CS 4644-DL / 7643-A
DANFEI XU

Topics:

- Backpropagation
- Computation Graph and Automatic Differentiation

Administrative

- PS1 / HW1 is out. Due by Sep 19th 11:59pm (+48hr grace period)
- Use Piazza for Q&A
- PS1 / HW1 tutorial 1pm Sep 6st (Friday) 3:15 PM (hosted by David He and Tony Tu)
- The tutorial will be recorded.
- **Start early!**
- Project proposal prompt posting soon. Due Sep 24th (no grace period)

Recap: Multiclass SVM loss

Given an example (x_i, y_i) where x_i is the image and where y_i is the (integer) label,

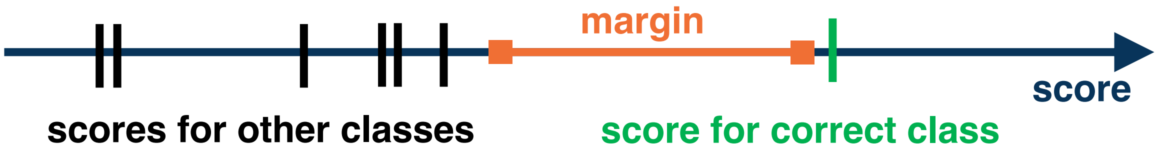
and using the shorthand for the scores vector: $s = f(x_i, W)$

the SVM loss has the form:

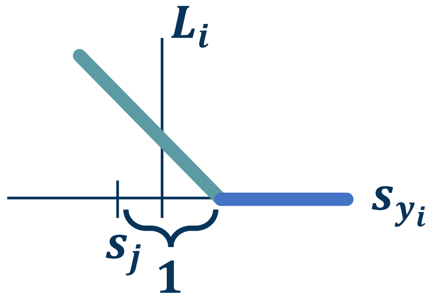
$$L_i = \sum_{j \neq y_i} \begin{cases} 0 & \text{if } s_{y_i} \geq s_j + 1 \\ s_j - s_{y_i} + 1 & \text{otherwise} \end{cases}$$

$$= \sum_{j \neq y_i} max(0, s_j - s_{y_i} + 1)$$

Loss = 0:



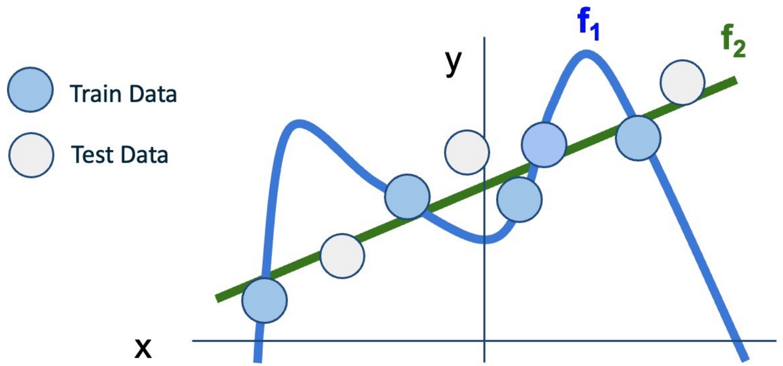
"Hinge Loss"



Recap: Regularization

Q: How do we pick between W and 2W?
A: Opt for simpler functions to avoid overfit

How? Regularization!



$$\underbrace{L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i)}_{} + \underbrace{\lambda R(W)}_{}$$

λ = regularization strength (hyperparameter)

Data loss: Model predictions should match training data

Regularization: Prevent the model from doing *too* well on training data

Recap: Softmax Classifier and Cross Entropy Loss

Want to interpret raw classifier scores as **probabilities**

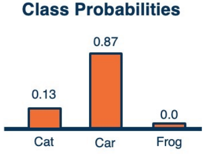
$$p_\theta(Y = y_i | X = x_i) = \frac{e^{s_{y_i}}}{\sum_j e^{s_j}}$$

Softmax Function

cat	3.2
car	5.1
frog	-1.7

Raw class scores

$\longrightarrow$



How do we optimize the classifier? We maximize the probability of $p_\theta(y_i|x_i)$

1. Maximum Likelihood Estimation (MLE):
Choose weights to maximize the likelihood of observed data. In this case, the loss function is the **Negative Log-Likelihood (NLL)**.

Finding a set of weights θ that maximizes the probability of correct prediction: $\underset{\theta}{\operatorname{argmax}} \prod p_\theta(y_i|x_i)$

This is equivalent to:

$$\underset{\theta}{\operatorname{argmax}} \sum \ln p_\theta(y_i|x_i)$$

$$L_i = -\ln p_\theta(y_i|x_i) = -\ln\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right)$$

2. Information theory view:
Derive NLL from the cross entropy measurement.
Also known as the cross-entropy loss

Cross Entropy: $H(p, q) = -\sum p(x) \ln q(x)$

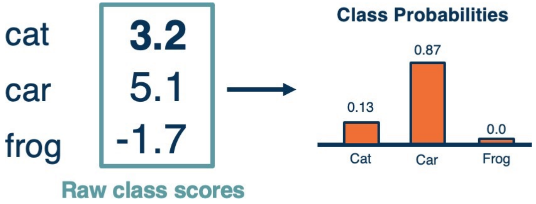
Cross Entropy Loss -> NLL

$$\boldsymbol{H_i(p, p_\theta) = -\sum_{y \in Y} p(y|x_i) \ln p_\theta(y|x_i)}$$

$$\boldsymbol{= -\ln p_\theta(y_i|x_i)}$$

$$\boldsymbol{L = \sum H_i(p, p_\theta) = -\sum \ln p_\theta(y_i|x_i) \equiv NLL}$$

Q: Why softmax?



Why this?

$$\boxed{p_\theta(Y = y_i | X = x_i) = \frac{e^{s_{y_i}}}{\sum_j e^{s_j}}}$$

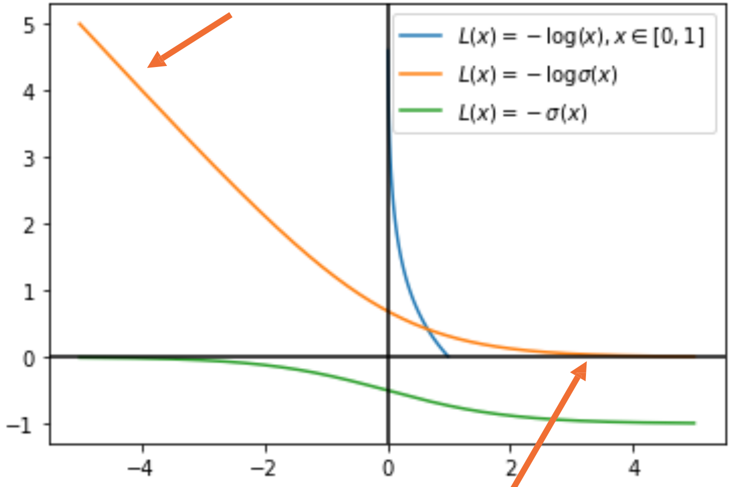
Use logistic function as example. Same as softmax but for binary classification

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

Consider the following three basis for NLL:

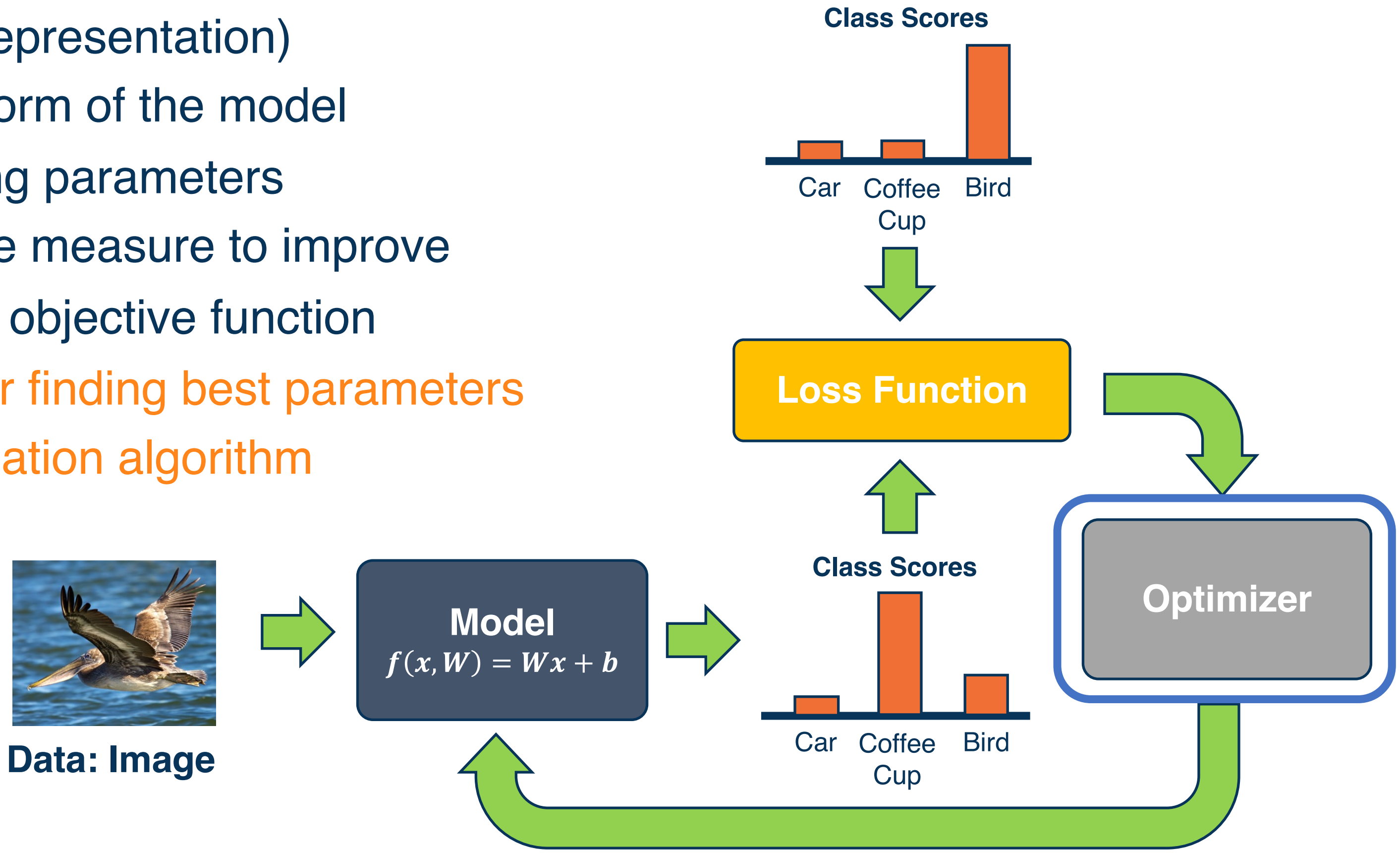
1. Squash and clip network value (x) to (0, 1]
2. (Negative) logistic function
3. NLL with logistic function

2. NLL w/ logistic: Strong guidance when classifier is wrong



Only saturate at convergence, e.g. $\sigma(3) \approx 0.95$

- Input (and representation)
- Functional form of the model
    - Including parameters
- Performance measure to improve
    - Loss or objective function
- Algorithm for finding best parameters
    - Optimization algorithm

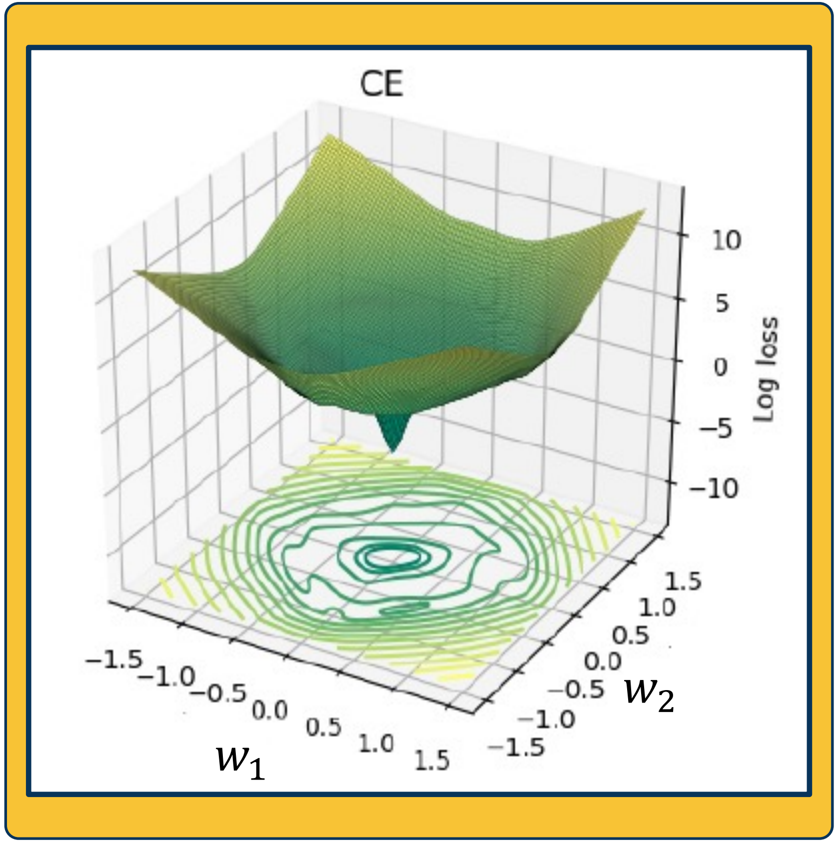


Gradient-based Optimization

As weights change, the gradients change as well

- This is often somewhat-smooth locally, so small changes in weights produce small changes in the loss

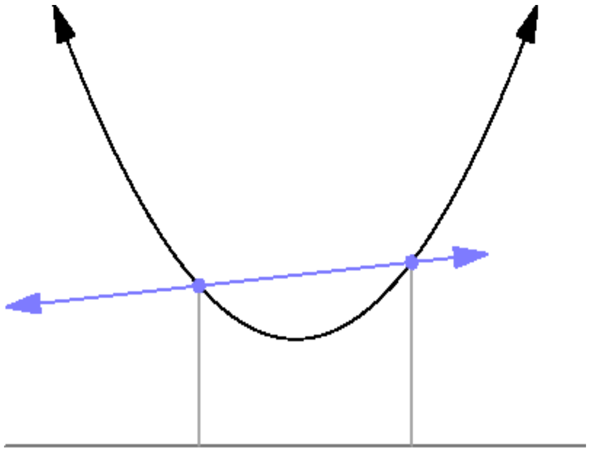
We can therefore think about **iterative algorithms** that take **current values of weights and modify them** a bit



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

$$\frac{\partial f}{\partial w} = \lim_{h \to 0} \frac{f(w+h) - f(w)}{h}$$

- **Gradient** is multi-dimensional derivatives
- Notation: $\frac{\partial f}{\partial w}$ is the gradient of f (e.g., a loss function) with respect to variable w (e.g., a weight vector).
- $\frac{\partial f}{\partial w}$ is of the **same shape** as w
- **Intuitively:** Measures how the function changes as the variable w changes by a small step size
- Steepest descent direction is the **negative gradient**
- **Gradient descent:** Minimize loss by changing parameters



Δx

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

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

$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{w}} = \lim_{\boldsymbol{h}\to 0} \frac{\boldsymbol{f}(\boldsymbol{w}+\boldsymbol{h}) - \boldsymbol{f}(\boldsymbol{w})}{\boldsymbol{h}}$$

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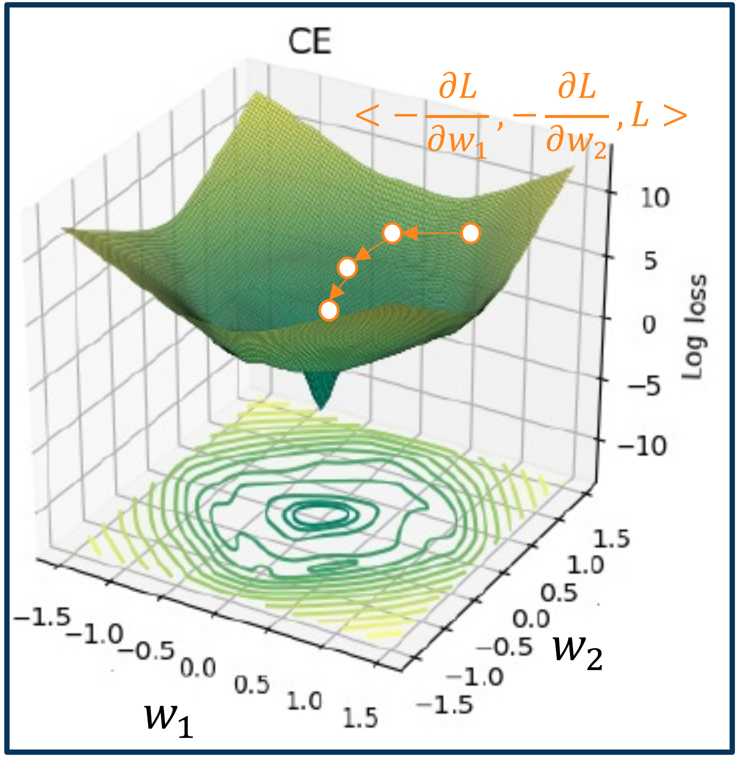


Calculate gradients: finite differences

current W:

[0.34,
-1.11,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25347

gradient dW:

[?,
?,
?,
?,
?,
?,
?,
?,
?,…]

Calculate gradients: finite differences

current W:	**W + h** (first dim)**:**	**gradient dW:**
[0.34,	[0.34 + **0.0001**,	[?,
-1.11,	-1.11,	?,
0.78,	0.78,	?,
0.12,	0.12,	?,
0.55,	0.55,	?,
2.81,	2.81,	?,
-3.1,	-3.1,	?,
-1.5,	-1.5,	?,
0.33,…]	0.33,…]	?,…]
loss 1.25347	**loss 1.25322**	

Calculate gradients: finite differences

current W:	**W + h** (first dim):	**gradient dW:**
[0.34,	[0.34 + **0.0001**,	[**-2.5**,
-1.11,	-1.11,	?,
0.78,	0.78,	?,
0.12,	0.12,	
0.55,	0.55,	
2.81,	2.81,	
-3.1,	-3.1,	
-1.5,	-1.5,	?,
0.33,…]	0.33,…]	?,…]
loss 1.25347	**loss 1.25322**	

(1.25322 - 1.25347)/0.0001
= -2.5

$$\boxed{\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}}$$

Calculate gradients: finite differences

current W:

[0.34,
-1.11,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25347

W + h (second dim)**:**

[0.34,
-1.11 + **0.0001**,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25353

gradient dW:

[-2.5,
?,
?,
?,
?,
?,
?,
?,
?,…]

Calculate gradients: finite differences

current W:

[0.34,
-1.11,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25347

W + h (second dim):

[0.34,
-1.11 + **0.0001**,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25353

gradient dW:

[-2.5,
0.6,
?,
?,
?,…]

(1.25353 - 1.25347)/0.0001
= 0.6

$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Calculate gradients: finite differences

current W:	**W + h** (third dim)**:**	**gradient dW:**
[0.34,	[0.34,	[-2.5,
-1.11,	-1.11,	0.6,
0.78,	0.78 + **0.0001**,	?,
0.12,	0.12,	?,
0.55,	0.55,	?,
2.81,	2.81,	?,
-3.1,	-3.1,	?,
-1.5,	-1.5,	?,
0.33,…]	0.33,…]	?,…]
loss 1.25347	**loss 1.25347**	

Calculate gradients: finite differences

current W:

[0.34,
-1.11,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25347

W + h (third dim)**:**

[0.34,
-1.11,
0.78 + **0.0001**,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25347

gradient dW:

[-2.5,
0.6,
0,
?,
?,…]

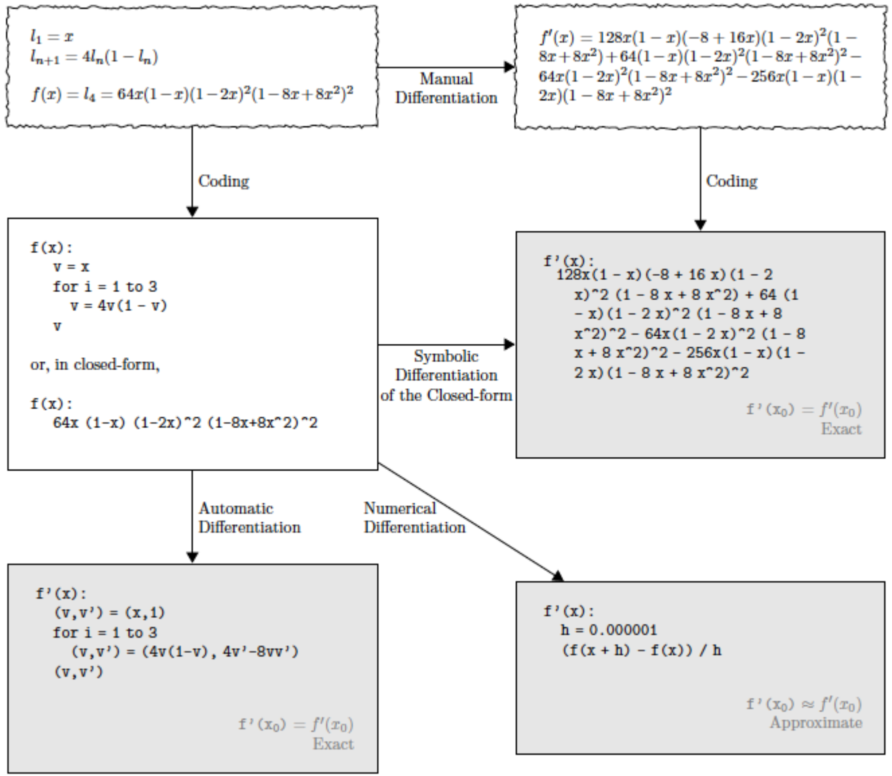
(1.25347 - 1.25347)/0.0001
= 0

$$\boxed{\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}}$$

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

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

More on **autodiff**:
https://www.cs.toronto.edu/~rgrosse/courses/csc421_2019/readings/L06%20Automatic%20Differentiation.pdf



Numerical vs Analytic Gradients

$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Numerical gradient: slow, approximate, easy to implement
Analytic gradient: fast, exact, error-prone (if implemented from scratch)

Almost all differentiable functions that you can think of have analytical gradients implemented in popular libraries, e.g., PyTorch, TensorFlow.

If you want to derive your own gradients, check your implementation with numerical gradient.
This is called a **gradient check.**

The gradient descent algorithm

- 1. Choose a model: $\boldsymbol{f(x, W)} = \mathrm{Wx}$
- 2. Choose loss function: $\boldsymbol{L_i = |y - Wx_i|^2}$
- 3. Calculate partial derivative for each parameter: $\boldsymbol{\frac{\partial L}{\partial w_i}}$
- 4. Update the parameters: $\boldsymbol{w_i = w_i - \frac{\partial L}{\partial w_i}}$
- 5. Add learning rate to prevent too big of a step: $\boldsymbol{w_i = w_i - \alpha \frac{\partial L}{\partial w_i}}$
- **Repeat 3-5**

How to compute gradients for deep neural networks?

$\sin(x)$ $\log(x)$ $\cos(x)$ x^3 $\exp(x)$

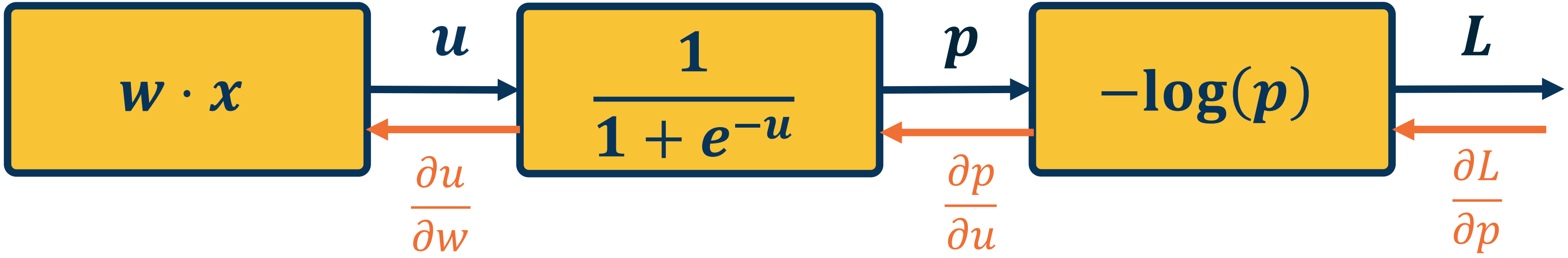
Compose into a complex function

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

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

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

Chain rule



$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial p}\frac{\partial p}{\partial u}\frac{\partial u}{\partial w}$$

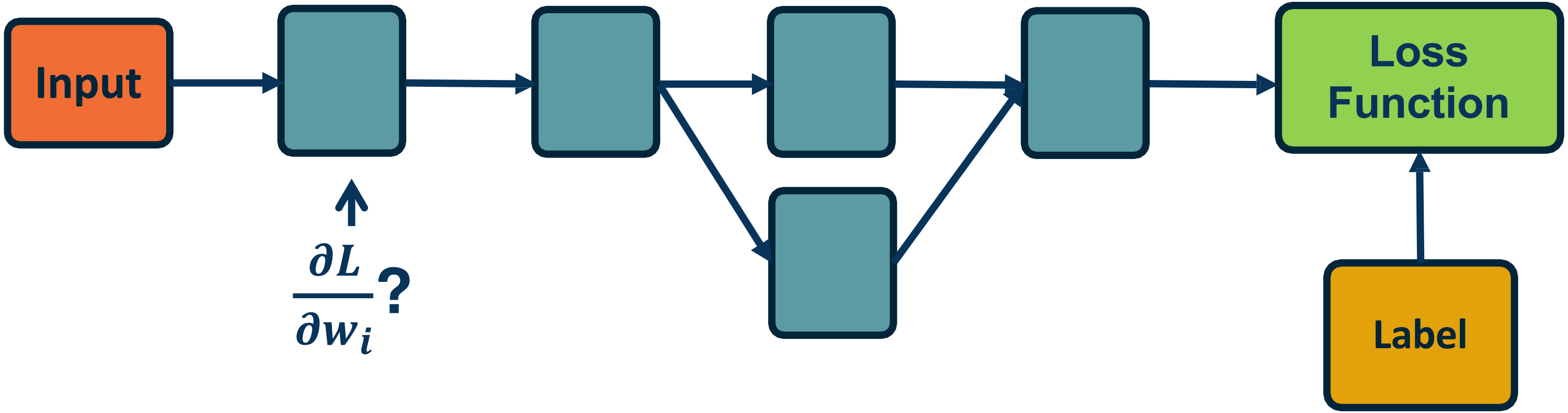
Backpropagation (roughly):

1. Calculate local gradients for each node (e.g., $\frac{\partial u}{\partial w}$)
2. Trace the computation graph (backward) to calculate the global gradients for each node w.r.t. to the loss function.

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!



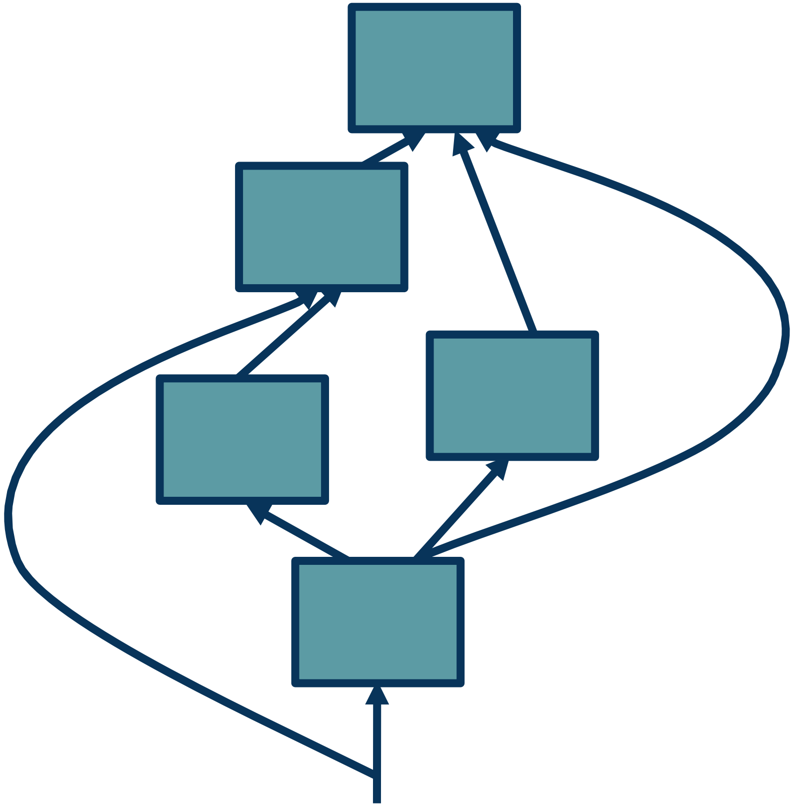
Computational Graph

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

The **backpropagation algorithm** will then process this graph, **one module at a time**



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

Backpropagation: a simple example

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

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

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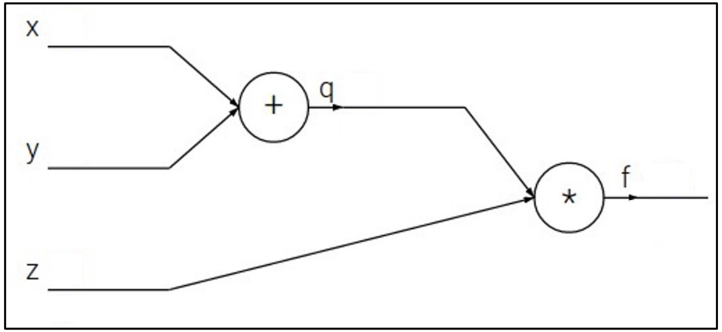

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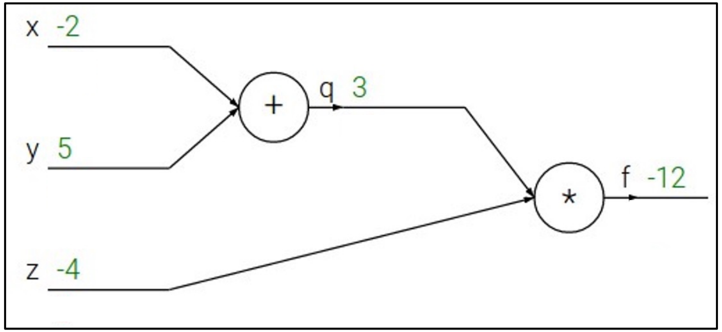
$$f(x, y, z) = (x + y)z$$

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



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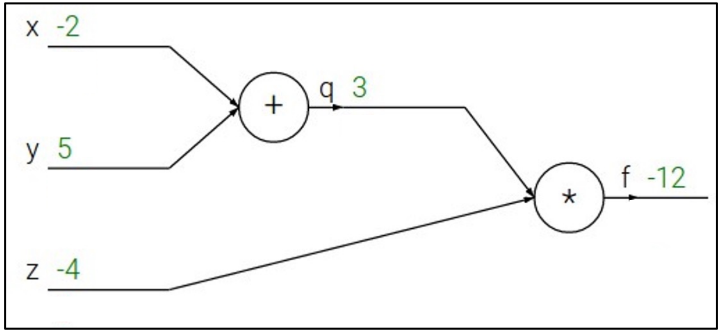

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

Backpropagation: a simple example

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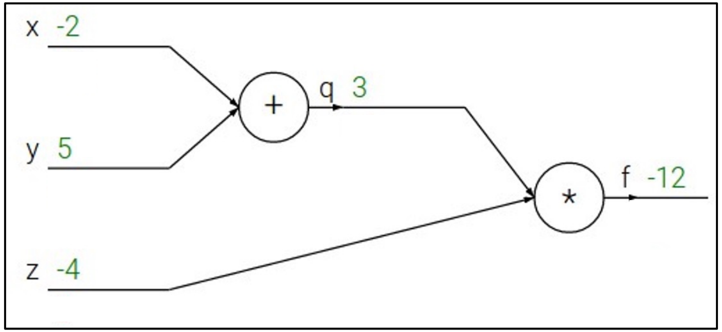
$$\boxed{q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1}$$



1. Calculate local gradients

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

Backpropagation: a simple example

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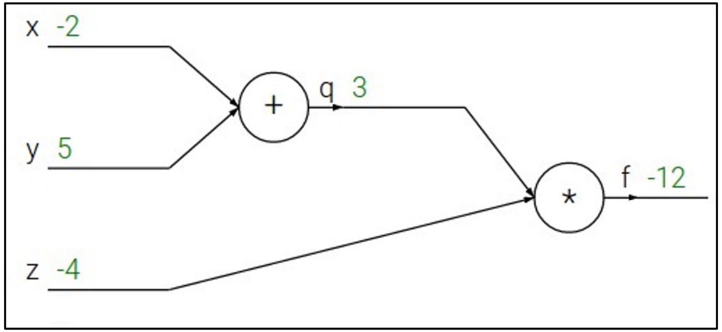
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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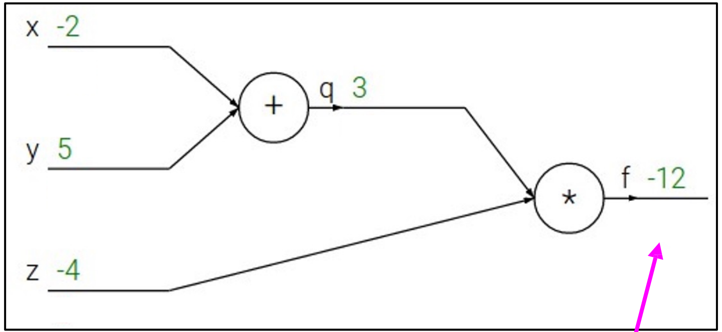

$\frac{\partial f}{\partial f}$

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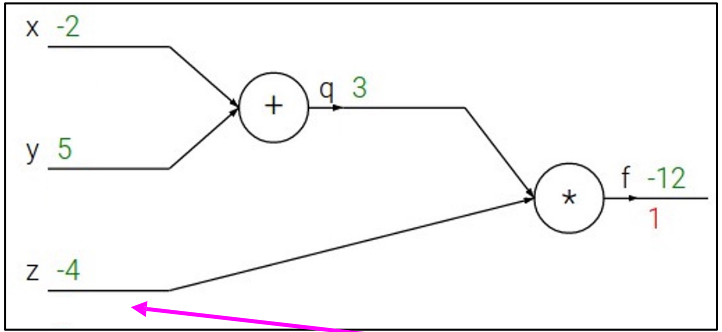

$\frac{\partial f}{\partial z}$

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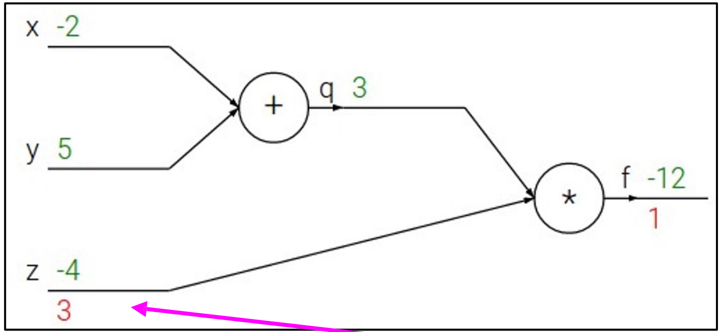

$$\frac{\partial f}{\partial z}$$

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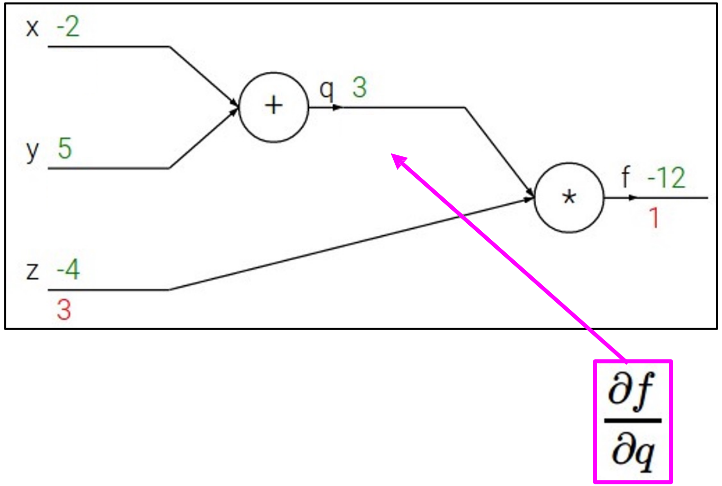

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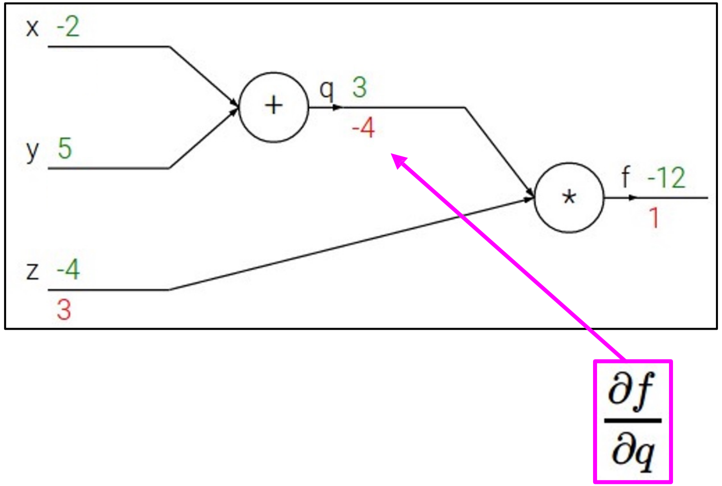

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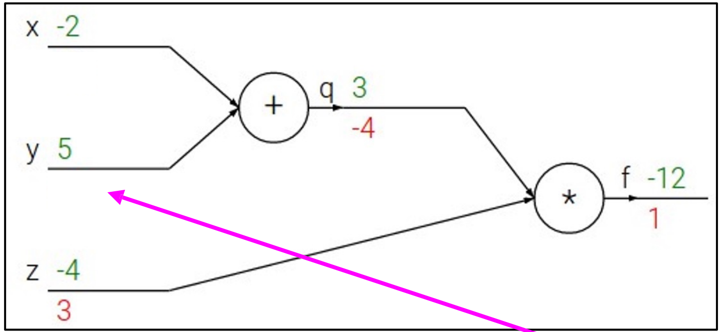
$$\boxed{f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q}$$

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

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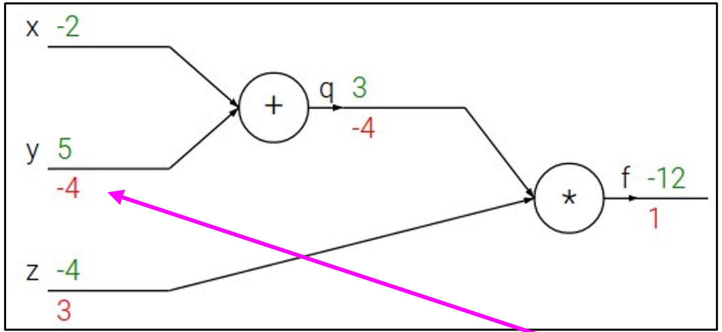
$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



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

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

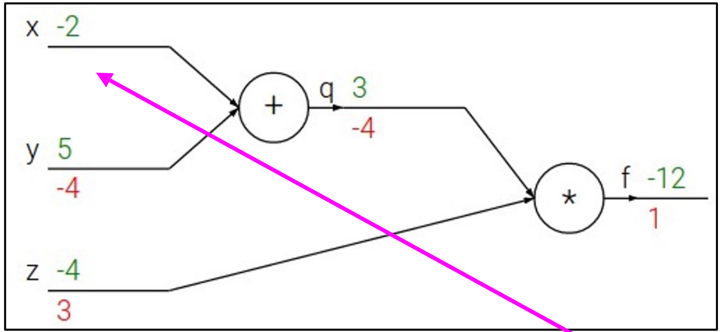
$$f(x, y, z) = (x + y)z$$

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

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

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

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



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

Chain rule:

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

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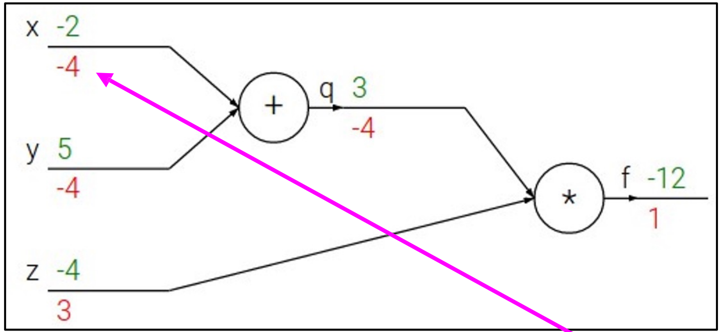

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

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

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

Chain rule:

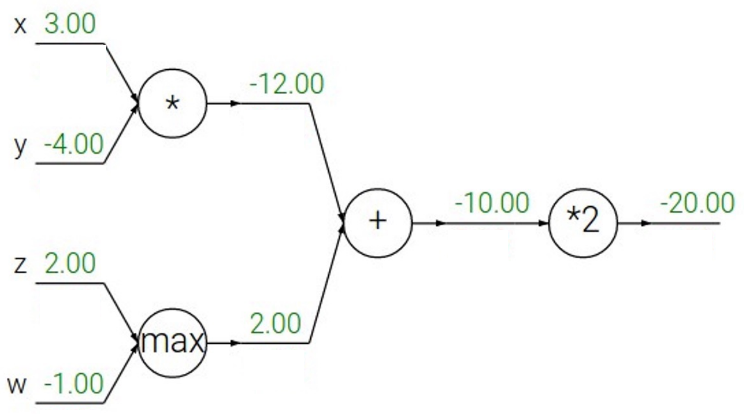
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

Upstream gradient

Local gradient

Patterns in backward flow

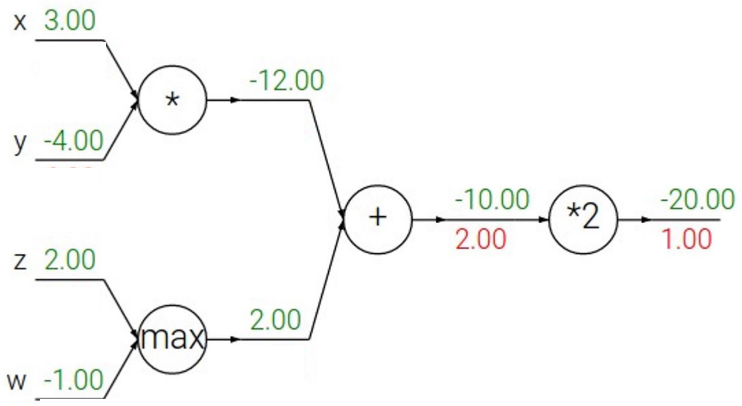
How does a local gradient modify the upstream gradient? $f = 2(xy + \max(z, w))$



Patterns in backward flow

How does a local gradient modify the upstream gradient? $f = 2(xy + \max(z, w))$

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

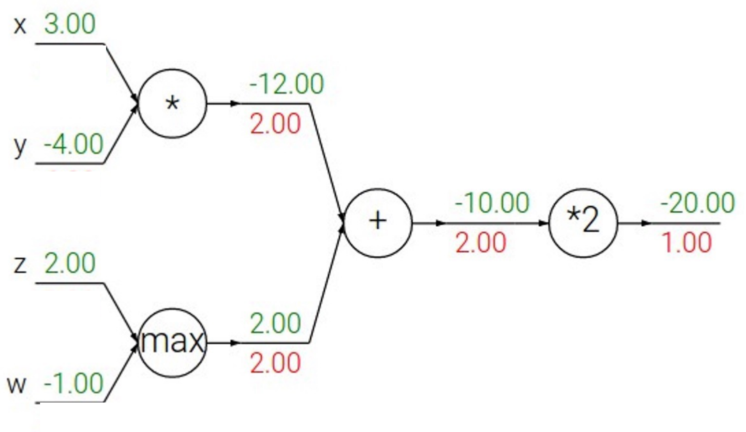


Patterns in backward flow

How does a local gradient modify the upstream gradient? $f = 2(xy + \max(z, w))$

add gate: gradient replicator

$$f = a + b$$
$$\frac{\partial f}{\partial a} = \frac{\partial f}{\partial b} = 1$$

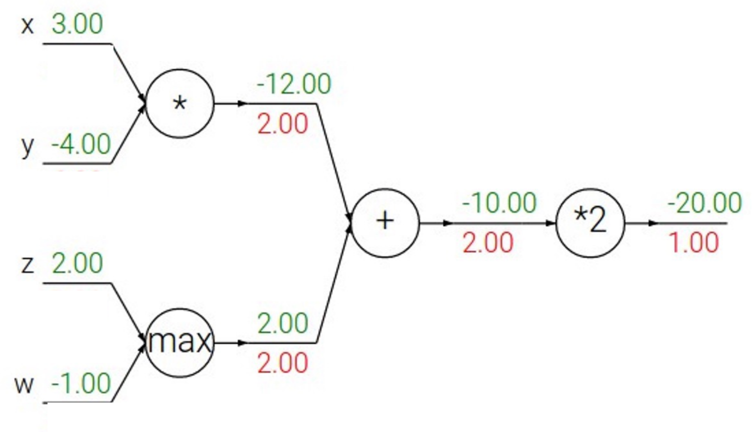


Patterns in backward flow

How does a local gradient modify the upstream gradient? $f = 2(xy + \max(z, w))$

add gate: gradient replicator

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



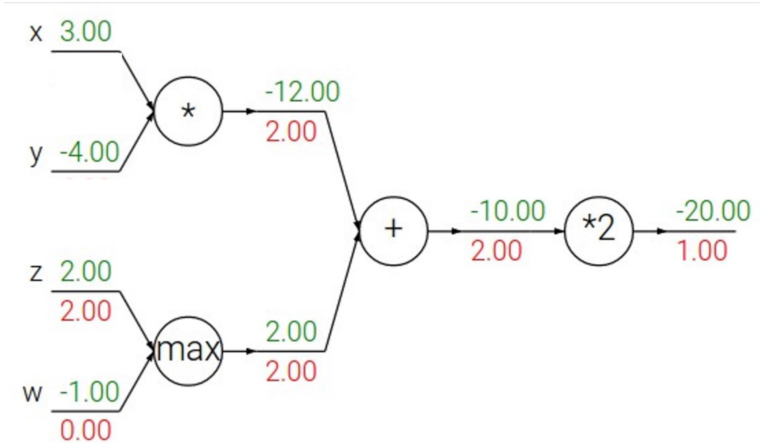
Patterns in backward flow

How does a local gradient modify the upstream gradient? $f = 2(xy + \max(z, w))$

add gate: gradient replicator

max gate: gradient router

only the path selected by the max operator gets the upstream gradient



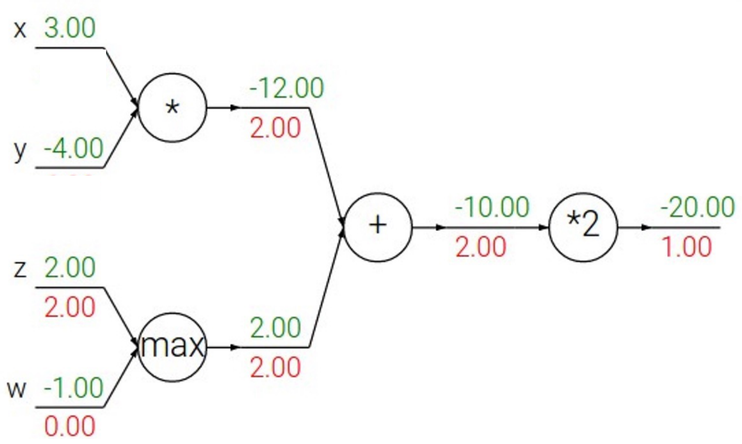
Patterns in backward flow

How does a local gradient modify the upstream gradient? $f = 2(xy + \max(z, w))$

add gate: gradient replicator

max gate: gradient router

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



Patterns in backward flow

How does a local gradient modify the upstream gradient? $f = 2(xy + \max(z, w))$

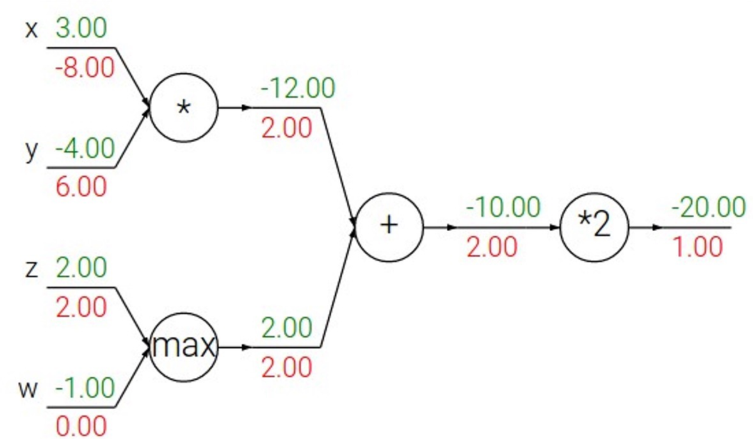
add gate: gradient replicator

max gate: gradient router

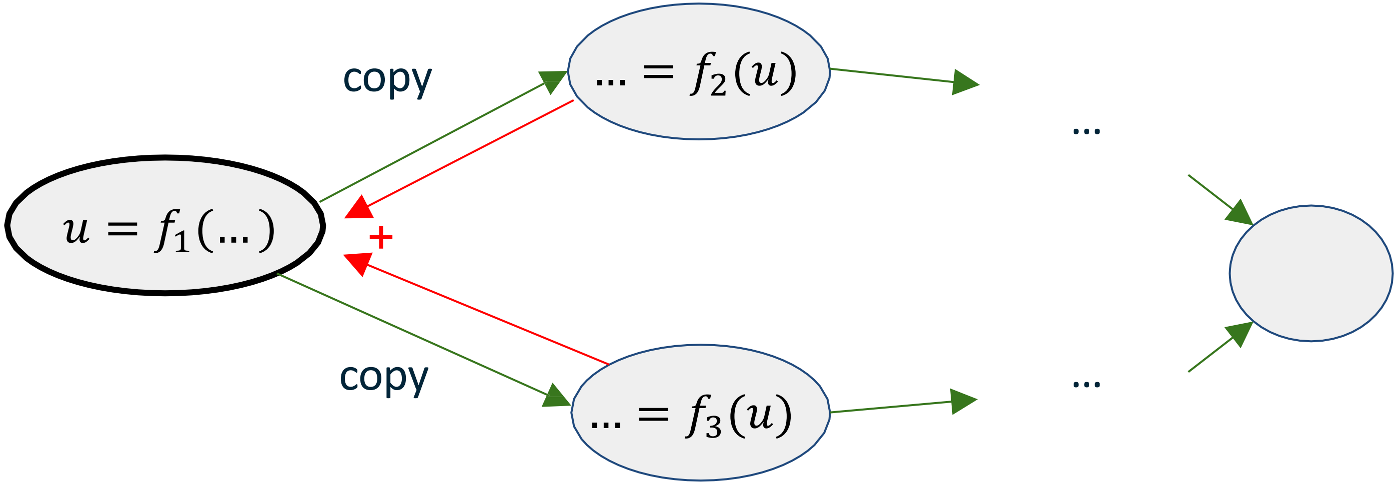
mul gate: gradient switcher

$$f = a \cdot b$$

$$\frac{\partial f}{\partial a} = b \quad \frac{\partial f}{\partial b} = a$$

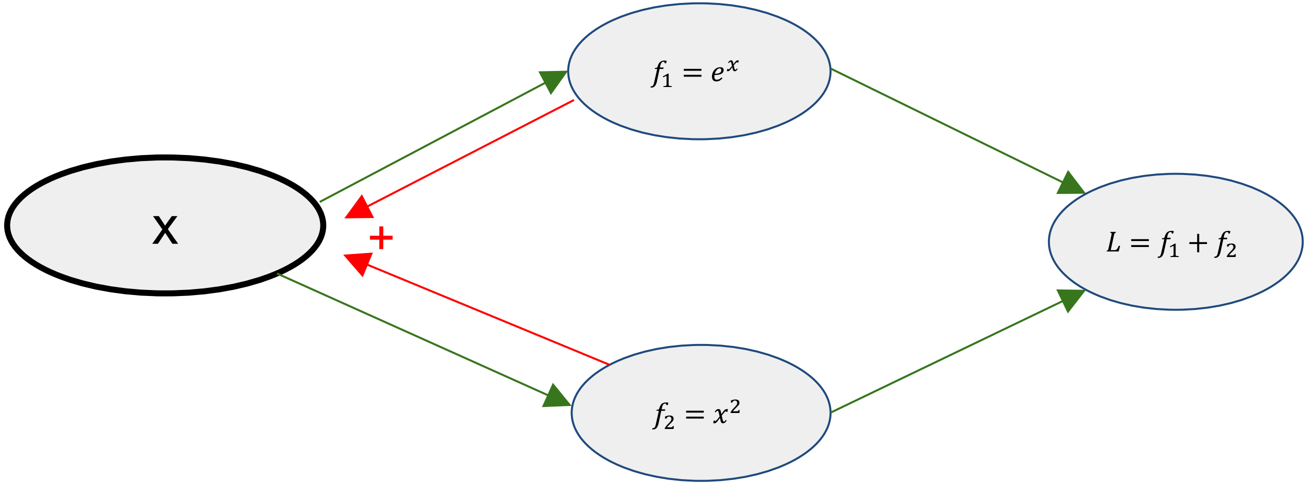


Upstream gradients add at fork branches



… as long as the branches join at some point in the graph

Upstream gradients add at fork branches



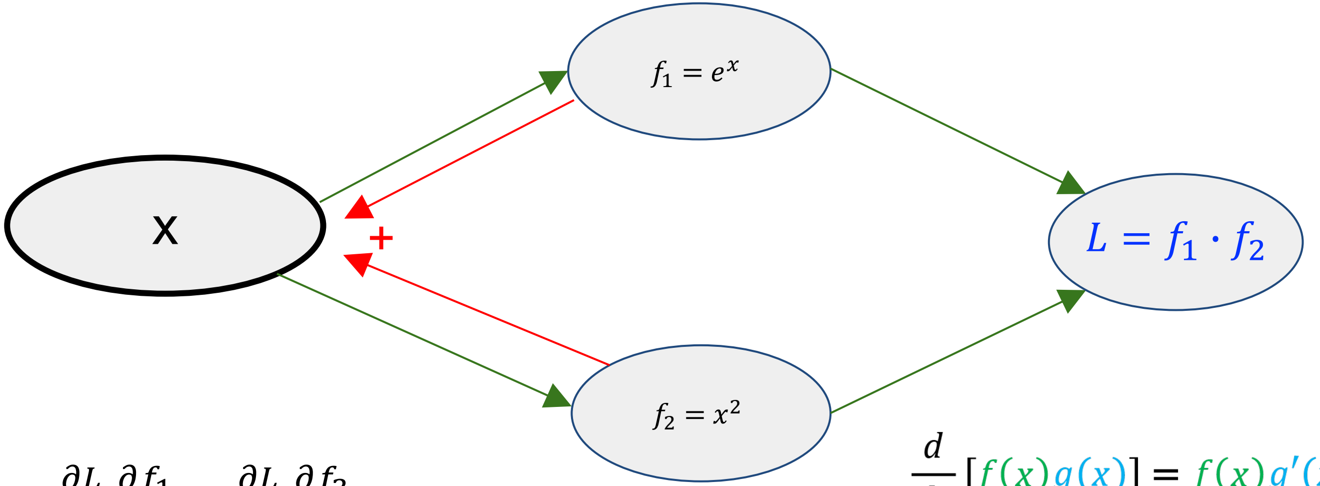
Claim: $\frac{\partial L}{\partial x} = \frac{\partial L}{\partial f_1}\frac{\partial f_1}{\partial x} + \frac{\partial L}{\partial f_2}\frac{\partial f_2}{\partial x}$

$= 1 \cdot e^x + 1 \cdot 2x = e^x + 2x$

Derivation: $L = e^x + x^2$

$$\frac{\partial L}{\partial x} = e^x + 2x$$

Upstream gradients add at fork branches



Claim: $\frac{\partial L}{\partial x} = \frac{\partial L}{\partial f_1}\frac{\partial f_1}{\partial x} + \frac{\partial L}{\partial f_2}\frac{\partial f_2}{\partial x}$

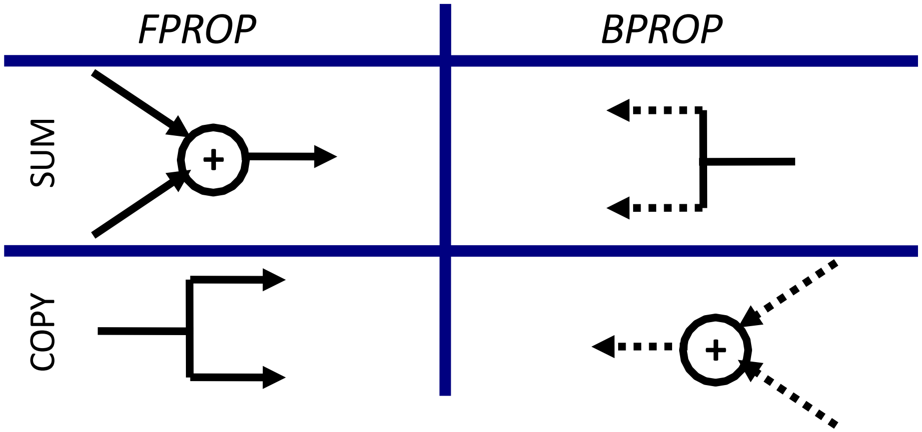
$= x^2 \cdot e^x + e^x \cdot 2x$

$$\frac{d}{dx}[f(x)g(x)] = f(x)g'(x) + f'(x)g(x)$$

Derivation: $L = e^x \cdot x^2$

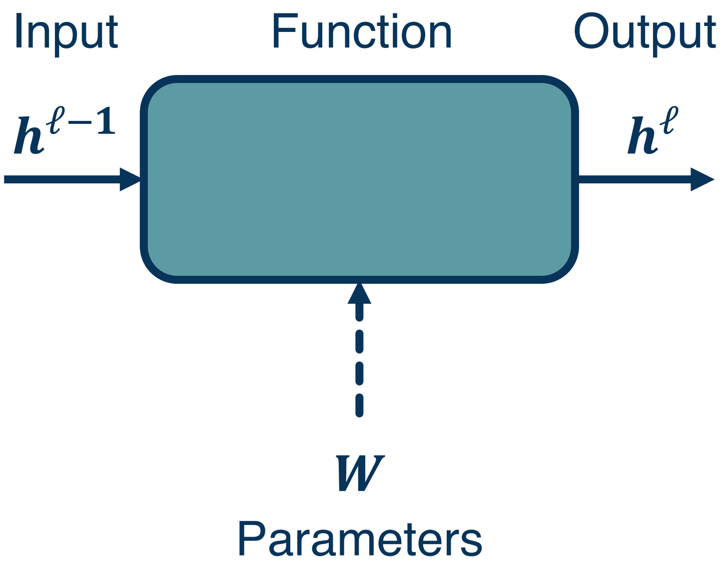
$$\frac{\partial L}{\partial x} = e^x \cdot 2x + e^x \cdot x^2$$

Duality in F(orward)prop and B(ack)prop



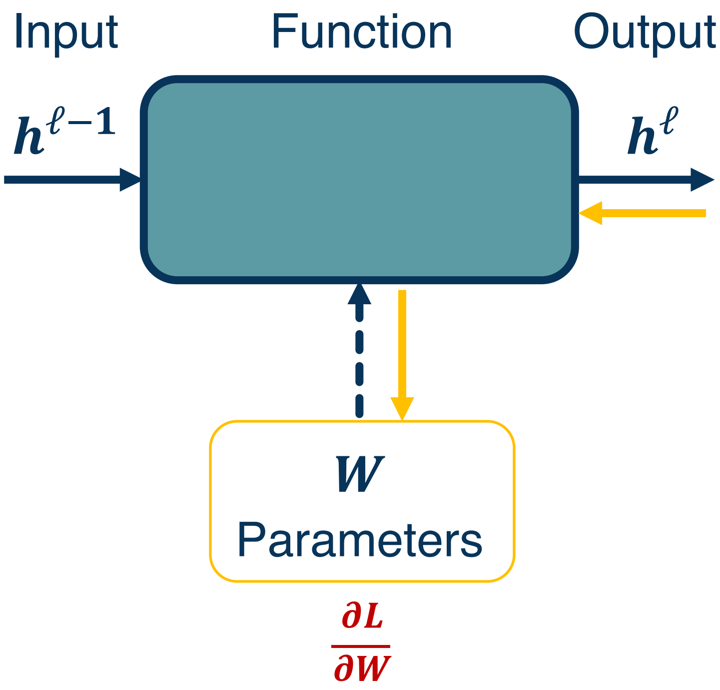
Given this computation graph, the training algorithm will:

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



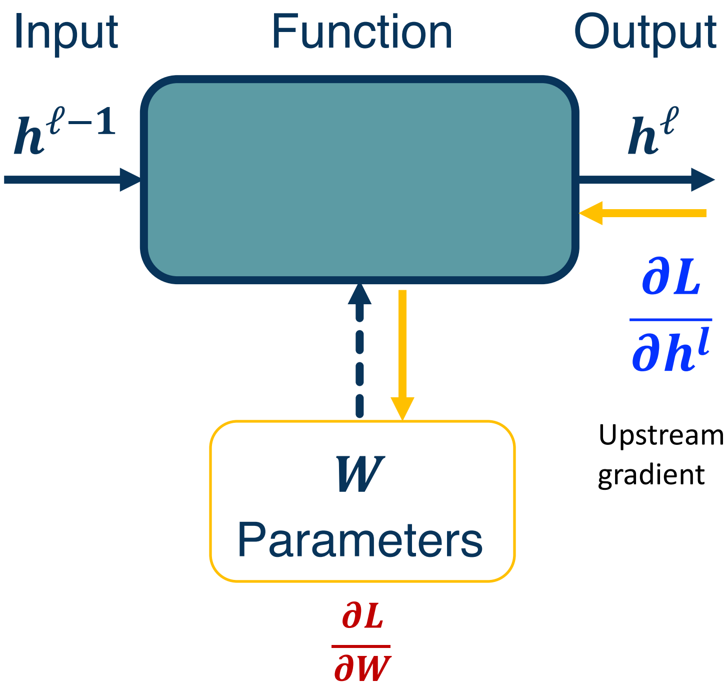
Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

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



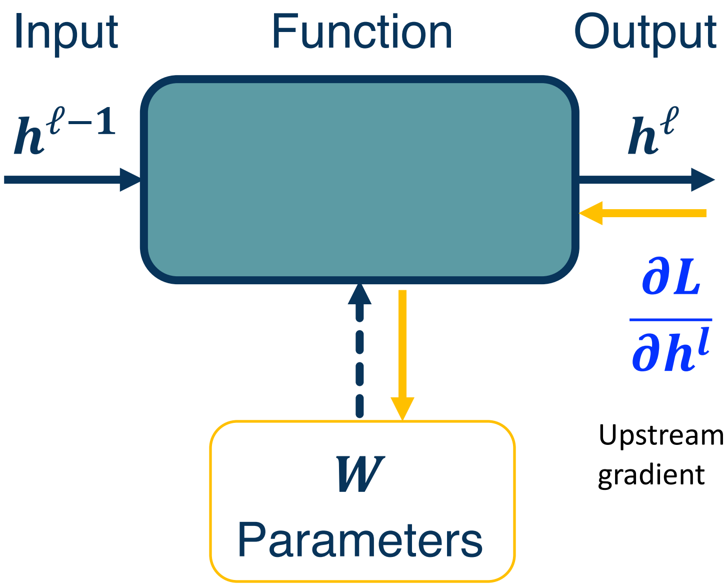
In the **backward pass**, we seek to calculate the gradients of the loss with respect to the module's parameters

- Assume that we have the gradient of the loss with respect to the **module's outputs** (given to us by upstream module)



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

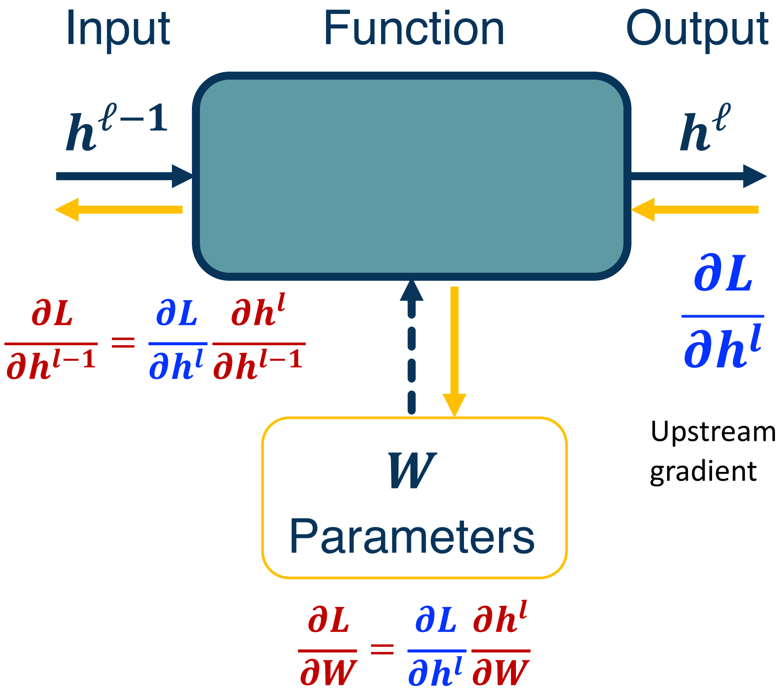
- Assume that we have the gradient of the loss with respect to the **module's outputs** (given to us by upstream module)
- We can calculate the gradient of the loss with respect to the module's weights



$$\frac{\partial L}{\partial W} = \frac{\partial L}{\partial h^l}\frac{\partial h^l}{\partial W}$$

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 can calculate the gradient of the loss with respect to the module's weights
- 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



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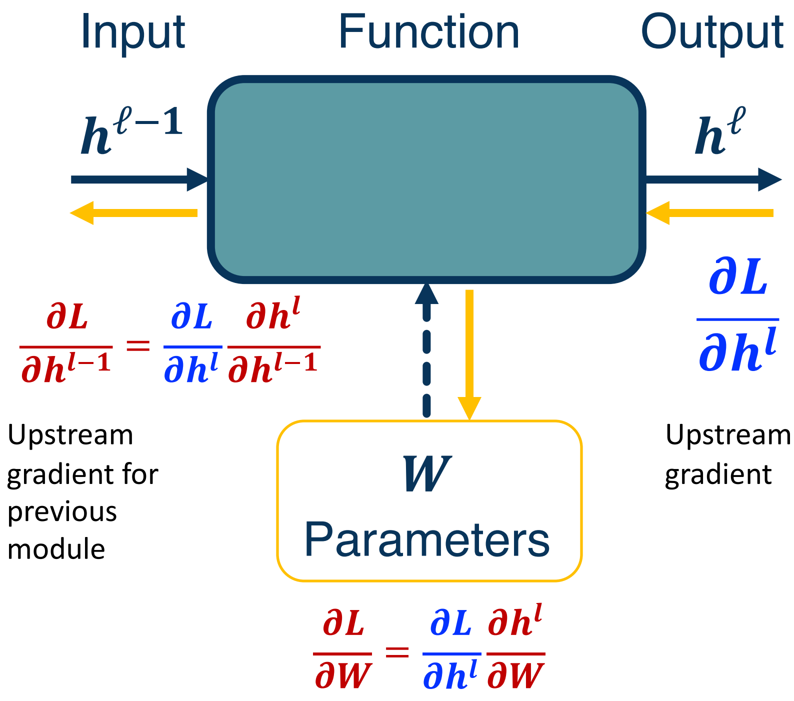
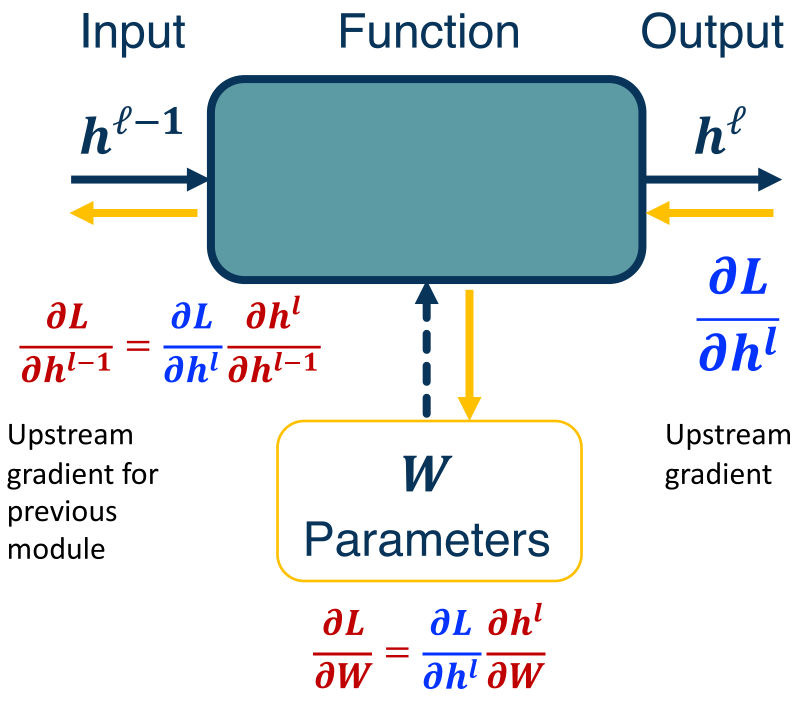
  - Becomes the **upstream gradient** for the previous module



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 can calculate the gradient of the loss with respect to the module's weights
- 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
  - Becomes the **upstream gradient** for the previous module
- **Gradient descent**: update weight with gradient with respect to loss



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

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

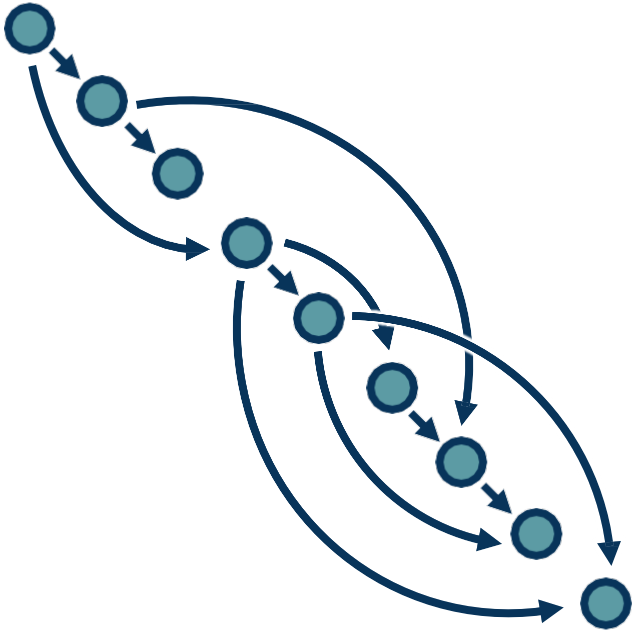
But the idea can be applied to **any directed acyclic graph (DAG)**

- Graph represents an **ordering constraining** which paths must be calculated first

Given an ordering, we can then iterate from the last module backwards, **applying the chain rule**

- We will store, for each node, its **gradient outputs for efficient computation**
- We will do this **automatically** by tracing the entire graph, aggregate and assign gradients at each function / parameters, from output to input.

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



A General Framework

Computation = Graph

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

Auto-Diff

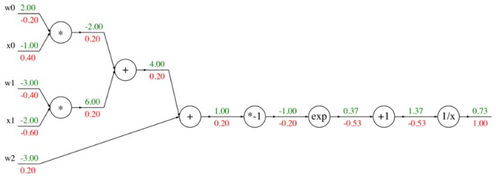
- A family of algorithms for implementing chain-rule on computation graphs

Deep Learning Framework = Differentiable Programming Engine

- 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)

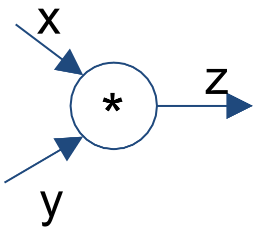
Modularized implementation: forward / backward API



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



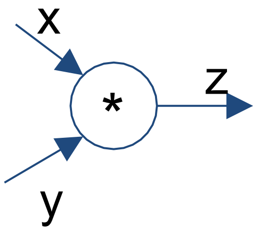
(x,y,z are scalars)

```
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]
```

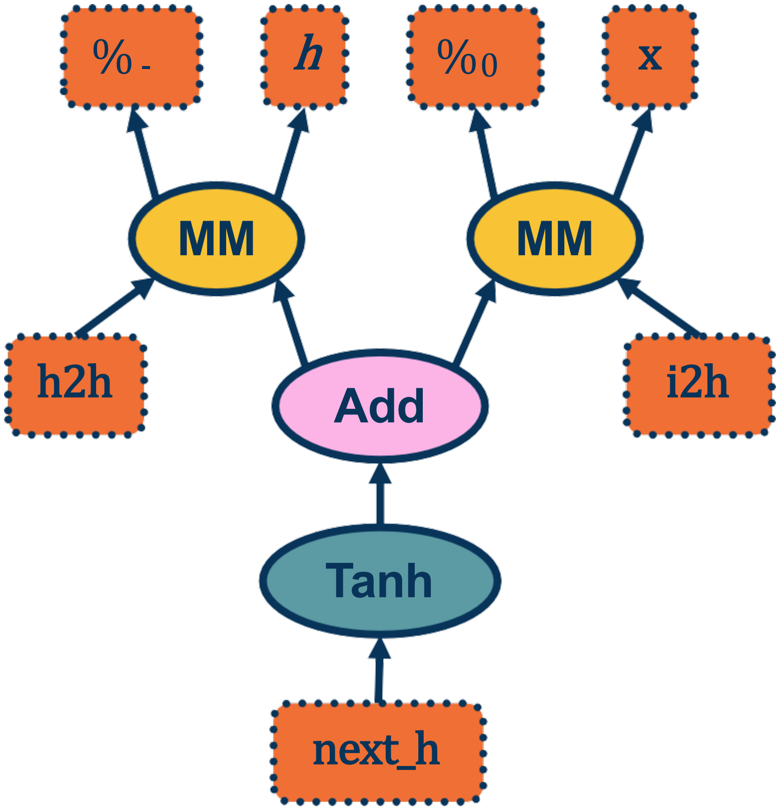
Writing code == building graph

```python
from torch.autograd import Variable

x = Variable(torch.randn(1, 20))
prev_h = Variable(torch.randn(1, 20))
W_h = Variable(torch.randn(20, 20))
W_x = Variable(torch.randn(20, 20))

i2h = torch.mm(W_x, x.t())
h2h = torch.mm(W_h, prev_h.t())
next_h = i2h + h2h
next_h = next_h.tanh()

next_h.backward(torch.ones(1, 20))
```



From pytorch.org

Neural Turing Machine

input image

loss

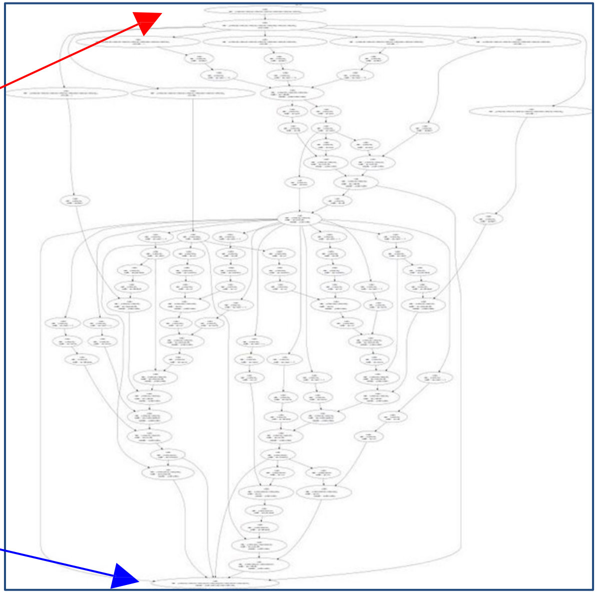
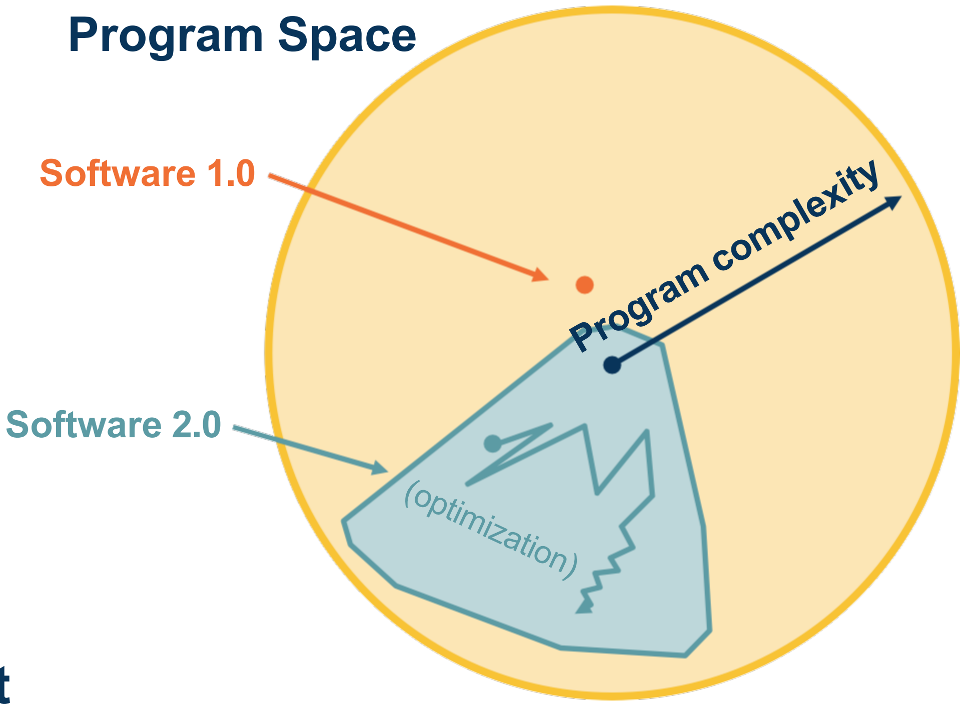


Figure reproduced with permission from a Twitter post by Andrej Karpathy.

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



Adapted from figure by Andrej Karpathy

- Autodiff from scratch: [micrograd repo](), [video tutorial]()

Next time:

- More on backprop but for (shallow) neural nets!
- Jacobians
- Activation functions