Topics:

- Backpropagation / Automatic Differentiation
- Jacobians

# CS 4644 / 7643-A
# ZSOLT KIRA

- **Assignment Due Feb 5th**
- Resources:
  - These lectures
  - Matrix calculus for deep learning
  - Gradients notes and MLP/ReLU Jacobian notes.
  - Assignment (@41) and matrix calculus (@46)

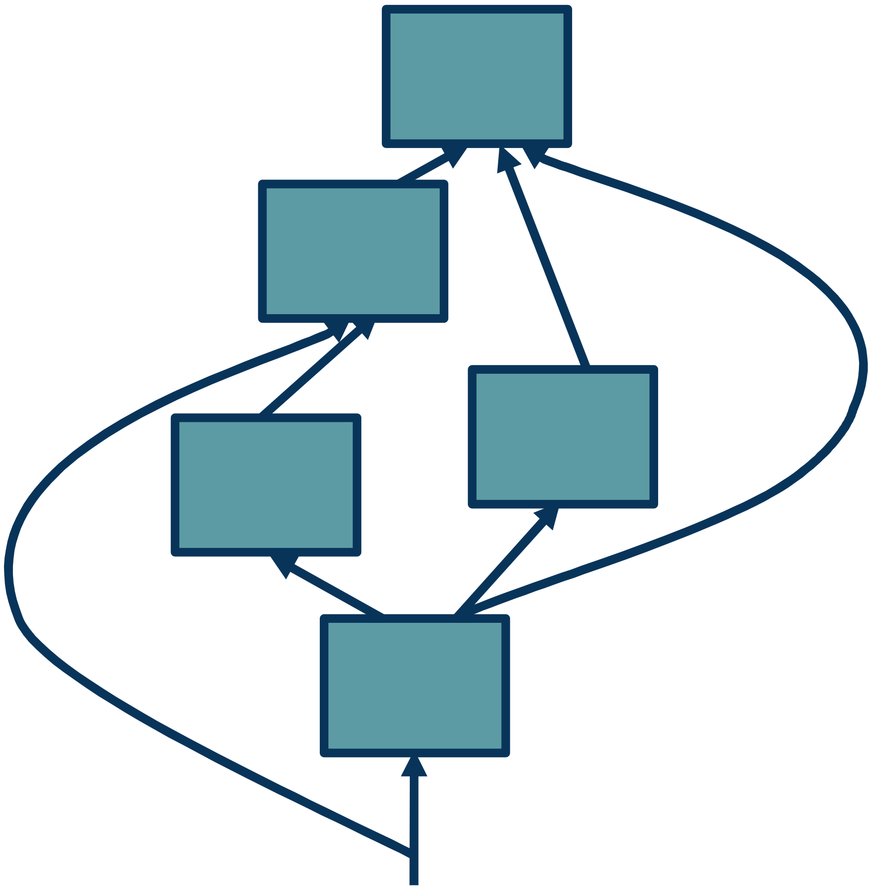
- **Project:** Teaming thread on piazza

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**

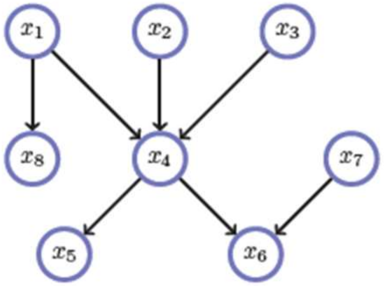


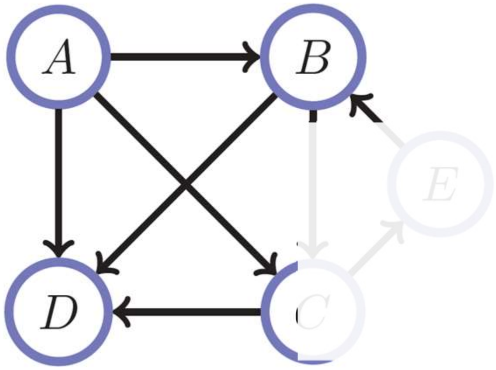
*Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun*

# A General Framework

# Directed Acyclic Graphs (DAGs)

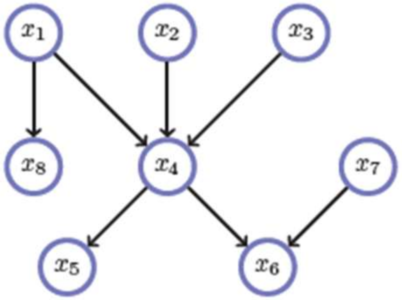
- Exactly what the name suggests
  - Directed edges
  - No (directed) cycles
  - Underlying undirected cycles okay

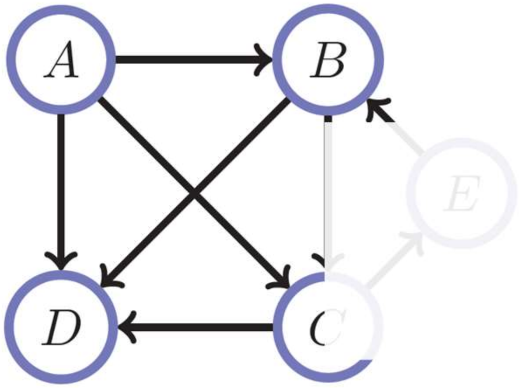




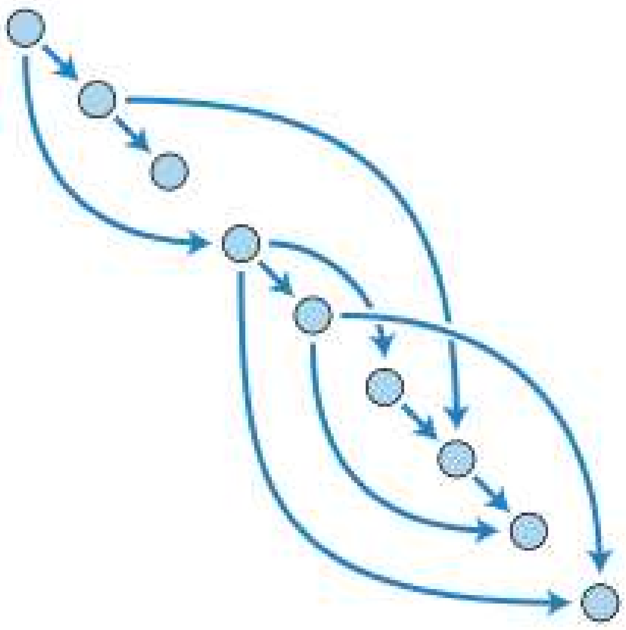
# Directed Acyclic Graphs (DAGs)

- Concept
  - Topological Ordering

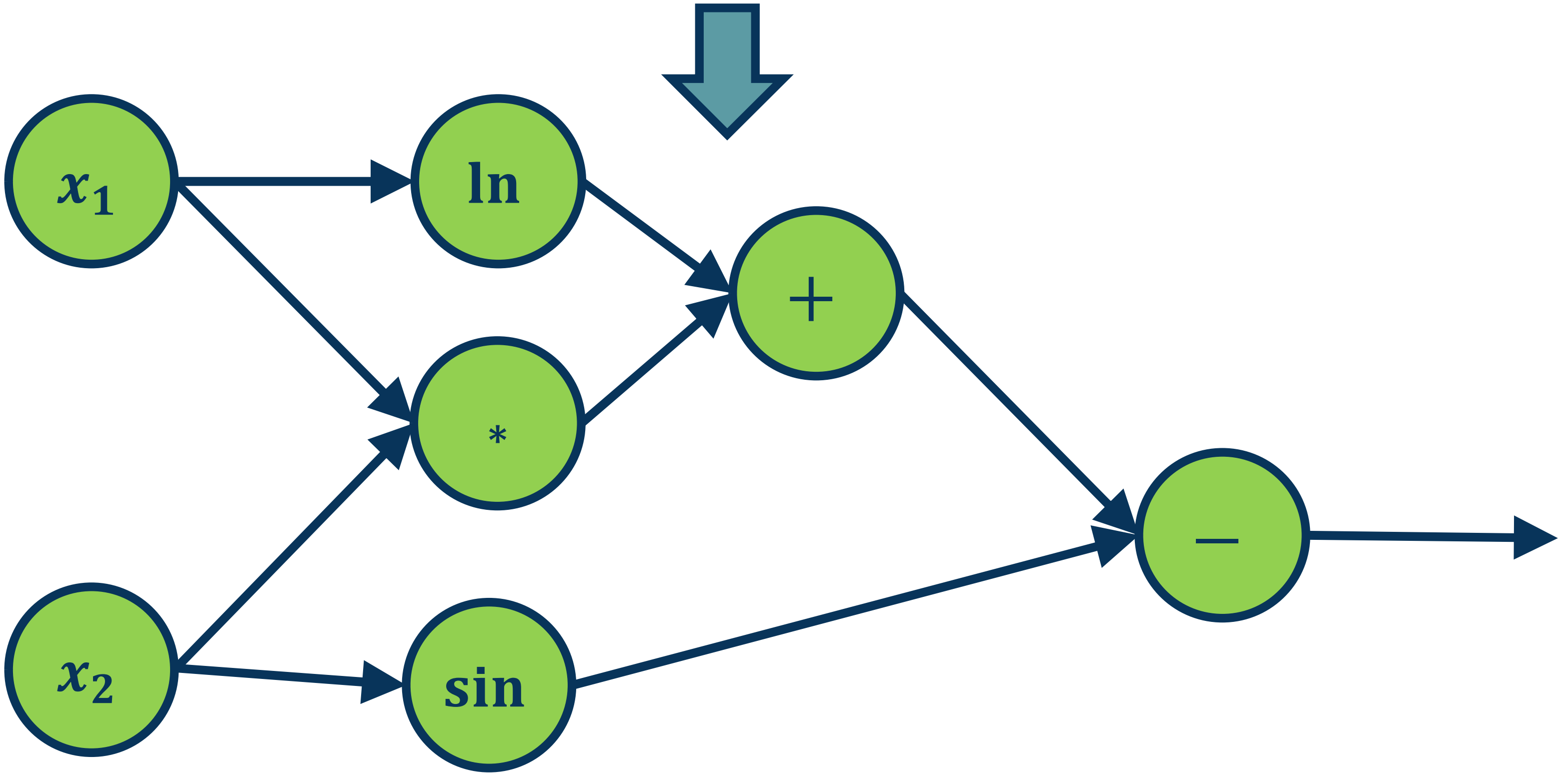




# Directed Acyclic Graphs (DAGs)

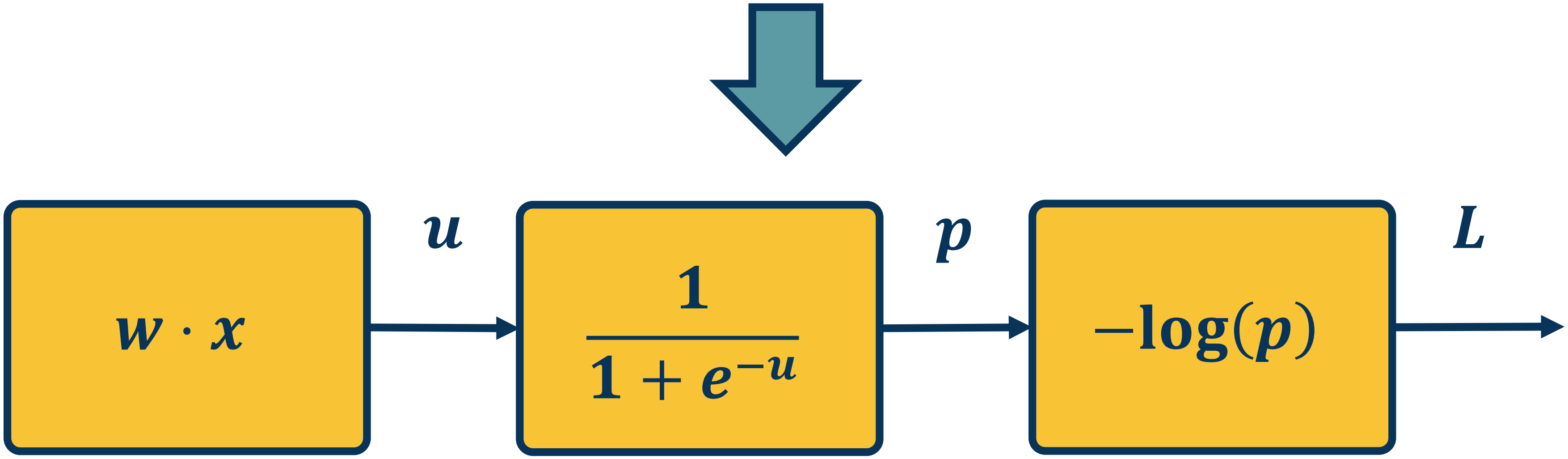


$$f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$$



# Example

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



$w \cdot x$

$u$

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

$p$

$-\log(p)$

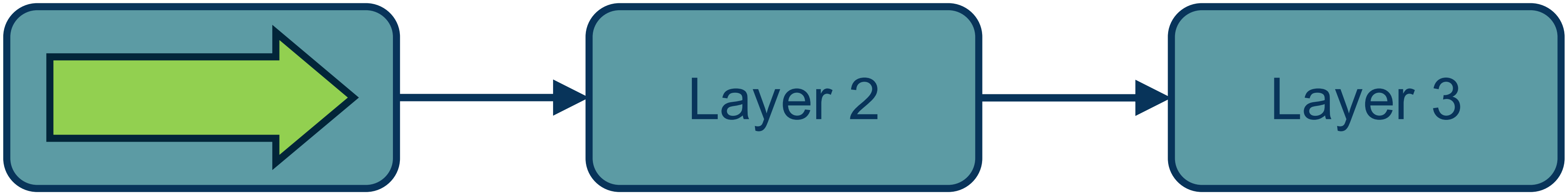
$L$

*Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun*

# Machine Learning Example

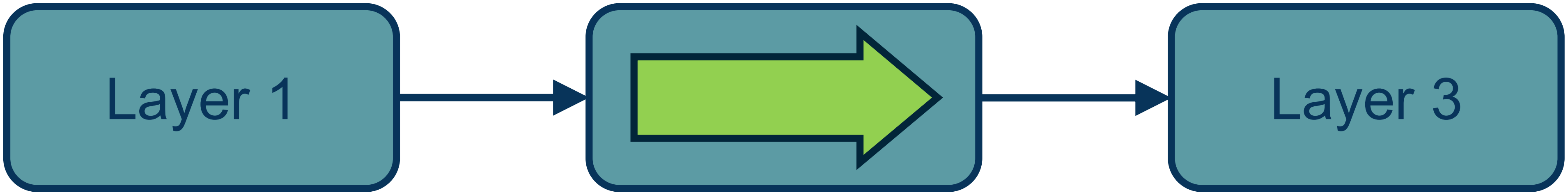
# Backpropagation

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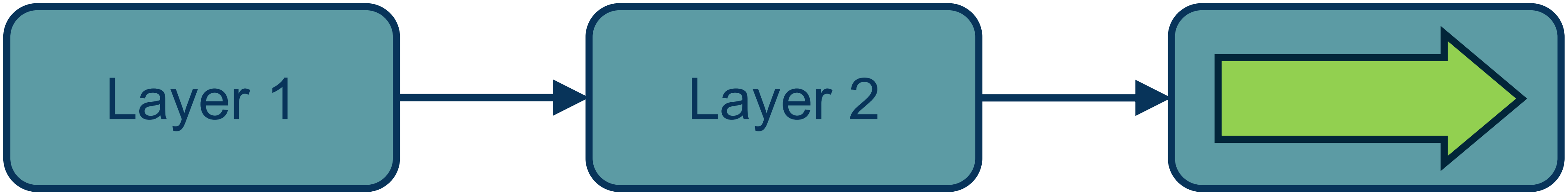
# **Step 1:** Compute Loss on Mini-Batch: **Forward Pass**



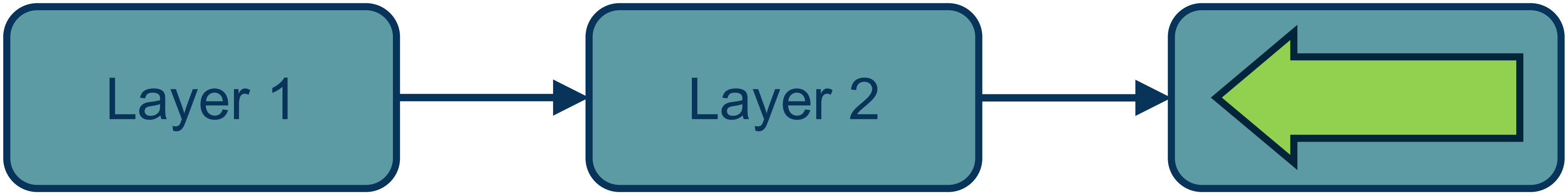
Note that we must store the **intermediate outputs of all layers**!

- 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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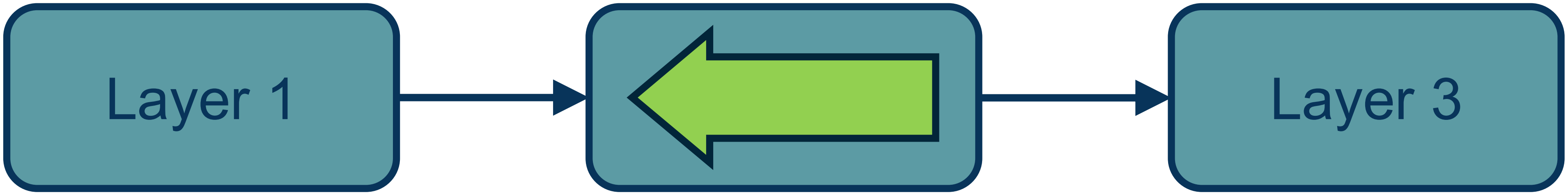

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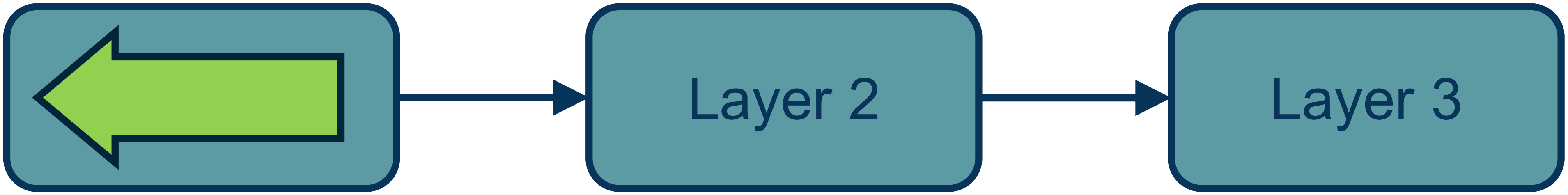
**Step 1:** Compute Loss on Mini-Batch: **Forward Pass**

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

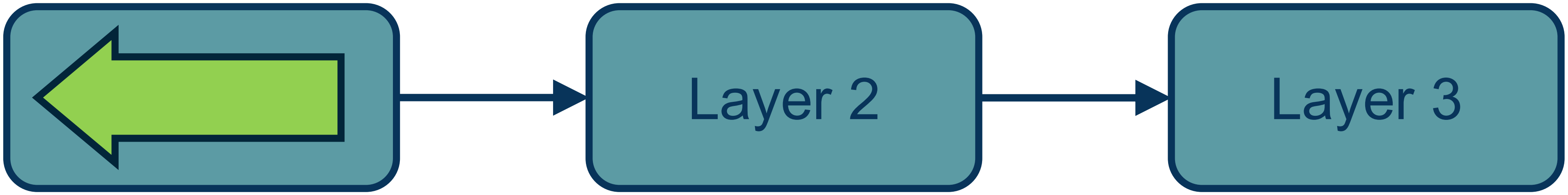


*Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun*

**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

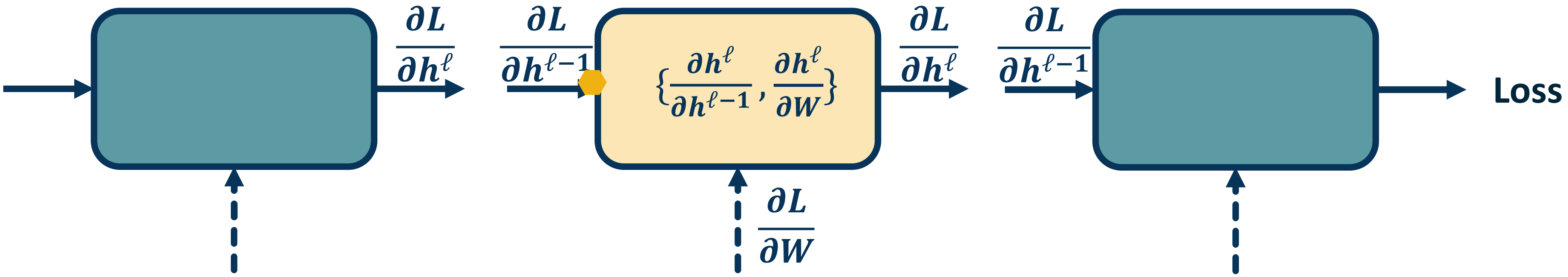


$$w_i = w_i - \alpha \frac{\partial L}{\partial w_i}$$

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

*Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun*

- 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:** $\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x}$

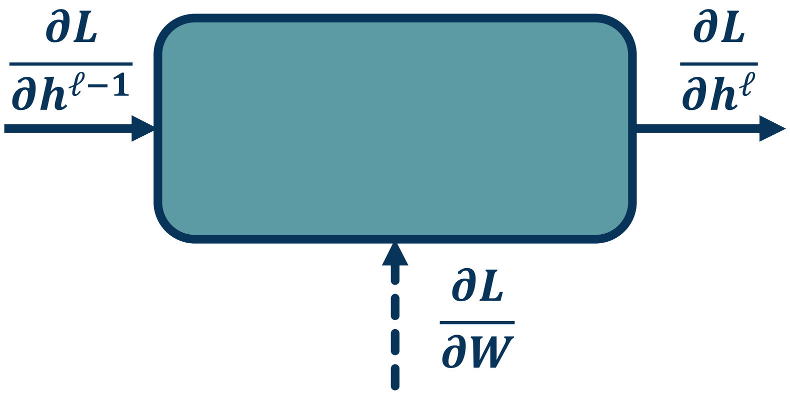
# Computing the Gradients of Loss

# 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:** $\frac{\partial L}{\partial h^{\ell-1}} = \frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial h^{\ell-1}}$
- **Gradient of loss w.r.t. weights:** $\frac{\partial L}{\partial W} = \frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial W}$

Given by upstream module **(upstream gradient)**

Calculated Analytically



*Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun*

# Backpropagation: a simple example

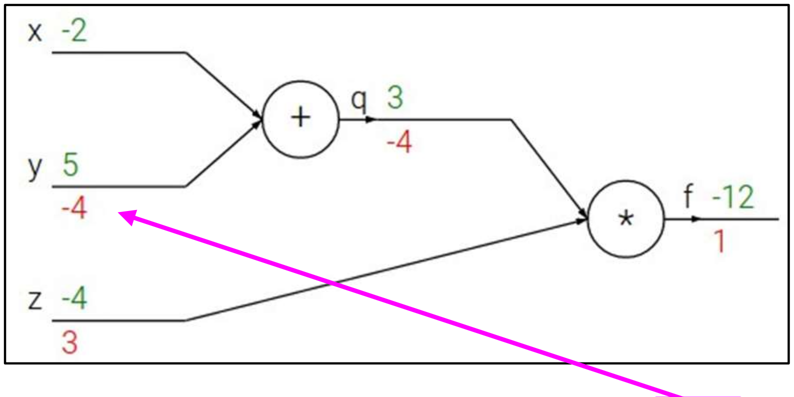
$$f(x, y, z) = (x + y)z$$

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:

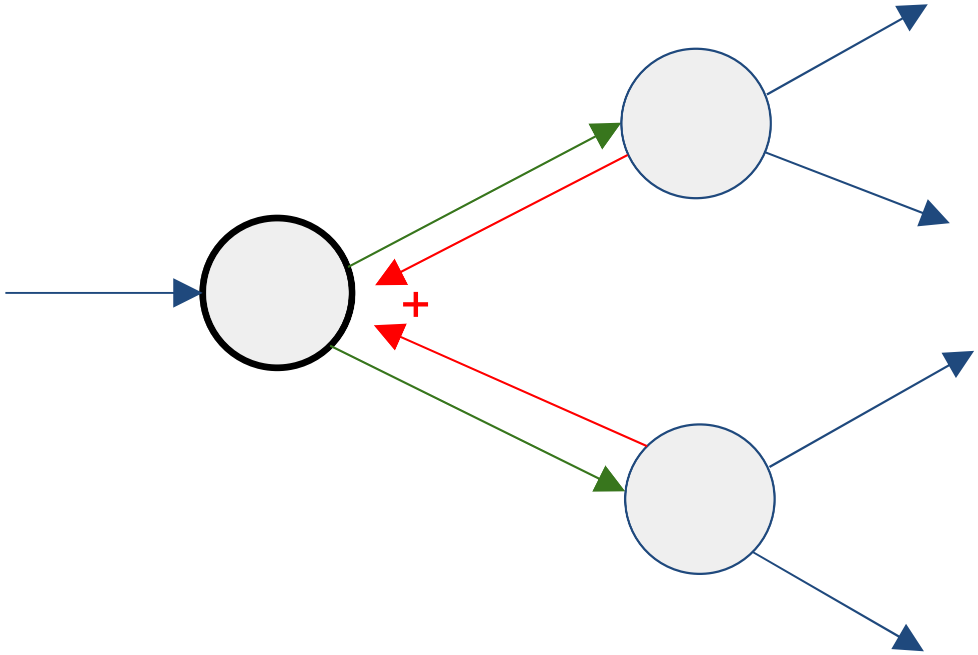
$$\boxed{\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial y}}$$

Upstream gradient

Local gradient

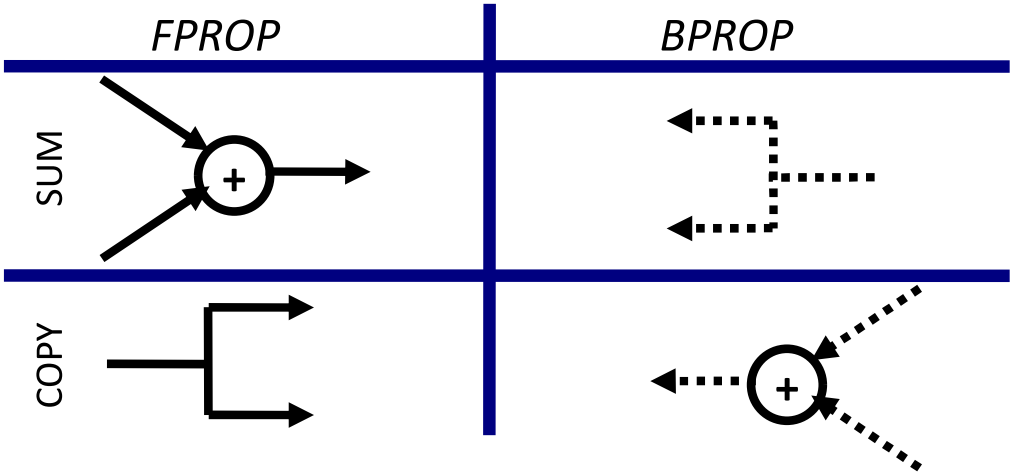
Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

# Gradients add at branches

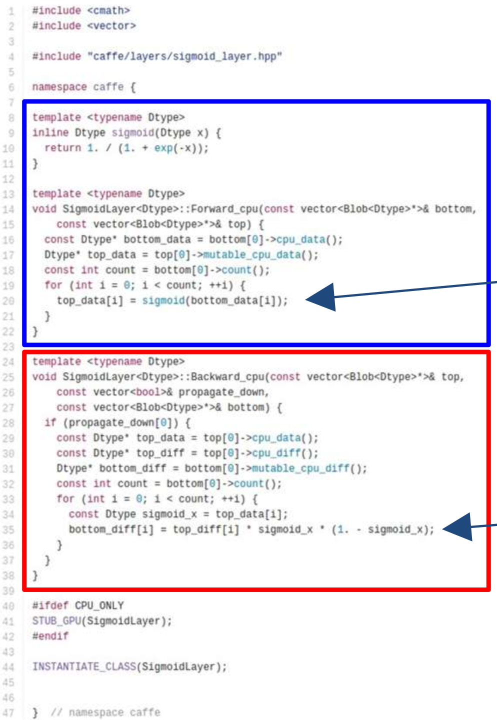


Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

# Duality in Fprop and Bprop



# 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
```

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

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

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

# Linear Algebra View: Vector and Matrix Sizes

# Closer Look at a Linear Classifier

$$\begin{bmatrix} \boldsymbol{w_{11}} & \boldsymbol{w_{12}} & \cdots & \boldsymbol{w_{1m}} & \boldsymbol{b1} \\ \boldsymbol{w_{21}} & \boldsymbol{w_{22}} & \cdots & \boldsymbol{w_{2m}} & \boldsymbol{b2} \\ \boldsymbol{w_{31}} & \boldsymbol{w_{32}} & \cdots & \boldsymbol{w_{3m}} & \boldsymbol{b3} \end{bmatrix} \begin{bmatrix} \boldsymbol{x_1} \\ \boldsymbol{x_2} \\ \vdots \\ \boldsymbol{x_m} \\ \boldsymbol{1} \end{bmatrix}$$

$$\boldsymbol{W} \qquad\qquad\qquad\qquad \boldsymbol{x}$$

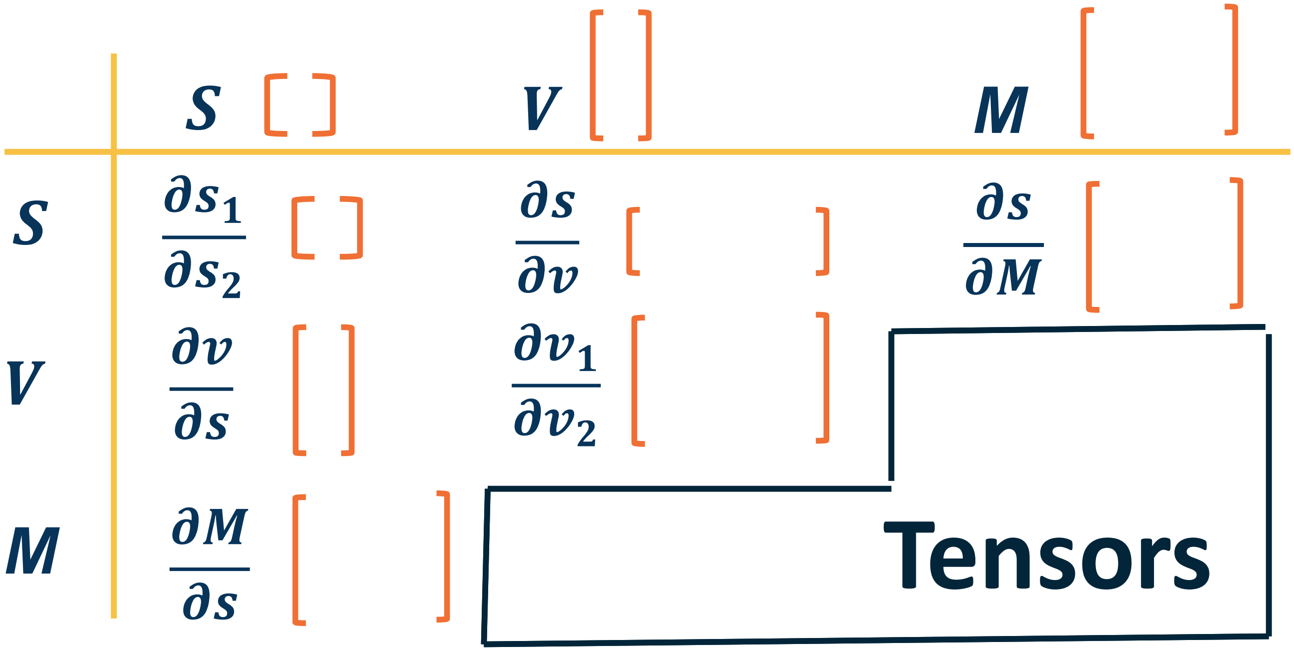
**Sizes:** $[\boldsymbol{c} \times (\boldsymbol{d}+\mathbf{1})]$ $\quad$ $[(\boldsymbol{d}+\mathbf{1}) \times \mathbf{1}]$

Where $c$ is number of classes

$d$ is dimensionality of input

## 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 $\boldsymbol{M} \in \mathbb{R}^{k \times \ell}$



| | $S$ | $V$ | $M$ |
|---|---|---|---|
| $S$ | $\frac{\partial s_1}{\partial s_2}$ | $\frac{\partial s}{\partial v}$ | $\frac{\partial s}{\partial M}$ |
| $V$ | $\frac{\partial v}{\partial s}$ | $\frac{\partial v_1}{\partial v_2}$ | |
| $M$ | $\frac{\partial M}{\partial s}$ | | Tensors |

## 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. $\boldsymbol{v} = [\boldsymbol{v_1}, \boldsymbol{v_2}, \ldots, \boldsymbol{v_m}]^{T}$
  and matrix $\boldsymbol{M} \in \mathbb{R}^{k \times \ell}$

- What is the size of $\frac{\partial v}{\partial s}$ ? $\mathbb{R}^{m \times 1}$ (column vector of size $m$)

$$\begin{bmatrix} \frac{\partial v_1}{\partial s} \\ \frac{\partial v_2}{\partial s} \\ \vdots \\ \frac{\partial v_m}{\partial s} \end{bmatrix}$$

- What is the size of $\frac{\partial s}{\partial v}$ ? $\mathbb{R}^{1 \times m}$ (row vector of size $m$)

$$\begin{bmatrix} \frac{\partial s}{\partial v_1} & \frac{\partial s}{\partial v_1} & \cdots & \frac{\partial s}{\partial v_m} \end{bmatrix}$$

# Dimensionality of Derivatives

# Conventions:

- What is the size of $\frac{\partial v^1}{\partial v^2}$ ? A matrix:

$$\begin{array}{cc} & \begin{array}{cccccc} & & \textbf{Col } j & & & \end{array} \\ \textbf{Row } i & \left[\begin{array}{cccccc} \frac{\partial v_1^1}{\partial v_1^2} & \cdots & \cdots & \cdots & \cdots & \\ \cdots & & \cdots & \cdots & \cdots & \cdots \\ \frac{\partial v_i^1}{\partial v_1^2} & \cdots & \frac{\partial v_i^1}{\partial v_j^2} & \cdots & \frac{\partial v_i^1}{\partial v_{m_2}^2} & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \end{array}\right]_{m_1 \times m_2} \end{array}$$

- This matrix of partial derivatives is called a **Jacobian**

(Note this is slightly different convention than on Wikipedia). Also, computationally other conventions are used.

## Conventions:

- What is the size of $\frac{\partial s}{\partial M}$ ? A matrix:

$$\begin{bmatrix} \frac{\partial s}{\partial m_{[1,1]}} & \cdots & \cdots & \cdots & \cdots & \\ \cdots & & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \frac{\partial s}{\partial m_{[i,j]}} & \cdots & \cdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \end{bmatrix}$$

# Example 1:

$$y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} x \\ x^2 \end{bmatrix} \qquad \frac{\partial y}{\partial x} = \begin{bmatrix} 1 \\ 2x \end{bmatrix}$$

# Example 2:

$$y = w^T x = \sum_k w_k x_k$$

$$\frac{\partial y}{\partial x} = \left[\frac{\partial y}{\partial x_1}, \dots, \frac{\partial y}{\partial x_m}\right]$$

$$= [w_1, \dots, w_m]$$ because $$\frac{\partial(\sum_k w_k x_k)}{\partial x_i} = w_i$$

$$= w^T$$

## Example 3:

$$\frac{\partial (wAw)}{\partial w} = 2w^T A \text{ (assuming A is symmetric)}$$

## Example 4:

$$y = Wx \qquad\qquad \frac{\partial y}{\partial x} = W$$

$$\begin{array}{cc} & \begin{array}{ccccc} & & \text{Col } j & & \end{array} \\ \text{Row } i & \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \cdots & \cdots & \cdots & \\ \cdots & & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \frac{\partial y_i}{\partial x_j} & \cdots & \cdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \end{bmatrix} \end{array} = \begin{bmatrix} \cdots & \cdots & \cdots & \cdots & \cdots & \\ \cdots & & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & w_{ij} & \cdots & \cdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \end{bmatrix}$$

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

- 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

# 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 $[\boldsymbol{B} \times \boldsymbol{C} \times \boldsymbol{W} \times \boldsymbol{H}]$

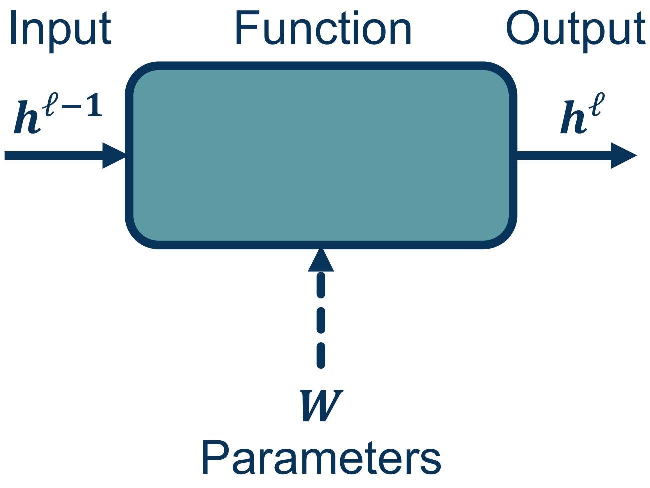
**Jacobians become tensors which is complicated**

- Instead, flatten input to a vector and get a vector of derivatives!
- This can also be done for partial derivatives between two vectors, two matrices, or two tensors

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

$$\textbf{Flatten} \ \Big\Downarrow$$

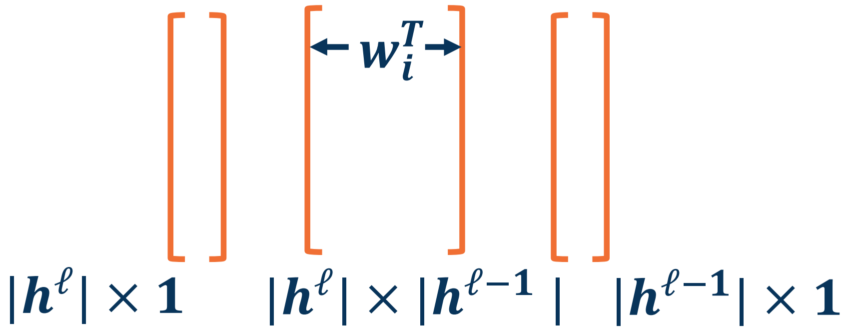
$$\begin{bmatrix} x_{11} \\ x_{12} \\ \vdots \\ x_{21} \\ x_{22} \\ \vdots \\ x_{n1} \\ \vdots \\ x_{nn} \end{bmatrix}$$



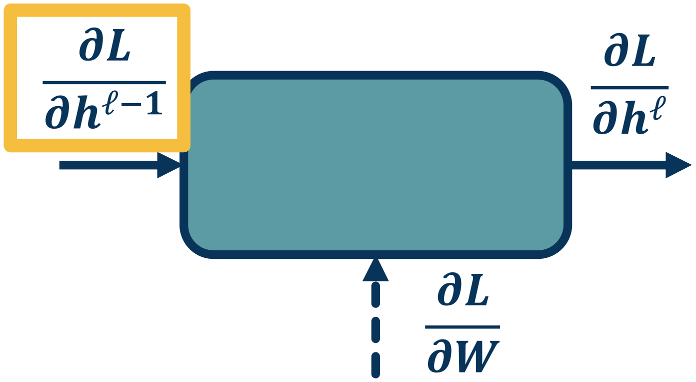
**Define:**

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

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



# Fully Connected (FC) Layer: Forward Function



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

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

**Define:**

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

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

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

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

# Fully Connected (FC) Layer

# Fully Connected (FC) Layer

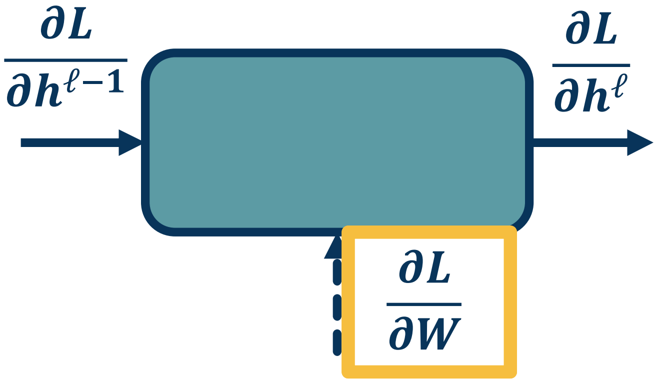
$$h^\ell = W h^{\ell-1}$$

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

**Define:**

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

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



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

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

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

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

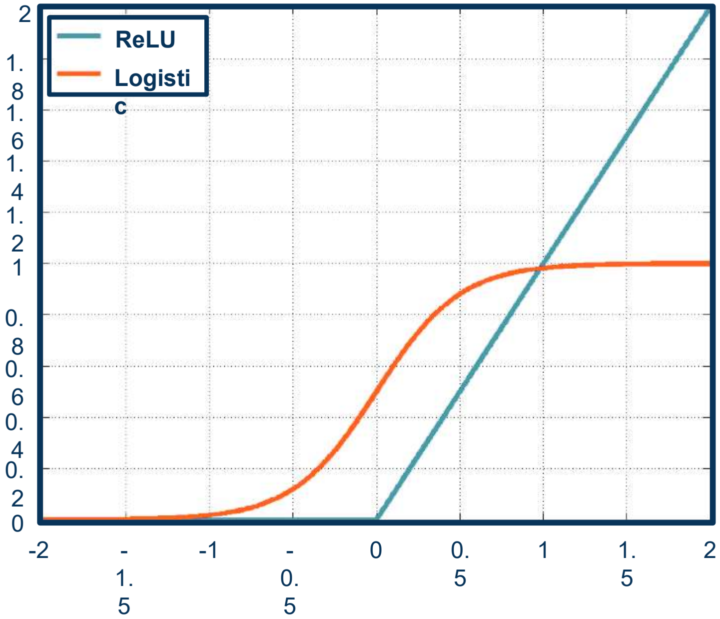
$$1 \times |h^{\ell-1}| \quad 1 \times |h^\ell| \quad |h^\ell| \times |h^{\ell-1}|$$

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

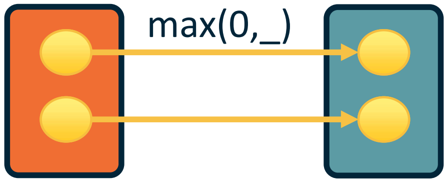
A common choice is the **Rectified Linear Unit**

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

**How many** parameters for this layer?



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



# Rectified Linear Unit (ReLU)

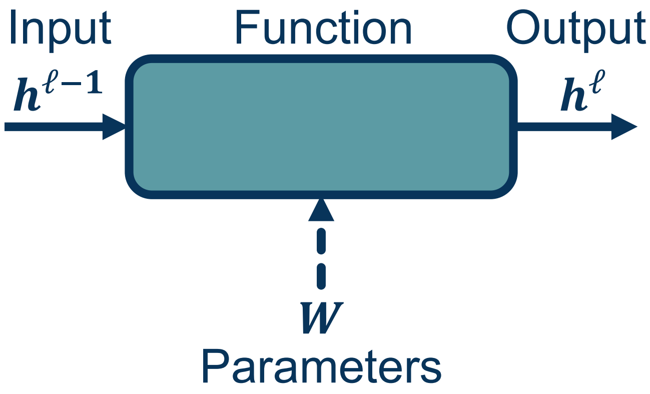
# Jacobian of ReLU

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**

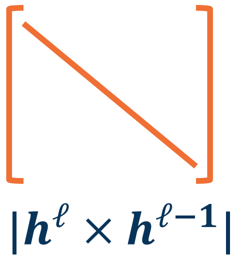
Max function **funnels gradients through selected max**

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



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

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



For diagonal

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

# Vectorization and Jacobians of Simple Layers

**Composition of Functions:** $f\big(g(x)\big) = (f \circ g)(x)$

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

$$f(x) = g_\ell\left(g_{\ell-1}\big(\ldots g_1(x)\big)\right)$$

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

(Many of these will be parameterized)

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

# Scalar Case

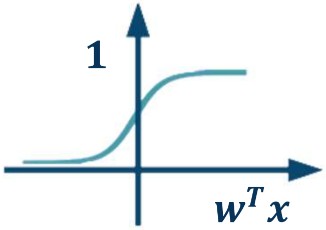
# Vector Case

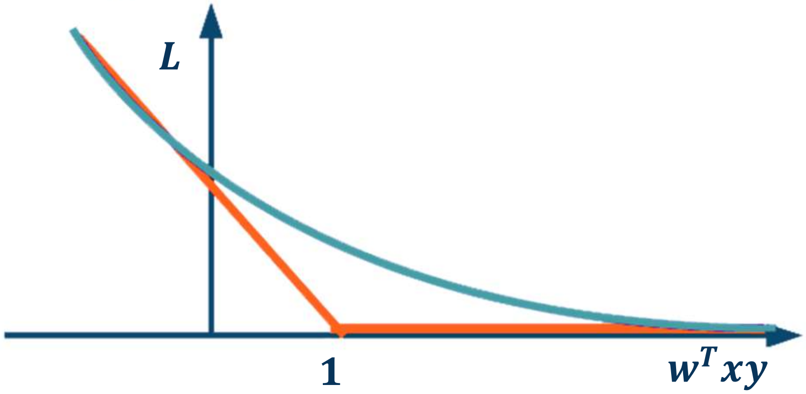
# Jacobian View of Chain Rule

# Graphical View of Chain Rule

# Chain Rule: Cascaded

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





**Log Loss**

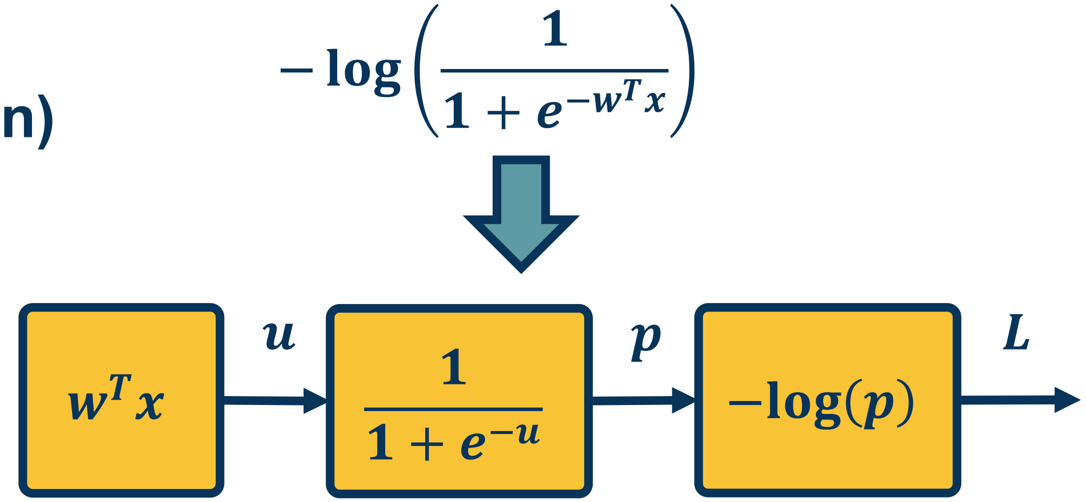
*Adapted from slide by Marc'Aurelio Ranzato*

# Linear Classifier: Logistic Regression

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

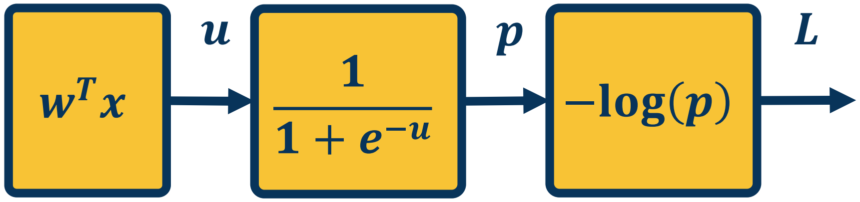
Machine Learning functions **(input -> model -> loss function)** is also a computation graph

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



# Neural Network Computation Graph

# Example Gradient Computations



$$\bar{L} = 1$$

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

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

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

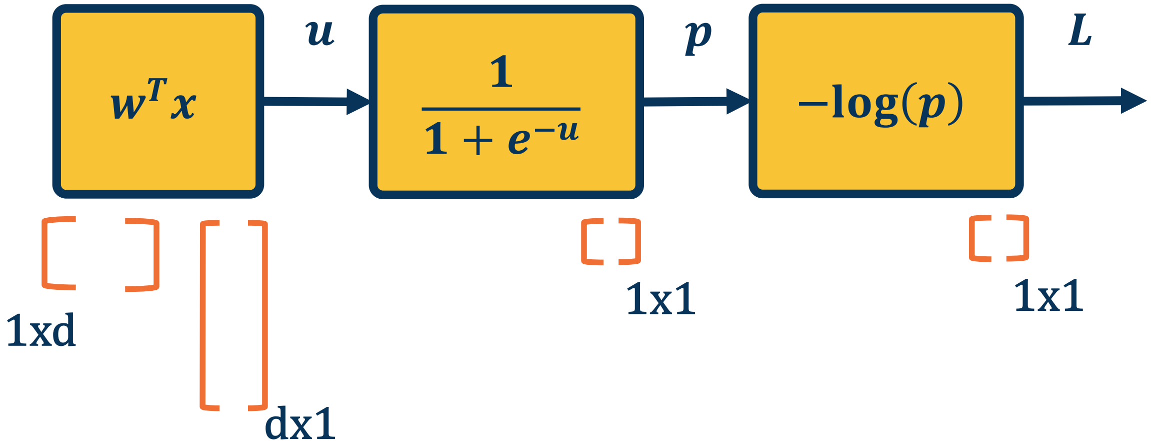
$$\bar{w} = \frac{\partial L}{\partial w} = \frac{\partial L}{\partial u}\,\frac{\partial u}{\partial w} = \bar{u}x^T$$

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

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

**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**

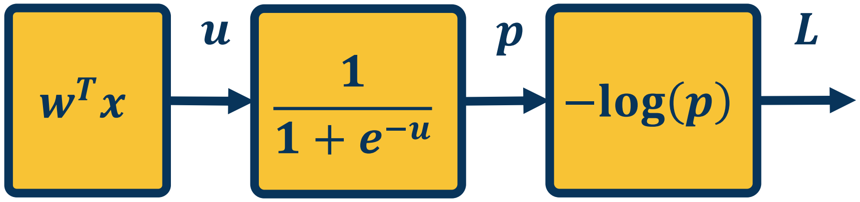


**Extremely efficient** in graphics processing units (GPUs)

$$\bar{w} = -\underset{1x1}{\frac{1}{\sigma(w^Tx)}}\,\underset{1x1}{\sigma(w^Tx)}\,\underset{1x1}{(1-\sigma(w^Tx))}\,\underset{1xd}{x^T}$$

## Vectorized Computations

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

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

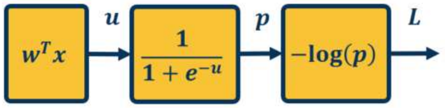
$$\bar{w} = \frac{\partial L}{\partial w} = \frac{\partial L}{\partial u}\,\frac{\partial u}{\partial w} = \bar{u}x^T$$

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

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

**This effectively shows gradient flow along path from** $L$ **to** $w$

# Different Views of Equivalent Ideas



$L = 1$

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

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

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

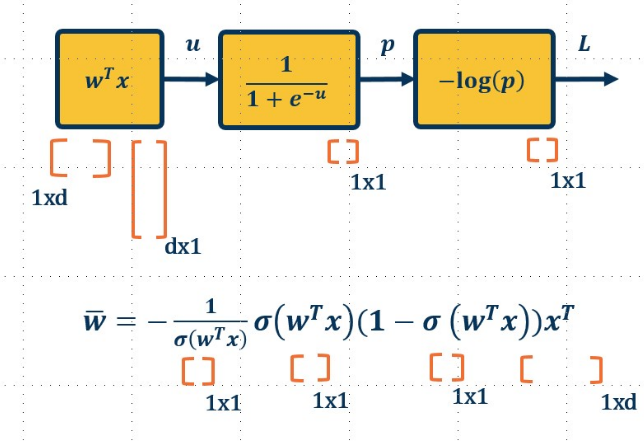
$\bar{w} = \frac{\partial L}{\partial w} = \frac{\partial L}{\partial u}\frac{\partial u}{\partial w} = \bar{u}x^T$

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

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

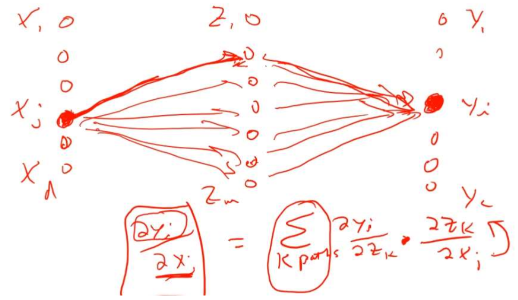
This effectively shows gradient flow along path from $L$ to $w$

**Computation Graph / Global View of Chain Rule**



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

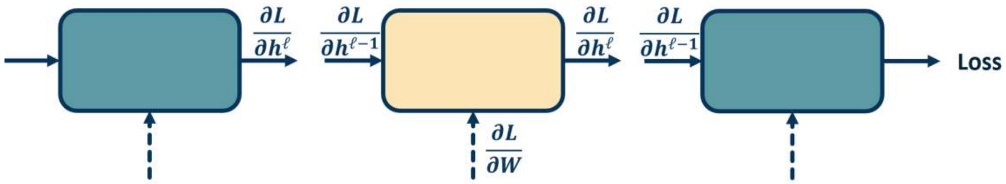
**Computational / Tensor View**



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

**Graph View**

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



**Backpropagation View (Recursive Algorithm)**

- **Backpropagation:** Recursive, modular algorithm for chain rule + gradient descent

- **When we move to vectors and matrices:**
  - Composition of functions (scalar)
  - Composition of functions (vectors/matrices)
  - Jacobian view of chain rule
  - Can view entire set of calculations as linear algebra operations (matrix-vector or matrix-matrix multiplication)

- **Automatic differentiation**:
  - Reduction of modules to simple operations we know (simple multiplication, etc.)
  - Automatically build computation graph in background as write code
  - Automatically compute gradients via backward pass

# Summary