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!

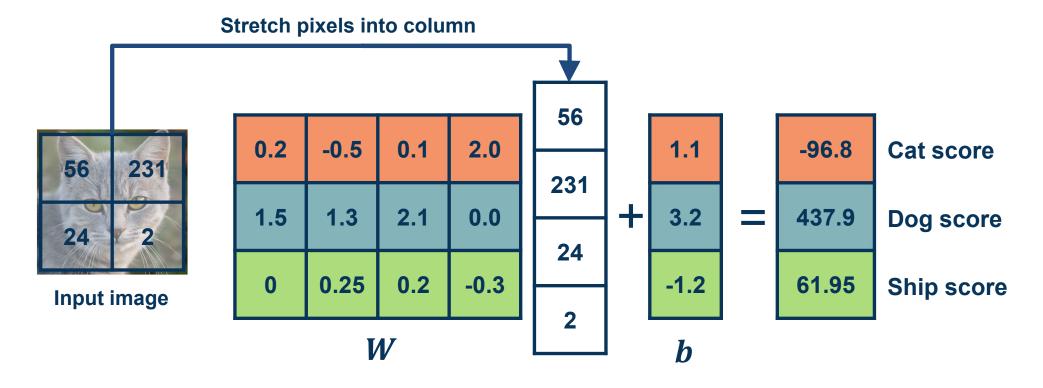
Piazza

- 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)



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



 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

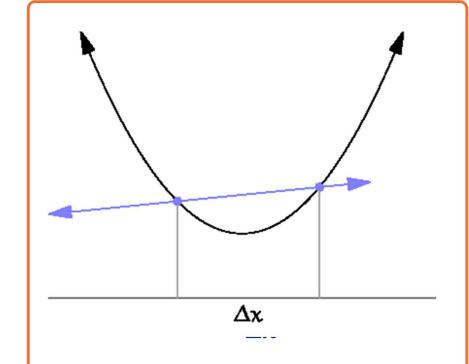


Image and equation from: https://en.wikipedia.org/wiki/Derivative#/media/ File:Tangent_animation.gif



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

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



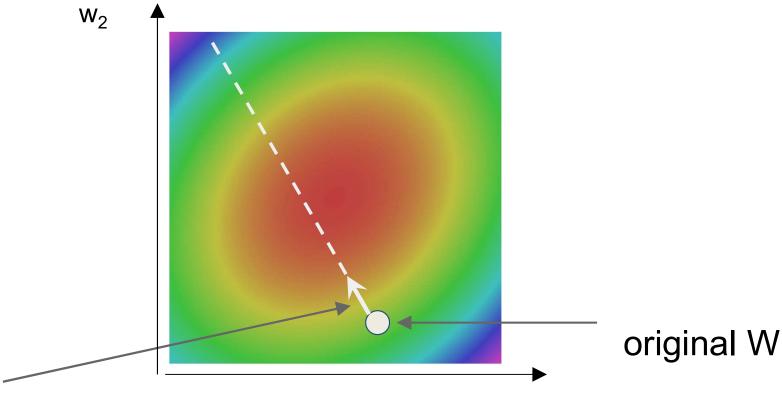
Often, we only compute the gradients across a small subset of data

$$L = \frac{1}{N} \sum_{i} L(f(x_i, W), y_i)$$

$$L = \frac{1}{M} \sum L(f(x_i, W), y_i)$$

- Where M is a subset of data
- We iterate over mini-batches:
 - Get mini-batch, compute loss, compute derivatives, and take a set

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



negative gradient direction

W



For some functions, we can analytically derive the partial derivative

Example:

Function

Loss

$$f(w, x_i) = w^T x_i \qquad (y_i - w^T x_i)^2$$

(Assume w and 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

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

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
$$\frac{\partial L}{\partial w_i}$$
?

$$\begin{aligned} \mathsf{L} &= \sum_{k=1}^{N} (y_k - w^T x_k)^2 & \frac{\partial L}{\partial w_j} = \sum_{k=1}^{N} \frac{\partial}{\partial w_j} (y_k - w^T x_k)^2 \\ &= \sum_{k=1}^{N} 2 \big(y_k - w^T x_k \big) \frac{\partial}{\partial w_j} (y_k - w^T x_k) \\ &= \sum_{k=1}^{N} 2 \big(y_k - w^T x_k \big) \frac{\partial}{\partial w_j} (y_k - w^T x_k) \\ &= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} w^T x_k \\ &= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} \sum_{i=1}^{m} w_i x_{ki} \\ &= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} \sum_{i=1}^{m} w_i x_{ki} \end{aligned}$$

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

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

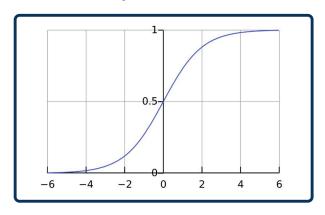
First, one can derive that: $\sigma'(x) = \sigma(x)(1 - \sigma(x))$

$$f(\mathbf{x}) = \sigma\left(\sum_{k} w_{k} x_{k}\right)$$

$$L = \sum_{i} \left(y_i - \sigma \left(\sum_{k} w_k x_{ik} \right) \right)^2$$

$$\frac{\partial L}{\partial w_j} = \sum_{i} 2 \left(y_i - \sigma \left(\sum_{k} w_k x_{ik} \right) \right) \left(-\frac{\partial}{\partial w_j} \sigma \left(\sum_{k} w_k x_{ik} \right) \right) \\
= \sum_{i} -2 \left(y_i - \sigma \left(\sum_{k} w_k x_{ik} \right) \right) \sigma' \left(\sum_{k} w_k x_{ik} \right) \frac{\partial}{\partial w_j} \sum_{k} w_k x_{ik} \\
= \sum_{i} -2 \delta_i \sigma(\mathbf{d}_i) (1 - \sigma(\mathbf{d}_i)) x_{ij}$$

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



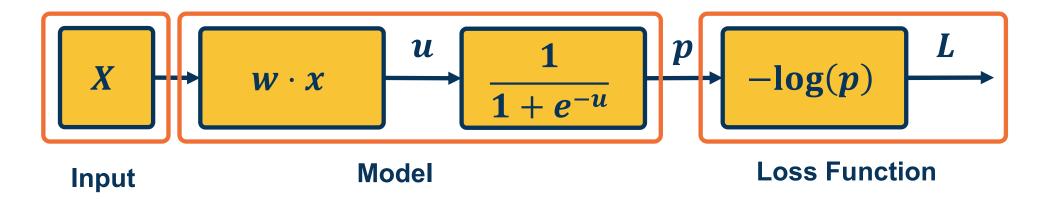
The sigmoid perception update rule:

$$w_j \leftarrow w_j + 2\eta \sum_{k=1}^N \delta_i \sigma_i (1-\sigma_i) x_{ij}$$
 where $\sigma_i = \sigma \Biggl(\sum_{j=1}^m w_j x_{ij}\Biggr)$ $\delta_i = y_i - \sigma_i$

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)

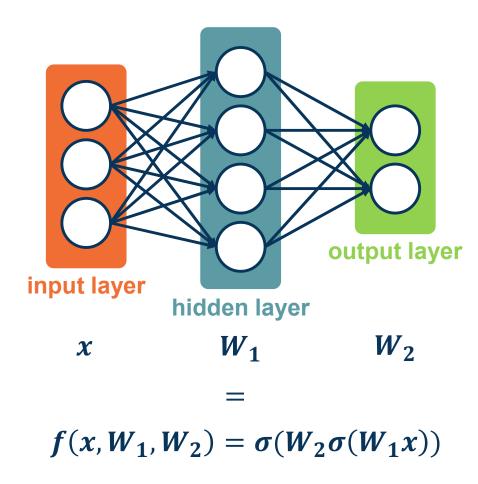


Figure adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

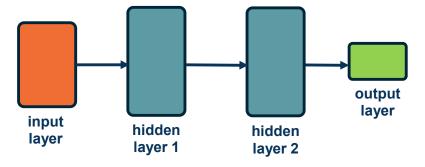


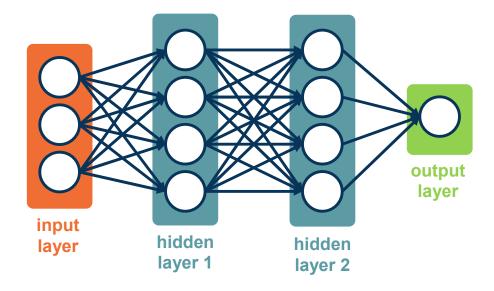
Large (deep) networks can be built by adding more and more layers

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**:





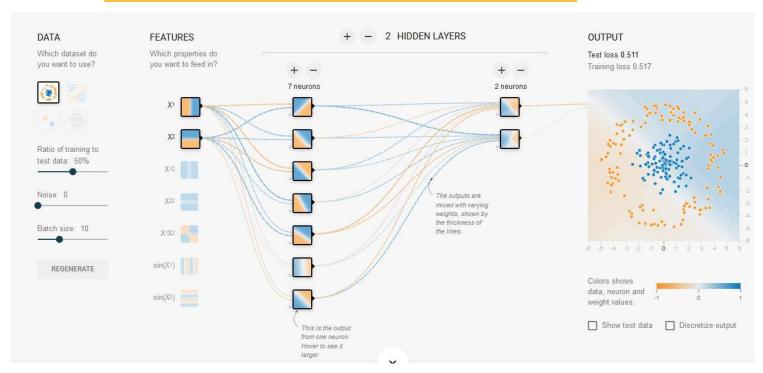
$$f(x, W_1, W_2, W_3) = \sigma(W_2 \sigma(W_1 x))$$

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



Demo

http://playground.tensorflow.org





Computation Graphs



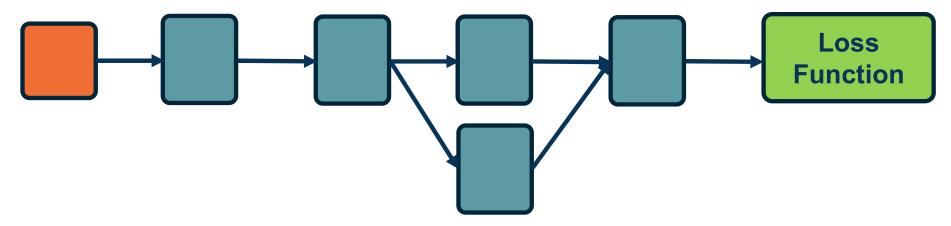
Functions can be made **arbitrarily complex** (subject to memory and computational limits), e.g.:

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

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

At the end, add the loss function

Composition can have some structure



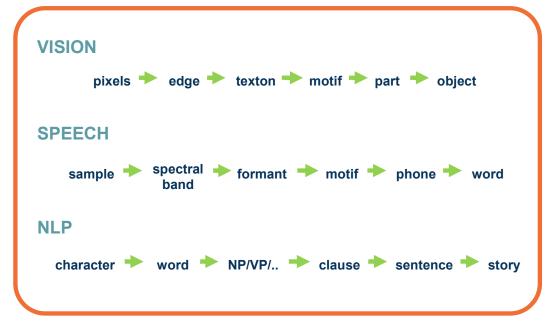


The world is **compositional!**

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

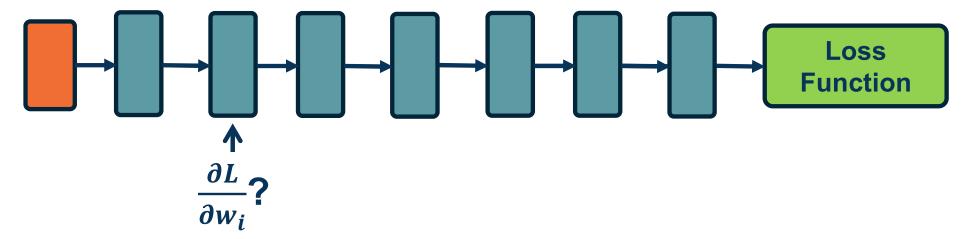


Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

Pixels -> edges -> object parts -> objects

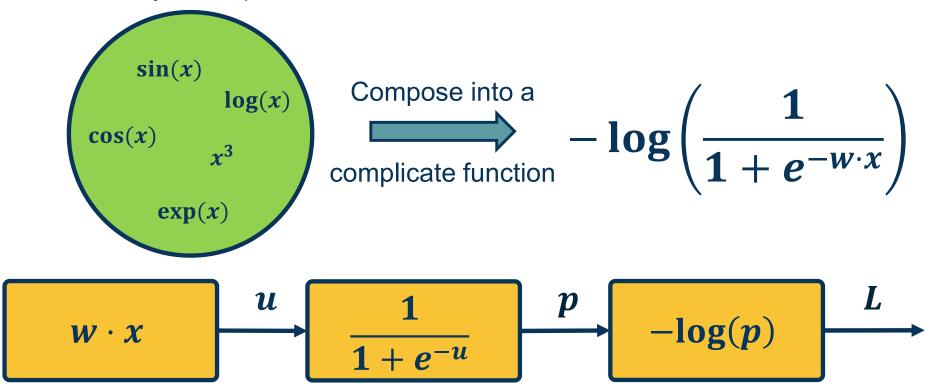


- We are learning complex models with significant amount of parameters (millions or billions)
- How do we compute the gradients of the loss (at the end) with respect to internal parameters?
- Intuitively, want to understand how small changes in weight deep inside are propagated to affect the loss function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





Given a library of simple functions



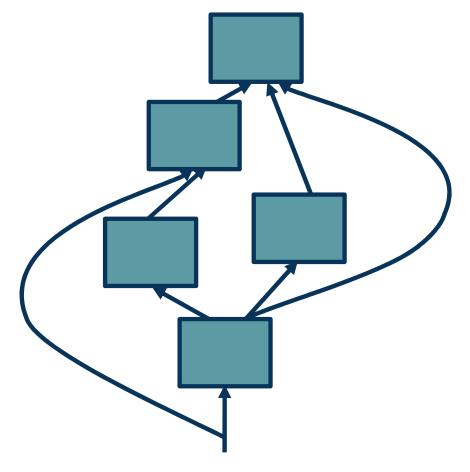


To develop a general algorithm for this, we will view the function as a **computation graph**

Graph can be any directed acyclic graph (DAG)

 Modules must be differentiable to support gradient computations for gradient descent

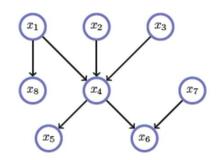
A training algorithm will then process this graph, one module at a time

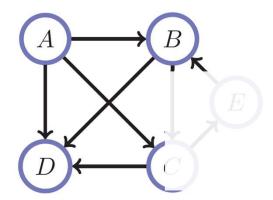




Directed Acyclic Graphs (DAGs)

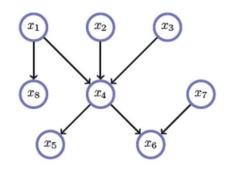
- Exactly what the name suggests
 - Directed edges
 - No (directed) cycles
 - Underlying undirected cycles okay

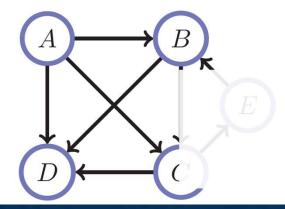




Directed Acyclic Graphs (DAGs)

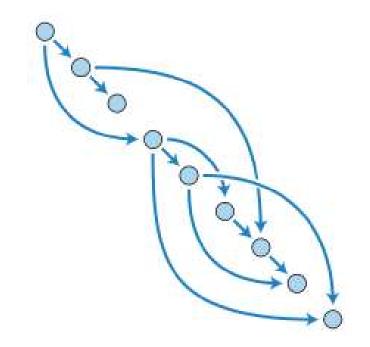
- Concept
 - Topological Ordering





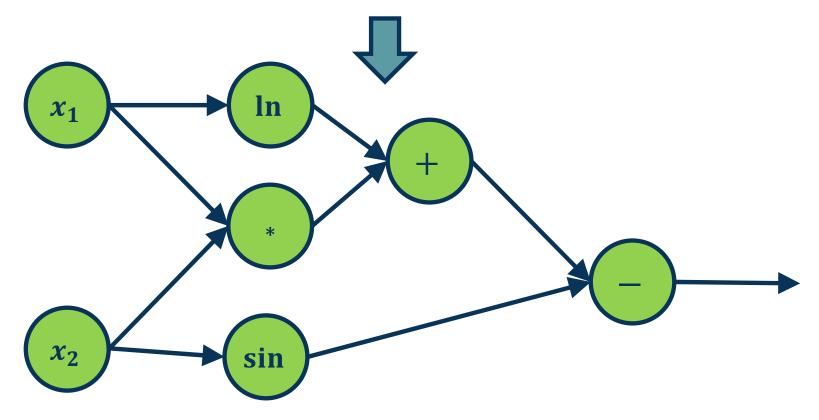


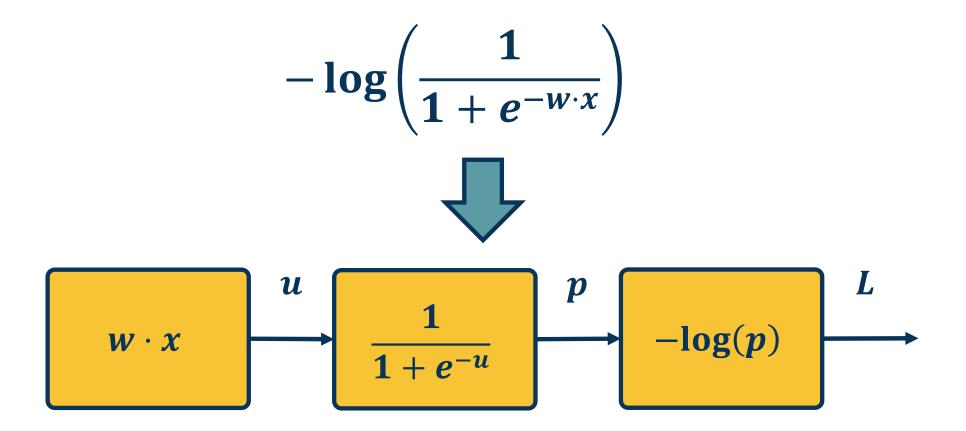
Directed Acyclic Graphs (DAGs)





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





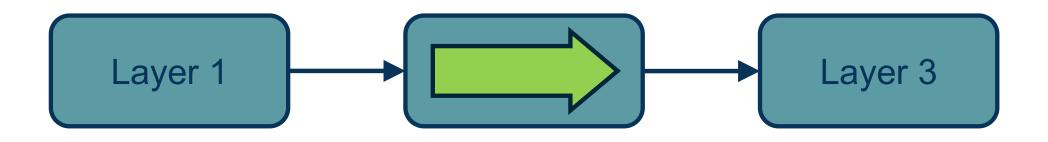


Backpropagation













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)

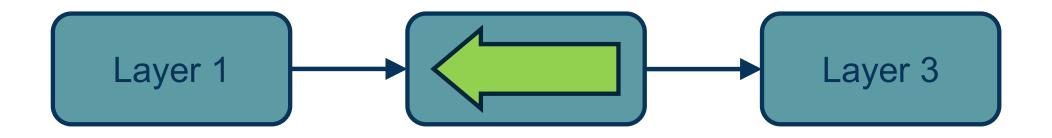


Step 2: Compute Gradients wrt parameters: Backward Pass





Step 2: Compute Gradients wrt parameters: Backward Pass



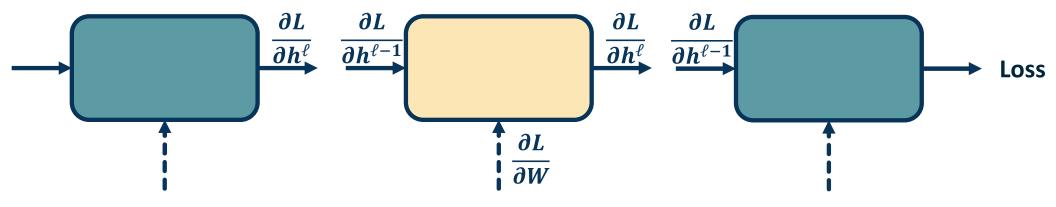


Step 2: Compute Gradients wrt parameters: Backward Pass





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



We will use the chain rule to do this:

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



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!





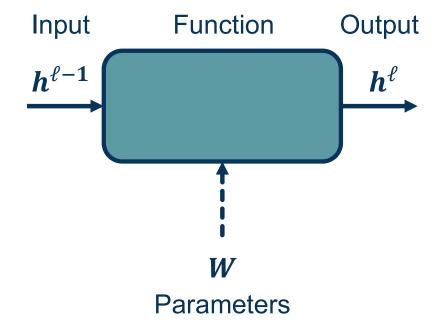
Given this computation graph, the training algorithm will:

- 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)

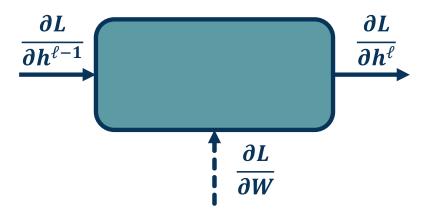
This algorithm is called backpropagation





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



• 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!

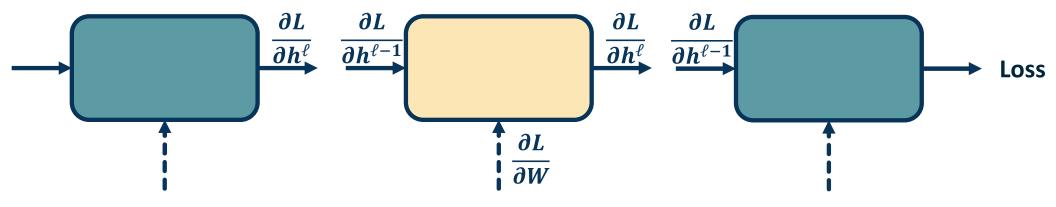
Example: If
$$h^{\ell} = Wh^{\ell-1}$$

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

and
$$\frac{\partial h^{\ell}}{\partial w_i} = h^{\ell-1,T}$$
 in the *i*-th row



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



We will use the chain rule to do this:

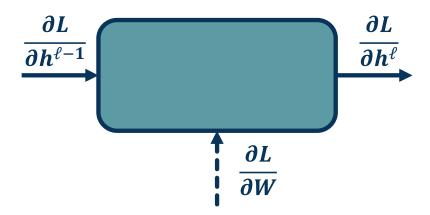
Chain Rule:
$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x}$$



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



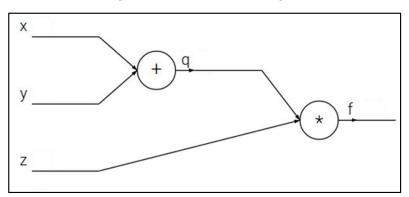
Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun



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

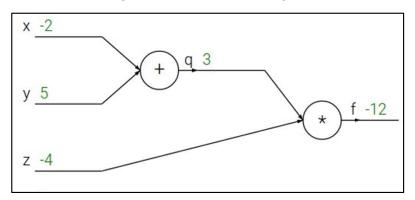


$$f(x,y,z) = (x+y)z$$



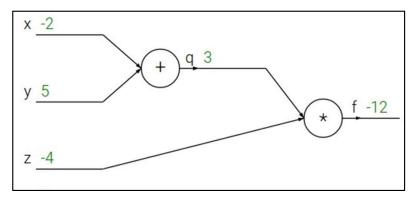
$$f(x,y,z) = (x+y)z$$

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



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

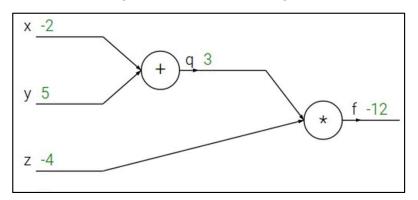
e.g. x = -2, y = 5, z = -4



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

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

$$q=x+y \hspace{0.5cm} rac{\partial q}{\partial x}=1, rac{\partial q}{\partial y}=1$$

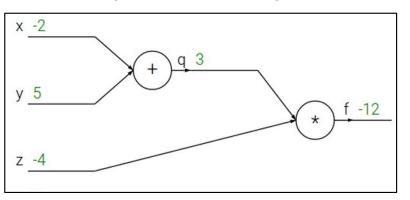


$$f(x,y,z) = (x+y)z$$

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

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

$$f=qz$$
 $rac{\partial f}{\partial q}=z, rac{\partial f}{\partial z}=q$

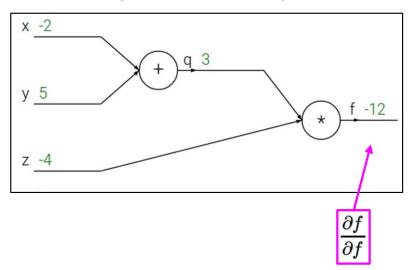


$$f(x,y,z) = (x+y)z$$

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

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

$$f=qz$$
 $rac{\partial f}{\partial q}=z, rac{\partial f}{\partial z}=q$

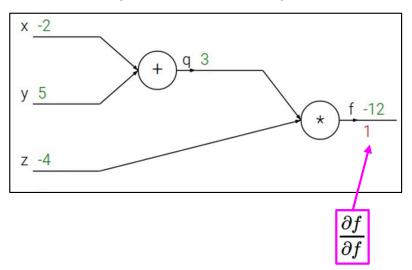


$$f(x,y,z) = (x+y)z$$

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

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

$$f=qz$$
 $rac{\partial f}{\partial q}=z, rac{\partial f}{\partial z}=q$



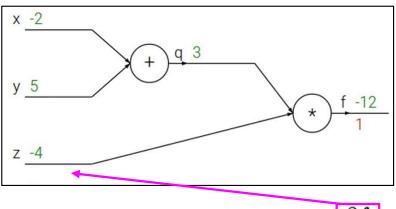
$$f(x,y,z) = (x+y)z$$

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

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

$$f=qz$$
 $rac{\partial f}{\partial q}=z, rac{\partial f}{\partial z}=q$

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



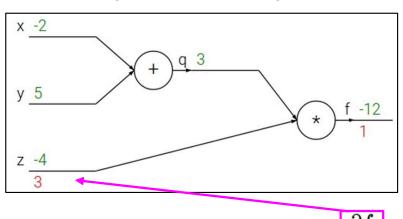
 $\frac{\partial f}{\partial z}$

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

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

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

$$f=qz$$
 $rac{\partial f}{\partial q}=z, rac{\partial f}{\partial z}=q$

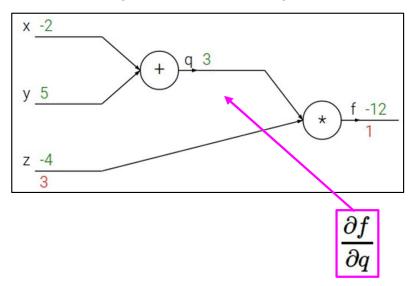


$$f(x,y,z) = (x+y)z$$

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

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

$$f=qz$$
 $rac{\partial f}{\partial q}=z, rac{\partial f}{\partial z}=q$

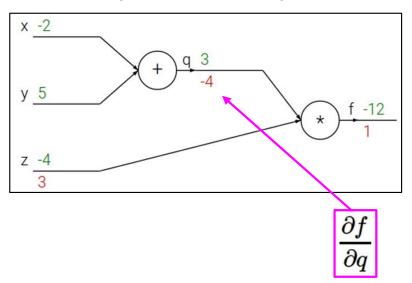


$$f(x,y,z) = (x+y)z$$

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

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

$$f=qz$$
 $rac{\partial f}{\partial q}=z, rac{\partial f}{\partial z}=q$

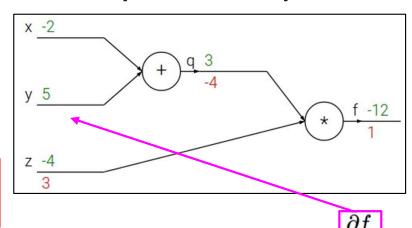


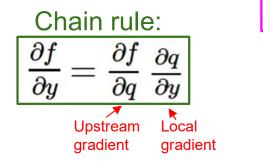
$$f(x,y,z) = (x+y)z$$

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

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

$$f=qz$$
 $rac{\partial f}{\partial q}=z, rac{\partial f}{\partial z}=q$



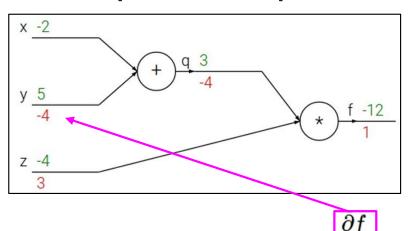


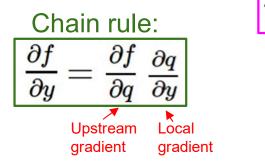
$$f(x, y, z) = (x + y)z$$

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

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

$$f=qz$$
 $rac{\partial f}{\partial q}=z, rac{\partial f}{\partial z}=q$



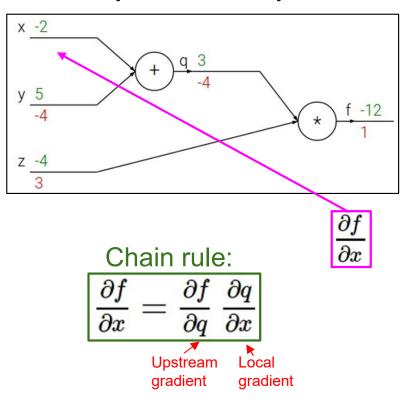


$$f(x, y, z) = (x + y)z$$

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

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

$$f=qz$$
 $rac{\partial f}{\partial q}=z, rac{\partial f}{\partial z}=q$

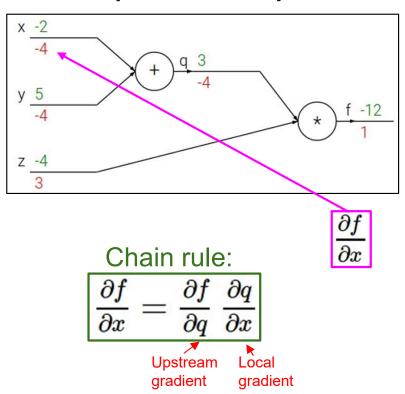


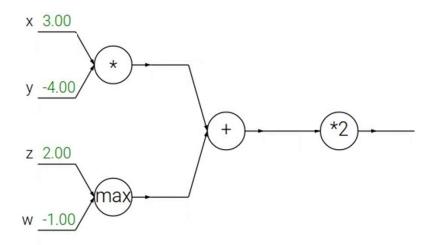
$$f(x, y, z) = (x + y)z$$

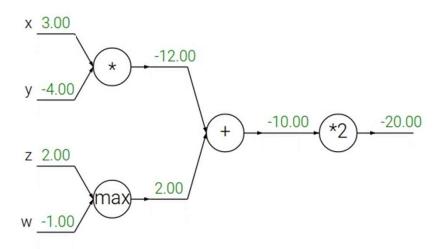
e.g. x = -2, y = 5, z = -4

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

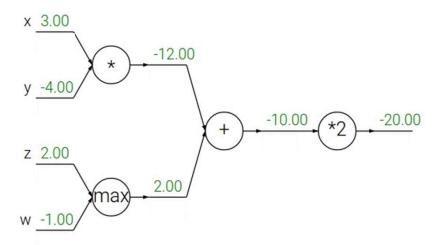
$$f=qz$$
 $rac{\partial f}{\partial q}=z, rac{\partial f}{\partial z}=q$



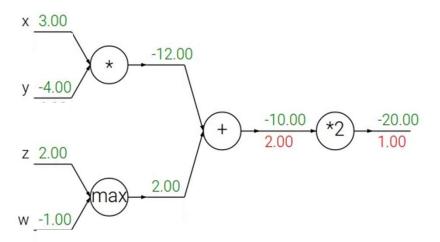




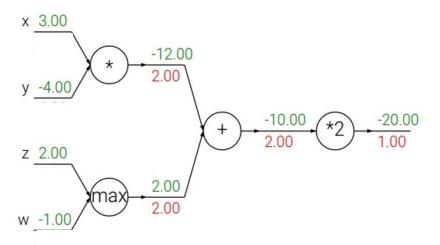




Q: What is an **add** gate?

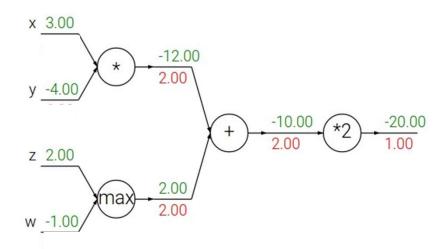


add gate: gradient distributor



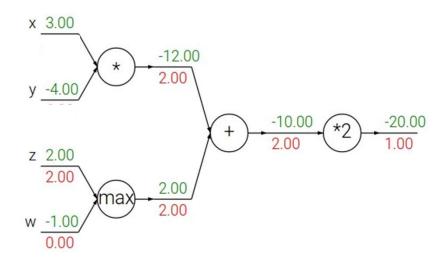
add gate: gradient distributor

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



add gate: gradient distributor

max gate: gradient router

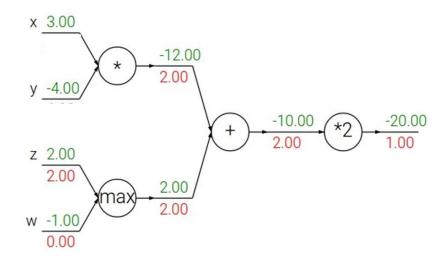




add gate: gradient distributor

max gate: gradient router

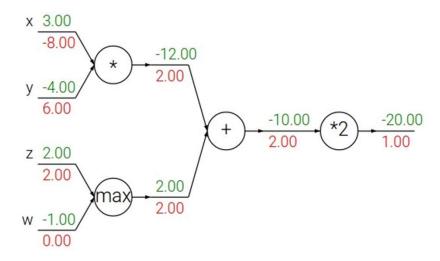
Q: What is a **mul** gate?



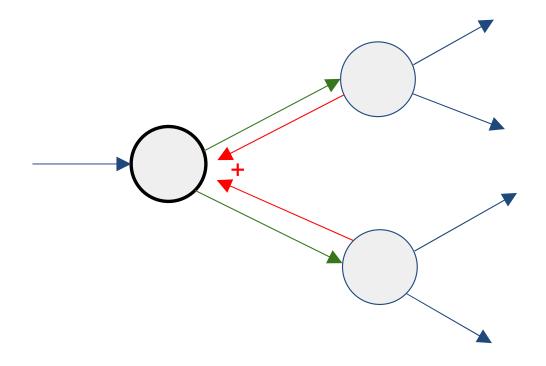
add gate: gradient distributor

max gate: gradient router

mul gate: gradient switcher

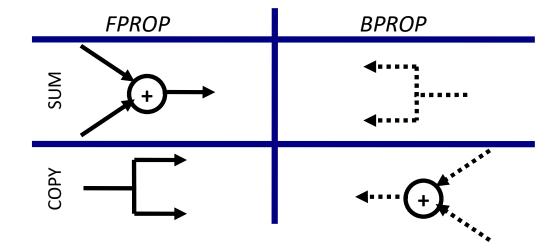


Gradients add at branches





Duality in Fprop and Bprop



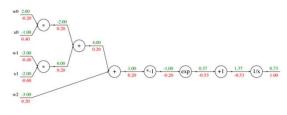


Deep Learning = Differentiable Programming

- 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...]

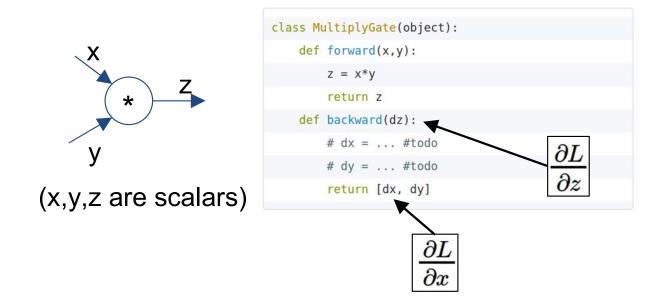
    # 2. forward the computational graph:
    for gate in self.graph.nodes_topologically_sorted():
        gate.forward()

    return loss # the final gate in the graph outputs the loss

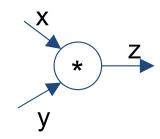
def backward():
    for gate in reversed(self.graph.nodes_topologically_sorted()):
        gate.backward() # little piece of backprop (chain rule applied)
    return inputs_gradients
```



Modularized implementation: forward / backward API



Modularized implementation: forward / backward API

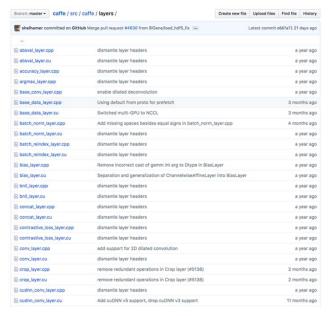


(x,y,z are scalars)

```
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



| 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 | dismantie 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 | dismantie 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 | dismantie layer headers | a year ago |
| dummy_data_layer.cpp | dismantle layer headers | a year ago |
| eltwise_layer.cpp | dismantie 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 is licensed under BSD 2-Clause



```
#include <cmath>
    #include <vector>
                                                                                                                                             Caffe Sigmoid Layer
    #include "caffe/layers/sigmoid_layer.hpp"
    namespace caffe {
    template <typename Dtype>
    inline Dtype sigmoid(Dtype x) {
     return 1. / (1. + exp(-x));
    void SigmoidLayer<Dtype>::Forward_cpu(const vector<Blob<Dtype>">& bottom,
     const Dtype* bottom_data = bottom[0]->cpu_data();
Dtype* top_data = top[0]->mutable_cpu_data();
                                                                                                             \sigma(x) = \frac{1}{1 + e^{-x}}
      const int count = bottom[0]->count();
      for (int i = 0; i < count; ++i) {
       top_data[i] = sigmoid(bottom_data[i]);
    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();
                                                                                                             (1 - \sigma(x)) \sigma(x) * top_diff (chain rule)
        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);
47 } // namespace caffe
  Caffe is licensed under BSD 2-Clause
```



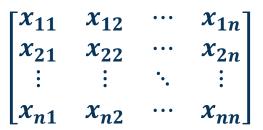
Batches of data are **matrices** or **tensors** (multi-dimensional matrices)

Examples:

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

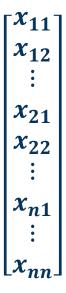
Jacobians become tensors which is complicated

- 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



Flatten





Jacobians of Batches



