Topics:

- Gradient Descent
- Neural Networks

CS 4803-DL / 7643-A

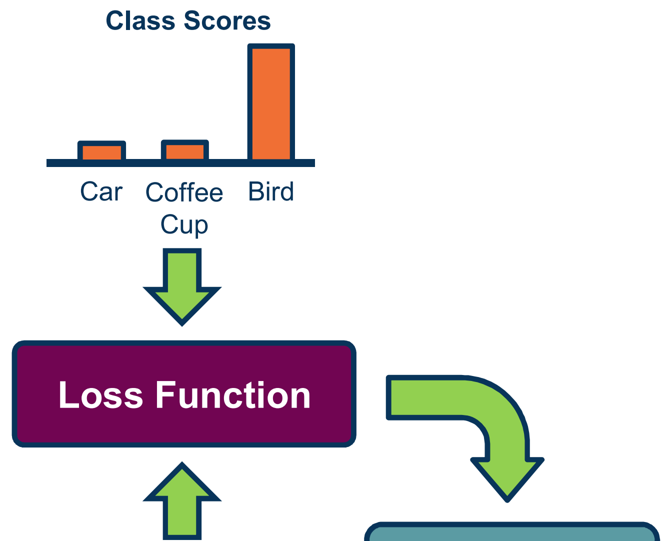
ZSOLT KIRA

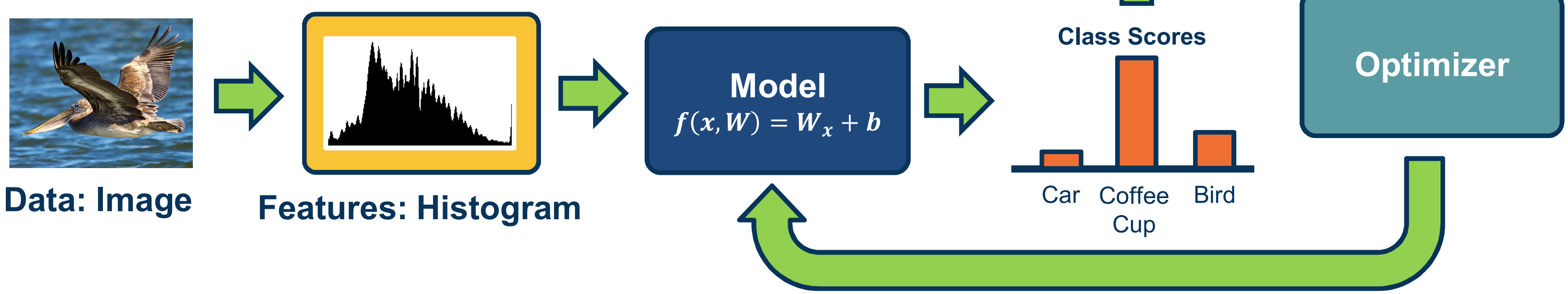
- **Assignment 1 out!**
  - **Due Feb 7th**
  - Start now, start now, start now!
  - Start now, start now, start now!
  - Start now, start now, start now!

- **Piazza**
  - Be active!!!

- **Office hours**
  - Let us know special topic requests (e.g. PS0, Assignment 1, research paper discussion, etc.)

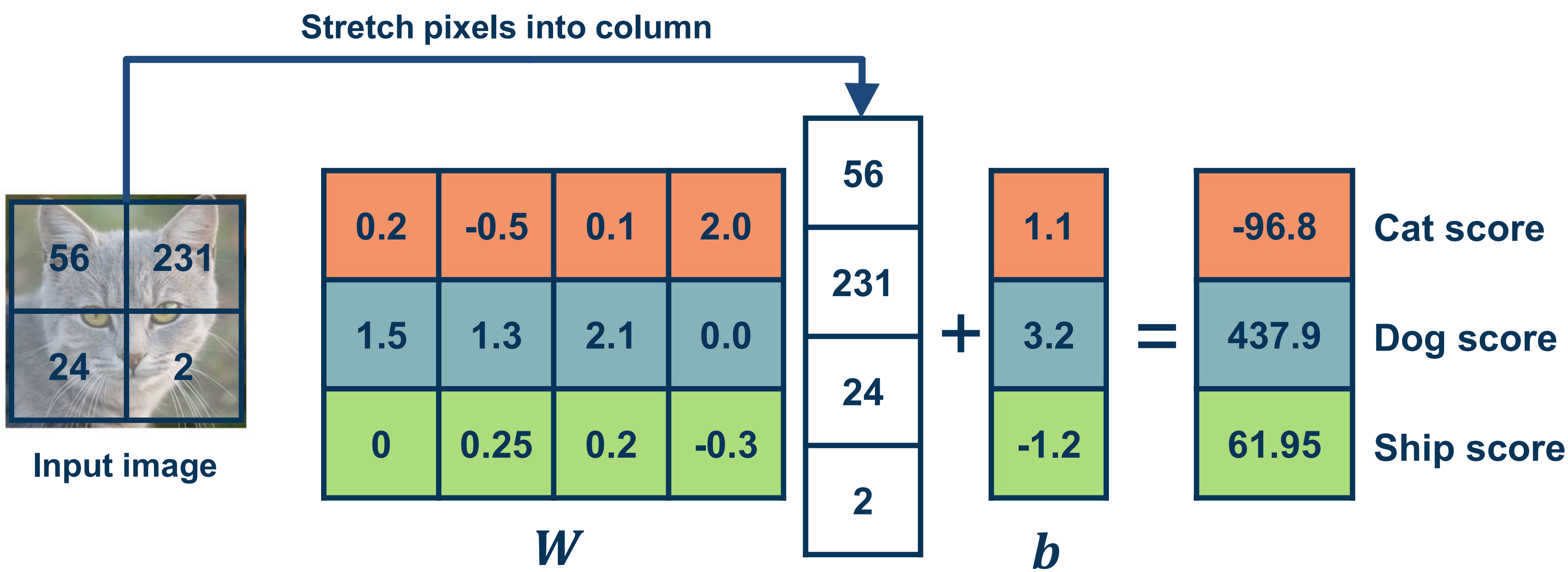
- Input (and representation)
- Functional form of the model
  - Including parameters
- Performance measure to improve
  - Loss or objective function
- Algorithm for finding best parameters
  - Optimization algorithm





Components of a Parametric Model

Example with an image with **4 pixels**, and **3 classes** (cat/dog/ship)



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

Softmax Classifier (Multinomial Logistic Regression)

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

$s = f(x_i; W)$

$P(Y = k|X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}$ **Softmax Function**

Probabilities must be >= 0

Probabilities must sum to 1

$L_i = -\log P(Y = y_i|X = x_i)$

	Unnormalized log-probabilities / logits	exp →	Unnormalized probabilities	normalize →	Probabilities
cat	**3.2**		**24.5**		**0.13**
car	5.1		164.0		0.87
frog	-1.7		0.18		0.00

→ $L_i = -\log(0.13)$

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

Often, we add a **regularization term** to the loss function

L1 Regularization

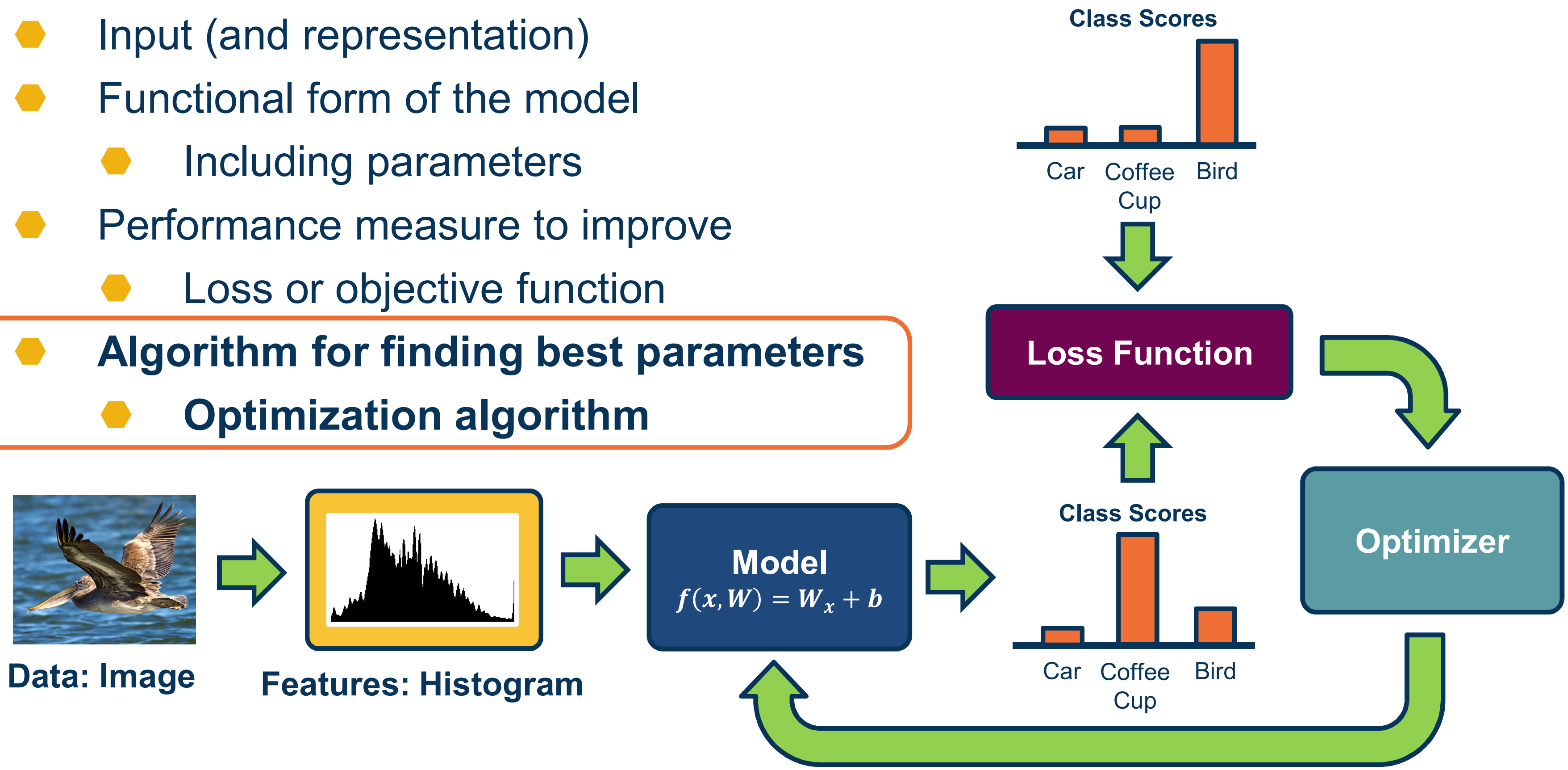
$$L_i = |y - Wx_i|^2 + |W|$$

Example regularizations:

- L1/L2 on weights (encourage small values)

Gradient Descent

- 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**



Components of a Parametric Model

Given a model and loss function, finding the best set of weights is a **search problem**

- Find the best combination of weights that minimizes our loss function

Several classes of methods:

- Random search
- Genetic algorithms (population-based search)
- Gradient-based optimization

In deep learning, **gradient-based methods are dominant** although not the only approach possible

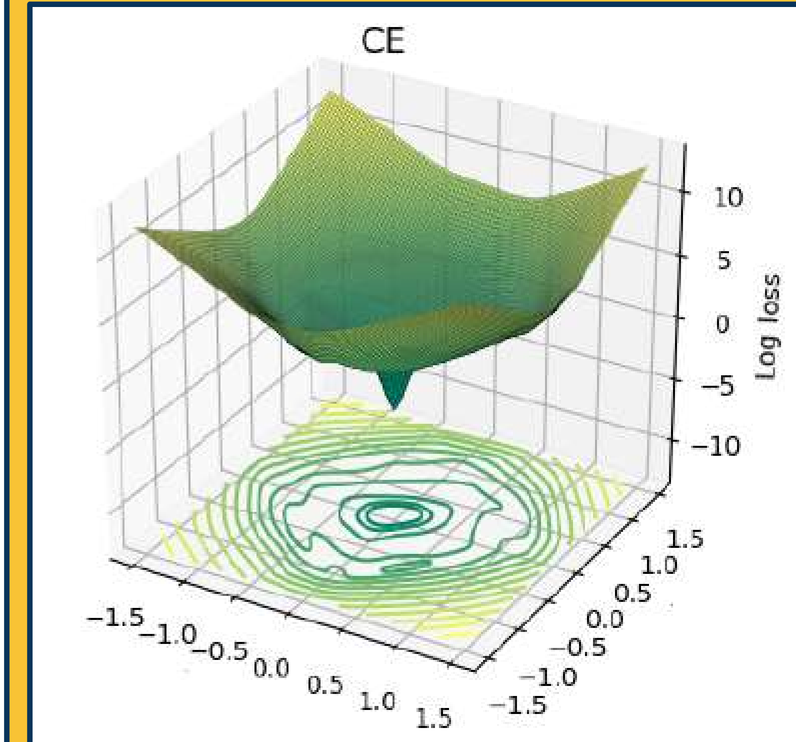
$$\begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1m} & b1 \\ w_{21} & w_{22} & \cdots & w_{2m} & b2 \\ w_{21} & w_{22} & \cdots & w_{3m} & b3 \end{bmatrix}$$

Loss

As weights change, the loss changes 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



Strategy: Follow the Slope!

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

$$f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}$$

- Steepest descent direction is the **negative gradient**
- **Intuitively:** Measures how the function changes as the argument a changes by a small step size
  - As step size goes to zero
- **In Machine Learning:** Want to know how the **loss function** changes **as weights** are varied
  - Can consider each parameter separately by taking **partial derivative** of loss function with respect to that parameter

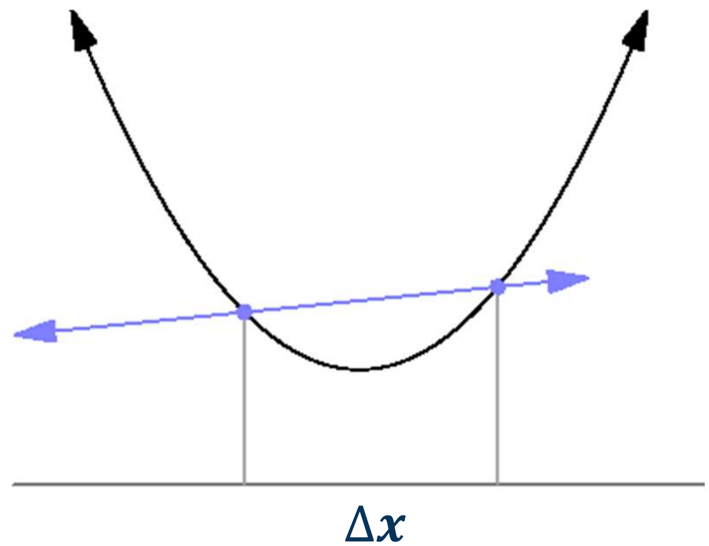


Image and equation from: https://en.wikipedia.org/wiki/Derivative#/media/File:Tangent_animation.gif

Derivatives

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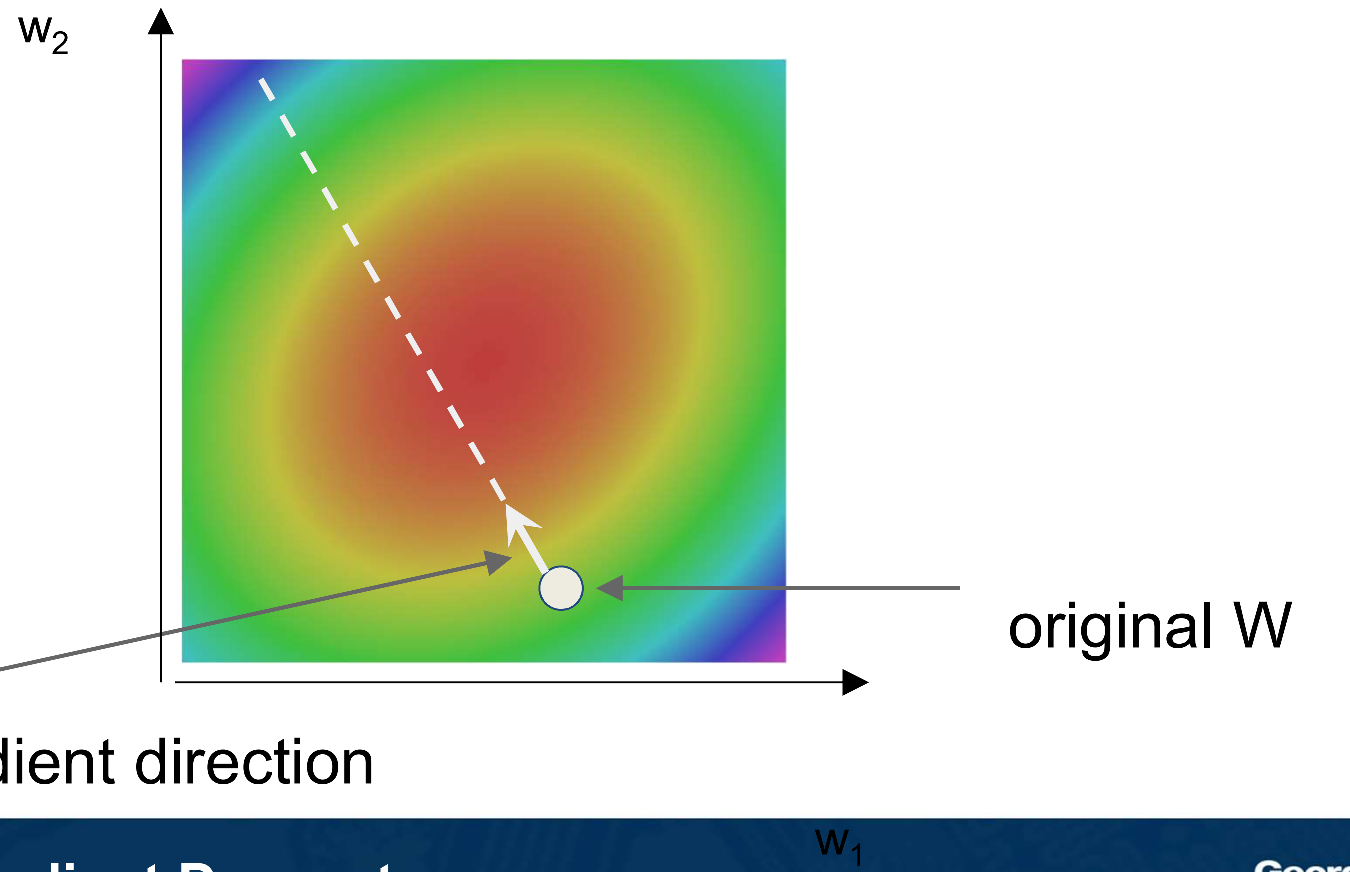
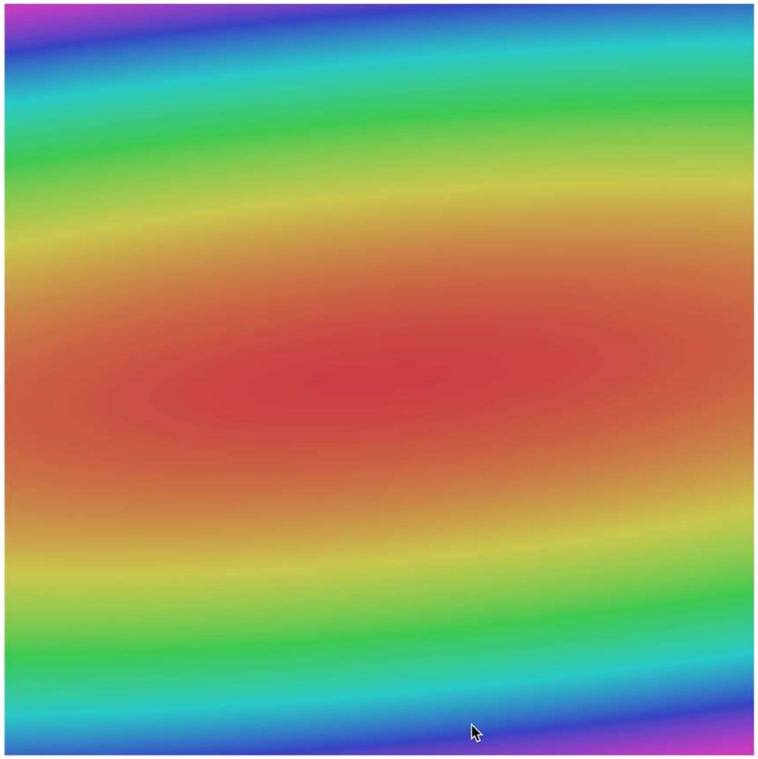
This idea can be turned into an **algorithm (gradient descent)**

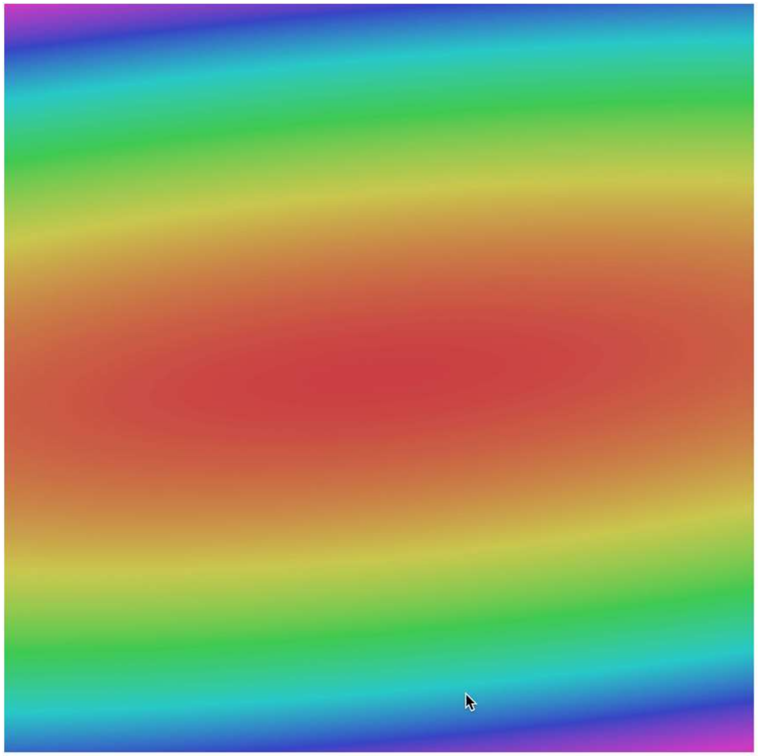
- Choose a model: $\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{W}) = \mathrm{Wx}$
- Choose loss function: $\boldsymbol{L_i} = |\boldsymbol{y} - \boldsymbol{W}\boldsymbol{x_i}|^2$
- Calculate partial derivative for each parameter: $\frac{\partial \boldsymbol{L}}{\partial \boldsymbol{w_i}}$
- Update the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

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



Gradient Descent





w_1

Gradient Descent

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

- Full Batch Gradient Descent $$\boldsymbol{L} = \frac{\mathbf{1}}{\boldsymbol{N}} \sum \boldsymbol{L}\left(\boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{W}), \boldsymbol{y}_i\right)$$
- Mini-Batch Gradient Descent $$\boldsymbol{L} = \frac{\mathbf{1}}{\boldsymbol{M}} \sum \boldsymbol{L}\left(\boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{W}), \boldsymbol{y}_i\right)$$
  - Where M is a *subset* of data
- We iterate over mini-batches:
  - Get mini-batch, compute loss, compute derivatives, and take a set

Mini-Batch Gradient Descent

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Gradient descent is guaranteed to converge under some conditions

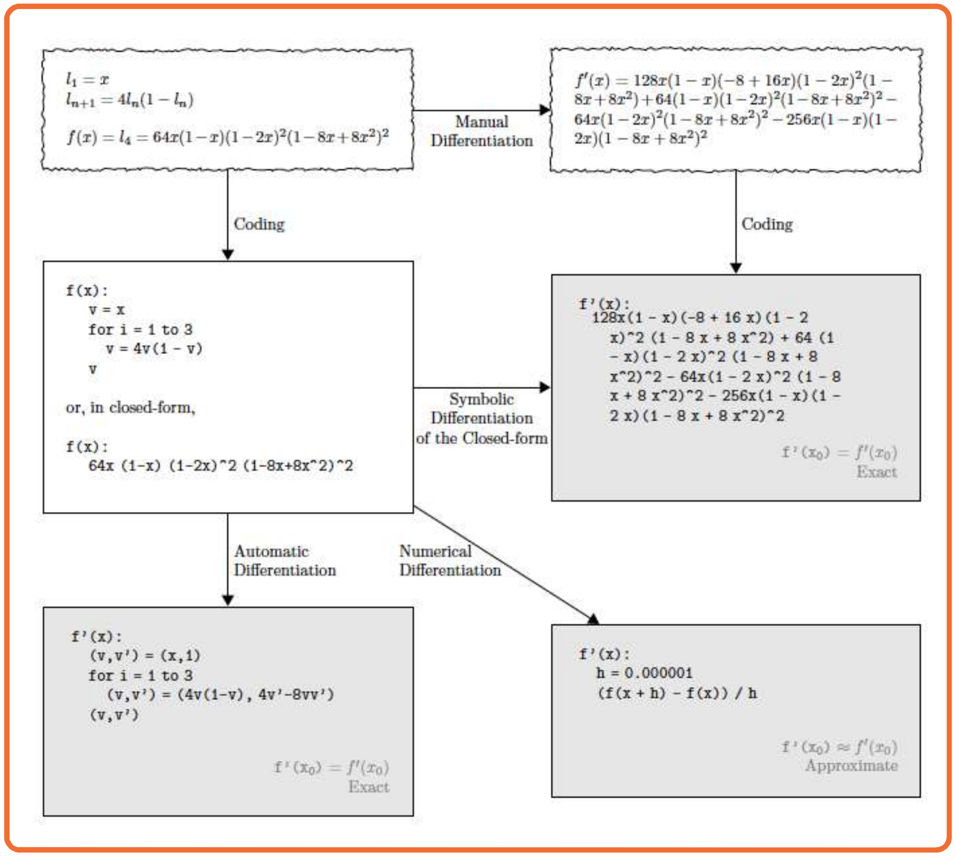
- For example, learning rate has to be appropriately reduced throughout training
- It will converge to a *local* minima
  - Small changes in weights would not decrease the loss
- It turns out that some of the local minima that it finds in practice (if trained well) are still pretty good!

Gradient Descent Properties

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

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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:

[?,
?,
?,
?,
?,
?,
?,
?,
?,…]

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**	

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 (first dim)**:**

[0.34 + **0.0001**,
-1.11,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25322

gradient dW:

[**-2.5**,
?,
?,

(1.25322 - 1.25347)/0.0001
= -2.5

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

?,
?,…]

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

current W:	**W + h** (second dim)**:**	**gradient dW:**
[0.34,	[0.34,	[-2.5,
-1.11,	-1.11 + **0.0001**,	?,
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 1.25353**	

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

current W:	**W + h** (second dim)**:**	**gradient dW:**
[0.34,	[0.34,	[-2.5,
-1.11,	-1.11 + **0.0001**,	**0.6**,
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 1.25353**	

(1.25353 - 1.25347)/0.0001
= 0.6

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

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

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**	

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**,
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**	

(1.25347 - 1.25347)/0.0001
= 0

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

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 write :)
Analytic gradient: fast :), exact :), error-prone :(

In practice: Derive analytic gradient, check your implementation with numerical gradient.
This is called a **gradient check.**

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

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

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- Manual differentiation
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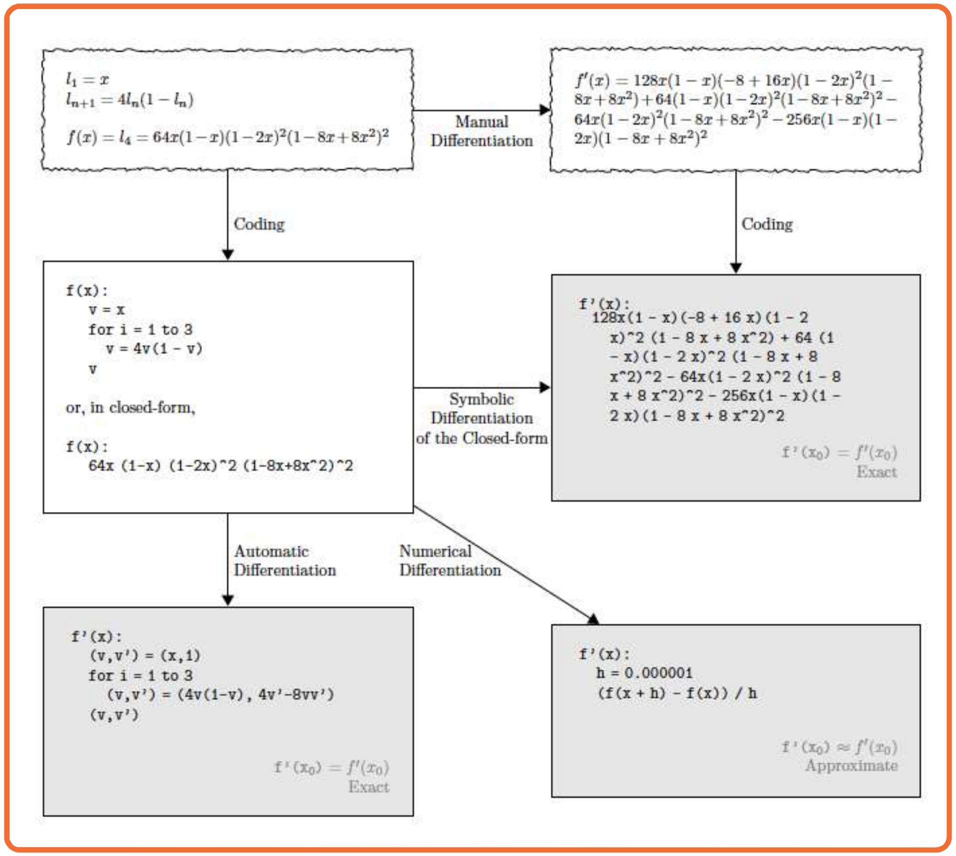
- Automatic differentiation



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For some functions, we can analytically derive the partial derivative

Example:

Function

$$f(w, x_i) = w^T x_i$$

Loss

$$(y_i - w^T x_i)^2$$

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

Update Rule

$$w_j \leftarrow w_j + 2\eta \sum_{k=1}^{N} \delta_k x_{kj}$$

Derivation of Update Rule

For some functions, we can analytically derive the partial derivative

Example:

Function

$$f(w, x_i) = w^T x_i$$

Loss

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

Update Rule

$$w_j \leftarrow w_j + 2\eta \sum_{k=1}^{N} \delta_k x_{kj}$$

Derivation of Update Rule

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

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

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

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

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

$$= \sum_{k=1}^{N} 2(y_k - w^T x_k) \frac{\partial}{\partial w_j} (y_k - w^T x_k)$$

$$= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} w^T x_k$$

…where… $\delta_k = y_k - w^T x_k$

$$= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} \sum_{i=1}^{m} w_i x_{ki}$$

$$= -2 \sum_{k=1}^{N} \delta_k x_{kj}$$

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

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

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

$$\mathrm{f(x)} = \sigma\left(\sum_k w_k x_k\right)$$

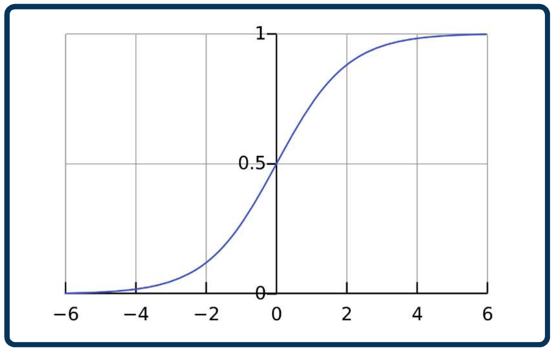
$$\mathrm{L} = \sum_i \left(y_i - \sigma\left(\sum_k w_k x_{ik}\right)\right)^2$$

$$\frac{\partial L}{\partial w_j} = \sum_i 2\left(y_i - \sigma\left(\sum_k w_k x_{ik}\right)\right)\left(-\frac{\partial}{\partial w_j}\sigma\left(\sum_k w_k x_{ik}\right)\right)$$

$$= \sum_i -2\left(y_i - \sigma\left(\sum_k w_k x_{ik}\right)\right)\sigma'\left(\sum_k w_k x_{ik}\right)\frac{\partial}{\partial w_j}\sum_k w_k x_{ik}$$

$$= \sum_i -2\delta_i \sigma(\mathrm{d}_i)(1-\sigma(\mathrm{d}_i))x_{ij}$$

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



The sigmoid perception update rule:

$$w_j \leftarrow w_j + 2\eta \sum_{k=1}^{N} \delta_i \sigma_i (1-\sigma_i) x_{ij}$$

where $\sigma_i = \sigma\left(\sum_{j=1}^{m} w_j x_{ij}\right)$

$$\delta_i = y_i - \sigma_i$$

Adding a Non-Linear Function

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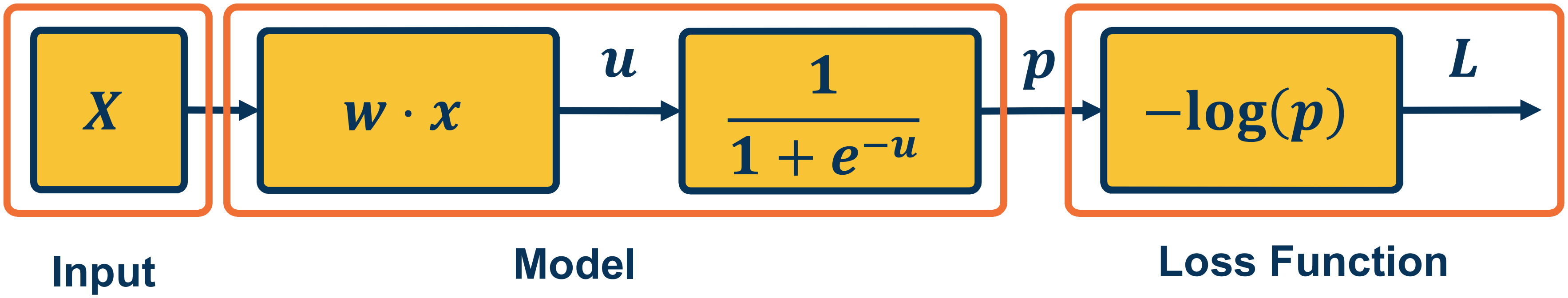
Neural Network View of a Linear Classifier

A **linear classifier** can be broken down into:

- Input
- A function of the input
- A loss function

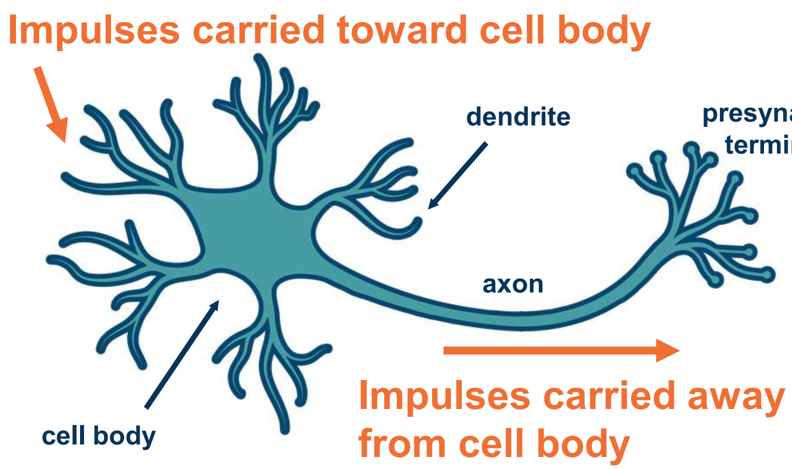
It's all just one function that can be **decomposed** into building blocks

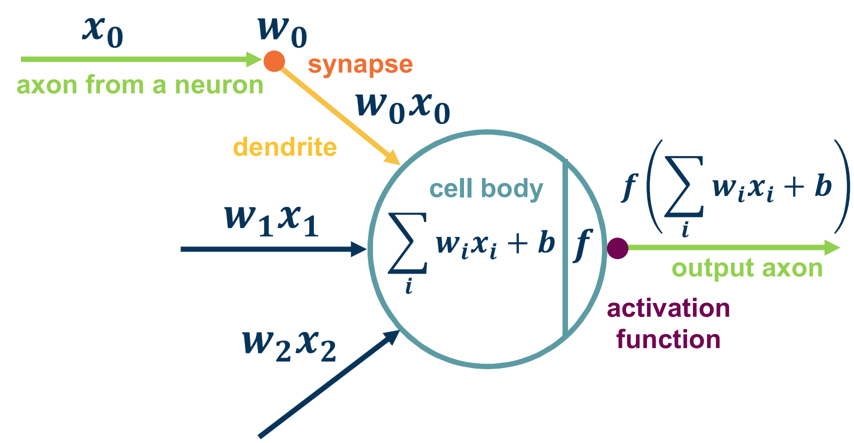


What Does a Linear Classifier Consist of?

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)

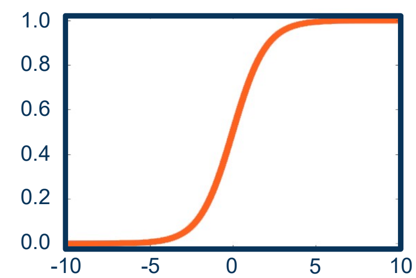




Figures adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

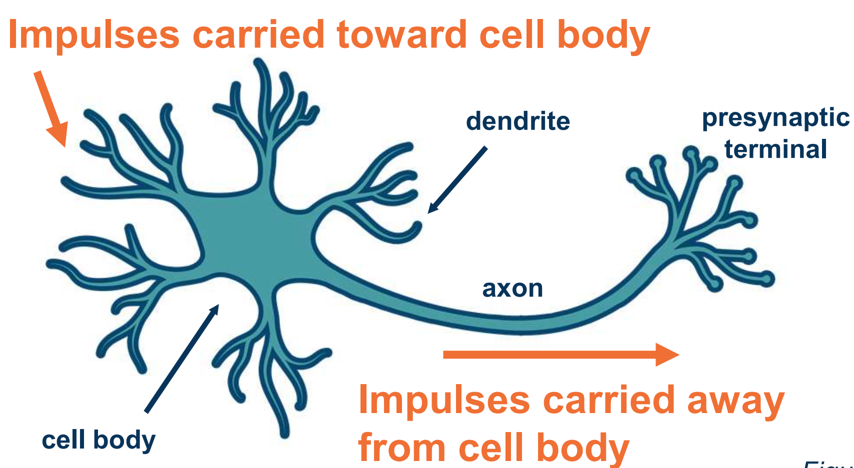
Origins of the Term Neural Network

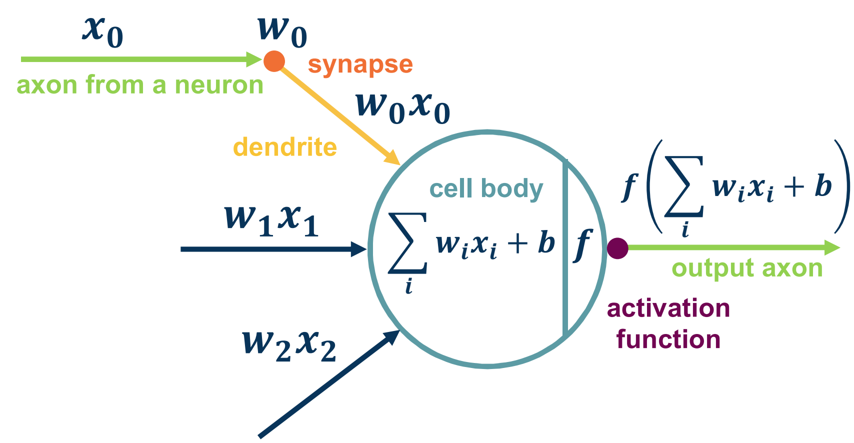
As we did before, the output of a neuron can be modulated by a non-linear function (e.g. sigmoid)



Sigmoid Activation Function

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





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

Adding Non-Linearities

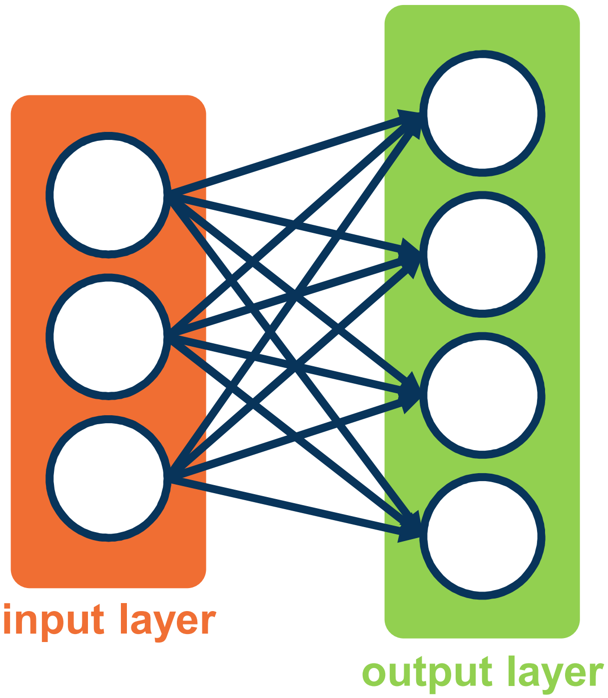
We can have **multiple** neurons connected to the same input

Corresponds to a multi-class classifier

- Each output node outputs the score for a class

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

- Often called fully connected layers
  - Also called a linear *projection layer*



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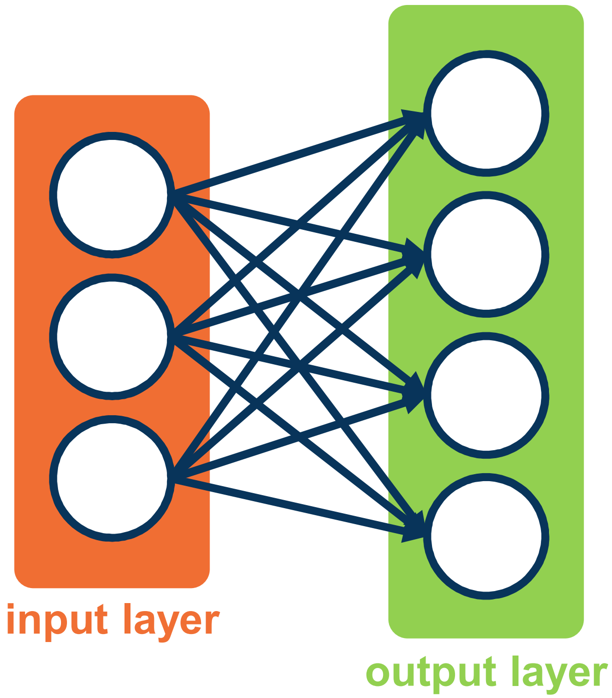
- Each input/output is a **neuron (node)**
- A linear classifier (+ optional non-linearity) is called a **fully connected** layer
- Connections are represented as **edges**
- Output of a particular neuron is referred to as **activation**
- This will be expanded as we view computation in a neural network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



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Neural Network Terminology

We can **stack** multiple layers together

- Input to second layer is output of first layer

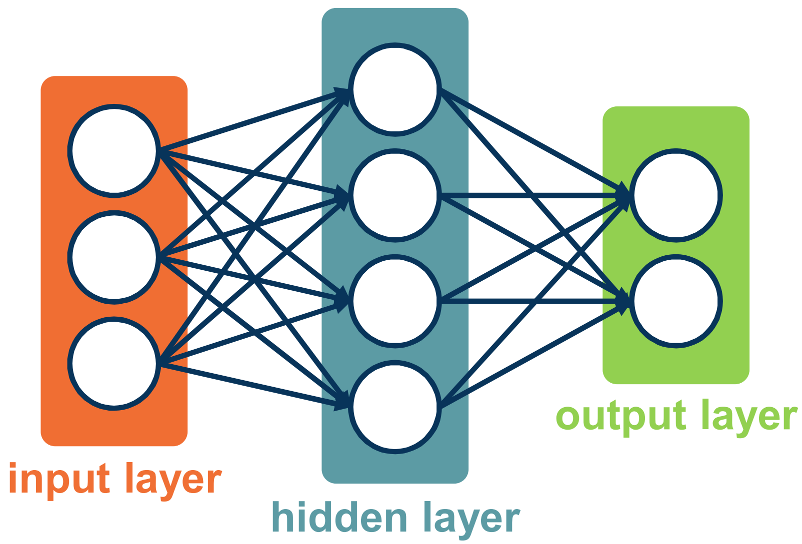
Called a **2-layered neural network** (input is not counted)

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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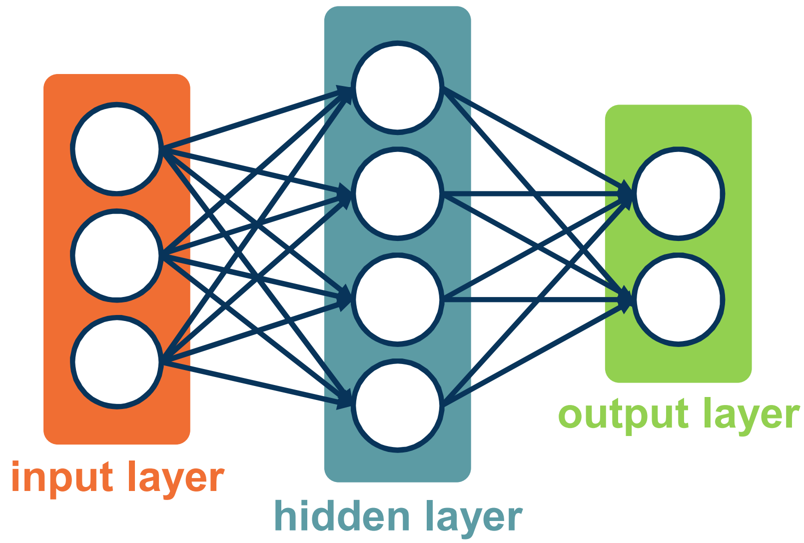
Connecting Many Layers

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)



$\boldsymbol{x}$ $\quad$ $\boldsymbol{W_1}$ $\quad$ $\boldsymbol{W_2}$

$$=$$

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

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

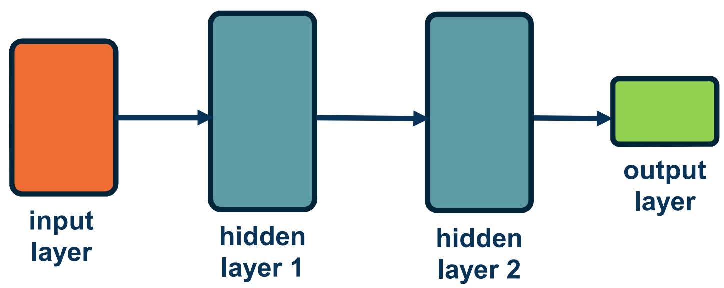
The Linear Algebra View

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**:



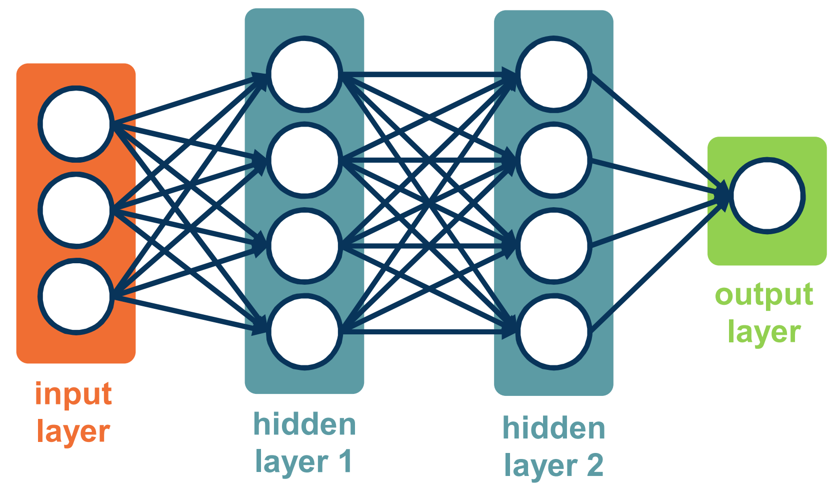


Figure adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Adding More Layers!

Computation Graphs

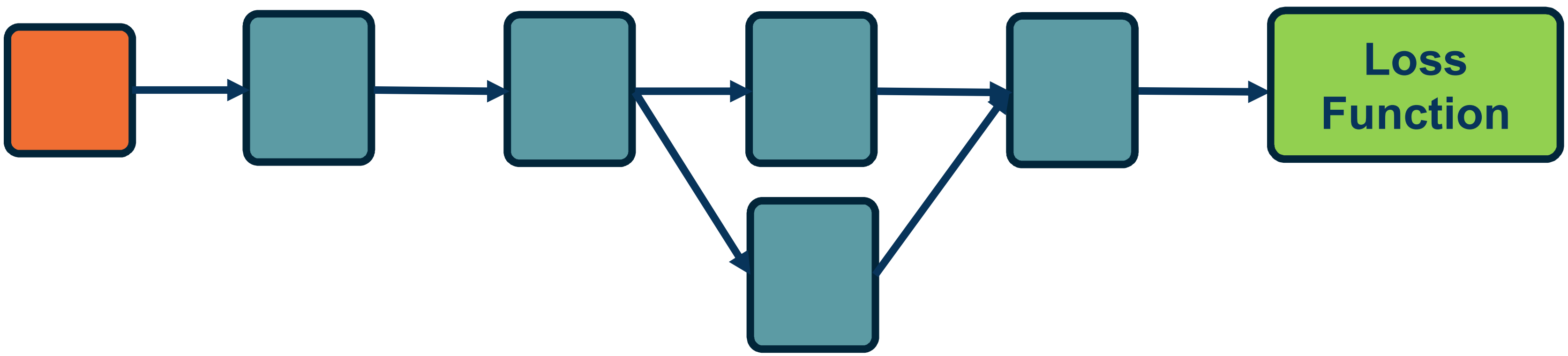
Functions can be made **arbitrarily complex** (subject to memory and computational limits), e.g.:

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

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

- At the end, **add the loss function**

Composition can have **some structure**



Adding Even More Layers

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

VISION

pixels → edge → texton → motif → part → object

SPEECH

sample → spectral band → formant → motif → phone → word

NLP

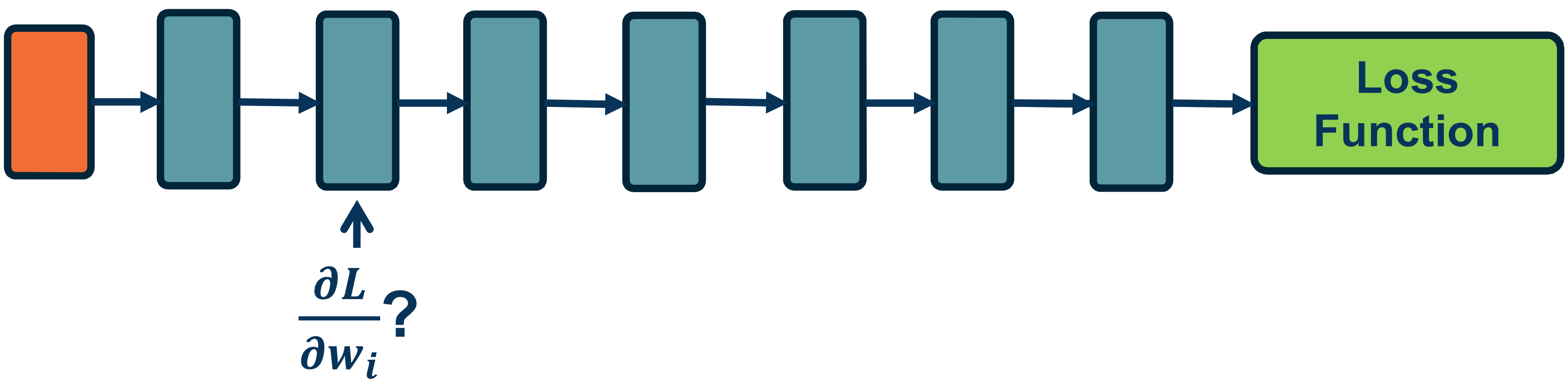
character → word → NP/VP/.. → clause → sentence → story

Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

- **Pixels -> edges -> object parts -> objects**

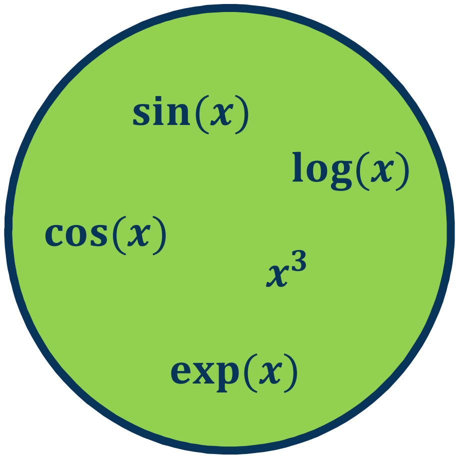
Compositionality

- 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



Computing Gradients in Complex Function

Given a library of simple functions



Compose into a complicate function

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

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

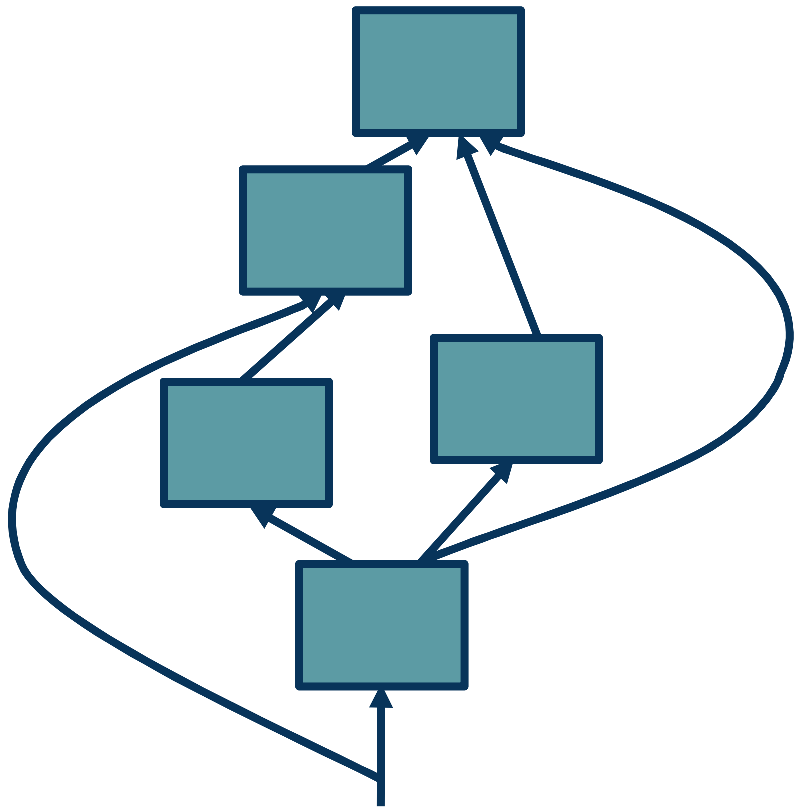
Decomposing a Function

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

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

- Modules must be differentiable to support gradient computations for gradient descent

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



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

A General Framework

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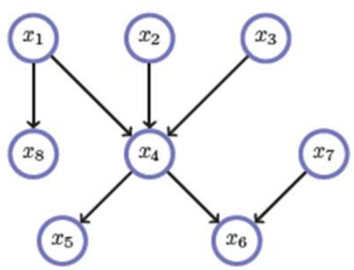
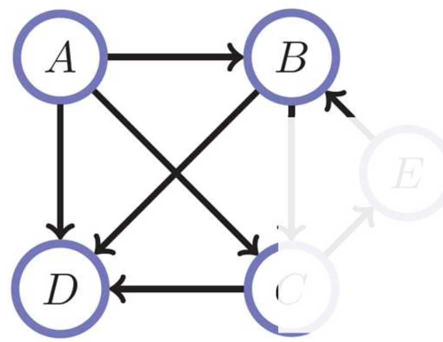
Directed Acyclic Graphs (DAGs)

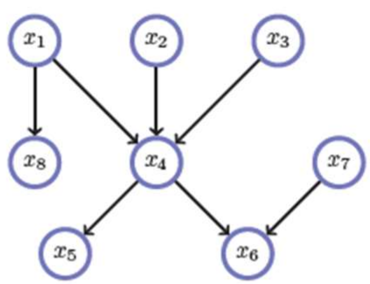
- Exactly what the name suggests
  - Directed edges
  - No (directed) cycles
  - Underlying undirected cycles okay

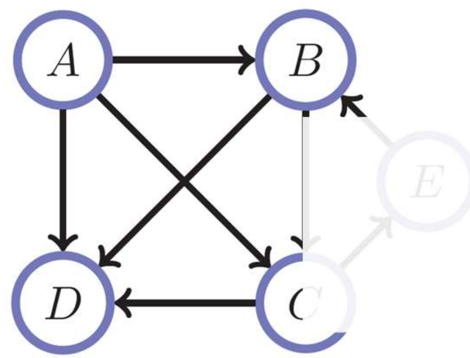




Directed Acyclic Graphs (DAGs)

- Concept
  - Topological Ordering





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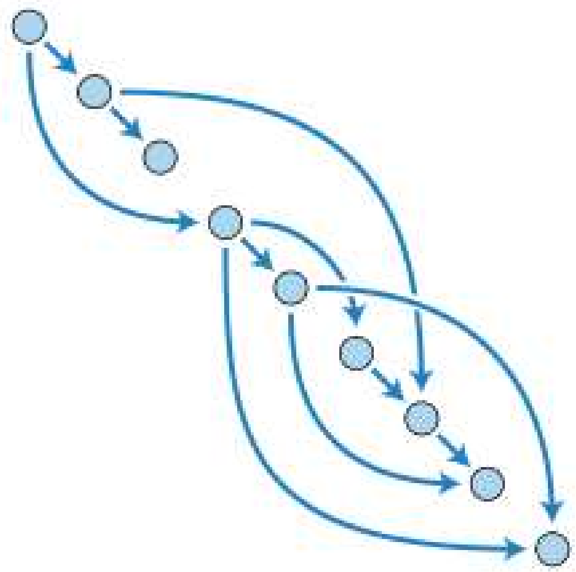
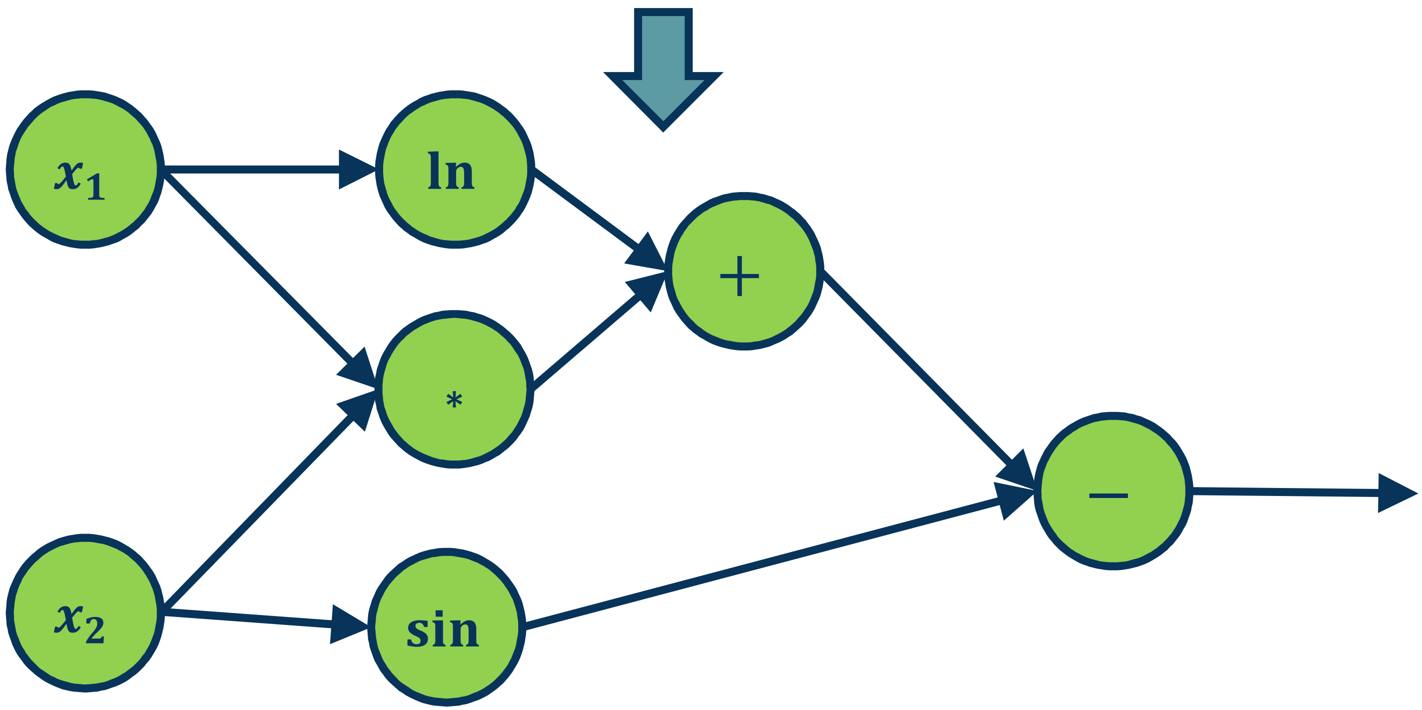
Directed Acyclic Graphs (DAGs)

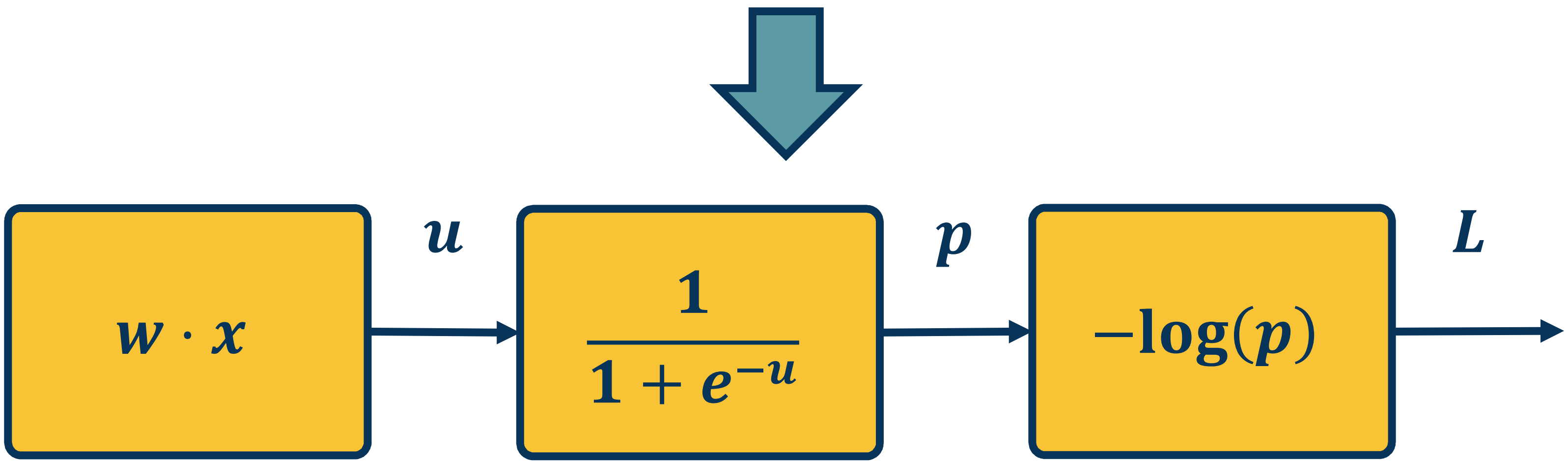


$$f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$$



Example

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



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Machine Learning Example

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Backpropagation

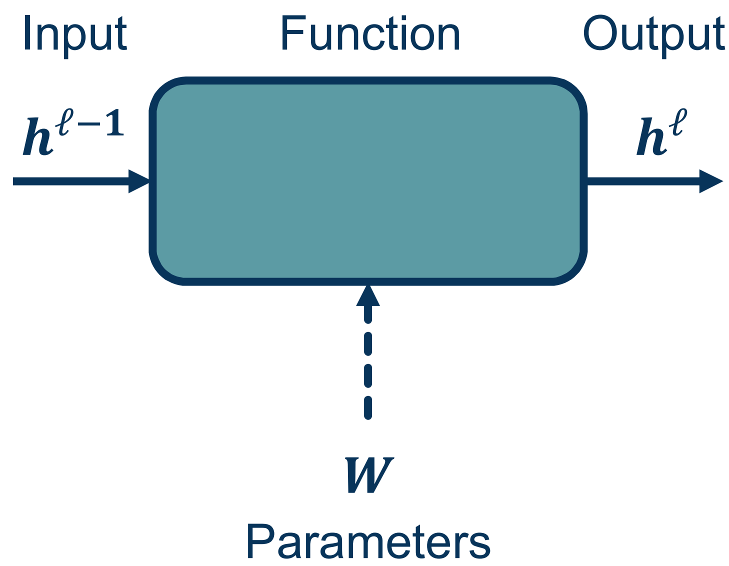
Given this computation graph, the training algorithm will:

- 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:

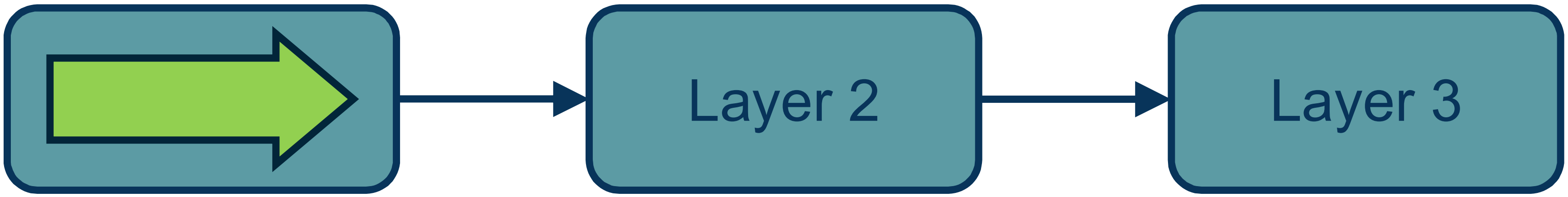
- Starts at **loss function** where we know how to calculate the gradients
- Progresses back through the modules
- Ends in the **input layer** where we do not need gradients (no parameters)

This algorithm is called **backpropagation**



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

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



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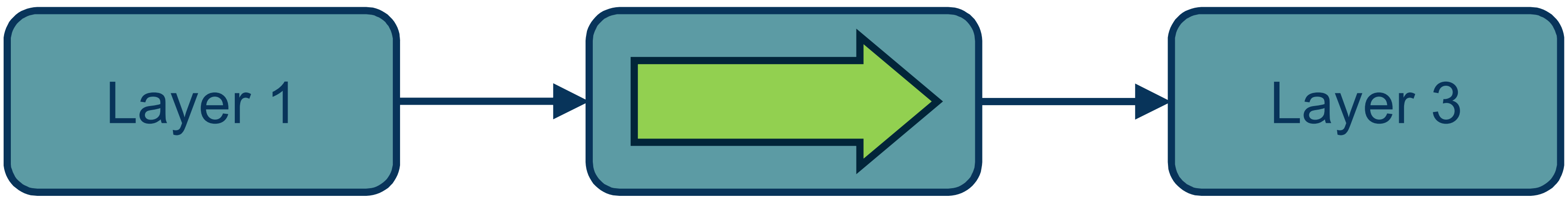

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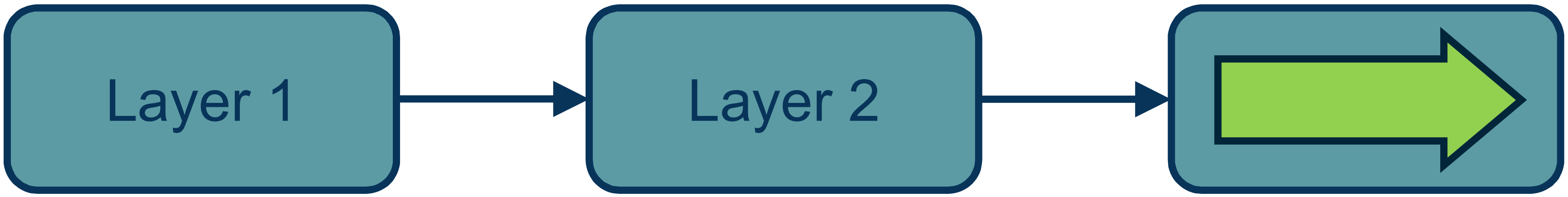


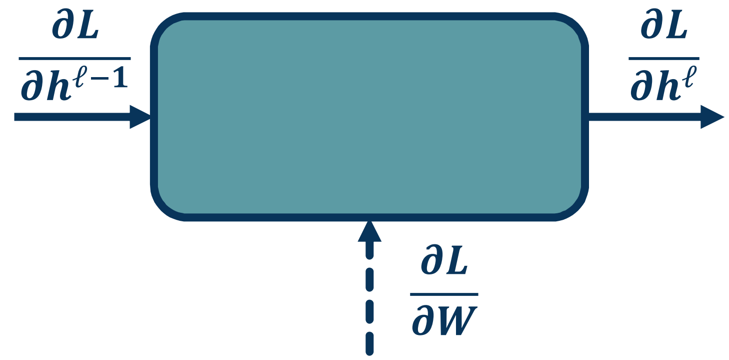
Note that we must store the **intermediate outputs of all layers**!

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

Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

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

Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

Backward Pass Computations

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

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

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

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

and $\frac{\partial \boldsymbol{h}_i^{\ell}}{\partial \boldsymbol{w}_i} = \boldsymbol{h}^{\ell-1,T}$

Computing the Local Gradients: Example

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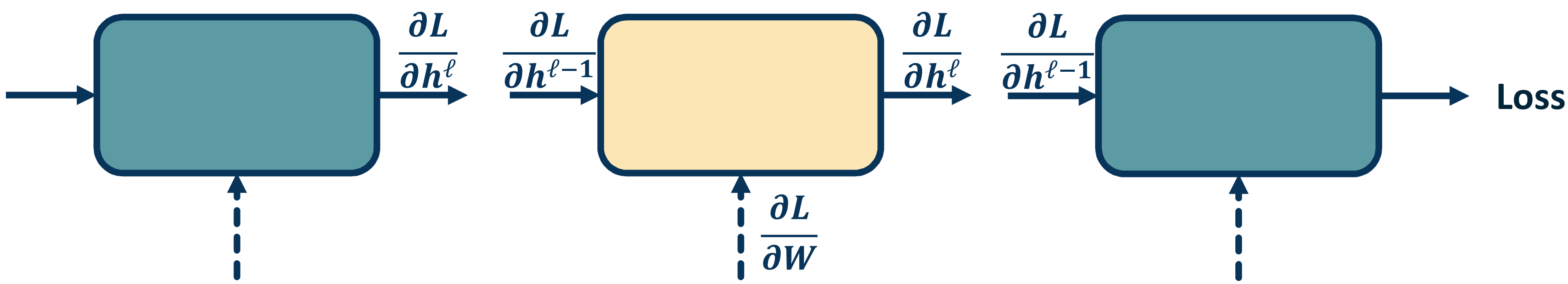
- We want to to compute: $\{\frac{\partial L}{\partial h^{\ell-1}}, \frac{\partial L}{\partial W}\}$



- We will use the *chain rule* to do this:

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

Computing the Gradients of Loss

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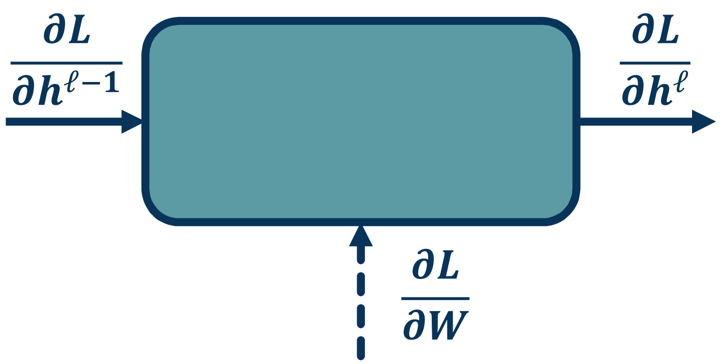
- We will use the **chain rule** to compute: $\{\frac{\partial L}{\partial h^{\ell-1}}, \frac{\partial L}{\partial W}\}$
- **Gradient of loss w.r.t. inputs:** $\frac{\partial L}{\partial h^{\ell-1}} = \frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial h^{\ell-1}}$

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

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



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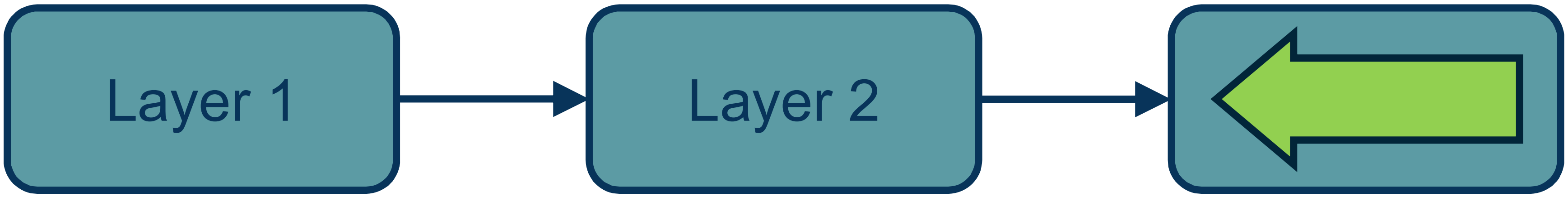
Computing the Gradients of Loss

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

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



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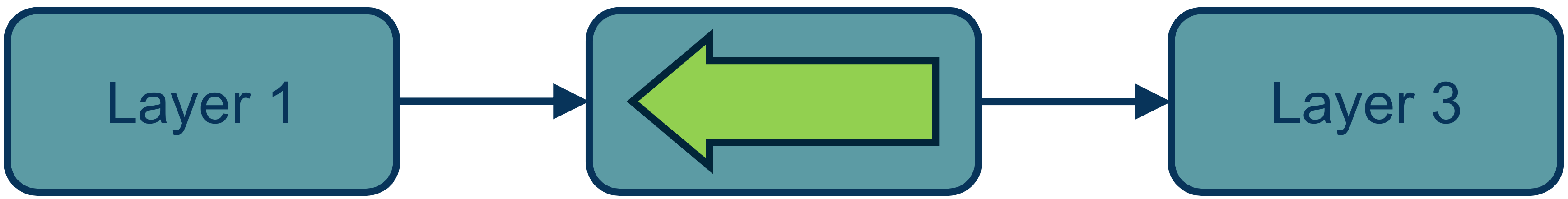

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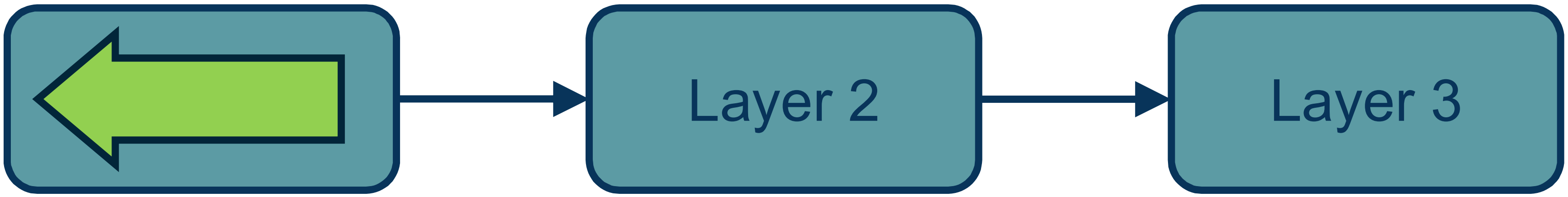

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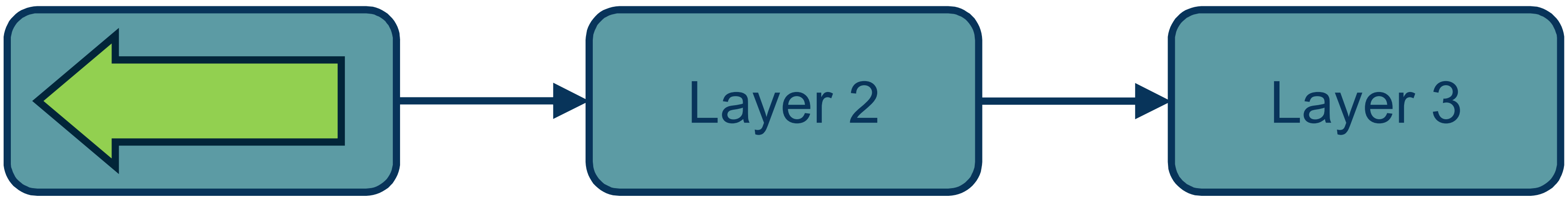
Step 1: Compute Loss on Mini-Batch: **Forward Pass**

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

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

Backpropagation: a simple example

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

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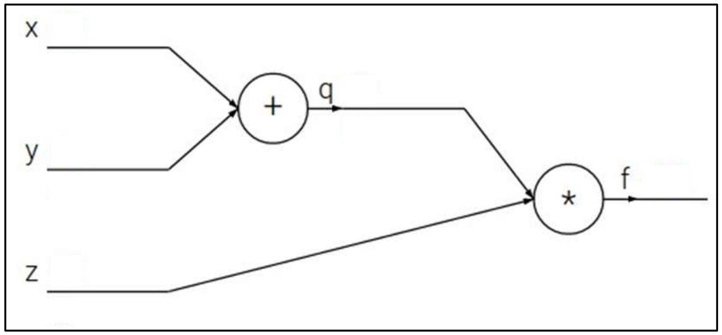
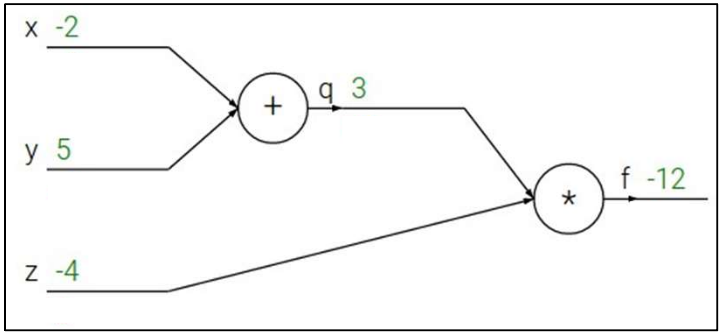


Backpropagation: a simple example

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

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



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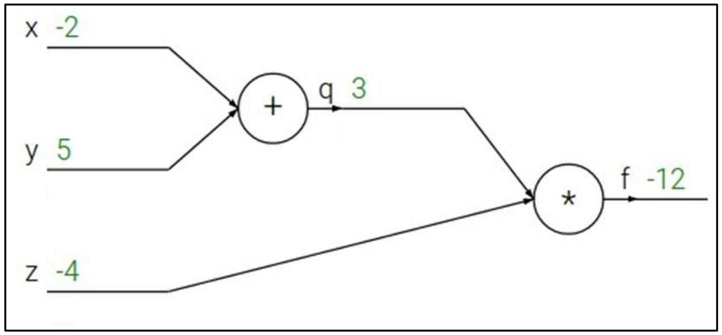

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

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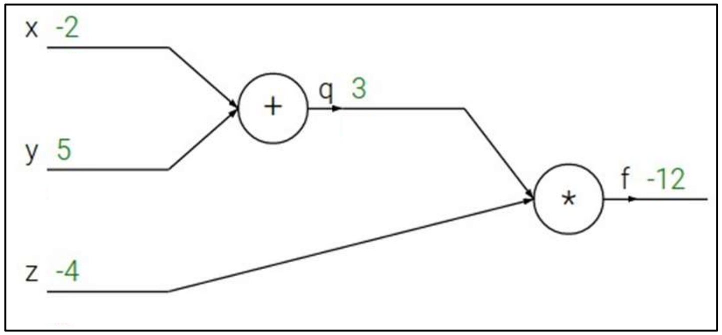

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

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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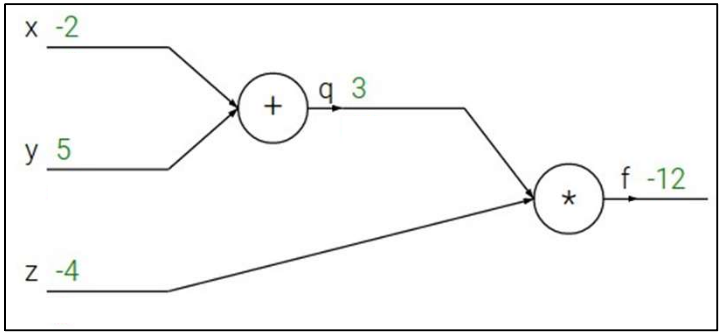

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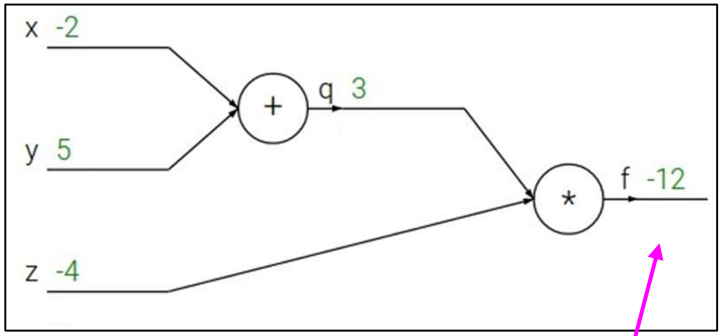

$\frac{\partial f}{\partial f}$

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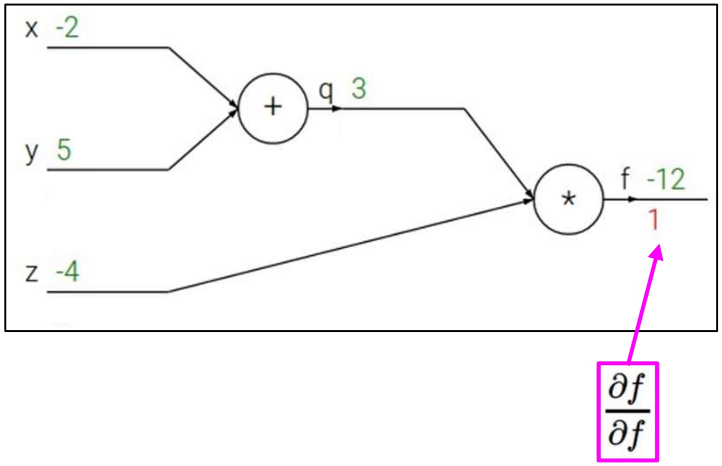

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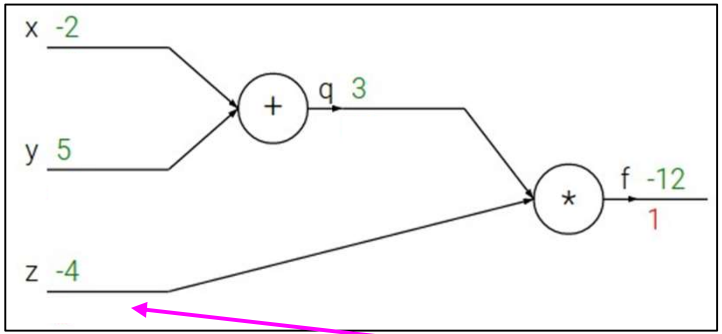

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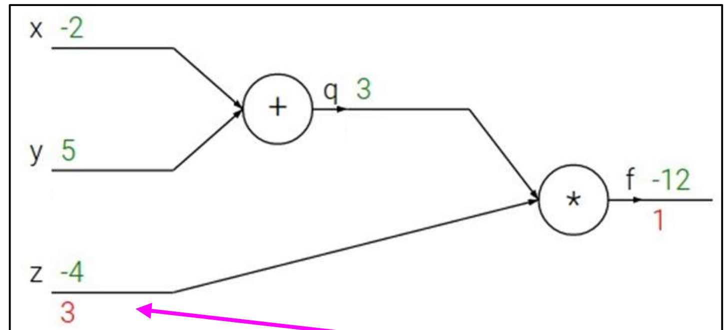

$$\frac{\partial f}{\partial z}$$

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

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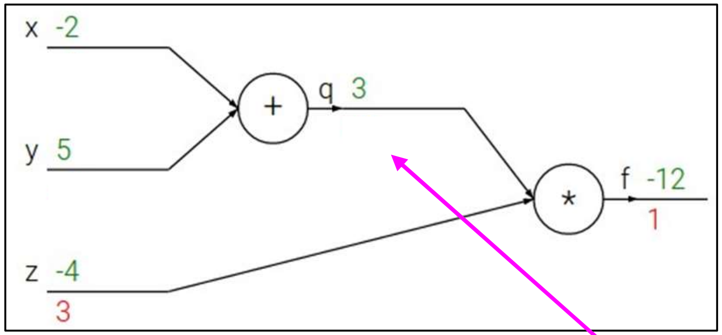

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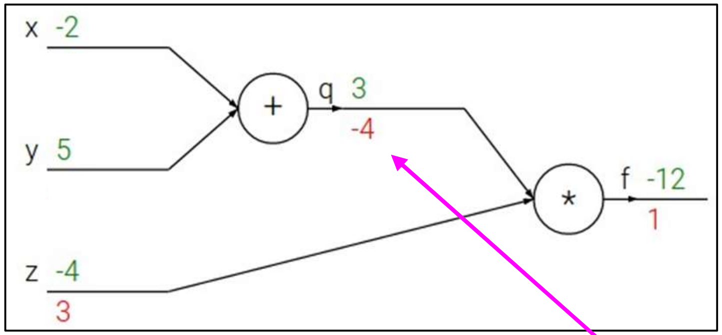

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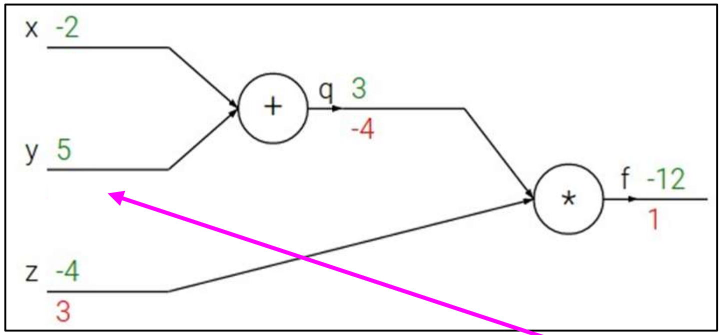

$$\frac{\partial f}{\partial y}$$

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

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

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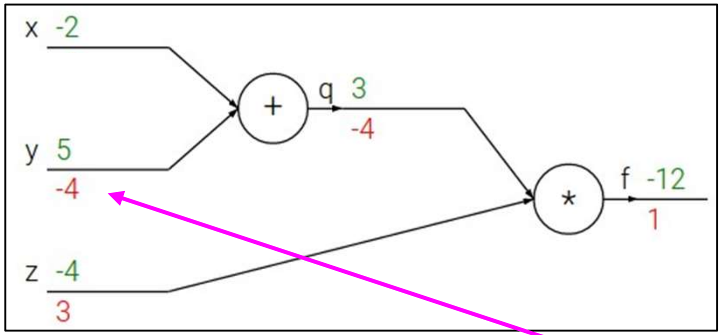

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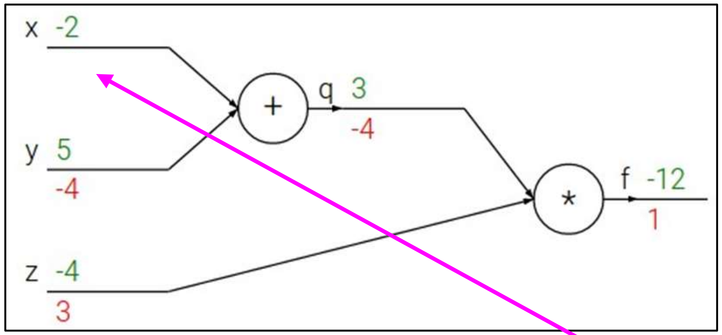

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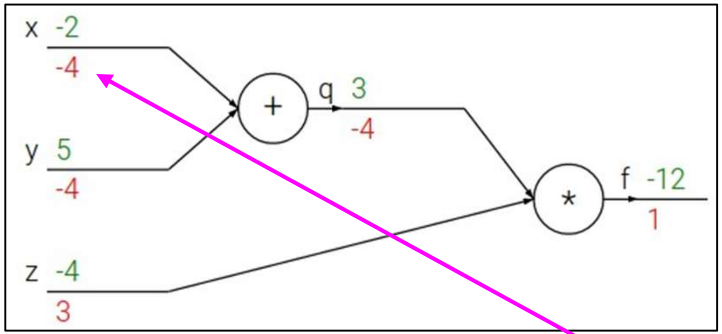

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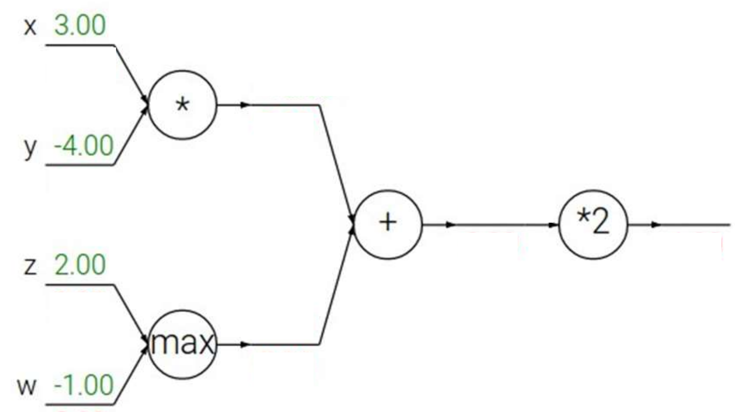
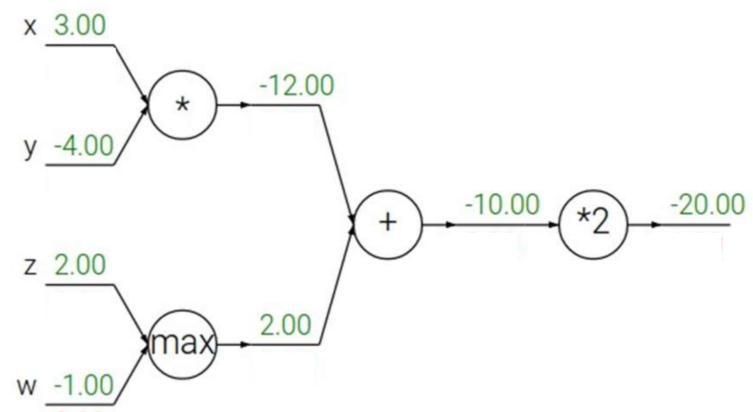
Upstream gradient

Local gradient

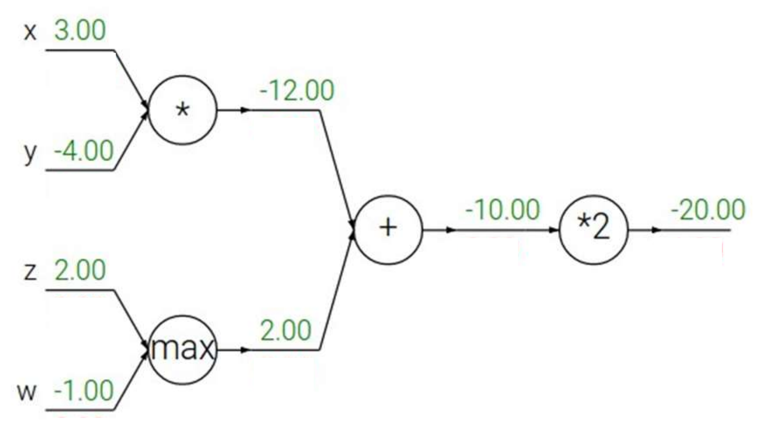
Backpropagation: a simple example



Backpropagation: a simple example

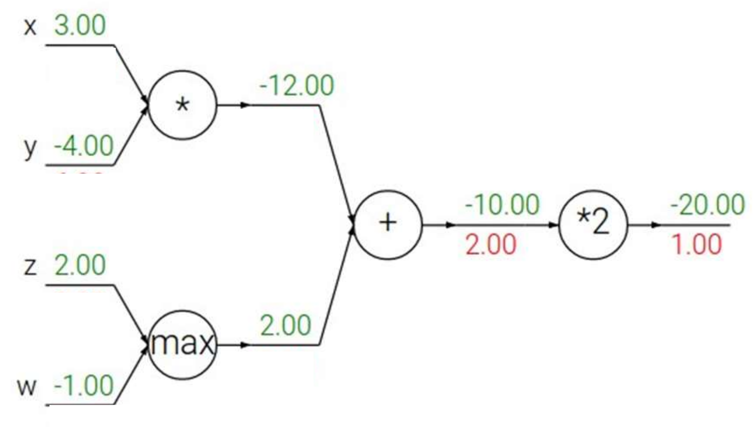


Patterns in backward flow



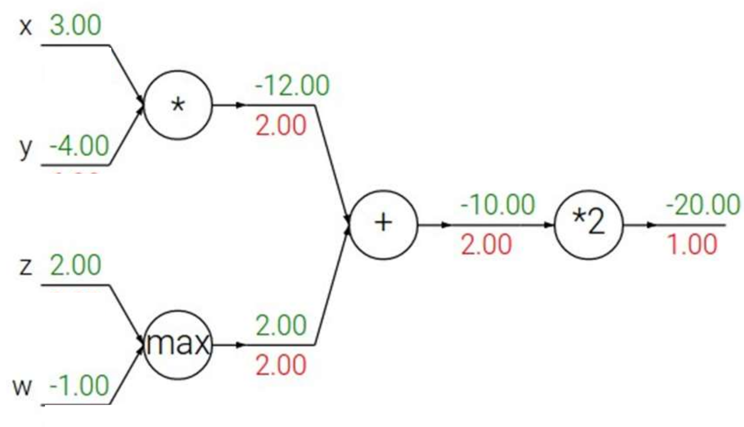
Patterns in backward flow

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



Patterns in backward flow

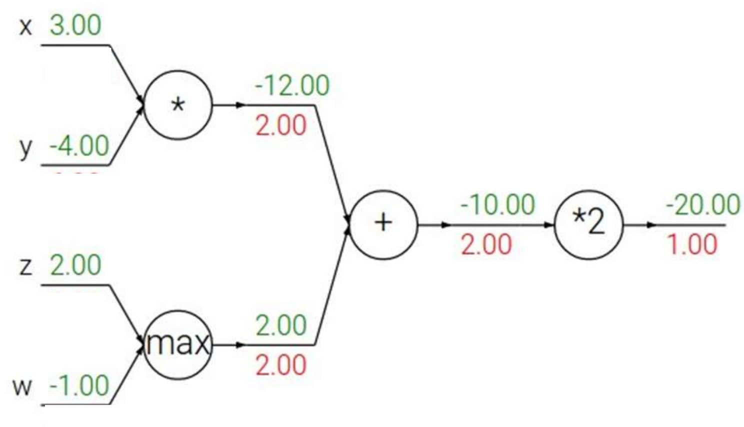
add gate: gradient distributor



Patterns in backward flow

add gate: gradient distributor

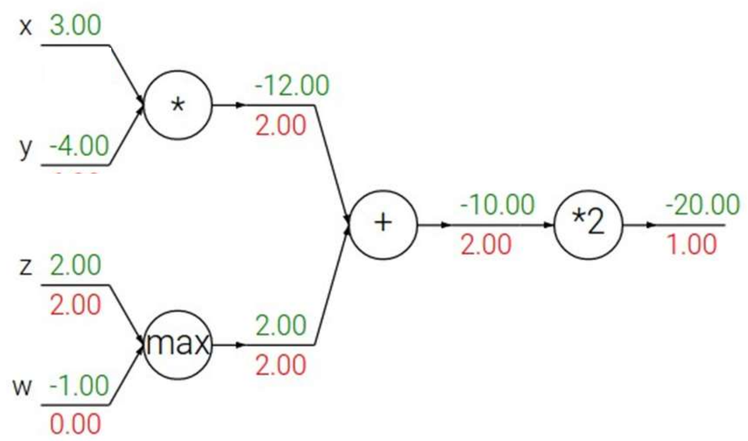
Q: What is a **max** gate?



Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

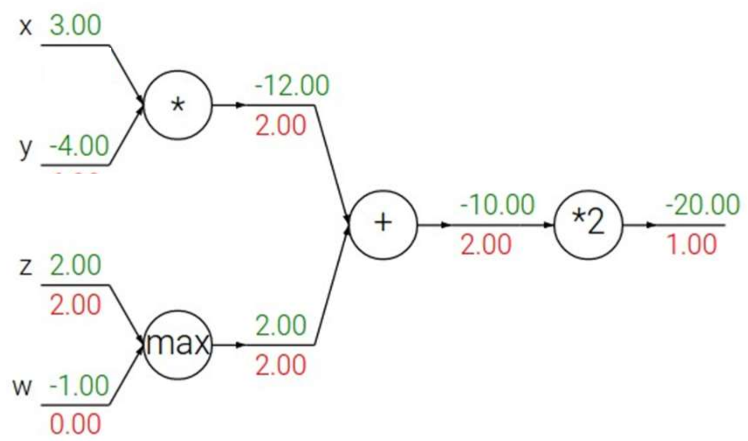


Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

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

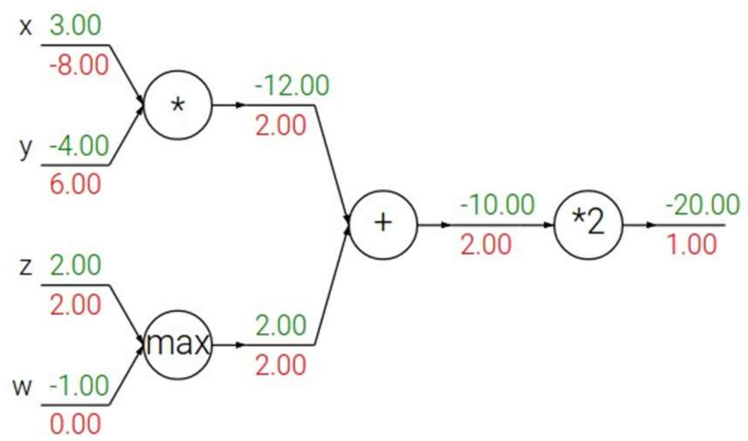


Patterns in backward flow

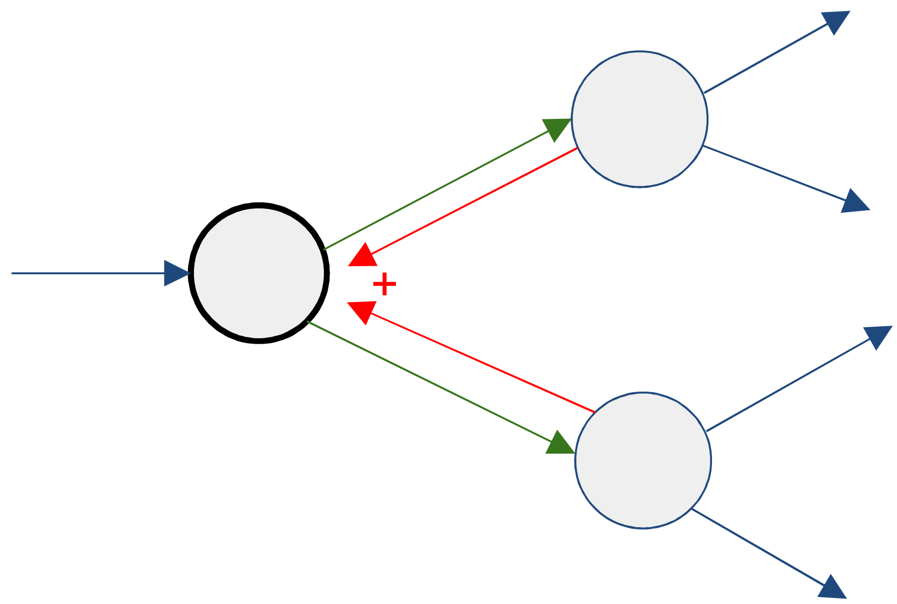
add gate: gradient distributor

max gate: gradient router

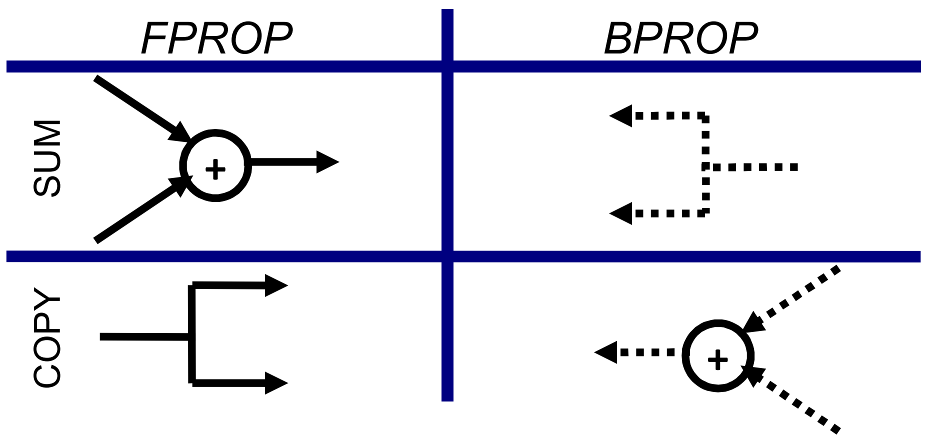
mul gate: gradient switcher



Gradients add at branches



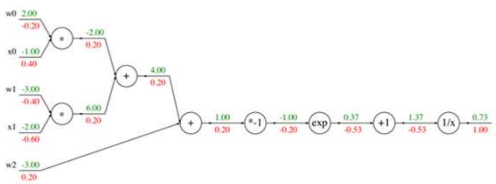
Duality in Fprop and Bprop



Deep Learning = Differentiable Programming

- Computation = Graph
  - Input = Data + Parameters
  - Output = Loss
  - Scheduling = Topological ordering
- What do we need to do?
  - Generic code for representing the graph of modules
  - Specify modules (both forward and backward function)

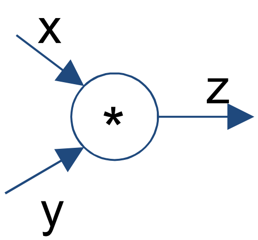
Modularized implementation: forward / backward API



Graph (or Net) object *(rough psuedo code)*

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

Modularized implementation: forward / backward API



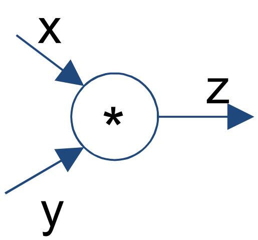
(x,y,z are scalars)

```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        return z
    def backward(dz):
        # dx = ... #todo
        # dy = ... #todo
        return [dx, dy]
```

$$\frac{\partial L}{\partial z}$$

$$\frac{\partial L}{\partial x}$$

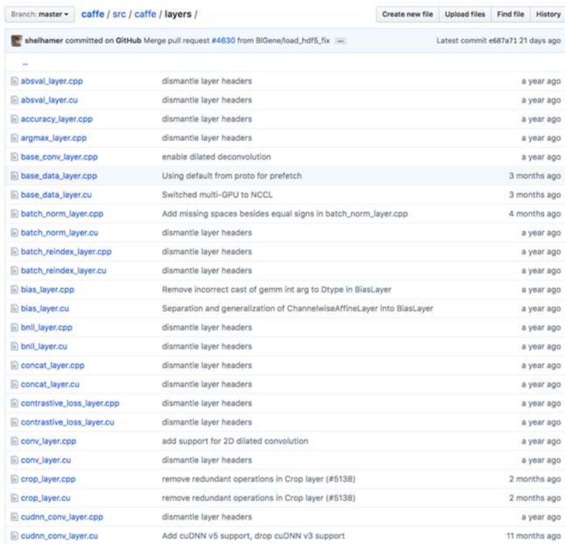
Modularized implementation: forward / backward API



(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]
```

Example: Caffe layers



Branch: master ▾ caffe / src / caffe / layers /

Create new file | Upload files | Find file | History

shelhamer committed on GitHub Merge pull request #4630 from BlGene/load_hdf5_fix … Latest commit e687a71 21 days ago

..		
absval_layer.cpp	dismantle layer headers	a year ago
absval_layer.cu	dismantle layer headers	a year ago
accuracy_layer.cpp	dismantle layer headers	a year ago
argmax_layer.cpp	dismantle layer headers	a year ago
base_conv_layer.cpp	enable dilated deconvolution	a year ago
base_data_layer.cpp	Using default from proto for prefetch	3 months ago
base_data_layer.cu	Switched multi-GPU to NCCL	3 months ago
batch_norm_layer.cpp	Add missing spaces besides equal signs in batch_norm_layer.cpp	4 months ago
batch_norm_layer.cu	dismantle layer headers	a year ago
batch_reindex_layer.cpp	dismantle layer headers	a year ago
batch_reindex_layer.cu	dismantle layer headers	a year ago
bias_layer.cpp	Remove incorrect cast of gemm int arg to Dtype in BiasLayer	a year ago
bias_layer.cu	Separation and generalization of ChannelwiseAffineLayer into BiasLayer	a year ago
bnll_layer.cpp	dismantle layer headers	a year ago
bnll_layer.cu	dismantle layer headers	a year ago
concat_layer.cpp	dismantle layer headers	a year ago
concat_layer.cu	dismantle layer headers	a year ago
contrastive_loss_layer.cpp	dismantle layer headers	a year ago
contrastive_loss_layer.cu	dismantle layer headers	a year ago
conv_layer.cpp	add support for 2D dilated convolution	a year ago
conv_layer.cu	dismantle layer headers	a year ago
crop_layer.cpp	remove redundant operations in Crop layer (#5138)	2 months ago
crop_layer.cu	remove redundant operations in Crop layer (#5138)	2 months ago
cudnn_conv_layer.cpp	dismantle layer headers	a year ago
cudnn_conv_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago

cudnn_lcn_layer.cpp	dismantle layer headers	a year ago
cudnn_lcn_layer.cu	dismantle layer headers	a year ago
cudnn_lrn_layer.cpp	dismantle layer headers	a year ago
cudnn_lrn_layer.cu	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 v5 support, drop cuDNN v3 support	11 months ago
cudnn_sigmoid_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_sigmoid_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_softmax_layer.cpp	dismantle layer headers	a year ago
cudnn_softmax_layer.cu	dismantle layer headers	a year ago
cudnn_tanh_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_tanh_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
data_layer.cpp	Switched multi-GPU to NCCL	3 months ago
deconv_layer.cpp	enable dilated deconvolution	a year ago
deconv_layer.cu	dismantle layer headers	a year ago
dropout_layer.cpp	supporting N-D Blobs in Dropout layer Reshape	a year ago
dropout_layer.cu	dismantle layer headers	a year ago
dummy_data_layer.cpp	dismantle layer headers	a year ago
eltwise_layer.cpp	dismantle layer headers	a year ago
eltwise_layer.cu	dismantle layer headers	a year ago
elu_layer.cpp	ELU layer with basic tests	a year ago
elu_layer.cu	ELU layer with basic tests	a year ago
embed_layer.cpp	dismantle layer headers	a year ago
embed_layer.cu	dismantle layer headers	a year ago
euclidean_loss_layer.cpp	dismantle layer headers	a year ago
euclidean_loss_layer.cu	dismantle layer headers	a year ago
exp_layer.cpp	Solving issue with exp layer with base e	a year ago
exp_layer.cu	dismantle layer headers	a year ago

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Caffe Sigmoid Layer

```cpp
#include <cmath>
#include <vector>

#include "caffe/layers/sigmoid_layer.hpp"

namespace caffe {

template <typename Dtype>
inline Dtype sigmoid(Dtype x) {
  return 1. / (1. + exp(-x));
}

template <typename Dtype>
void SigmoidLayer<Dtype>::Forward_cpu(const vector<Blob<Dtype>*>& bottom,
    const vector<Blob<Dtype>*>& top) {
  const Dtype* bottom_data = bottom[0]->cpu_data();
  Dtype* top_data = top[0]->mutable_cpu_data();
  const int count = bottom[0]->count();
  for (int i = 0; i < count; ++i) {
    top_data[i] = sigmoid(bottom_data[i]);
  }
}

template <typename Dtype>
void SigmoidLayer<Dtype>::Backward_cpu(const vector<Blob<Dtype>*>& top,
    const vector<bool>& propagate_down,
    const vector<Blob<Dtype>*>& bottom) {
  if (propagate_down[0]) {
    const Dtype* top_data = top[0]->cpu_data();
    const Dtype* top_diff = top[0]->cpu_diff();
    Dtype* bottom_diff = bottom[0]->mutable_cpu_diff();
    const int count = bottom[0]->count();
    for (int i = 0; i < count; ++i) {
      const Dtype sigmoid_x = top_data[i];
      bottom_diff[i] = top_diff[i] * sigmoid_x * (1. - sigmoid_x);
    }
  }
}

#ifdef CPU_ONLY
STUB_GPU(SigmoidLayer);
#endif

INSTANTIATE_CLASS(SigmoidLayer);


}  // namespace caffe
```

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

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