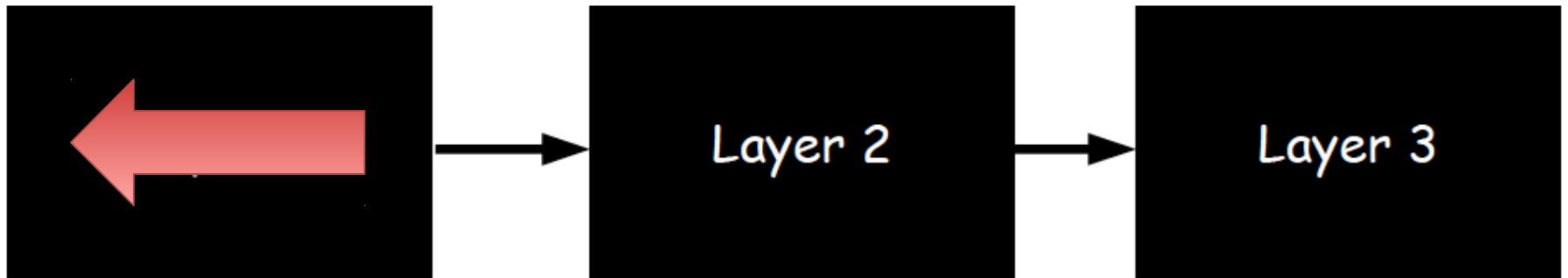
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- Step 1: Compute Loss on mini-batch [F-Pass]
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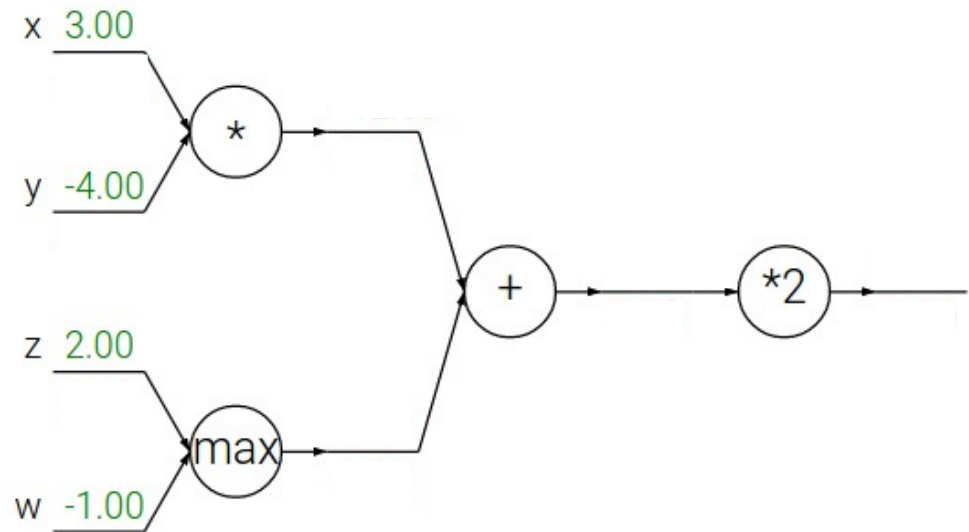
Neural Network Training

- Step 1: Compute Loss on mini-batch [F-Pass]
- Step 2: Compute gradients wrt parameters [B-Pass]
- Step 3: Use gradient to update parameters

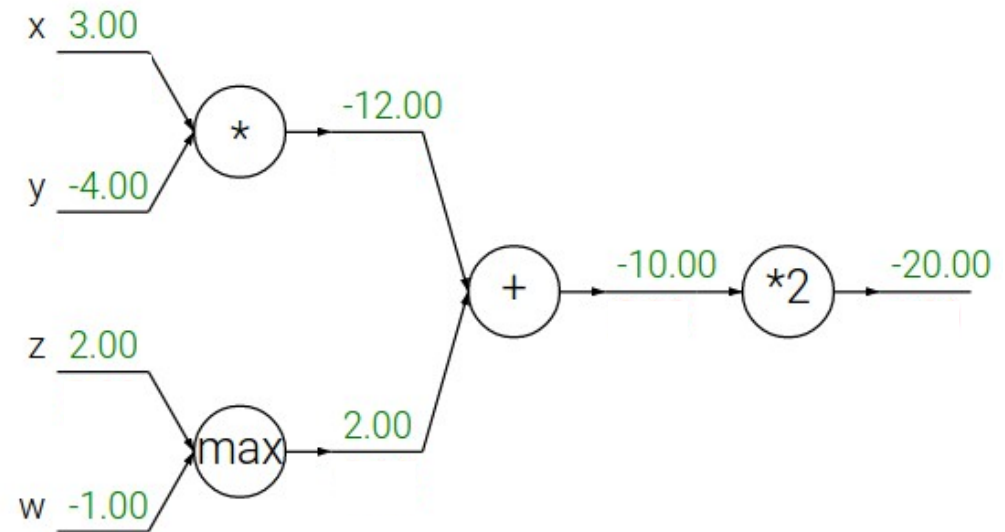


$$\theta \leftarrow \theta - \eta \frac{dL}{d\theta}$$

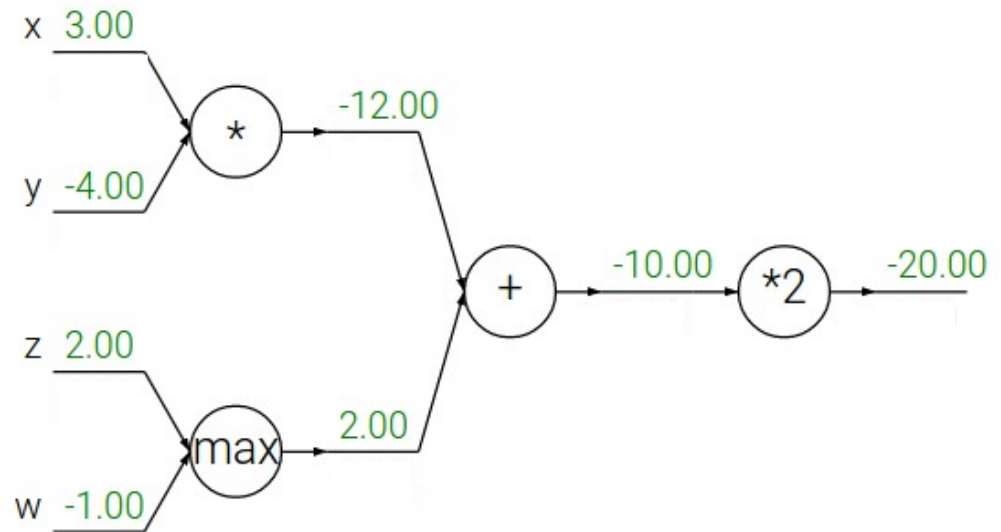
Backpropagation: a simple example



Backpropagation: a simple example

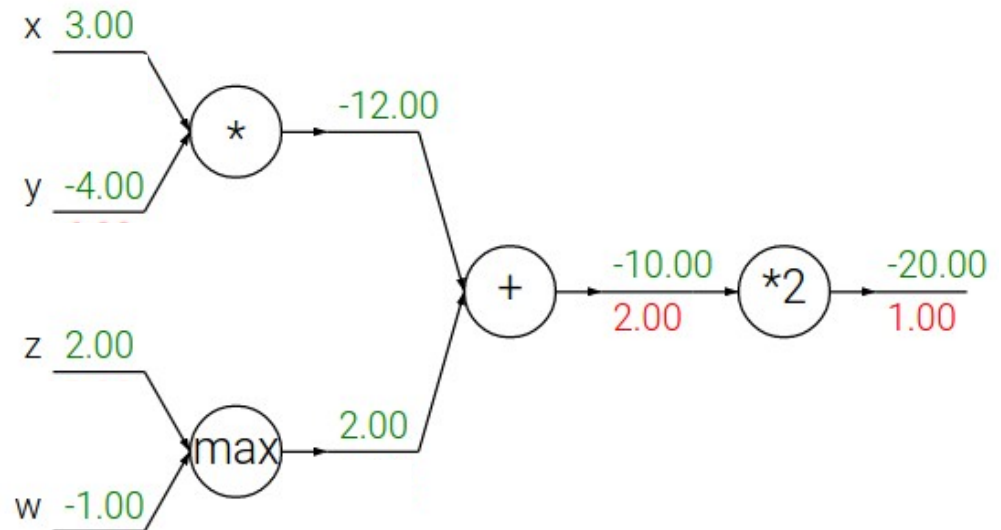


Patterns in backward flow



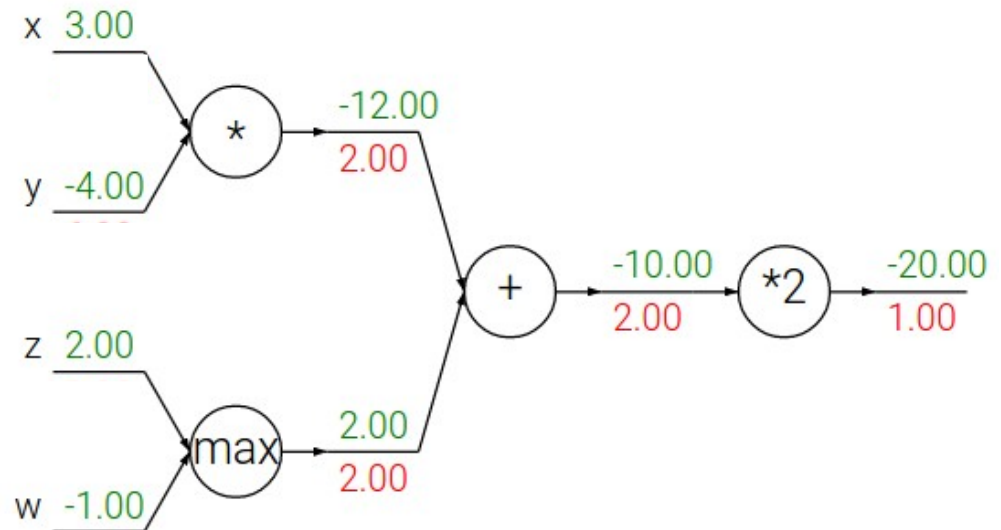
Patterns in backward flow

Q: What is an **add** gate?



Patterns in backward flow

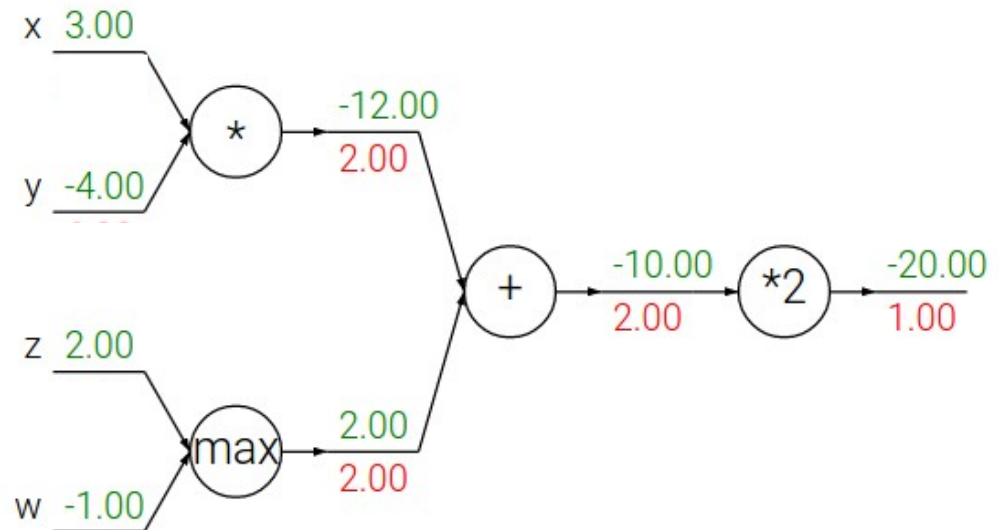
add gate: gradient distributor



Patterns in backward flow

add gate: gradient distributor

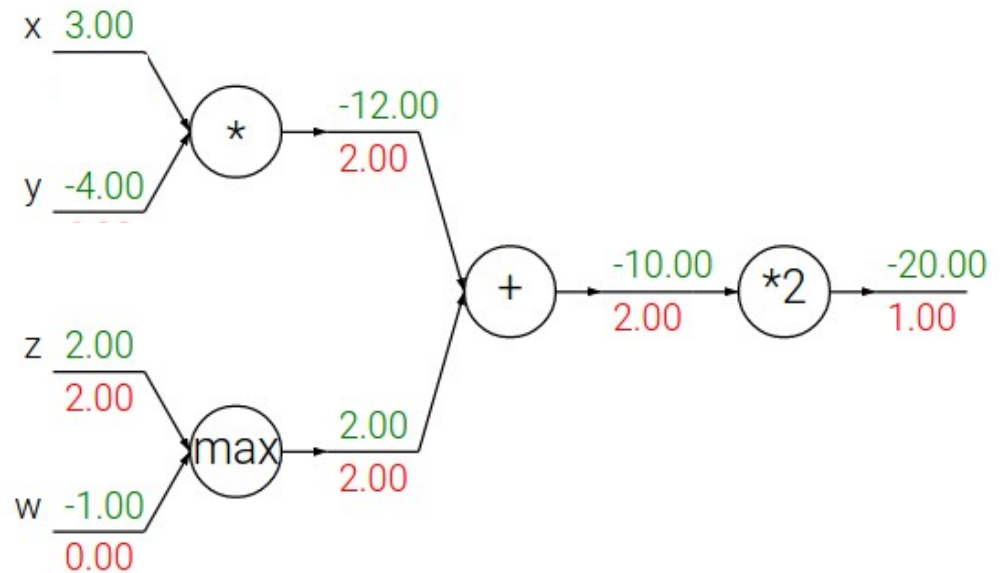
Q: What is a **max** gate?



Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

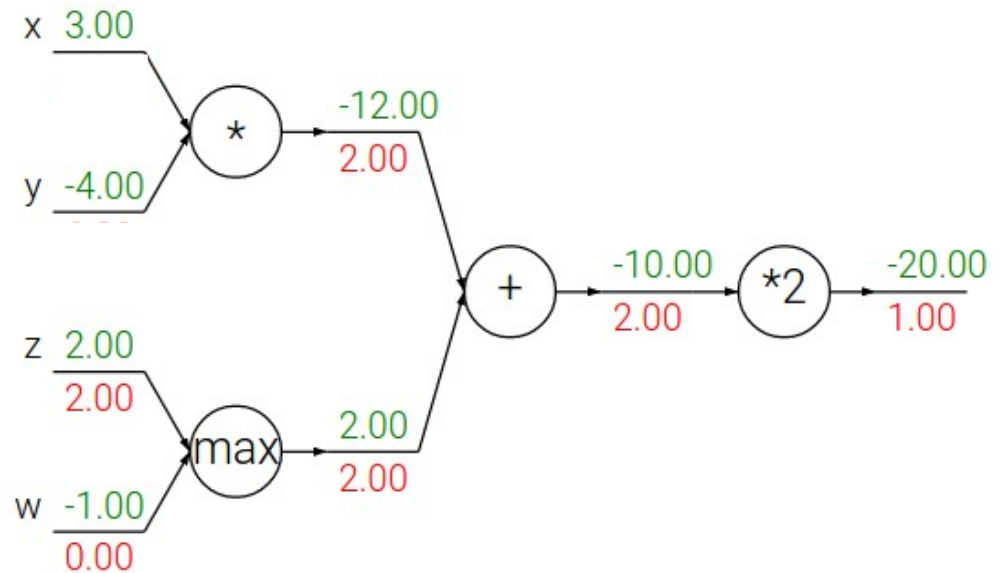


Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

Q: What is a **mul** gate?

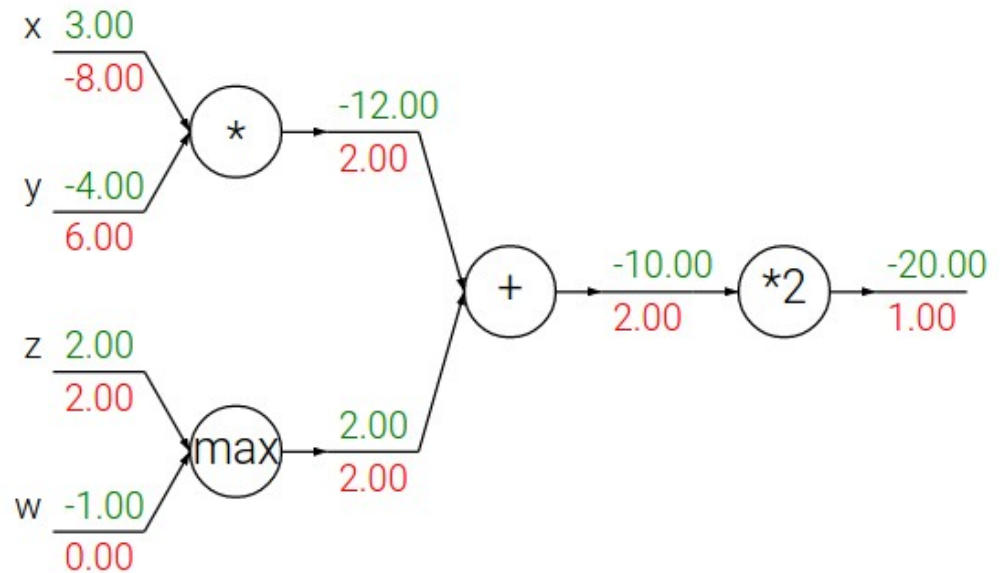


Patterns in backward flow

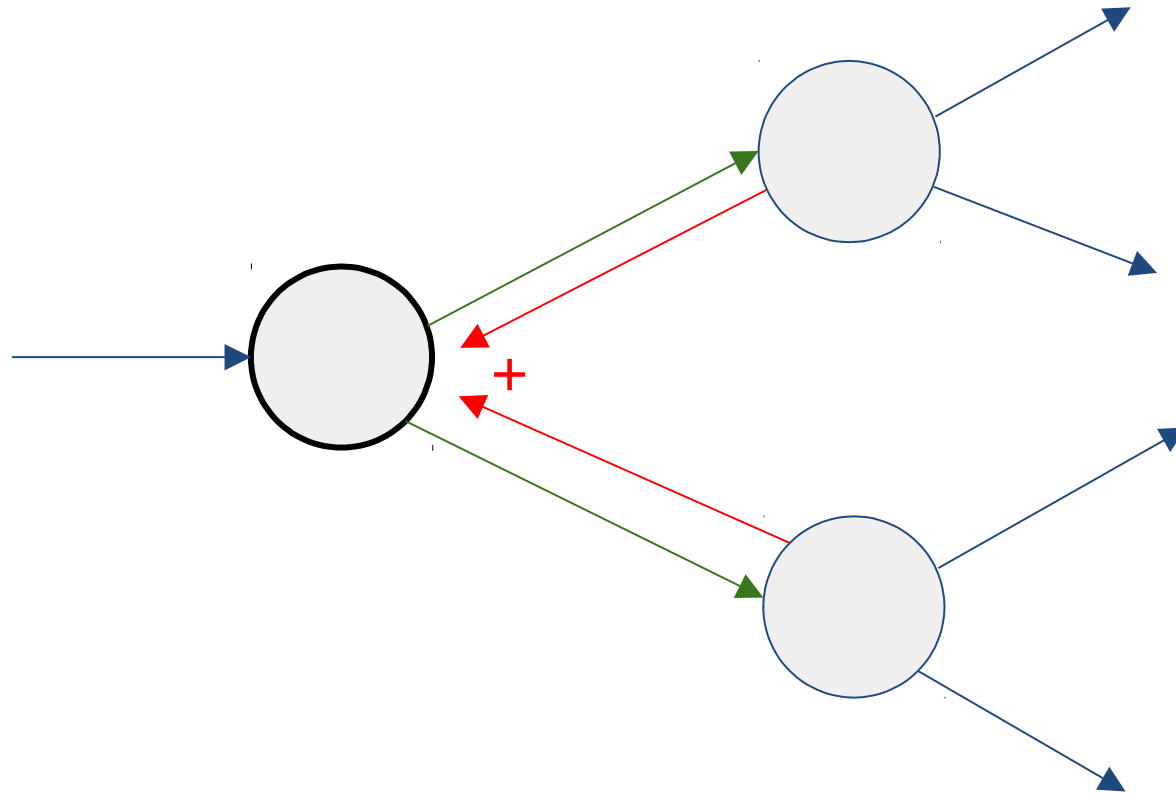
add gate: gradient distributor

max gate: gradient router

mul gate: gradient switcher



Gradients add at branches



Duality in Fprop and Bprop

