Topics:

- Gradient Descent
- Neural Networks

CS 4644-DL / 7643-A ZSOLT KIRA

• Assignment 1 out!

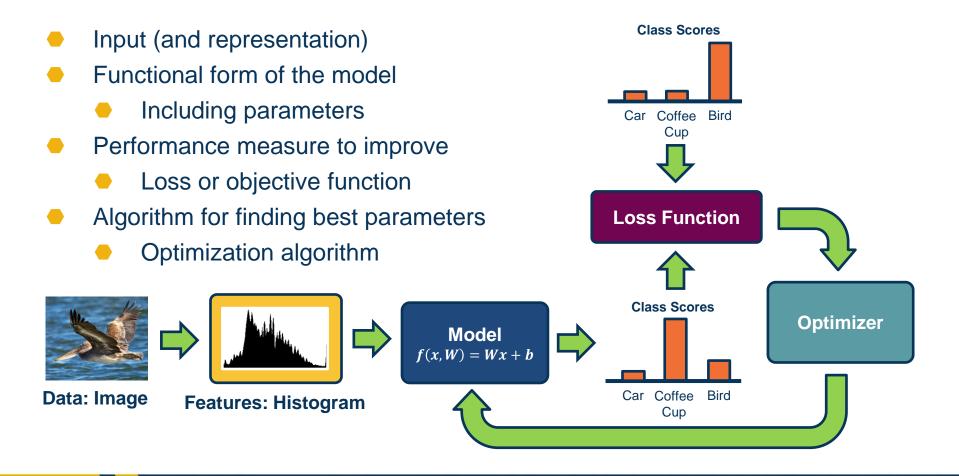
- Due Feb 2nd (with grace period Feb 4th)
- Start now, start now, start now!
- Start now, start now, start now!
- Start now, start now, start now!

• Piazza

• Be active!!!

Office hours

- Lots of special topics (e.g. Assignment 1, Matrix Calculus, etc.)
- Note: Course will start to get math heavy!



Components of a Parametric Model



Input: Vector

- Functional form of the model: Softmax(Wx)
- Performance measure to improve: Cross-Entropy
- Algorithm for finding best parameters: **Gradient Descent**

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

• Update Weights
$$w_i = w_i - \alpha \frac{\partial L}{\partial w_i}$$

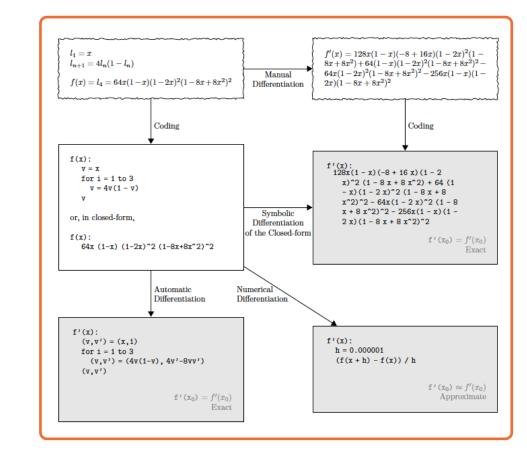




We know how to compute the **model output and loss** function

Several ways to compute $\frac{\partial L}{\partial w_i}$

- Manual differentiation
- Symbolic differentiation
- Numerical differentiation
- Automatic differentiation



Computing Gradients



For some functions, we can analytically derive the partial derivative

Example:

FunctionLoss $f(w, x_i) = w^T x_i$ $\sum_{i=1}^{N} (y_i - w^T x_i)^2$

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

Dataset: N examples (indexed by *i*)

Update Rule $w_j \leftarrow w_j + 2\alpha \sum_{i=1}^N \delta_i x_{ij}$

$$\mathbf{L} = \sum_{i=1}^{N} (y_i - w^T x_i)^2$$

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

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

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

Derivation of Update Rule

 $\frac{\partial L}{\partial w_j} = \sum_{i=1}^{N} \frac{\partial}{\partial w_j} (y_i - w^T x_i)^2$ $=\sum_{i=1}^{N}2(y_{i}-w^{T}x_{i})\frac{\partial}{\partial w_{i}}(y_{i}-w^{T}x_{i})$ $= -2\sum_{i=1}^{N} \delta_{i} \frac{\partial}{\partial w_{j}} w^{T} x_{i}$...where... $\delta_{i} = y_{i} - w^{T} x_{i}$ $= -2\sum_{i=1}^{n} \delta_i \frac{\partial}{\partial w_j} \sum_{k=1}^{n} w_k x_{ik}$ $=-2\sum_{i=1}^{N}\delta_{i}x_{ij}$

Manual Differentiation



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

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

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

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

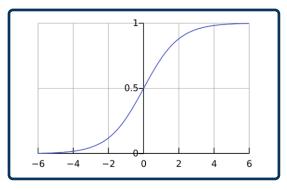
$$L = \sum_{i} \left(y_{i} - \sigma\left(\sum_{k} w_{k} x_{ik}\right)\right)^{2}$$

$$\frac{\partial L}{\partial w_{j}} = \sum_{i} 2\left(y_{i} - \sigma\left(\sum_{k} w_{k} x_{ik}\right)\right) \left(-\frac{\partial}{\partial w_{j}} \sigma\left(\sum_{k} w_{k} x_{ik}\right)\right)$$

$$= \sum_{i} -2\left(y_{i} - \sigma\left(\sum_{k} w_{k} x_{ik}\right)\right) \sigma'\left(\sum_{k} w_{k} x_{ik}\right) \frac{\partial}{\partial w_{j}} \sum_{k} w_{k} x_{ik}$$

$$= \sum_{i} -2\delta_{i}\sigma(\mathbf{d}_{i})(1 - \sigma(\mathbf{d}_{i}))x_{ij}$$
where $\delta_{i} = y_{i} - \mathbf{f}(x_{i})$

$$d_{i} = \sum_{i} w_{k} x_{ik}$$



The sigmoid perception update rule:

$$w_{j} \leftarrow w_{j} + 2\alpha \sum_{k=1}^{N} \delta_{i} \sigma_{i} (1 - \sigma_{i}) x_{ij}$$

where $\sigma_{i} = \sigma \left(\sum_{j=1}^{d} w_{j} x_{ij} \right)$
 $\delta_{i} = y_{i} - \sigma_{i}$

Adding a Non-Linear Function

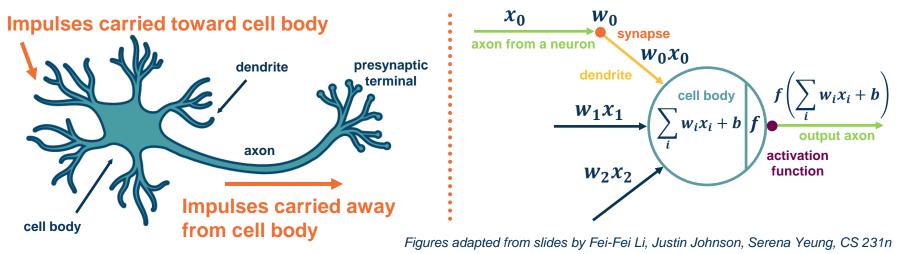


Neural Network View of a Linear **Classifier**



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

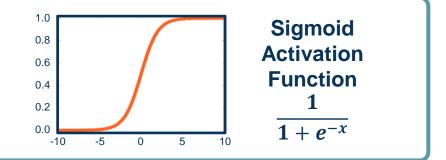
- A neuron takes input (firings) from other neurons (-> input to linear classifier)
- The inputs are summed in a weighted manner (-> weighted sum)
 - Learning is through a modification of the weights
- If it receives enough input, it "fires" (threshold or if weighted sum plus bias is high enough)

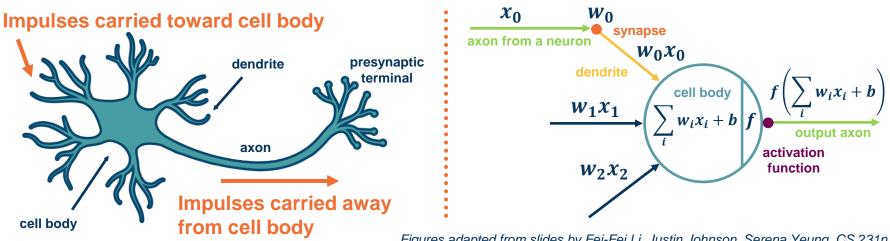


Origins of the Term Neural Network



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





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

Adding Non-Linearities

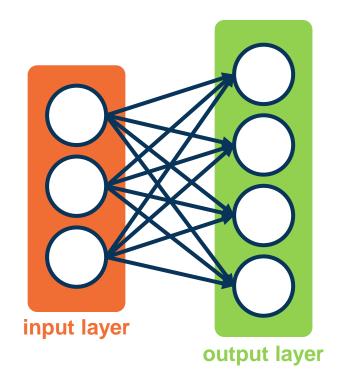


We can have **multiple** neurons connected to the same input

Corresponds to a multi-class classifier

 Each output node outputs the score for a class

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



- Often called fully connected layers
 - Also called a linear projection layer
 Figure adapt

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

Connecting Many Neurons



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

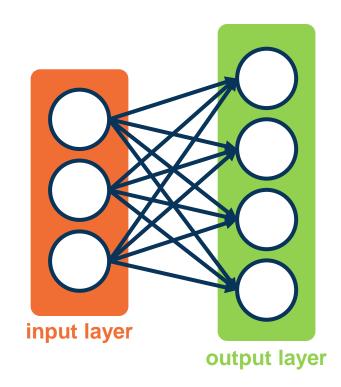


Figure adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Neural Network Terminology



We can stack multiple layers together

- Input to second layer is output of first layer
- Called a **2-layered neural network** (input is not counted)

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

- We will see that they end up learning effective features
- This **increases** the representational power of the function!
- Two layered networks can represent any continuous function

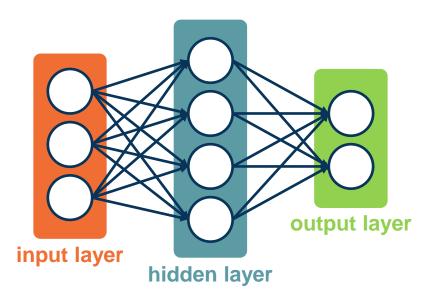


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Connecting Many Layers



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)

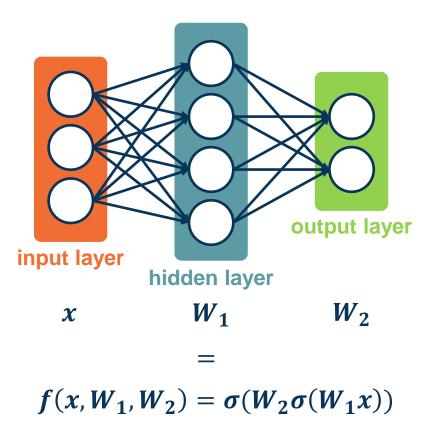


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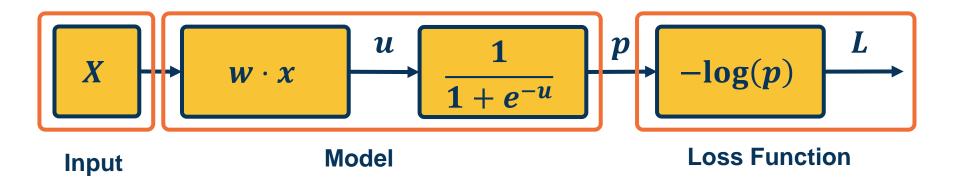




A linear classifier can be broken down into:

- lnput
- A function of the input
- A loss function

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





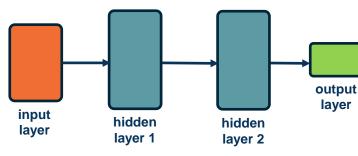


Large (deep) networks can be built by adding more and more layers

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:



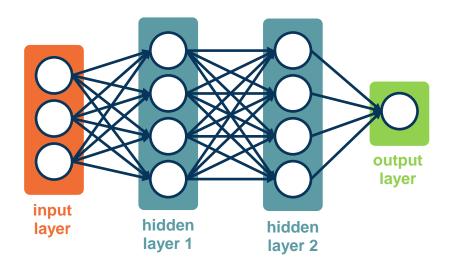


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Computation Graphs



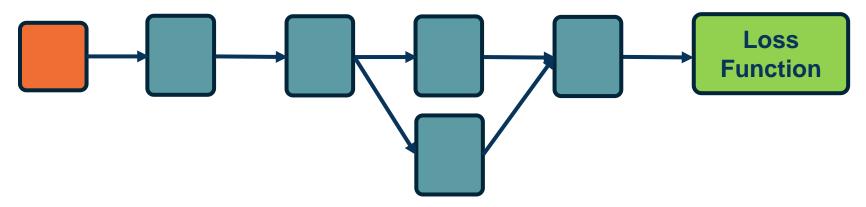
Functions can be made **arbitrarily complex** (subject to memory and computational limits), e.g.:

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

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

At the end, add the loss function

Composition can have some structure





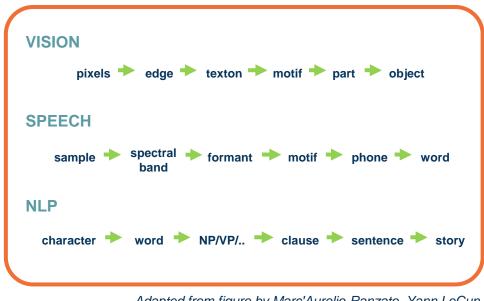


The world is **compositional**!

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



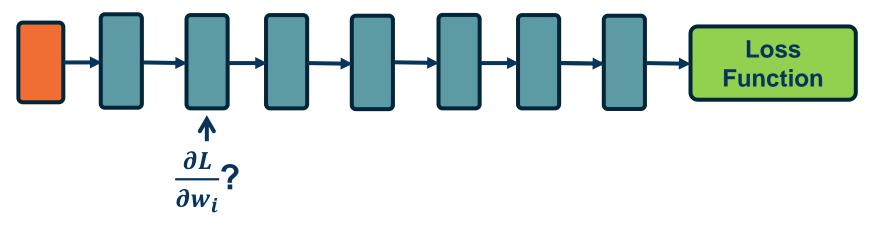
Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

Pixels -> edges -> object parts -> objects





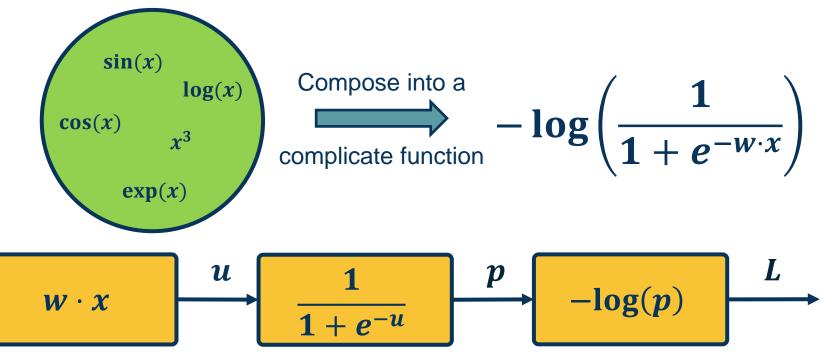
- We are learning complex models with significant amount of parameters (millions or billions)
- How do we compute the gradients of the loss (at the end) with respect to internal parameters?
- Intuitively, want to understand how small changes in weight deep inside are propagated to affect the loss function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







Given a library of simple functions





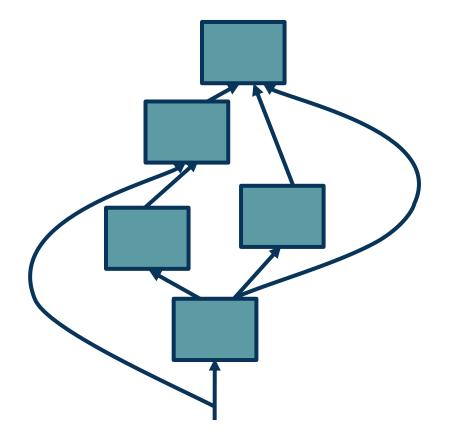


To develop a general algorithm for this, we will view the function as a **computation graph**

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**

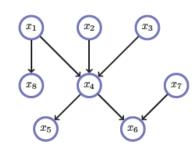


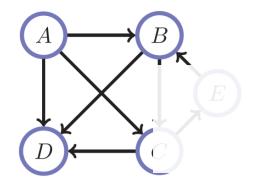




Directed Acyclic Graphs (DAGs)

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



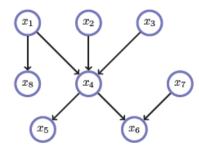


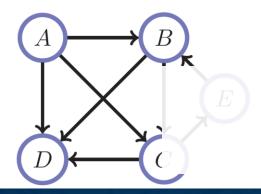


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Directed Acyclic Graphs (DAGs)

- Concept
 - Topological Ordering

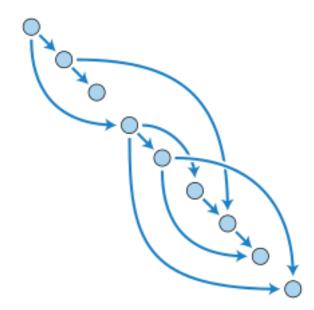






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Directed Acyclic Graphs (DAGs)





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Backpropagation



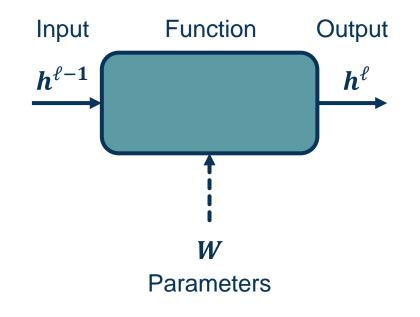
Given this computation graph, the training algorithm will:

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

Backward pass is a recursive algorithm that:

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

This algorithm is called **backpropagation**



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

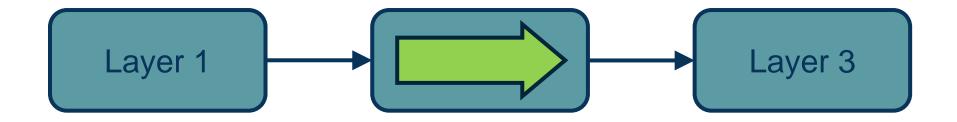


Overview of Training















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

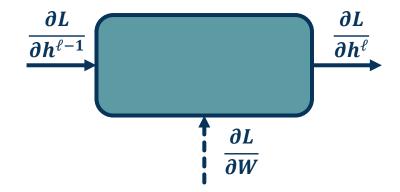
This is because we will need them to compute the gradients (the gradient equations will have terms with the output values in them)





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

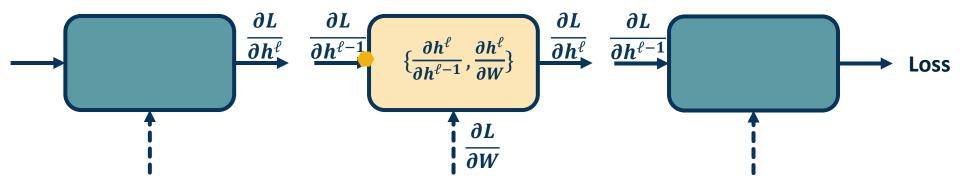
• We are given:
$$\frac{\partial L}{\partial h^{\ell}}$$

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









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

1

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

Example:

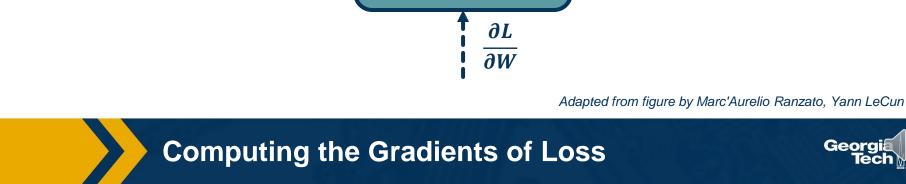
If
$$h^\ell = Wh^{\ell-1}$$

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

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

Computing the Local Gradients: Example





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)

 $\overline{\partial h^\ell}$

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

 $\overline{\partial h^{\ell-1}}$

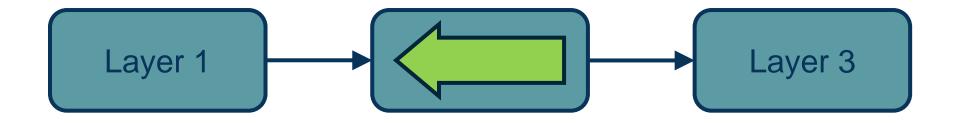
Step 2: Compute Gradients wrt parameters: Backward Pass







Step 2: Compute Gradients wrt parameters: Backward Pass







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

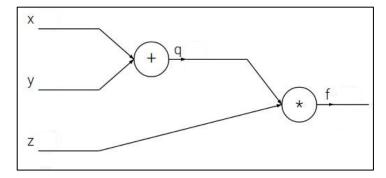


$$f(x,y,z) = (x+y)z$$



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

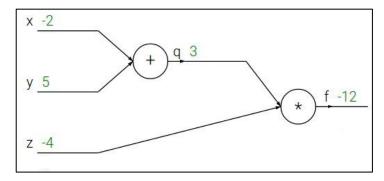






$$f(x, y, z) = (x + y)z$$

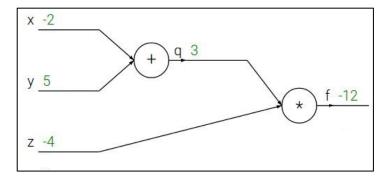
e.g. x = -2, y = 5, z = -4





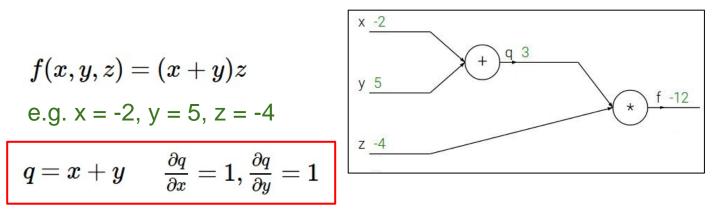
$$f(x, y, z) = (x + y)z$$

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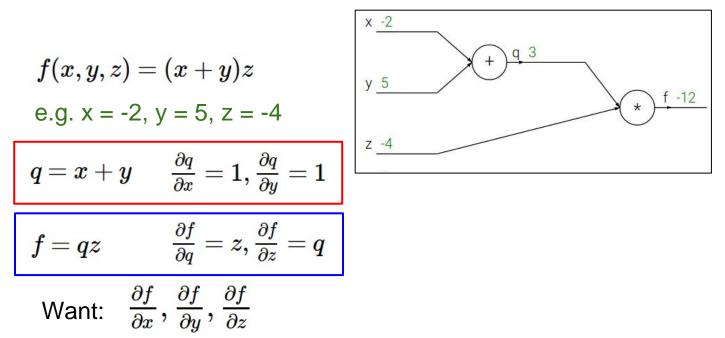
Want:
$$\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$$



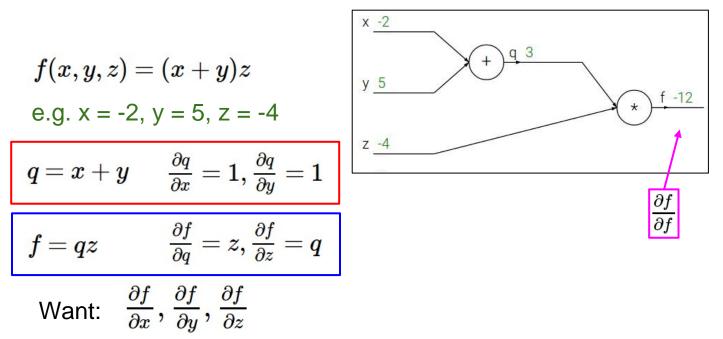


Want:
$$\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$$

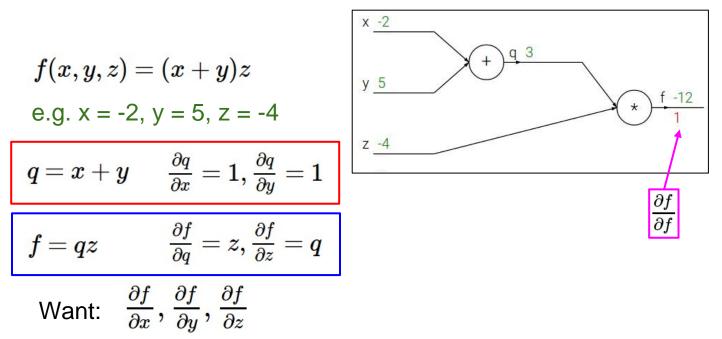




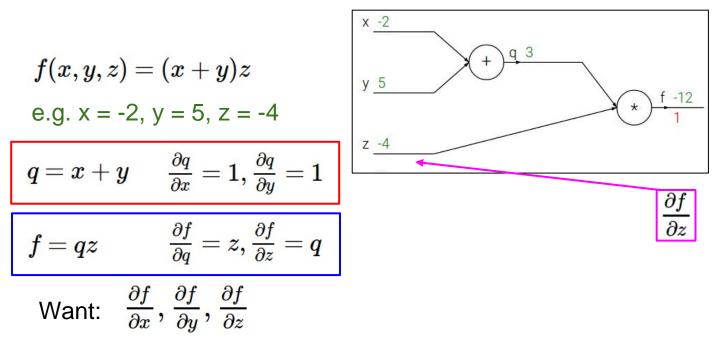




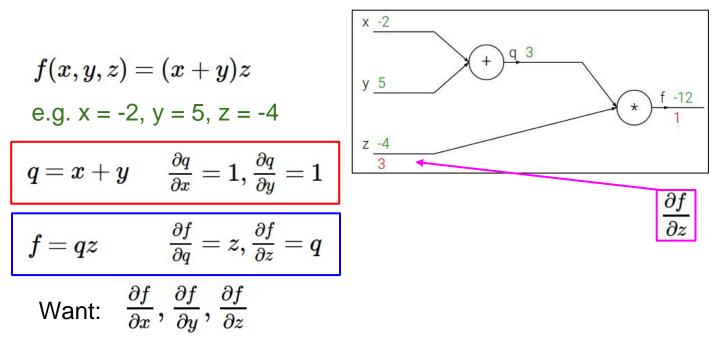




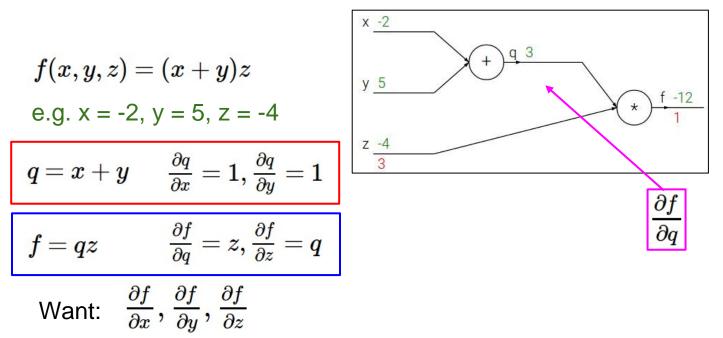




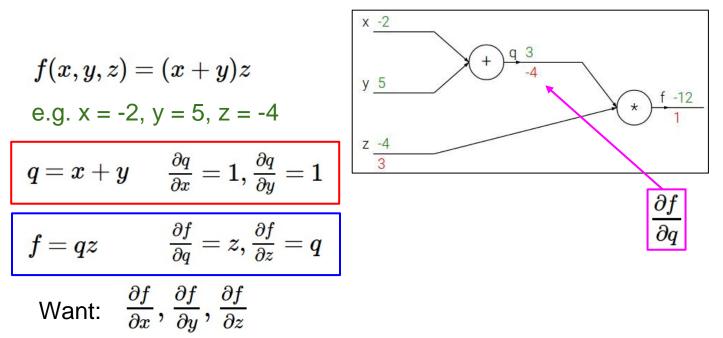




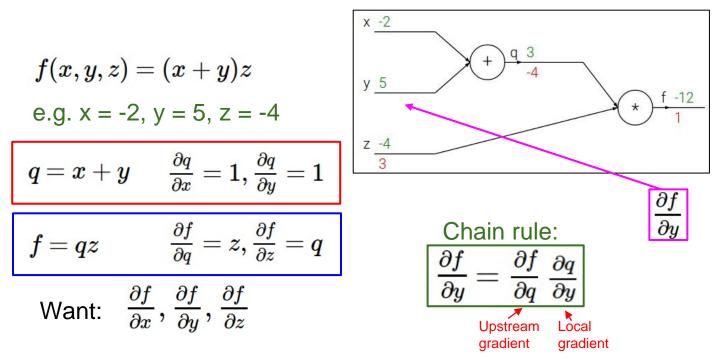






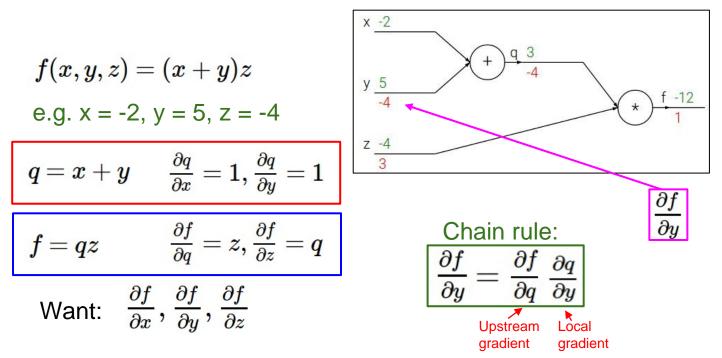






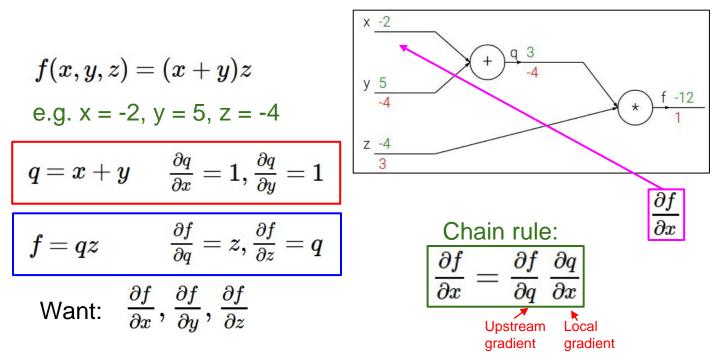


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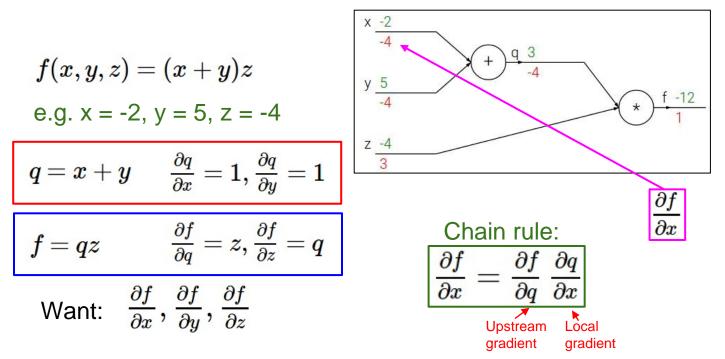






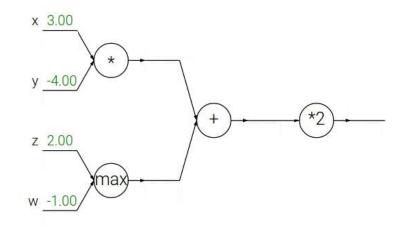


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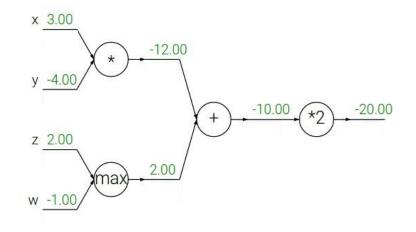




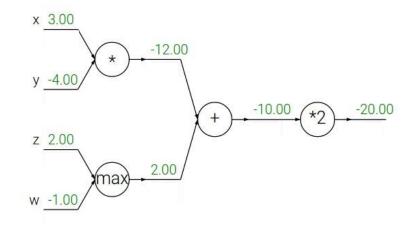






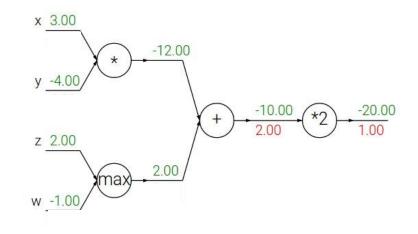






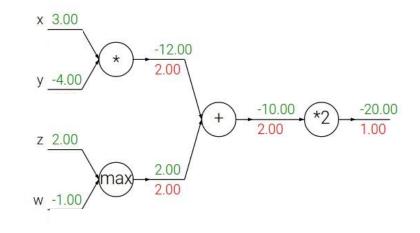


Q: What is an **add** gate?



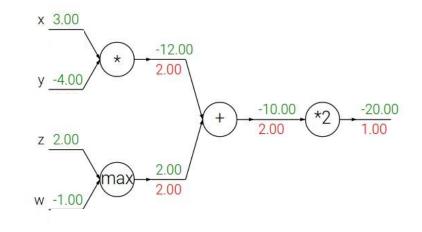


add gate: gradient distributor



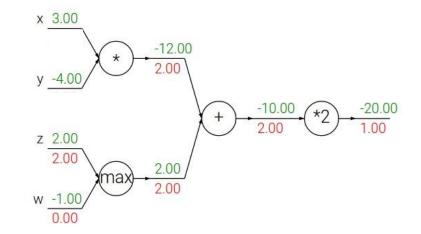


add gate: gradient distributor Q: What is a max gate?



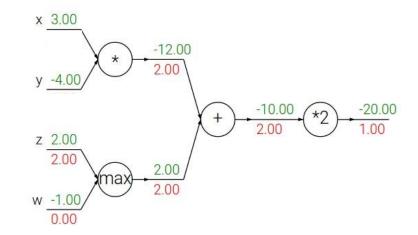


add gate: gradient distributormax gate: gradient router



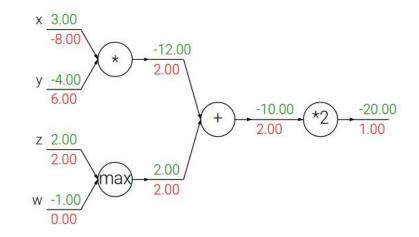


add gate: gradient distributormax gate: gradient routerQ: What is a mul gate?



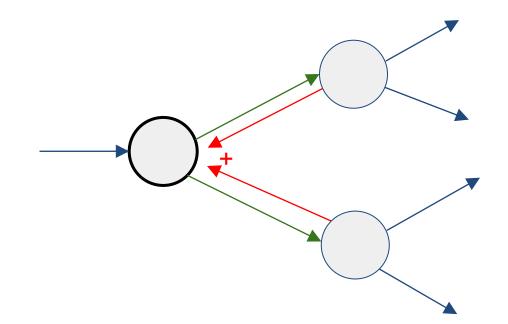


add gate: gradient distributormax gate: gradient routermul gate: gradient switcher



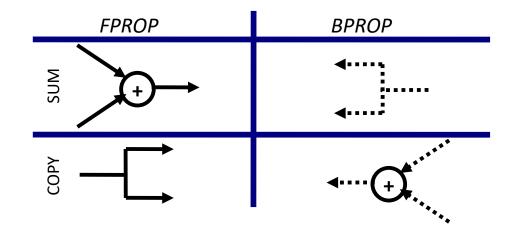


Gradients add at branches





Duality in Fprop and Bprop





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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



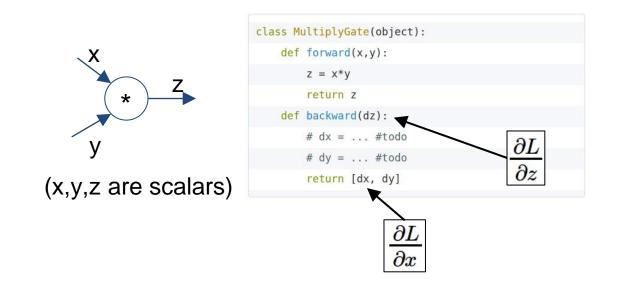
Graph (or Net) object (rough psuedo code)

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



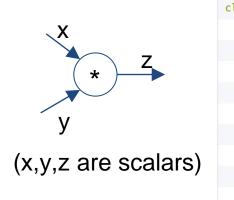


Modularized implementation: forward / backward API





Modularized implementation: forward / backward API



lass M	<pre>ultiplyGate(object):</pre>
def	forward(x,y):
	z = x*y
	<pre>self.x = x # must keep these around!</pre>
	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 GitHul	b Merge pull request #4630 from BiGene/load_hdf5_fix		Latest commit	e687a71 21	days ago
1. ¹⁰ 1					
absval_layer.cpp	dismantle layer headers			. 0	year ago
🖹 absval_layer.cu	dismantle layer headers			а	year ago
accuracy_layer.cpp	dismantle layer headers			a	year ago
argmax_layer.cpp	dismantle layer headers			8	year ago
base_conv_layer.cpp	enable dilated deconvolution			а	year ago
base_data_layer.cpp	Using default from proto for prefetch			3 mo	nths ago
base_data_layer.cu	Switched multi-GPU to NCCL			3 mo	nths ago
batch_norm_layer.cpp	Add missing spaces besides equal signs in batch_norm_lays	er.cpp		4 mo	nths ago
batch_norm_layer.cu	dismantle layer headers			а	year ago
batch_reindex_layer.cpp	dismantle layer headers.			а	year ago
batch_reindex_layer.cu	dismantle layer headers			а	year ago
bias_layer.cpp	Remove incorrect cast of gemm int arg to Dtype in BlasLaye	IF.		a	year ago
blas_layer.cu	Separation and generalization of ChannelwiseAffineLayer in	to BiasLayer		а	year ago
E bnll_layer.cpp	dismantle layer headers				year ago
) bnll_layer.cu	dismantie layer headers			a	year ago
concat_layer.cpp	dismantie layer headers			a	year ago
E concat_layer.cu	dismantie layer headers				year ago
Contrastive_loss_layer.cpp	dismantle layer headers			a	year ago
contrastive_loss_layer.cu	dismantle layer headers				year ago
conv_layer.cpp	add support for 2D dilated convolution			а	year ago
conv_layer.cu	dismantle layer headers			а	year ago
) crop_layer.cpp	remove redundant operations in Crop layer (#5138)			2 mo	nths ago
erop_layer.cu	remove redundant operations in Crop layer (#5138)			2 mo	nths ago
Cudnn_conv_layer.cpp	dismantie layer headers			a	year ago
cudnn.conv.layer.cu	Add cuDNN v5 support, drop cuDNN v3 support			11 mo	nths ago

E cudnn_lcn_layer.cpp	dismantle layer headers	a year ago
Cudnn_lcn_layer.cu	dismantle layer headers	a year ago
Cudnn_Irn_layer.cpp	dismantle layer headers	a year ago
Cudnn_Irn_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 v6 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 v6 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 ag
Cudnn_tanh_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months age
E cudnn_tanh_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months age
ata_layer.cpp	Switched multi-GPU to NCCL	3 months age
deconv_layer.cpp	enable dilated deconvolution	a year ag
deconv_layer.cu	dismantle layer headers	a year ag
🖹 dropout_layer.cpp	supporting N-D Blobs in Dropout layer Reshape	a year ag
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 ag
eltwise_layer.cu	dismantle layer headers	a year ago
elu_layer.cpp	ELU layer with basic tests	a year ag
⊫ elu_layer.cu	ELU layer with basic tests	a year ago
embed_layer.cpp	dismantle layer headers	a year ag
embed_layer.cu	dismantle layer headers	a year ago
euclidean_loss_layer.cpp	dismantle layer headers	a year ag
euclidean_loss_layer.cu	dismantle layer headers	a year ag
exp_layer.cpp	Solving issue with exp layer with base e	a year ago
exp_layer.cu	dismantle layer headers	a year ag

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