Topics:

- Jacobians/Matrix Calculus continued
- Backpropagation / Automatic Differentiation

CS 4644 / 7643-A

ZSOLT KIRA

- **Assignment 1 out!**
  - **Due Jan 31st (with grace period Feb 2nd)**
  - Hopefully you have started!

- Resources:
  - These lectures
  - Matrix calculus for deep learning
  - Gradients notes and MLP/ReLU Jacobian notes.
  - Assignment 1 and matrix calculus (@93, @109)

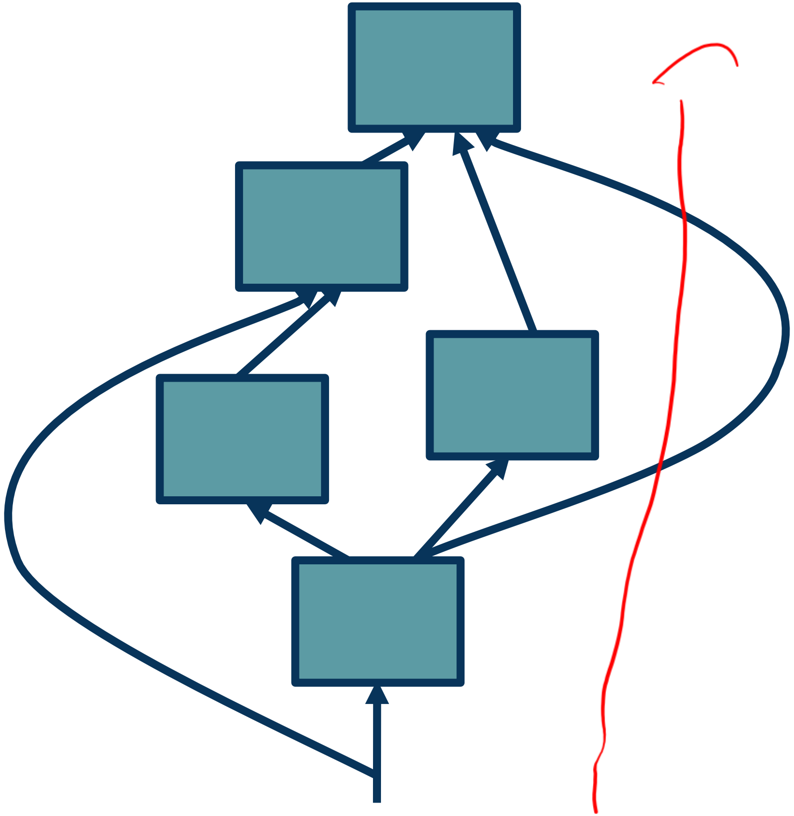
- Project:
  - Project proposal overview out, due by **Feb 14th**
  - See recorded office hours for discussion about requirements, answers to some questions, etc.
  - Groups of 5 requires permission: Start private piazza thread

To develop a general algorithm for this, we will view the function as a **computation graph**

Graph can be any **directed acyclic graph (DAG)**

- Modules must be differentiable to support gradient computations for gradient descent

A **training algorithm** will then process this graph, **one module at a time**

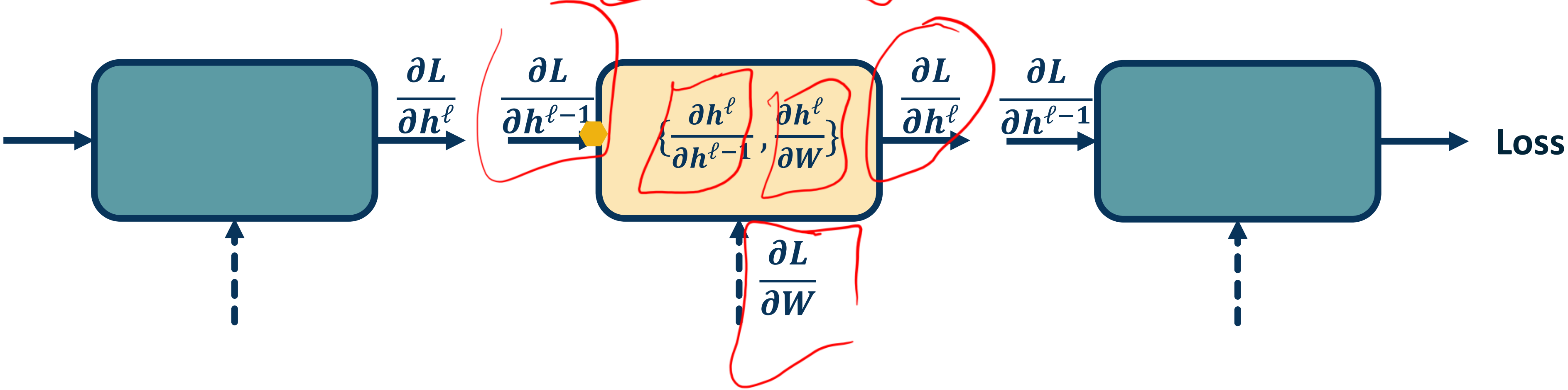


Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

A General Framework

Computing the Gradients of Loss

- We want to to compute: $\left\{\frac{\partial L}{\partial h^{\ell-1}}, \frac{\partial L}{\partial W}\right\}$

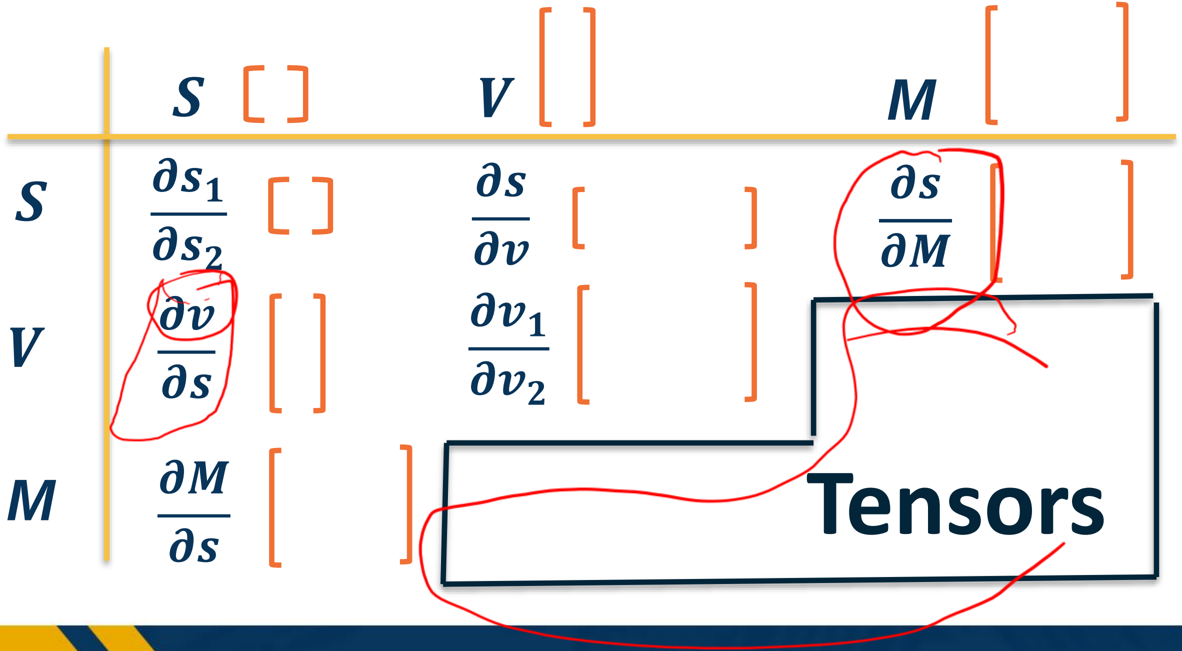


- We will use the *chain rule* to do this:

Chain Rule: $\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x}$

Conventions:

- Size of derivatives for scalars, vectors, and matrices:
  Assume we have scalar $\boldsymbol{s} \in \mathbb{R}^1$, vector $\boldsymbol{v} \in \mathbb{R}^m$, i.e. $\boldsymbol{v} = [v_1, v_2, \ldots, v_m]^T$ and matrix $\boldsymbol{M} \in \mathbb{R}^{k\times\ell}$



	s	v	M
s	$\frac{\partial s_1}{\partial s_2}$	$\frac{\partial s}{\partial v}$	$\frac{\partial s}{\partial M}$
v	$\frac{\partial v}{\partial s}$	$\frac{\partial v_1}{\partial v_2}$	Tensors
M	$\frac{\partial M}{\partial s}$		

- What is the size of $\frac{\partial L}{\partial W}$?
  - Remember that loss is a **scalar** and W is a matrix:

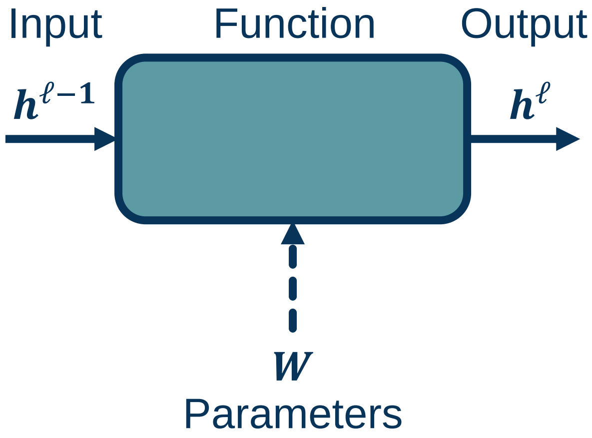
$$\begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1m} & b1 \\ w_{21} & w_{22} & \cdots & w_{2m} & b2 \\ w_{31} & w_{32} & \cdots & w_{3m} & b3 \end{bmatrix}$$

Jacobian is also a matrix:

$$W$$

$$\begin{bmatrix} \frac{\partial L}{\partial w_{11}} & \frac{\partial L}{\partial w_{12}} & \cdots & \frac{\partial L}{\partial w_{1m}} & \frac{\partial L}{\partial b_1} \\ \frac{\partial L}{\partial w_{21}} & \cdots & \cdots & \frac{\partial L}{\partial w_{2m}} & \frac{\partial L}{\partial b_2} \\ \cdots & \cdots & \cdots & \frac{\partial L}{\partial w_{3m}} & \frac{\partial L}{\partial b_3} \end{bmatrix}$$

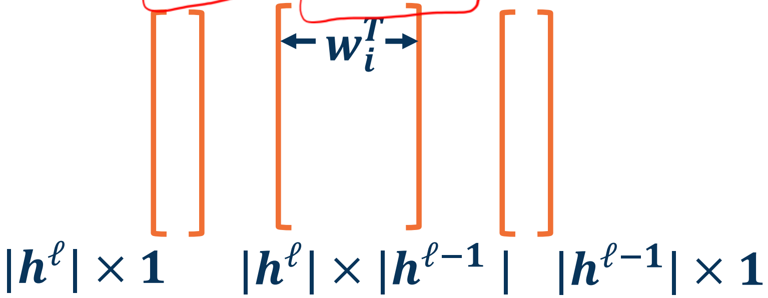
Dimensionality of Derivatives in ML



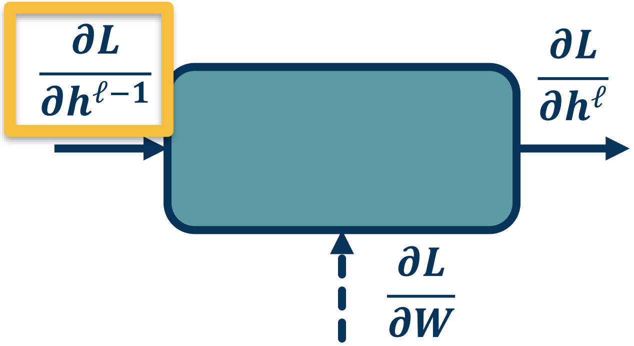
Define:

$$h_i^{\ell} = w_i^T h^{\ell-1}$$

$$h^{\ell} = W h^{\ell-1}$$



Fully Connected (FC) Layer: Forward Function



$$h^{\ell} = W h^{\ell-1}$$

$$\frac{\partial h^{\ell}}{\partial h^{\ell-1}} = W$$

Define:

$$h_i^{\ell} = w_i^T h^{\ell-1}$$

$$\boxed{\frac{\partial L}{\partial h^{\ell-1}}} = \frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial h^{\ell-1}}$$

$$1 \times |h^{\ell-1}| \quad 1 \times |h^{\ell}| \quad |h^{\ell}| \times |h^{\ell-1}|$$

Fully Connected (FC) Layer

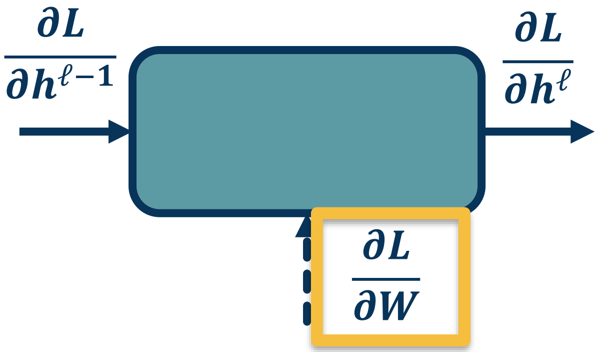
$$h^{\ell} = W h^{\ell-1}$$

$$\frac{\partial h^{\ell}}{\partial h^{\ell-1}} = W$$

Define:

$$h_i^{\ell} = w_i^T h^{\ell-1}$$

$$\frac{\partial h_i^{\ell}}{\partial w_i^T} = h^{(\ell-1),T}$$



$$\frac{\partial L}{\partial w_i^T} = \frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial w_i^T}$$

$$\begin{bmatrix} \quad \end{bmatrix} \begin{bmatrix} \quad \end{bmatrix} \begin{bmatrix} \leftarrow & 0 & \rightarrow \\ \leftarrow & \frac{\partial h_i^{\ell}}{\partial w_i^T} & \rightarrow \\ \leftarrow & 0 & \rightarrow \end{bmatrix}$$

$1 \times |h^{\ell-1}|$ $1 \times |h^{\ell}|$ $|h^{\ell}| \times |h^{\ell-1}|$

$$\frac{\partial L}{\partial W} \begin{bmatrix} \quad \end{bmatrix}$$

Note doing this on full W matrix would result in Jacobian tensor!

But it is *sparse* – each output only affected by corresponding weight row

$\frac{\partial L}{\partial w} = \frac{\partial h}{\partial w}$

Iterate and populate

Note can simplify/vectorize!

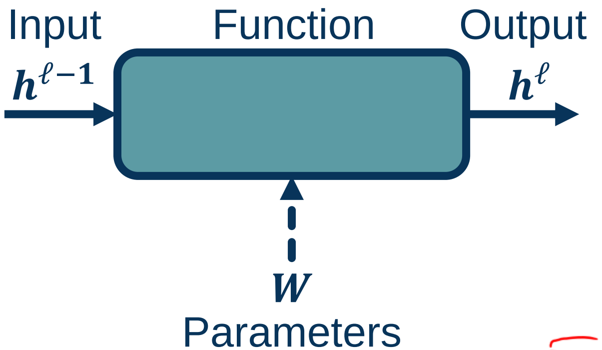
Fully Connected (FC) Layer

Full Jacobian of ReLU layer is **large** (output dim x input dim)

- But again it is **sparse**
- Only **diagonal values non-zero** because it is element-wise
- An output value affected only by **corresponding input value**

Max function **funnels gradients through selected max**

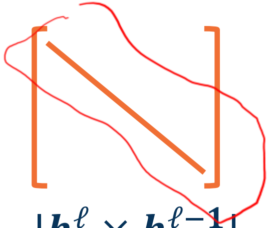
- Gradient will be **zero** if input **<= 0**



100

Forward: $h^{\ell} = \max(0, h^{\ell-1})$

Backward: $\frac{\partial L}{\partial h^{\ell-1}} = \frac{\partial L}{\partial h^{\ell}} \; \frac{\partial h^{\ell}}{\partial h^{\ell-1}}$



$|h^{\ell} \times h^{\ell-1}|$

For diagonal

$$\frac{\partial h^{\ell}}{\partial h^{\ell-1}} = \begin{cases} 1 & if\ h^{\ell-1} > 0 \\ 0 & otherwise \end{cases}$$

Jacobian of ReLU

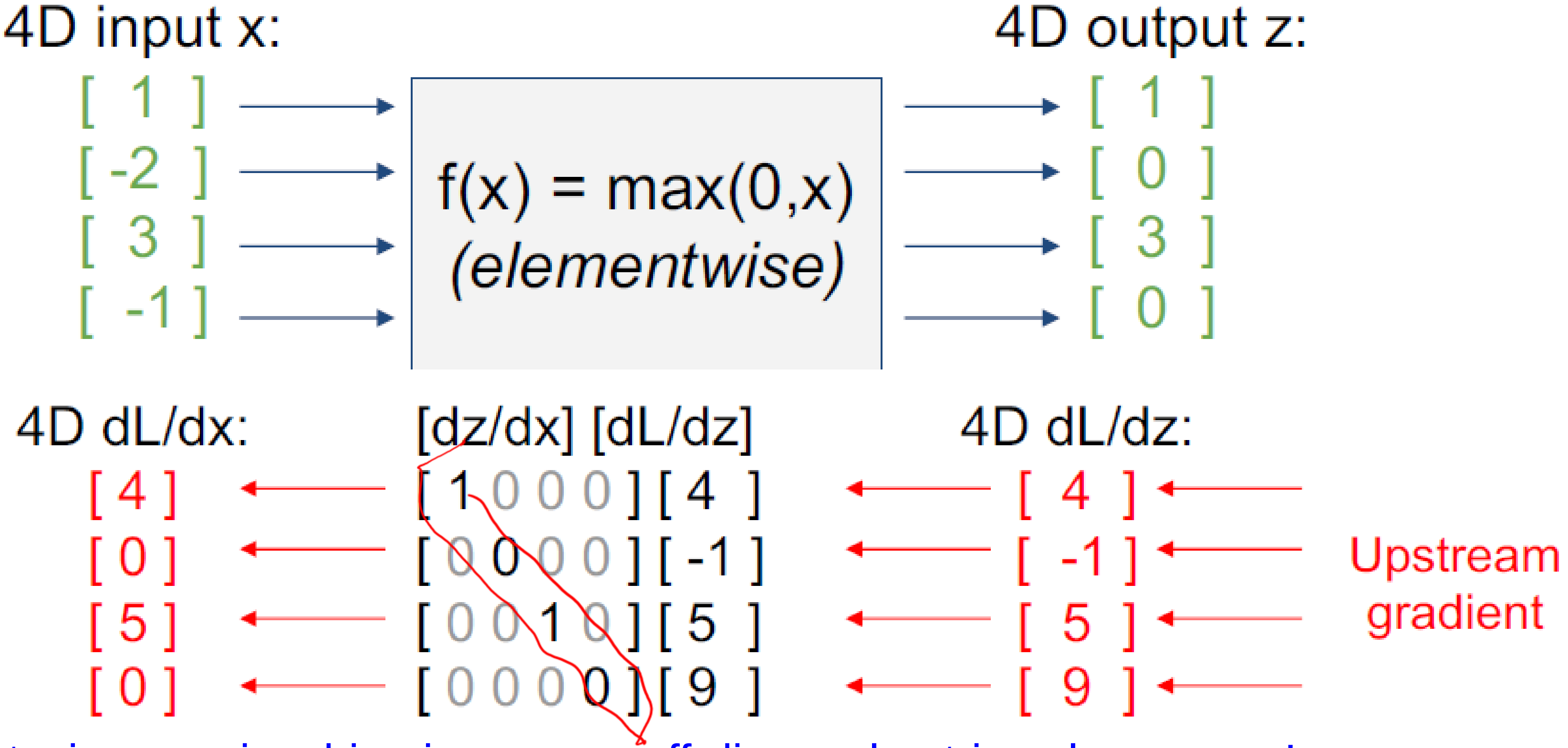


Figure adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

4D input x:

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix}$$

$f(x) = \max(0,x)$
(elementwise)

4D output z:

$$\begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

4D dL/dx: [dz/dx] [dL/dz] 4D dL/dz:

$$\begin{bmatrix} 4 \\ 0 \\ 5 \\ 0 \end{bmatrix} \leftarrow \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \leftarrow \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \leftarrow$$

Upstream gradient

For element-wise ops, jacobian is **sparse**: off-diagonal entries always zero!
Never **explicitly** form Jacobian -- instead use elementwise multiplication

- Neural networks involves composing simple functions into a **computation graph**

- Optimization (updating weights) of this graph is through backpropagation
  - Recursive algorithm: Gradient descent (partial derivatives) plus chain rule

- Remaining questions:
  - How does this work with vectors, matrices, tensors?
    - Across a composed function? **This Time!**
  - How can we implement this algorithmically to make these calculations automatic? **Automatic Differentiation**

Summary

Vectorization in Function Compositions

Composition of Functions: $f(g(x)) = \boxed{(f \circ g)(x)}$

A complex function (e.g. defined by a neural network):

$$f(x) = \boxed{g_\ell}(g_{\ell-1}(\dots \boxed{g_1(x)}))$$

$$\underline{f(x) = g_\ell \circ g_{\ell-1} \dots \circ g_1(x)}$$

(Many of these will be parameterized)

(Note you might find the opposite notation as well!)

Scalar Case

$$x \in \mathbb{R}^1 \xrightarrow[g_1]{} z \in \mathbb{R}^1 \xrightarrow[g_2]{} y \in \mathbb{R}^1$$

$$y = g_2(g_1(x))$$

$$\frac{\partial y}{\partial x} = \frac{\partial y}{\boxed{\partial z}} \cdot \frac{\partial z}{\boxed{\partial x}}$$

scalar
mult

$$\vec{x} \in \mathbb{R}^d \xrightarrow[\substack{g_1 \\ \mathbb{R}^d \to \mathbb{R}^m}]{} z \in \mathbb{R}^m \xrightarrow[\substack{g_2 \\ \mathbb{R}^m \to \mathbb{R}^c}]{} y \in \mathbb{R}^c$$

$$\left[\frac{\partial \vec{y}}{\partial \vec{x}}\right] = \boxed{\frac{\partial \vec{y}}{\partial \vec{z}}} \cdot \frac{\partial \vec{z}}{\partial \vec{x}}$$

$$\left[\qquad\right] \uparrow \left[\qquad\right]$$

matrix multiplication

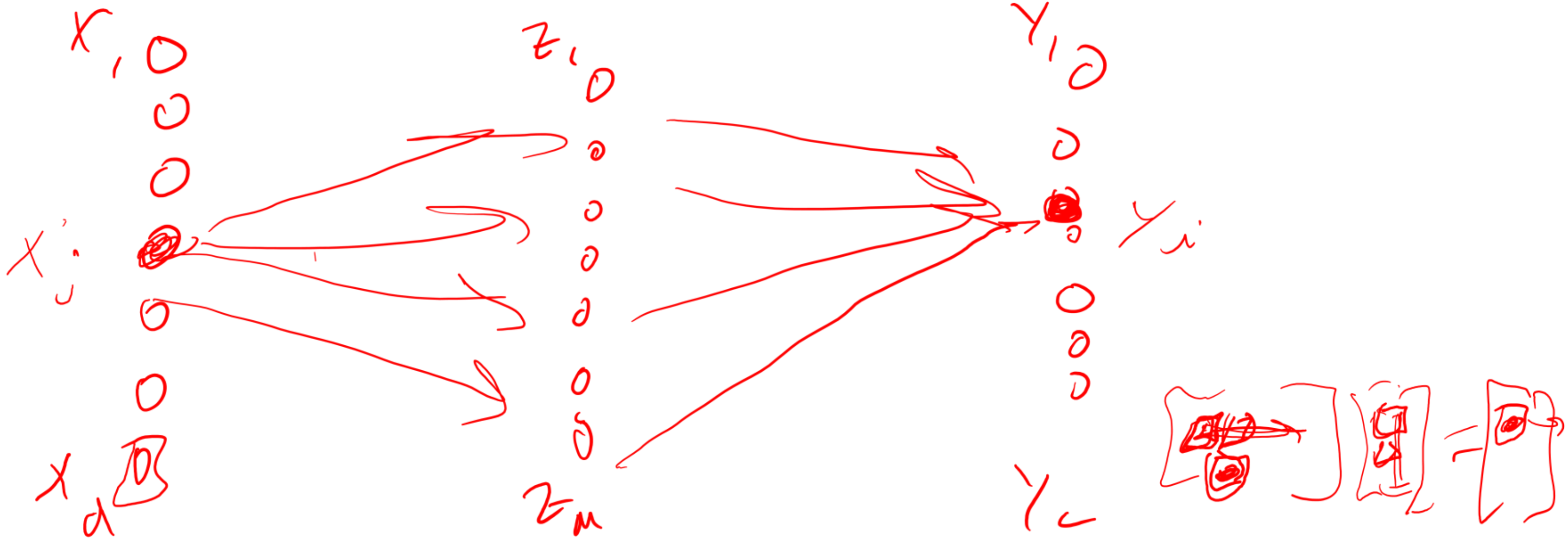
Vector Case

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

$$\left[\frac{\partial y_i}{\partial x_j} \right] = \left[\frac{\partial y_i}{\partial z_k} \right] \left[\frac{\partial z_k}{\partial x_j} \right]$$

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

Jacobian View of Chain Rule

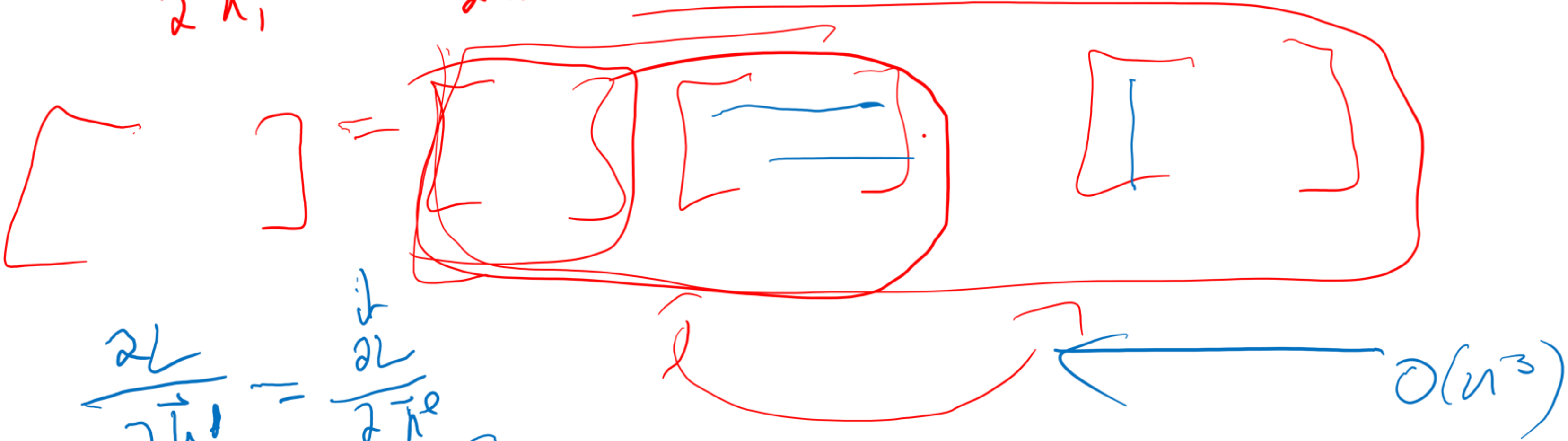


$$\frac{\partial y_i}{\partial x_j} = \sum_{k \text{ paths}} \frac{\partial y_i}{\partial z_k} \cdot \frac{\partial z_k}{\partial x_j}$$

Graphical View of Chain Rule

$$\vec{h}^1 \in \mathbb{R}^d \rightarrow \vec{h}^2 \rightarrow \dots \rightarrow \vec{h}^\ell \rightarrow L$$

$$\frac{\partial \vec{h}^\ell}{\partial \vec{h}_1} = \frac{\partial \vec{h}^\ell}{\partial \vec{h}^{\ell-1}} \cdot \frac{\partial \vec{h}^{\ell-1}}{\partial \vec{h}^{\ell-2}} \cdot \dots \frac{\partial \vec{h}^2}{\partial \vec{h}^1}$$



$$\frac{\partial L}{\partial \vec{h}^1} = \frac{\partial L}{\partial \vec{h}^\ell}$$

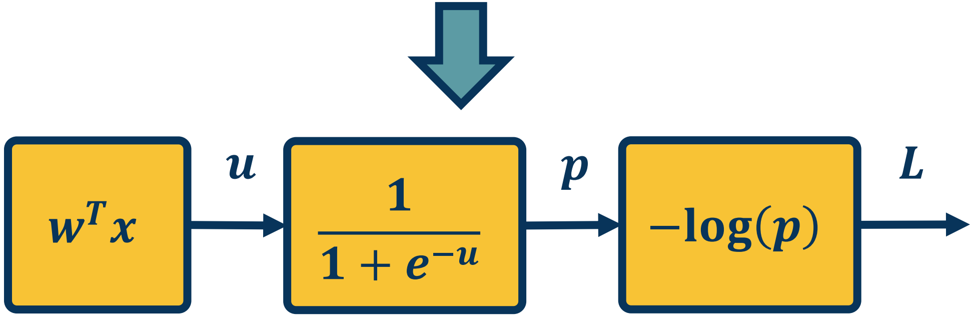
Chain Rule: Cascaded

We have discussed **computation graphs for generic functions**

Machine Learning functions **(input -> model -> loss function)** is also a computation graph

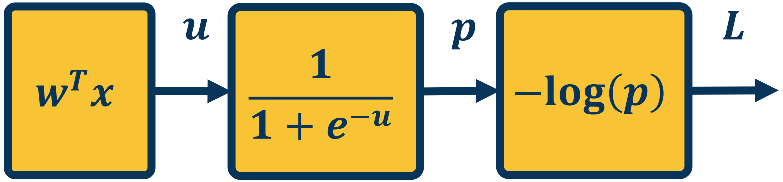
We can use the **computed gradients from backprop/automatic differentiation** to update the weights!

$$-\log\left(\frac{1}{1+e^{-w^T x}}\right)$$



Neural Network Computation Graph

Example Gradient Computations



$$\bar{L} = 1$$

$$\bar{p} = \frac{\partial L}{\partial p} = -\frac{1}{p}$$

where $p = \sigma\left(w^Tx\right)$ and $\sigma(x) = \frac{1}{1+e^{-x}}$

$$\bar{u} = \frac{\partial L}{\partial u} = \frac{\partial L}{\partial p}\,\frac{\partial p}{\partial u} = \bar{p}\,\sigma(1-\sigma)$$

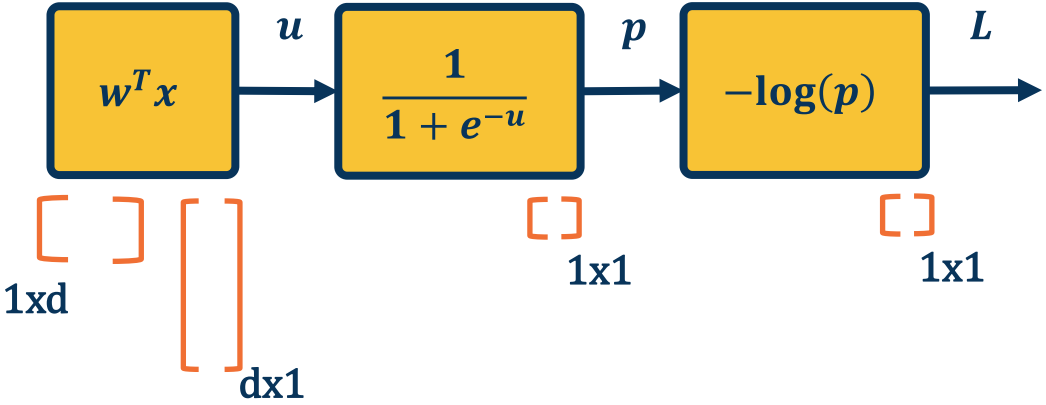
$$\bar{w} = \frac{\partial L}{\partial w} = \frac{\partial L}{\partial u}\,\frac{\partial u}{\partial w} = \bar{u}x^T$$

We can do this in a combined way to see all terms together:

$$\bar{w} = \frac{\partial L}{\partial p}\,\frac{\partial p}{\partial u}\,\frac{\partial u}{\partial w} = \bar{L}\,\bar{p}\,\bar{u} = -\frac{1}{\sigma(w^Tx)}\sigma\left(w^Tx\right)(1-\sigma\left(w^Tx\right))x^T$$
$$= -\left(1-\sigma\left(w^Tx\right)\right)x^T$$

This effectively shows gradient flow along path from L to w

The chain rule can be computed as a **series of scalar, vector, and matrix linear algebra operations**



Extremely efficient in graphics processing units (GPUs)

$$\bar{w} = -\underbrace{\frac{1}{\sigma(w^T x)}}_{\text{1x1}}\underbrace{\sigma(w^T x)}_{\text{1x1}}\underbrace{(1-\sigma(w^T x))}_{\text{1x1}}\underbrace{x^T}_{\text{1xd}}$$

Many **standard regularization methods** still apply!

L1 Regularization

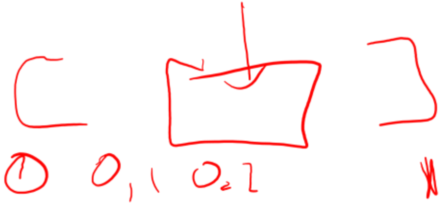
$$L = |y - Wx_i|^2 + \boxed{\lambda}|W|$$

where $|W|$ is element-wise

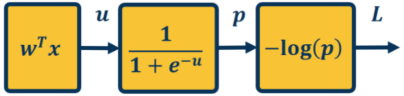
0.1

Example regularizations:

- L1/L2 on weights (encourage small values)
- L2: $L = |y - Wx_i|^2 + \lambda|W|^2$ (weight decay)
- Elastic L1/L2: $|y - Wx_i|^2 + \alpha|W|^2 + \beta|W|$



Different Views of Equivalent Ideas



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where $p = \sigma(w^T x)$ and $\sigma(x) = \frac{1}{1+e^{-x}}$

$\bar{u} = \frac{\partial L}{\partial u} = \frac{\partial L}{\partial p}\frac{\partial p}{\partial u} = \bar{p}\,\sigma(1-\sigma)$

$\bar{w} = \frac{\partial L}{\partial w} = \frac{\partial L}{\partial u}\frac{\partial u}{\partial w} = \bar{u}x^T$

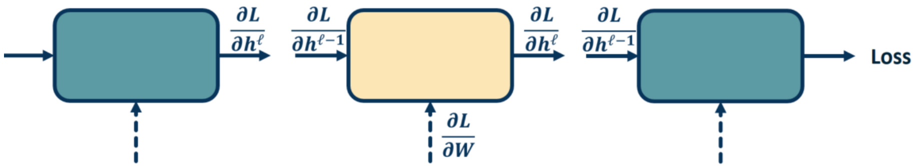
We can do this in a combined way to see all terms together:

$$\bar{w} = \frac{\partial L}{\partial p}\frac{\partial p}{\partial u}\frac{\partial u}{\partial w} = -\frac{1}{\sigma(w^T x)}\sigma(w^T x)(1-\sigma(w^T x))x^T$$
$$= -\left(1-\sigma(w^T x)\right)x^T$$

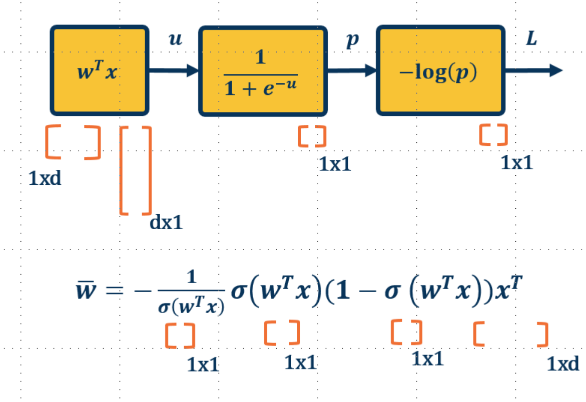
This effectively shows gradient flow along path from L to w

Computation Graph of primitives (automatic differentiation)

- We want to to compute: $\{\frac{\partial L}{\partial h^{\ell-1}}, \frac{\partial L}{\partial W}\}$

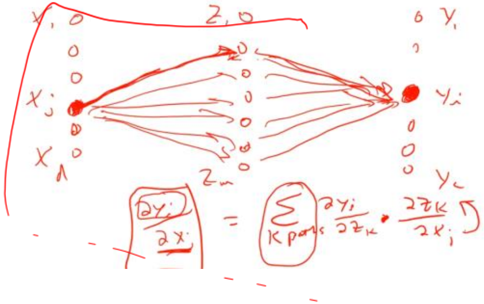


Backpropagation View (Recursive Algorithm)



$$\bar{w} = -\frac{1}{\sigma(w^T x)}\sigma(w^T x)(1-\sigma(w^T x))x^T$$

Computational / Tensor View



Graph View

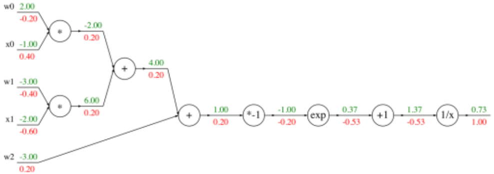
Backpropagation and Automatic Differentiation

Deep Learning = Differentiable Programming

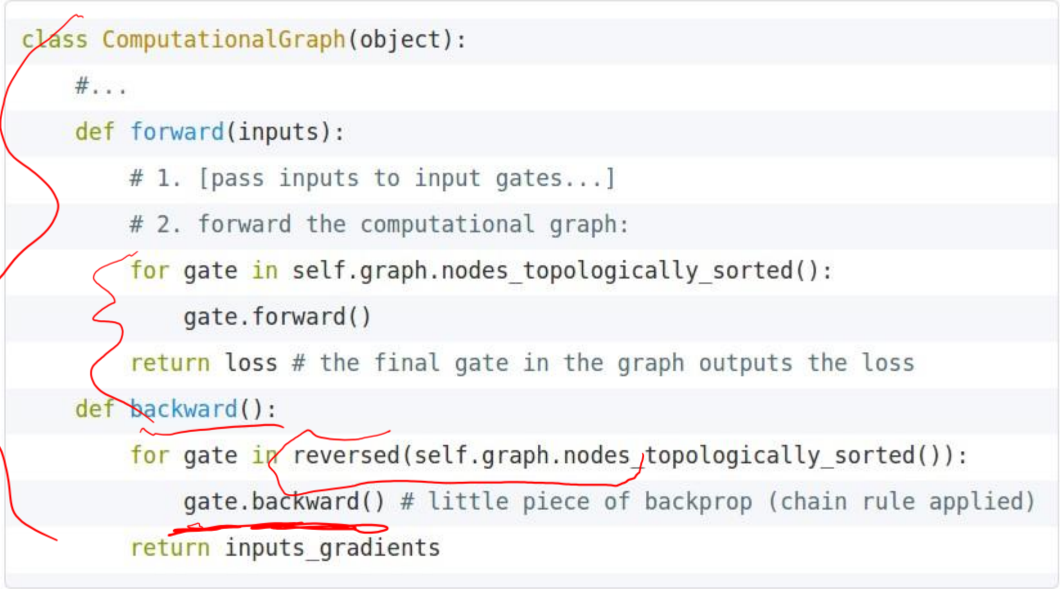
- Computation = Graph
  - Input = Data + Parameters
  - Output = Loss
  - Scheduling = Topological ordering

- What do we need to do?
  - Generic code for representing the graph of modules ←
  - Specify modules (both forward and backward function)

Modularized implementation: forward / backward API



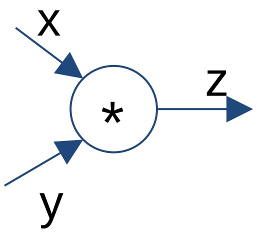
Graph (or Net) object *(rough psuedo code)*



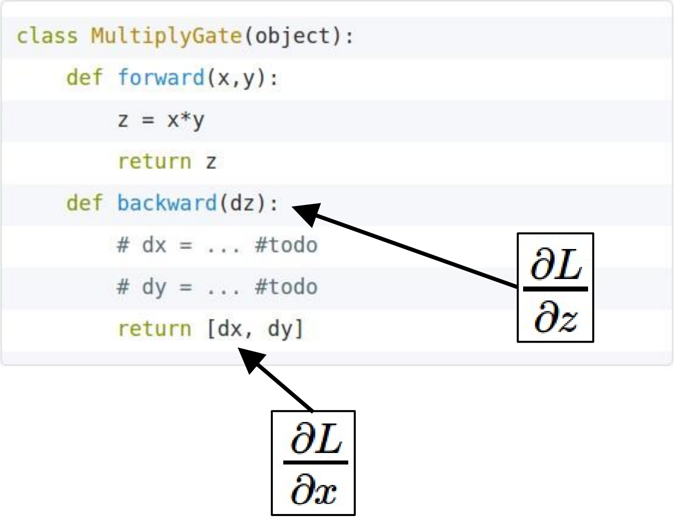
```
class ComputationalGraph(object):
    #...
    def forward(inputs):
        # 1. [pass inputs to input gates...]
        # 2. forward the computational graph:
        for gate in self.graph.nodes_topologically_sorted():
            gate.forward()
        return loss # the final gate in the graph outputs the loss
    def backward():
        for gate in reversed(self.graph.nodes_topologically_sorted()):
            gate.backward() # little piece of backprop (chain rule applied)
        return inputs_gradients
```

Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Modularized implementation: forward / backward API



(x,y,z are scalars)



```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        return z
    def backward(dz):
        # dx = ... #todo
        # dy = ... #todo
        return [dx, dy]
```

$\boxed{\frac{\partial L}{\partial z}}$

$\boxed{\frac{\partial L}{\partial x}}$

Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Backpropagation does not really spell out how to **efficiently** carry out the necessary computations

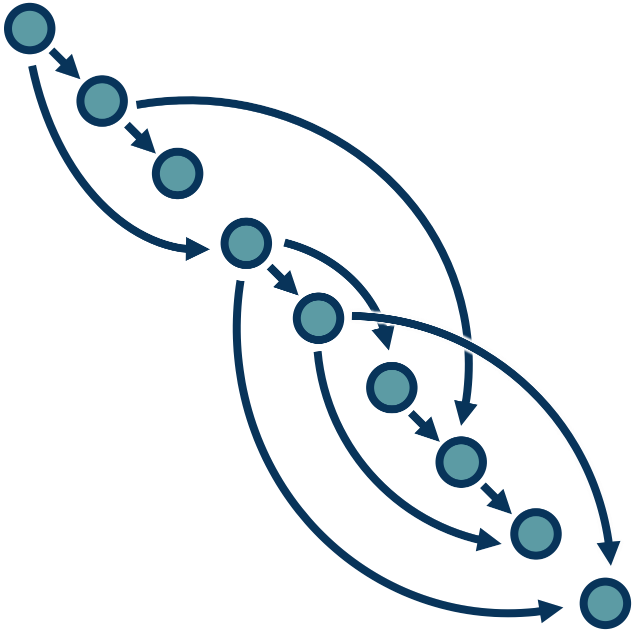
But the idea can be applied to **any directed acyclic graph (DAG)**

- Graph represents an **ordering constraining** which paths must be calculated first

Given an ordering, we can then iterate from the last module backwards, **applying the chain rule**

- We will store, for each node, its **local gradient function/computation for efficiency**
- We will do this **automatically** by computing backwards function for primitives and as you write code, express the function with them

This is called reverse-mode **automatic differentiation**



A General Framework

Computation = Graph

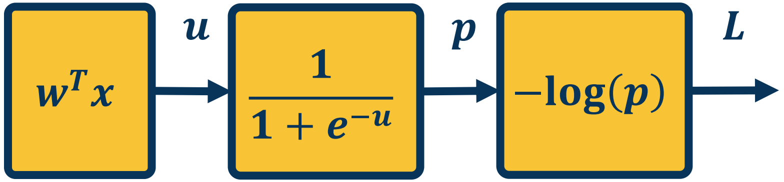
- Input = Data + Parameters
- Output = Loss
- Scheduling = Topological ordering

Auto-Diff

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

Deep Learning = Differentiable Programming

Example Gradient Computations



Automatic differentiation:

- Carries out this procedure for us on arbitrary graphs
- Knows derivatives of primitive functions
- As a result, we just define these (forward) functions **and don't even need to specify the gradient (backward) functions!**

$$\bar{L} = 1$$

$$\bar{p} = \frac{\partial L}{\partial p} = -\frac{1}{p}$$

where $p = \sigma\left(w^T x\right)$ **and** $\sigma(x) = \frac{1}{1+e^{-x}}$

$$\bar{u} = \frac{\partial L}{\partial u} = \frac{\partial L}{\partial p}\,\frac{\partial p}{\partial u} = \bar{p}\,\sigma(1-\sigma)$$

$$\bar{w} = \frac{\partial L}{\partial w} = \frac{\partial L}{\partial u}\,\frac{\partial u}{\partial w} = \bar{u}x^T$$

We can do this in a combined way to see all terms together:

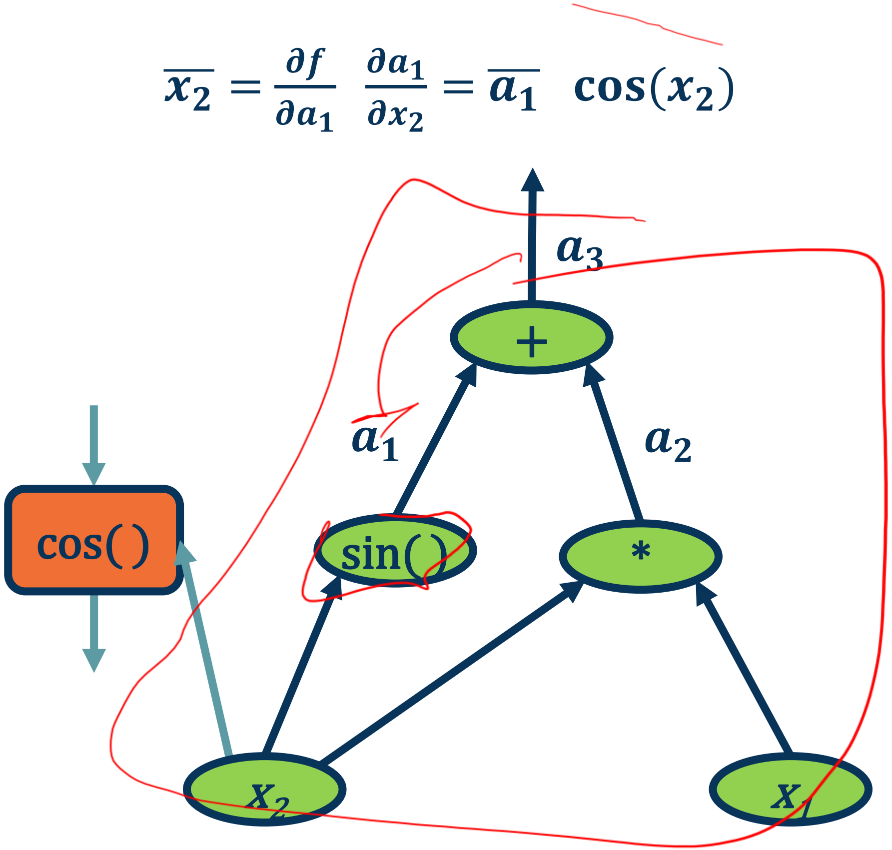
$$\bar{w} = \frac{\partial L}{\partial p}\,\frac{\partial p}{\partial u}\,\frac{\partial u}{\partial w} = -\frac{1}{\sigma(w^T x)}\sigma\left(w^T x\right)\left(1-\sigma\left(w^T x\right)\right)x^T$$
$$= -\left(1-\sigma\left(w^T x\right)\right)x^T$$

This effectively shows gradient flow along path from L to w

- Key idea is to **explicitly store computation graph** in memory and **corresponding gradient functions**

- **Nodes** broken down to **basic primitive computations** (addition, multiplication, log, etc.) for which **corresponding derivative is known**

$$\overline{x_2} = \frac{\partial f}{\partial a_1}\frac{\partial a_1}{\partial x_2} = \overline{a_1}\ \cos(x_2)$$



Computational Implementation

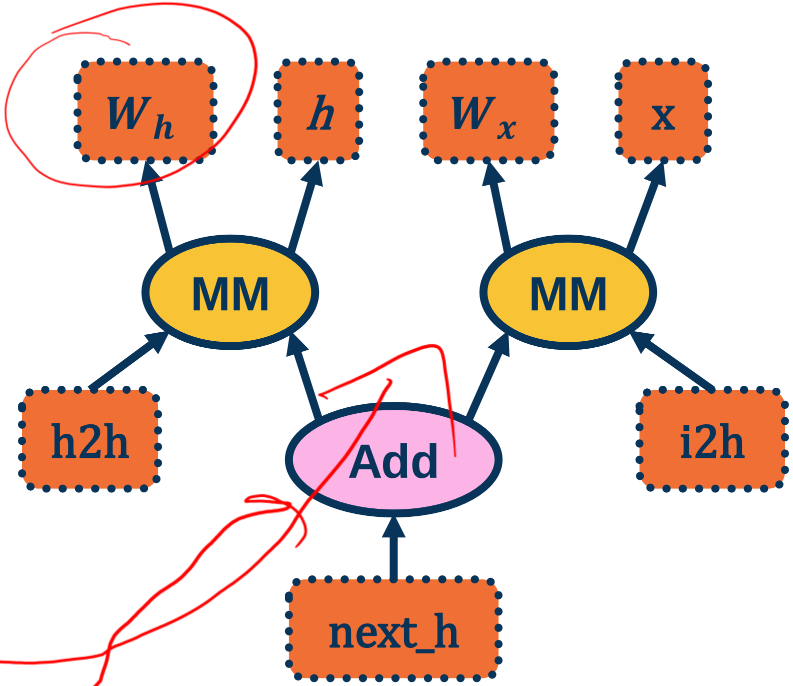
A graph is created on the fly

```
from torch.autograd import Variable

x = Variable(torch.randn(1, 20))
prev_h = Variable(torch.randn(1, 20))
W_h = Variable(torch.randn(20, 20))
W_x = Variable(torch.randn(20, 20))

i2h = torch.mm(W_x, x.t())
h2h = torch.mm(W_h, prev_h.t())
next_h = i2h + h2h
```

(Note above)



Back-propagation uses the dynamically built graph

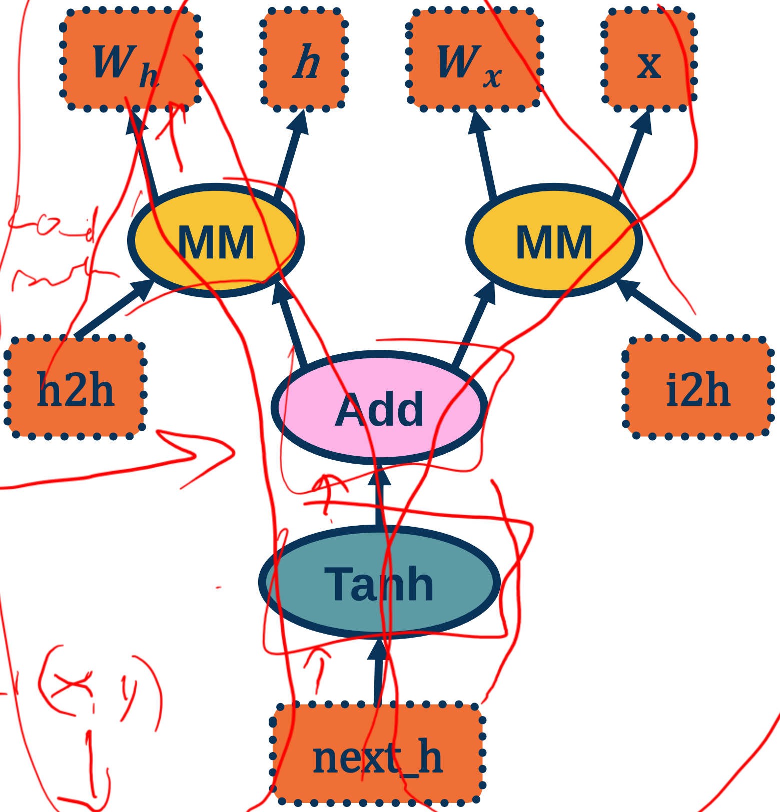
```
from torch.autograd import Variable

x = Variable(torch.randn(1, 20))
prev_h = Variable(torch.randn(1, 20))
W_h = Variable(torch.randn(20, 20))
W_x = Variable(torch.randn(20, 20))

i2h = torch.mm(W_x, x.t())
h2h = torch.mm(W_h, prev_h.t())
next_h = i2h + h2h
next_h = next_h.tanh()

next_h.backward(torch.ones(1, 20))
```

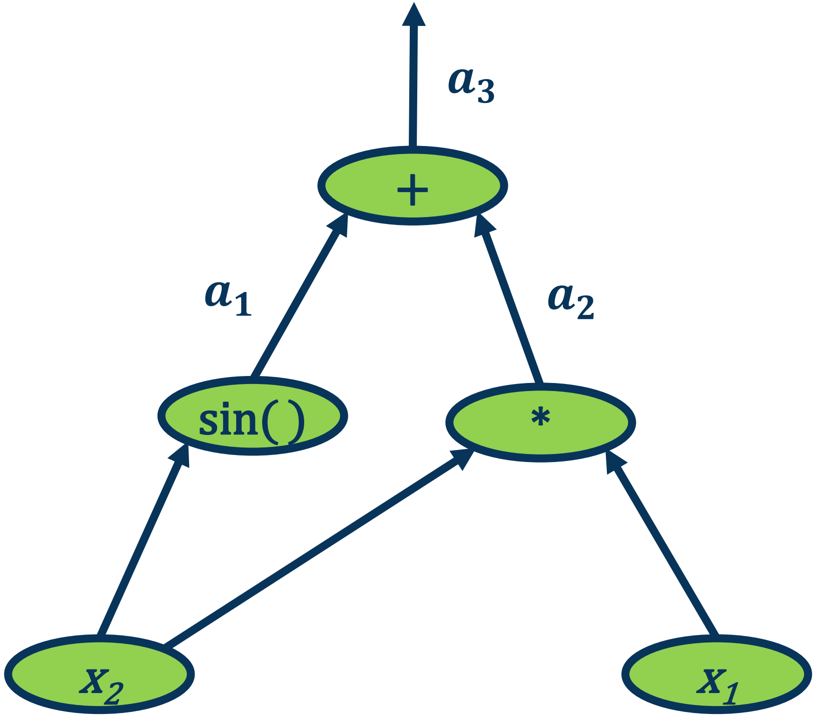
module_1(x, y)



From pytorch.org

Computation Graphs in PyTorch

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



We want to find the **partial derivative of output f** (output) with respect to **all intermediate variables**

- Assign intermediate variables

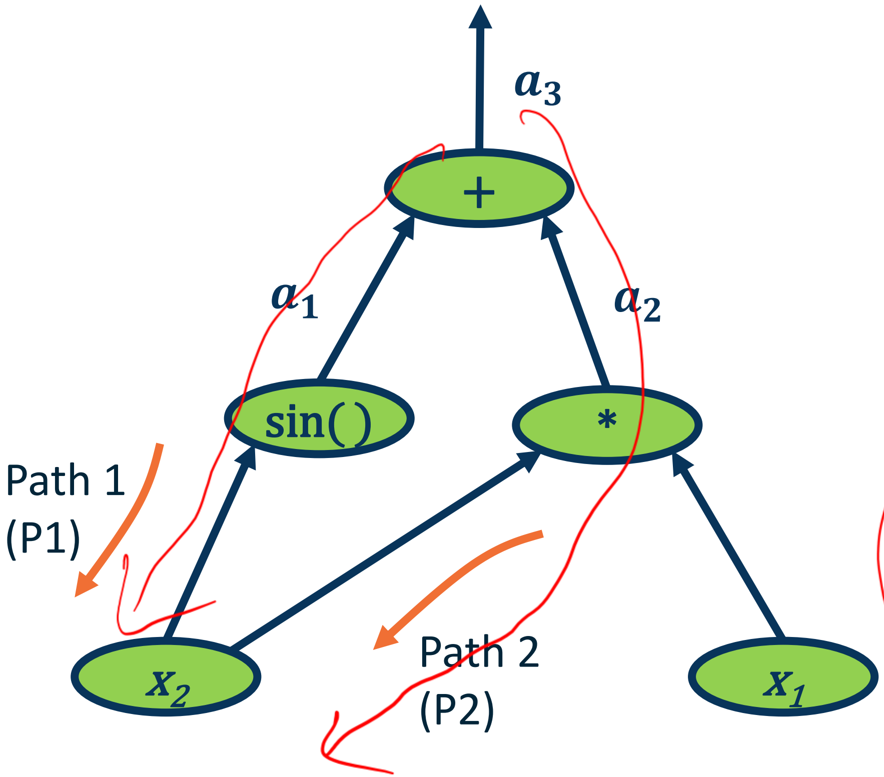
  Simplify notation:

  Denote bar as: $\overline{a_3} = \frac{\partial f}{\partial a_3}$

- Start at **end** and move **backward**

Example

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



$$\overline{a_3} = \frac{\partial f}{\partial a_3} = 1$$

$$\overline{a_1} = \frac{\partial f}{\partial a_1} = \frac{\partial f}{\partial a_3}\frac{\partial a_3}{\partial a_1} = \frac{\partial f}{\partial a_3}\frac{\partial(a_1+a_2)}{\partial a_1} = \frac{\partial f}{\partial a_3}\,1 = \overline{a_3}$$

$$\overline{a_2} = \frac{\partial f}{\partial a_2} = \frac{\partial f}{\partial a_3}\frac{\partial a_3}{\partial a_2} = \overline{a_3}$$

$$\overline{x_2^{P1}} = \frac{\partial f}{\partial a_1}\frac{\partial a_1}{\partial x_2} = \overline{a_1}\,\cos(x_2)$$

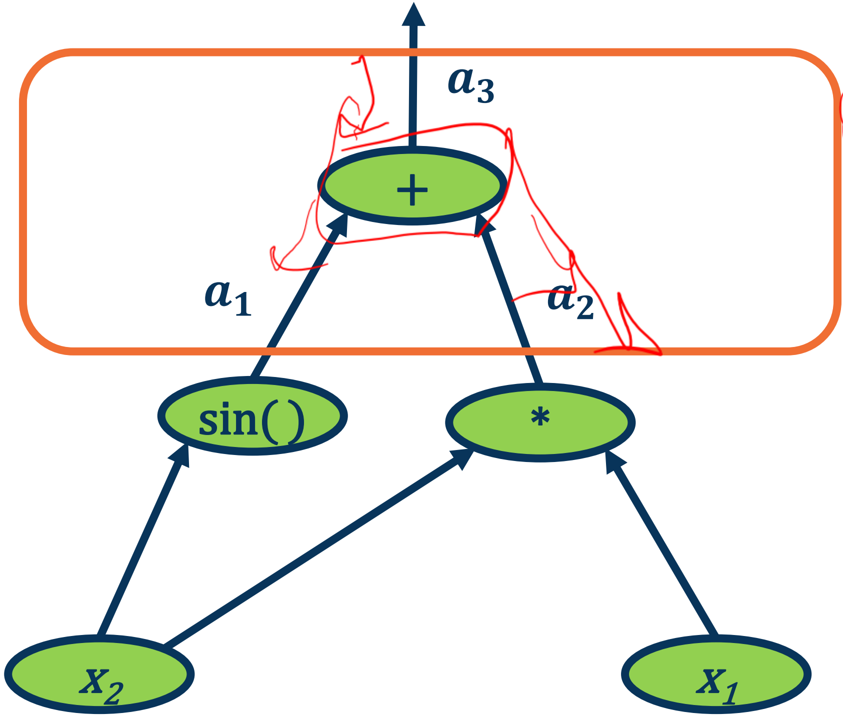
$$\overline{x_2^{P2}} = \frac{\partial f}{\partial a_2}\frac{\partial a_2}{\partial x_2} = \frac{\partial f}{\partial a_2}\frac{\partial(x1x2)}{\partial x_2} = \overline{a_2}x_1$$

$$\overline{x_1} = \frac{\partial f}{\partial a_2}\frac{\partial a_2}{\partial x_1} = \overline{a_2}x_2$$

Gradients from multiple paths **summed**

Example

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



$$\boxed{\bar{a}_1} = \boxed{\frac{\partial f}{\partial a_1}} = \frac{\partial f}{\partial a_3} \frac{\partial a_3}{\partial a_1} = \frac{\partial f}{\partial a_3} \frac{\partial (a_1 + a_2)}{\partial a_1} = \frac{\partial f}{\partial a_3} 1 = \boxed{\bar{a}_3}$$

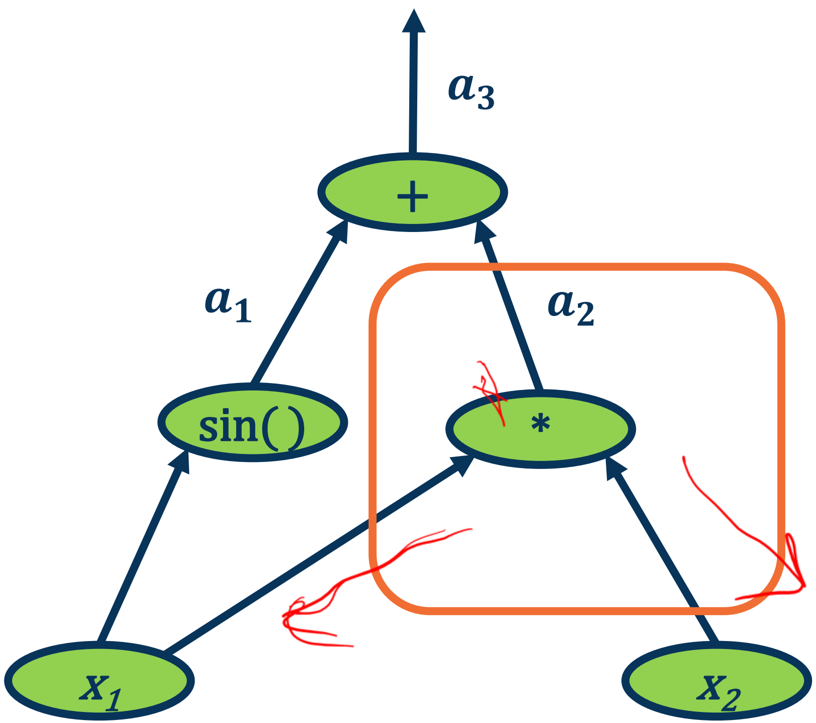
$$\boxed{\bar{a}_2} = \frac{\partial f}{\partial a_2} = \frac{\partial f}{\partial a_3} \frac{\partial a_3}{\partial a_2} = \boxed{\bar{a}_3}$$

Addition operation distributes gradients along all paths!

Patterns of Gradient Flow: Addition

Patterns of Gradient Flow: Multiplication

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

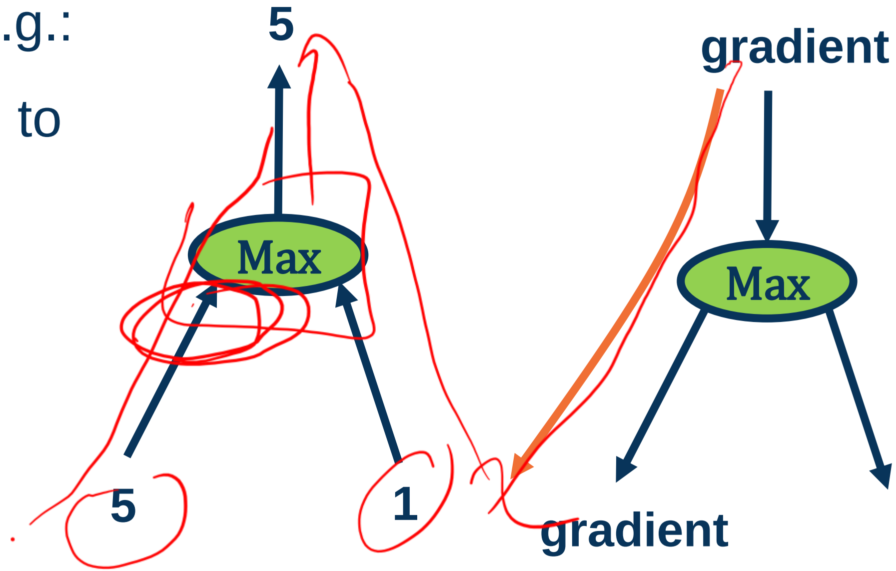


Multiplication operation is a gradient switcher (multiplies it by the values of the other term)

$$\boxed{\overline{x_2}} = \frac{\partial f}{\partial a_2}\frac{\partial a_2}{\partial x_2} = \frac{\partial f}{\partial a_2}\frac{\partial (x1x2)}{\partial x_2} = \boxed{\overline{a_2}}\,x_1$$

$$\overline{x_1} = \frac{\partial f}{\partial a_2}\frac{\partial a_2}{\partial x_1} = \boxed{\overline{a_2}x_2}$$

Several other patterns as well, e.g.:



Max operation **selects** which path to push the gradients through

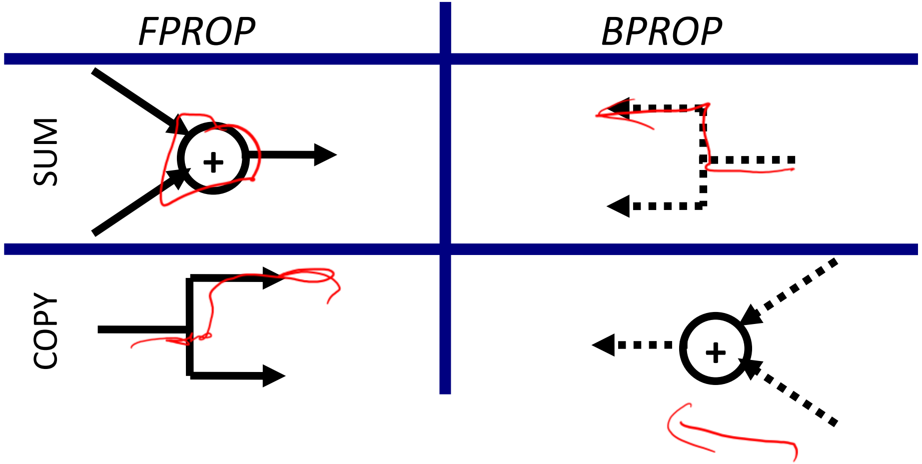
- Gradient flows along the path that was "selected" to be max
- This information must be recorded in the forward pass

The flow of gradients is one of the **most important aspects** in deep neural networks

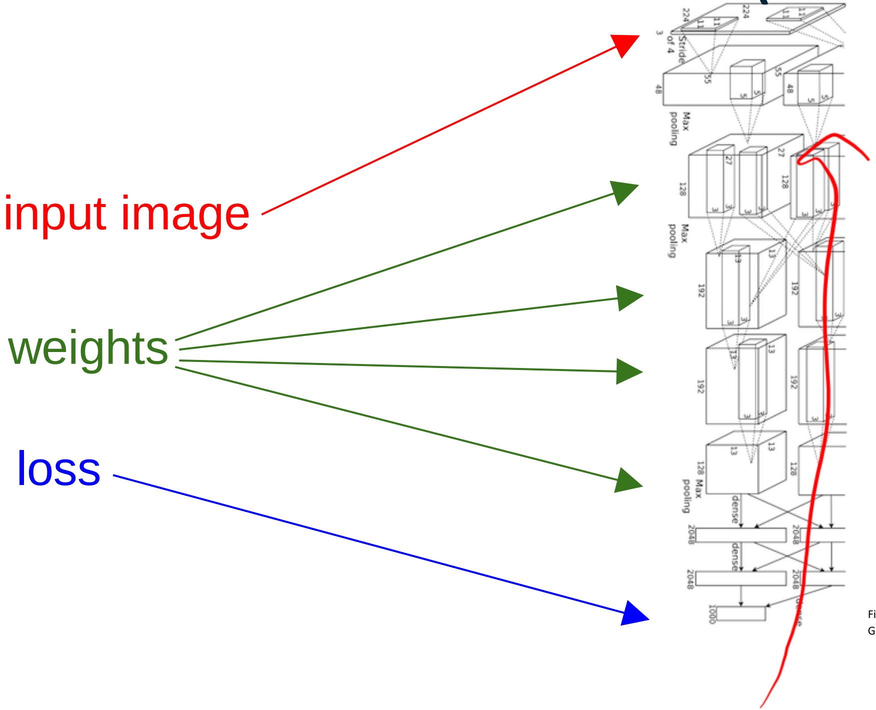
- If gradients **do not flow backwards properly,** learning slows or stops!

Patterns of Gradient Flow: Other

Duality in Fprop and Bprop



Convolutional network (AlexNet)



input image

weights

loss

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Neural Turing Machine

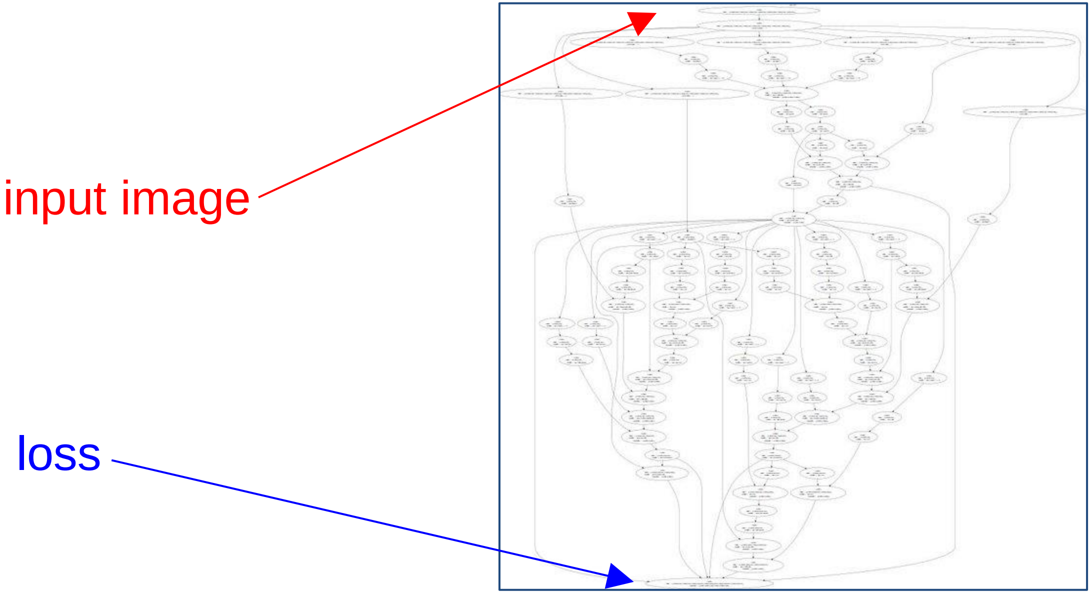
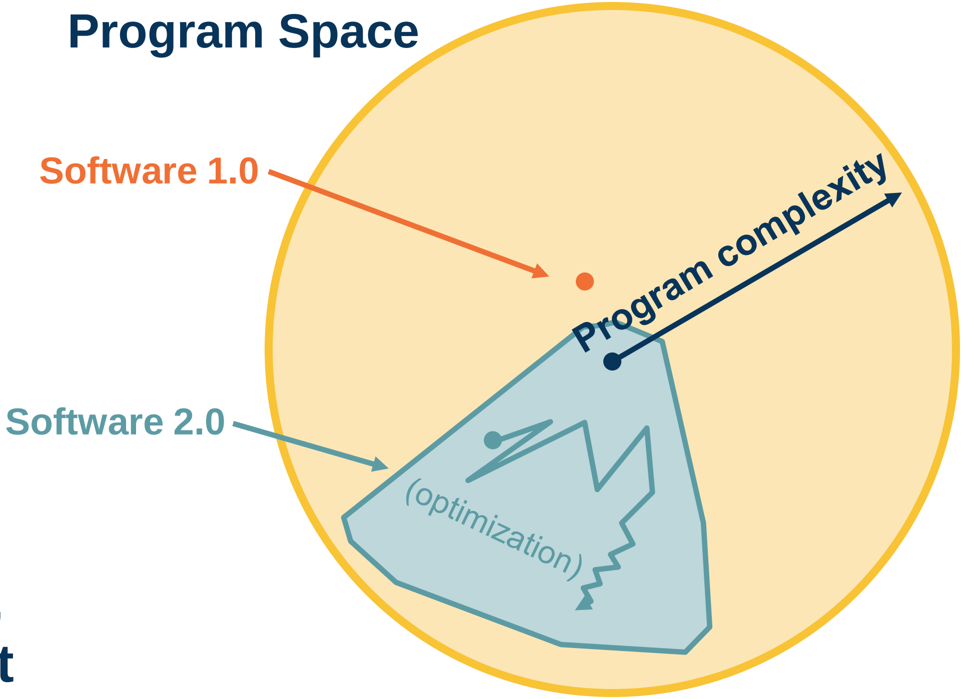


Figure reproduced with permission from a Twitter post by Andrej Karpathy.

Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

- Computation graphs are **not limited to mathematical functions!**
- Can have **control flows** (if statements, loops) and **backpropagate** through **algorithms**!
- Can be done **dynamically** so that **gradients are computed**, then **nodes are added, repeat**
- **Differentiable programming**



Adapted from figure by Andrej Karpathy

Power of Automatic Differentiation