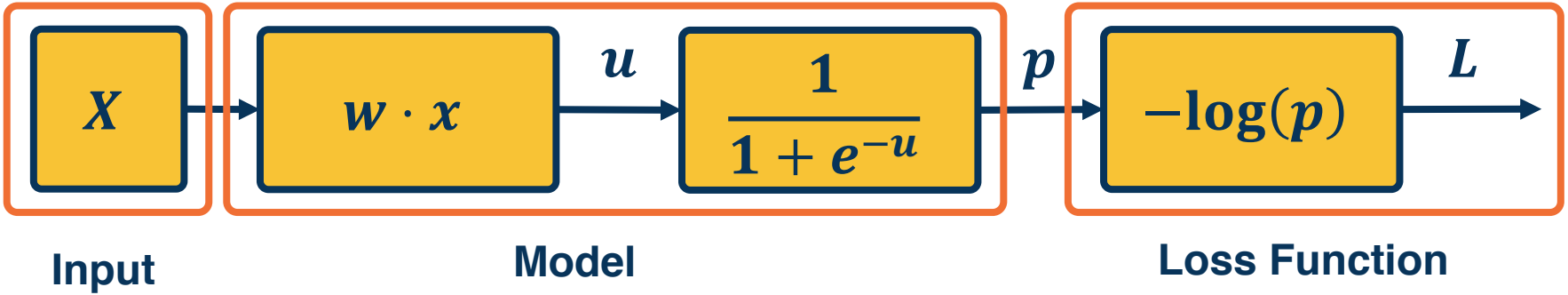
Neural Network View of a Linear Classifier

A **linear classifier** can be broken down into:

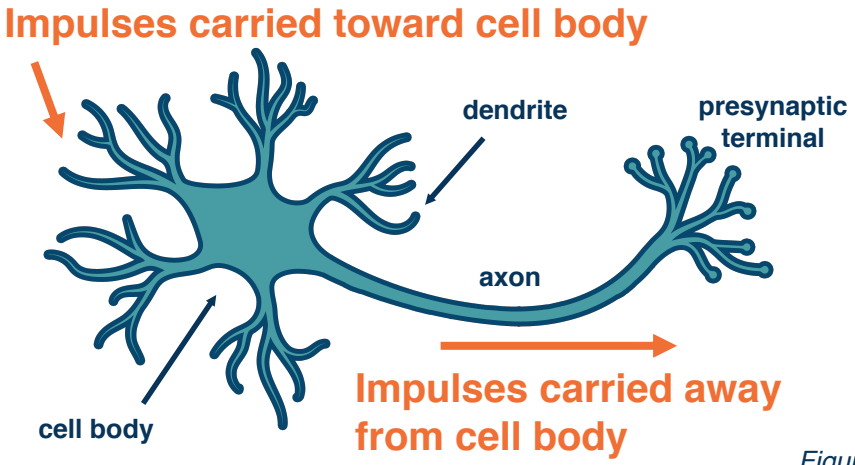
- Input
- A function of the input
- A loss function

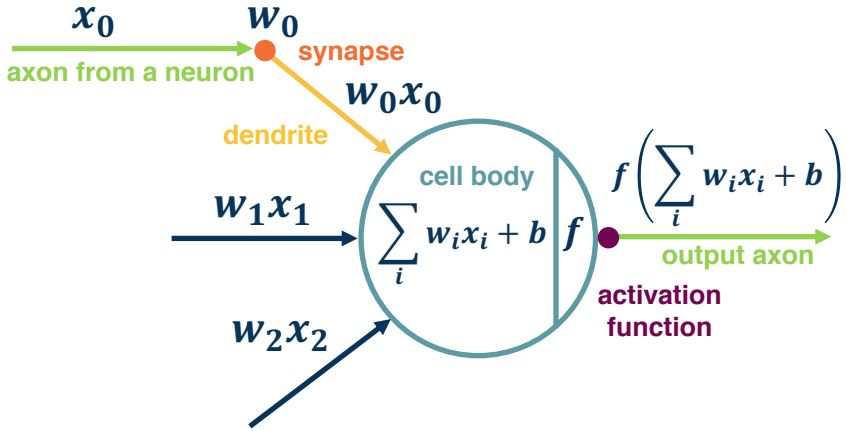
It's all just one function that can be **decomposed** into building blocks



A simple **neural network** has similar structure as our linear classifier:

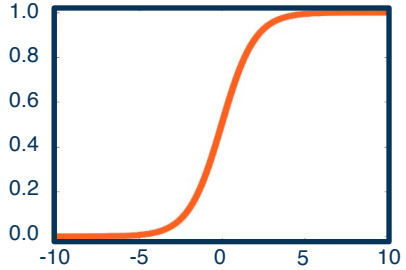
- A neuron takes input (firings) from other neurons **(-> input to linear classifier)**
- The inputs are summed in a weighted manner **(-> weighted sum)**
  - Learning is through a modification of the weights
- If it receives enough input, it "fires" (threshold or if weighted sum plus bias is high enough)





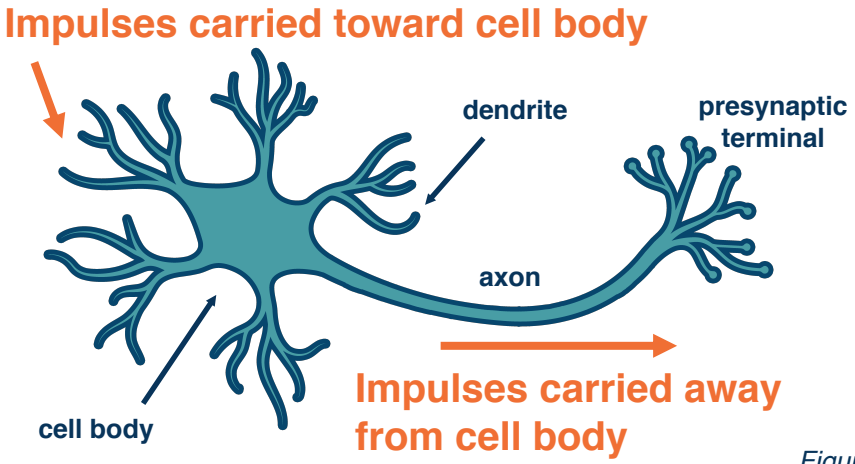
Figures adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

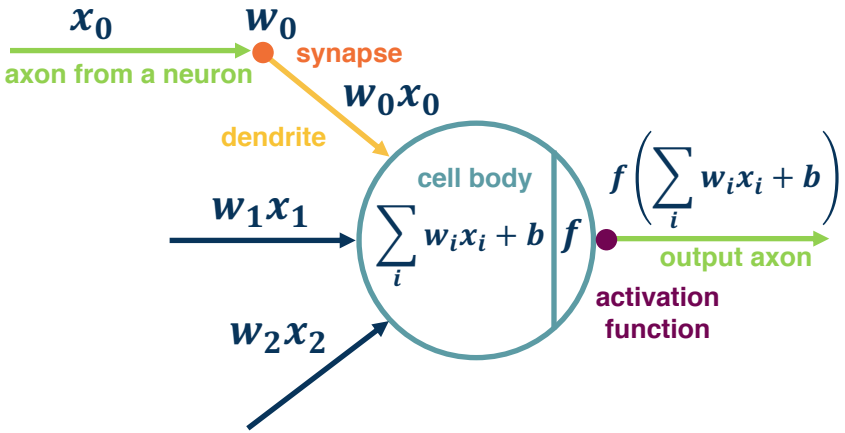
As we did before, the output of a neuron can be modulated by a non-linear function (e.g. sigmoid)



Sigmoid Activation Function

$$\frac{1}{1+e^{-x}}$$





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

We can have **multiple** neurons connected to the same input

Corresponds to a multi-class classifier

- Each output node outputs the score for a class

$$f(x, W) = \sigma(Wx + b) \quad \begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1m} & b1 \\ w_{21} & w_{22} & \cdots & w_{2m} & b2 \\ w_{21} & w_{22} & \cdots & w_{3m} & b3 \end{bmatrix}$$

- Often called fully connected layers
  - Also called a linear *projection layer*

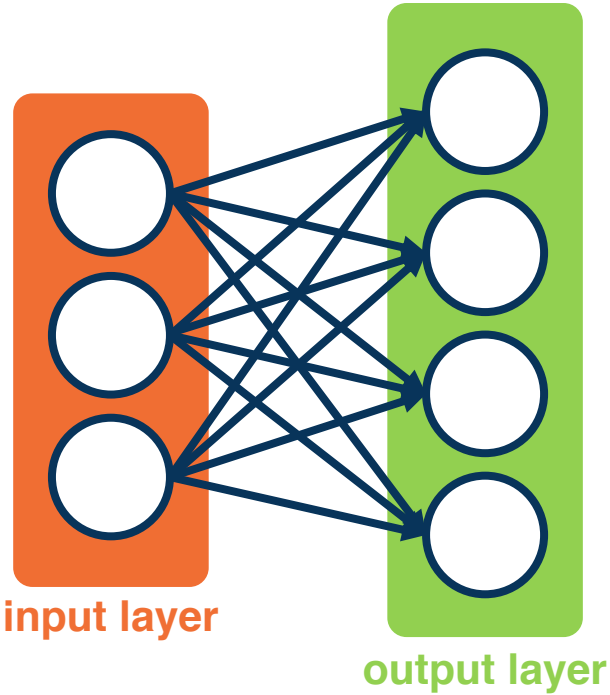
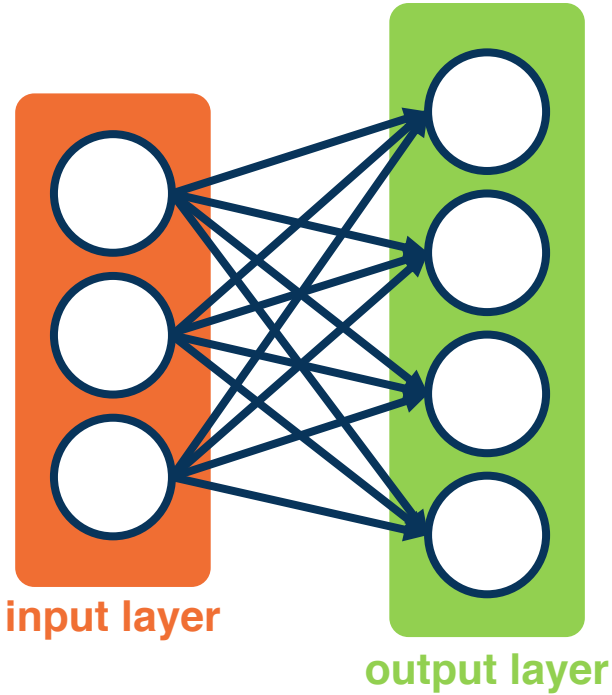


Figure adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

- Each input/output is a **neuron (node)**
- A linear classifier is called a **fully connected** layer
- Connections are represented as **edges**
- Output of a particular neuron is referred to as **activation**
- This will be expanded as we view computation in a neural network as a **graph**



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We can **stack** multiple layers together

- Input to second layer is output of first layer

Called a **2-layered neural network** (input is not counted)

Because the middle layer is neither input or output, and we don't know what their values represent, we call them **hidden** layers

- We will see that they end up learning effective features

This **increases** the representational power of the function!

- Two layered networks can represent any continuous function

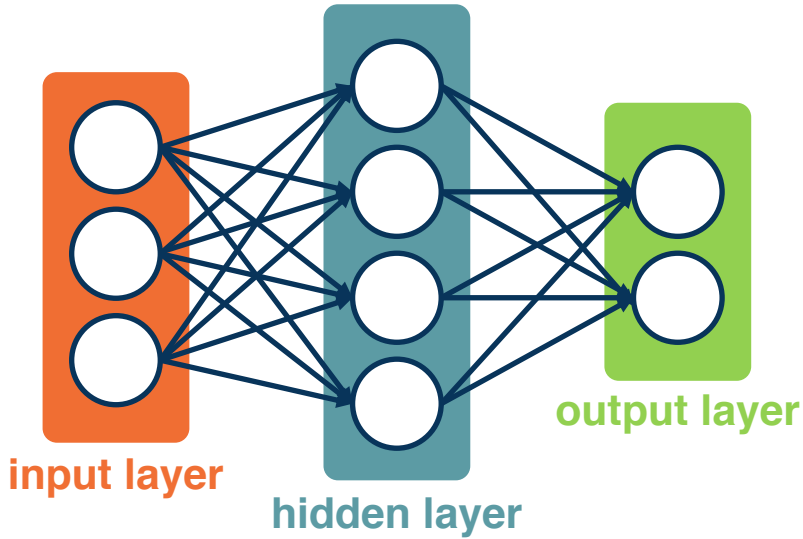
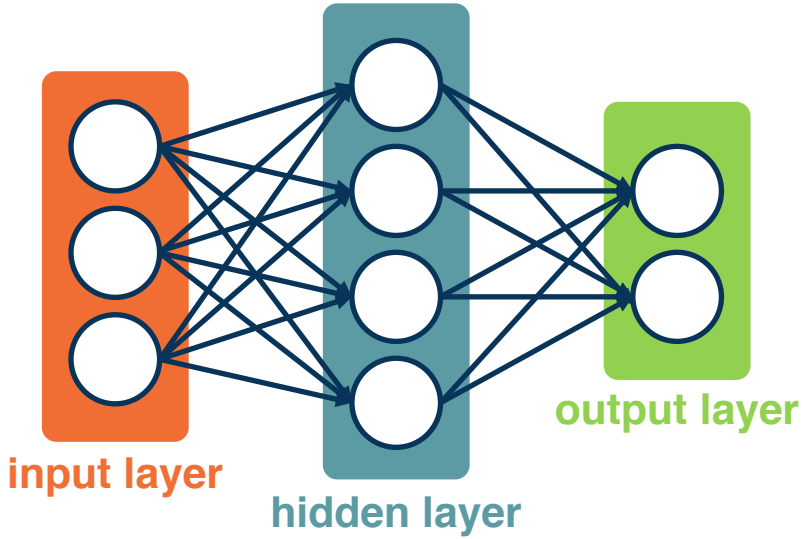


Figure adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

The same two-layered neural network **corresponds to adding another weight matrix**

- We will prefer the linear algebra view, but use some terminology from neural networks (& biology)



$$x \quad W_1 \quad W_2$$

$$=$$

$$f(x, W_1, W_2) = \sigma(W_2\sigma(W_1 x))$$

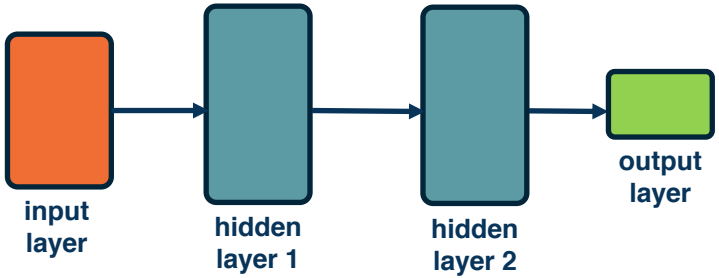
Figure adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Large (deep) networks can be built by adding more and more layers

Three-layered neural networks can represent **any function**

- The number of nodes could grow unreasonably (exponential or worse) with respect to the complexity of the function

We will show them **without edges**:



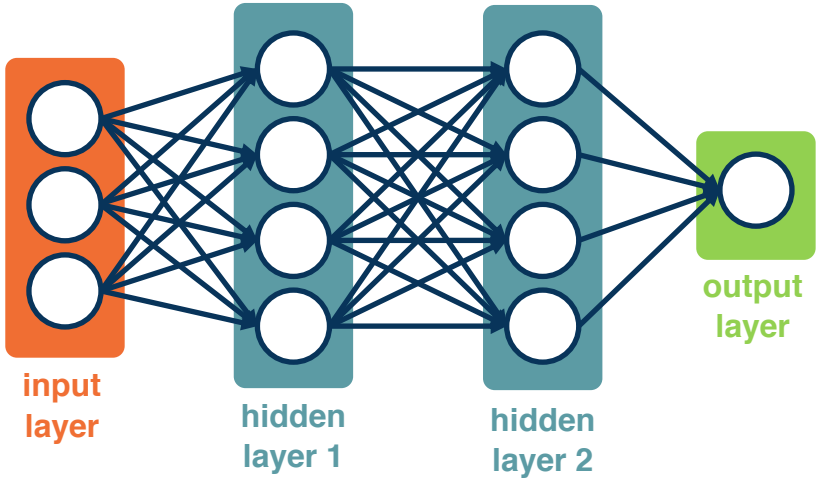


Figure adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Adding More Layers!

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Computation Graphs

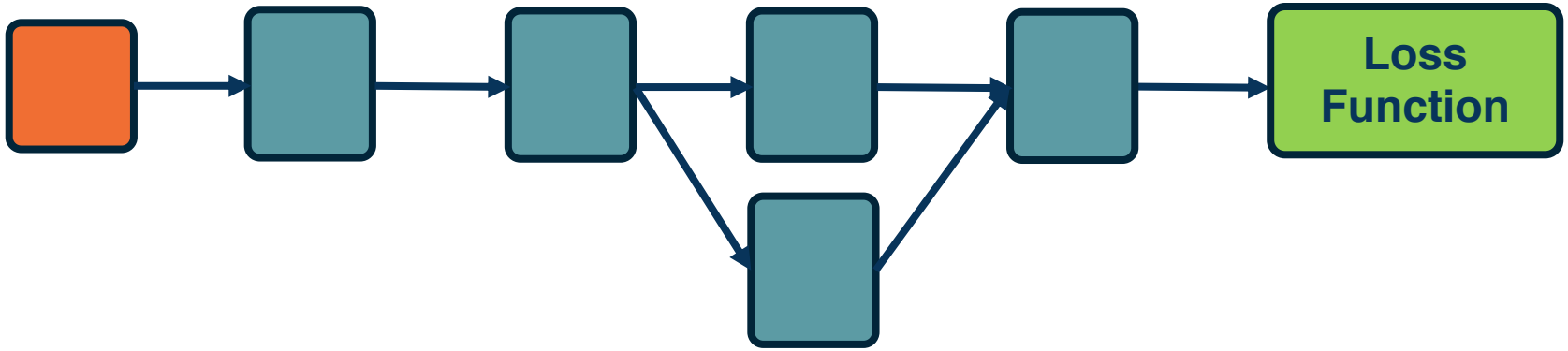
Functions can be made **arbitrarily complex** (subject to memory and computational limits), e.g.:

$$f(x, W) = \sigma(W_5\sigma(W_4\sigma(W_3\sigma(W_2\sigma(W_1 x))$$

We can use **any type of differentiable function (layer)** we want!

- At the end, **add the loss function**

Composition can have **some structure**



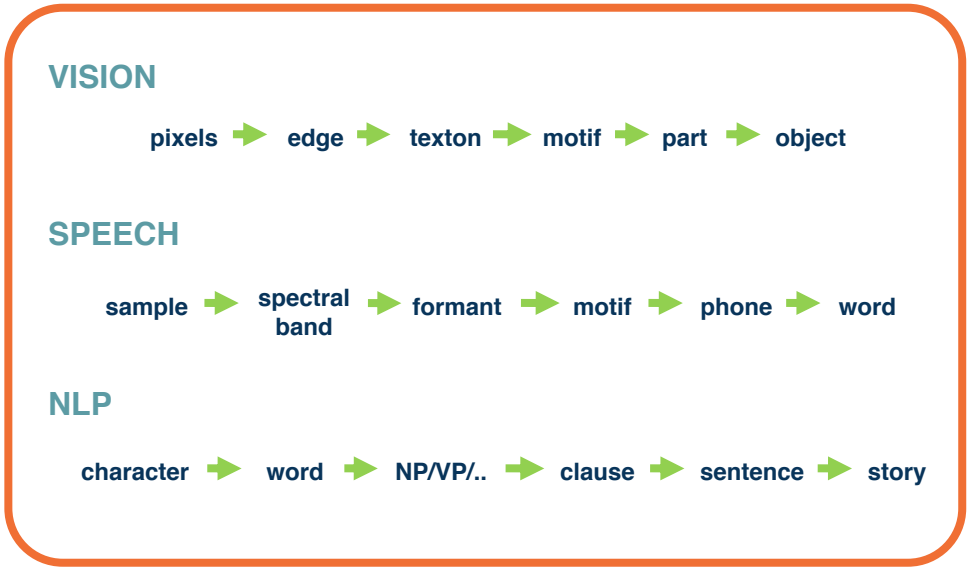
Adding Even More Layers

The world is **compositional**!

We want our **model** to reflect this

Empirical and theoretical evidence that it makes **learning complex functions easier**

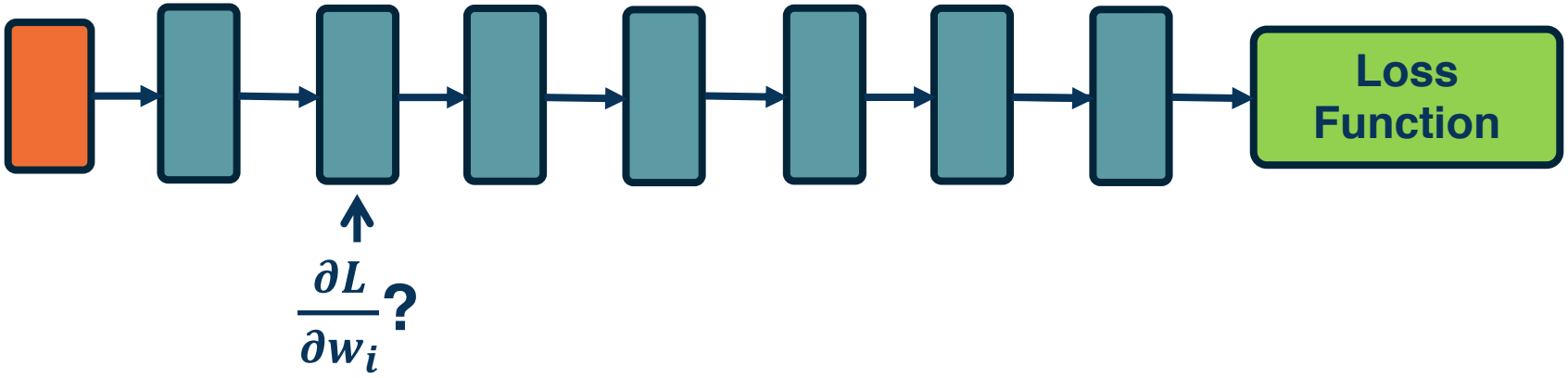
Note that **prior state of art engineered features** often had this compositionality as well



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

- **Pixels -> edges -> object parts -> objects**

- We are learning **complex models** with significant amount of parameters (millions or billions)
- How do we compute the gradients of the **loss** (at the end) with respect to **internal** parameters?
- Intuitively, want to understand how **small changes** in weight deep inside **are propagated** to affect the **loss function** at the end

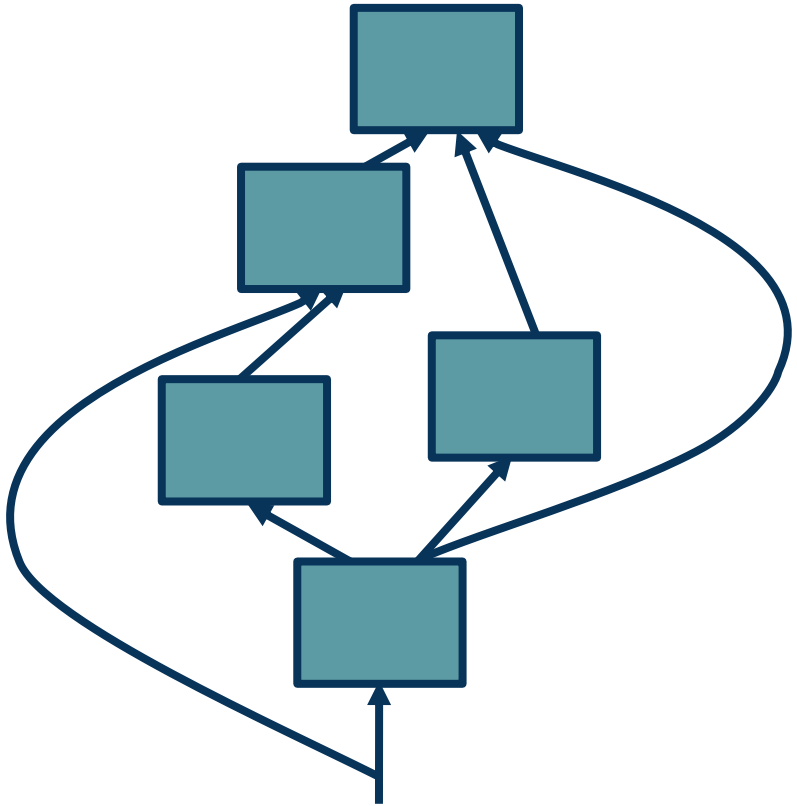


To develop a general algorithm for this, we will view the function as a **computation graph**

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

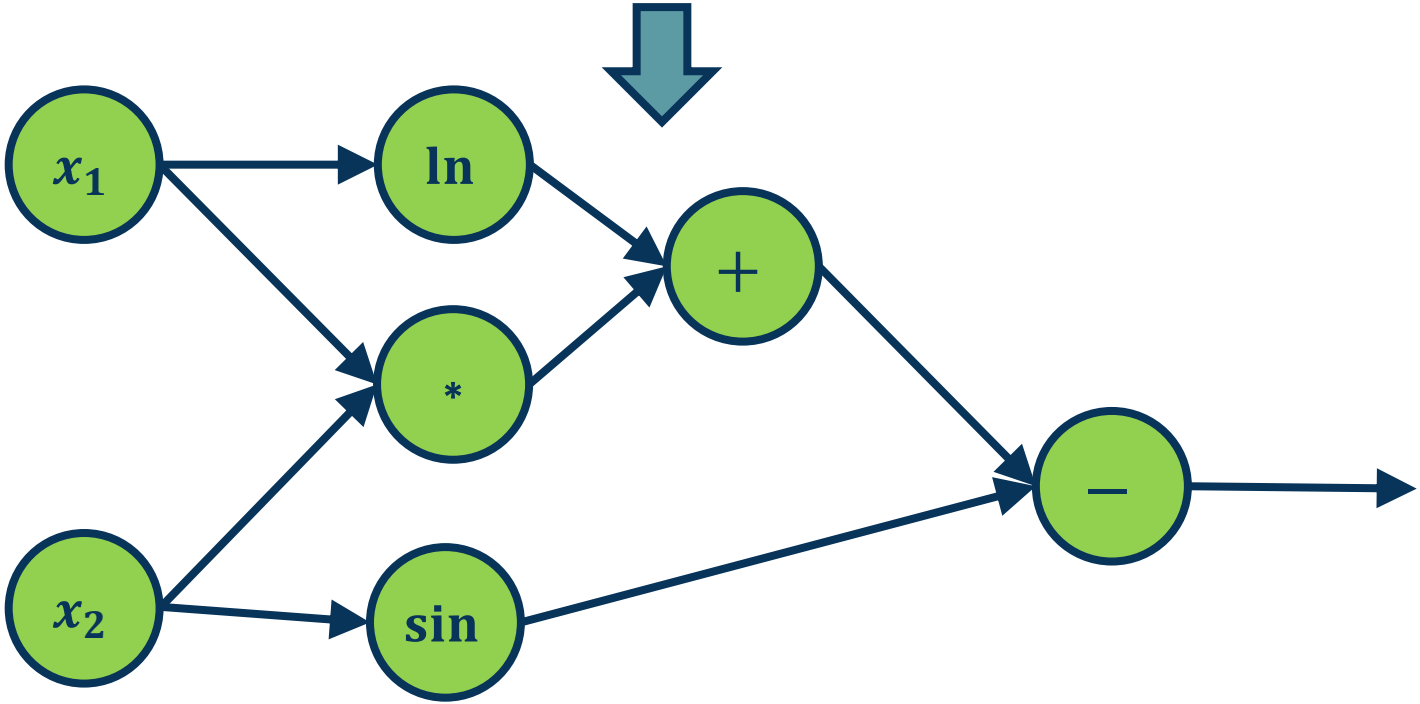
- Modules must be differentiable to support gradient computations for gradient descent

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



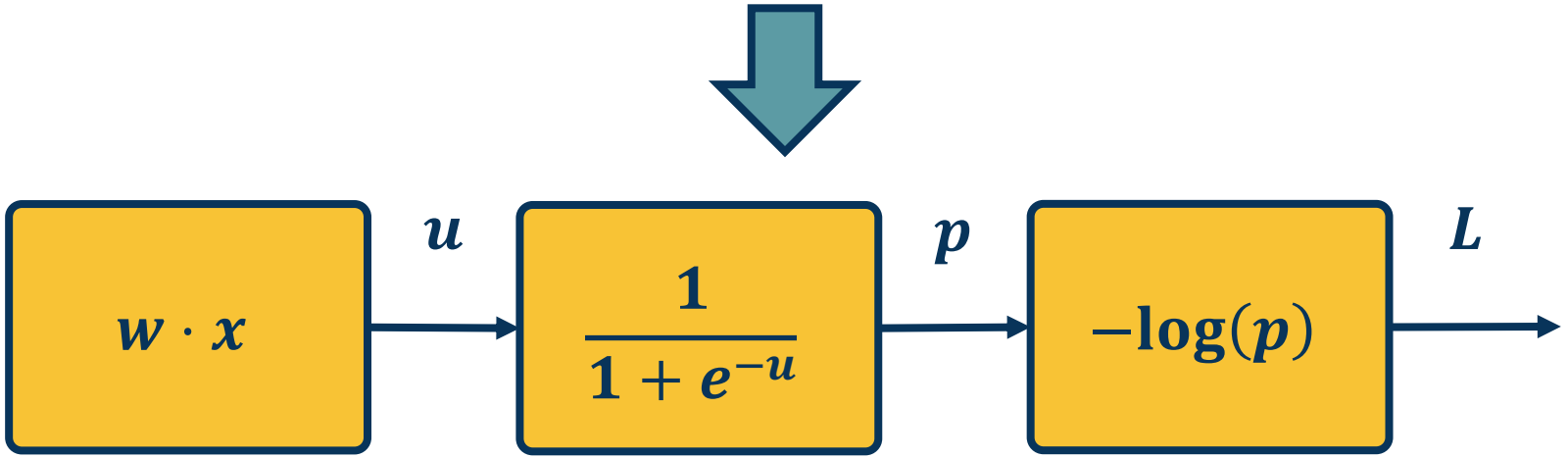
Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

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



Example

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



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

Backpropagation

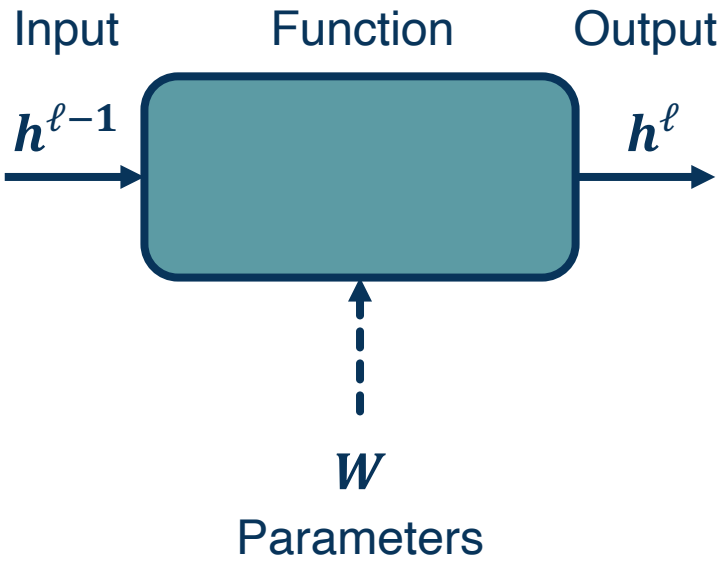
Given this computation graph, the training algorithm will:

- Calculate the current model's outputs (called the **forward pass**)
- Calculate the gradients for each module (called the **backward pass**)

Backward pass is a recursive algorithm that:

- Starts at **loss function** where we know how to calculate the gradients
- Progresses back through the modules
- Ends in the **input layer** where we do not need gradients (no parameters)

This algorithm is called **backpropagation**



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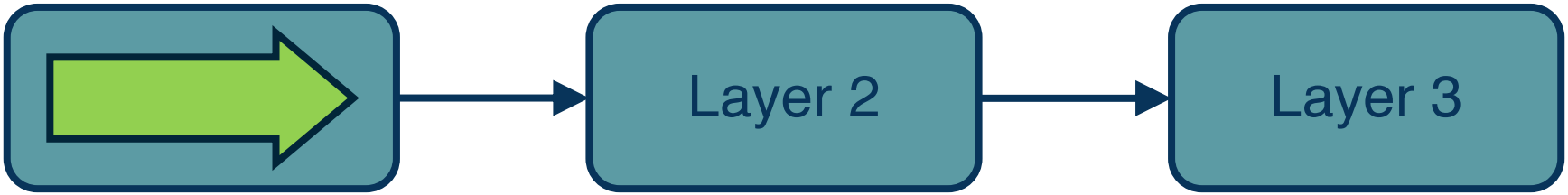
Step 1: Compute Loss on Mini-Batch: **Forward Pass**



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Step 1: Compute Loss on Mini-Batch: **Forward Pass**

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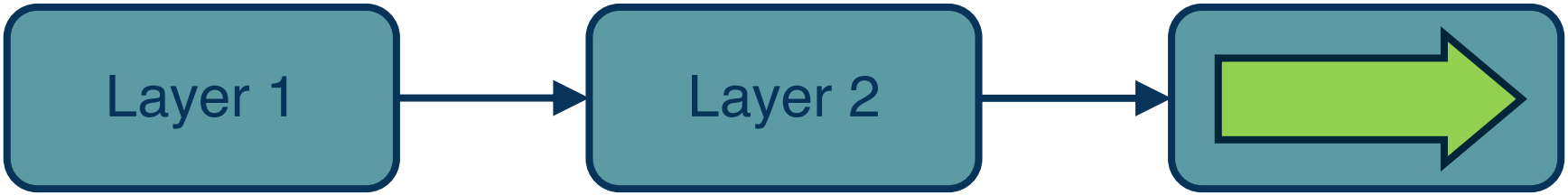


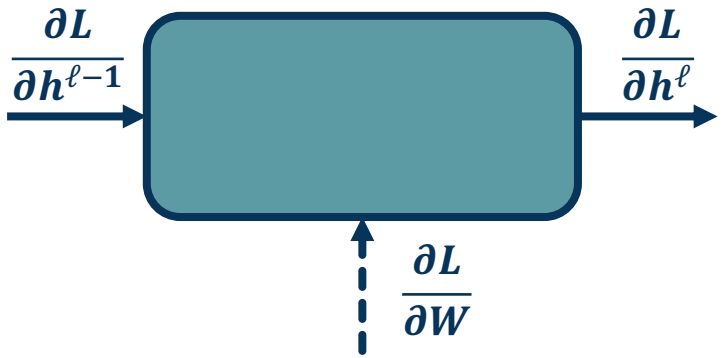
Note that we must store the **intermediate outputs of all layers**!

- This is because we will need them to **compute the gradients** (the gradient equations will have terms with the output values in them)

Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

In the **backward pass**, we seek to calculate the gradients of the loss with respect to the module's parameters

- Assume that we have the gradient of the loss with respect to the **module's outputs** (given to us by upstream module)
- We will also pass the gradient of the loss with respect to the **module's inputs**
  - This is not required for update the module's weights, but passes the gradients back to the previous module



Problem:

- We can compute local gradients: $\{\frac{\partial h^{\ell}}{\partial h^{\ell-1}}, \frac{\partial h^{\ell}}{\partial W}\}$
- We are given: $\frac{\partial L}{\partial h^{\ell}}$
- Compute: $\{\frac{\partial L}{\partial h^{\ell-1}}, \frac{\partial L}{\partial W}\}$

Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

- We can compute **local gradients**: $\{\frac{\partial h^{\ell}}{\partial h^{\ell-1}}, \frac{\partial h^{\ell}}{\partial W}\}$

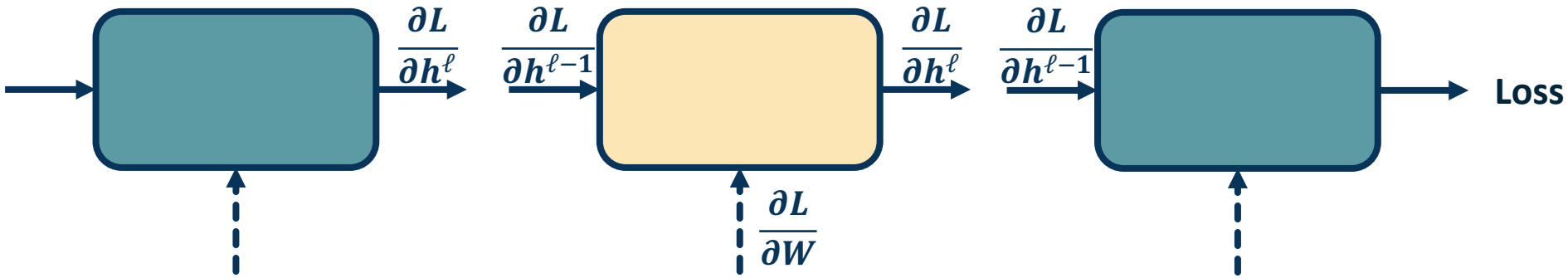
- This is just the **derivative of our function** with respect to its parameters and inputs!

Example: If $h^{\ell} = W h^{\ell-1}$

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

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

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

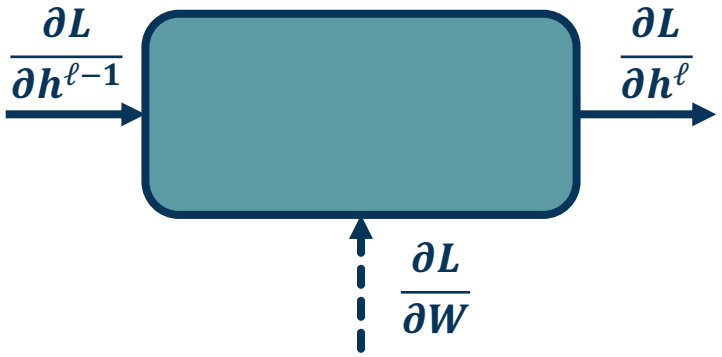


- We will use the *chain rule* to do this:

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

- We will use the **chain rule** to compute: $\{\frac{\partial L}{\partial h^{\ell-1}}, \frac{\partial L}{\partial W}\}$
- **Gradient of loss w.r.t. inputs:** $\frac{\partial L}{\partial h^{\ell-1}} = \frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial h^{\ell-1}}$

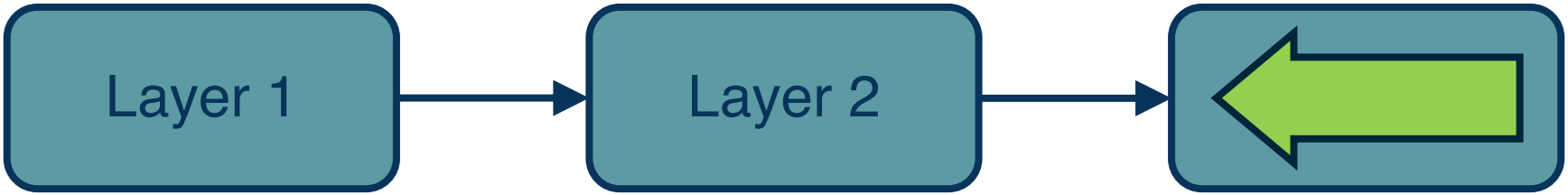
  Given by upstream module **(upstream gradient)**
- **Gradient of loss w.r.t. weights:** $\frac{\partial L}{\partial W} = \frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial W}$



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

Step 1: Compute Loss on Mini-Batch: **Forward Pass**

Step 2: Compute Gradients wrt parameters: **Backward Pass**



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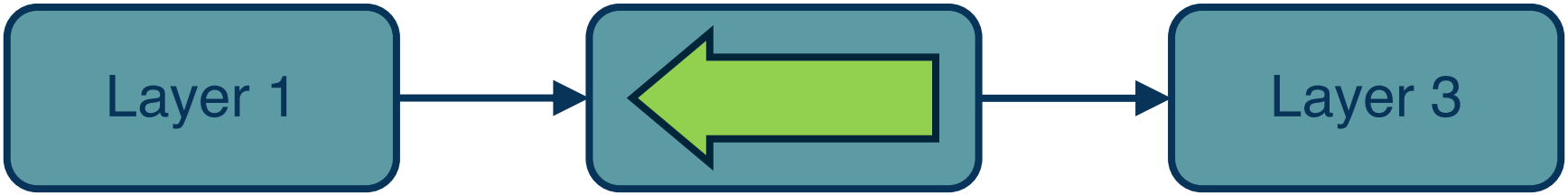

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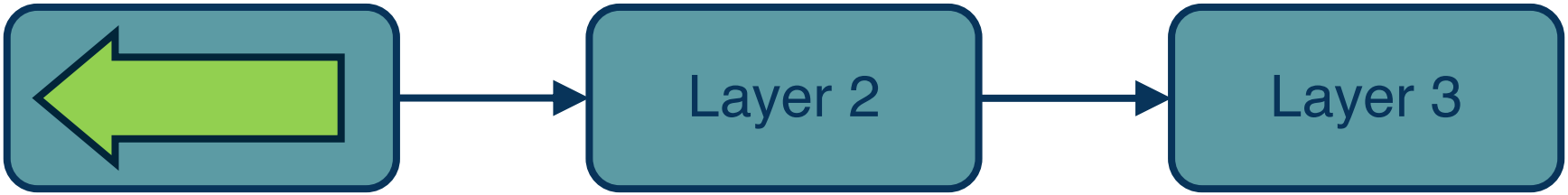

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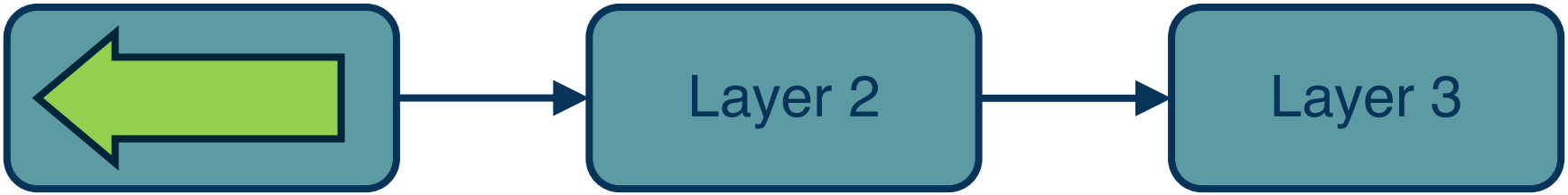
Step 1: Compute Loss on Mini-Batch: **Forward Pass**

Step 2: Compute Gradients wrt parameters: **Backward Pass**

Step 3: Use **gradient** to update **all parameters** at the end



$$w_i = w_i - \alpha \frac{\partial L}{\partial w_i}$$

Backpropagation is the application of gradient descent to a computation graph via the chain rule!

Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

Backpropagation and Automatic Differentiation

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

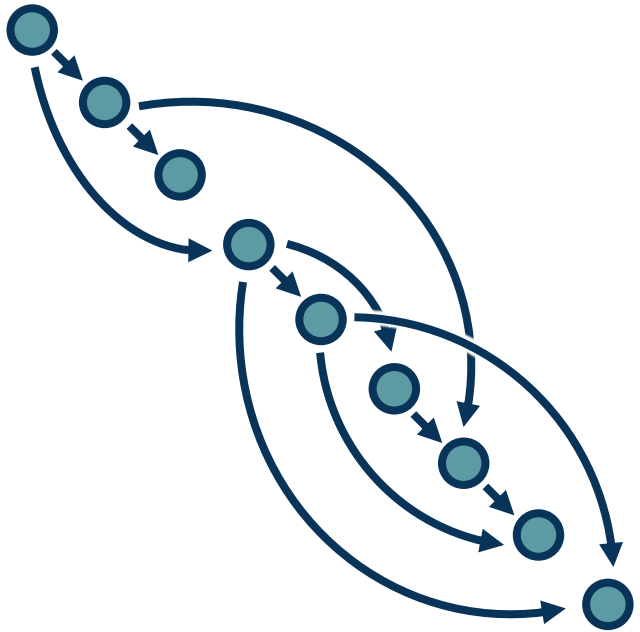
But the idea can be applied to **any directed acyclic graph (DAG)**

- 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 **gradient outputs for efficient computation**

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



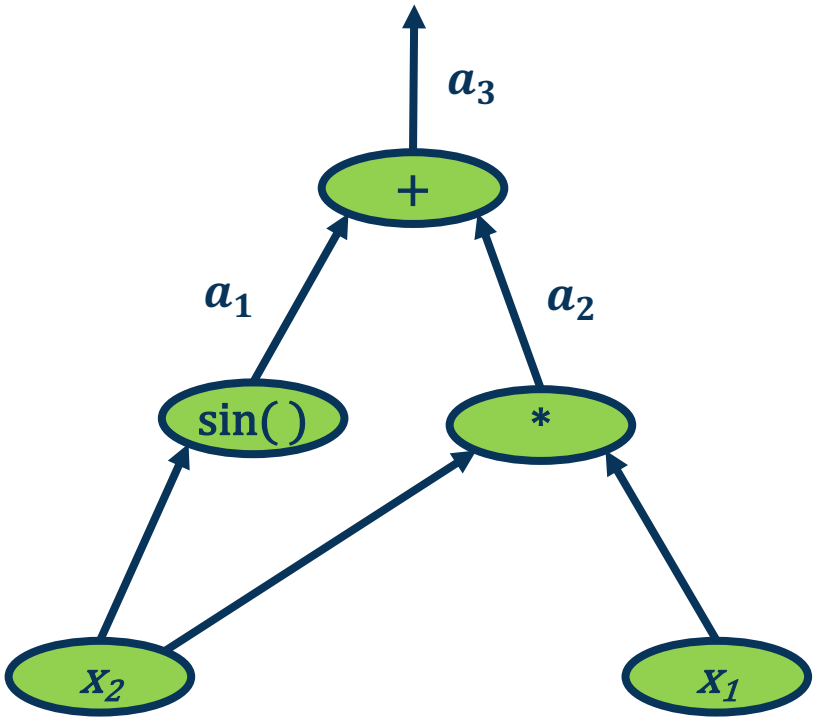
Computation = Graph

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

Auto-Diff

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

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



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

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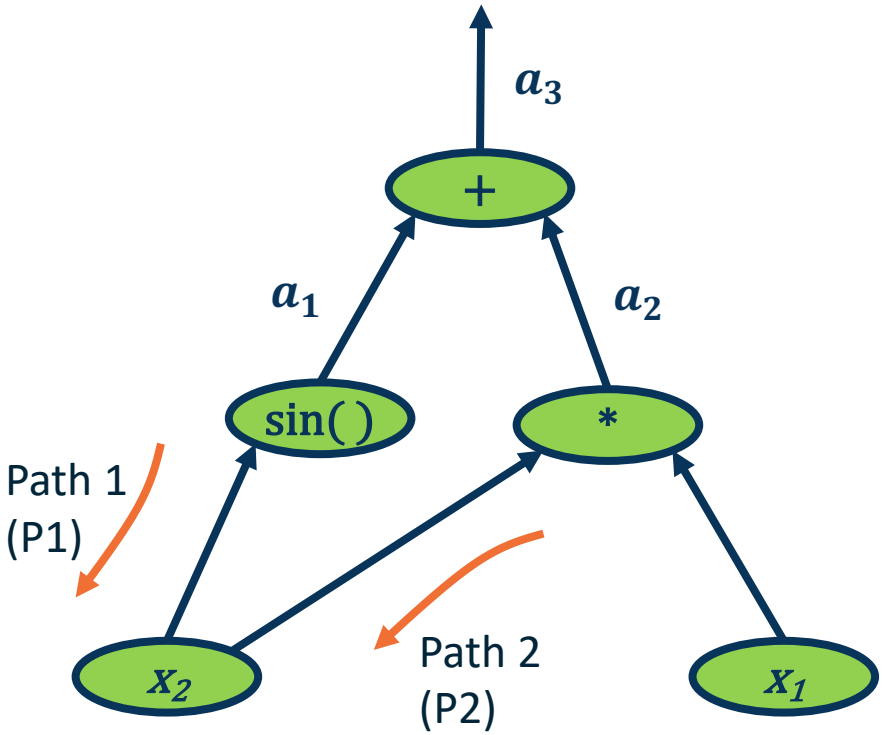
$$f(x_1, x_2) = x_1 x_2 + \sin(x_2)$$



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

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

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

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

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

Gradients from multiple paths **summed**

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

Example

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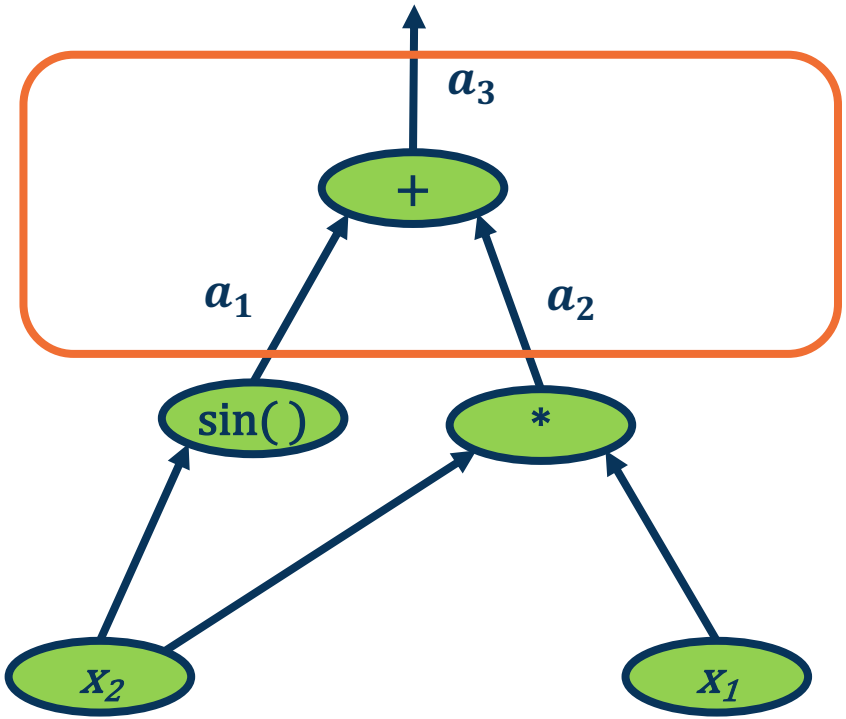
$$f(x_1, x_2) = x_1 x_2 + \sin(x_2)$$



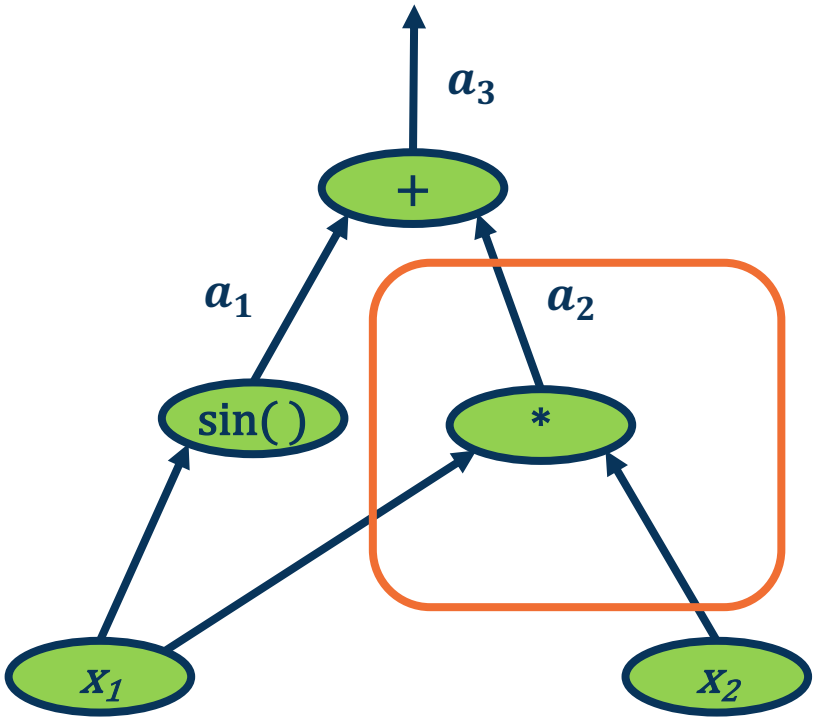
$$\overline{a_1} = \frac{\partial f}{\partial a_1} = \frac{\partial f}{\partial a_3}\frac{\partial a_3}{\partial a_1} = \frac{\partial f}{\partial a_3}\frac{\partial (a_1 + a_2)}{\partial a_1} = \frac{\partial f}{\partial a_3}\,1 = \overline{a_3}$$

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

Addition operation distributes gradients along all paths!

Patterns of Gradient Flow: Addition

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



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

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

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

Patterns of Gradient Flow: Multiplication

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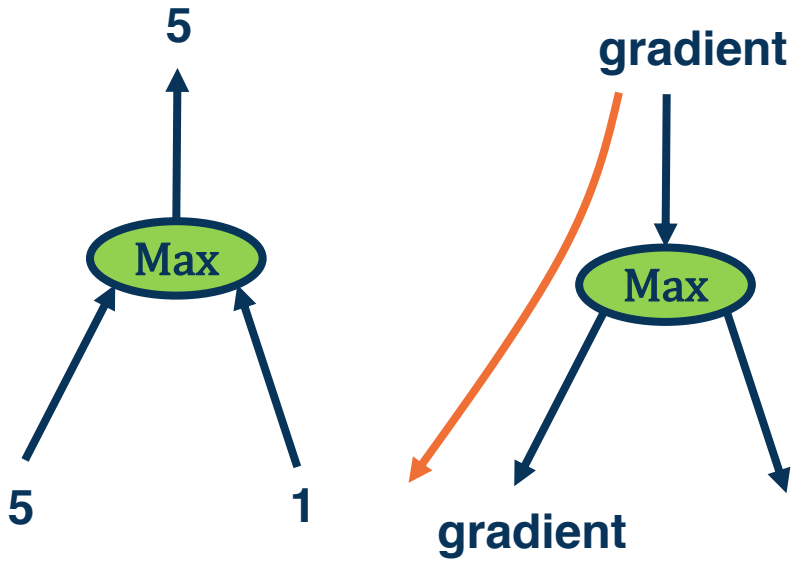
Several other patterns as well, e.g.:

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



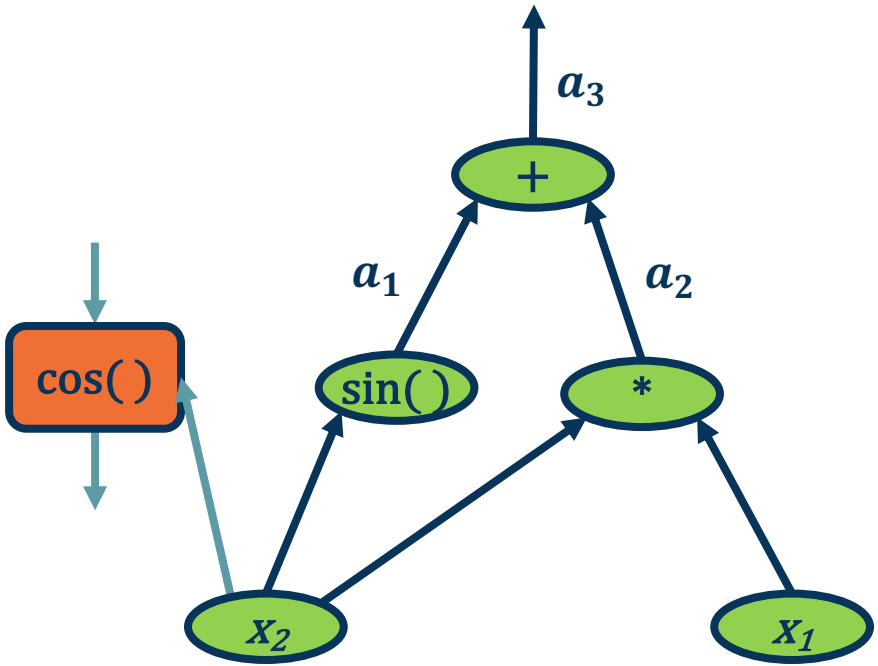
The flow of gradients is one of the **most important aspects** in deep neural networks

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

- 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**

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

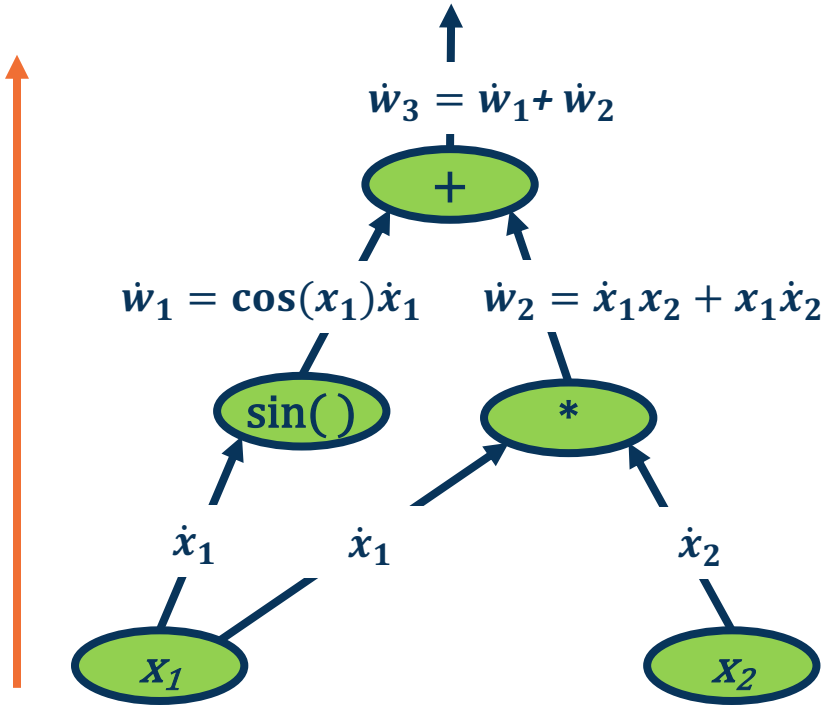


Note that we can also do **forward mode** automatic differentiation

Start from **inputs** and propagate gradients forward

Complexity is proportional to input size

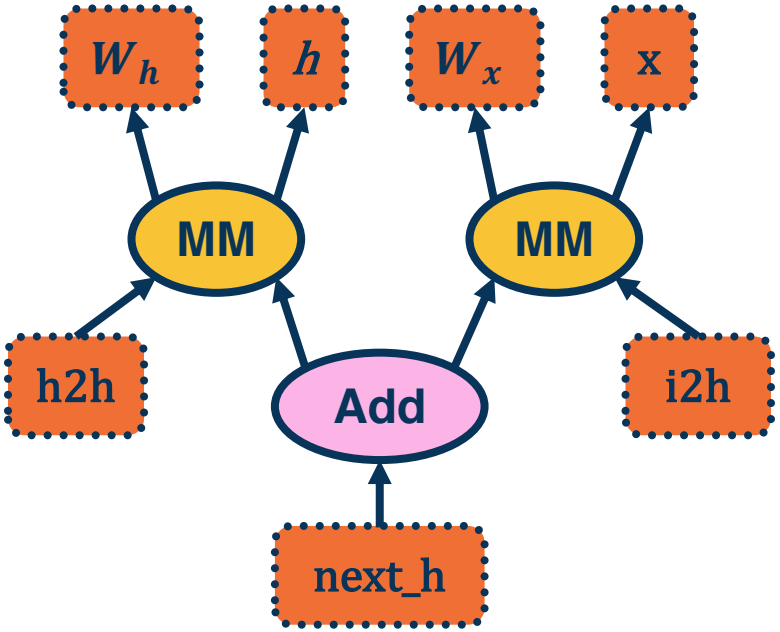
- However, in most cases our **inputs** (images) are large and **outputs** (loss) are small



A graph is created on the fly

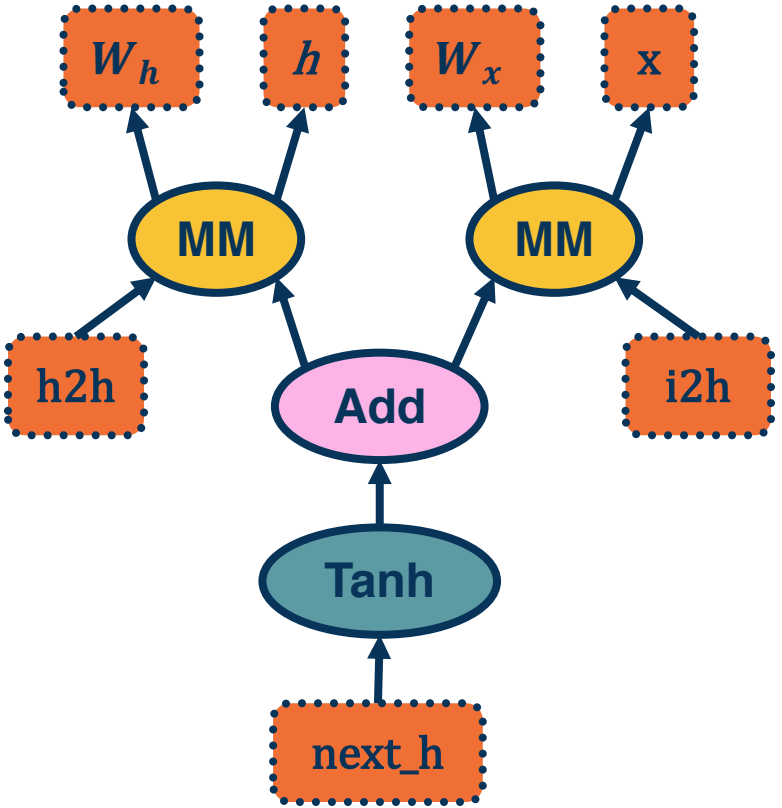
```
from torch.autograd import Variable

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)



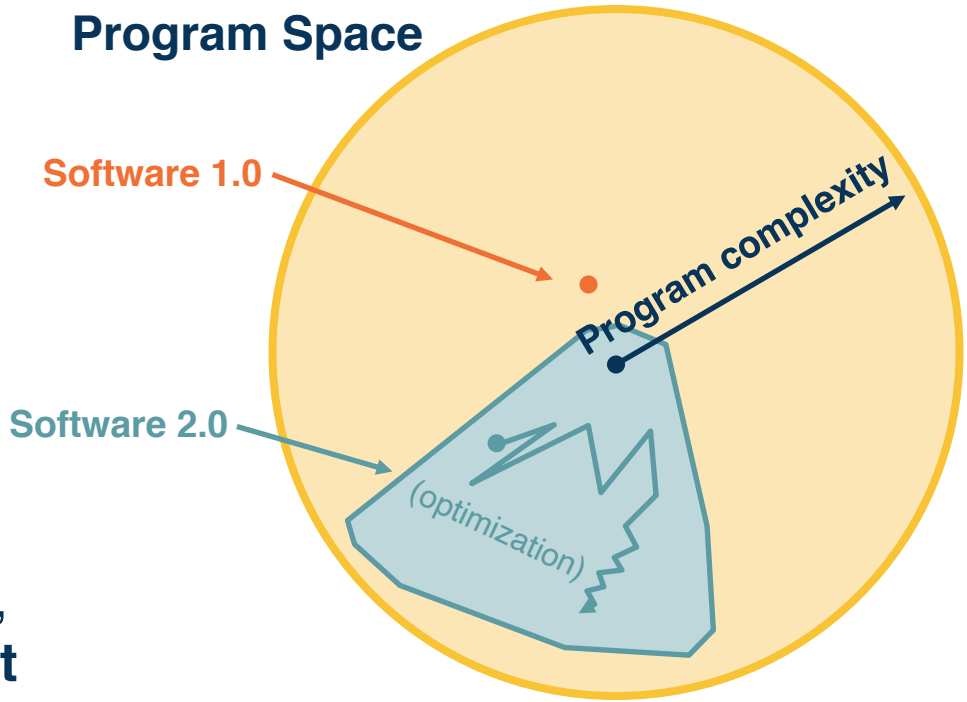
Back-propagation uses the dynamically built graph

```
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))
```



From pytorch.org

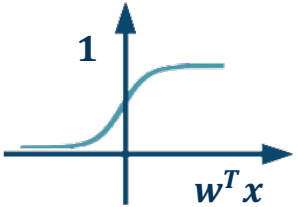
- Computation graphs are **not limited to mathematical functions!**
- Can have **control flows** (if statements, loops) and **backpropagate** through **algorithms**!
- Can be done **dynamically** so that **gradients are computed**, then **nodes are added, repeat**
- **Differentiable programming**

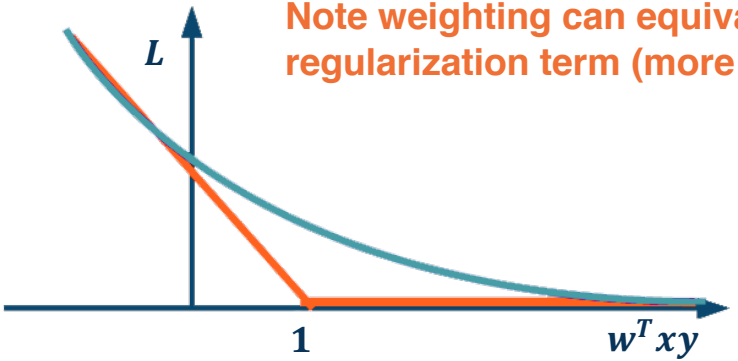


Adapted from figure by Andrej Karpathy

Computation Graph Example for Logistic Regression

- Input: $\boldsymbol{x} \in \boldsymbol{R^D}$
- Binary label: $\boldsymbol{y} \in \{-\mathbf{1}, +\mathbf{1}\}$
- Parameters: $\boldsymbol{w} \in \boldsymbol{R^D}$
- Output prediction: $\boldsymbol{p(y=1|x) = \frac{1}{1+e^{-w^T x}}}$
- Loss: $\boldsymbol{L = \frac{1}{2}\|w\|^2 - \lambda \log\big(p(y|x)\big)}$





Note weighting can equivalently be on regularization term (more standard)!

Log Loss

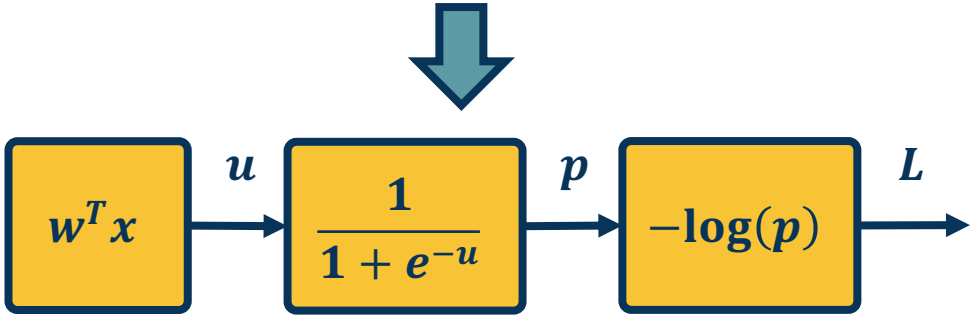
Adapted from slide by Marc'Aurelio Ranzato

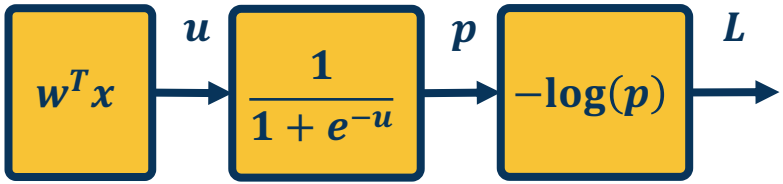
We have discussed **computation graphs for generic functions**

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!

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





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

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

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

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

Example Gradient Computations

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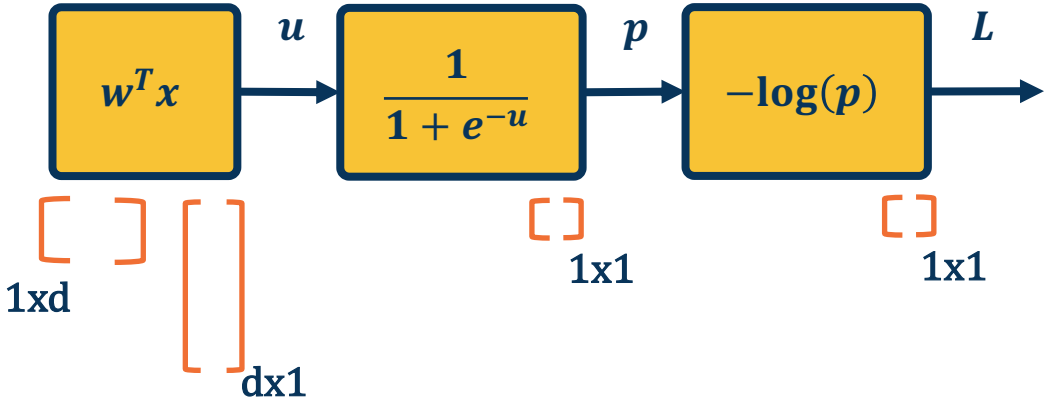
Vectorization and Jacobians of Simple Layers

Georgia Tech

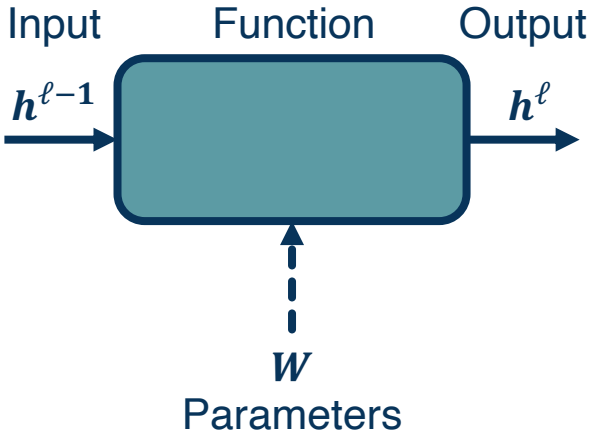
The chain rule can be computed as a **series of scalar, vector, and matrix linear algebra operations**



Extremely efficient in graphics processing units (GPUs)

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

1x1 1x1 1x1 1xd



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

$$\begin{bmatrix} \\ \\ \end{bmatrix} \quad \begin{bmatrix} \leftarrow w_i^T \rightarrow \\ \\ \end{bmatrix} \quad \begin{bmatrix} \\ \\ \end{bmatrix}$$

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

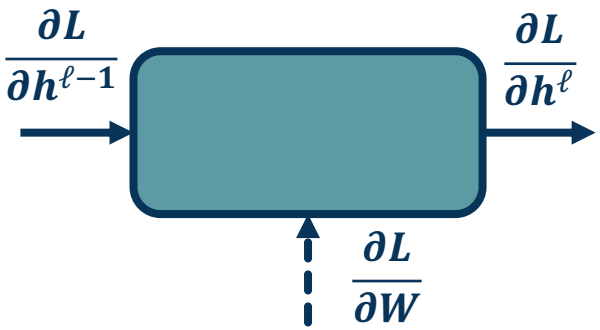
Fully Connected (FC) Layer: Forward Function

Georgia Tech

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

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

(other elements zeros)



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

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

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

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

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

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

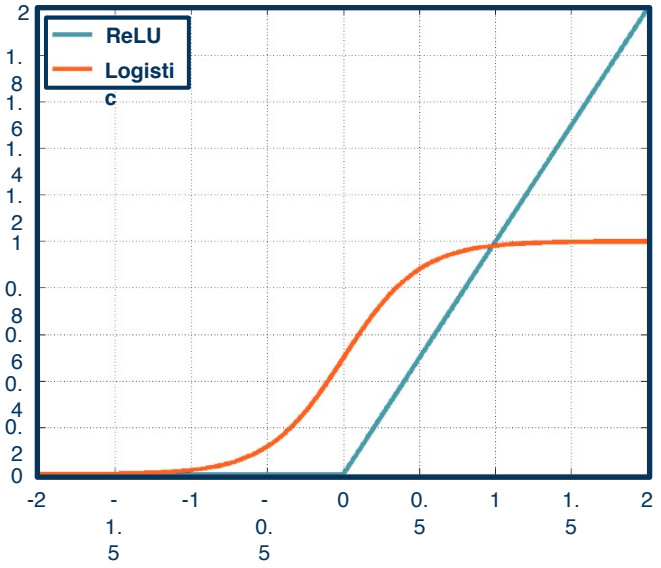
$$1 \times |h^{\ell-1}| \quad 1 \times |h^{\ell}| \quad |h^{\ell}| \times |h^{\ell-1}|$$

We can employ **any differentiable (or piecewise differentiable) function**

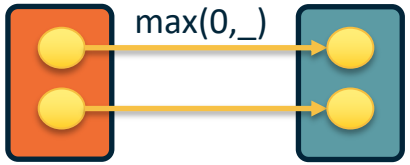
A common choice is the **Rectified Linear Unit**

- Provides non-linearity but better gradient flow than sigmoid
- Performed **element-wise**

How many parameters for this layer?



$$\boldsymbol{h^{\ell} = \max\left(0, h^{\ell-1}\right)}$$

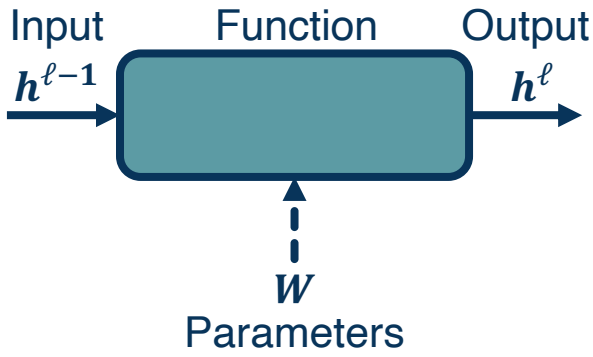


Full Jacobian of ReLU layer is **large** (output dim x input dim)

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

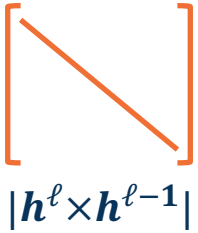
Max function **funnels gradients through selected max**

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



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

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



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