CS 4644-DL / 7643-A
DANFEI XU

Topics:

- Backpropagation
- Computation Graph and Automatic Differentiation

Administrative

- PS1 / HW1 is out. Due by Sep 15^{th} 11:59pm (+48hr late days)
- Use Piazza for Q&A
- **Start early!**
- How to pick a project lecture (Sep 10)
- Project helping session (Sep 29)
- Project proposal due Oct 1 (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,

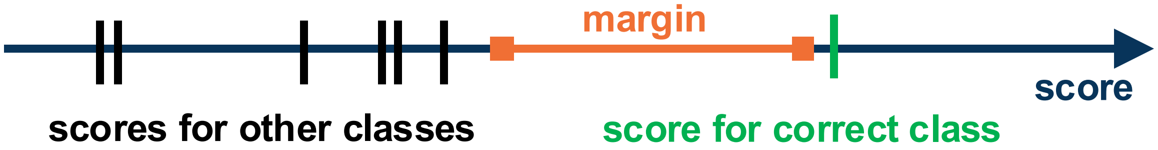
and using the shorthand for the scores vector: $s = f(x_i, W)$

the SVM loss has the form:

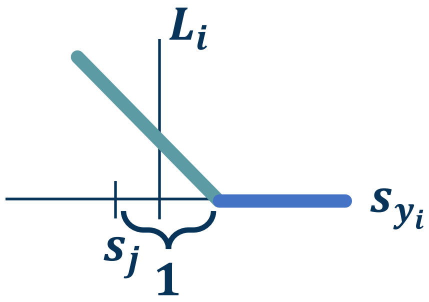
$$L_i = \sum_{j \neq y_i} \begin{cases} \boxed{0 \quad \text{if } s_{y_i} \geq s_j + 1} \\ \boxed{s_j - s_{y_i} + 1 \quad \text{otherwise}} \end{cases}$$

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

Loss = 0:



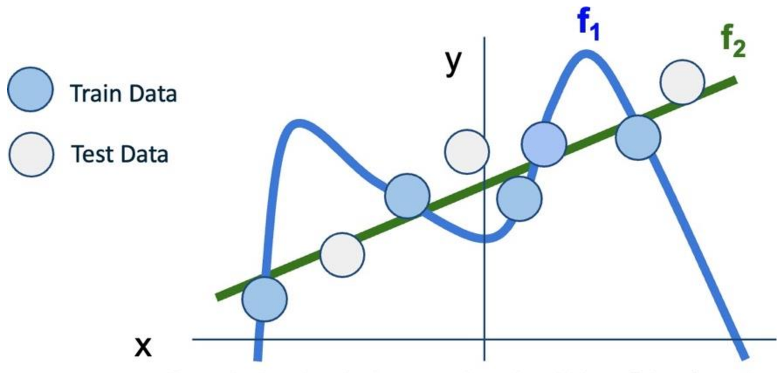
"Hinge Loss"



Recap: Regularization

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

How? Regularization!



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

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**

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

Softmax Function

	Raw class scores
cat	3.2
car	5.1
frog	-1.7

→

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

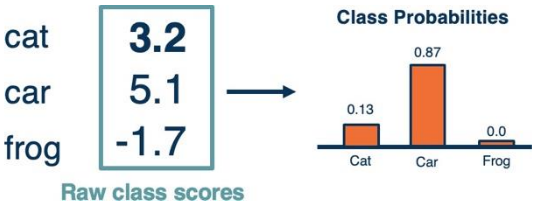
Cross Entropy: $H(p,q) = -\sum p(x) \ln q(x)$

Cross Entropy Loss -> NLL

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

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

Q: Why softmax?



Why this?

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

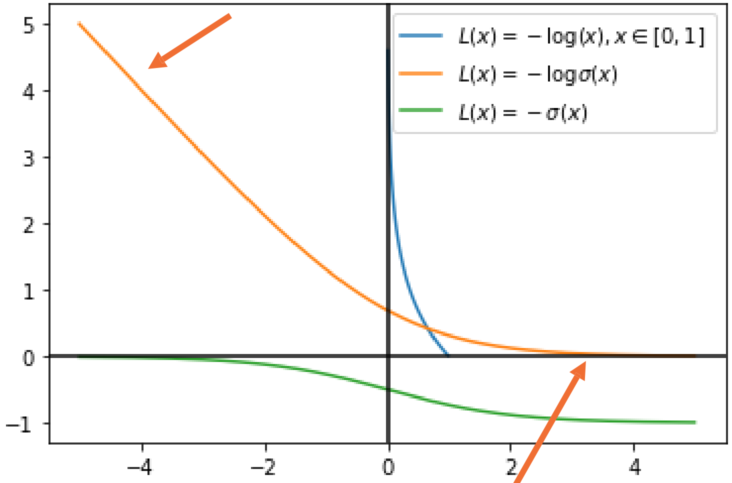
Use logistic function as example. Same as softmax but for binary classification

$$: (;) = \frac{<\%}{1 + <\%}$$

Consider the following three basis for NLL:

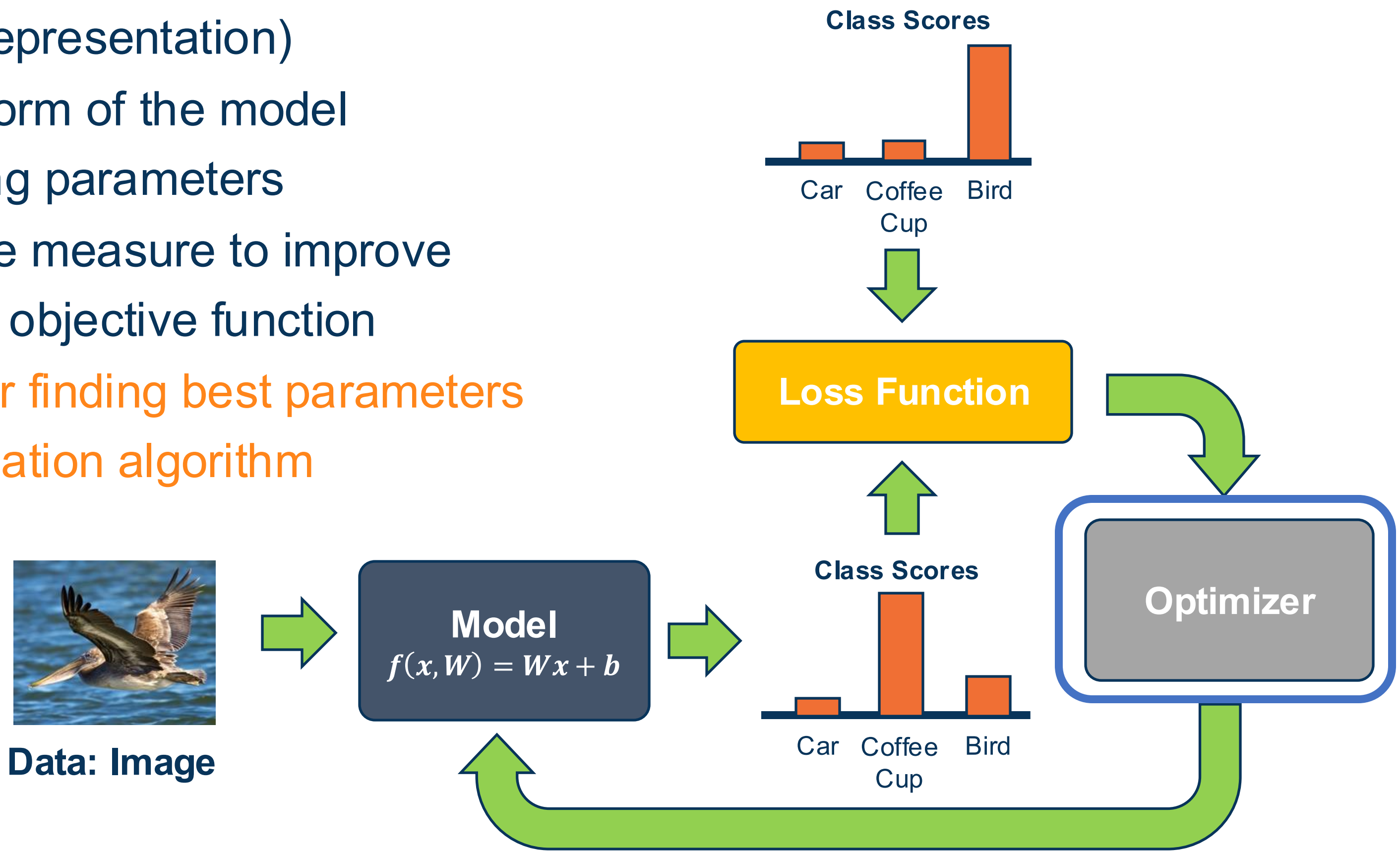
1. Squash and clip network value (x) to (0, 1]
2. (Negative) logistic function
3. NLL with logistic function

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

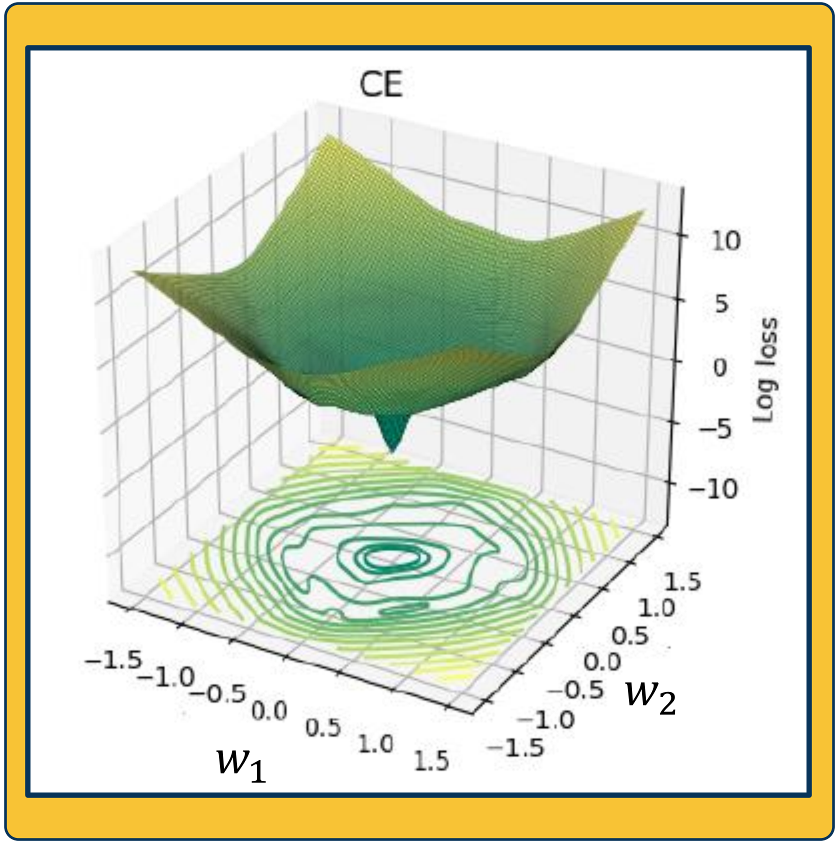


Gradient-based Optimization

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

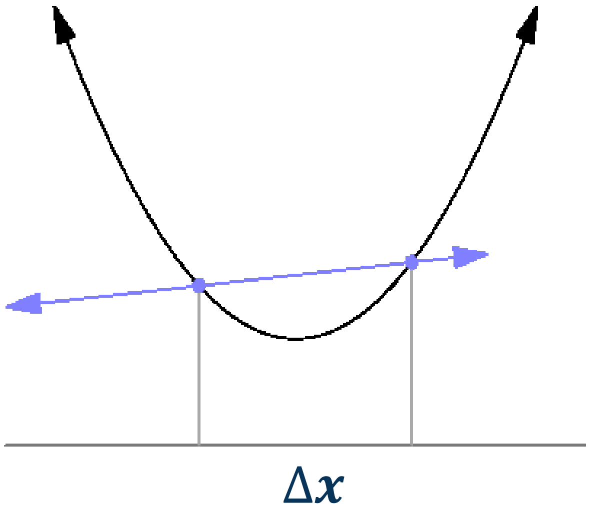


Image and equation from: https://en.wikipedia.org/wiki/Derivative#/media/File:Tangent_animation.gif

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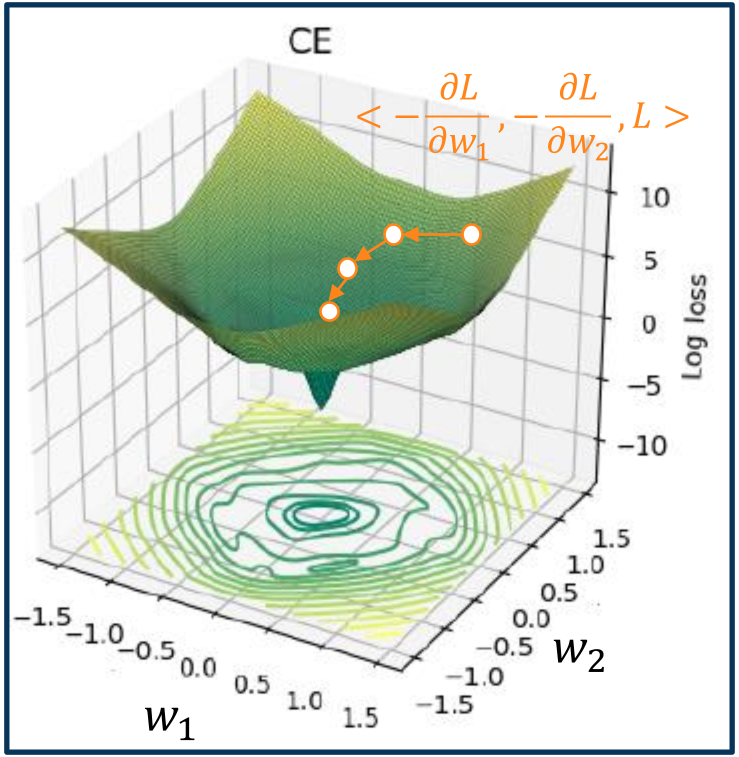


Calculate gradients: finite differences

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**	

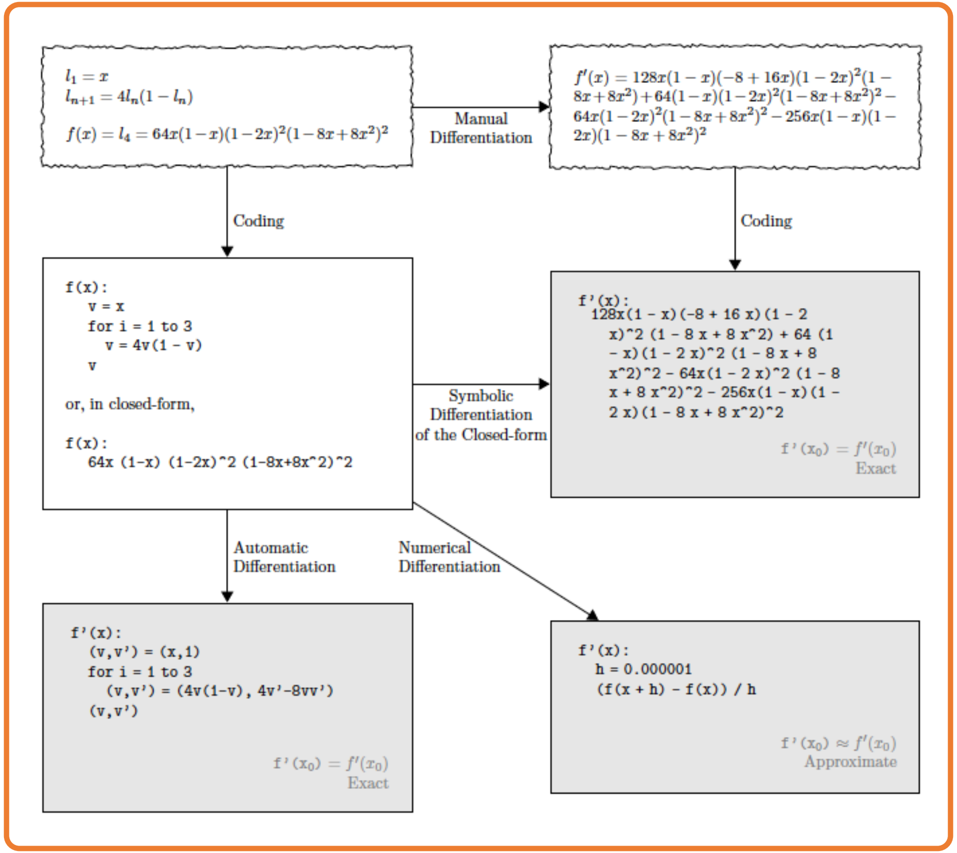
(1.25322 - 1.25347)/0.0001
= -2.5

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

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



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**

Gradient Descent on Softmax Classifier!

$\xrightarrow{f_\theta}$

	s	softmax →	NLL →
cat	**3.2**	**0.13**	0.886
car	5.1	0.87	
frog	-1.7	0.00	

$$s$$

$$p = \frac{e^{s}}{\sum_j e^{s_j}}$$

$$L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right)$$

$$\frac{\partial L}{\partial s_i} = ?$$

Gradient Descent on Softmax Classifier!

f_θ

	s		
cat	**3.2**	**0.13**	
car	5.1	0.87	0.886
frog	-1.7	0.00	

softmax: $p = \frac{e^{s}}{\sum_j e^{s_j}}$

NLL: $L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right)$

$$\frac{\partial L}{\partial s_{y_i}} = p_{y_i} - 1 \qquad \frac{\partial L}{\partial s_{j \neq y_i}} = p_j$$

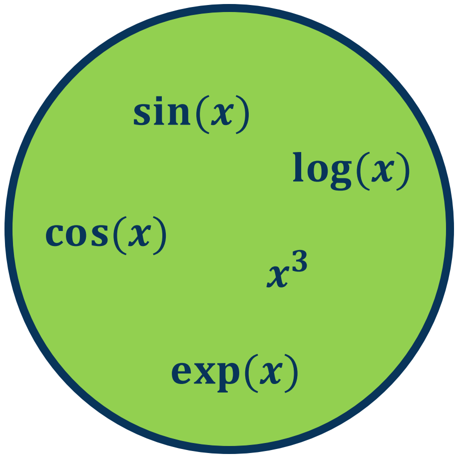
$\frac{\partial L}{\partial s}$:

-0.87
0.87
0.00

$$\frac{\partial L}{\partial \theta} = ?$$

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

How to compute gradients for deep neural networks?

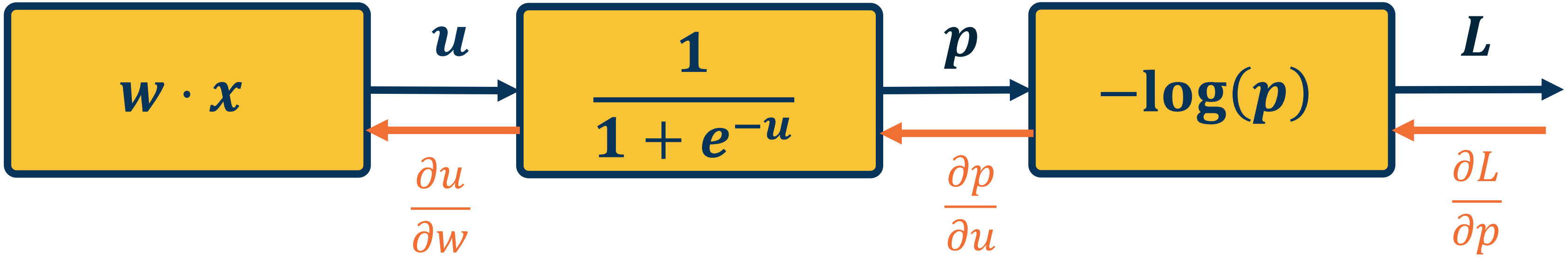


Compose into a complex function

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

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

Backpropagation via chain rule



$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial p}\frac{\partial p}{\partial u}\frac{\partial u}{\partial w} \qquad \frac{\partial L}{\partial \theta} = \frac{\partial L}{\partial s}\frac{\partial s}{\partial \theta}$$

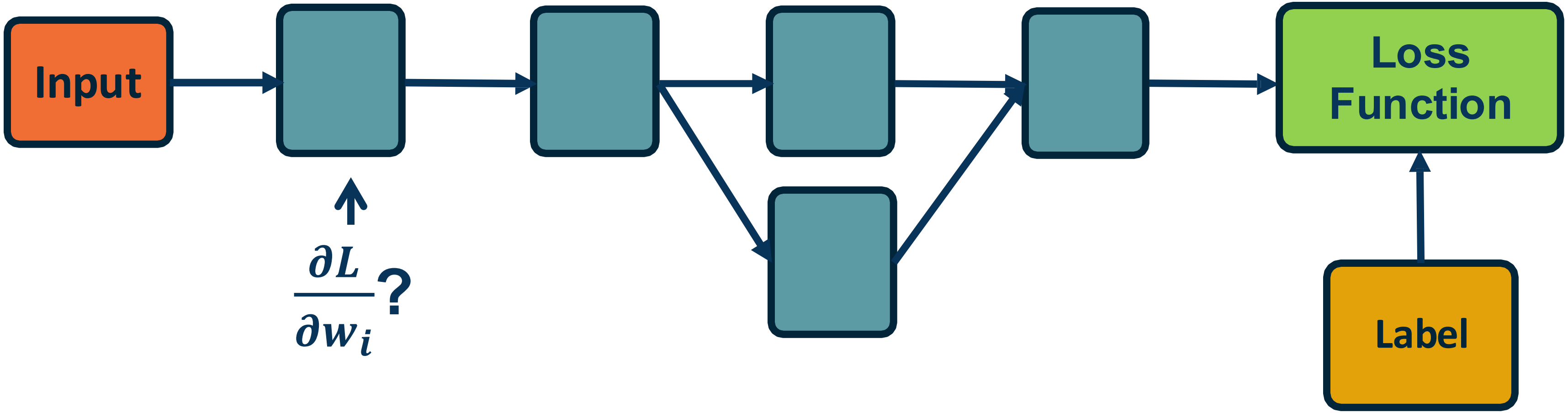
Backpropagation (roughly):

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!



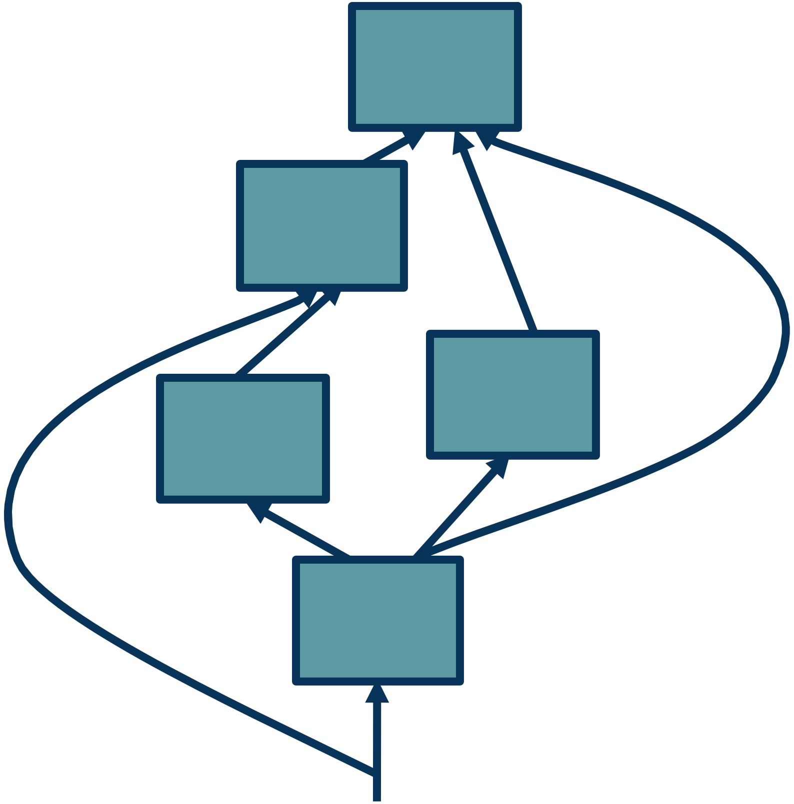
Computational Graph

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 node at a time**



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Backpropagation: a simple example

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

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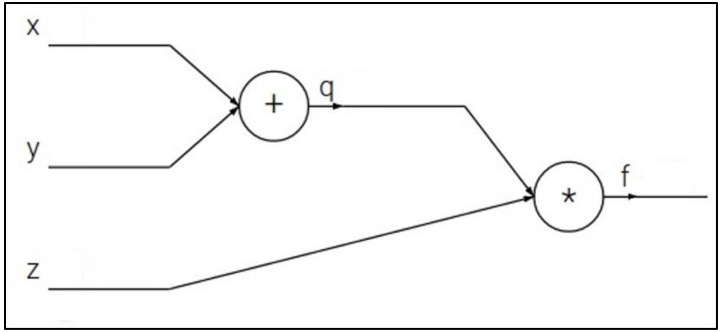

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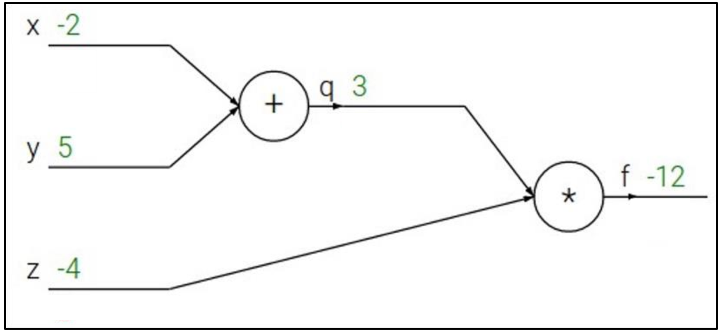
e.g. x = -2, y = 5, z = -4



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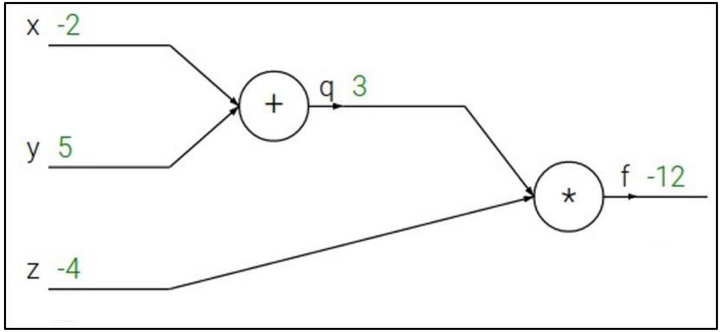

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

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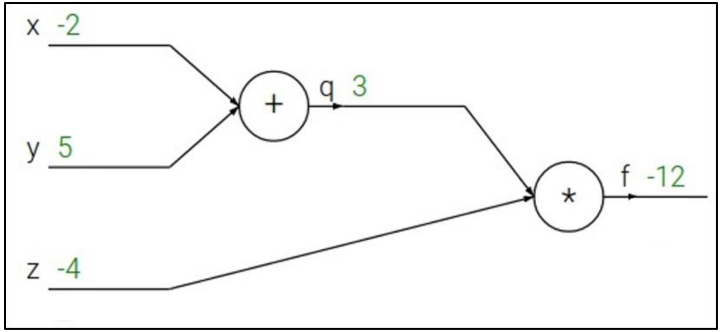

1. Calculate local gradients

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

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

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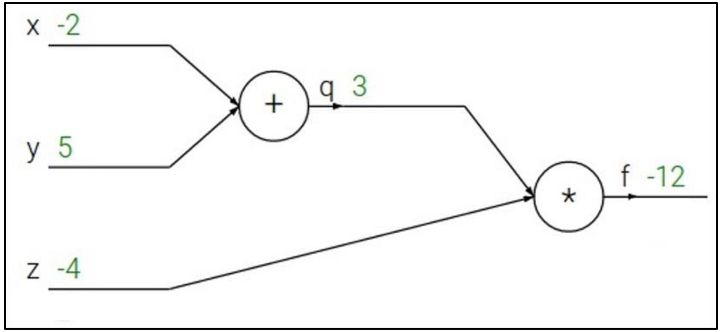

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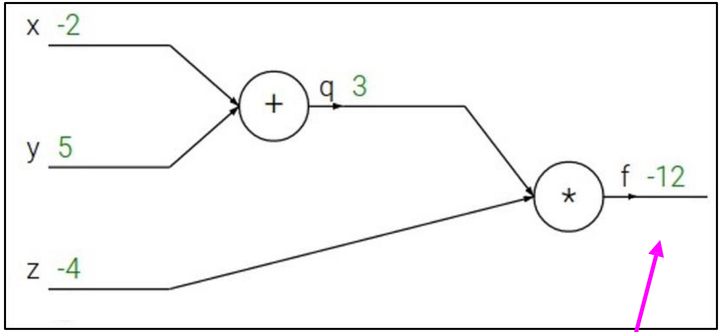

$$\frac{\partial f}{\partial f}$$

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

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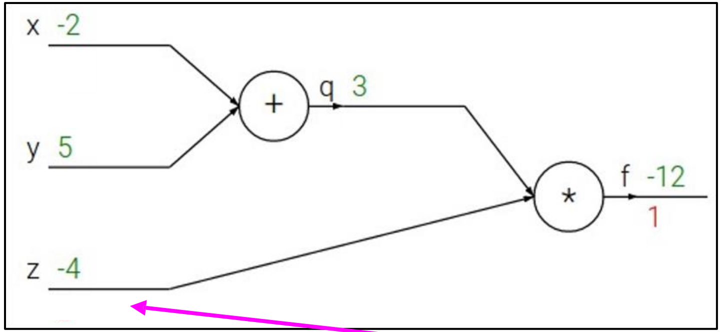

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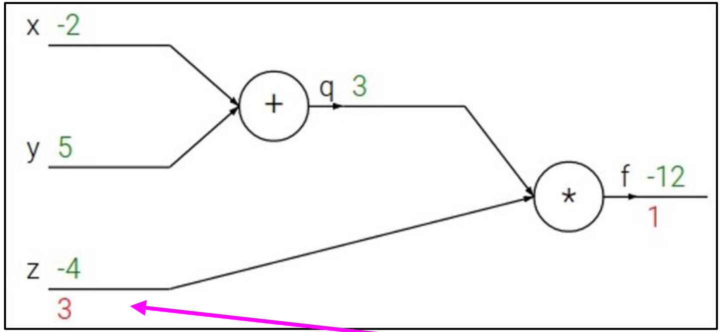

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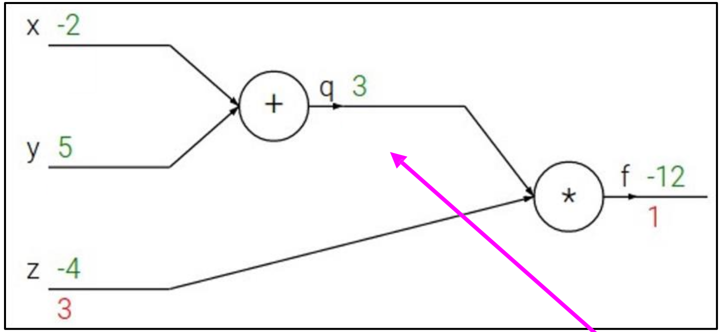

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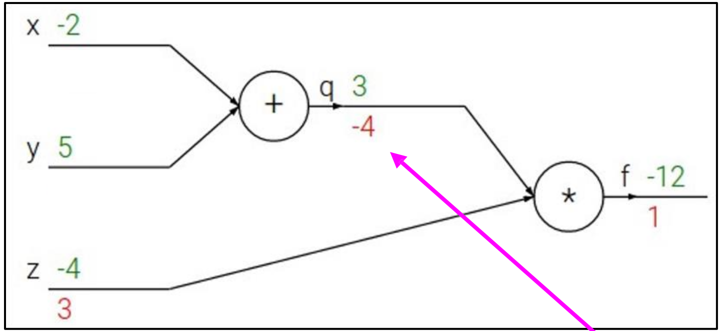

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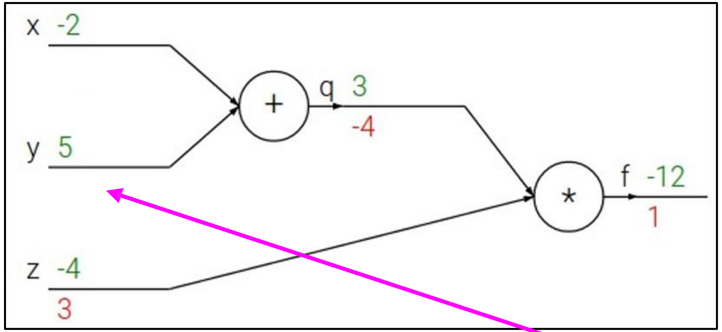

$$\frac{\partial f}{\partial y}$$

Chain rule:

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

Upstream gradient

Local gradient

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

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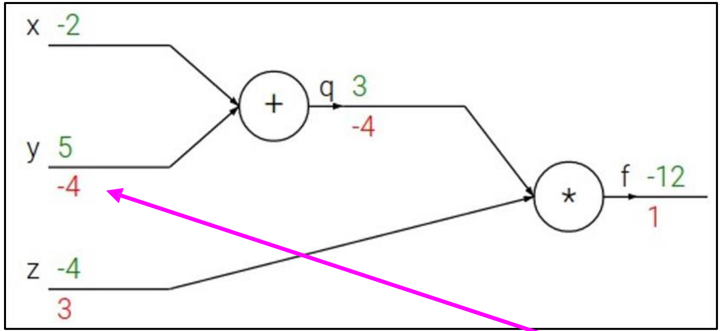

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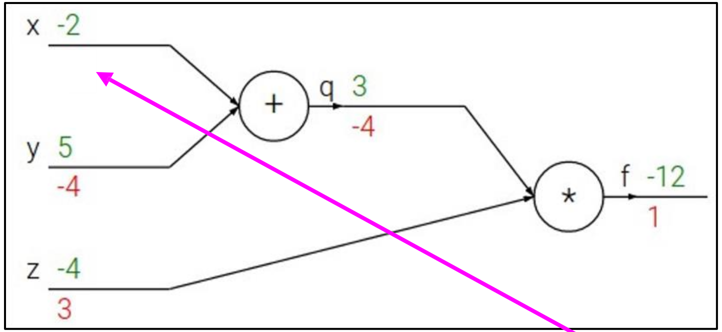

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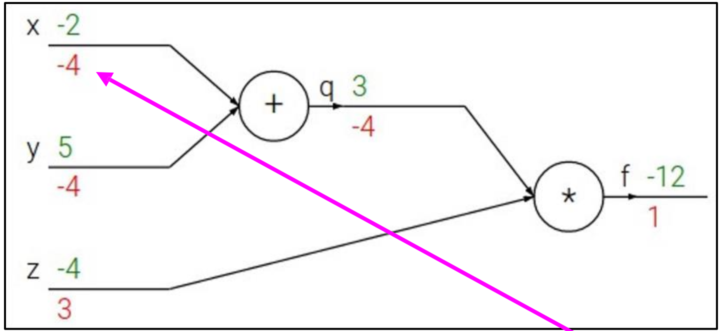
$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

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

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



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

Chain rule:

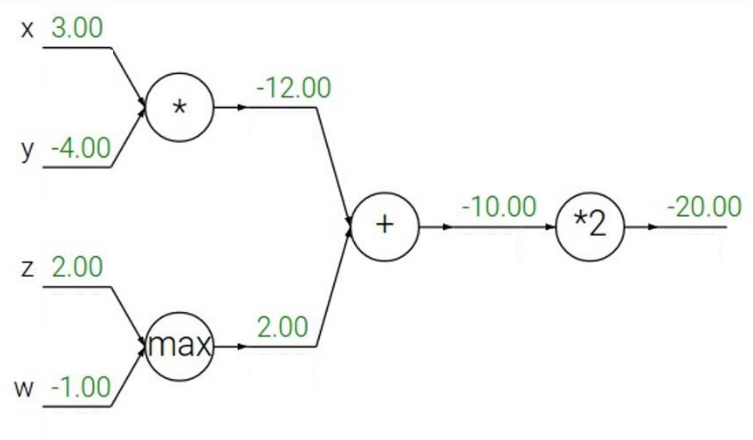
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

Upstream gradient

Local gradient

Patterns in *backward flow*

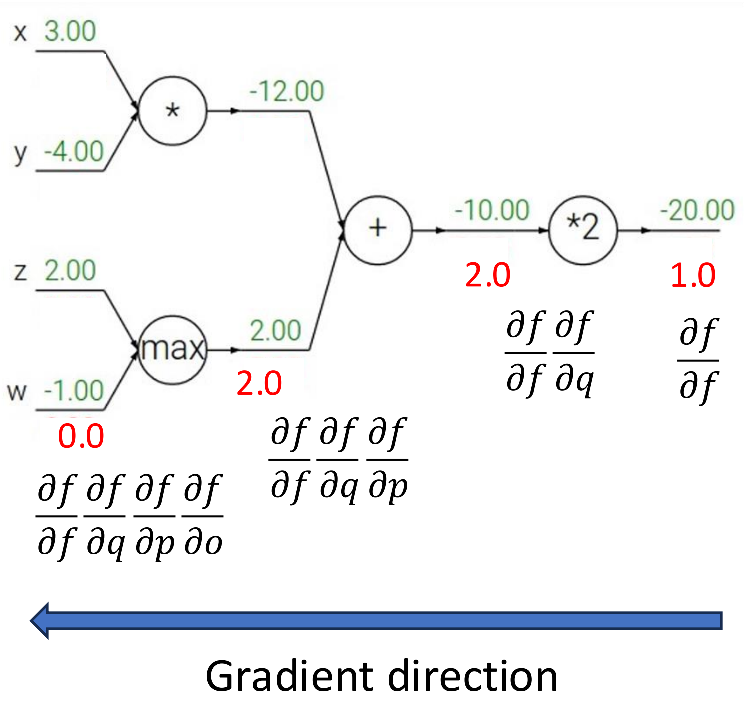
How does **a local gradient** modify the **upstream gradient**? $f = 2(xy + \max(z, w))$



Patterns in *backward flow*

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

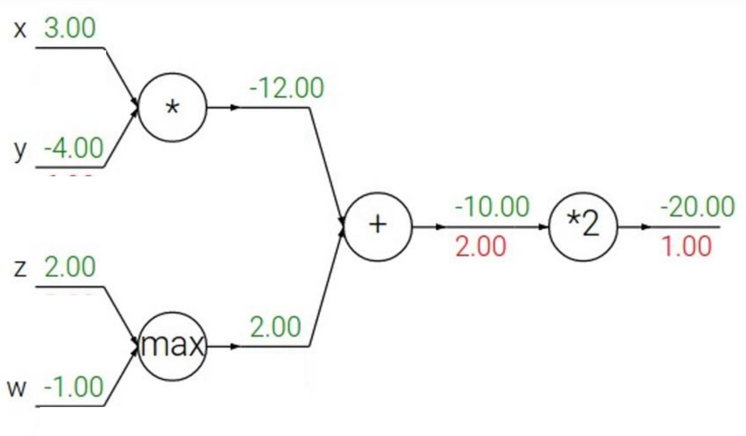
Each forward flow function (gate) determines how the gradient will be modified during backpropagation (chain rule)



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?



Gradient direction

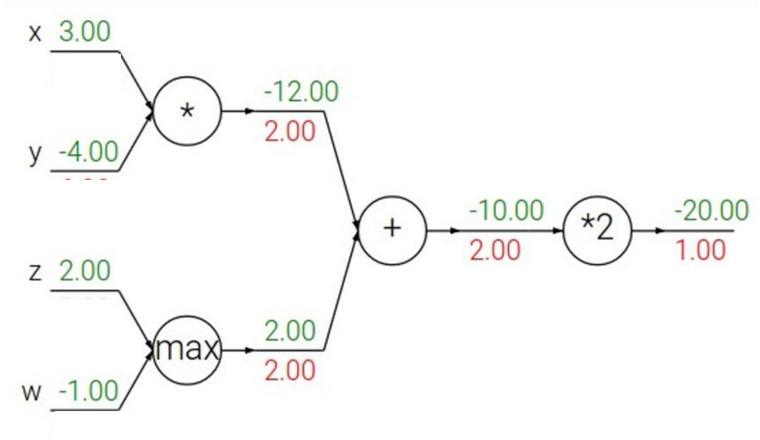
Patterns in backward flow

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

add gate: gradient replicator

$$S = T + U$$

$$\frac{NS}{NT} = \frac{NS}{NU} = 1$$



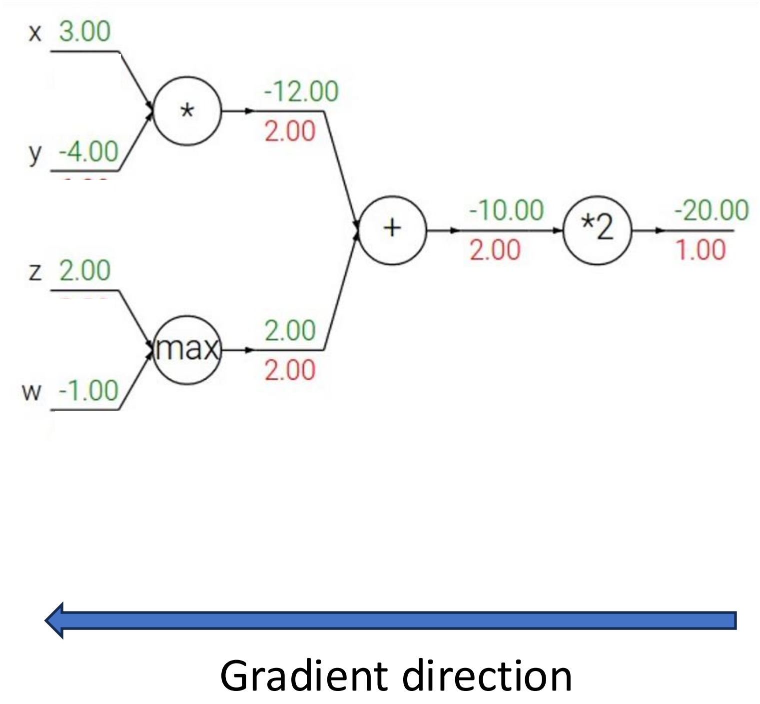
Gradient direction

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?



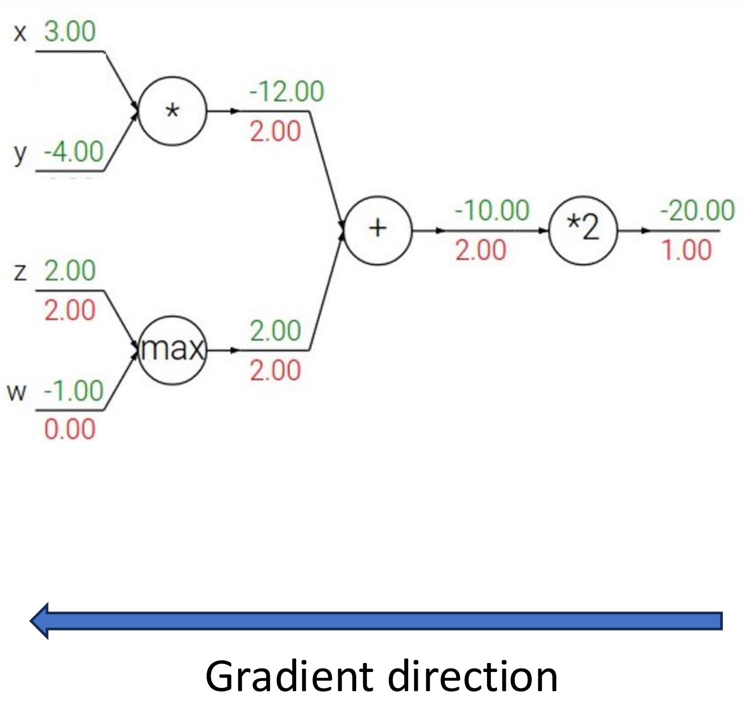
Patterns in backward flow

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



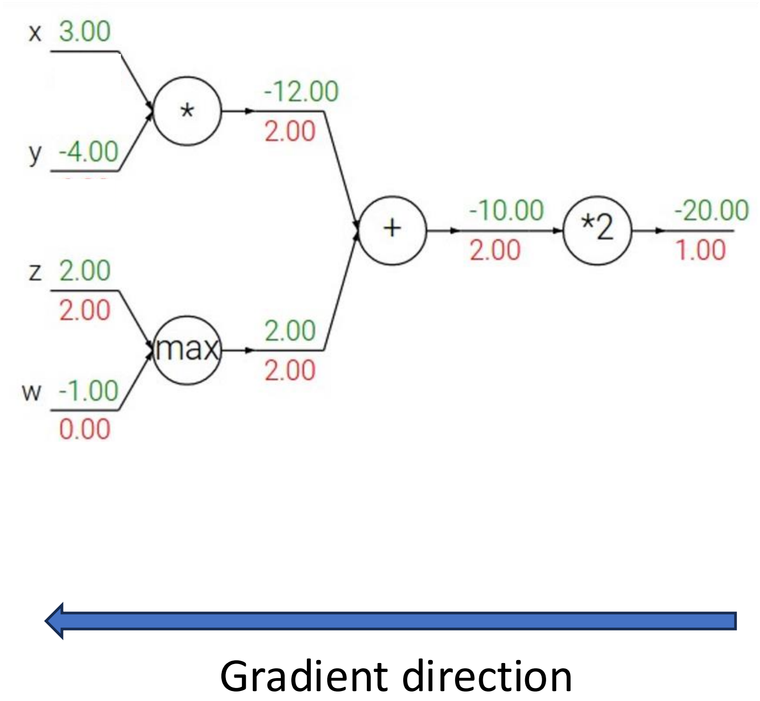
Patterns in backward flow

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? $f = 2(xy + \max(z, w))$

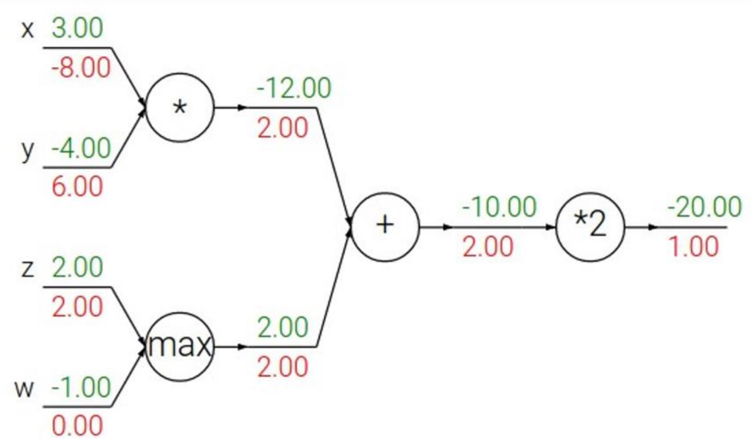
add gate: gradient replicator

max gate: gradient router

mul gate: gradient switcher

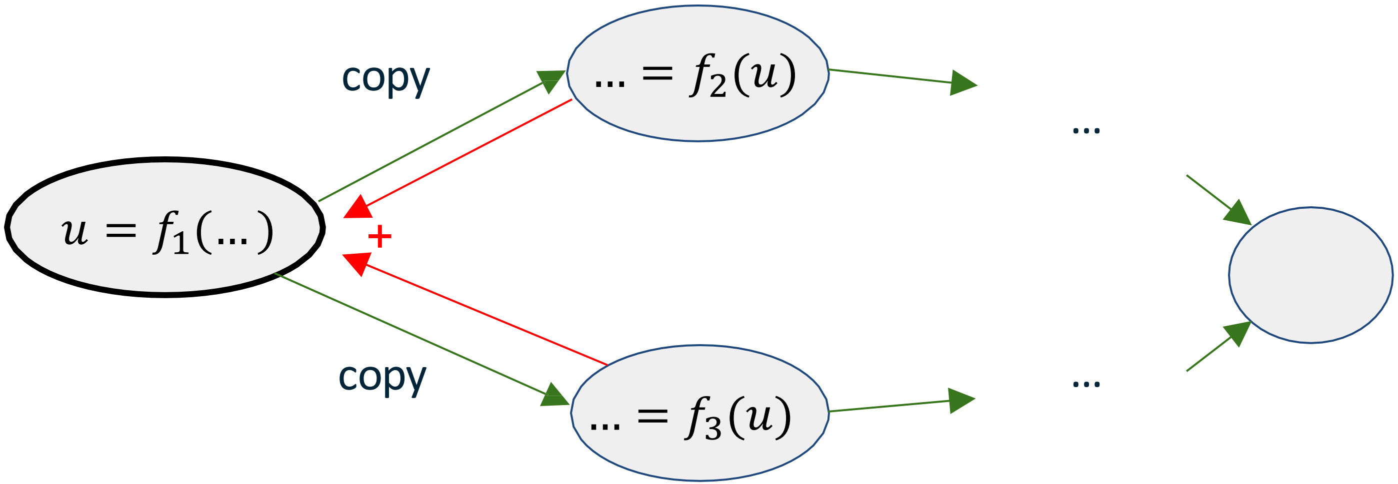
$$S = T\,VU$$

$$\frac{NS}{NT} = U \qquad \frac{NS}{NU} = T$$



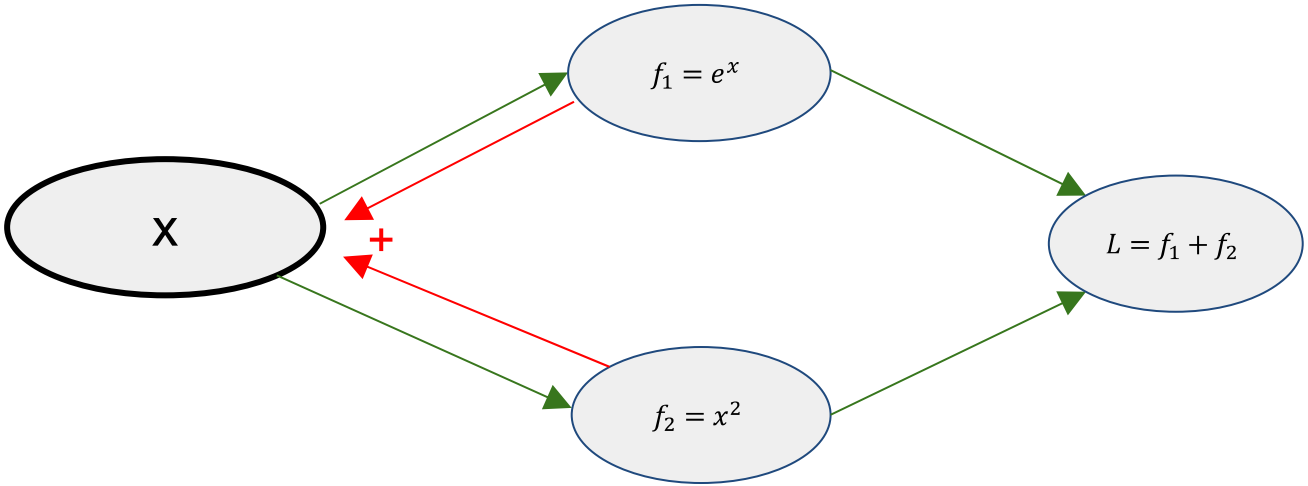
Gradient direction

Upstream gradients add at fork branches



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

Upstream gradients add at fork branches

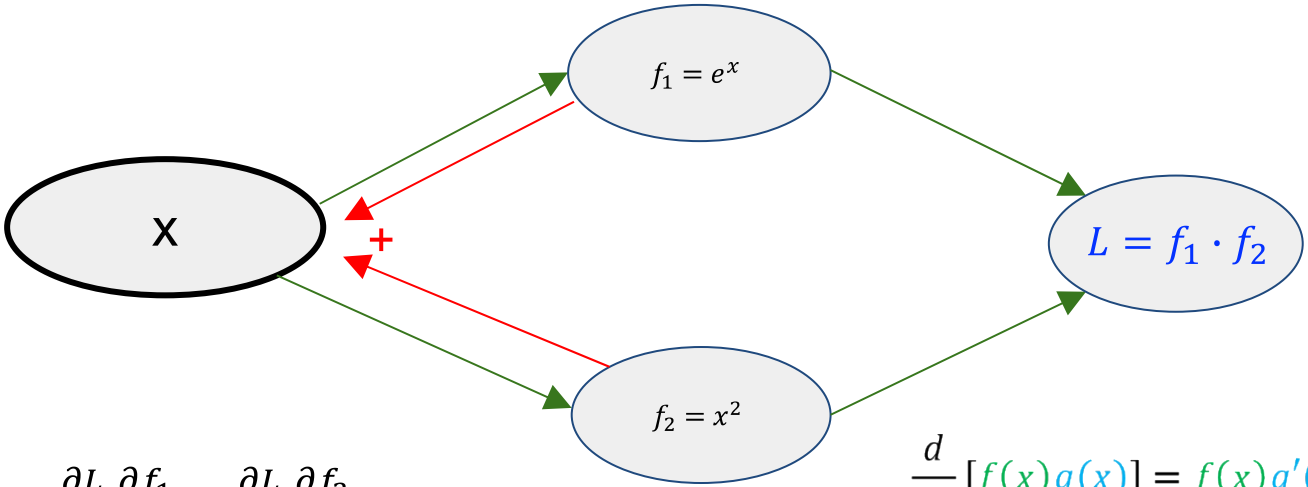


Claim: $\frac{\partial L}{\partial x} = \frac{\partial L}{\partial f_1}\frac{\partial f_1}{\partial x} + \frac{\partial L}{\partial f_2}\frac{\partial f_2}{\partial x}$
$= 1 \cdot e^x + 1 \cdot 2x = e^x + 2x$

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

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

Upstream gradients add at fork branches



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

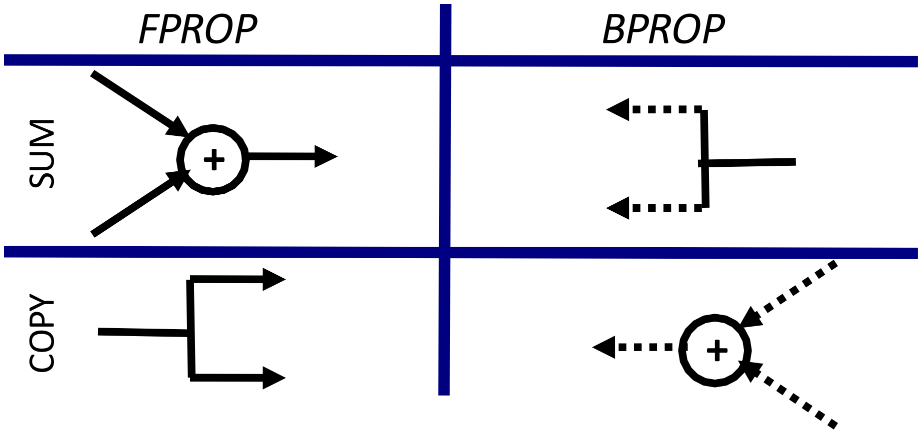
$= x^2 \cdot e^x + e^x \cdot 2x$

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

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

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

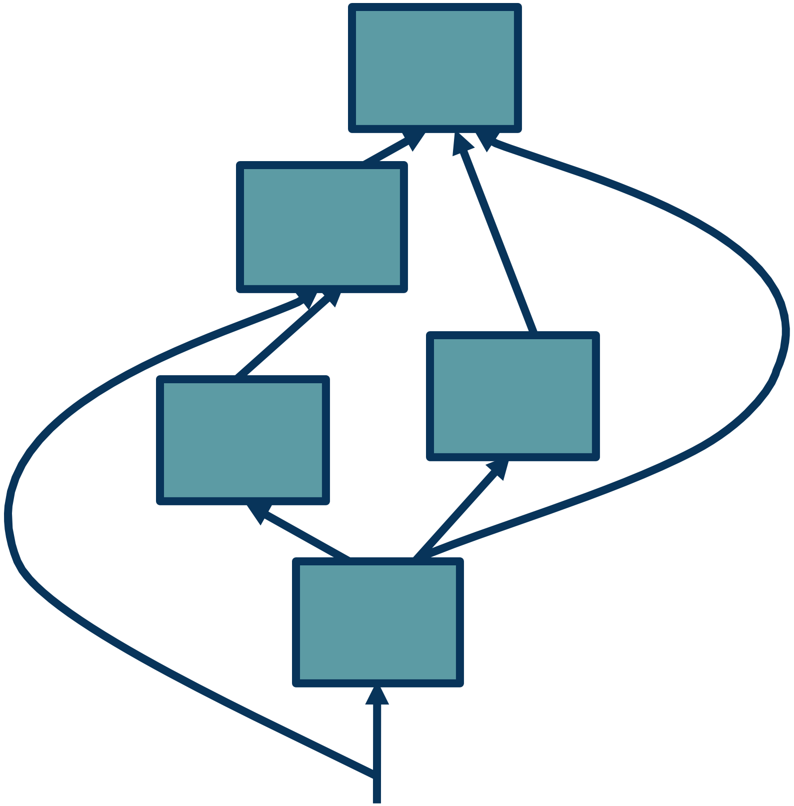
Duality in F(orward)prop and B(ack)prop



Can we backpropagate on *any* computation graph?

Graph can be any **directed acyclic graph (DAG)**

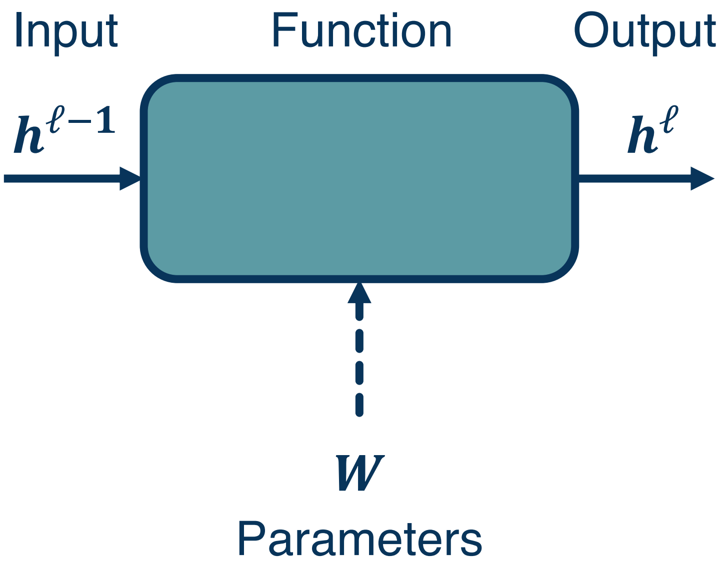
The **backpropagation algorithm** will then process this graph, **one node at a time**



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

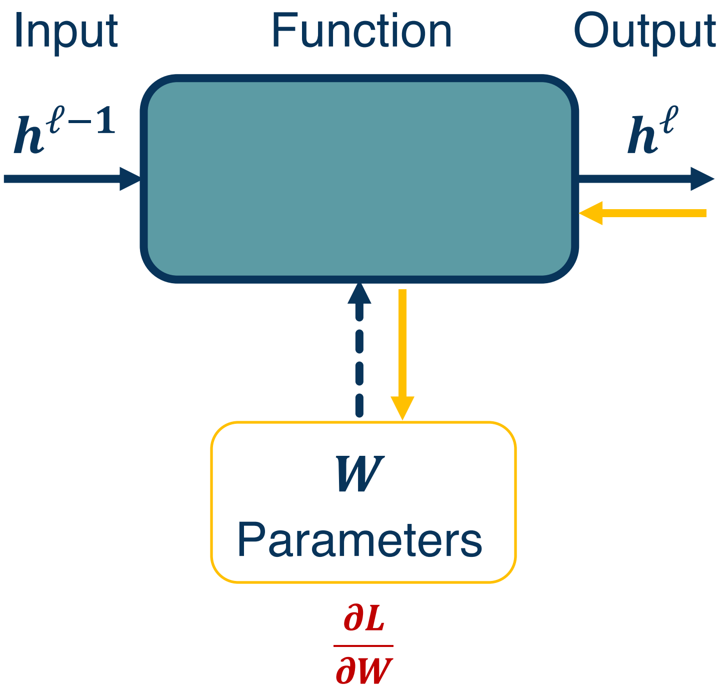
Given this computation graph, the training algorithm will:

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



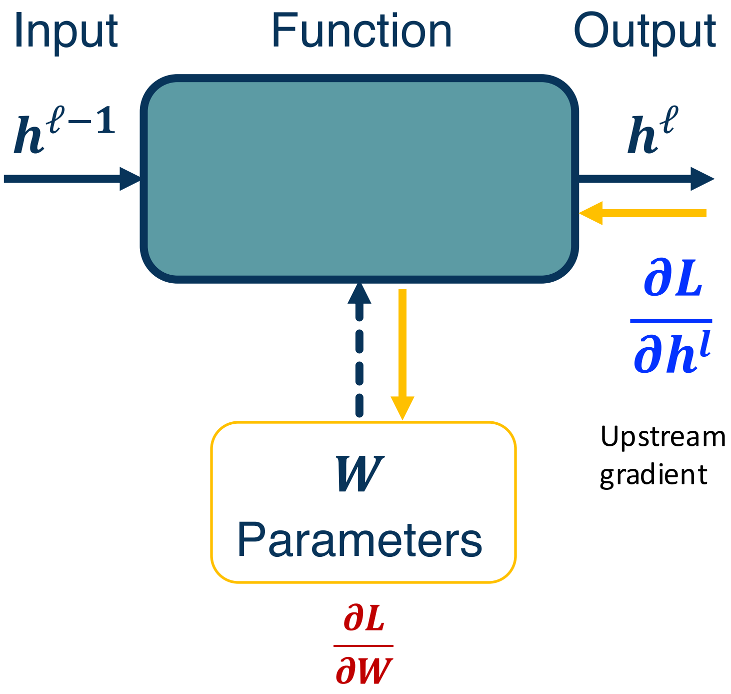
Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

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



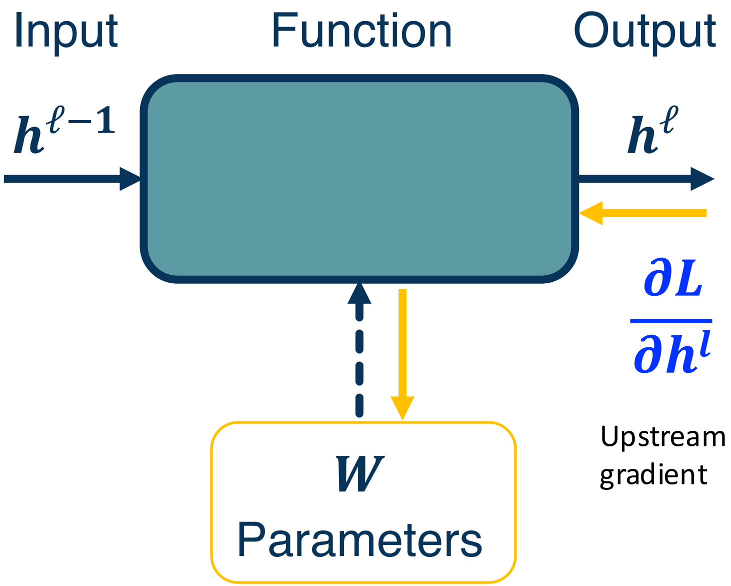
In the **backward pass**, we seek to calculate the gradients of the loss with respect to the module's parameters

- 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

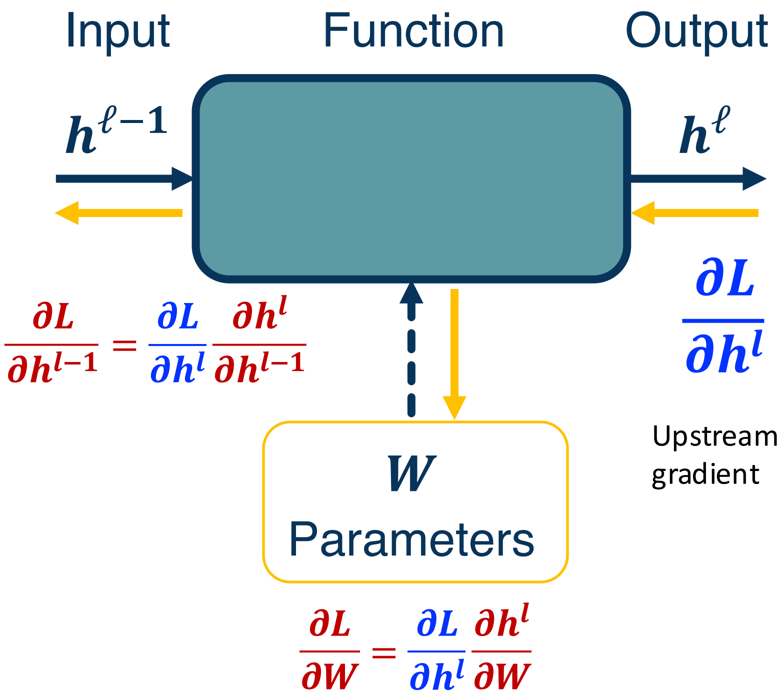
- Assume that we have the gradient of the loss with respect to the **module's outputs** (given to us by upstream module)
- We can calculate the gradient of the loss with respect to the module's weights



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

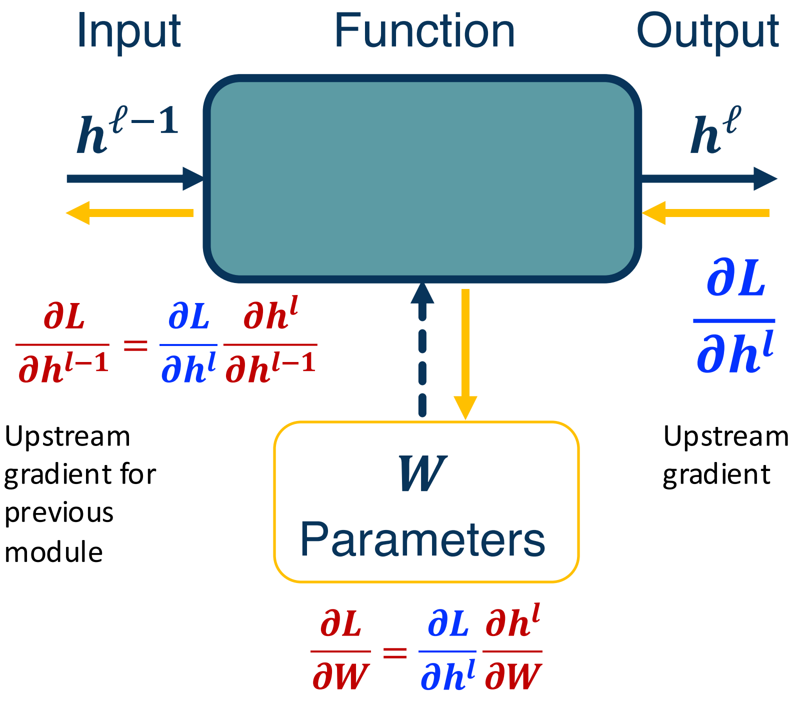
In the **backward pass**, we seek to calculate the gradients of the loss with respect to the module's parameters

- 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



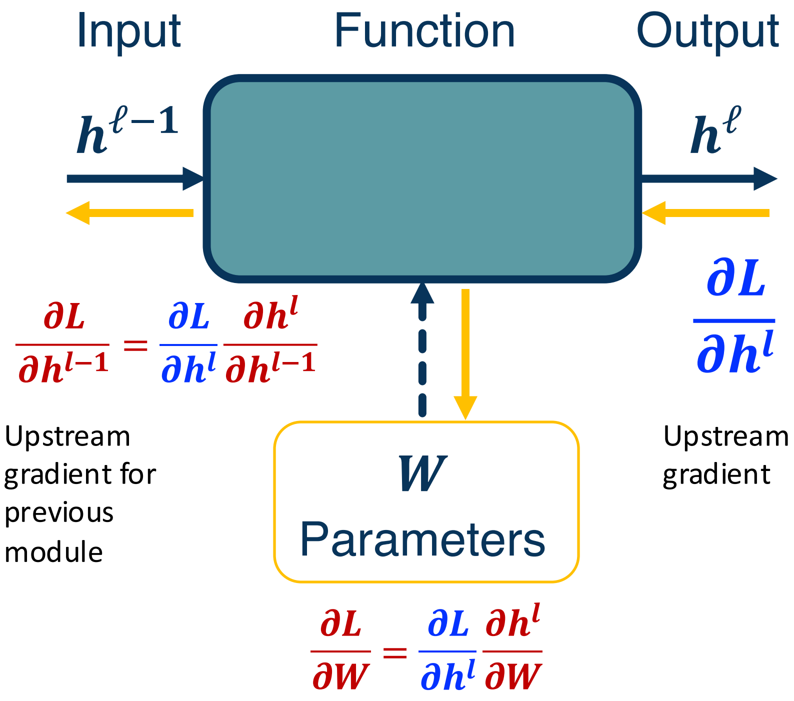
In the **backward pass**, we seek to calculate the gradients of the loss with respect to the module's parameters

- 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



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)**

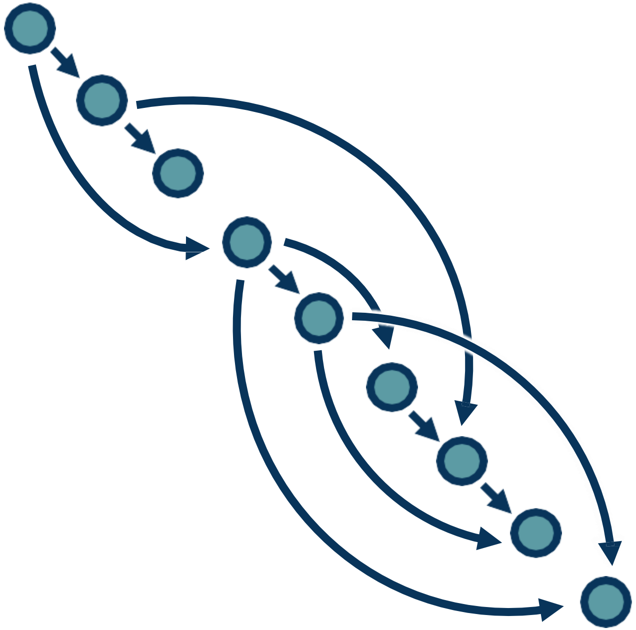
- Graph represents an **ordering constraining** which paths must be calculated first

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**



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)

PyTorch: Computational Graphs

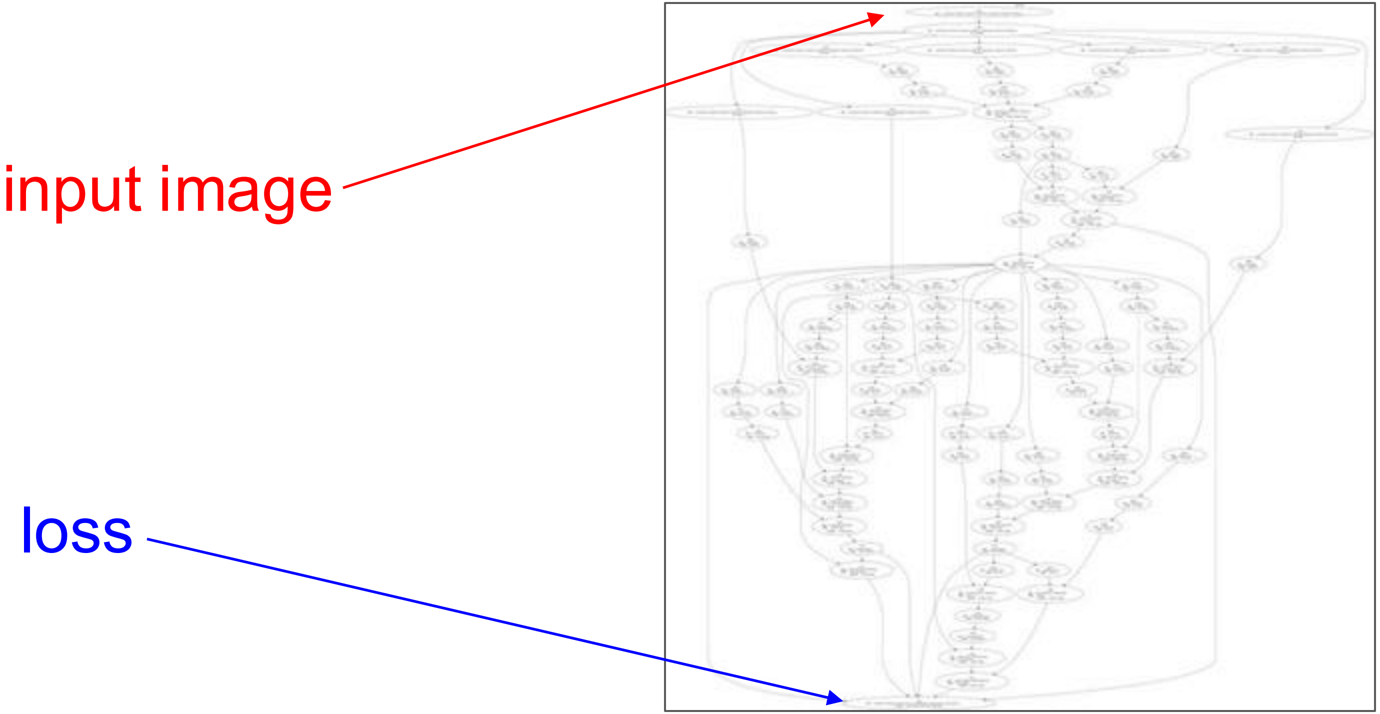


Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

PyTorch: Tensors

Running example: Train a two-layer ReLU network on random data with L2 loss

```python
import torch

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()

    with torch.no_grad():
        w1 -= learning_rate * w1.grad
        w2 -= learning_rate * w2.grad
        w1.grad.zero_()
        w2.grad.zero_()
```

PyTorch: Tensors

Create random tensors for data and weights

```python
import torch

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()

    with torch.no_grad():
        w1 -= learning_rate * w1.grad
        w2 -= learning_rate * w2.grad
        w1.grad.zero_()
        w2.grad.zero_()
```

PyTorch: Tensors

Forward pass: compute predictions and loss

```
import torch

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()

    with torch.no_grad():
        w1 -= learning_rate * w1.grad
        w2 -= learning_rate * w2.grad
        w1.grad.zero_()
        w2.grad.zero_()
```

PyTorch: Autograd

Calculate gradient for each node (weight and intermediate variables) in the graph

```
import torch

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()

    with torch.no_grad():
        w1 -= learning_rate * w1.grad
        w2 -= learning_rate * w2.grad
        w1.grad.zero_()
        w2.grad.zero_()
```

PyTorch: Autograd

```
import torch

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()

    with torch.no_grad():
        w1 -= learning_rate * w1.grad
        w2 -= learning_rate * w2.grad
        w1.grad.zero_()
        w2.grad.zero_()
```

Make gradient step on weights, then zero them. Torch.no_grad means "don't build a computational graph for this part"

PyTorch: Autograd

```
import torch

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()

    with torch.no_grad():
        w1 -= learning_rate * w1.grad
        w2 -= learning_rate * w2.grad
        w1.grad.zero_()
        w2.grad.zero_()
```

PyTorch methods that end in underscore modify the Tensor in-place; methods that don't return a new Tensor

PyTorch: New Autograd Functions

Define your own autograd functions by writing forward and backward functions for Tensors

Use ctx object to “cache” values for the backward pass

```
class MyReLU(torch.autograd.Function):
    @staticmethod
    def forward(ctx, x):
        ctx.save_for_backward(x)
        return x.clamp(min=0)

    @staticmethod
    def backward(ctx, grad_y):
        x, = ctx.saved_tensors
        grad_input = grad_y.clone()
        grad_input[x < 0] = 0
        return grad_input
```

PyTorch: New Autograd Functions

Define your own autograd functions by writing forward and backward functions for Tensors

Use ctx object to “cache” values for the backward pass

Define a helper function to make it easy to use the new function

```
class MyReLU(torch.autograd.Function):
    @staticmethod
    def forward(ctx, x):
        ctx.save_for_backward(x)
        return x.clamp(min=0)

    @staticmethod
    def backward(ctx, grad_y):
        x, = ctx.saved_tensors
        grad_input = grad_y.clone()
        grad_input[x < 0] = 0
        return grad_input

def my_relu(x):
    return MyReLU.apply(x)
```

PyTorch: New Autograd Functions

```python
class MyReLU(torch.autograd.Function):
    @staticmethod
    def forward(ctx, x):
        ctx.save_for_backward(x)
        return x.clamp(min=0)

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        grad_input = grad_y.clone()
        grad_input[x < 0] = 0
        return grad_input

def my_relu(x):
    return MyReLU.apply(x)
```

```python
N, D_in, H, D_out = 64, 1000, 100, 10

x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
for t in range(500):
    y_pred = my_relu(x.mm(w1)).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()

    with torch.no_grad():
        w1 -= learning_rate * w1.grad
        w2 -= learning_rate * w2.grad
        w1.grad.zero_()
        w2.grad.zero_()
```

Can use our new autograd function in the forward pass

PyTorch: New Autograd Functions

```
def my_relu(x):
    return x.clamp(min=0)
```

In practice you almost never need to define new autograd functions! Only do it when you need custom backward. In this case we can just use a normal PyTorch function

```
N, D_in, H, D_out = 64, 1000, 100, 10

x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
for t in range(500):
    y_pred = my_relu(x.mm(w1)).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()

    with torch.no_grad():
        w1 -= learning_rate * w1.grad
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        w1.grad.zero_()
        w2.grad.zero_()
```

PyTorch: **Dynamic** Computation Graphs

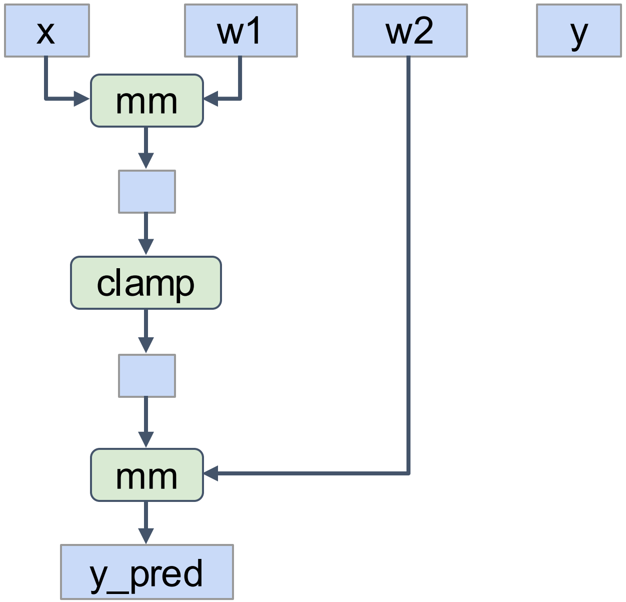
```
import torch

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()
```

PyTorch: **Dynamic** Computation Graphs


```python
import torch

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()
```

Create Tensor objects

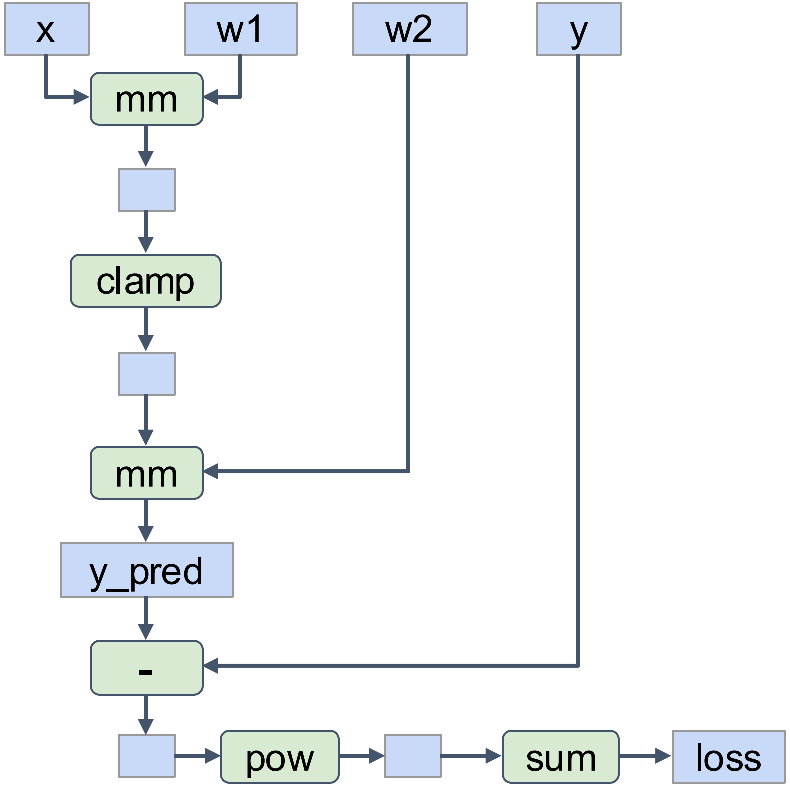
PyTorch: **Dynamic** Computation Graphs




```python
import torch

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()
```

Build graph data structure AND perform computation

PyTorch: **Dynamic** Computation Graphs




```python
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N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
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w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()
```
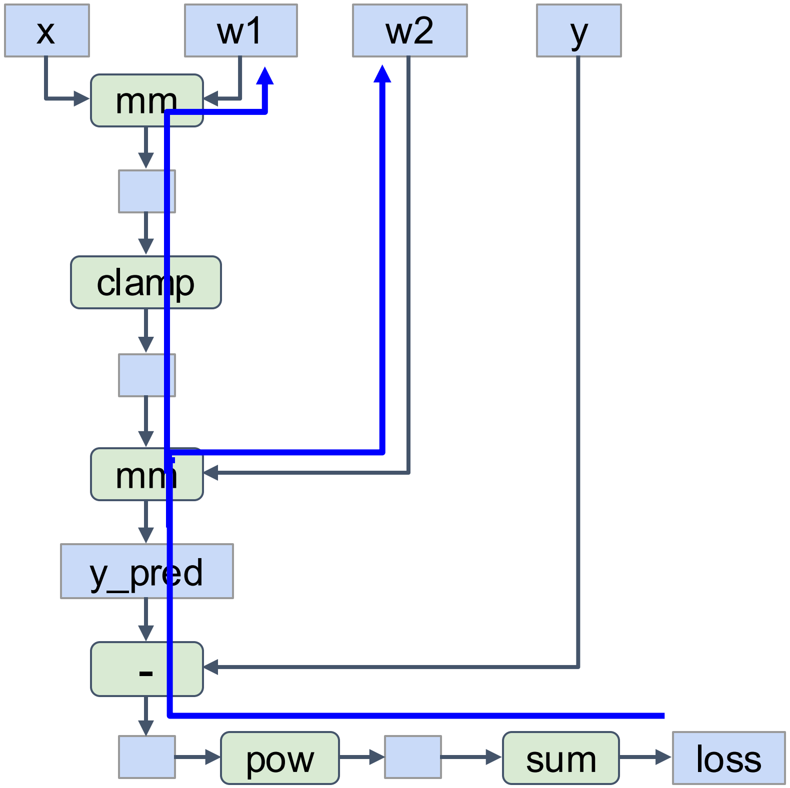

Build graph data structure AND perform computation

PyTorch: **Dynamic** Computation Graphs




```
import torch

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()
```

Search for path between loss and w1, w2 (for backprop) AND perform computation

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Throw away the graph, backprop path, and rebuild it from scratch on every iteration

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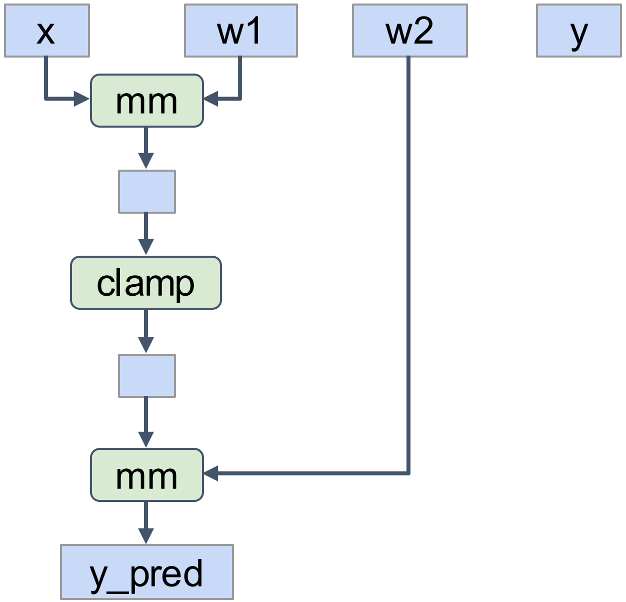


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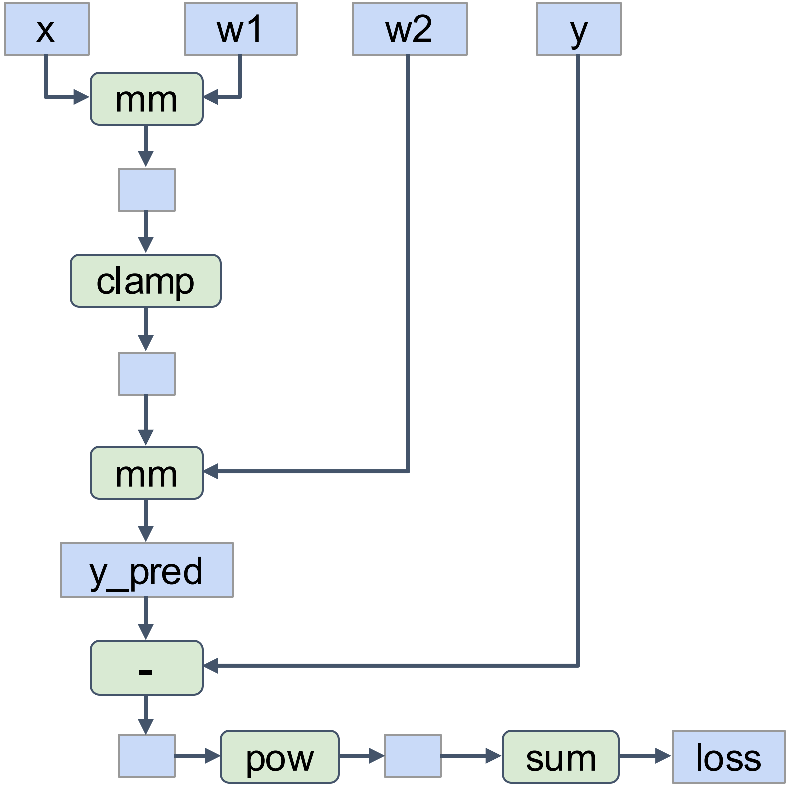


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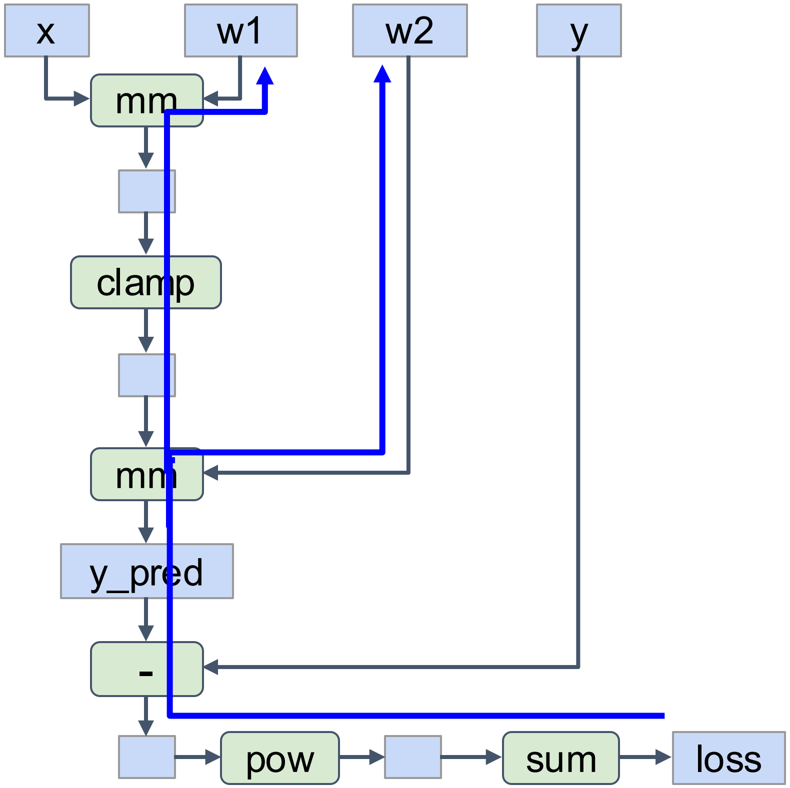


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Search for path between loss and w1, w2 (for backprop) AND perform computation

PyTorch: **Dynamic** Computation Graphs

Building the graph and **computing** the graph happen at the same time.

Seems inefficient, especially if we are building the same graph over and over again...

```
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w1 = torch.randn(D_in, H, requires_grad=True)
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```
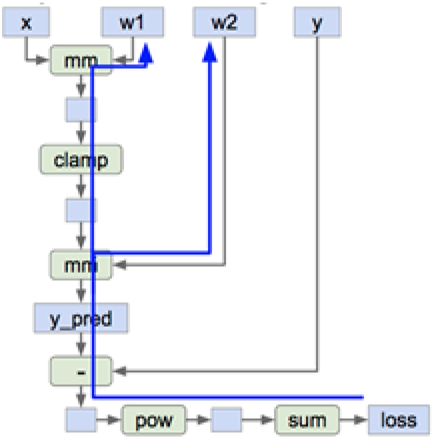

Static Computation Graphs



Alternative: **Static** graphs

Step 1: Build computational graph describing our computation (including finding paths for backprop)

Step 2: Reuse the same graph on every iteration

```
graph = build_graph()

for x_batch, y_batch in loader:
    run_graph(graph, x=x_batch, y=y_batch)
```

@tf.function: compile static graph

tf.function decorator (implicitly) compiles python functions to static graph for better performance

```
N, D, H = 64, 1000, 100
x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
model = tf.keras.Sequential()
model.add(tf.keras.layers.Dense(H, input_shape=(D,),
                                activation=tf.nn.relu))
model.add(tf.keras.layers.Dense(D))
optimizer = tf.optimizers.SGD(1e-1)

@tf.function
def model_func(x, y):
  y_pred = model(x)
  loss = tf.losses.MeanSquaredError()(y_pred, y)
  return y_pred, loss

for t in range(50):
  with tf.GradientTape() as tape:
    y_pred, loss = model_func(x, y)
  gradients = tape.gradient(
      loss, model.trainable_variables)
  optimizer.apply_gradients(
      zip(gradients, model.trainable_variables))
```

@tf.function: compile static graph

Ran on Google Colab, April 2020

Here we compare the forward-pass time of the same model under dynamic graph mode and static graph mode

```
N, D, H = 64, 1000, 100
x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
model = tf.keras.Sequential()
model.add(tf.keras.layers.Dense(H, input_shape=(D,), activation=tf.nn.relu))
model.add(tf.keras.layers.Dense(D))
optimizer = tf.optimizers.SGD(1e-1)

@tf.function
def model_static(x, y):
  y_pred = model(x)
  loss = tf.losses.MeanSquaredError()(y_pred, y)
  return y_pred, loss


def model_dynamic(x, y):
  y_pred = model(x)
  loss = tf.losses.MeanSquaredError()(y_pred, y)

print("dynamic graph: ", timeit.timeit(lambda: model_dynamic(x, y), number=10))
print("static graph: ", timeit.timeit(lambda: model_static(x, y), number=10))
```

```
dynamic graph:  0.02520249200000535
static graph:  0.03932226699998864
```

@tf.function: compile static graph

Ran on Google Colab, April 2020

```
N, D, H = 64, 1000, 100
x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
model = tf.keras.Sequential()
model.add(tf.keras.layers.Dense(H, input_shape=(D,), activation=tf.nn.relu))
model.add(tf.keras.layers.Dense(D))
optimizer = tf.optimizers.SGD(1e-1)

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def model_static(x, y):
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```

```
def model_dynamic(x, y):
  y_pred = model(x)
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print("dynamic graph: ", timeit.timeit(lambda: model_dynamic(x, y), number=10))
print("static graph: ", timeit.timeit(lambda: model_static(x, y), number=10))
```

```
dynamic graph:  0.02520249200000535
static graph:  0.03932226699998864
```

Static graph is *in theory* faster than dynamic graph, but the performance gain depends on the type of model / layer / computation graph.

@tf.function: compile static graph

Ran on Google Colab, April 2020

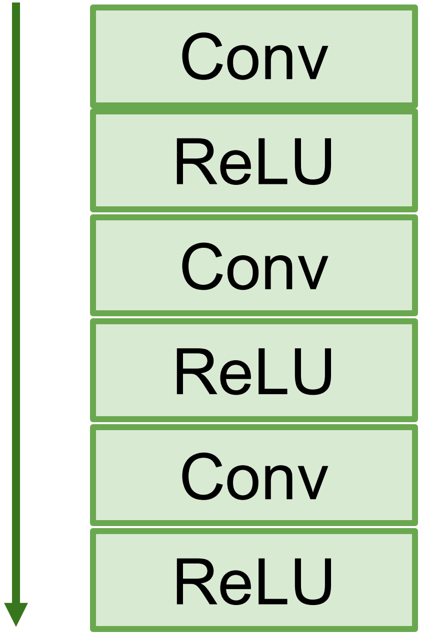
```
N, D, H = 64, 1000, 100
x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
model = tf.keras.Sequential()
model.add(tf.keras.layers.Dense(H, input_shape=(D,), activation=tf.nn.relu))
model.add(tf.keras.layers.Dense(D))
optimizer = tf.optimizers.SGD(1e-1)

@tf.function
def model_static(x, y):
  y_pred = model(x)
  loss = tf.losses.MeanSquaredError()(y_pred, y)
  return y_pred, loss


def model_dynamic(x, y):
  y_pred = model(x)
  loss = tf.losses.MeanSquaredError()(y_pred, y)

print("dynamic graph:", timeit.timeit(lambda: model_dynamic(x, y), number=1000))
print("static graph:", timeit.timeit(lambda: model_static(x, y), number=1000))

dynamic graph: 2.3648411540000325
static graph: 1.1723986679999143
```

Static graph is *in theory* faster than dynamic graph, but the performance gain depends on the type of model / layer / computation graph.

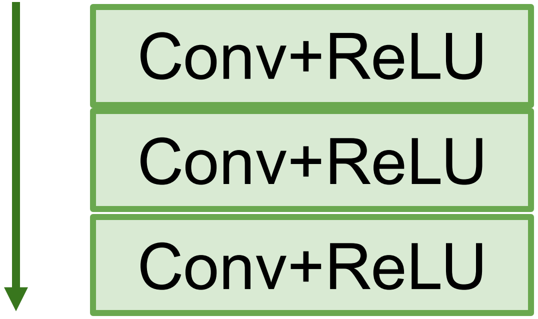
Static vs Dynamic: Optimization

With static graphs, framework can **optimize** the graph for you before it runs!

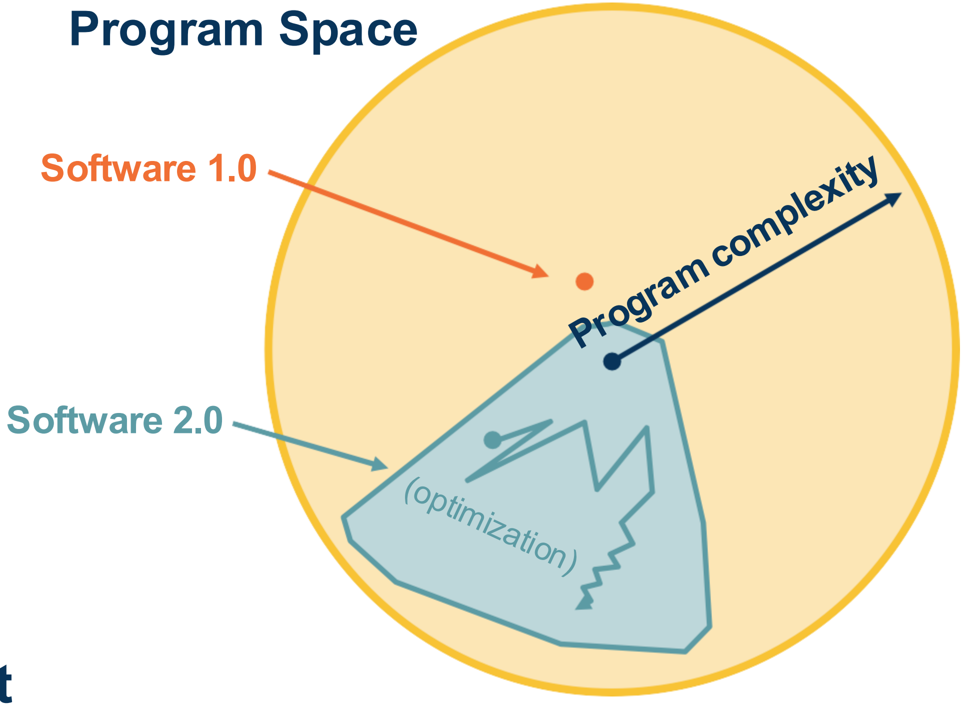
The graph you wrote



Equivalent graph with **fused operations**



- 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

Power of Automatic Differentiation

- Autodiff from scratch: micrograd repo, video tutorial

Next time:

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