Topics:

- Neural Networks
- Backpropagation

CS 4644-DL / 7643-A

ZSOLT KIRA

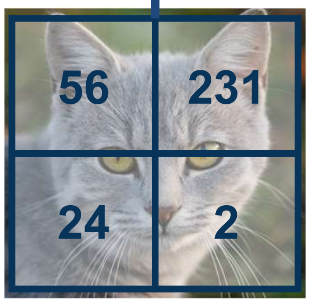
- **Assignment 1 out!**
  - **Due Feb 5th**
  - Start now, start now, start now!
  - Start now, start now, start now!
  - Start now, start now, start now!

- **Piazza**
  - Be active!!!
  - Extra credit!

- **Office hours**
  - Assignment (@41) and matrix calculus (@46)

Example with an image with **4 pixels**, and **3 classes** (cat/dog/ship)

Stretch pixels into column



Input image

$$\underbrace{\begin{bmatrix}0.2 & -0.5 & 0.1 & 2.0\\ 1.5 & 1.3 & 2.1 & 0.0\\ 0 & 0.25 & 0.2 & -0.3\end{bmatrix}}_{W}\begin{bmatrix}56\\ 231\\ 24\\ 2\end{bmatrix}+\underbrace{\begin{bmatrix}1.1\\ 3.2\\ -1.2\end{bmatrix}}_{b}=\begin{bmatrix}-96.8\\ 437.9\\ 61.95\end{bmatrix}\begin{array}{l}\textbf{Cat score}\\ \textbf{Dog score}\\ \textbf{Ship score}\end{array}$$

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

Derivatives

- We can find the steepest descent direction by computing the **derivative (gradient):**

$$f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}$$

- Steepest descent direction is the **negative gradient**
- **Intuitively:** Measures how the function changes as the argument a changes by a small step size
  - As step size goes to zero
- **In Machine Learning:** Want to know how the **loss function** changes **as weights** are varied
  - Can consider each parameter separately by taking **partial derivative** of loss function with respect to that parameter

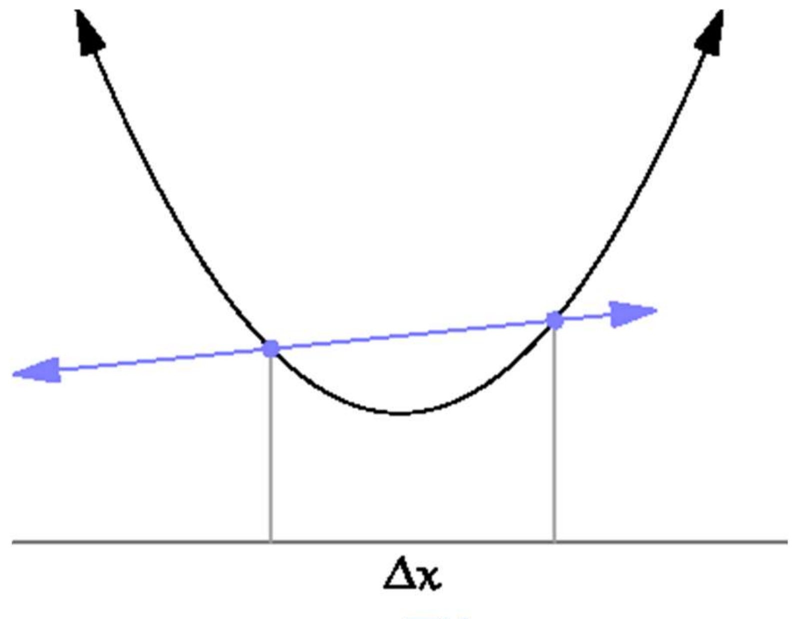


Image and equation from: https://en.wikipedia.org/wiki/Derivative#/media/File:Tangent_animation.gif

This idea can be turned into an **algorithm (gradient descent)**

- Choose a model: $\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{W}) = \mathrm{Wx}$
- Choose loss function: $\boldsymbol{L_i} = |\boldsymbol{y} - \boldsymbol{W}\boldsymbol{x_i}|^{\mathbf{2}}$
- Calculate partial derivative for each parameter: $\frac{\partial \boldsymbol{L}}{\partial \boldsymbol{w_i}}$
- Update the parameters: $\boldsymbol{w_i} = \boldsymbol{w_i} - \frac{\partial \boldsymbol{L}}{\partial \boldsymbol{w_i}}$
- Add learning rate to prevent too big of a step: $\boldsymbol{w_i} = \boldsymbol{w_i} - \boldsymbol{\alpha}\frac{\partial \boldsymbol{L}}{\partial \boldsymbol{w_i}}$
- Repeat (from Step 3)

Often, we only compute the gradients across a small subset of data

- Full Batch Gradient Descent $$L = \frac{1}{N} \sum L\left(f(x_i, W), y_i\right)$$

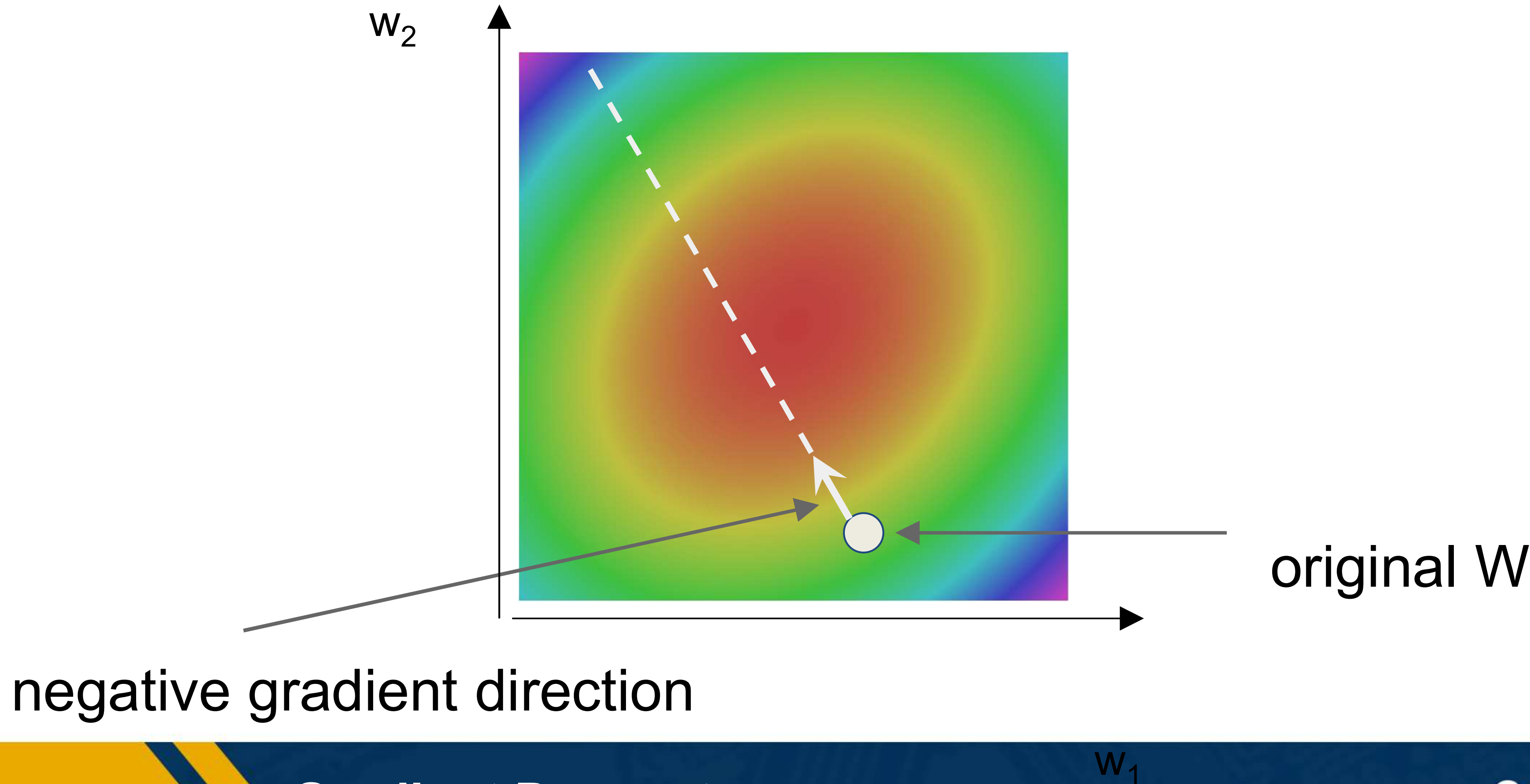
- Mini-Batch Gradient Descent $$L = \frac{1}{M} \sum L\left(f(x_i, W), y_i\right)$$
  - Where M is a *subset* of data

- We iterate over mini-batches:
  - Get mini-batch, compute loss, compute derivatives, and take a set

Mini-Batch Gradient Descent

Georgia Tech

http://demonstrations.wolfram.com/VisualizingTheGradientVector/



Gradient Descent

For some functions, we can analytically derive the partial derivative

Example:

Function

$$f(w, x_i) = w^T x_i$$

Loss

$$(y_i - w^T x_i)^2$$

(Assume w and $\mathbf{x_i}$ are column vectors, so same as $w \cdot x_i$)

Dataset: N examples (indexed by k)

Update Rule

$$w_j \leftarrow w_j + 2\eta \sum_{k=1}^{N} \delta_k x_{kj}$$

Derivation of Update Rule

L$= \sum_{k=1}^{N} (y_k - w^T x_k)^2$

Gradient descent tells us we should update w as follows to minimize L:

$$w_j \leftarrow w_j - \eta \frac{\partial L}{\partial w_j}$$

So what's $\frac{\partial L}{\partial w_j}$?

$$\frac{\partial L}{\partial w_j} = \sum_{k=1}^{N} \frac{\partial}{\partial w_j} (y_k - w^T x_k)^2$$

$$= \sum_{k=1}^{N} 2(y_k - w^T x_k) \frac{\partial}{\partial w_j} (y_k - w^T x_k)$$

$$= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} w^T x_k$$

…where… $\boxed{\delta_k = y_k - w^T x_k}$

$$= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} \sum_{i=1}^{m} w_i x_{ki}$$

$$= -2 \sum_{k=1}^{N} \delta_k x_{kj}$$

If we add a **non-linearity (sigmoid),** derivation is more complex

$$\sigma(x) = \frac{1}{1+e^{-x}}$$

First, one can derive that: $\sigma'(x) = \sigma(x)(1-\sigma(x))$

$$\mathrm{f}(\mathrm{x}) = \sigma\left(\sum_k w_k x_k\right)$$

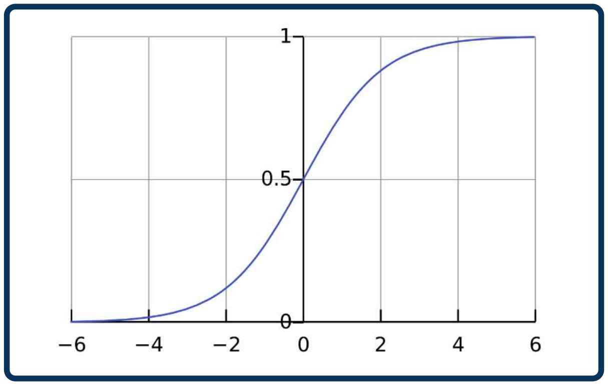
$$\mathrm{L} = \sum_i \left(y_i - \sigma\left(\sum_k w_k x_{ik}\right)\right)^2$$

$$\frac{\partial L}{\partial w_j} = \sum_i 2\left(y_i - \sigma\left(\sum_k w_k x_{ik}\right)\right)\left(-\frac{\partial}{\partial w_j}\sigma\left(\sum_k w_k x_{ik}\right)\right)$$

$$= \sum_i -2\left(y_i - \sigma\left(\sum_k w_k x_{ik}\right)\right)\sigma'\left(\sum_k w_k x_{ik}\right)\frac{\partial}{\partial w_j}\sum_k w_k x_{ik}$$

$$= \sum_i -2\delta_i \sigma(\mathrm{d}_i)(1-\sigma(\mathrm{d}_i))x_{ij}$$

where $\delta_i = y_i - \mathrm{f}(x_i)$ $\quad d_i = \sum w_k x_{ik}$



The sigmoid perception update rule:

$$w_j \leftarrow w_j + 2\eta \sum_{k=1}^{N} \delta_i \sigma_i (1-\sigma_i) x_{ij}$$

where $\sigma_i = \sigma\left(\sum_{j=1}^{m} w_j x_{ij}\right)$

$$\delta_i = y_i - \sigma_i$$

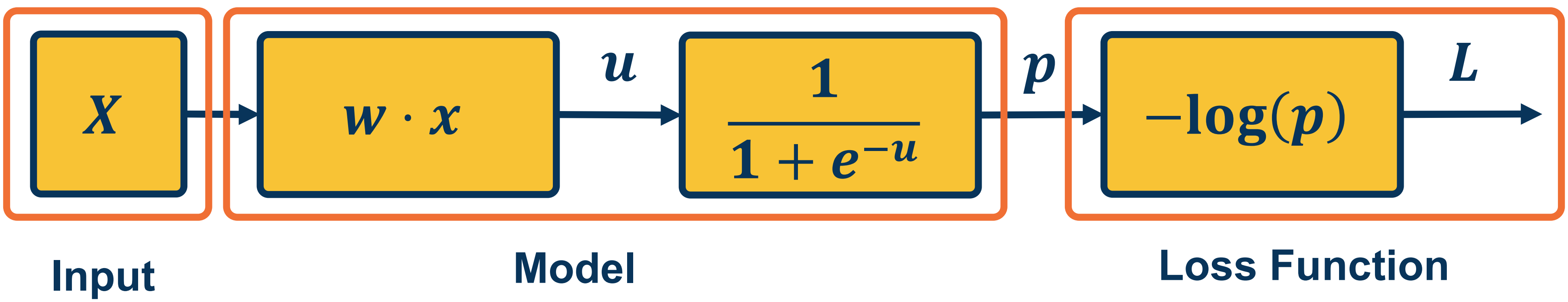
Adding a Non-Linear Function

What Does a Linear Classifier Consist of?

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

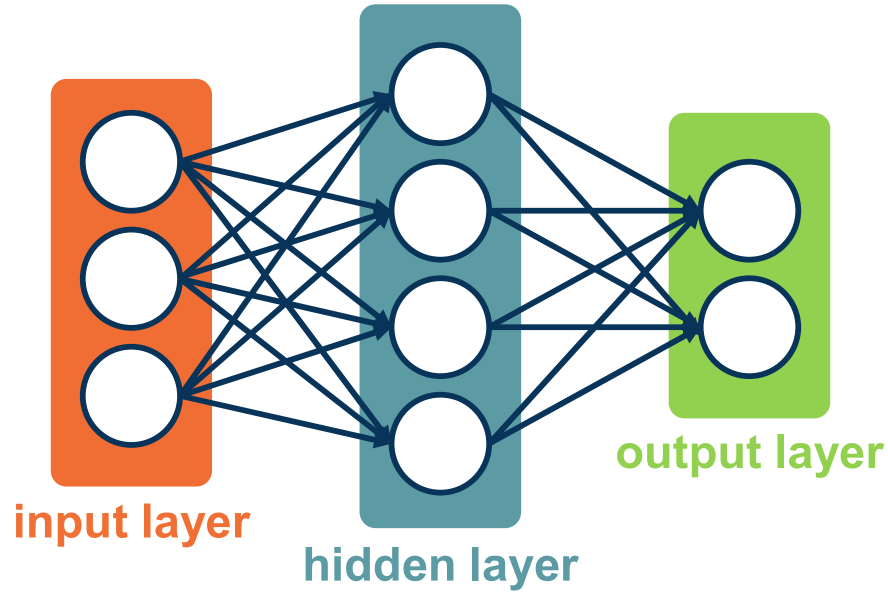
- Input
- A function of the input
- A loss function

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



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)



$$x \qquad W_1 \qquad W_2$$

$$=$$

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

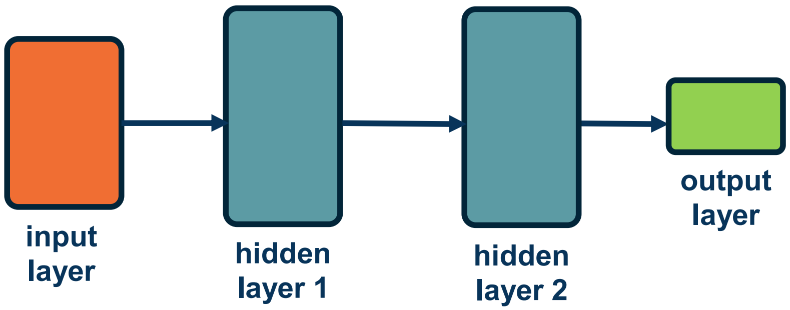
Figure adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

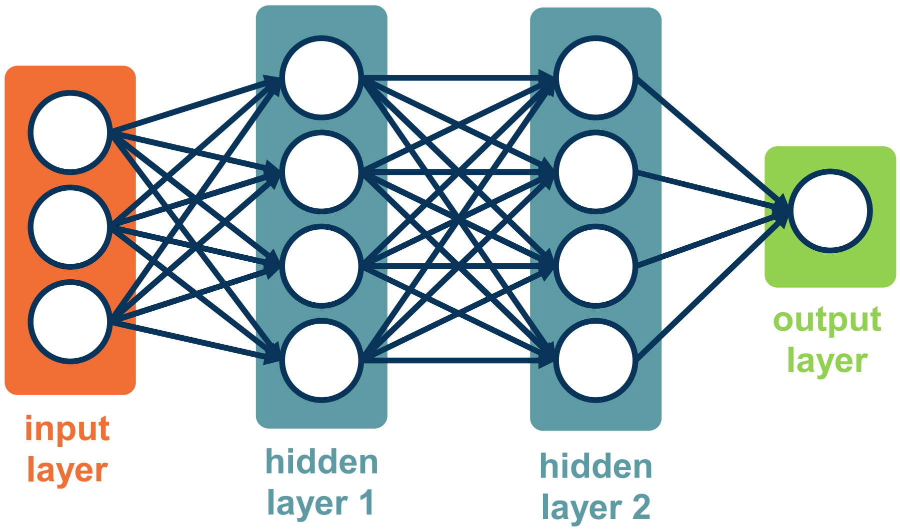
Large (deep) networks can be built by adding more and more layers

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**:





$$f(x, W_1, W_2, W_3) = \sigma(W_2\sigma(W_1x))$$

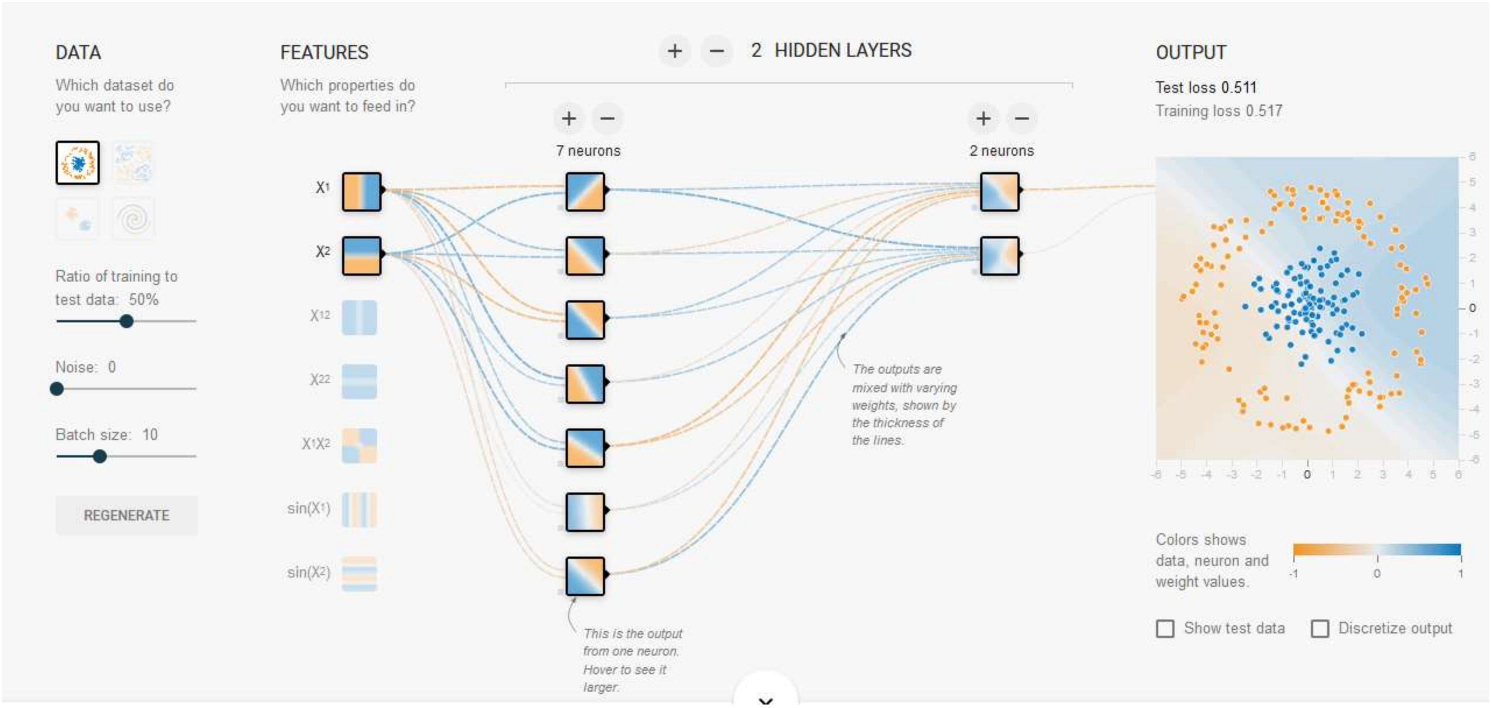
Figure adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Adding More Layers!

Georgia Tech

Demo

- http://playground.tensorflow.org



Computation Graphs

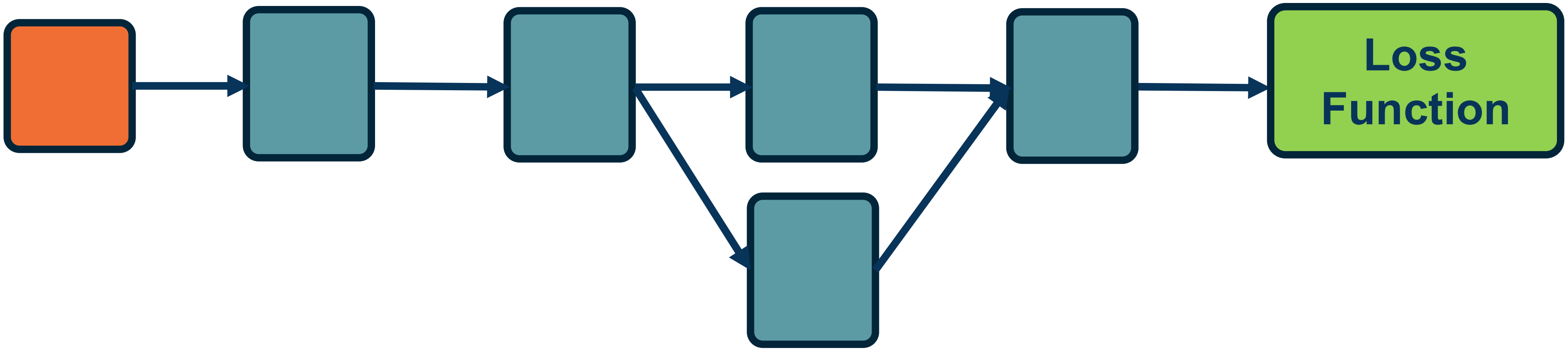
Functions can be made **arbitrarily complex** (subject to memory and computational limits), e.g.:

$$f(x, W) = \sigma(W_5\sigma(W_4\sigma(W_3\sigma(W_2\sigma(W_1x))$$

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

VISION

pixels → edge → texton → motif → part → object

SPEECH

sample → spectral band → formant → motif → phone → word

NLP

character → word → NP/VP/.. → clause → sentence → story

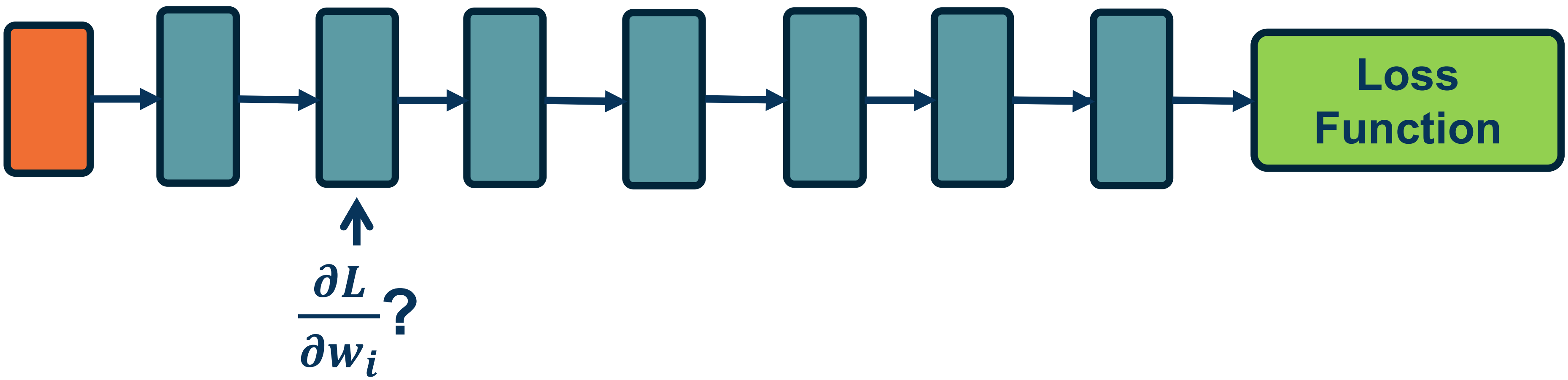
Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

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

Compositionality

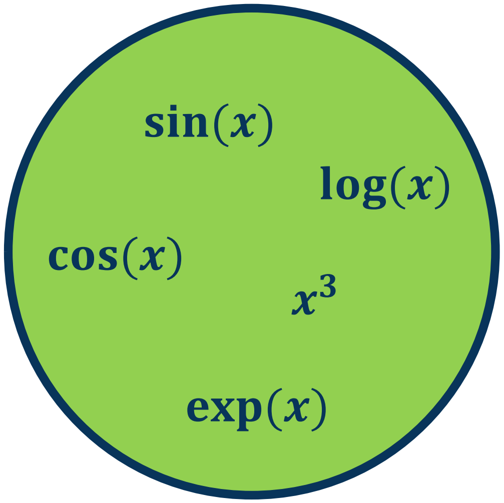
Computing Gradients in Complex Function

- 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



Decomposing a Function

Given a library of simple functions



Compose into a complicate function

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

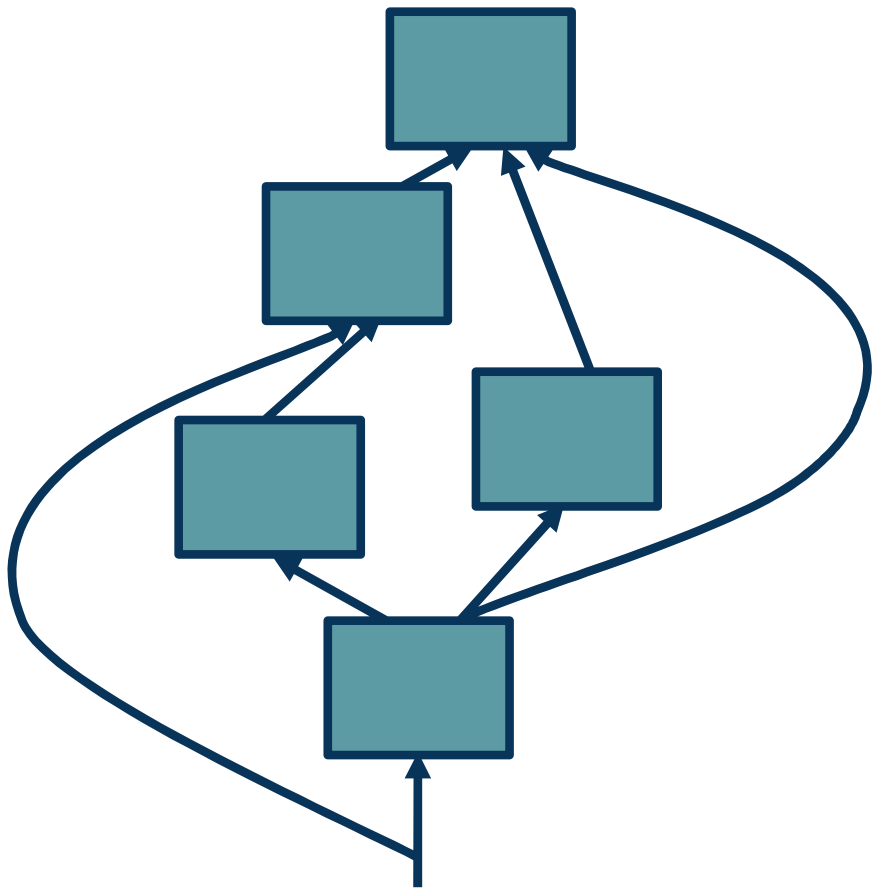
Adapted from slides by: Marc'Aurelio Ranzato, Yann LeCun

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**

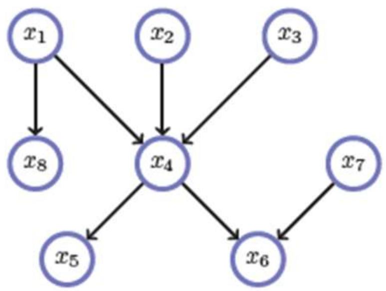


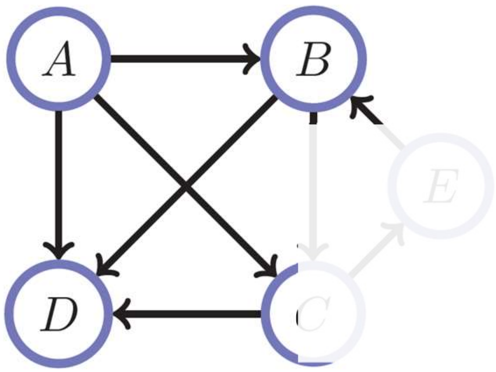
Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

A General Framework

Directed Acyclic Graphs (DAGs)

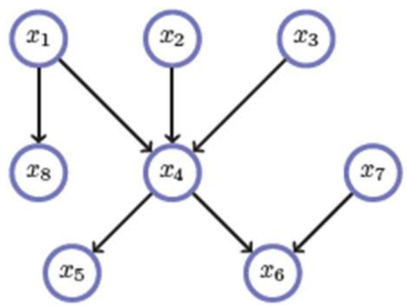
- Exactly what the name suggests
  - Directed edges
  - No (directed) cycles
  - Underlying undirected cycles okay

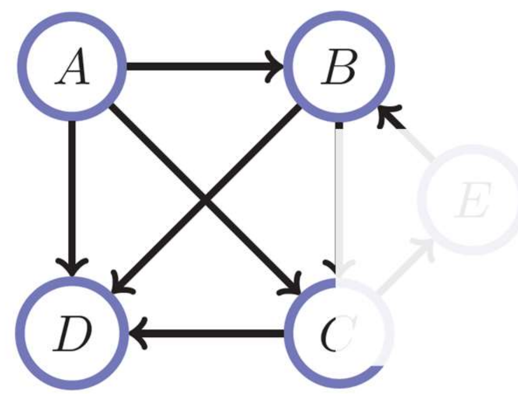




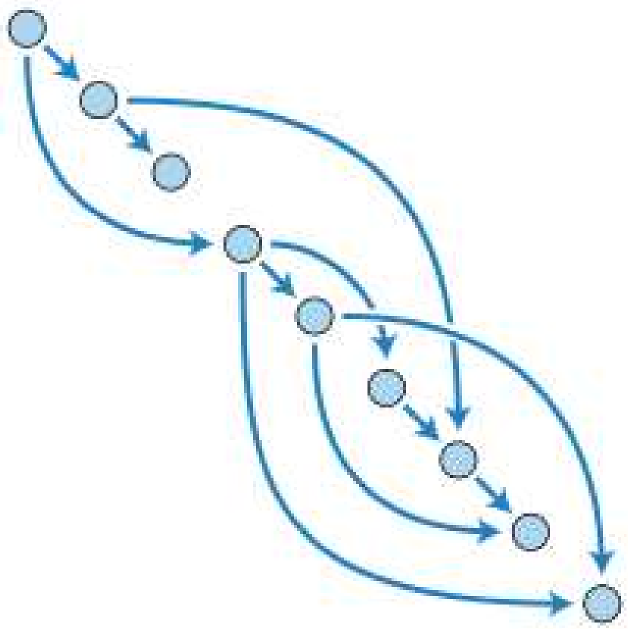
Directed Acyclic Graphs (DAGs)

- Concept
  - Topological Ordering

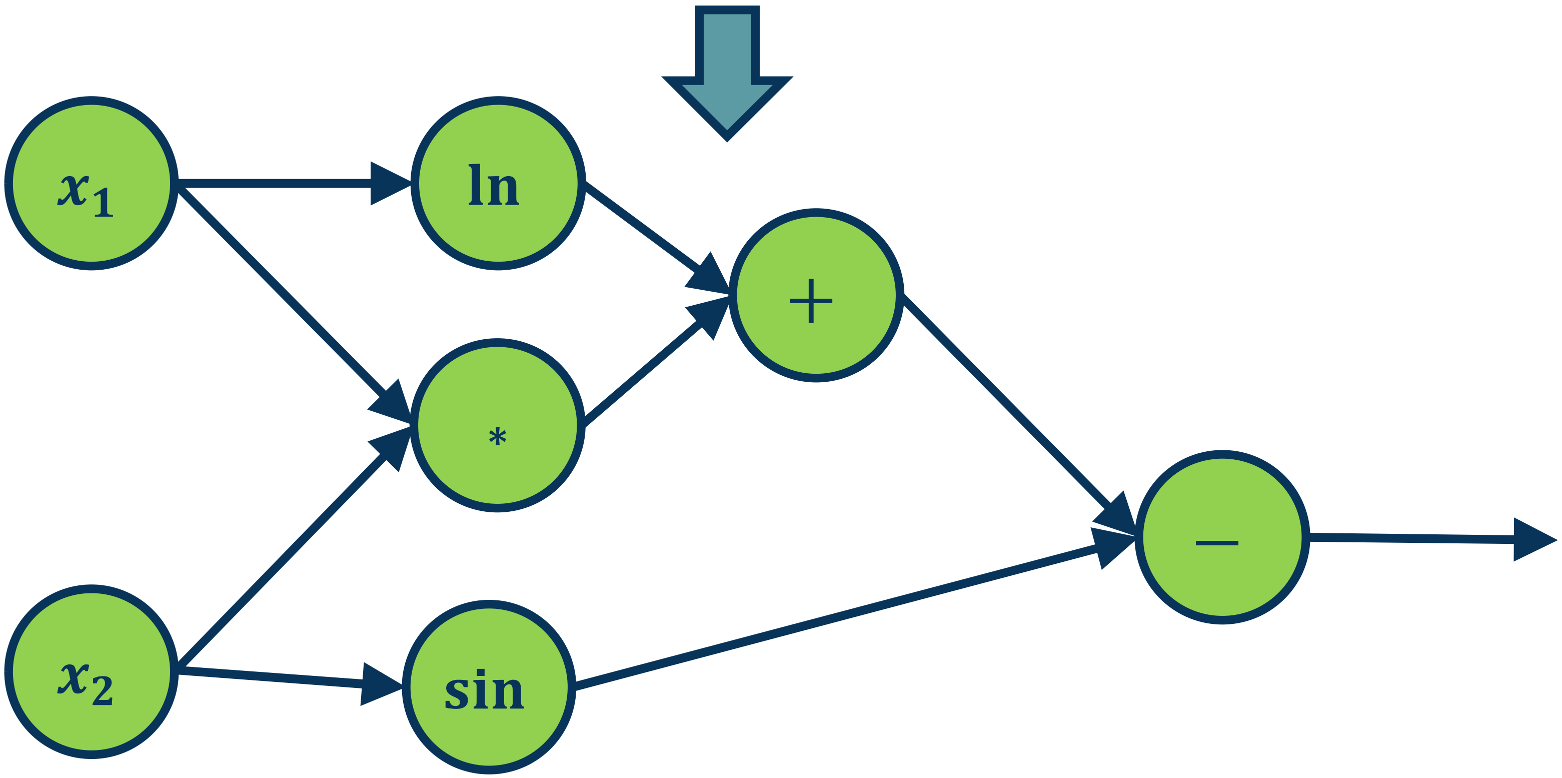




Directed Acyclic Graphs (DAGs)



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



Example

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

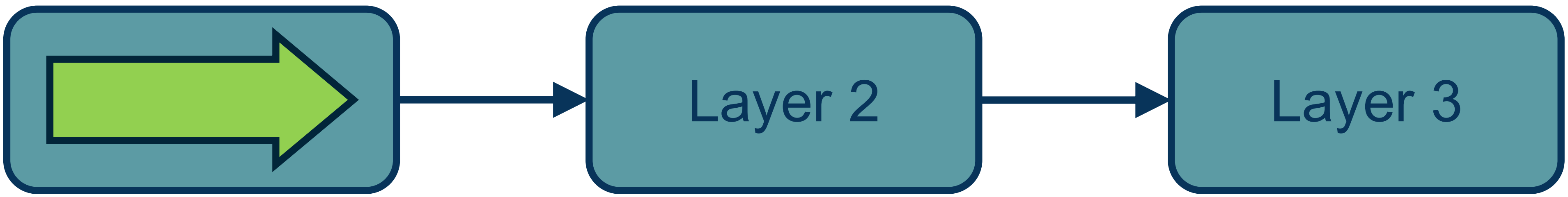
$$\downarrow$$

$$\boxed{w\cdot x} \xrightarrow{u} \boxed{\frac{1}{1+e^{-u}}} \xrightarrow{p} \boxed{-\log(p)} \xrightarrow{L}$$

Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

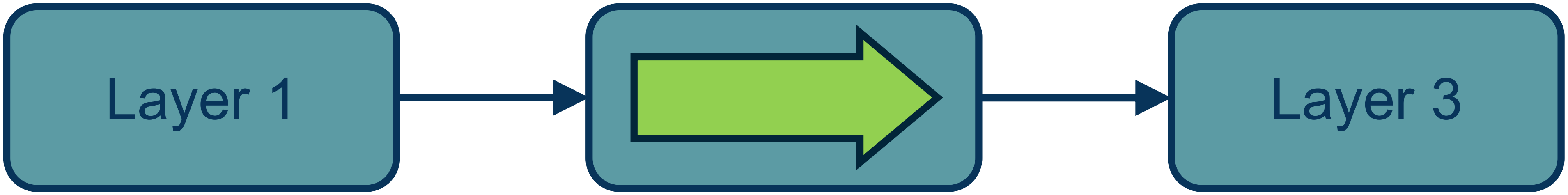
Backpropagation

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



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

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



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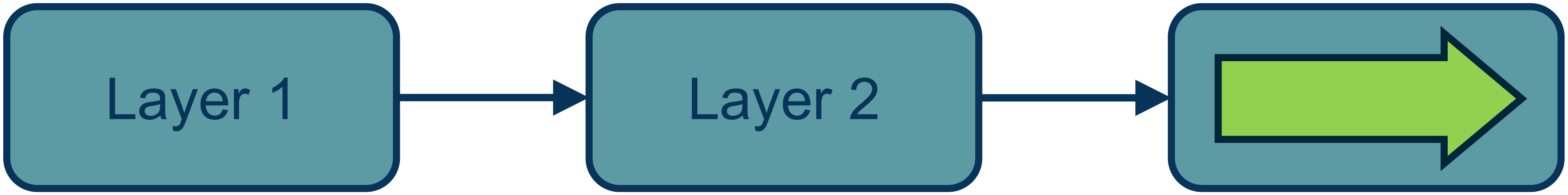
Step 1: Compute Loss on Mini-Batch: **Forward Pass**



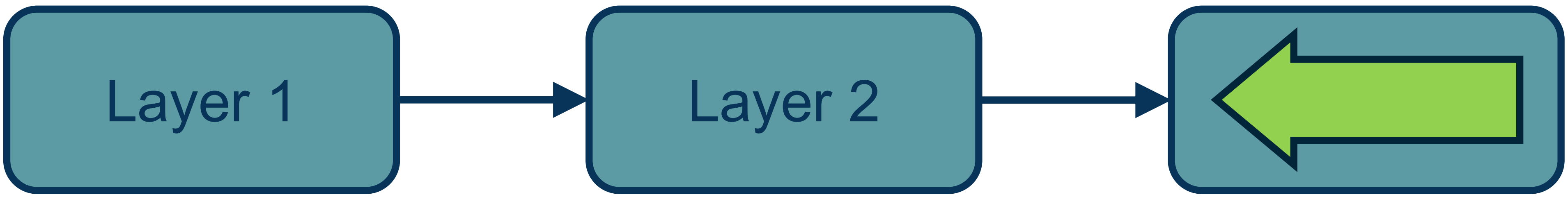
Note that we must store the **intermediate outputs of all layers**!

- 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

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

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



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

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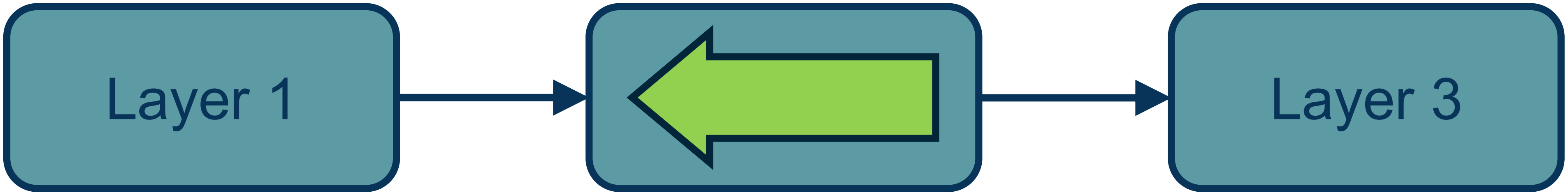

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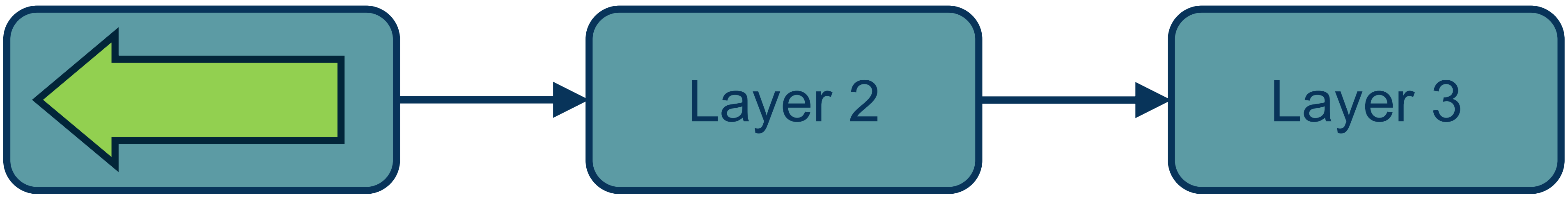
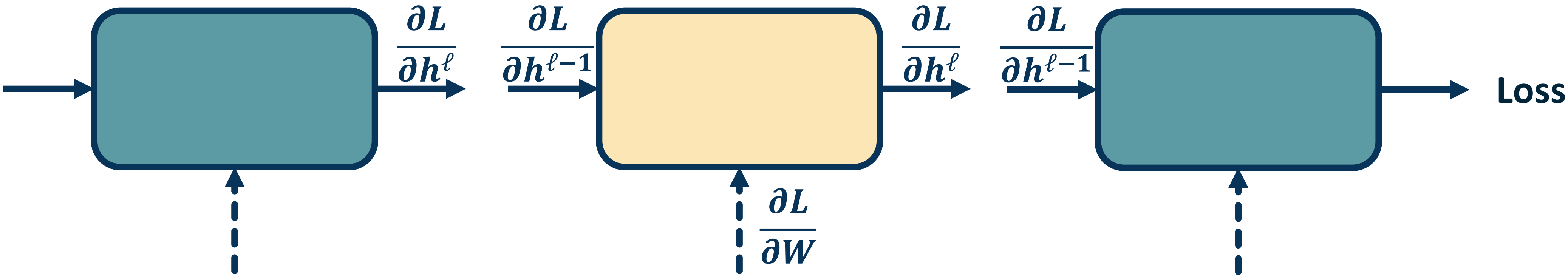
Step 1: Compute Loss on Mini-Batch: **Forward Pass**

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



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

- We want 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:

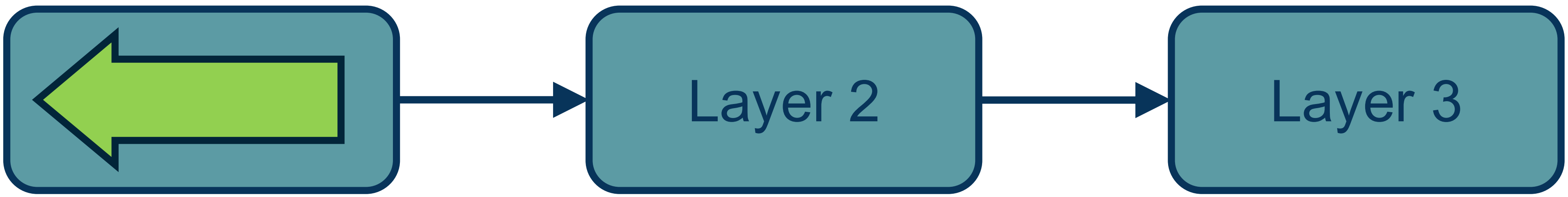
Chain Rule: $\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x}$

Computing the Gradients of Loss

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

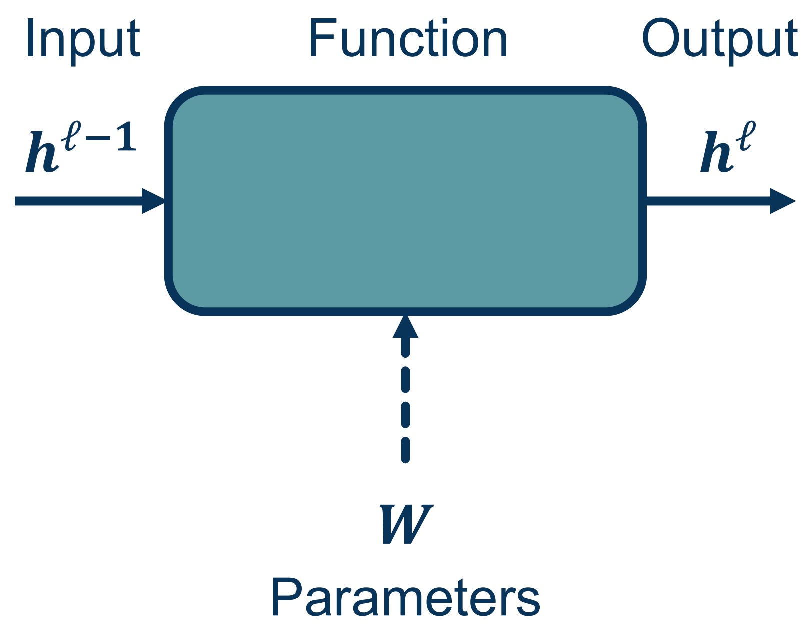
Given this computation graph, the training algorithm will:

- 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**

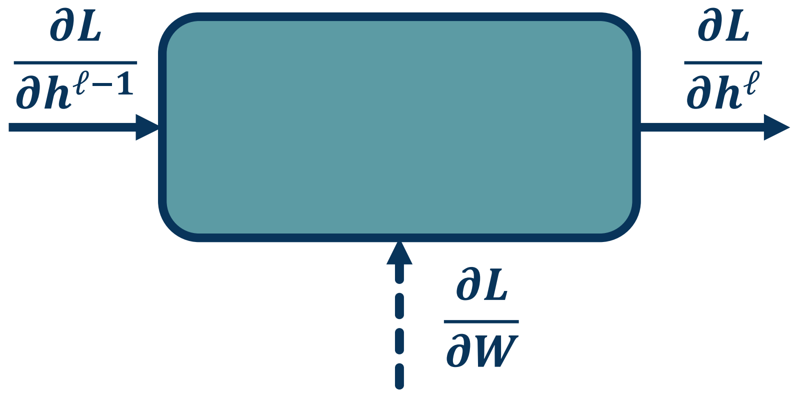


Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

Backward Pass Computations

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**: $\{\frac{\partial \boldsymbol{h}^{\ell}}{\partial \boldsymbol{h}^{\ell-1}}, \frac{\partial \boldsymbol{h}^{\ell}}{\partial \boldsymbol{W}}\}$

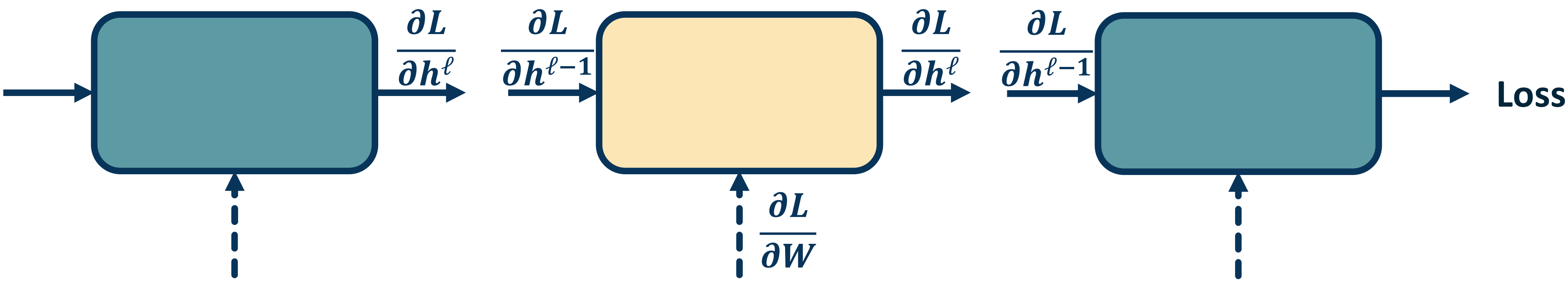
- This is just the **derivative of our function** with respect to its parameters and inputs!

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

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

and $\frac{\partial \boldsymbol{h}^{\ell}}{\partial \boldsymbol{w}_i} = \boldsymbol{h}^{\ell-1,T}$ (a sparse matrix with $\boldsymbol{h}^{\ell-1,T}$ in the *i*-th row)

- 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:

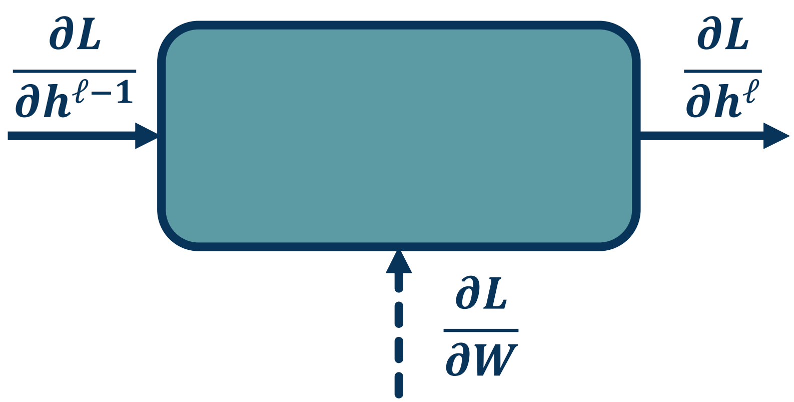
Chain Rule: $\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x}$

Computing the Gradients of Loss

- 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

Computing the Gradients of Loss

Backpropagation: a simple example

$$f(x, y, z) = (x + y)z$$

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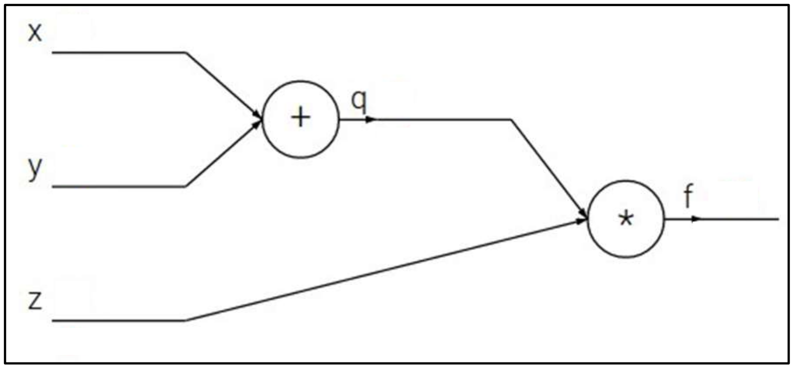
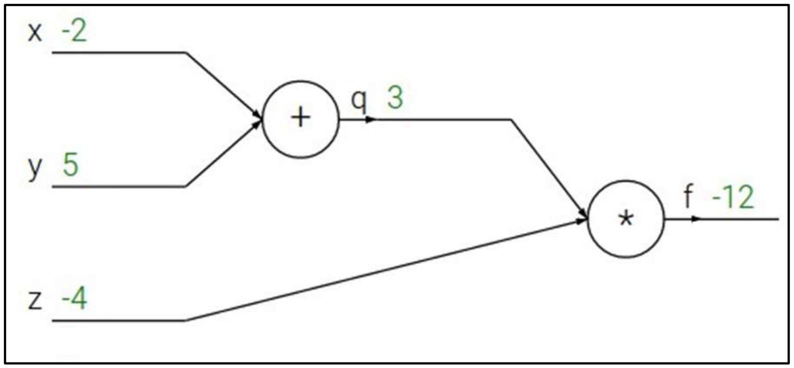


Backpropagation: a simple example

$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4



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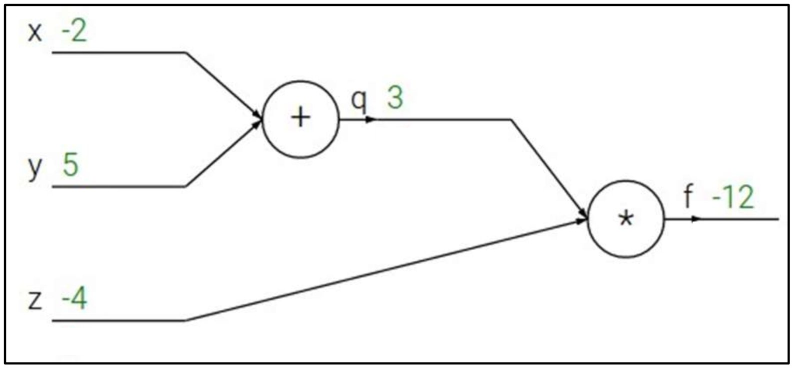


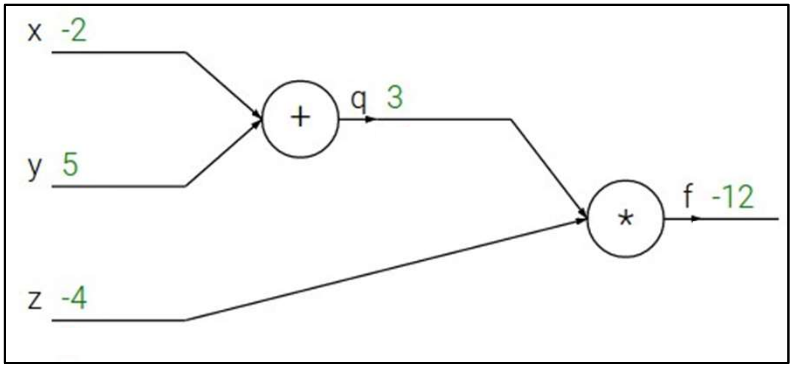
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

Backpropagation: a simple example

$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$\boxed{q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1}$$



Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

Backpropagation: a simple example

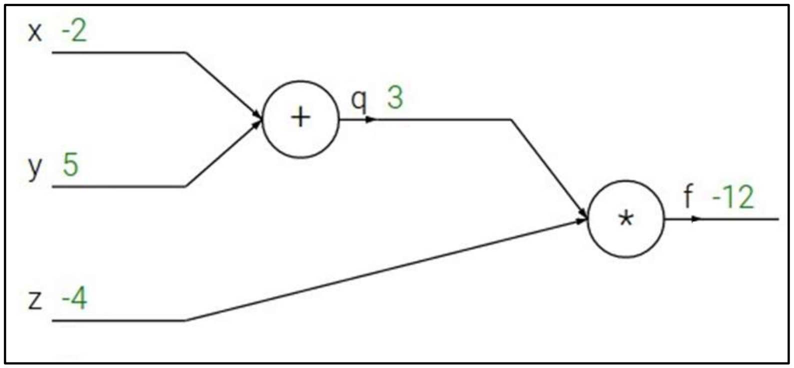
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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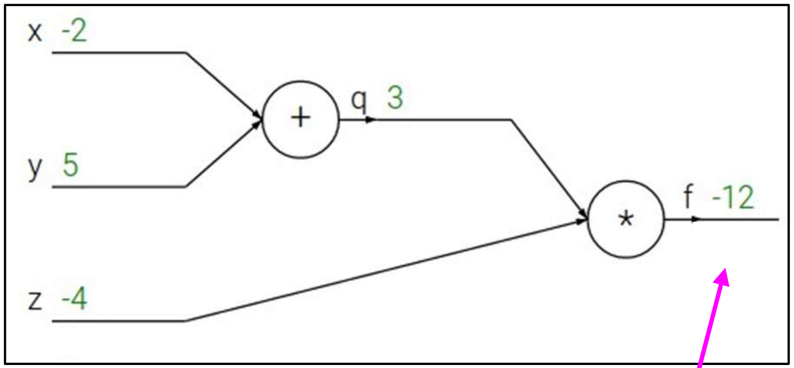
$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\boxed{\frac{\partial f}{\partial f}}$$

Backpropagation: a simple example

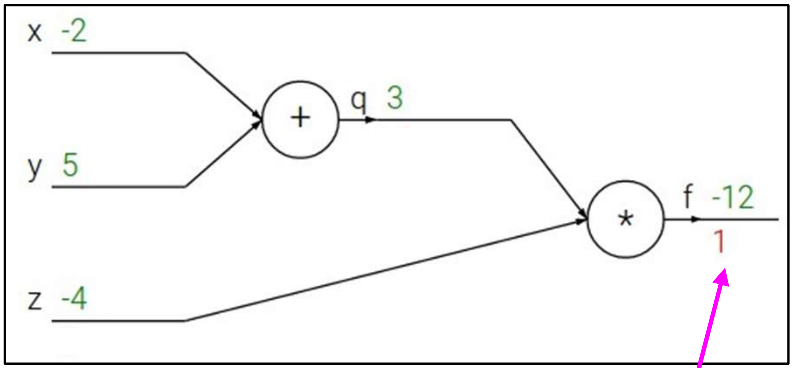
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Backpropagation: a simple example

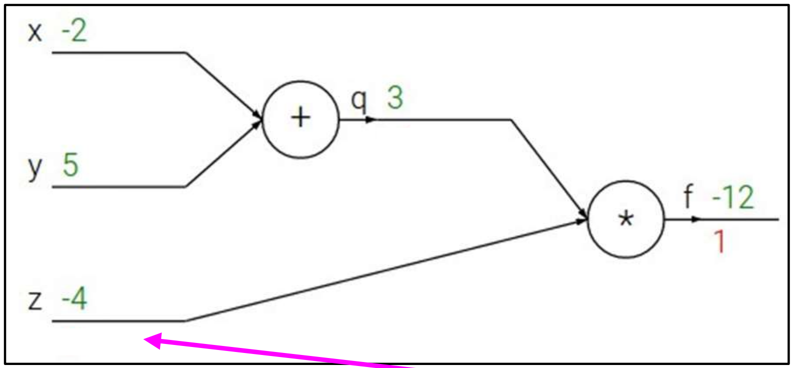
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$\frac{\partial f}{\partial z}$

Backpropagation: a simple example

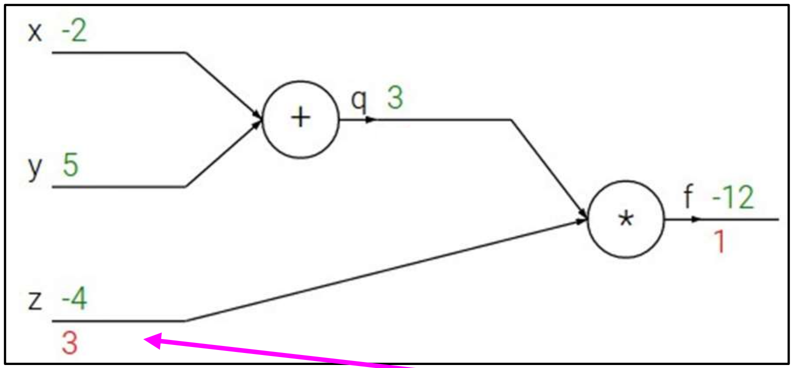
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$\frac{\partial f}{\partial z}$

Backpropagation: a simple example

$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

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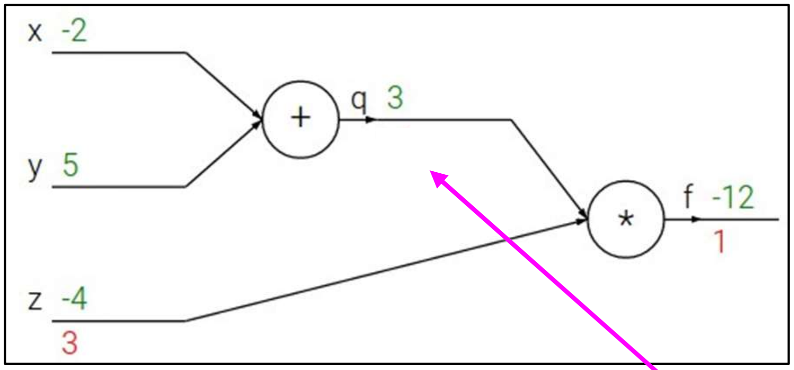
$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\frac{\partial f}{\partial q}$$

Backpropagation: a simple example

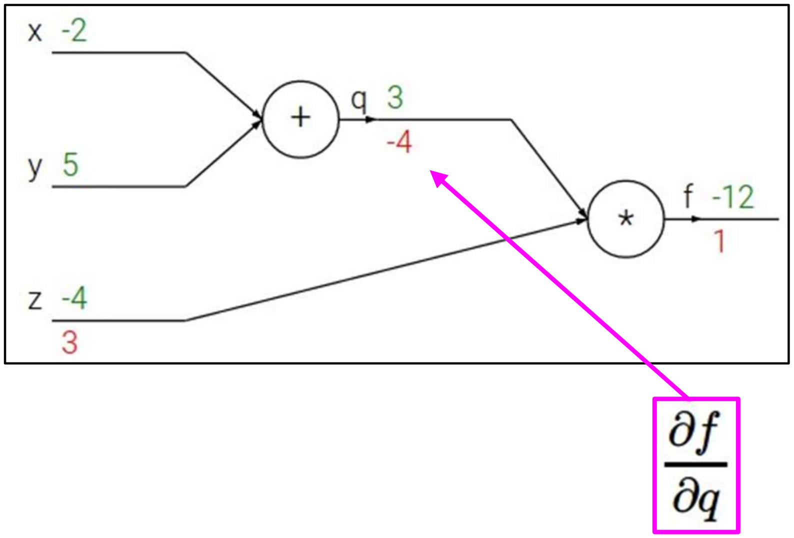
$$f(x,y,z) = (x+y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



Backpropagation: a simple example

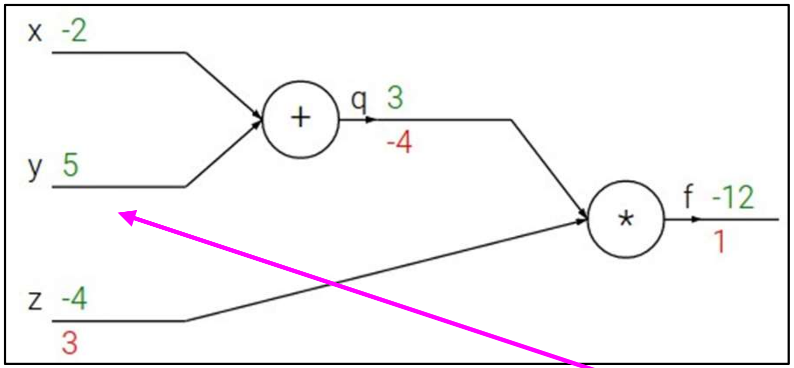
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$\boxed{q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1}$$

$$\boxed{f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q}$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\boxed{\frac{\partial f}{\partial y}}$$

Chain rule:

$$\boxed{\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial y}}$$

Upstream gradient

Local gradient

Backpropagation: a simple example

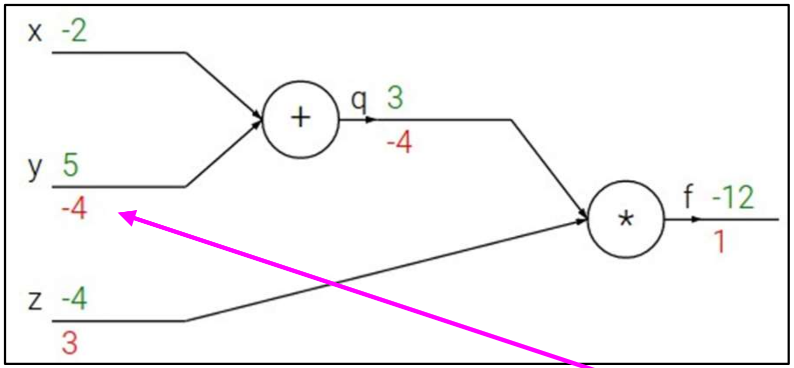
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$\frac{\partial f}{\partial y}$

Chain rule:

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial y}$$

Upstream gradient

Local gradient

Backpropagation: a simple example

$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

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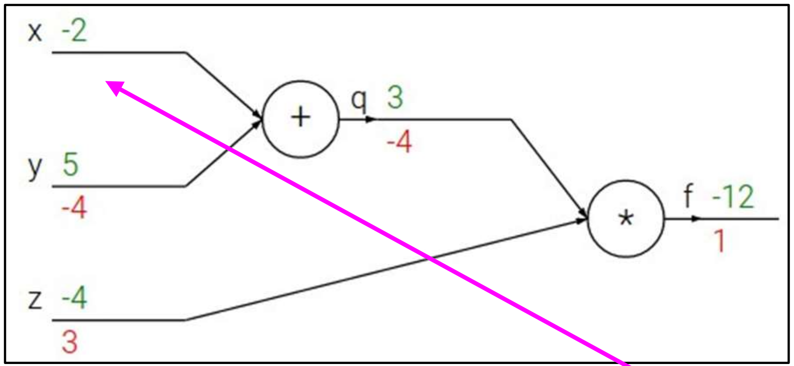
$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Chain rule:

$$\boxed{\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial x}}$$

Upstream gradient

Local gradient

Backpropagation: a simple example

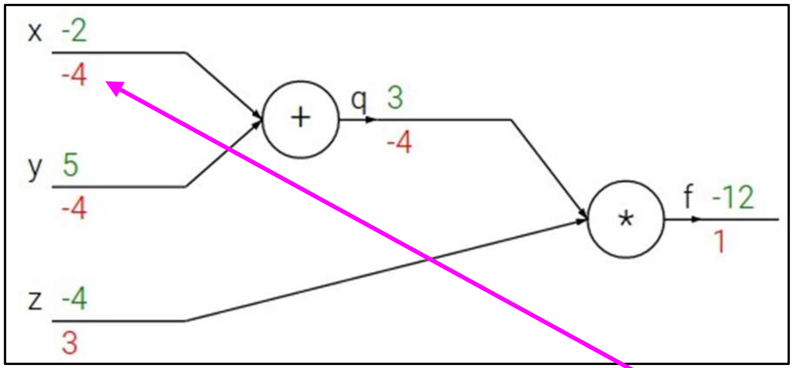
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

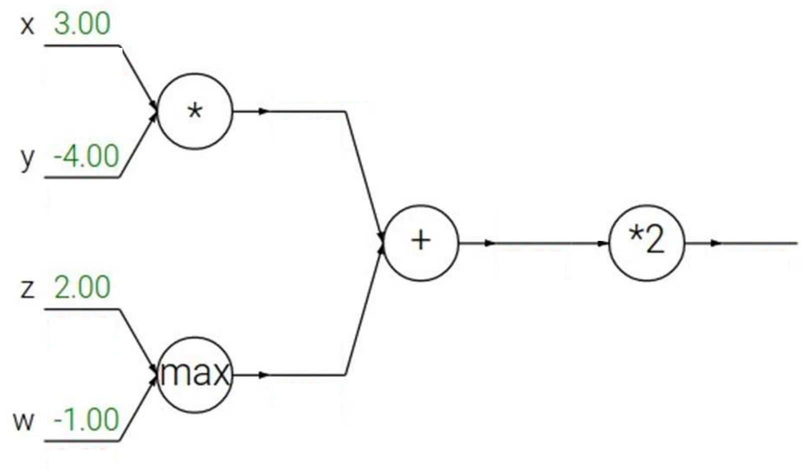
Chain rule:

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

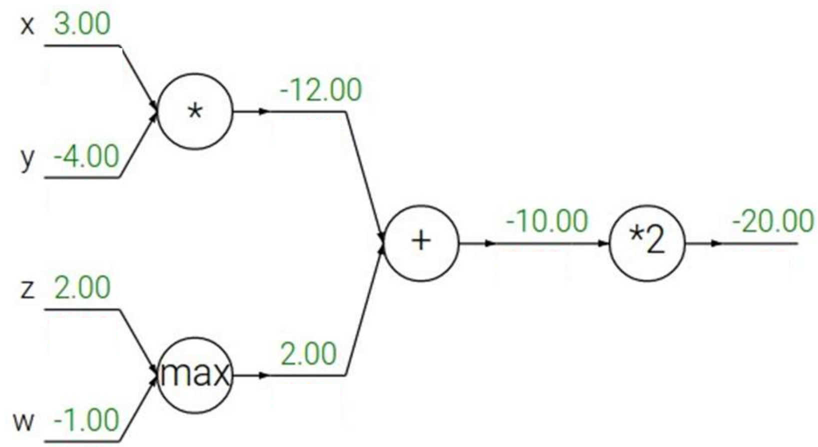
Upstream gradient

Local gradient

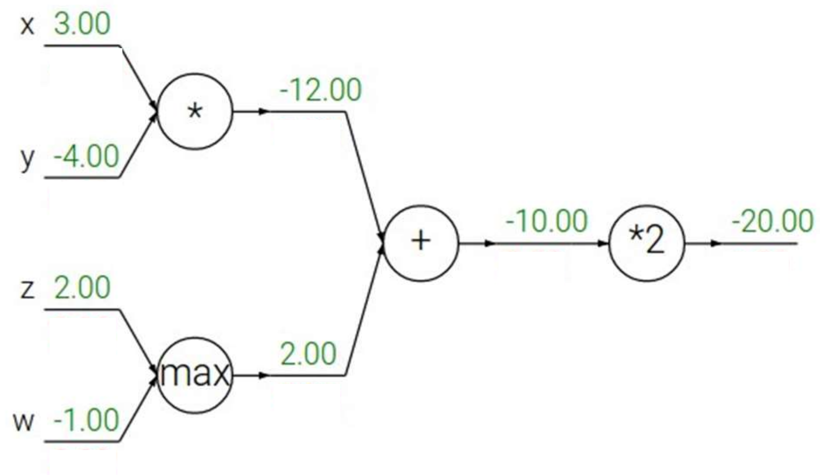
Backpropagation: a simple example



Backpropagation: a simple example

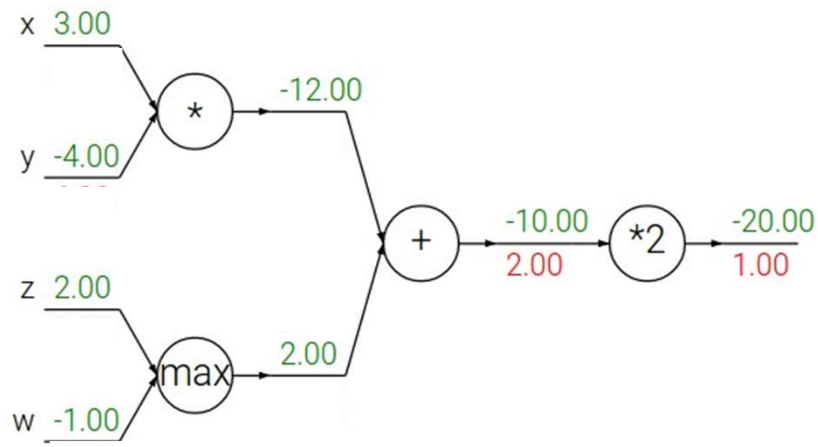


Patterns in backward flow



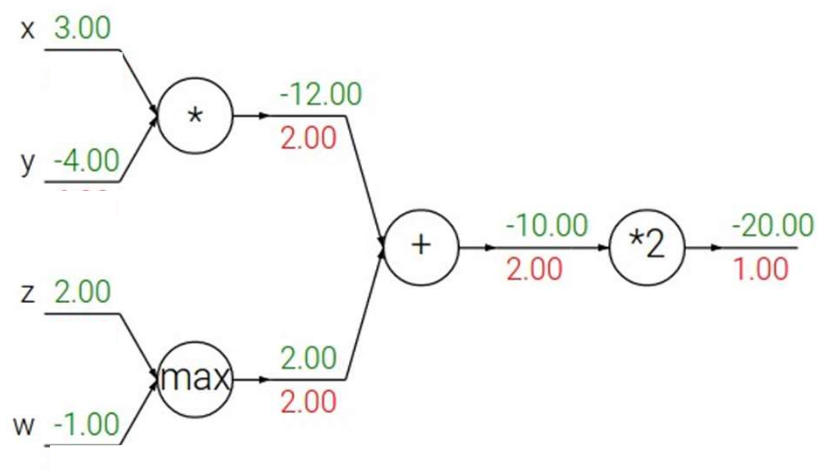
Patterns in backward flow

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



Patterns in backward flow

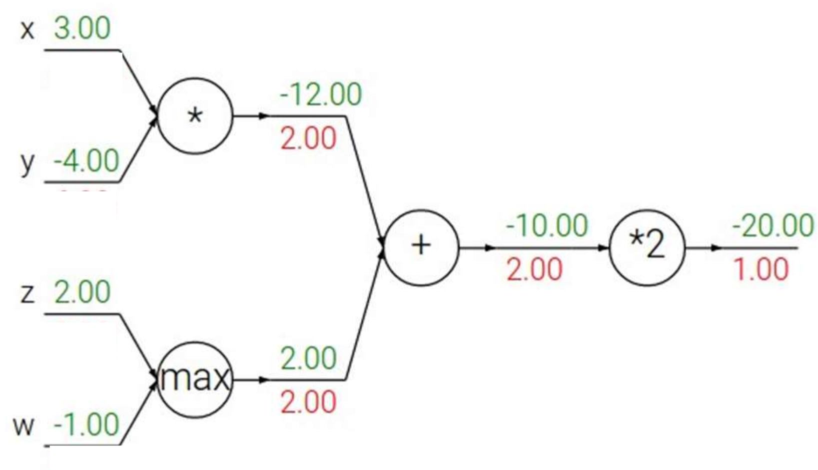
add gate: gradient distributor



Patterns in backward flow

add gate: gradient distributor

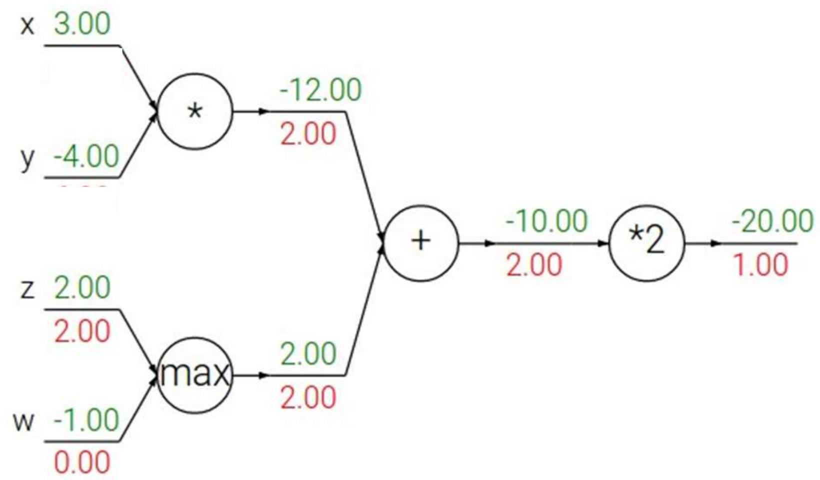
Q: What is a **max** gate?



Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

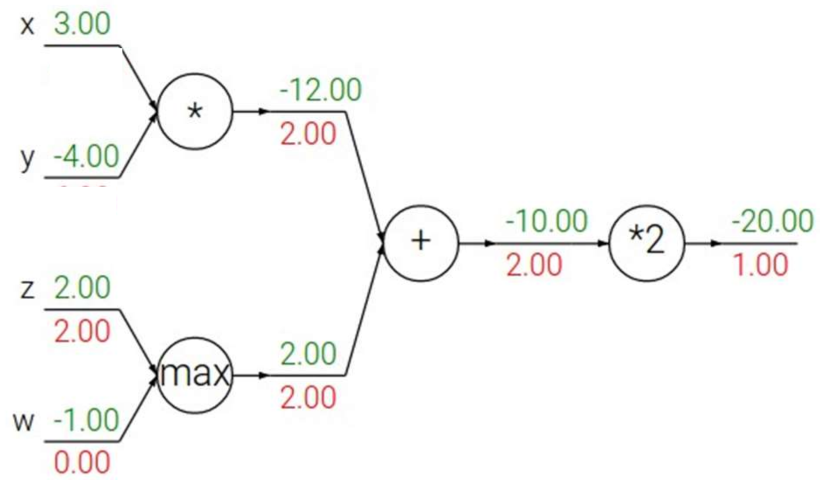


Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

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

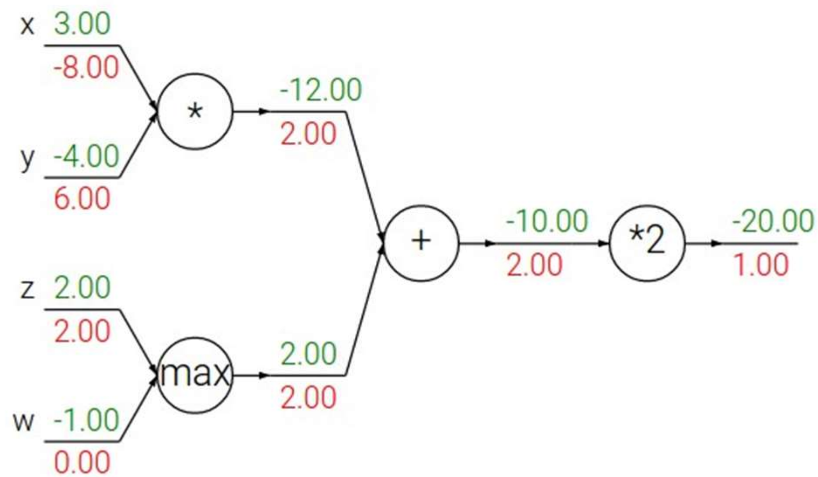


Patterns in backward flow

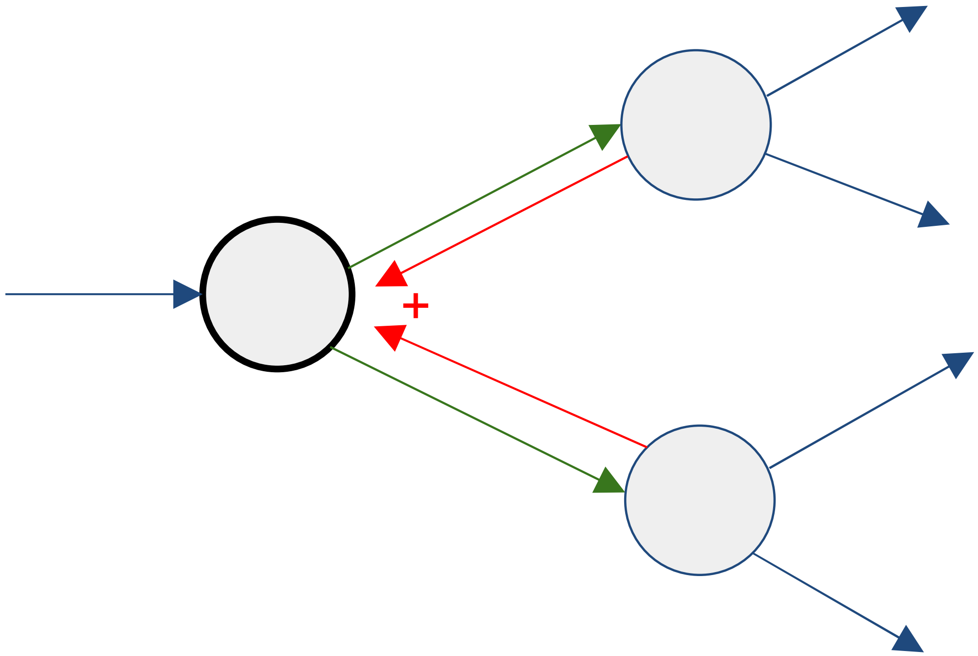
add gate: gradient distributor

max gate: gradient router

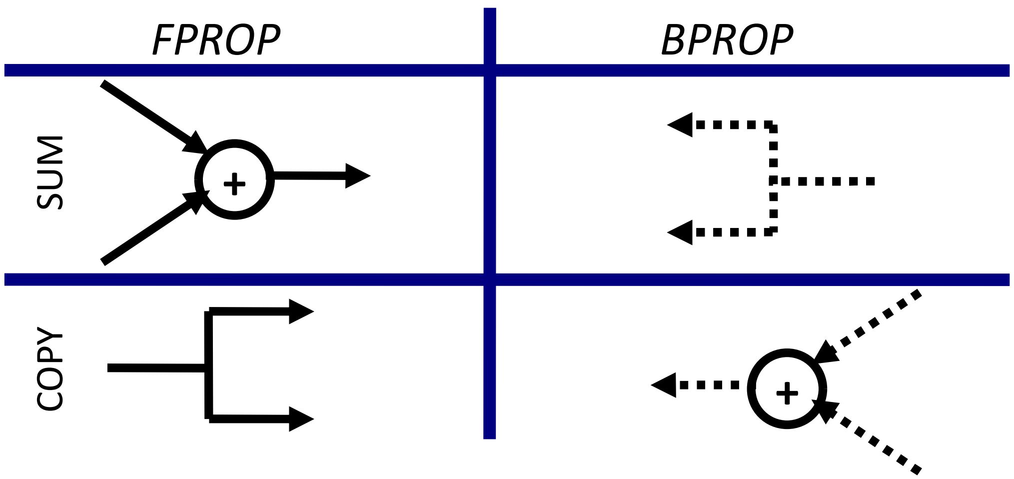
mul gate: gradient switcher



Gradients add at branches



Duality in Fprop and Bprop

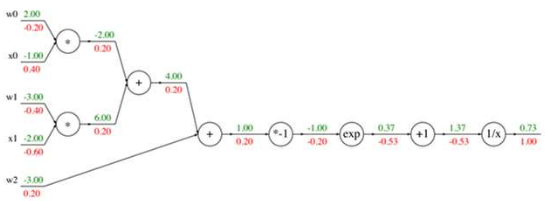


Deep Learning = Differentiable Programming

- 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)

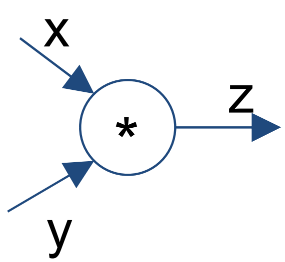
Modularized implementation: forward / backward API



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
```

Modularized implementation: forward / backward API



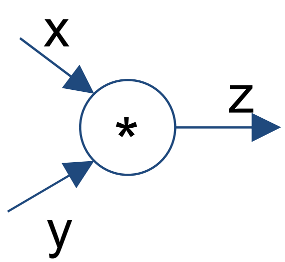
(x,y,z are scalars)

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

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

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

Modularized implementation: forward / backward API



(x,y,z are scalars)

```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        self.x = x # must keep these around!
        self.y = y
        return z
    def backward(dz):
        dx = self.y * dz # [dz/dx * dL/dz]
        dy = self.x * dz # [dz/dy * dL/dz]
        return [dx, dy]
```

Example: Caffe layers

Branch: master ▾ caffe / src / caffe / layers / Create new file | Upload files | Find file | History

shelhamer committed on GitHub Merge pull request #4630 from BIGene/load_hdf5_fix … Latest commit e687a71 21 days ago

..		
absval_layer.cpp	dismantle layer headers	a year ago
absval_layer.cu	dismantle layer headers	a year ago
accuracy_layer.cpp	dismantle layer headers	a year ago
argmax_layer.cpp	dismantle layer headers	a year ago
base_conv_layer.cpp	enable dilated deconvolution	a year ago
base_data_layer.cpp	Using default from proto for prefetch	3 months ago
base_data_layer.cu	Switched multi-GPU to NCCL	3 months ago
batch_norm_layer.cpp	Add missing spaces besides equal signs in batch_norm_layer.cpp	4 months ago
batch_norm_layer.cu	dismantle layer headers	a year ago
batch_reindex_layer.cpp	dismantle layer headers	a year ago
batch_reindex_layer.cu	dismantle layer headers	a year ago
bias_layer.cpp	Remove incorrect cast of gemm int arg to Dtype in BiasLayer	a year ago
bias_layer.cu	Separation and generalization of ChannelwiseAffineLayer into BiasLayer	a year ago
bnll_layer.cpp	dismantle layer headers	a year ago
bnll_layer.cu	dismantle layer headers	a year ago
concat_layer.cpp	dismantle layer headers	a year ago
concat_layer.cu	dismantle layer headers	a year ago
contrastive_loss_layer.cpp	dismantle layer headers	a year ago
contrastive_loss_layer.cu	dismantle layer headers	a year ago
conv_layer.cpp	add support for 2D dilated convolution	a year ago
conv_layer.cu	dismantle layer headers	a year ago
crop_layer.cpp	remove redundant operations in Crop layer (#5138)	2 months ago
crop_layer.cu	remove redundant operations in Crop layer (#5138)	2 months ago
cudnn_conv_layer.cpp	dismantle layer headers	a year ago
cudnn_conv_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago

cudnn_lcn_layer.cpp	dismantle layer headers	a year ago
cudnn_lcn_layer.cu	dismantle layer headers	a year ago
cudnn_lrn_layer.cpp	dismantle layer headers	a year ago
cudnn_lrn_layer.cu	dismantle layer headers	a year ago
cudnn_pooling_layer.cpp	dismantle layer headers	a year ago
cudnn_pooling_layer.cu	dismantle layer headers	a year ago
cudnn_relu_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_relu_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_sigmoid_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_sigmoid_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_softmax_layer.cpp	dismantle layer headers	a year ago
cudnn_softmax_layer.cu	dismantle layer headers	a year ago
cudnn_tanh_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_tanh_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
data_layer.cpp	Switched multi-GPU to NCCL	3 months ago
deconv_layer.cpp	enable dilated deconvolution	a year ago
deconv_layer.cu	dismantle layer headers	a year ago
dropout_layer.cpp	supporting N-D Blobs in Dropout layer Reshape	a year ago
dropout_layer.cu	dismantle layer headers	a year ago
dummy_data_layer.cpp	dismantle layer headers	a year ago
eltwise_layer.cpp	dismantle layer headers	a year ago
eltwise_layer.cu	dismantle layer headers	a year ago
elu_layer.cpp	ELU layer with basic tests	a year ago
elu_layer.cu	ELU layer with basic tests	a year ago
embed_layer.cpp	dismantle layer headers	a year ago
embed_layer.cu	dismantle layer headers	a year ago
euclidean_loss_layer.cpp	dismantle layer headers	a year ago
euclidean_loss_layer.cu	dismantle layer headers	a year ago
exp_layer.cpp	Solving issue with exp layer with base e	a year ago
exp_layer.cu	dismantle layer headers	a year ago

Caffe Sigmoid Layer

```cpp
#include <cmath>
#include <vector>

#include "caffe/layers/sigmoid_layer.hpp"

namespace caffe {

template <typename Dtype>
inline Dtype sigmoid(Dtype x) {
  return 1. / (1. + exp(-x));
}

template <typename Dtype>
void SigmoidLayer<Dtype>::Forward_cpu(const vector<Blob<Dtype>*>& bottom,
    const vector<Blob<Dtype>*>& top) {
  const Dtype* bottom_data = bottom[0]->cpu_data();
  Dtype* top_data = top[0]->mutable_cpu_data();
  const int count = bottom[0]->count();
  for (int i = 0; i < count; ++i) {
    top_data[i] = sigmoid(bottom_data[i]);
  }
}

template <typename Dtype>
void SigmoidLayer<Dtype>::Backward_cpu(const vector<Blob<Dtype>*>& top,
    const vector<bool>& propagate_down,
    const vector<Blob<Dtype>*>& bottom) {
  if (propagate_down[0]) {
    const Dtype* top_data = top[0]->cpu_data();
    const Dtype* top_diff = top[0]->cpu_diff();
    Dtype* bottom_diff = bottom[0]->mutable_cpu_diff();
    const int count = bottom[0]->count();
    for (int i = 0; i < count; ++i) {
      const Dtype sigmoid_x = top_data[i];
      bottom_diff[i] = top_diff[i] * sigmoid_x * (1. - sigmoid_x);
    }
  }
}

#ifdef CPU_ONLY
STUB_GPU(SigmoidLayer);
#endif

INSTANTIATE_CLASS(SigmoidLayer);


}  // namespace caffe
```


$$\boxed{\sigma(x) = \frac{1}{1+e^{-x}}}$$

$$\boxed{(1-\sigma(x))\,\sigma(x)}$$ * top_diff (chain rule)

Jacobians of Batches

Batches of data are **matrices** or **tensors** (multi-dimensional matrices)

Examples:

- Each instance is a vector of size m, our batch is of size $[\boldsymbol{B} \times \boldsymbol{m}]$
- Each instance is a matrix (e.g. grayscale image) of size $\boldsymbol{W} \times \boldsymbol{H}$, our batch is $[\boldsymbol{B} \times \boldsymbol{W} \times \boldsymbol{H}]$
- Each instance is a multi-channel matrix (e.g. color image with R,B,G channels) of size $\boldsymbol{C} \times \boldsymbol{W} \times \boldsymbol{H}$, our batch is $[\boldsymbol{B} \times \boldsymbol{C} \times \boldsymbol{W} \times \boldsymbol{H}]$

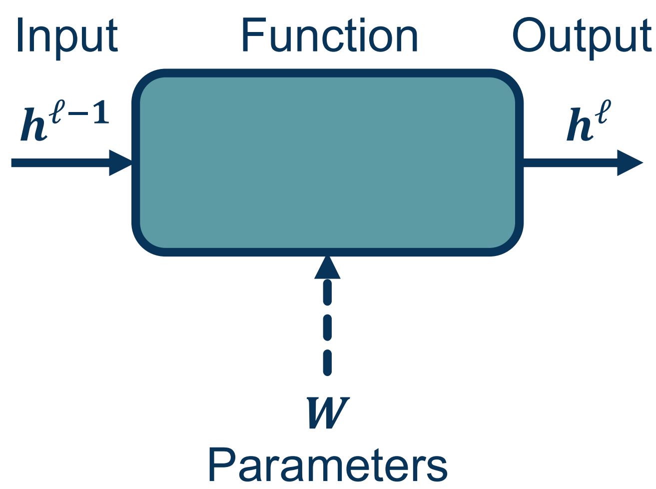
Jacobians become tensors which is complicated

- Instead, flatten input to a vector and get a vector of derivatives!
- In practice, figure out Jacobians for simpler items (scalars, vectors), figure out pattern, and *slice* or index appropriate elements to create Jacobians

$$\begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nn} \end{bmatrix}$$

Flatten ⇓

$$\begin{bmatrix} x_{11} \\ x_{12} \\ \vdots \\ x_{21} \\ x_{22} \\ \vdots \\ x_{n1} \\ \vdots \\ x_{nn} \end{bmatrix}$$

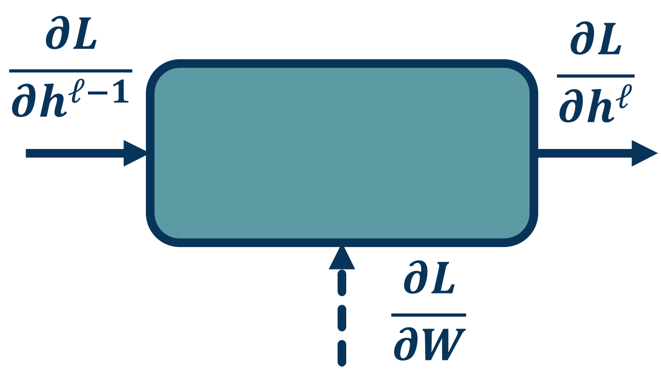


$$\boldsymbol{h}^{\ell} = \boldsymbol{W}\boldsymbol{h}^{\ell-1}$$

$\leftarrow w_i^T \rightarrow$

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

Fully Connected (FC) Layer: Forward Function



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

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

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

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

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

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

$$\frac{\partial L}{\partial w_i} = \frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial w_i} \qquad \begin{bmatrix} \leftarrow & 0 & \rightarrow \\ \leftarrow & \frac{\partial h^{\ell}}{\partial w_i} & \rightarrow \\ \leftarrow & 0 & \rightarrow \end{bmatrix}$$

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

Fully Connected (FC) Layer