Neural Networks

CSCI 601-471/671 (NLP: Self-Supervised Models)

https://self-supervised.cs.jhu.edu/sp2025/

How was HW1

- With a show of hand, which one best applies to you:
  1. It was smooth sailing through things I knew; my hamster nearly finished it.
  2. it was familiar stuff but I had to learn or refresh a few things.
  3. It was like shoveling snow in the middle of a blizzard, it just kept getting worse
  4. It was so challenging, it felt like climbing Mount Everest with slippers on.

"Can I use external libraries?" No, unless specified!

- Use the basic Python functions (no external libraries), unless explicitly specified.
- In almost all places, you're not expected to write more than 3-4 lines of code.

```
[ ] # a function that resturns the top `k` most similar words to `input_word`
    def my_most_similar(input_word, k):
      words = embeddings.vocab.keys() # list of words covered by this word embedding
      input_word_emd = embeddings[input_word]

      ### START CODE HERE ###
      ### END CODE HERE ###

      return top_k_most_similar_words


    my_most_similar('cat', 10)
```

“I can’t install ….”

- It may be frustrating to deal with software dependencies…
- But it’s [going to be] part of your job’s reality …
- Embrace it! 🤗

HW2 is released

- Have you seen it?
- Due next Tuesday noon.
  - Feels like a long time away?
  - it's due in 120 hours!

Recap: Language Modeling

- **Language Modeling:** estimating distributions over language.

- **One approach** we previously saw: counting word co-occurrences.
  - **Pro:** easy — just count!
  - **Con:** difficult to scale to longer context due to the sparsity challenge.

- Another approach:
  - Using a learnable function that can estimate word transition probabilities.
    - **Now:** What are these learnable functions and how can we train them.

Neural Networks: Chapter Plan

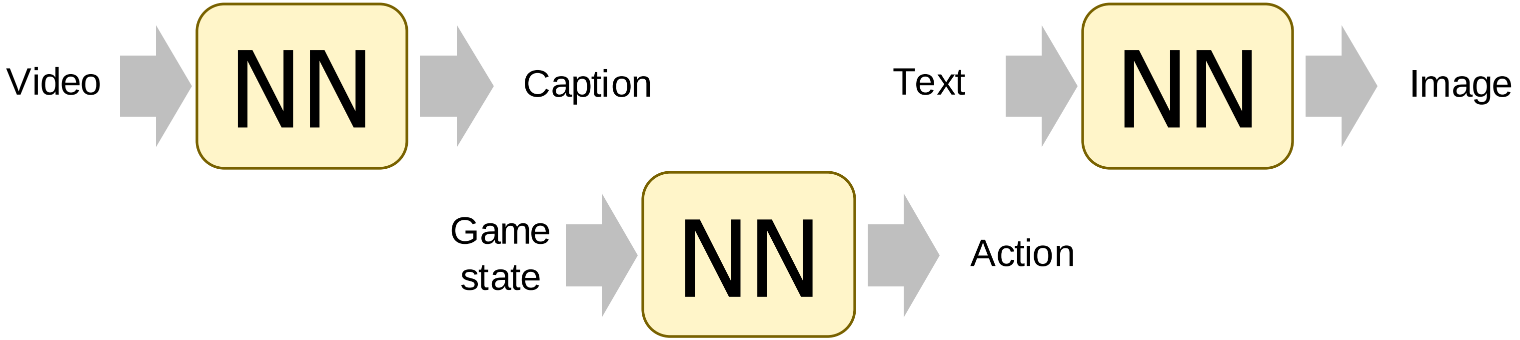
1. Defining neural networks (feedforward nets)
2. Neural nets: brief history
3. Algebra background for training neural nets
4. Training neural networks: analytical backpropagation
5. Backprop in practice

Chapter goal: Get comfortable with thinking, designing and building neural networks — very powerful modeling tools.

Feedforward Neural Nets

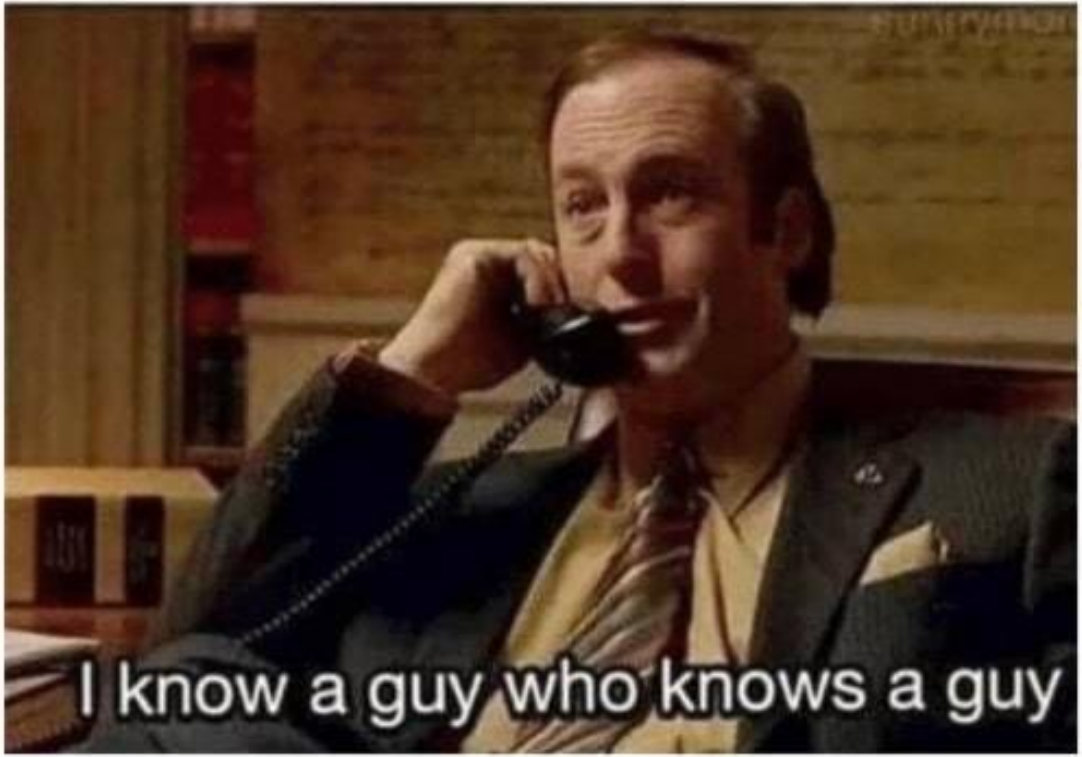
Neural Networks

- What are neural networks?
  - Functions that take an input and produce an output.



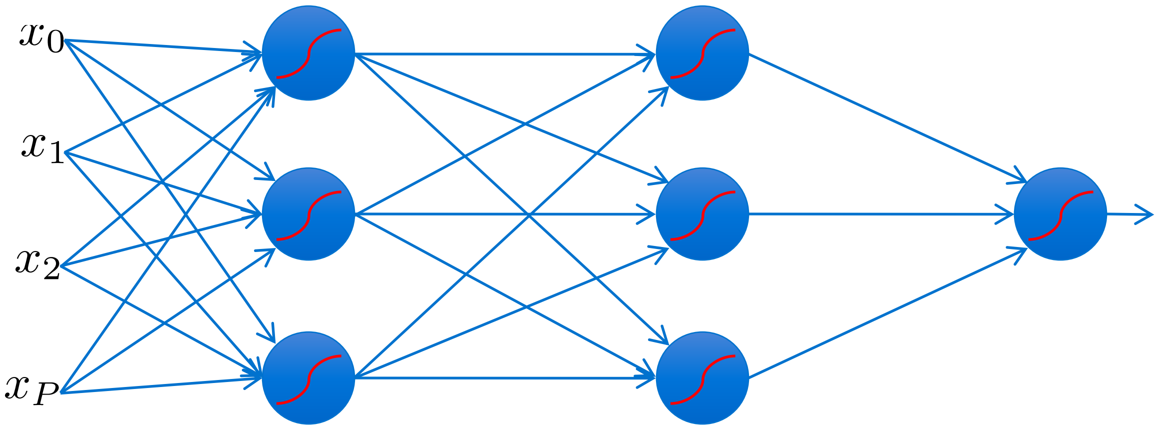
- What is inside this box?

What's Inside Neural Nets?



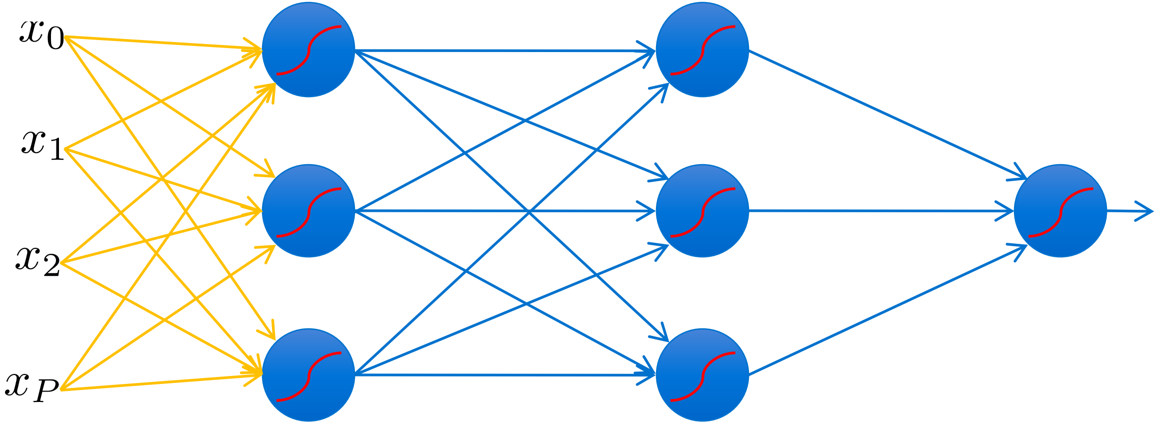
Feedforward networks

- This is a particular class called "feedforward" networks.
    - Cascade neurons together



Feedforward networks

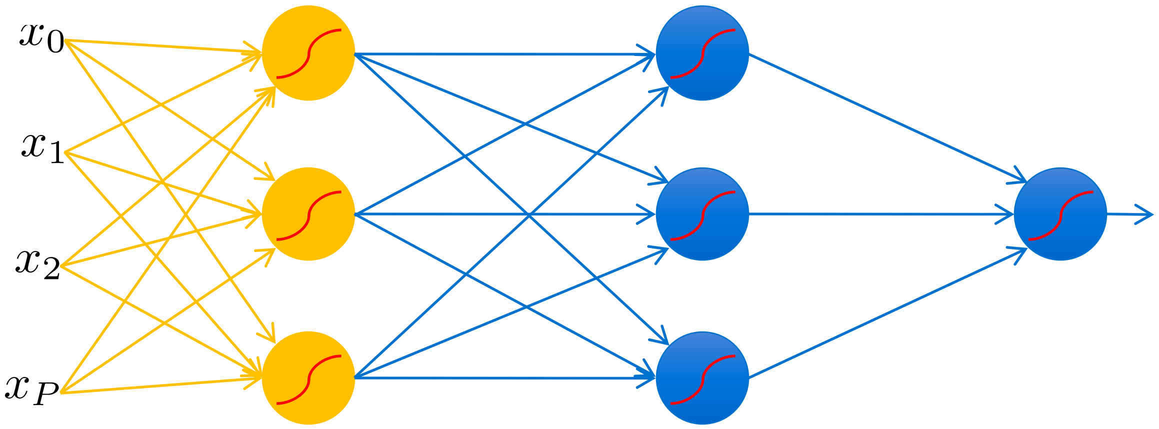
- Inputs multiplied by initial set of weights



[Slide: HKUST]

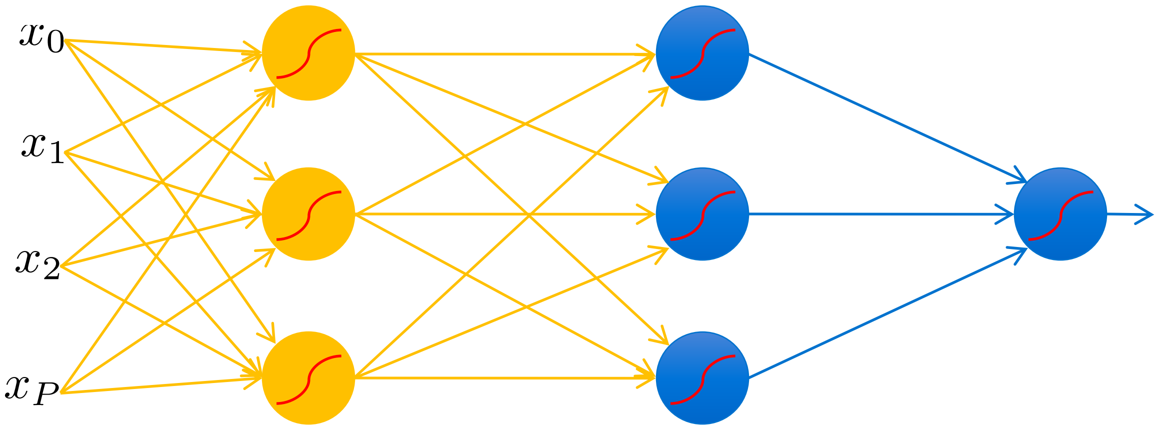
Feedforward networks

- Intermediate "predictions" computed at first hidden layer



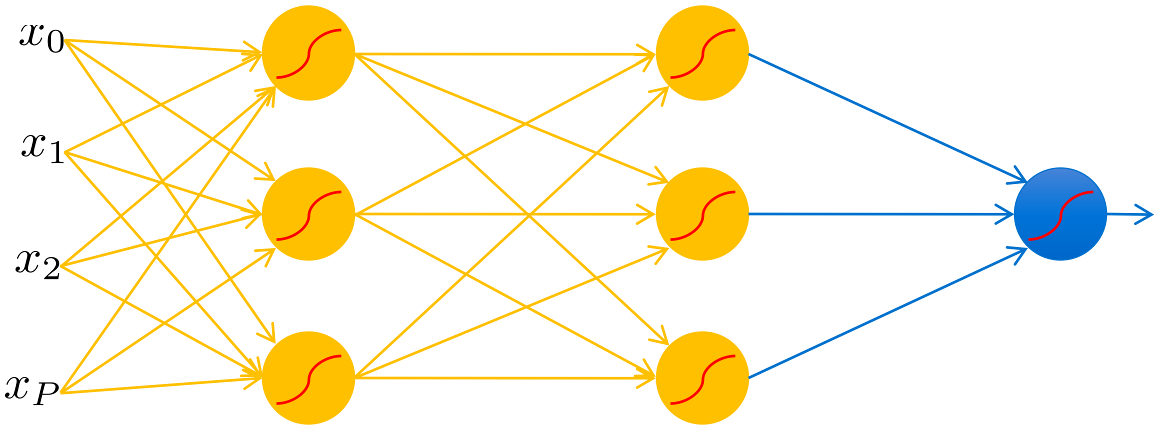
Feedforward networks

- Intermediate predictions multiplied by second layer of weights
- Predictions are fed forward through the network



Feedforward networks

- Compute second set of intermediate predictions



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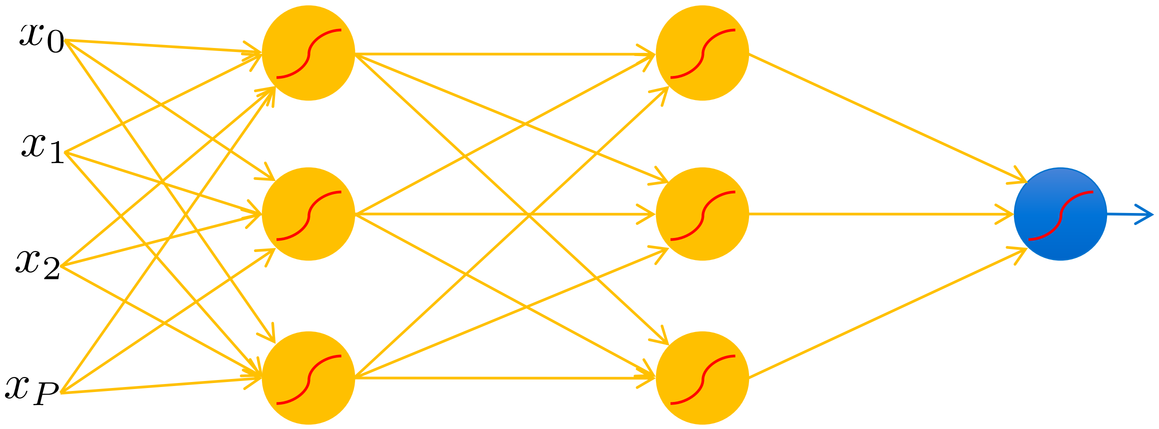
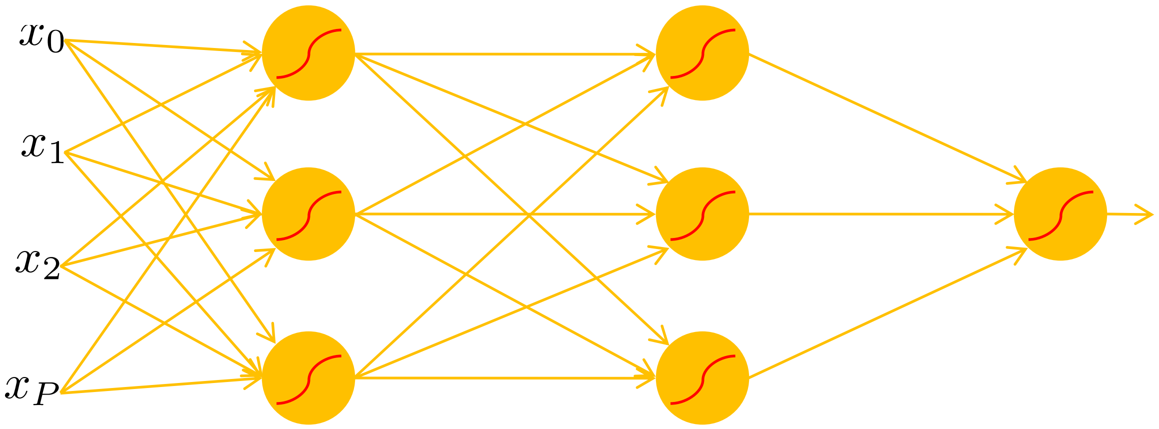
Feedforward networks

- Multiply by final set of weights



Feedforward networks

- Aggregate all the computations in the output
  - e.g. probability of a particular class



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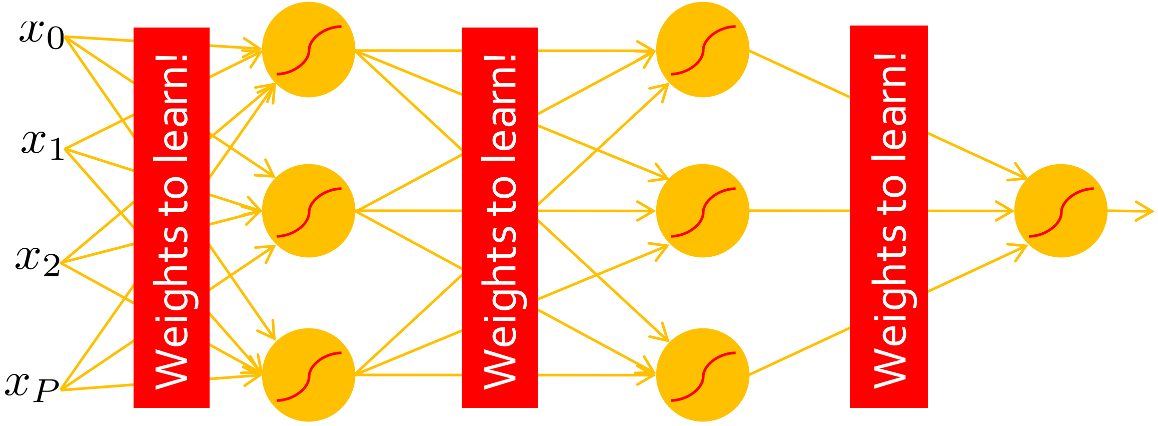
Feedforward networks

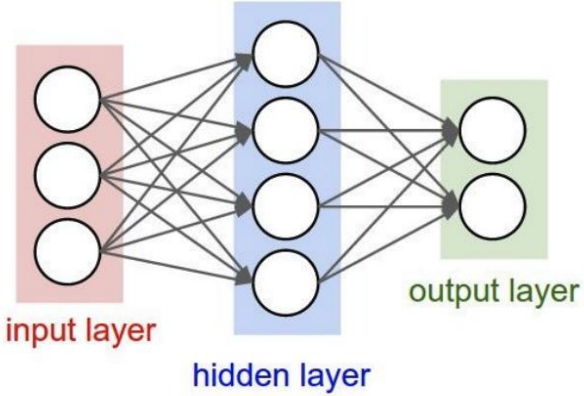
- All the intermediate parameters are ought to be learned.



Feedforward Neural Network

- Neural Networks are functions!
  - Function class for approximating real-valued, discrete-valued and vector valued target functions.
  - $\mathrm{NN}: \boldsymbol{X} \rightarrow \boldsymbol{Y}$ where $\boldsymbol{X} = [0,1]^n$, or $\mathbb{R}^n$ and $\boldsymbol{Y} = [0,1]^d, \{0,1\}^d$

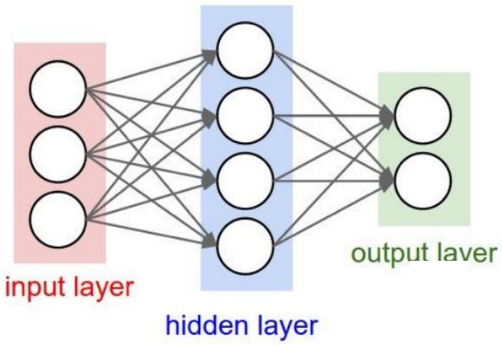
- Example: A **2-layer** neural network
  - The input, hidden and output variables are represented by nodes
  - The links are the weight parameters
  - Arrows denote direction of information flow through the network



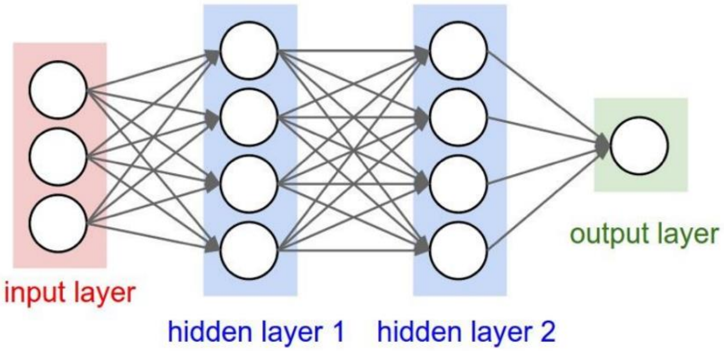
Neural Network: Making it bigger

Add more layers, or wider layers!

A **2-layer** neural network

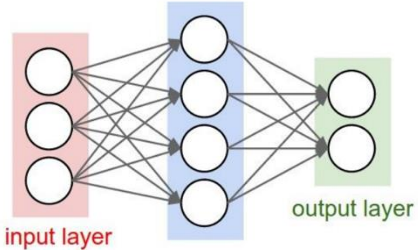


A **3-layer** neural network



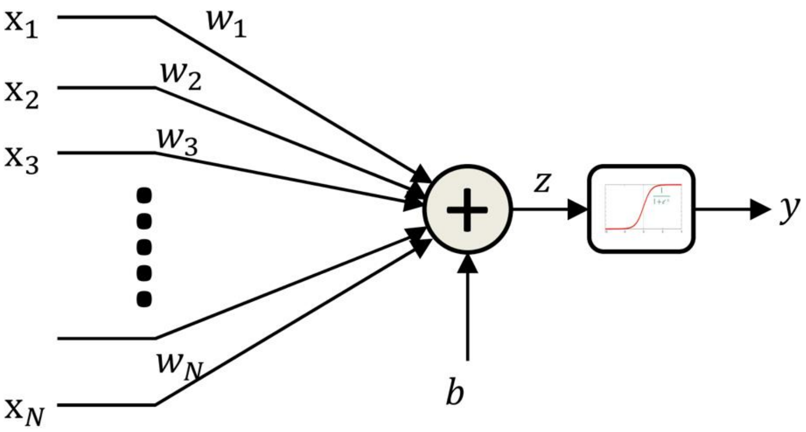
Feedforward Neural Network: The Neurons

- A mathematical model of neuron is "**perceptron**".
- It consists of a non-linear function that "fires" if the affine (linear) function of inputs is above a threshold.



$$y = \sigma\left(b + \sum_{i=1}^{N} w_i x_i\right)$$

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

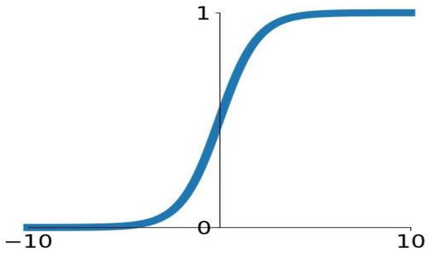


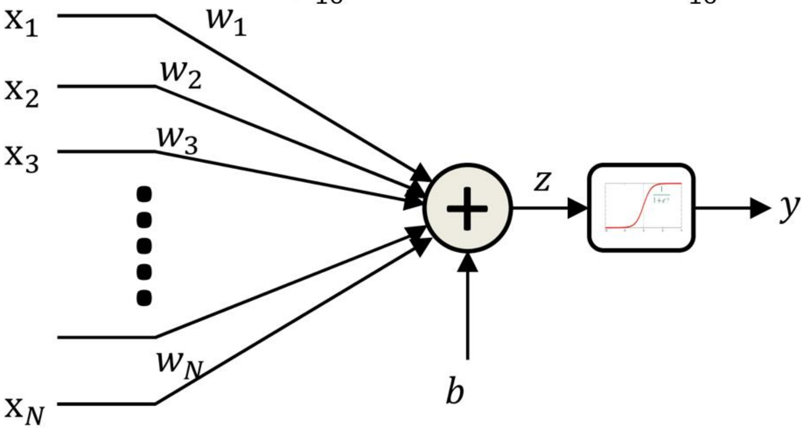
Feedforward Neural Network: The Neurons

- Sigmoid is a "squashing" function.
  - It maps small inputs to zero.
  - It maps large inputs to one.

$$y = \sigma\left(b + \sum_{i=1}^{N} w_i x_i\right)$$

$$\sigma(z) = \frac{1}{1+e^{-x}} \text{ (sigmoid function)}$$



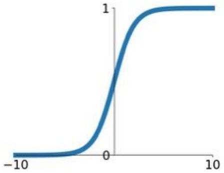


Other Activation Functions

Does not always have to be a squashing function

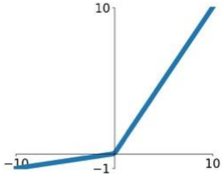
Sigmoid

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



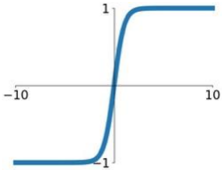
Leaky ReLU

$\max(0.1x, x)$



tanh

$\tanh(x)$

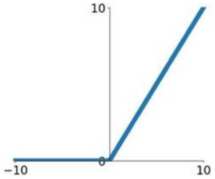


Maxout

$\max(w_1^T x + b_1, w_2^T x + b_2)$

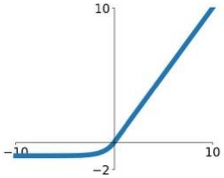
ReLU

$\max(0, x)$



ELU

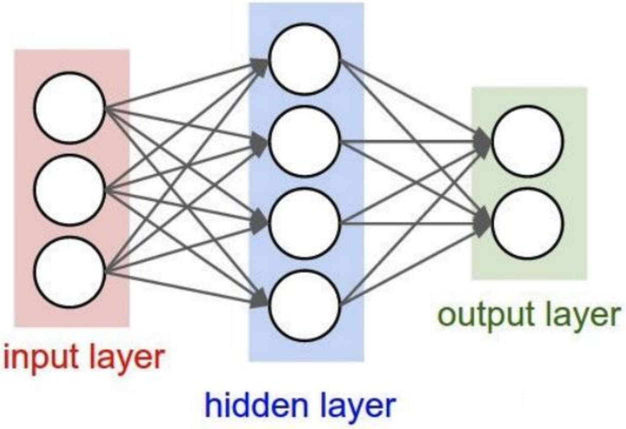
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



We will talk about their pro/cons later!

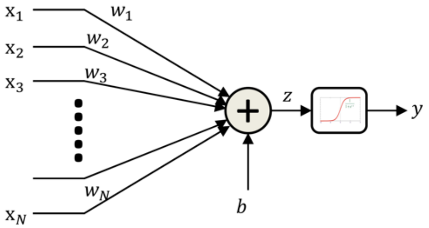
Terminology: Multi-Layer Perceptron (MLP)

- Multi-layer Perceptron (MLP):
  - A feedforward network with perceptron as its nodes.

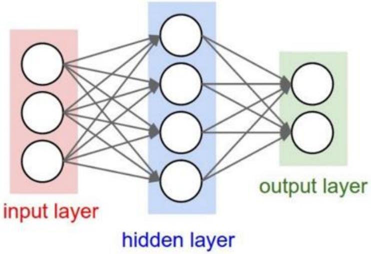


- A feedforward network does **not** have to be an MLP.
  - But people sometimes use the names interchangeably! 🤷‍♀️

- The original MLP [McCulloch–Pitts] was based on “threshold” activation.



Formally Defining a 2 Layer Network



- Example: A **2-layer** MLP network
  - The input, hidden and output variables are represented by nodes
  - The links are the weight parameters
  - Arrows denote direction of information flow through the network

$$f(\mathbf{x}) = W_2\, g(W_1\mathbf{x}) \quad \mathbf{x} \in \mathbb{R}^n, \mathbf{y} \in \mathbb{R}^d$$

$$g(\mathbf{z}) = [\sigma(z_1), \dots, \sigma(z_h)] \text{ (nonlinearity)} \qquad \sigma(z_i) = \frac{1}{1+e^{-x}} \text{ (sigmoid function)}$$

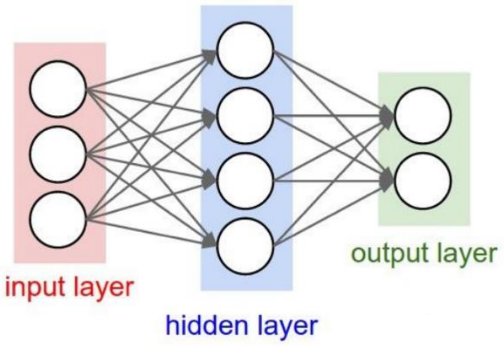
- $W_1 \in \mathbb{R}^{h\times n}$ and $W_2 \in \mathbb{R}^{d\times h}$ are the parameters that need to be learned.

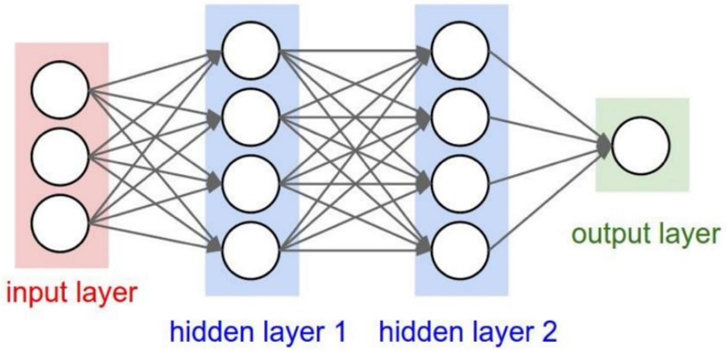
Quiz Time (1)

- What is needed to fully specify a neural network?
  1. Architecture (which input goes through what function etc.)
  2. Parameters of the function (the weights)
  3. Both

Quiz Time (2)

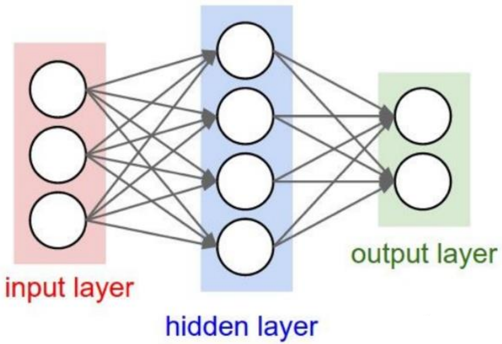
- Which of the followings has more parameters?

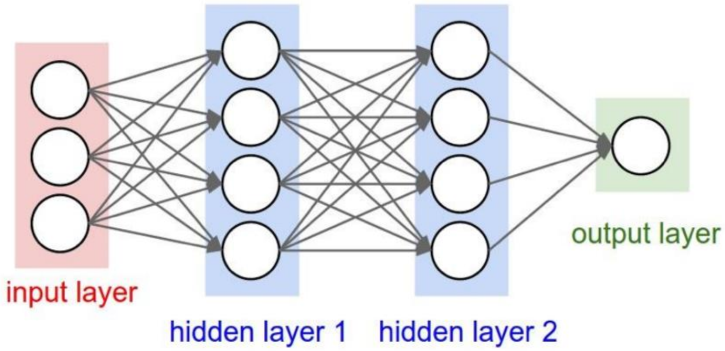




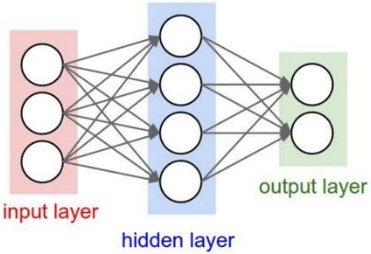
Quiz Time (3)

- Given an input to these models, which of them take longer to compute an output?





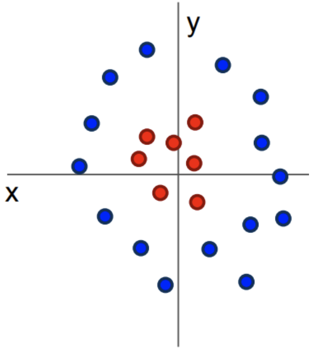
Why Add Non-linearity?



- Without non-linearity, the overall model amounts to a linear model.

$$f(\mathbf{x}) = W_2\, g(W_1\mathbf{x}) \xrightarrow{\text{drop } g} \tilde{f}(\mathbf{x}) = W_2 W_1 \mathbf{x} = W_3 \mathbf{x} \quad \text{(a linear function)}$$

- A linear function cannot approximate complex tasks.

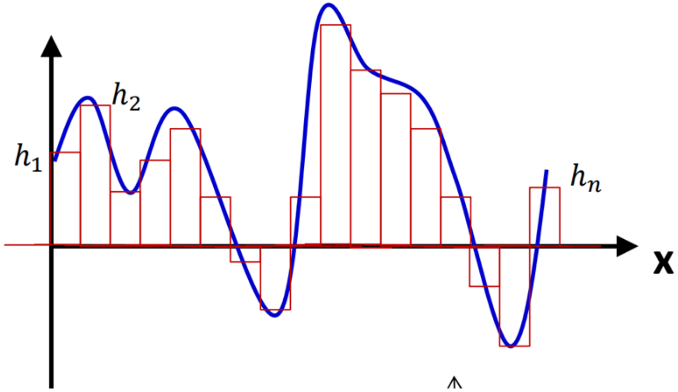


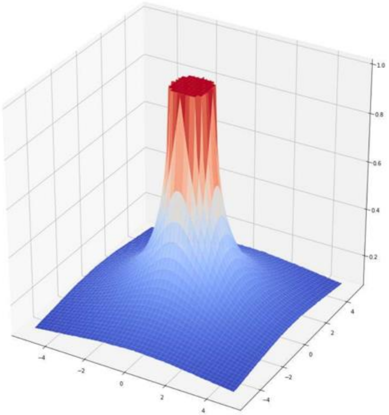
Cannot separate red and blue points with linear classifier

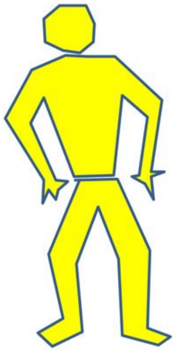
- Non-linearity adds capacity to the model to approximate any continuous function to arbitrary accuracy given sufficiently many hidden units.
  - See [“universal approximation theorem”]

Universal Approximation

- An MLP **can** represent **any function**, with **enough** expressivity.







Maiorov & Pinkus. Lower bounds for approximation by MLP neural networks, 1999.

Quiz Time

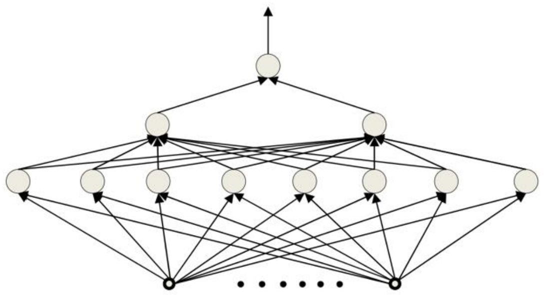
- What makes neural networks expressive functions?
    1. Activations (non-linearities)
    2. Depth (number of hidden layers)
    3. Width (number of variables in each hidden layer)
    4. All the above

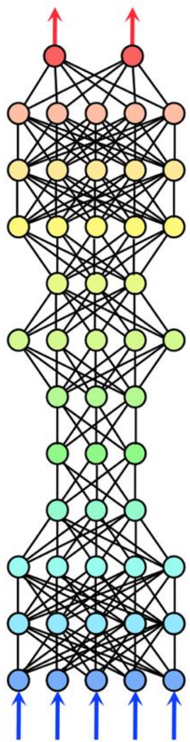
Demo time!

- Link: https://playground.tensorflow.org/

What is a good architecture? Depth vs. Width

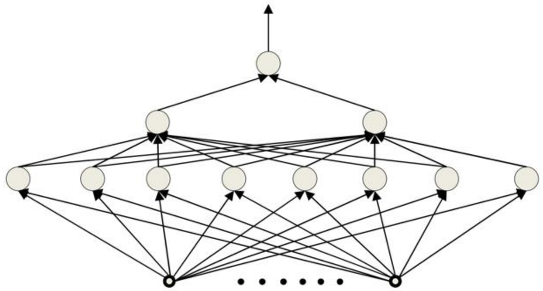
- Architectural parameters of a neural network affect its capacity to learn.
  - Deep vs. wide

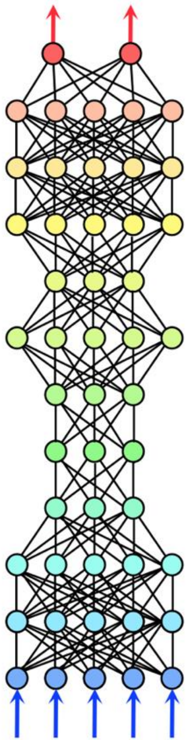




Depth vs Width on Boolean functions

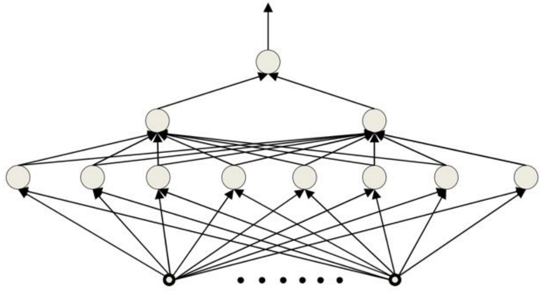
- An MLP is a universal **Boolean** function.
- A **shallow** (single hidden layer) is a universal Boolean machine
  - But it may require an **exponentially large** number of units.
- **Deeper** networks may require far **fewer** neurons than shallower networks to express the same function

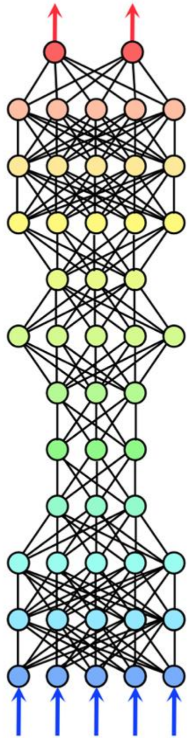




Depth vs Width on Boolean functions

- **Theorem:** There are certain class of functions with n inputs that can be represented with **deep** neural network with $O(n)$ units, whereas it would require $O(2^{\sqrt{n}})$ units for a **shallow** network.





Hastad, Almost optimal lower bounds for small depth circuits, 1986.
Delalleau & Bengio. Shallow vs. deep sum-product networks, 2011.

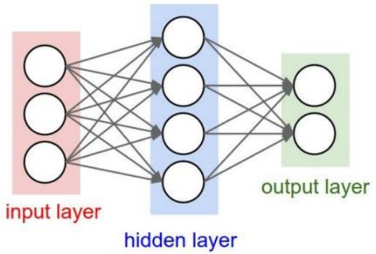
Summary

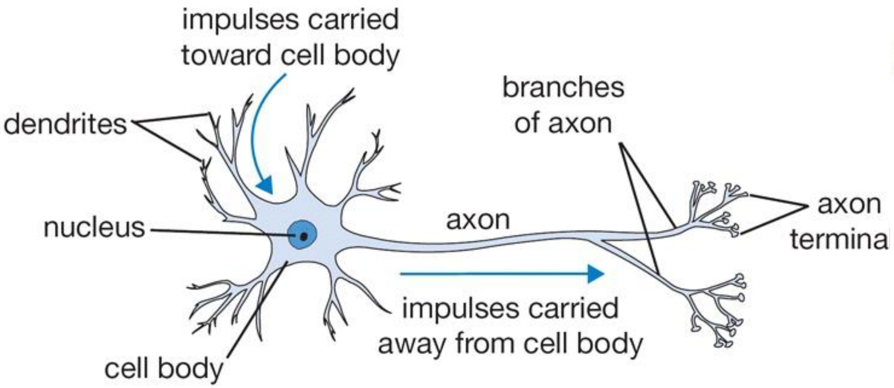
- An MLP is a universal function
- But can represent a given function only if
  - It is sufficiently wide
  - It is sufficiently deep
  - Depth can be traded off for (sometimes) exponential growth of the width of the network
- Optimal width and depth depend on the complexity of the problem.
- **Next:** A bit of history.

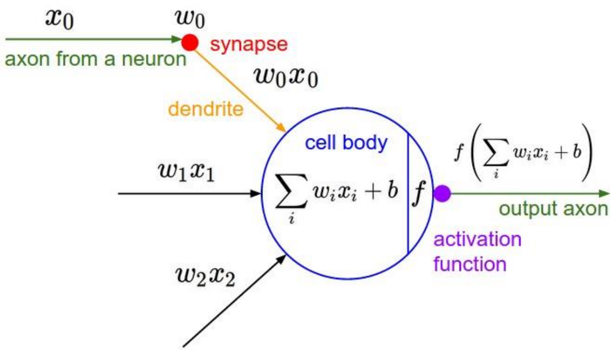
Neural Nets:
Origin and History

Artificial Neurons: An Inspiration from Nature

- A single node in your neural network
  - Accept information from multiple inputs
  - Transmit information to other neurons
- A neuron's function is inspired by its biological counterpart:
  - Apply some function on inputs signals
  - If output of function over threshold, neuron "fires"

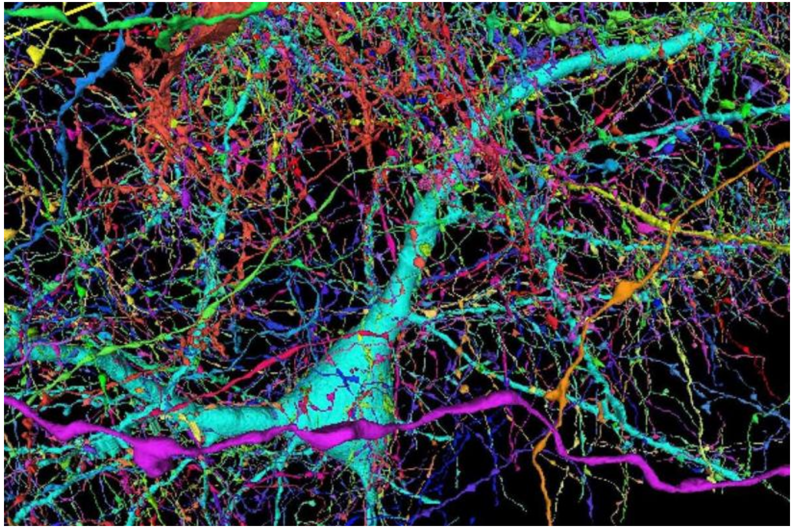






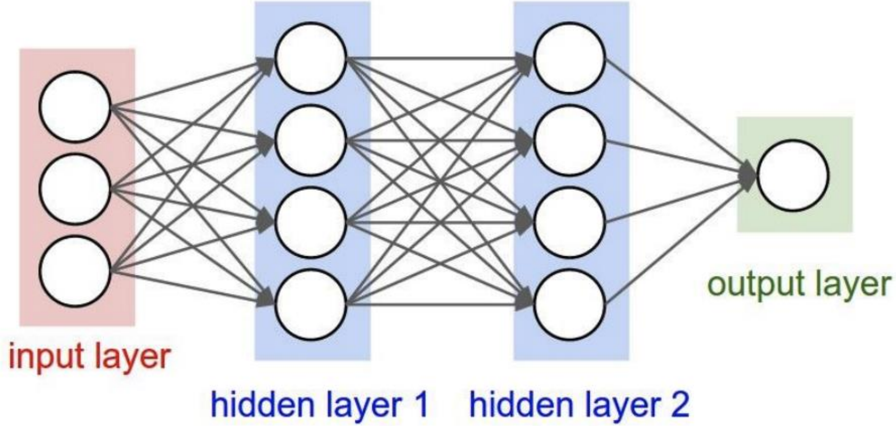
Artificial Neurons: Not Quite Analogous to Nature

Biological neurons:
complex connectivity



Source: Google Brain Map

Neurons in an artificial neural network: organized based on a highly regular structure for computational efficiency



Very Brief History of Neural Networks

1. Single-layer neural networks (1943-1969)
2. Symbolic AI & knowledge engineering (1970-1985)
3. Multi-layer NNs and symbolic learning (1985-1995)
4. Shallow statistical learning/probabilistic models (1995-2010)
5. Deep networks and self-supervised learning (2010-?)

Very Brief History of Neural Networks

1. **Single-layer neural networks (1943-1969)**
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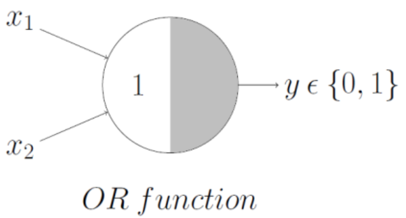
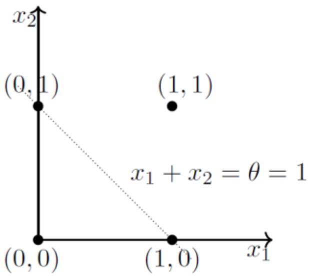
A Neuron as a Mathematical Model of Computation

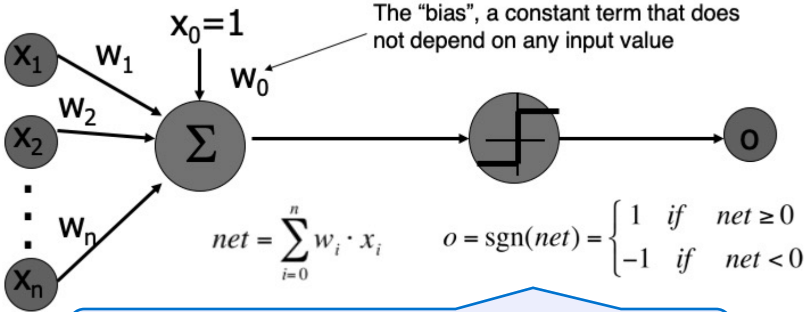
- McCulloch and Pitts (1943) showed how linear threshold units can be used to compute logical functions



OR function

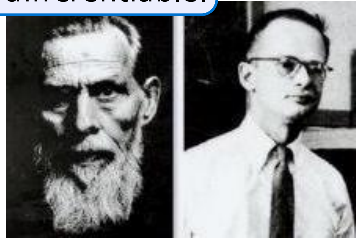
$$x_1 + x_2 = \sum_{i=1}^{2} x_i \geq 1$$





Notice the step function (threshold)!
Early models didn't need to be differentiable.

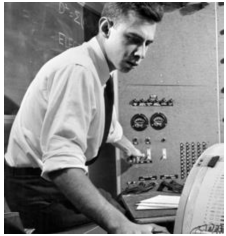
- An alternative model of computation (comparable to "Turing Machine")



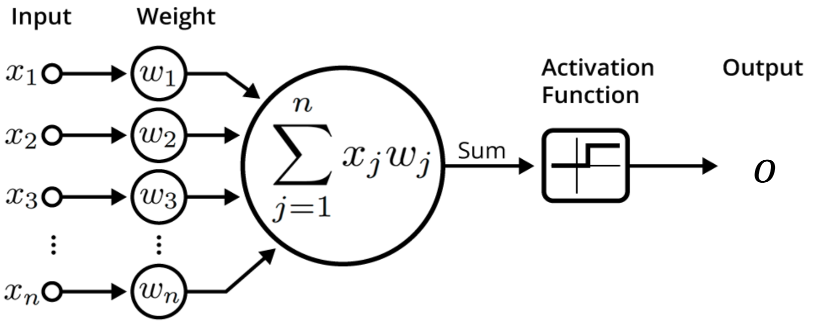
Johns Hopkins Whiting School of Engineering

[A Logical Calculus of Ideas Immanent in Nervous Activity, McCulloch and Pitts 1943]

Perceptron Learning Rule — Imitating Nature's Learning Process



- Rosenblatt (1959) developed the **Perceptron** algorithm —
  - An iterative algorithm for learning the weights of a **linear threshold unit**.



- A single neuron with a fixed input, it can incrementally change weights and learn to produce a fixed output using the Perceptron learning rule.
- Update each weights by: $$w_i = w_i + \eta(t - o)x_i$$

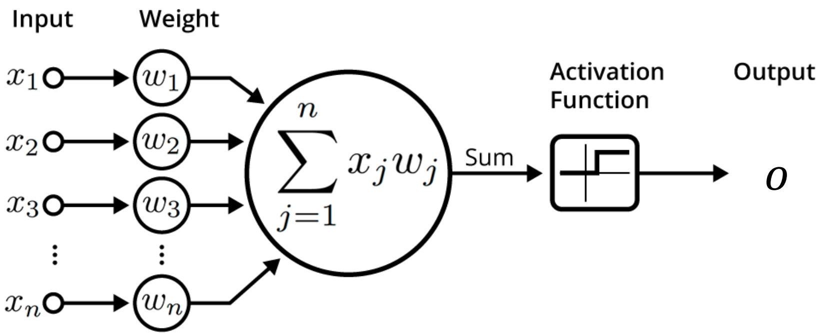
t: the target value

[The perceptron: a probabilistic model for information storage and organization in the brain, Rosenblatt 1959]

Quiz (1): Understanding Perceptron Update Rule

- Suppose the inputs $x_i \in \{0, 1\}$ and $\eta = 1$. If LTU's output o exactly matches the target value t, How would the update rule change the weights?
  1. Would increase them
  2. Would decrease them
  3. Would not change them

$$w_i = w_i + \eta(t - o)x_i$$

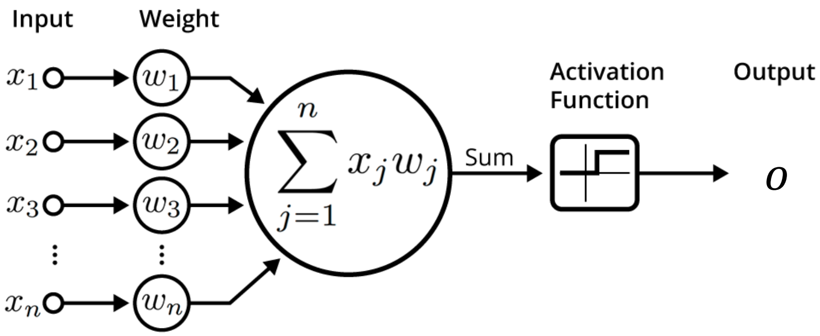


Quiz (2): Understanding Perceptron Update Rule

- Suppose the inputs $x_i \in \{0, 1\}$ and $\eta = 1$. If LTU's output o is smaller than the target value t, how would the update rule change the weights?
  1. Would increase them
  2. Would increase the weights for active inputs
  3. Would decrease them
  4. Would not change them

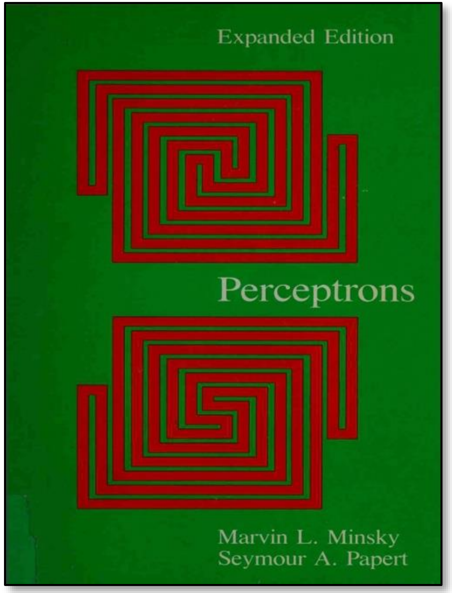
$$w_i = w_i + \eta(t - o)x_i$$

- After this update, the new output o would be:
  1. Larger
  2. Smaller
  3. Unchanged



Perceptron: Demise

- "Perceptrons" (1969) by Minsky and Papert illuminated few limitations of the perceptron.
- It showed that:
  - Shallow (2-layer) networks are unable to learn or represent many classification functions (e.g. XOR)
  - Only the linearly separable functions are learnable.
- Also, there was an understanding that deeper networks were infeasible to train.
- Result: research on NNs dissipated during the 70's and early 80's!



[slide: Ray Mooney]

Very Brief History of Neural Networks

1. Single-layer neural networks (1943-1969)
2. Symbolic AI & knowledge engineering (1970-1985)
3. Multi-layer NNs and symbolic learning (1985-1995)
4. Shallow statistical learning/probabilistic models (1995-2010)
5. Deep networks and self-supervised learning (2010-?)

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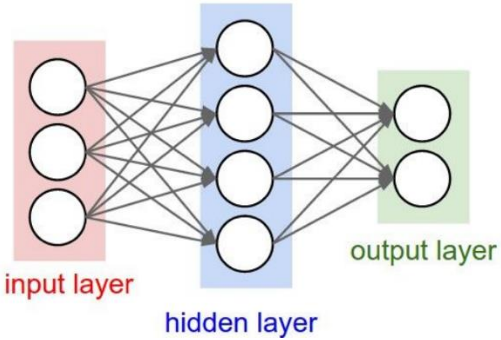
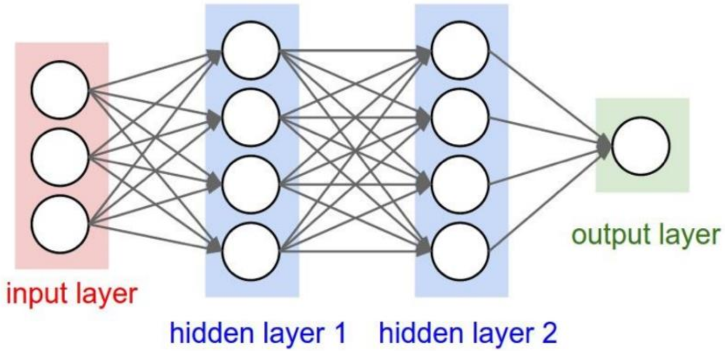
Neural Networks Resurgence (1986)

- Interest in NNs revived in the mid 1980's due to the rise of "connectionism."
- Backpropagation algorithm was [re-]introduced for training three-layer NN's.
  - Generalized the iterative "hill climbing" method to approximate networks with multiple layers, but no convergence guarantees.

what was possible to train in 1970's



what became possible to train via BP in 1980's



[Learning representations by back-propagating errors, Rumelhart, Hinton & Williams 1986; for a broader context, see: http://people.idsia.ch/~juergen/who-invented-backpropagation.html]

Second NN Demise (1995-2010)

- Generic backpropagation did not generalize that well to training deeper networks.
  - Overfitting / underfitting remained an issue.
  - Computers were still quite slow
- Little theoretical justification for underlying methods.
- Machine learning research moved to graphical/probabilistic models and kernel methods.

[slide: Ray Mooney]

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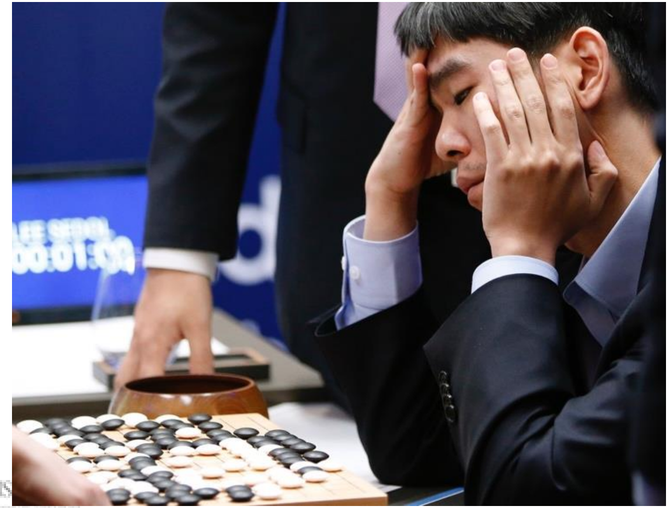
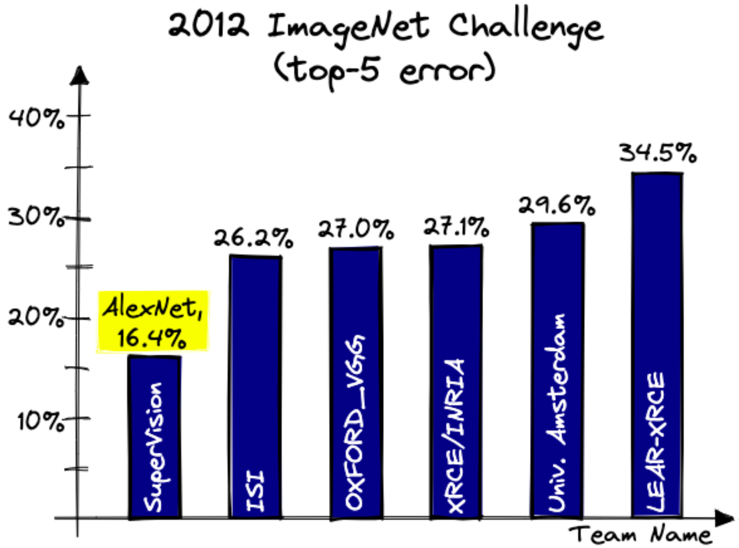
Deep Learning Revolution (2010…)

- Various successes with training deep neural works.
  - Convolutional neural nets (CNNs) for vision — 2012 AlexNet showed 16% error reduction on ImageNet benchmark.
  - Rise of deep reinforcement learning for games—AlphaGo beat human players.





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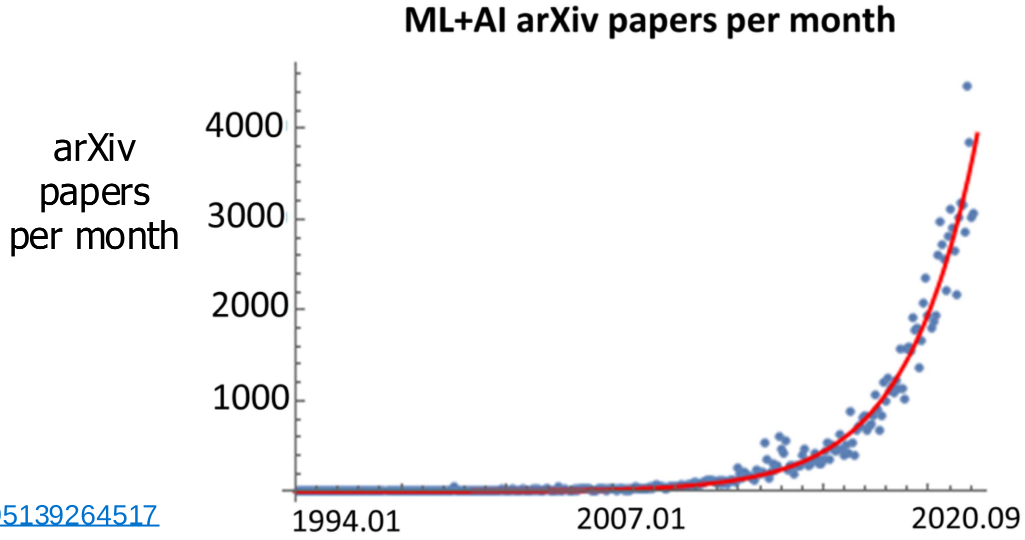
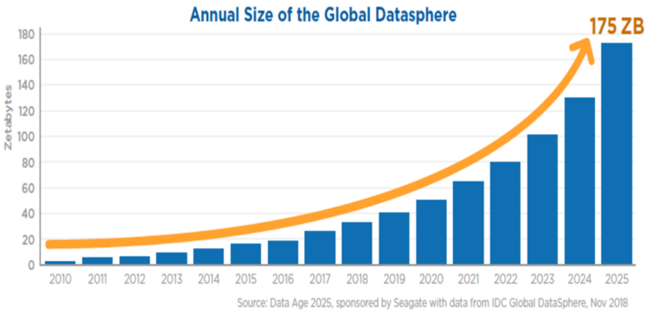
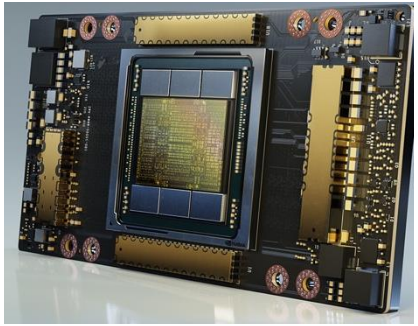


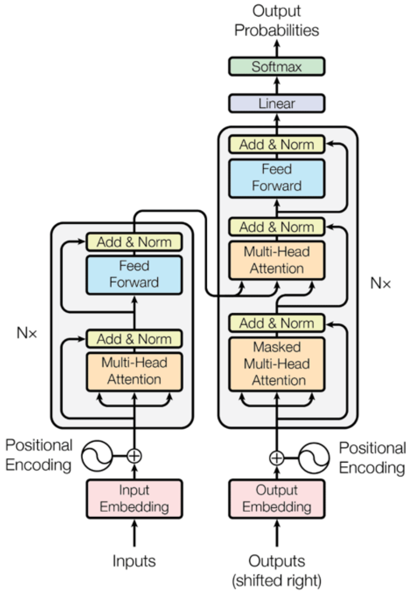
Figure credit:
https://twitter.com/MarioKrenn6240/status/1314622995139264517

Deep Learning Revolution (2010…)

- The success continued enabled by 3 forces:
  - Availability of massive [unlabeled] data — the data on Internet.
  - Faster computing technologies — specialized hardware (e.g., GPUs)
  - Algorithmic innovations — architectures, optimization, etc.







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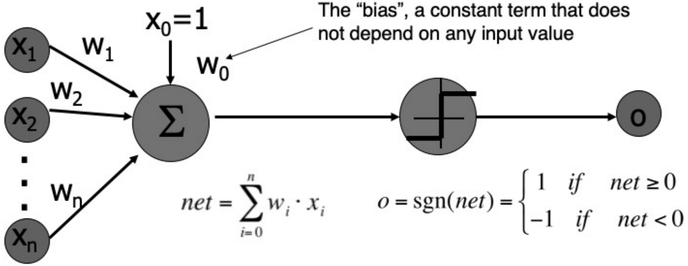
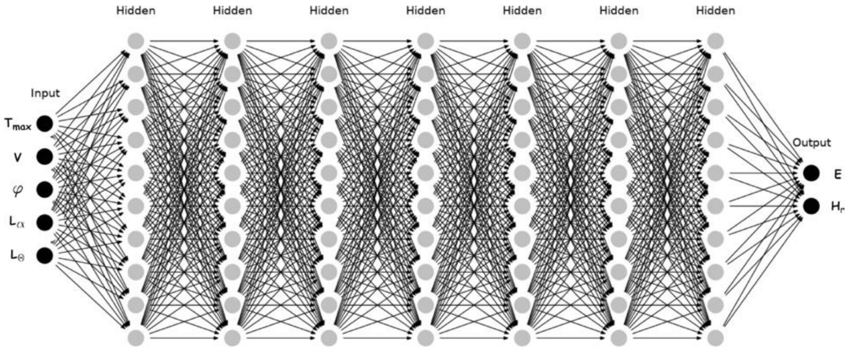
https://en.wikipedia.org/wiki/Big_Bounce

How it started



How it's going



[slide: Ray Mooney]

Summary

- Neural networks have been long in the making since 1950s.
- It’s a remarkable journey of science with many ups and downs.
- **Next:** How do you train NNs? We will start with some algebra refreshers.

Background for Training NNs
The Refreshers 🍹

Machine Learning Problems

- **Training data:** Given a set of inputs and output labels:
  - Inputs: $X = (x_1, \dots, x_n)$
  - Outputs: $Y = (y_1, \dots, y_n)$
- **Goal:** Find a function $f(x; \theta)$ with parameters θ that maps inputs in X to output to Y
- **Empirical risk:** measure the quality of the predictions with a loss function:

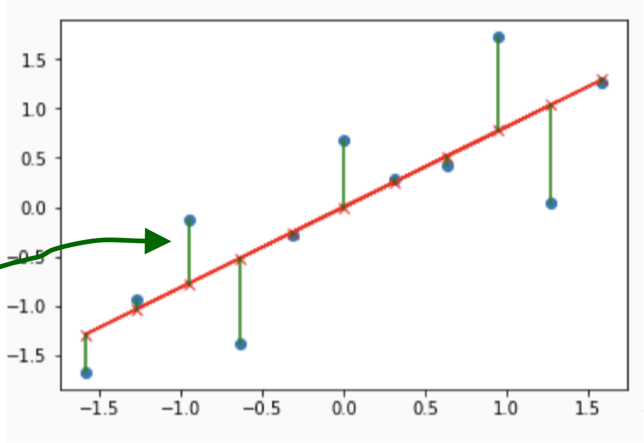
$$J(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i; \theta), y_i)$$

A Special Case: Linear Regression

- **Training data:** Given a set of inputs and output labels:
  - Inputs: $X = (x_1, \dots, x_n)$
  - Outputs: $Y = (y_1, \dots, y_n)$
- **Goal:** Find a linear function $f(x;\theta) = \theta . x$ that is best predictive of observations
- **Empirical risk:** measure the quality of the predictions with a loss function:

$$J(\theta) = \frac{1}{n}\sum_{i=1}^{n} \ell(\theta . x_i, y_i)$$

What are good choices for loss function?



Quiz: Loss functions

- Remember the objective function of our learning problem:

$$J(\theta) = \frac{1}{n}\sum_{i=1}^{n} \ell(f(x_i;\theta), y_i)$$

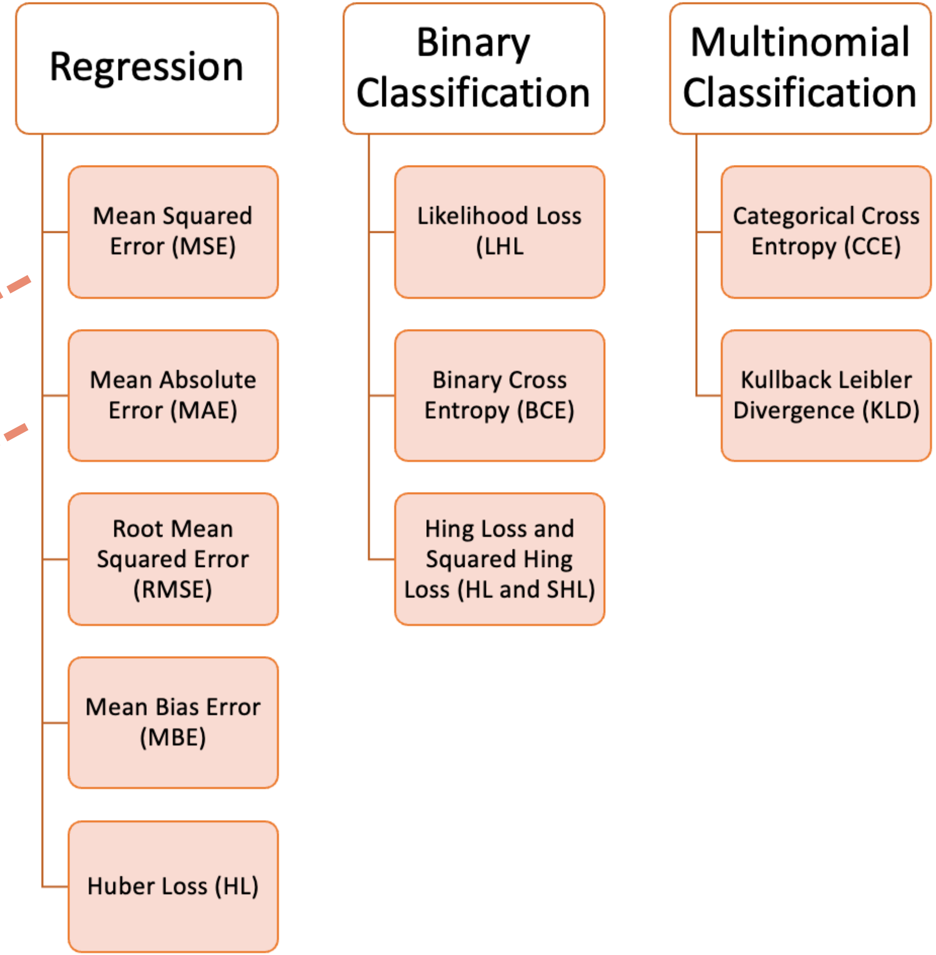
- Which of the followings is a more reasonable loss function $\ell(z, w)$?
  1. If z and w are far apart, the loss value should be higher
  2. If z and w are far apart, the loss value should be lower
  3. Neither

Loss Functions

- The choice of loss function depends on the problem

$$\ell(y,\hat{y}) = (y-\hat{y})^2$$

$$\ell(y,\hat{y}) = |y-\hat{y}|$$



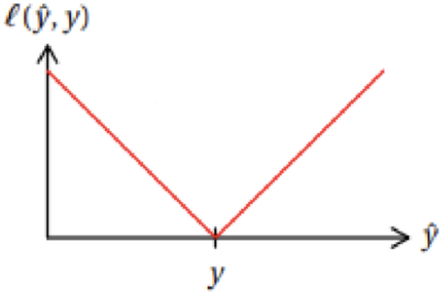
Quiz: MSE vs. MAE loss

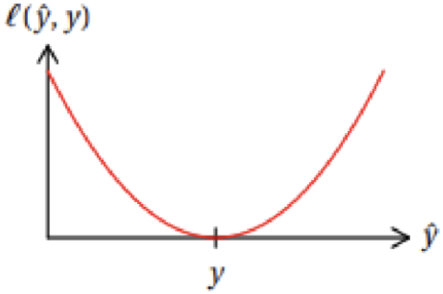
- Remember MSE and MAE loss:

MSE: $\ell(y, \hat{y}) = (y - \hat{y})^2$

MAE: $\ell(y, \hat{y}) = |y - \hat{y}|$

1. Which visualization corresponds to which loss?





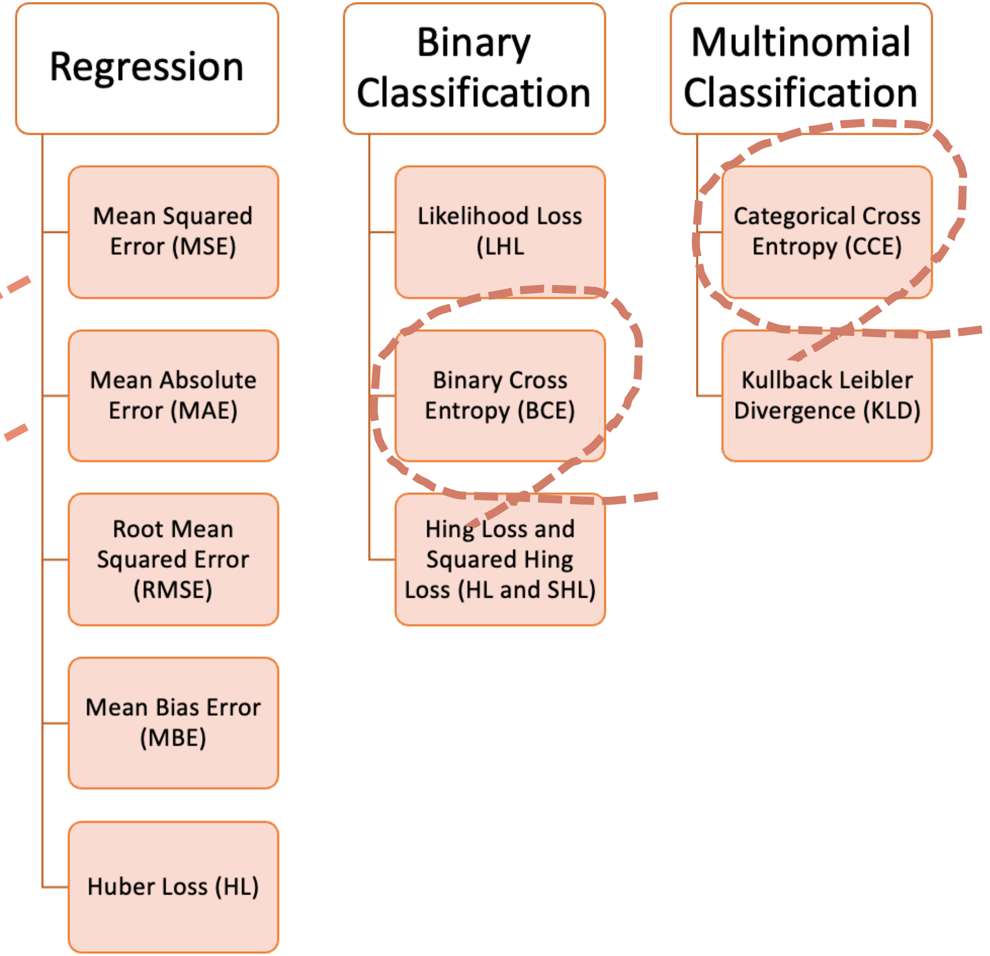
2. Which loss is more sensitive to outlier data (noisy outputs)?
3. Which loss is more difficult to compute gradients for?

Loss Functions

- The choice of loss function depends on the problem

$$\ell(y,\hat{y}) = (y-\hat{y})^2$$

$$\ell(y,\hat{y}) = |y-\hat{y}|$$



Loss Functions: Cross-Entropy

- A binary classification example: Without loss of generality:
  - Gold labels: $y = [1, 0]$ (i.e., first class is correct)
  - Predictions: $\hat{y} = [p, 1 - p]$

$$\ell(\boldsymbol{y}, \hat{\boldsymbol{y}}) = -\sum_{j}^{n} y_j \log(\hat{y}_j)$$

Summation over the dimensions of $\boldsymbol{y}$

- CE loss: $\ell(y, \hat{y}) = -1 \times \log p - 0 \times \log(1 - p) = -\log p$

Quiz: CE for Binary Classification

- A binary classification example: Without loss of generality:
  - Gold labels: $y = [1, 0]$ (i.e., first class is correct)
  - Predictions: $\hat{y} = [p, 1 - p]$

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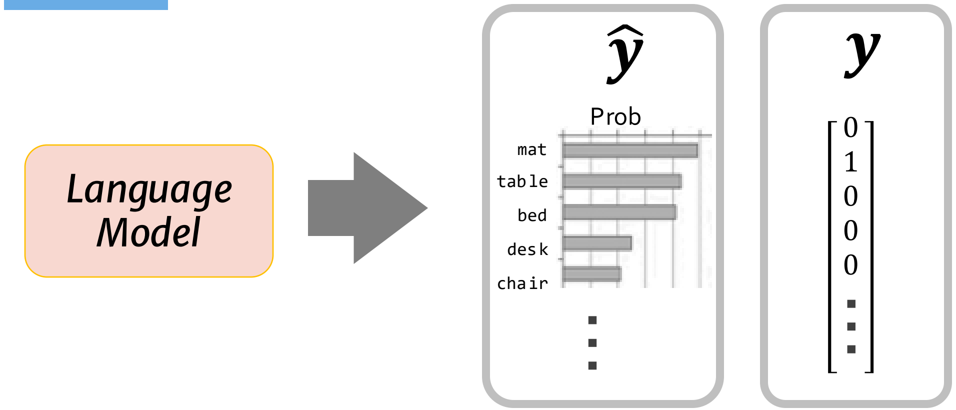
Summation over the dimensions of $\boldsymbol{y}$

- CE loss: $\ell(y, \hat{y}) = -1 \times \log p - 0 \times \log(1 - p) = -\log p$

- **Question 1:** Why the negative sign?
- **Question 2:** If the model prediction is miraculously accurate ($p = 1$), what is CE loss?
- **Question 3:** If the model prediction is embarrassingly off ($p = 0$), what is the CE loss?

Cross-Entropy Over Next-Word Distribution



$$\ell(\boldsymbol{y}, \hat{\boldsymbol{y}}) = -\sum_{j}^{n} y_j \log(\hat{y}_j)$$

Summation over the dimensions of $\boldsymbol{y}$

- Suppose for a fixed j, $y_j = 1$.
- **Question:** Then CE is the probability is? ….
  - It is the probability that our language model assigns to the jth term.

Machine Learning Problems

- **Training data:** Given a set of inputs and output labels:
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$$J(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i; \theta), y_i)$$

- Machine learning as optimization:

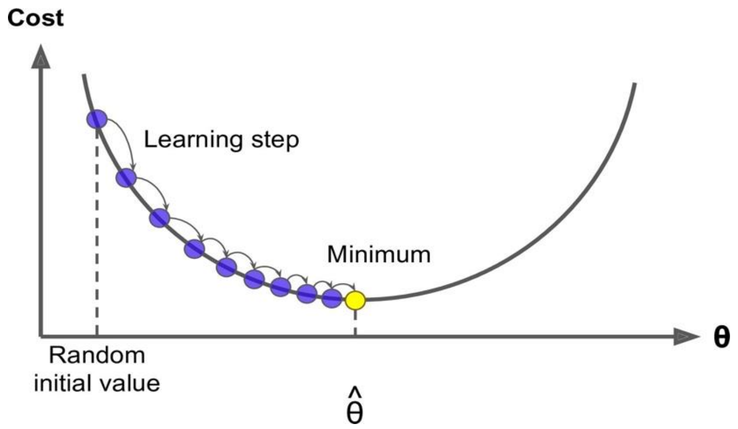
$$\operatorname*{argmin}_{\theta} J(\theta)$$

How do you solve this optimization?

Gradient Descent

- We have a cost function $J(\theta)$ we want to minimize
  - We can use Gradient Descent algorithm!

- **Idea:** for current value of θ, calculate gradient of $J(\theta)$, then take small step in direction of negative gradient. Repeat.



- Note: Our objectives may not be convex like this. But life turns out to be okay!

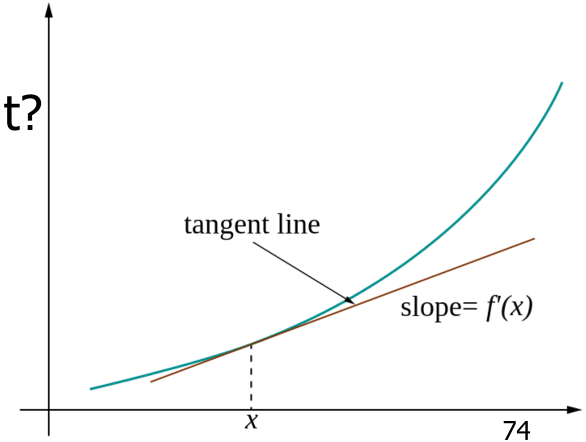
Gradient Descent (1): Intuition

- Imagine you're blindfolded
- Need to walk down a hill
- You can use your hands to find the directions that may be downhill

[slide: Andrej Karpathy]

Gradient Descent (2): Intuition

- In 1-dimension, the **derivative** of a function: $\frac{\partial J}{\partial \theta_j} = \lim_{h \to 0} \frac{J(\theta_j + h) - J(\theta_j)}{h}$
- **Gradient** is the vector of derivatives: $\nabla_\theta J = \left[\frac{\partial J}{\partial \theta_1}, \dots, \frac{\partial J}{\partial \theta_n}\right]$
- Gradient descent involves iterative steps in in direction of negative gradient.
- **Question:** Why step in direction of negative gradient?
  - Gradient quantifies how rapidly the function $L(\theta)$ varies when we change the argument θ_j by a tiny amount.



Gradient Descent (3)

- Iteratively subtract the gradient with respect to the model parameters (θ)

$$\theta^{new} \leftarrow \theta^{old} - \alpha \, \nabla_\theta J(\theta^{old})$$

α = Step size or learning rate

- We're moving in a direction opposite to the gradient of the loss $J(\theta)$
- I.e., we're moving towards smaller loss $J(\theta)$

- In PyTorch:

```
while True:
    theta_grad = evaluate_gradient(J,corpus,theta)
    theta = theta - alpha * theta_grad
```

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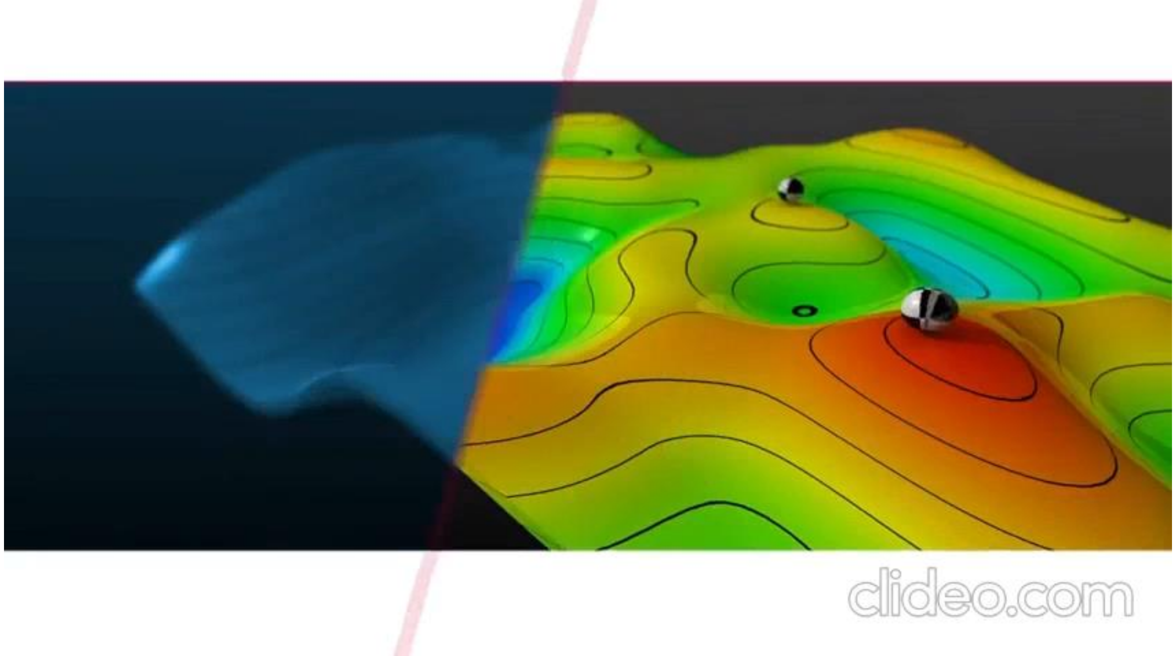
Gradient Descent (4)

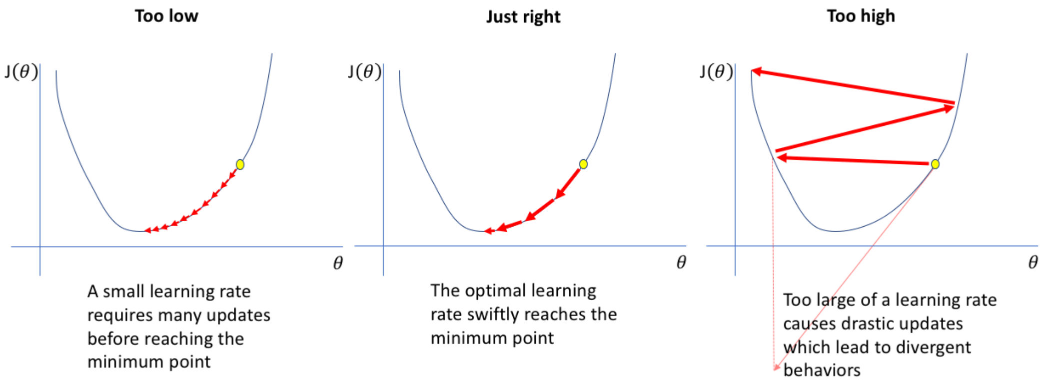
- Update equation (in matrix notation): $\theta^{new} = \theta^{old} - \alpha \nabla_{\theta} J(\theta)$



[demo credit: ICMS YouTube channel]

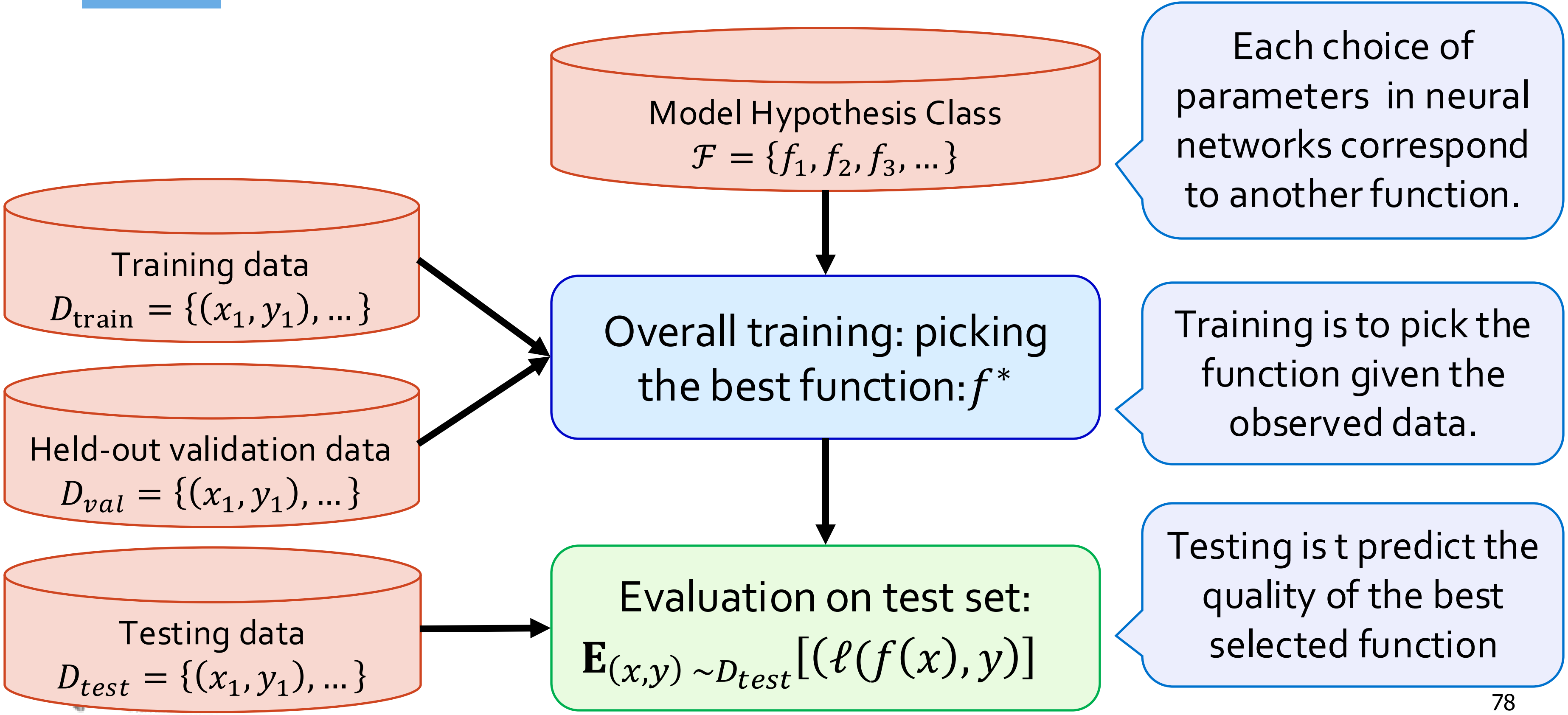
Gradient Descent: Setting the Step Size

- What is a good value for step size α?
  - If α = too small, it may be too slow
  - If α = too large, it may oscillate



- It may take trial-and-errors to find the sweet spot.
- Another trick is to define a "schedule" for gradually reducing the learning rate starting from a large number.

A Typical Learning and Evaluation Protocol



Summary Thus Far

- A statistical learning problem can be formulated as an optimization problem.

- The objective of this optimization consists of:
  - Learning data (input/outputs)
  - Predictive model architecture (encoding how an input gets mapped to an output)
  - Loss function (quantifying quality of predictions)

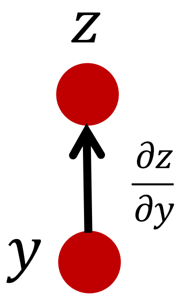
- Soon, we will use see how to use Neural Nets as the predictive model.

Algebra Refresher
(Needed for Backpropagation)

Derivatives

- First let's get the notation right:

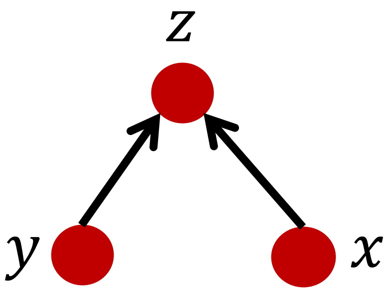
- The arrow shows functional dependence of z on y, i.e. given y, we can calculate z.
  - For example: $z(y) = 2y^2$



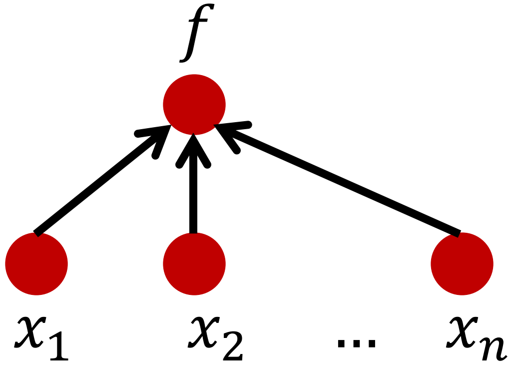
- The derivative of z, with respect to y: $\frac{\partial z}{\partial y}$

Quiz time!

- If $z(x,y) = y^4x^5$ what is the following derivative $\frac{\partial z}{\partial y}$?
  1. $\frac{\partial \mathrm{z}}{\partial \mathrm{y}} = 4\mathrm{y}^3\mathrm{x}^5$
  2. $\frac{\partial \mathrm{z}}{\partial \mathrm{y}} = 5\mathrm{y}^4\mathrm{x}^4$
  3. $\frac{\partial \mathrm{z}}{\partial \mathrm{y}} = 20\mathrm{y}^3\mathrm{x}^4$
  4. None of the above



Gradient



- Given a function with 1 output and n inputs

$$f(\mathbf{x}) = f(x_1, x_2, \dots, x_n) \in \mathbb{R}$$

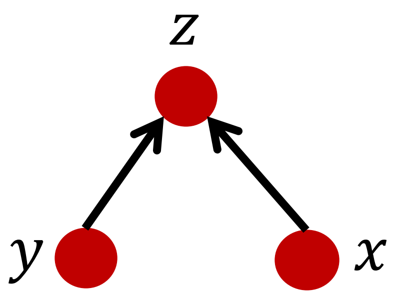
- Its gradient is a vector of partial derivatives with respect to each input

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix} \in \mathbb{R}^n$$

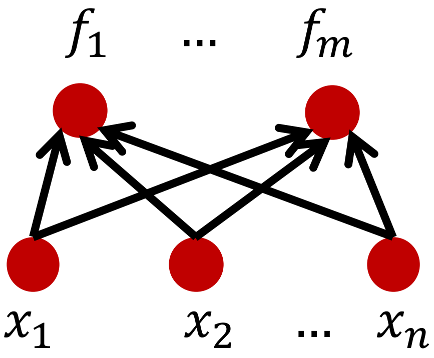
(always assume vectors are column vectors, i.e., they're in $\mathbb{R}^{n \times 1}$)

Quiz time!

- If $z(x, y) = y^4 x^5$ what is the following gradient ∇z?
  1. $\nabla z(x, y) = 4y^3 x^5$
  2. $\nabla z(x, y) = (5y^4 x^4, 20y^3 x^4)$
  3. $\nabla z(x, y) = (5y^4 x^4, 4y^3 x^5)$
  4. None of the above



Jacobian Matrix: Generalization of the Gradient



- Given a function with ***m* outputs** and ***n* inputs**

$$\mathbf{f}(\mathbf{x}) = [f_1(x_1, x_2, \dots, x_n), \dots, f_m(x_1, x_2, \dots, x_n)] \in \mathbb{R}^m$$

- It's Jacobian is an ***m* x *n* matrix** of partial derivatives: $\left(\mathbf{J_f}(\mathbf{x})\right)_{ij} = \frac{\partial f_i}{\partial x_j}$

$$\mathbf{J_f}(\mathbf{x}) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix} \in \mathbb{R}^{m \times n}$$

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Quiz: Jacobian's special case (1)

- Remember Jacobians:

$$\mathbf{f}(\mathbf{x}) = [f_1(x_1, x_2, \dots, x_n), \dots, f_m(x_1, x_2, \dots, x_n)] \in \mathbb{R}^m$$

$$\mathbf{J}_\mathbf{f}(\mathbf{x}) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix} \in \mathbb{R}^{m \times n} \quad \text{or} \quad \left(\mathbf{J}_\mathbf{f}(\mathbf{x})\right)_{ij} = \frac{\partial f_i}{\partial x_j}$$

- When m=1 (scalar-valued function), Jacobian reduces to …?

$\nabla^{\mathrm{T}} \mathbf{f}(\mathbf{x})$ (gradient transpose)

Quiz: Jacobian's special case (2)

- Remember Jacobians:

$$\mathbf{f}(\mathbf{x}) = [f_1(x_1, x_2, \dots, x_n), \dots, f_m(x_1, x_2, \dots, x_n)] \in \mathbb{R}^m$$

$$\mathbf{J_f}(\mathbf{x}) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix} \in \mathbb{R}^{m \times n} \quad \text{or} \quad \left(\mathbf{J_f}(\mathbf{x})\right)_{ij} = \frac{\partial f_i}{\partial x_j}$$

- When m=n=1 (single-variable function), Jacobian reduces to …?

the derivative of $\mathbf{f}$

Jacobian for Matrix Inputs

- Given a function with $\boldsymbol{m}$ **outputs** and $\boldsymbol{n} \times \boldsymbol{p}$ **inputs**

$$\mathbf{f}(\mathbf{X}) = [f_1(\mathbf{X}), \dots, f_m(\mathbf{X})] \in \mathbb{R}^m, \text{ where } \mathbf{X} = \begin{bmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{bmatrix} \in \mathbb{R}^{n \times p}$$

- Jacobian is a $\mathrm{m} \times n \times p$ **tensor** (i.e., matrix of matrices) of partial derivatives:

$$\left(\mathbf{J}_{\mathbf{f}}(\mathbf{X})\right)_{ijk} = \frac{\partial f_i}{\partial x_{jk}}$$

- The dimension of the Jacobian:= output dim x input dims.
- The Jacobian math holds if you keep adding more dimensions to the input or output.

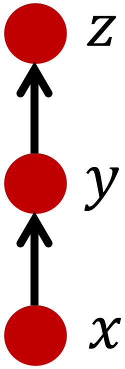
Why Use Matrix/Tensor Form?

In essence, matrix form (multi-variate calculus) is just an extension of single-variable calculus.

Two reasons:

- Compact derivations: with matrix form calculations we can compute a concise statements.
- Implementing algorithms in matrix form is much faster.
  - GPUs are optimized for VERY FAST matrix/tensor operations.

Chain Rule



- Function composition:

$$z \circ y(x) = z\big(y(x)\big) = z(x)$$

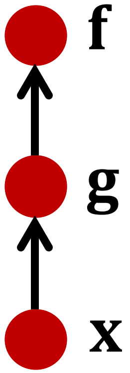
If z is a function of y, and
y is a function of x, then
z is a function of x, as well.

Then:

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} \frac{\partial y}{\partial x}$$

Chain Rule for Multivariable Functions

- Let $\mathbf{x} \in \mathbb{R}^d$, $\mathbf{g}\colon \mathbb{R}^d \rightarrow \mathbb{R}^n$, $\mathbf{f}\colon \mathbb{R}^n \rightarrow \mathbb{R}^m$
- Composing them: $\mathbf{f} \circ \mathbf{g}(\mathbf{x}) = \mathbf{f}\big(\mathbf{g}(\mathbf{x})\big)\colon \mathbb{R}^d \rightarrow \mathbb{R}^m$



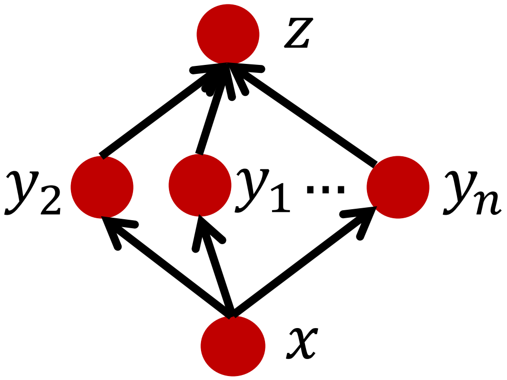
The result looks similar to the single-variable setup:

$$\mathbf{J}_{\mathbf{f}\circ\mathbf{g}}(\mathbf{x}) = \mathbf{J}_{\mathbf{f}}(\mathbf{g}(\mathbf{x}))\ \mathbf{J}_{\mathbf{g}}(\mathbf{x})$$

Note, the above statement is a **matrix** multiplication!

Function $\mathbf{f} \circ \mathbf{g}$ has *m* outputs and *d* inputs → Jacobian's dims: *m* by *d*

Quiz Time!



Let $x \in \mathbb{R}$, $\mathbf{y}: \mathbb{R} \to \mathbb{R}^n$, $\mathbf{z}: \mathbb{R}^n \to \mathbb{R}$

What is the Jacobean of $z \circ \mathbf{y}(x) = z(y_1(x), \ldots, y_n(x))$?

1. $\mathbf{J}_{z\circ\mathbf{y}}(x) = \mathbf{J}_z(\mathbf{y}(x))\ \mathbf{J}_\mathbf{y}(x)$
2. $\mathbf{J}_{z\circ\mathbf{y}}(x) = \left[\frac{\partial z}{\partial y_1}, \ldots, \frac{\partial z}{\partial y_n}\right]\left[\frac{\partial y_1}{\partial x}, \ldots, \frac{\partial y_n}{\partial x}\right]^{\mathrm{T}}$
3. $\mathbf{J}_{z\circ\mathbf{y}}(x) = \sum_{\mathrm{i}=1}^{n} \frac{\partial z}{\partial y_i} \ \frac{\partial y_i}{\partial x}$
4. All the above!

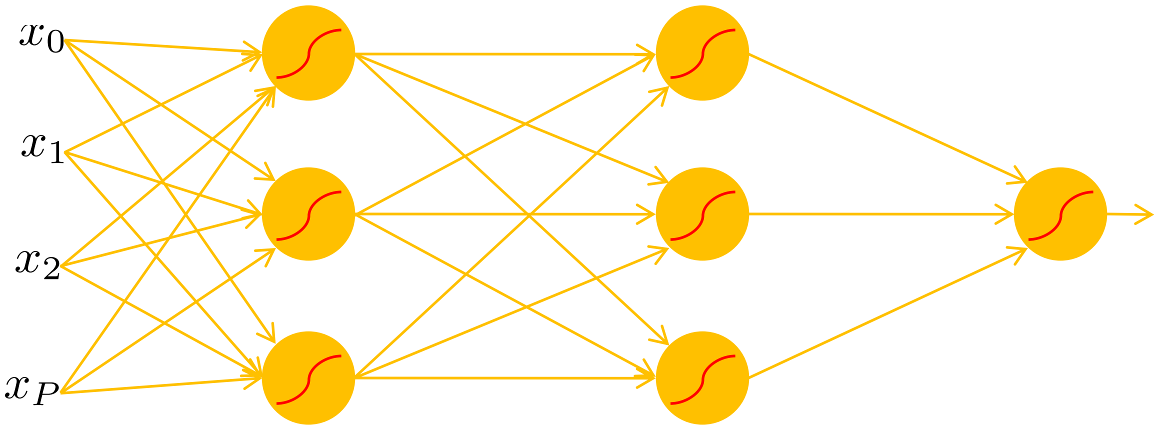
Summary

- We reviewed lots of background about neural networks!
  - Linear algebra foundation
  - Gradient descent
  - Extending gradients to tensor form: Jacobians

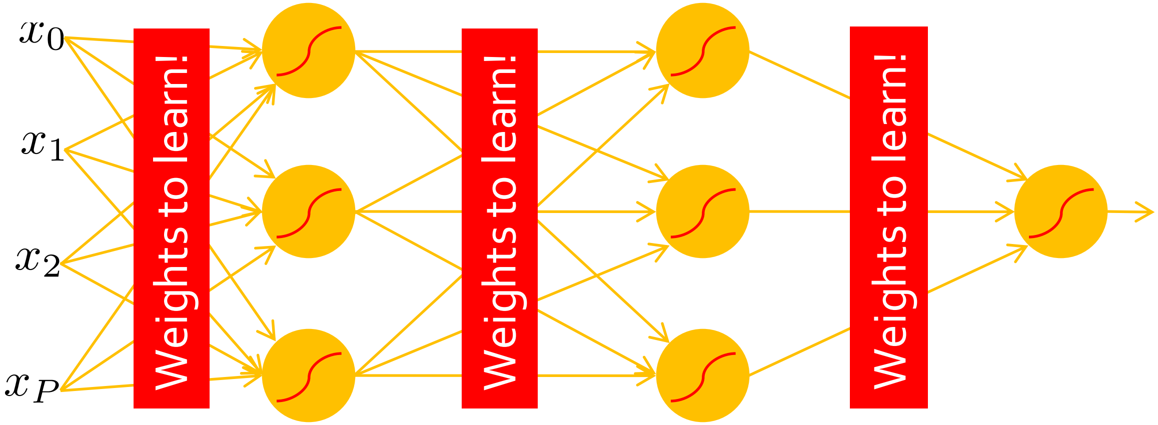
- **Next:** training a neural net!

Training Neural Networks: Analytical Backprop

Recap: Multi-Layer Perceptron



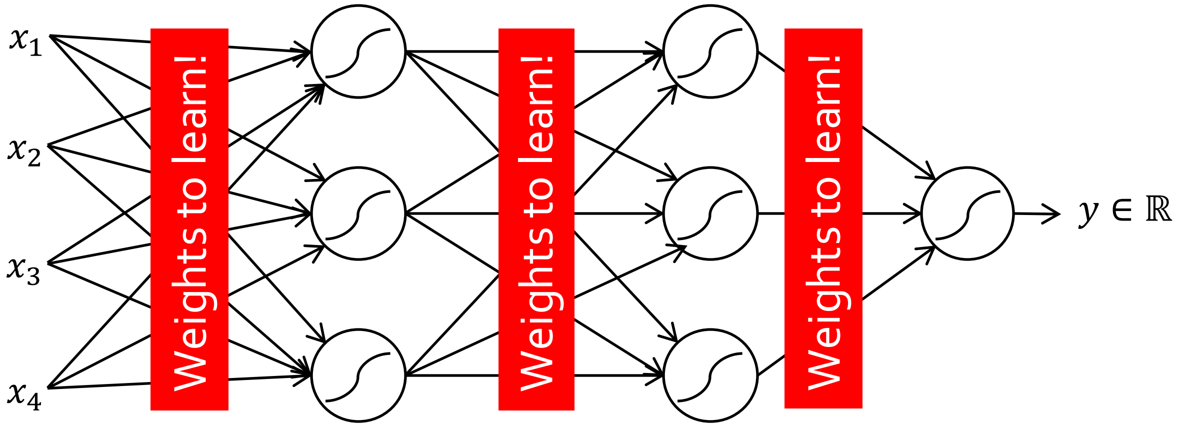
Recap: Multi-Layer Perceptron



Training Neural Networks: Setup

- We are given an architecture though its weights $\mathbf{W}$.
- We are given a training data $D = \{(\mathbf{x}_i, y_i^*)\}$
- We are given a loss function $\ell: \mathbb{R} \times \mathbb{R} \to (0, 1)$
  - $\ell(y^*, y)$ quantifies distance between an answer y^* and prediction $\mathrm{y} = \mathrm{NN}(\mathbf{x}; \mathbf{W})$ — lower is better.
- Overall objective to optimize: $\mathcal{L}(D; \mathbf{W}) = \sum_{(\mathbf{x}_i, y_i^*) \in D} \ell(\mathrm{NN}(\mathbf{x}_i; \mathbf{W}), y_i^*)$

$\mathbf{x} = (x_1, x_2, x_3, x_4) \in \mathbb{R}^4$



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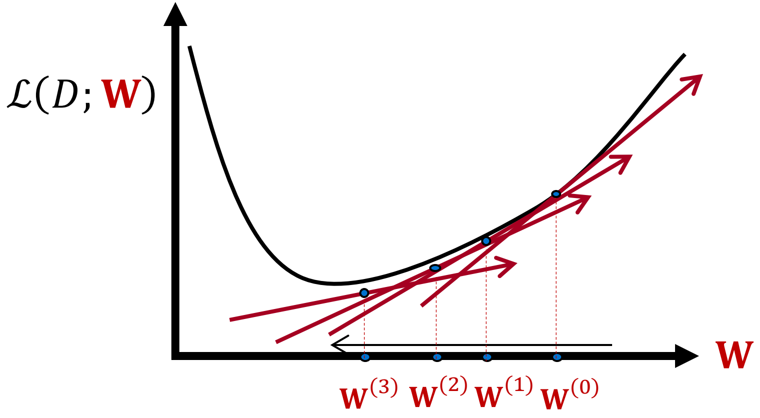
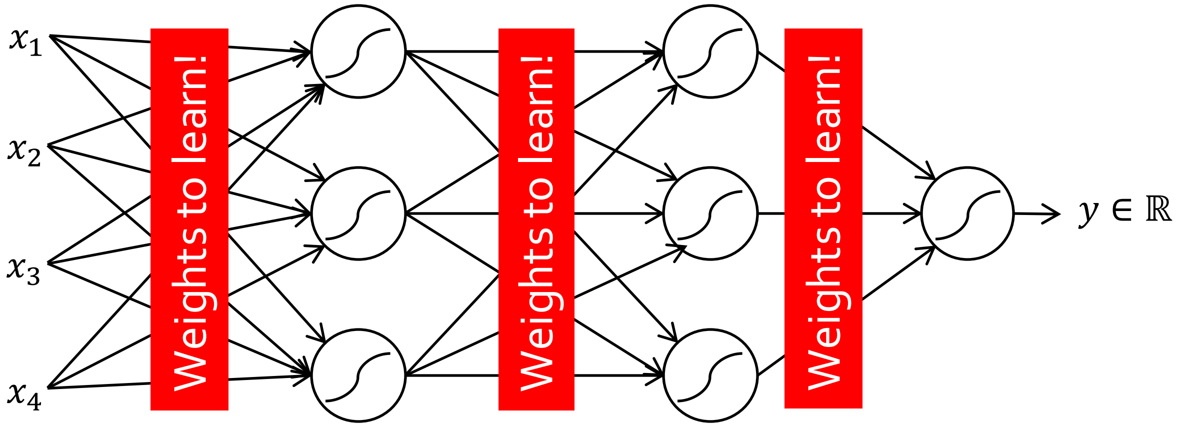
Training Neural Networks ~ Optimizing Parameters

- We can use gradient descent to minimizes the loss.
- At each step, the weight vector is modified in the direction that produces the steepest descent along the error surface.



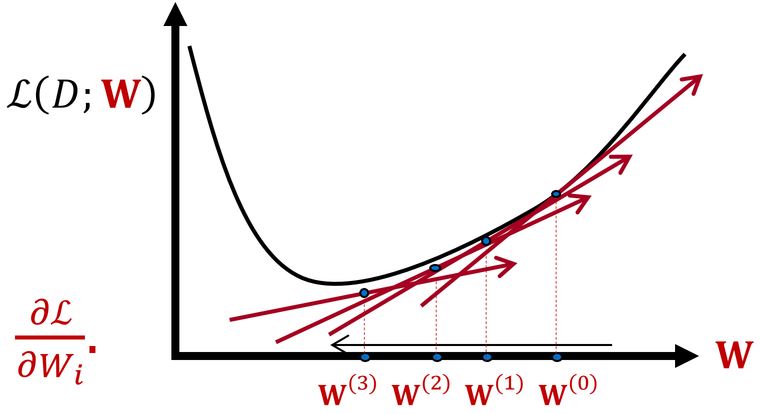
$\mathbf{x} = (x_1, x_2, x_3, x_4) \in \mathbb{R}^4$



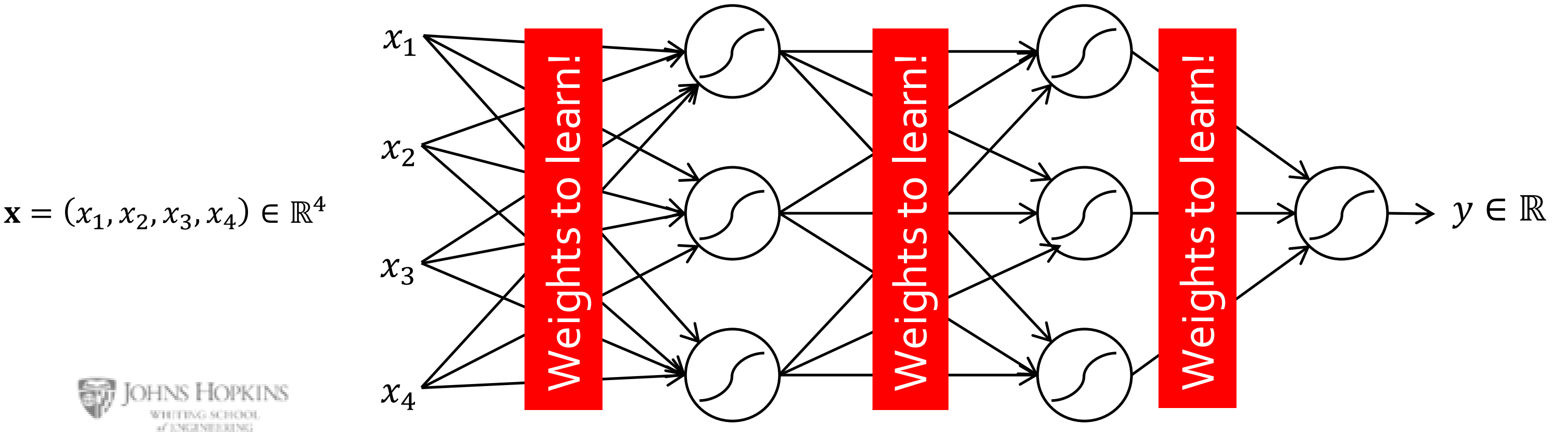
Training Neural Networks ~ Optimizing Parameters

For each sub-parameter $W_i \in \mathbf{W}$:

$$W_i^{(t+1)} = W_i^{(t)} - \alpha \frac{\partial \mathcal{L}}{\partial W_i}$$



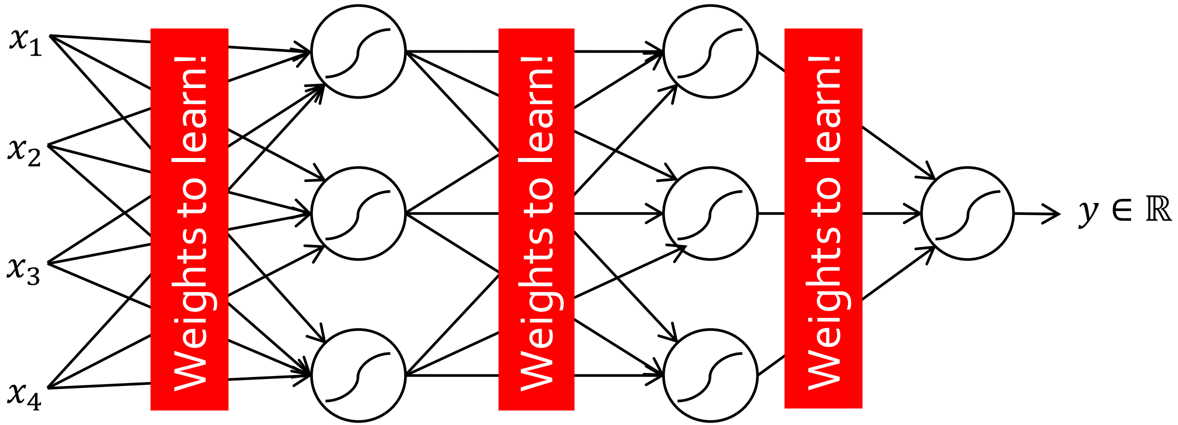
It all comes down to **efficiently** computing $\frac{\partial \mathcal{L}}{\partial W_i}$.



Training Neural Networks ~ Computing the Gradients

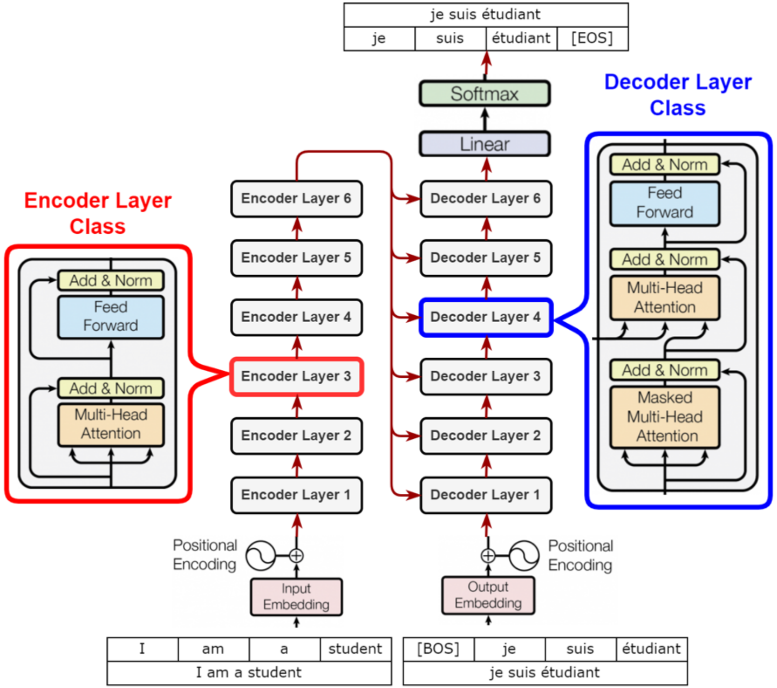
- How do you efficiently compute $\frac{\partial \mathcal{L}}{\partial W_i}$ for all parameters?
- It's easy to learn the final layer – it's just a linear unit.
- How about the weights in the earlier layers (i.e., before the final layer)?

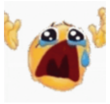
$\mathbf{x} = (x_1, x_2, x_3, x_4) \in \mathbb{R}^4$



Necessity of a Principled Algorithm for Gradient Computation

- Depth gives more representational capacity to neural networks.
- However, computing gradients for deeper layers is not trivial and tedious.
- Even if we have analytical formula for gradient, if they're architecture-specific, they must be repeated for each new architecture.
- The solution is "Backpropagation" algorithm!





Architecture of the BERT model with over 24 layers and millions of parameters — we will study get to this model in a few weeks!

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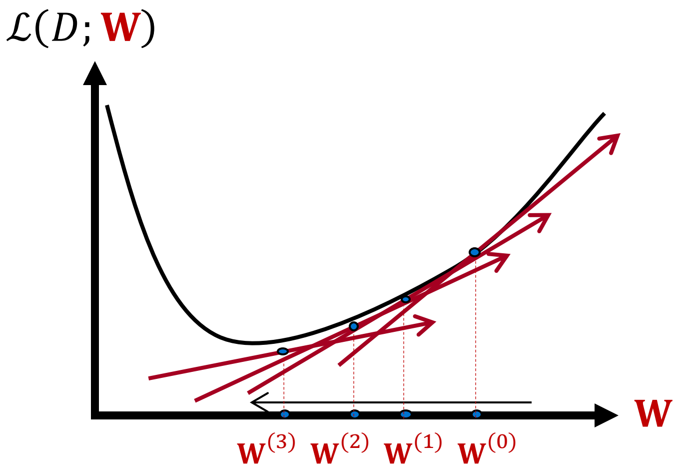
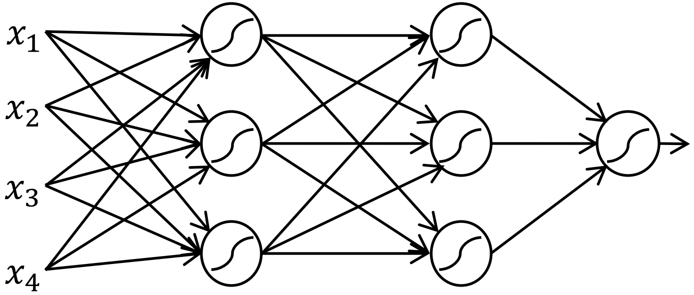
BP: Required Intuitions

1. Gradient Descent
   - Change the weights $\mathbf{W}$ in the direction of gradient to minimize the error function.



2. Chain Rule
   - Use the chain rule to calculate the weights of the intermediate weights



3. Dynamic Programming (Memoization)
   - Memoize the weight updates to make the updates faster.

A Generic Multi-Layer Perceptron

- Given the following definition:

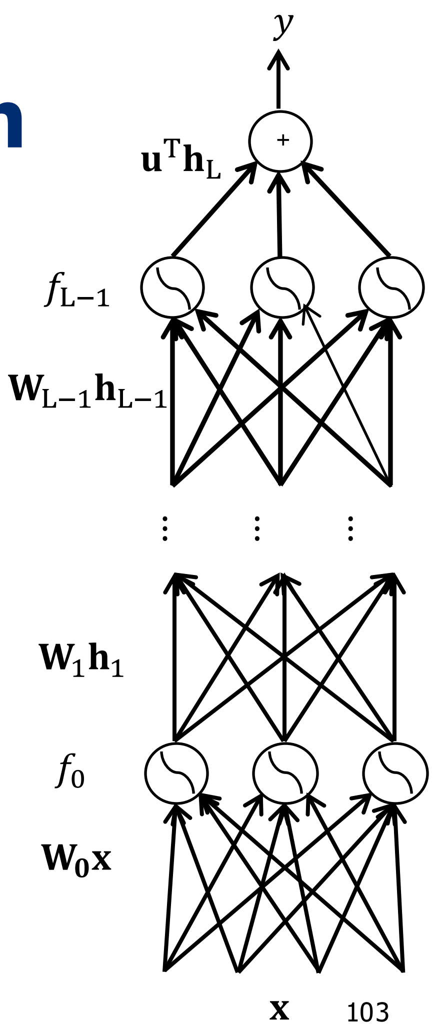
$$\mathbf{x} = \mathbf{h}_0 \in \mathbb{R}^{d_0} \quad \text{(input)}$$

$$\mathbf{h}_{i+1} = f_i(\mathbf{W}_i \mathbf{h}_i) \in \mathbb{R}^{d_i} \quad \text{(hidden layer } i\text{, } 0 \le i \le L-1\text{)}$$

$$y = \mathbf{u}^{\mathrm{T}} \mathbf{h}_L \in \mathbb{R} \quad \text{(output)}$$

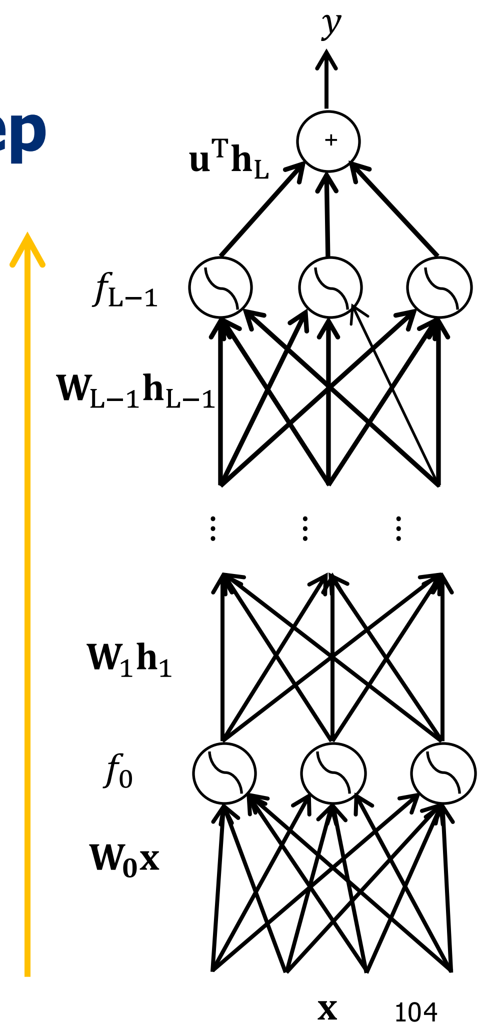
$$\mathcal{L} = \ell(y, y^*) \in \mathbb{R} \quad \text{(loss)}$$

- Trainable parameters: $\mathbf{W} = \{\mathbf{W}_0, \mathbf{W}_1, \dots, \mathbf{W}_L, \mathbf{u}\}$



A Generic Neural Network: Forward Step

- Given some [initial] values for the parameters, we can compute the forward pass, layer by layer.
- Forward pass is basically L matrix multiplications, each followed by an activation function.
- Matrix multiplication can be done efficiently with GPUs.
  - Therefore, forward pass is somewhat fast.
- Complexity of forward pass is …. linear of depth $O(L)$.



A Generic Neural Network: Direct Gradients

$\mathbf{x} = \mathbf{h}_0 \in \mathbb{R}^{d_0}$ (input)

$\mathbf{h}_{i+1} = f_i(\mathbf{W}_i \mathbf{h}_i) \in \mathbb{R}^{d_i}$

$(0 \leq i \leq L-1)$

$y = \mathbf{u}^{\mathrm{T}} \mathbf{h}_L \in \mathbb{R}$ (output)

$\mathcal{L} = \ell(y, y^*) \in \mathbb{R}$ (loss)

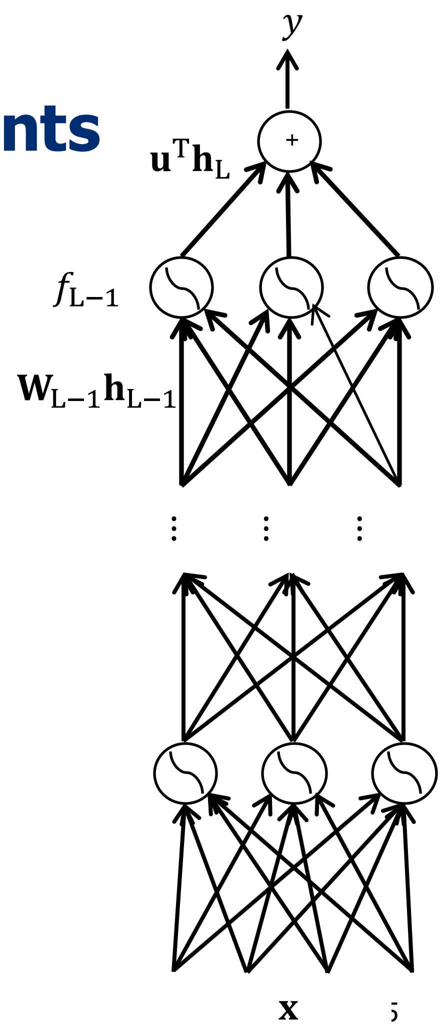
$\mathbf{W} = \{\mathbf{W}_0, \mathbf{W}_1, \dots, \mathbf{W}_L, \mathbf{u}\}$

We want the gradients of $\mathcal{L}$ with respect to model parameters.

Use the chain rule to simplify the following term:

$$\nabla_{\mathbf{W}_{L-1}} \mathcal{L} = \left(\mathbf{J}_{\mathcal{L}}(\mathbf{W}_{L-1})\right)^{\mathrm{T}} =$$

$$\left(\mathbf{J}_{\mathcal{L}}(\mathrm{y})\, \mathbf{J}_y(\mathbf{h}_{\mathrm{L}})\, \mathbf{J}_{\mathbf{h}_{\mathrm{L}}}(\mathbf{W}_{\mathrm{L}-1})\right)^{\mathrm{T}}$$



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$(0 \leq i \leq L-1)$

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$\mathcal{L} = \ell(y, y^*) \in \mathbb{R}$ (loss)

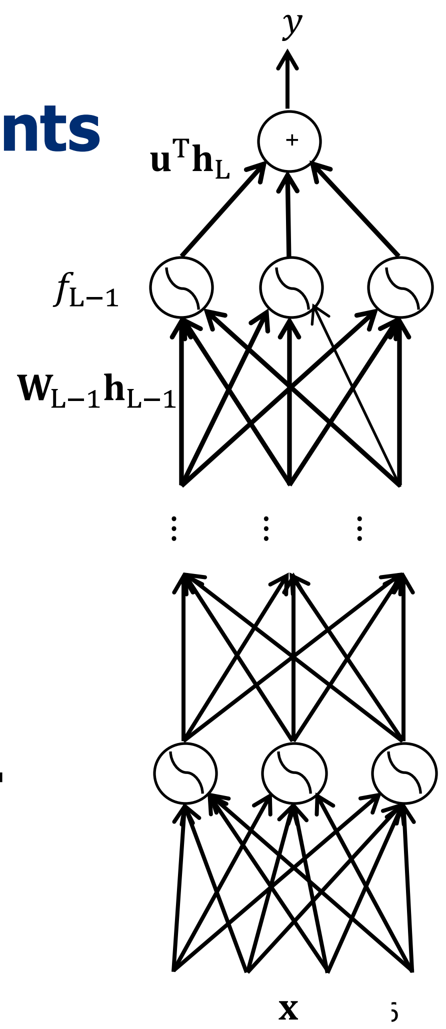
$\mathbf{W} = \{\mathbf{W}_0, \mathbf{W}_1, \dots, \mathbf{W}_L, \mathbf{u}\}$

We want the gradients of $\mathcal{L}$ with respect to model parameters.

Use the chain rule to simplify the following term:

$$\nabla_{\mathbf{W}_{L-2}} \mathcal{L} = \left(\mathbf{J}_{\mathcal{L}}(\mathbf{W}_{L-2})\right)^{\mathrm{T}} =$$

$$\left(\mathbf{J}_{\mathcal{L}}(\mathrm{y})\, \mathbf{J}_{y}(\mathbf{h}_{\mathrm{L}})\, \mathbf{J}_{\mathbf{h}_{\mathrm{L}}}(\mathbf{h}_{\mathrm{L}-1})\, \mathbf{J}_{\mathbf{h}_{\mathrm{L}-1}}(\mathbf{W}_{\mathrm{L}-2})\right)^{\mathrm{T}}$$



A Generic Neural Network: Direct Gradients

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$\mathbf{h}_{i+1} = f_i(\mathbf{W}_i \mathbf{h}_i) \in \mathbb{R}^{d_i}$

$(0 \leq i \leq L-1)$

$y = \mathbf{u}^{\mathrm{T}} \mathbf{h}_L \in \mathbb{R}$ (output)

$\mathcal{L} = \ell(y, y^*) \in \mathbb{R}$ (loss)

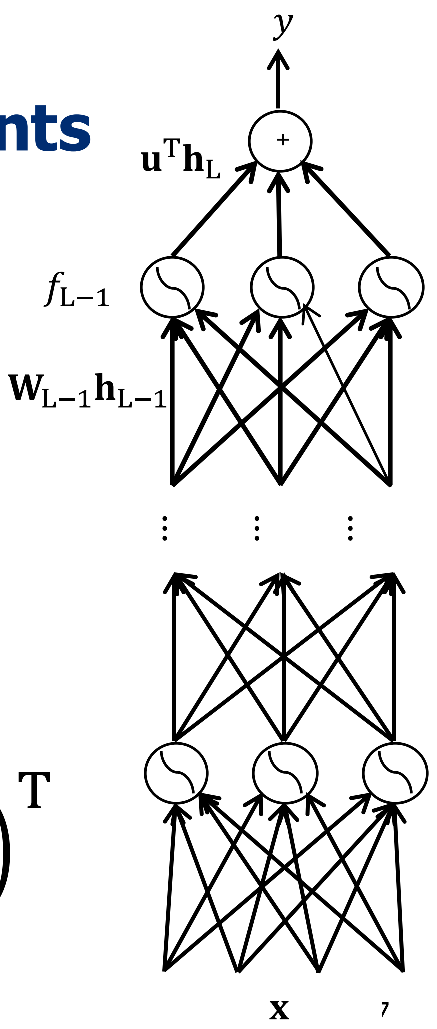
$\mathbf{W} = \{\mathbf{W}_0, \mathbf{W}_1, \ldots, \mathbf{W}_L, \mathbf{u}\}$

We want the gradients of $\mathcal{L}$ with respect to model parameters.

Use the chain rule to simplify the following term:

$$\nabla_{\mathbf{W}_{L-i}} \mathcal{L} = \left(\mathbf{J}_{\mathcal{L}}(\mathbf{W}_{L-i})\right)^{\mathrm{T}} =$$

$$\left(\mathbf{J}_{\mathcal{L}}(\mathrm{y})\, \mathbf{J}_{y}(\mathbf{h}_{\mathrm{L}})\, \mathbf{J}_{\mathbf{h}_{\mathrm{L}}}(\mathbf{h}_{\mathrm{L}-1}) \ldots \mathbf{J}_{\mathbf{h}_{\mathrm{L}-i+1}}(\mathbf{W}_{\mathrm{L}-i})\right)^{\mathrm{T}}$$



A Generic Neural Network: Direct Gradients

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$(0 \le i \le L-1)$

$y = \mathbf{u}^{\mathrm{T}} \mathbf{h}_L \in \mathbb{R}$ (output)

$\mathcal{L} = \ell(y, y^*) \in \mathbb{R}$ (loss)

$\mathbf{W} = \{\mathbf{W}_0, \mathbf{W}_1, \dots, \mathbf{W}_L, \mathbf{u}\}$

We want the gradients of $\mathcal{L}$ with respect to model parameters.

- $\nabla_{\mathbf{W}_{L-1}} \mathcal{L} = \left(\mathbf{J}_{\mathcal{L}}(\mathbf{W}_{L-1})\right)^{\mathrm{T}} = \left(\mathbf{J}_{\mathcal{L}}(\mathrm{y})\, \mathbf{J}_y(\mathbf{h}_{\mathrm{L}})\, \mathbf{J}_{\mathbf{h}_{\mathrm{L}}}(\mathbf{W}_{\mathrm{L}-1})\right)^{\mathrm{T}}$
- $\nabla_{\mathbf{W}_{L-2}} \mathcal{L} = \left(\mathbf{J}_{\mathcal{L}}(\mathbf{W}_{L-2})\right)^{\mathrm{T}} = \left(\mathbf{J}_{\mathcal{L}}(\mathrm{y})\, \mathbf{J}_y(\mathbf{h}_{\mathrm{L}})\, \mathbf{J}_{\mathbf{h}_{\mathrm{L}}}(\mathbf{h}_{\mathrm{L}-1})\, \mathbf{J}_{\mathbf{h}_{\mathrm{L}-1}}(\mathbf{W}_{\mathrm{L}-2})\right)^{\mathrm{T}}$
- **…**
- $\nabla_{\mathbf{W}_0} \mathcal{L} = \left(\mathbf{J}_{\mathcal{L}}(\mathbf{W}_{L-3})\right)^{\mathrm{T}} = \left(\mathbf{J}_{\mathcal{L}}(\mathrm{y})\, \mathbf{J}_y(\mathbf{h}_{\mathrm{L}})\, \mathbf{J}_{\mathbf{h}_{\mathrm{L}}}(\mathbf{h}_{\mathrm{L}-1}) \dots \mathbf{J}_{\mathbf{h}_1}(\mathbf{W}_0)\right)^{\mathrm{T}}$

3 matrix multiplications

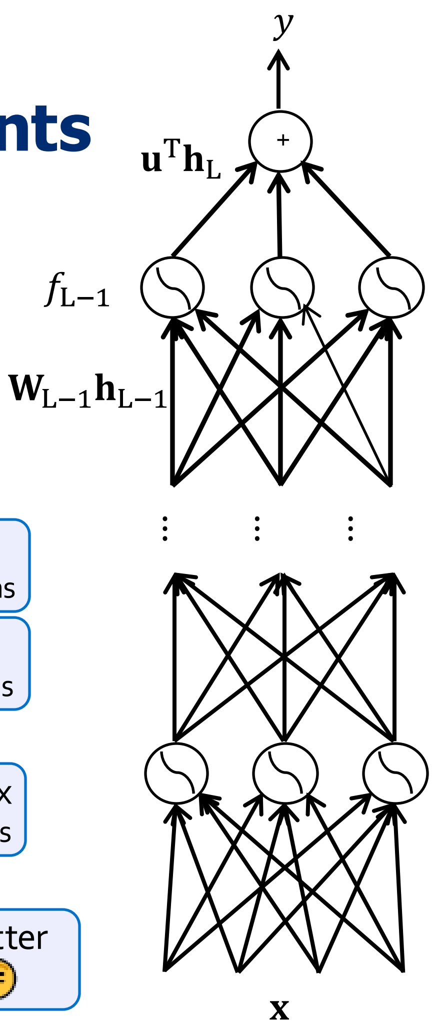
4 matrix multiplications

$L+2$ matrix multiplications

In total, how many matrix multiplications are done here?

(A) $O(L)$ (B) $O(L^2)$ (C) $O(L^3)$ (C) $O(\exp(L))$

Can we do better than this? 🤨



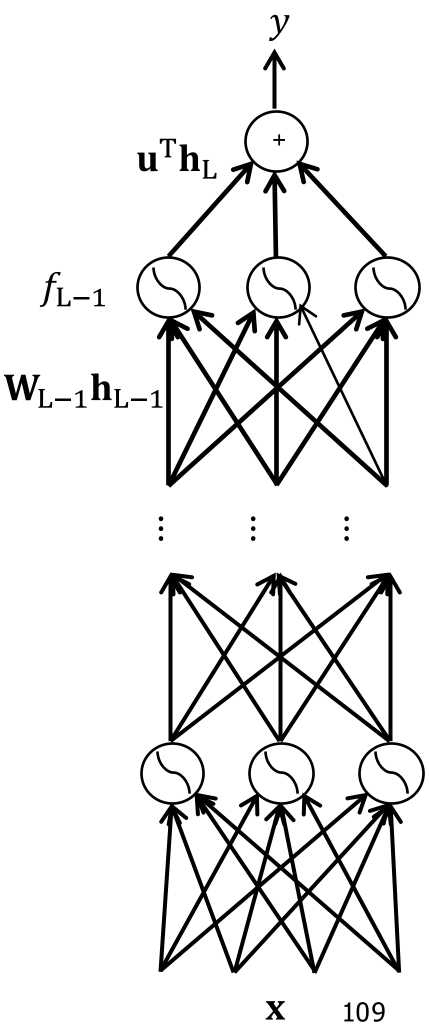
Caching Gradients to Turn $O(L^2)$ into $O(L)$

- Suppose we're computing:

$$\nabla_{\mathbf{W}_{L-1}}\mathcal{L} = \left(\mathbf{J}_{\mathcal{L}}(\mathrm{y})\,\mathbf{J}_{y}(\mathbf{h}_{\mathrm{L}})\,\mathbf{J}_{\mathbf{h}_{\mathrm{L}}}(\mathbf{W}_{\mathrm{L}-1})\right)^{\mathrm{T}}$$

$$\nabla_{\mathbf{W}_{L-2}}\mathcal{L} = \left(\mathbf{J}_{\mathcal{L}}(\mathrm{y})\,\mathbf{J}_{y}(\mathbf{h}_{\mathrm{L}})\,\mathbf{J}_{\mathbf{h}_{\mathrm{L}}}(\mathbf{h}_{\mathrm{L}-1})\,\mathbf{J}_{\mathbf{h}_{\mathrm{L}-1}}(\mathbf{W}_{\mathrm{L}-2})\right)^{\mathrm{T}}$$

- Parameter gradients depend on the gradients of the earlier layers!
- So, when computing gradients at each layer, we don't need to start from scratch!
- I can **reuse** gradients computed for higher layers for lower layers (i.e., memoization).



Caching Gradients to Turn $O(L^2)$ into $O(L)$

- First, precompute these cache values:

$O(L)$ matrix multiplications

First layer: $\delta_L = \mathbf{J}_{\mathcal{L}}(\mathrm{y})\ \mathbf{J}_y(\mathbf{h}_\mathrm{L})$

Subsequent layers: $\delta_i = \delta_{i+1}\ \mathbf{J}_{\mathbf{h}_i}(\mathbf{h}_{i-1}), \forall i: 0 \le i \le L-1$

- Now, let's go back to the gradients:

One matrix multiplications

$$\nabla_{\mathbf{W}_{L-1}}\mathcal{L} = \left(\mathbf{J}_{\mathcal{L}}(\mathrm{y})\ \mathbf{J}_y(\mathbf{h}_\mathrm{L})\ \mathbf{J}_{\mathbf{h}_\mathrm{L}}(\mathbf{W}_{\mathrm{L}-1})\right)^\mathrm{T} = \left(\delta_L\ \mathbf{J}_{\mathbf{h}_\mathrm{L}}(\mathbf{W}_{\mathrm{L}-1})\right)^\mathrm{T}$$

One matrix multiplications

$$\nabla_{\mathbf{W}_{L-2}}\mathcal{L} = \left(\mathbf{J}_{\mathcal{L}}(\mathrm{y})\ \mathbf{J}_y(\mathbf{h}_\mathrm{L})\ \mathbf{J}_{\mathbf{h}_\mathrm{L}}(\mathbf{h}_{\mathrm{L}-1})\ \mathbf{J}_{\mathbf{h}_{\mathrm{L}-1}}(\mathbf{W}_{\mathrm{L}-2})\right)^\mathrm{T} = \left(\delta_{L-1}\ \mathbf{J}_{\mathbf{h}_{\mathrm{L}-1}}(\mathbf{W}_{\mathrm{L}-2})\right)^\mathrm{T}$$

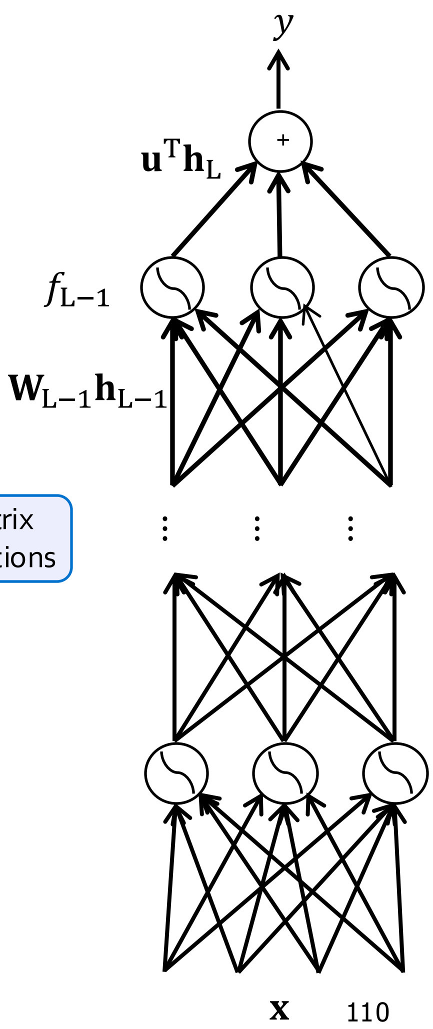
...

One matrix multiplications

$$\nabla_{\mathbf{W}_0}\mathcal{L} = \left(\mathbf{J}_{\mathcal{L}}(\mathrm{y})\ \mathbf{J}_y(\mathbf{h}_\mathrm{L})\ \mathbf{J}_{\mathbf{h}_\mathrm{L}}(\mathbf{h}_{\mathrm{L}-1}) \ldots \mathbf{J}_{\mathbf{h}_1}(\mathbf{W}_0)\right)^\mathrm{T} = \left(\delta_1\ \mathbf{J}_{\mathbf{h}_1}(\mathbf{W}_0)\right)$$

In total, how many matrix multiplications are done here when using caching?

(A) $O(L)$ (B) $O(L^2)$ (C) $O(L^3)$ (C) $O(\exp(L))$



Gradient: Local Grad + Upstream Grad

- Gradients at each layer computed by

$$\nabla_{\mathbf{W}_{L-i}}\mathcal{L} = \left(\delta_{L-i+1}\,\mathbf{J}_{\mathbf{h}_{L-i+1}}(\mathbf{W}_{L-i})\right)^{T}$$

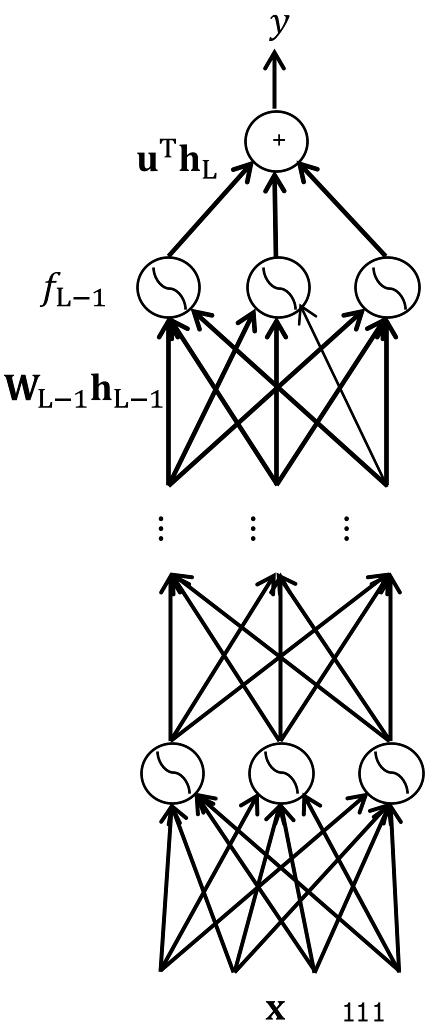
Upstream gradient ~ We lookup from the layer above.

Local Gradient

Let δ_i denote Jacobian at the output of layer i:

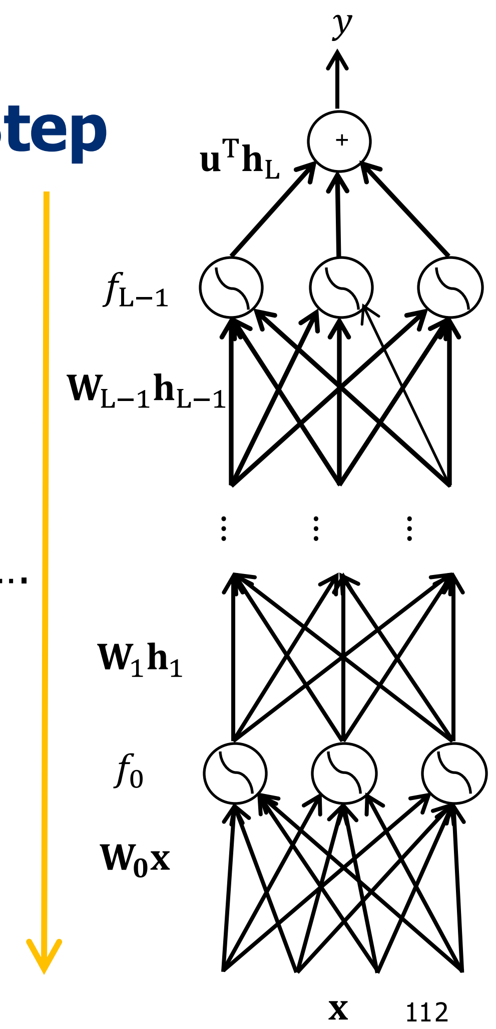
$$\delta_L = \mathbf{J}_{\mathcal{L}}(\mathrm{y})\,\mathbf{J}_y(\mathbf{h}_L)$$

$$\delta_i = \delta_{i+1}\;\mathbf{J}_{\mathbf{h}_i}(\mathbf{h}_{i-1})$$



A Generic Neural Network: Backward Step

- Backward step computes the gradients starting from the end to the beginning, layer by layer.
- Start by computing local gradients: $\mathbf{J}_{\mathbf{h}_{\mathrm{L}-i+1}}(\mathbf{W}_{\mathrm{L}-i})$
- Use then to compute upstream gradients δ_L, then δ_{L-1}, then δ_{L-2}, ….
- Use these to compute global gradients: $\nabla_{\mathbf{W}_i}\mathcal{L}$
- Computational cost as a function of depth:
  - With memoization, gradient computation is a **linear** function of depth L
    - (same cost as the forward process!!)
  - Without memorization, gradients computation would grow **quadratic** with L



A Generic Neural Network: Back Propagation

Initialize network parameters with random values

Loop until convergence

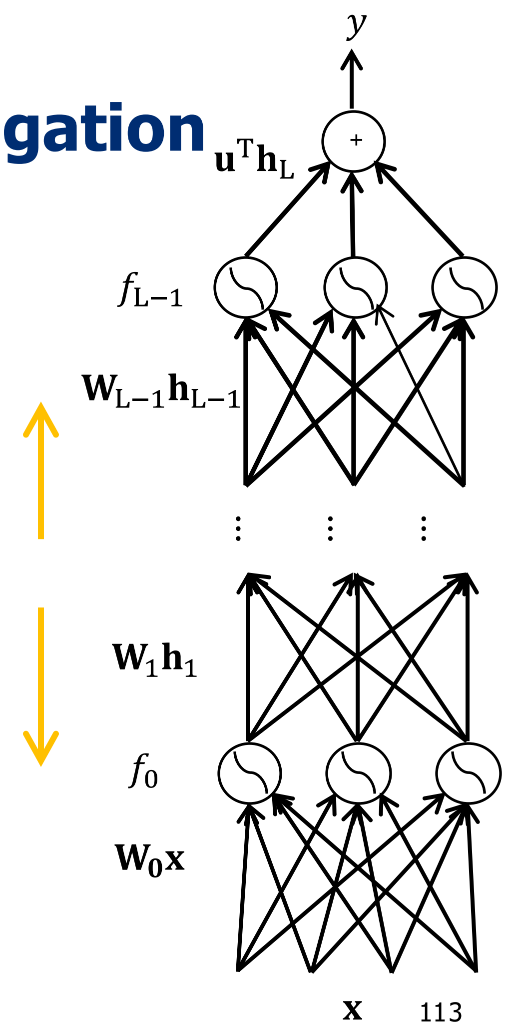
Loop over training instances

In practice, this step is done over **batches** of instances!

i. Forward step:
Start from the input and compute all the layers till the end (loss $\mathcal{L}$)

ii. Backward step:
Compute local gradients, starting from the last layer
Compute upstream gradients δ_i values, starting from the last layer
Use δ_i values to compute global gradients $\nabla_{\mathcal{L}}(\mathbf{W}_i)$ at each layer

iii. Gradient update:
Update each parameter: $\mathbf{W}_i^{(t+1)} \leftarrow \mathbf{W}_i^{(t)} - \alpha \, \nabla_{\mathbf{W}_i}\mathcal{L}$



Summary

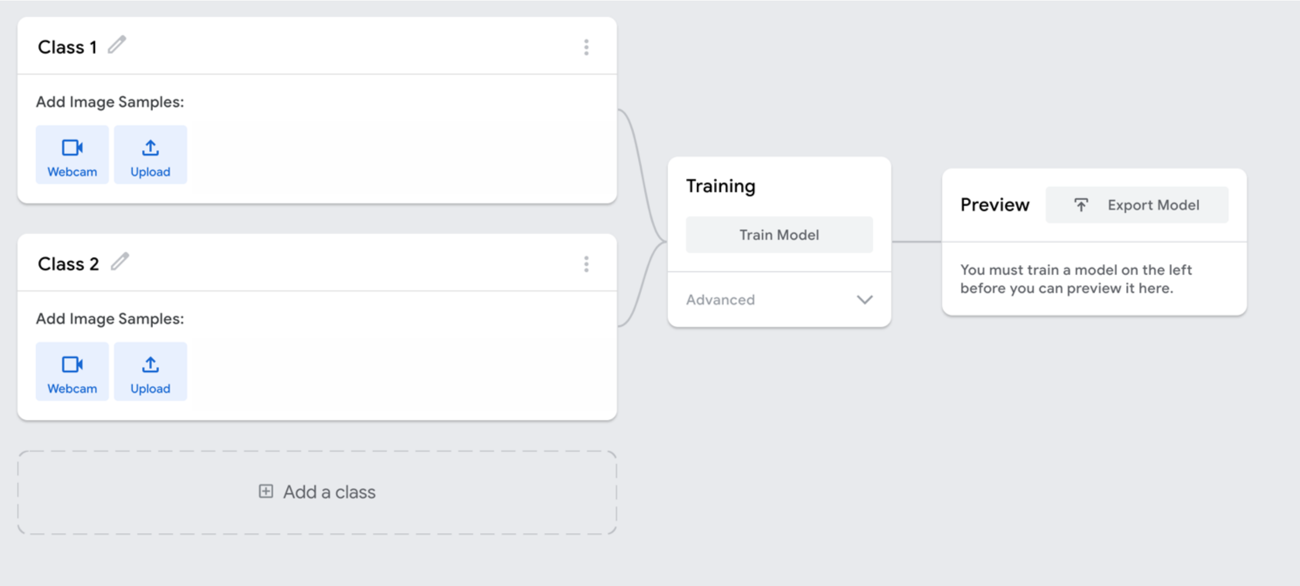
- Backpropagation: an algorithm for training neural networks.
- Using Dynamic Programming for efficient computation of gradients.
- **Next:** Backprop in real practice.

Quick Pulse Check

- How is **Backprop** different from/related to **Gradient Descent**?
  - **Backpropagation** is an algorithm used to compute the gradient of the loss function with respect to each weight in the network.
  - **Gradient descent**, on the other hand, is an optimization algorithm that uses these computed gradients to update the network's weights.
  - *Basically, backpropagation provides the necessary gradients for gradient descent to perform the weight updates.*

Demo Time!

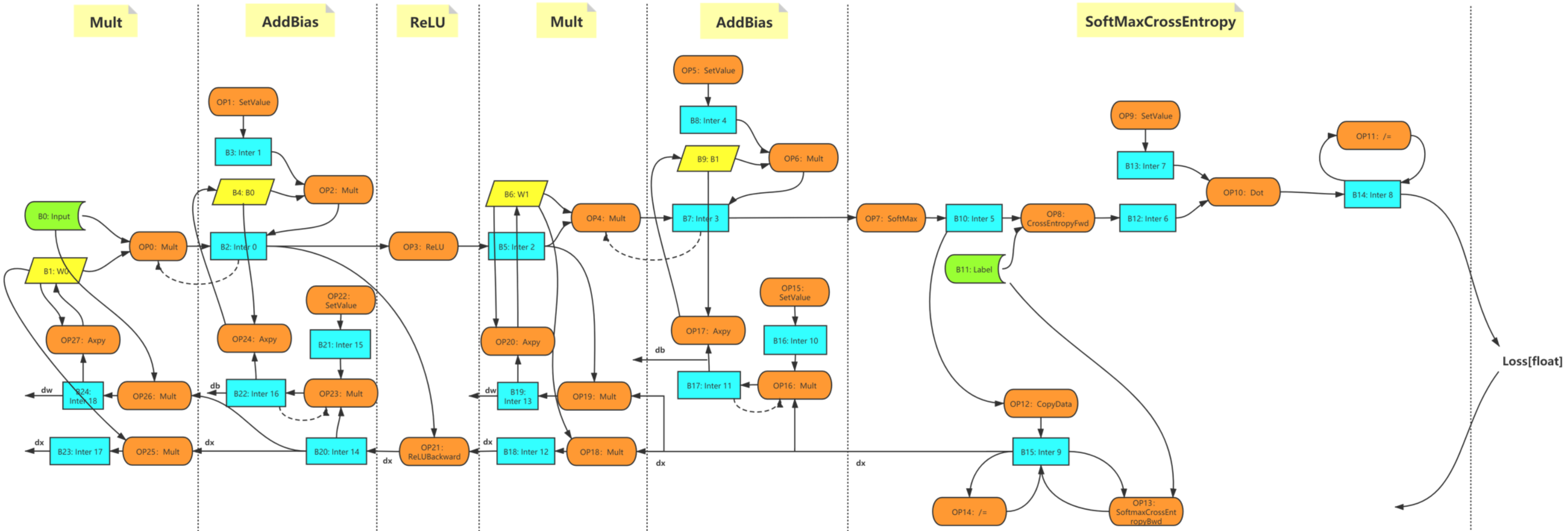
- https://teachablemachine.withgoogle.com/



Backprop in Real Practice: Computation Graph

Computation Graph: Example

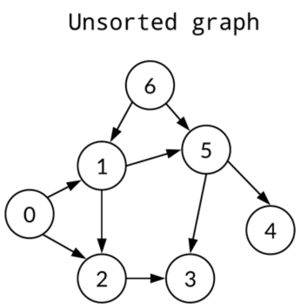
- In reality, neural networks are not as regular as the previous example …

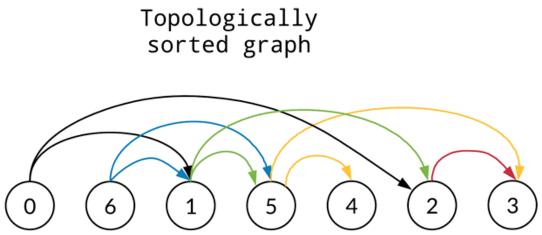


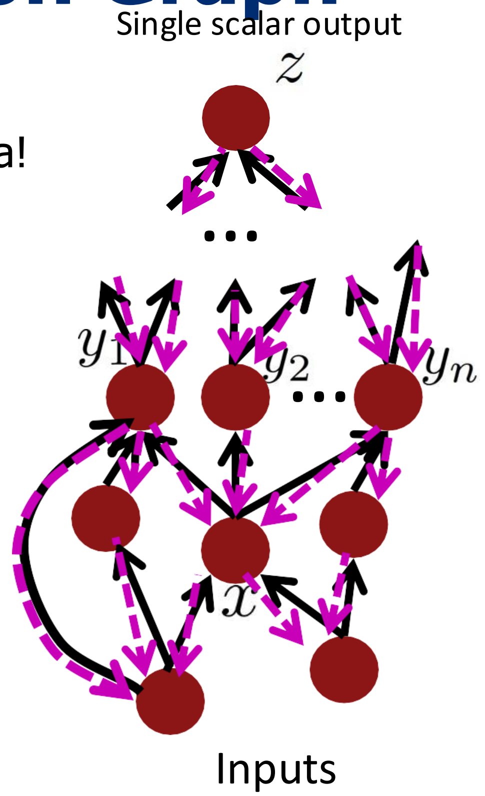
Backprop in General Computation Graph

- What if the network does not have a regular structure? Same idea!

1. Sort the nodes in topological order (what depends on what)
   - **Cost:** Linear in the number of nodes/edges.







Backprop in General Computation Graph

- What if the network does not have a regular structure? Same idea!

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2. Forward-Propagation:
   - Visit nodes in topological sort order and compute value of node given predecessors
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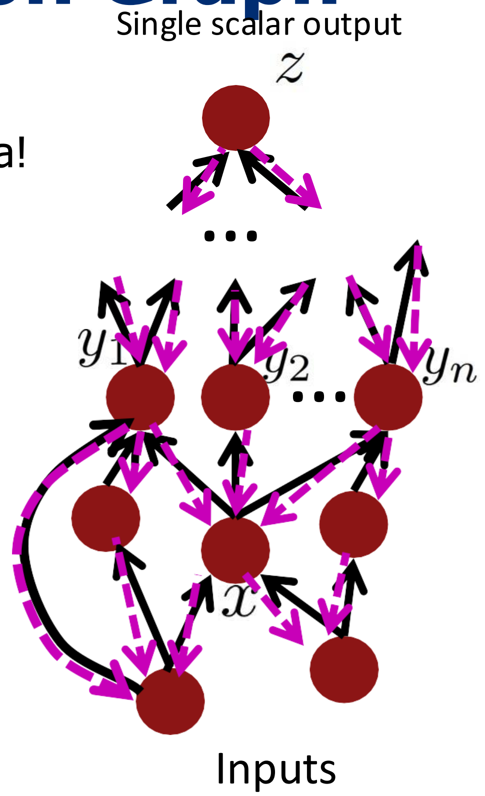
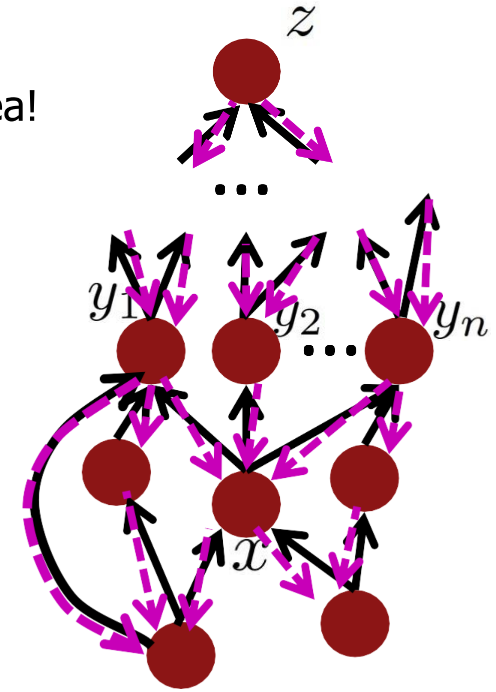


Backprop in General Computation Graph

- What if the network does not have a regular structure? Same idea!

1. Sort the nodes in topological order (what depends on what)
2. Forward-Propagation:
   - Visit nodes in topological sort order and compute value of node given predecessors
3. Backward-Propagation:
   - Compute local gradients
   - Visit nodes in reverse order and compute global gradients using gradients of successors
   - **Cost:** <u>Linear</u> in the number of nodes/edges.

Single scalar output



Inputs

Computation Graph:
👀 View inside each node

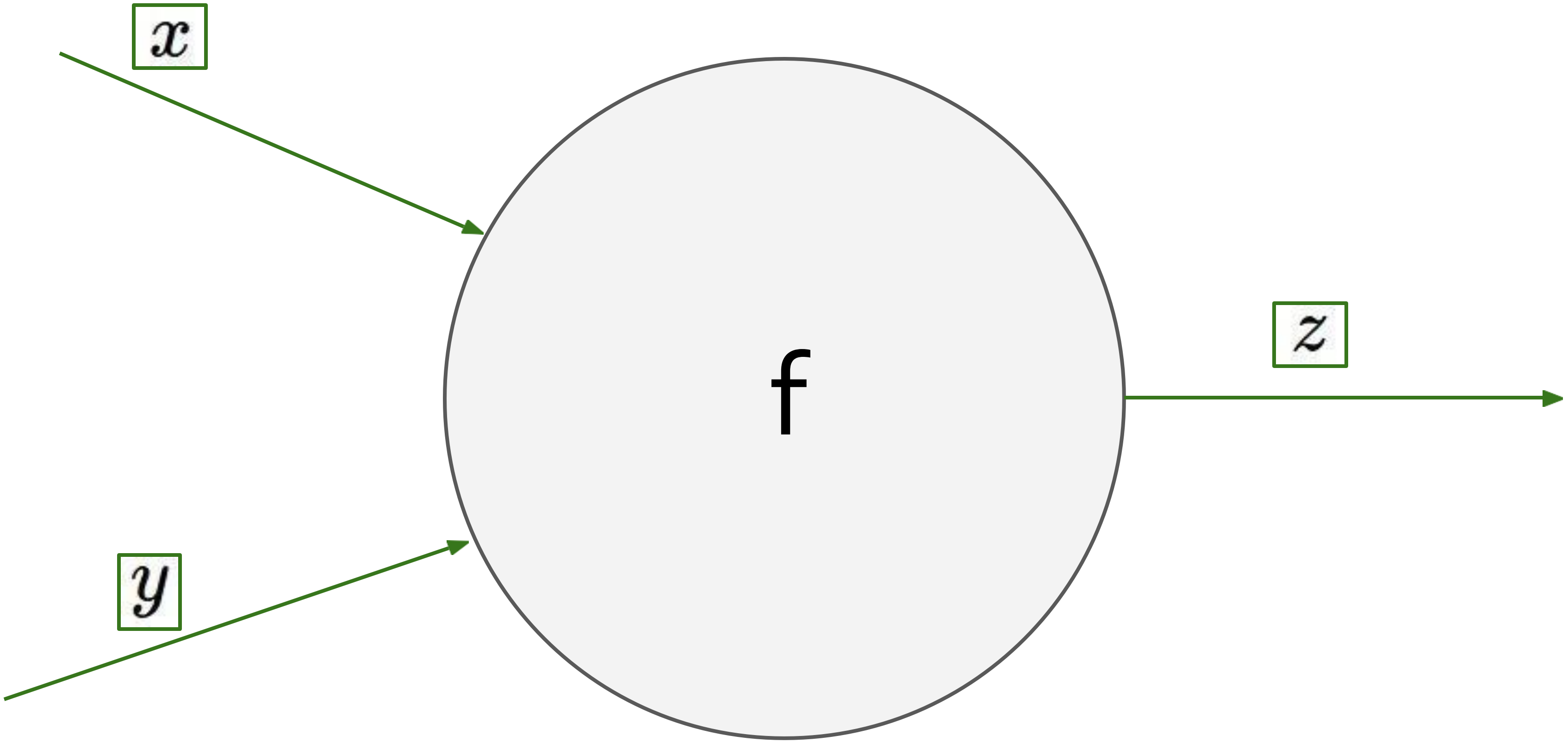
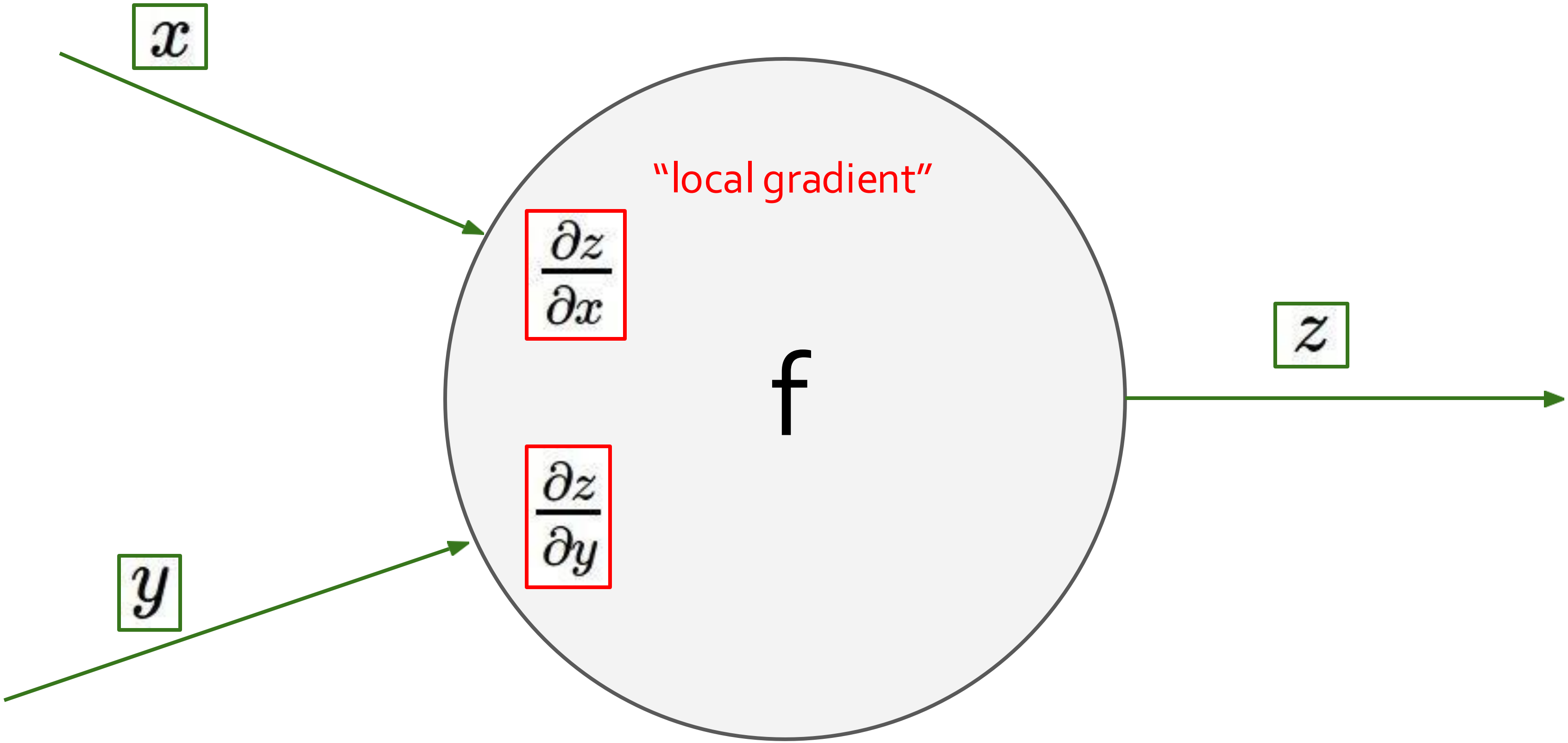


Figure from Andrej Karpathy



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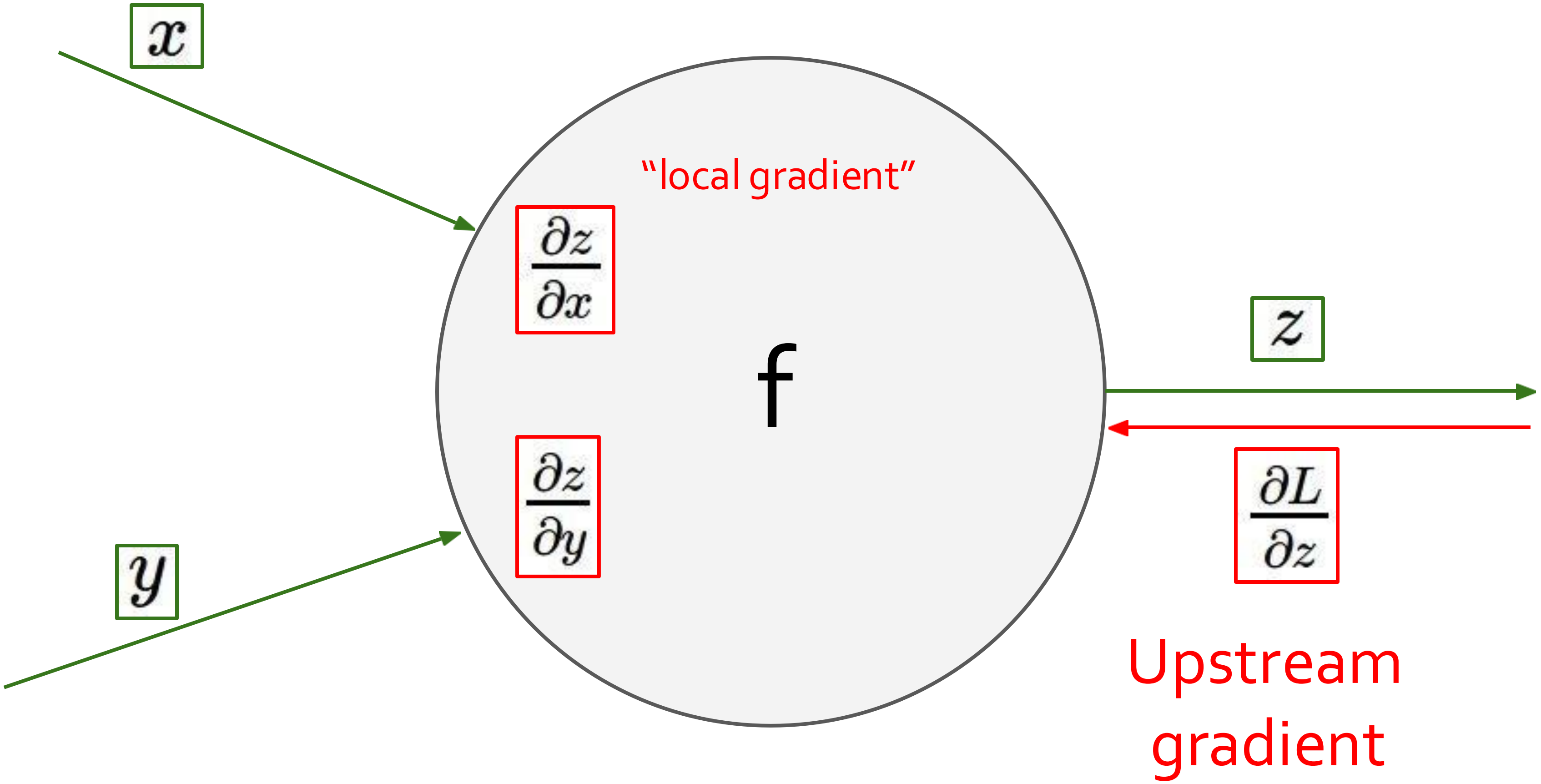

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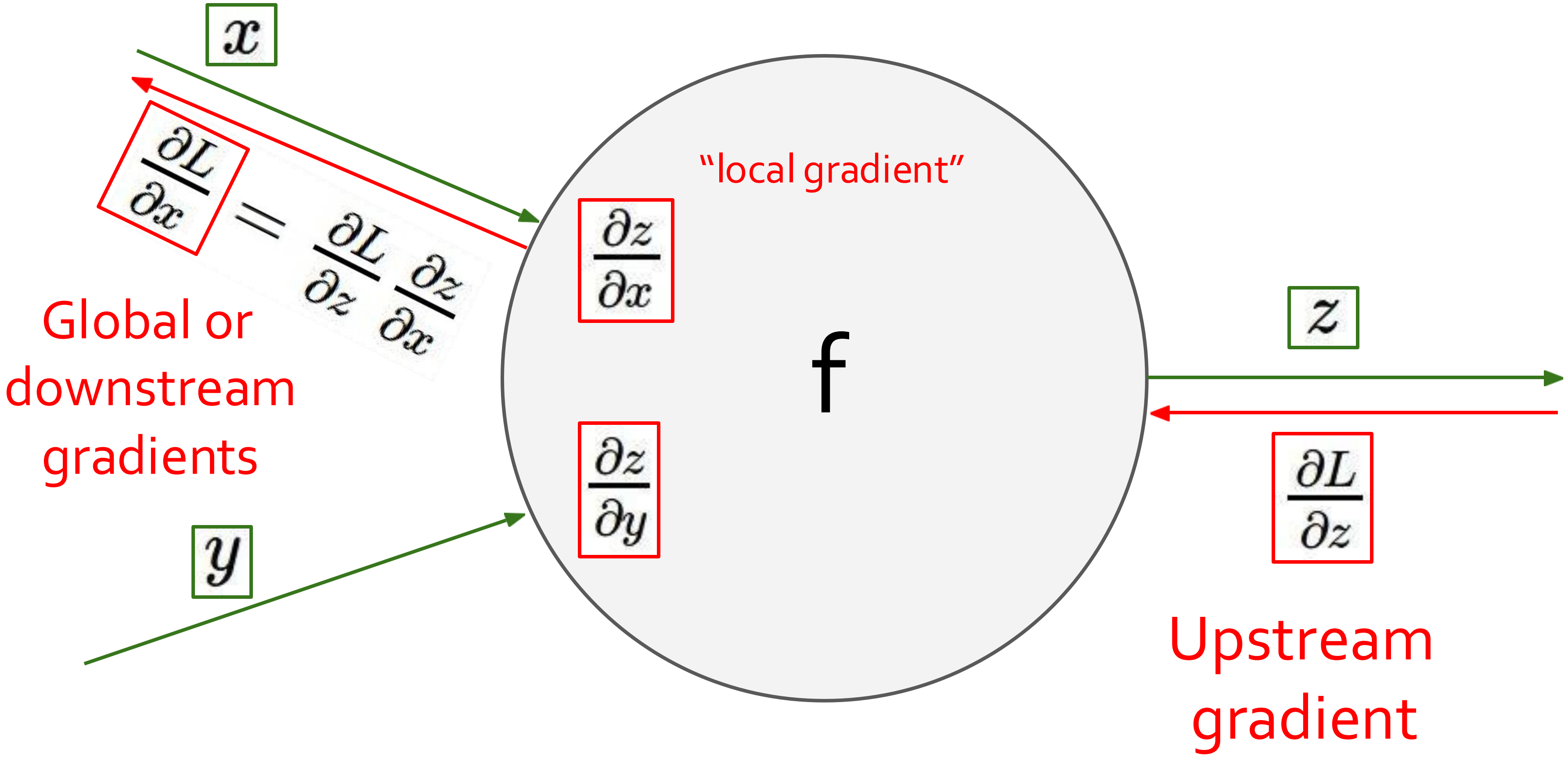

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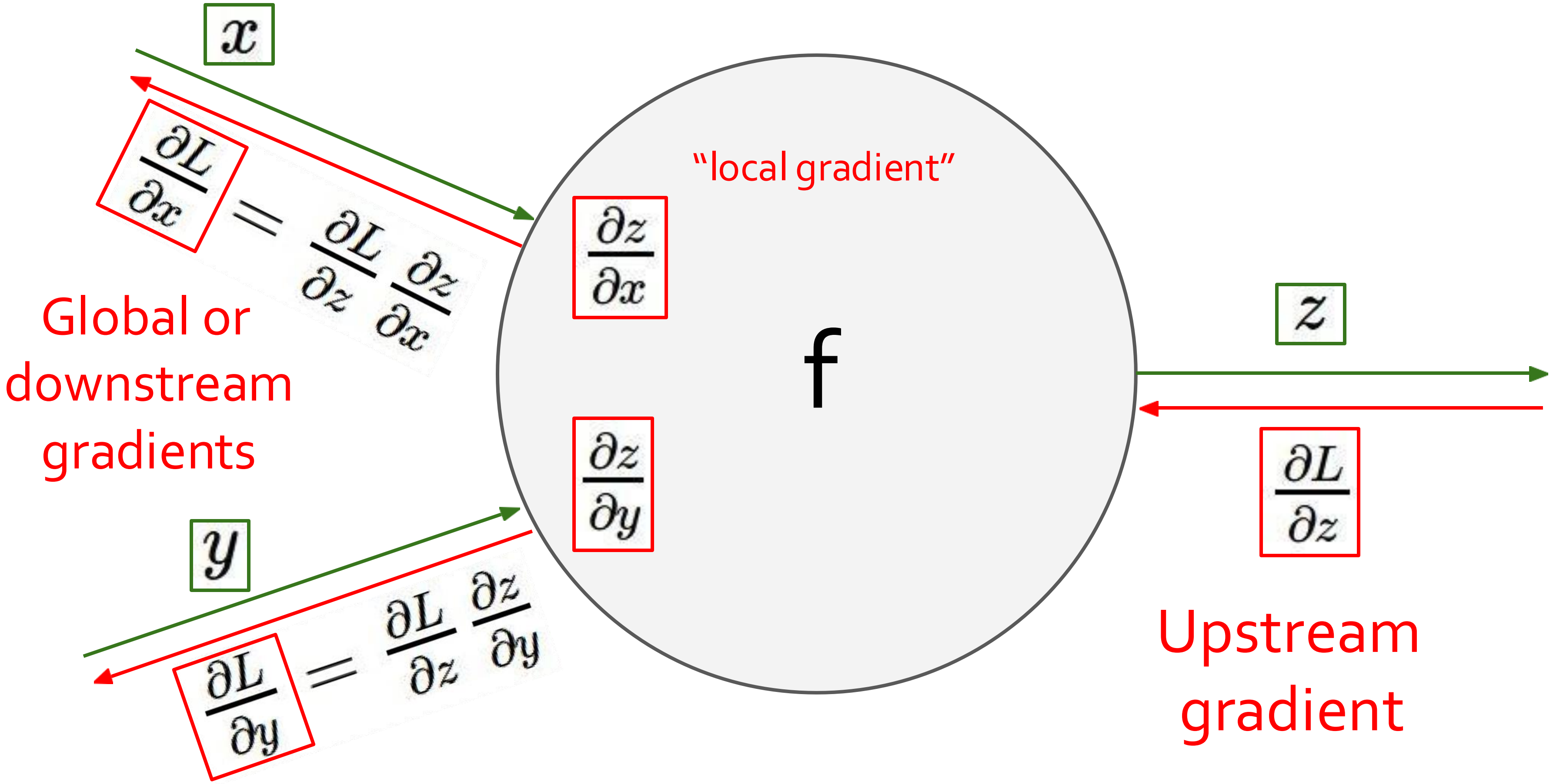

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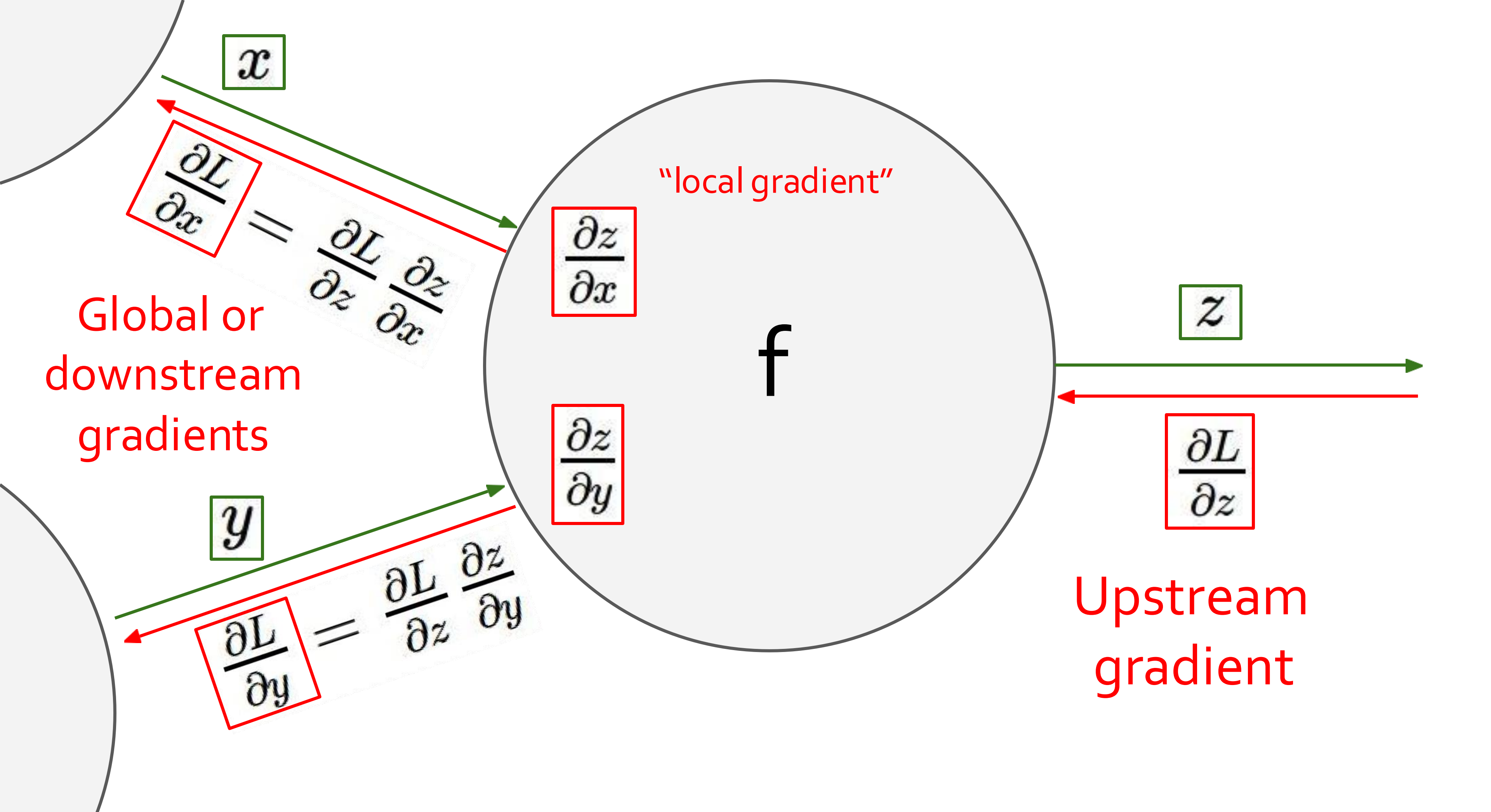
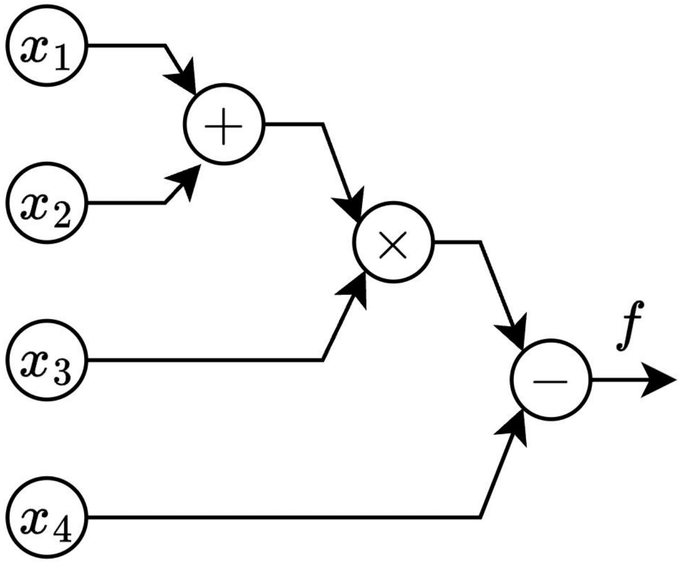


Figure from Andrej Karpathy

Computation Graph: An Example

$$f(x_1, x_2, x_3, x_4, x_5) = (x_1 + x_2)x_3 - x_4$$

Evaluated at: $(x_1, x_2, x_3, x_4) = (5, 4, 3, 2)$



Want: $\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \frac{\partial f}{\partial x_3}, \frac{\partial f}{\partial x_4}$

In what order should we process the **forward** step?

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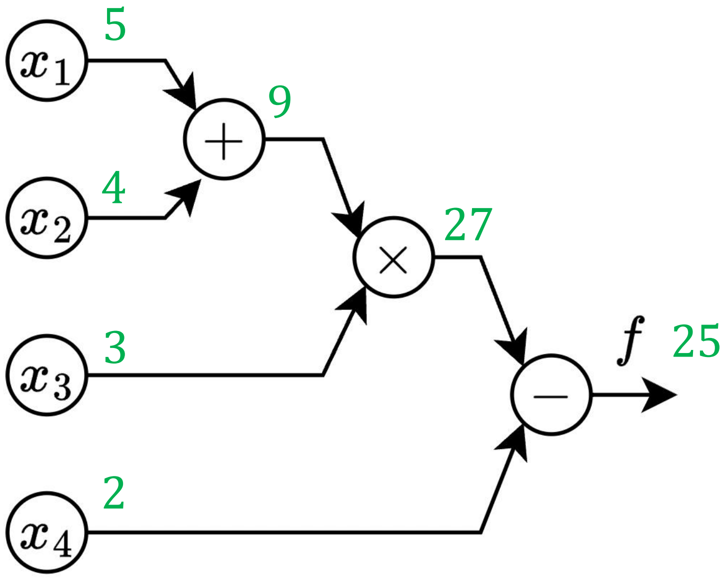

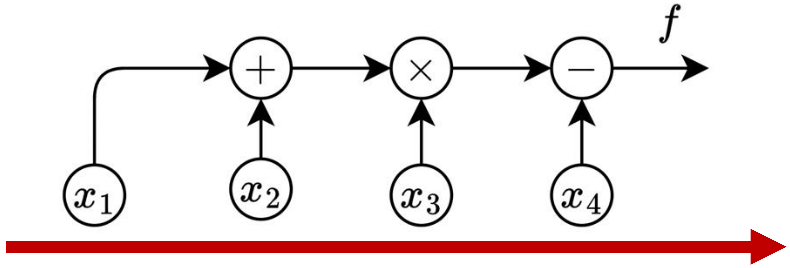

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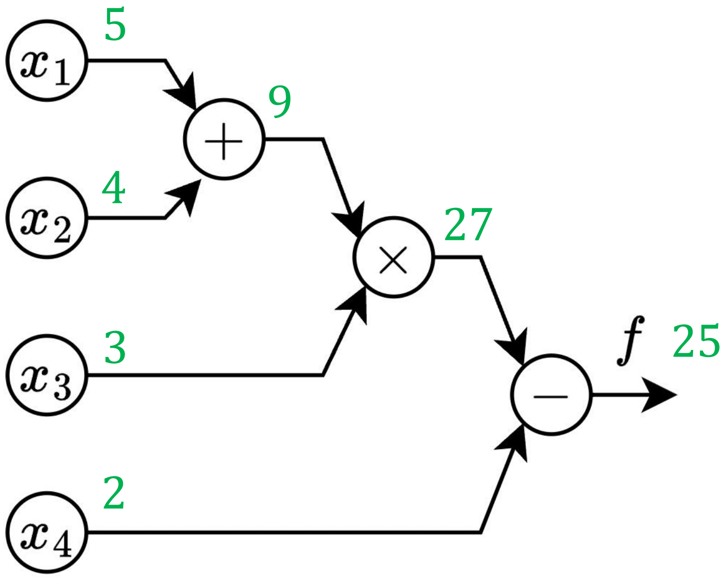

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In what order should we process the **backward** step?

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$$f(x_1, x_2, x_3, x_4, x_5) = (x_1 + x_2)x_3 - x_4$$

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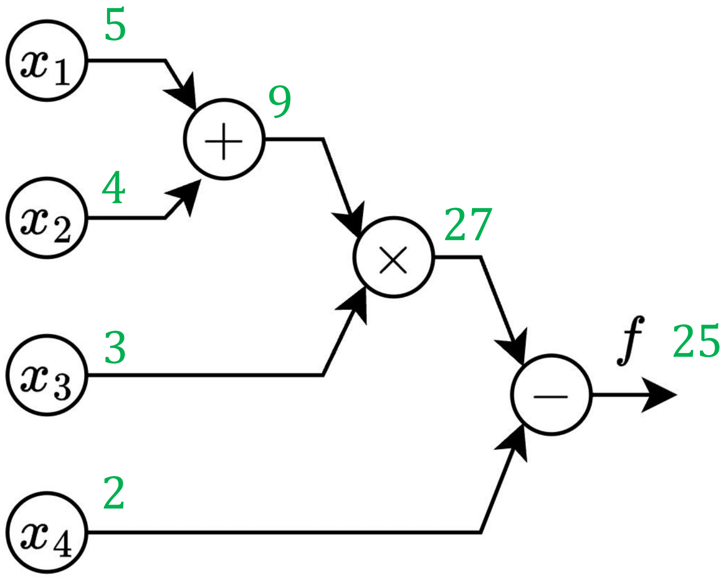
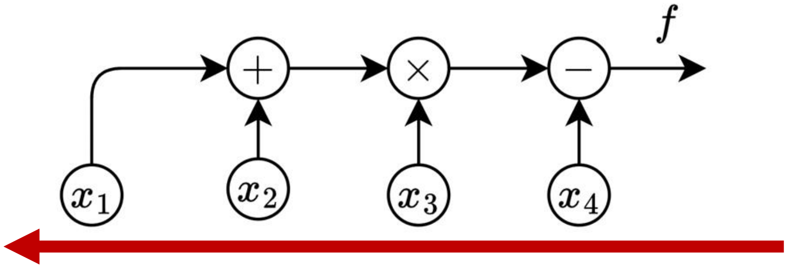
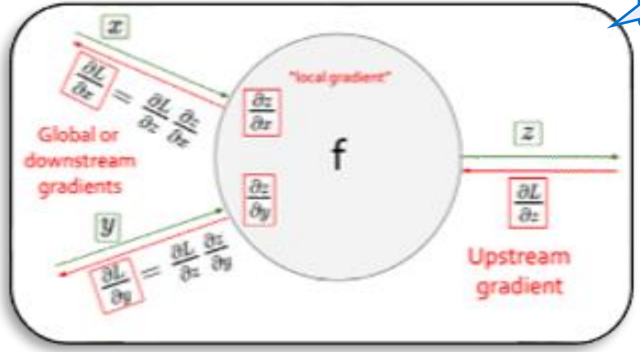




In what order should we process the **backward** step?

Graph: An Example

Remember this!



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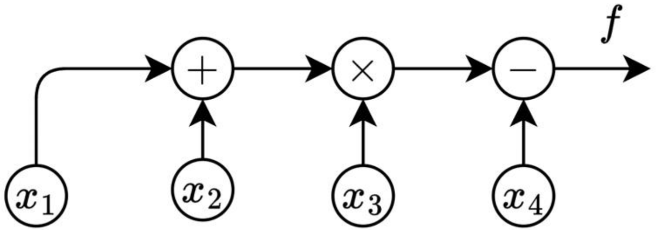

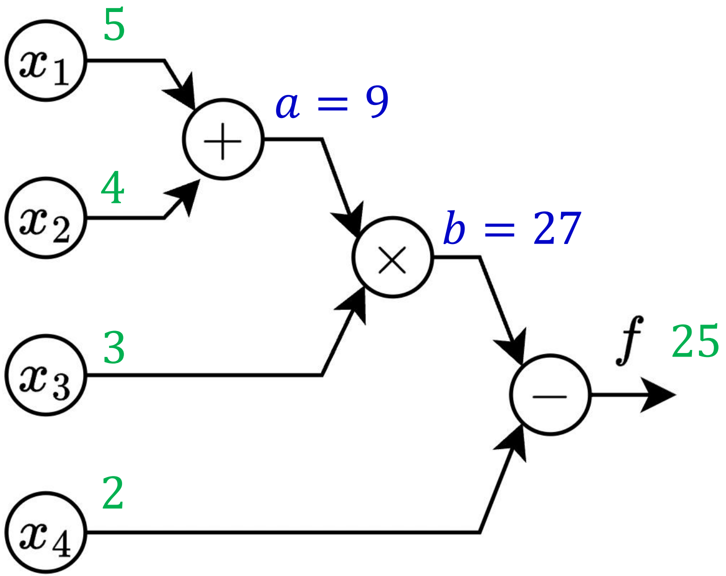

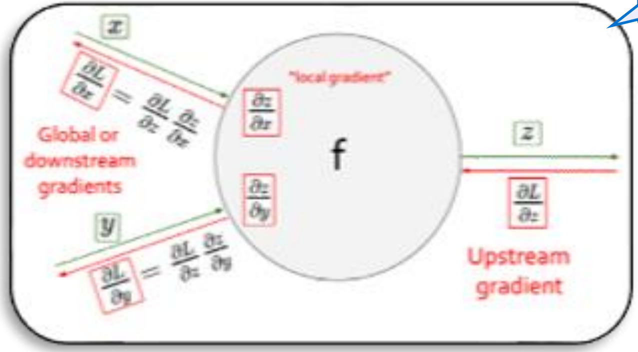

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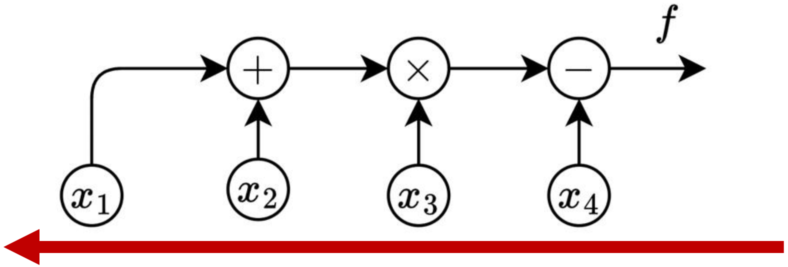
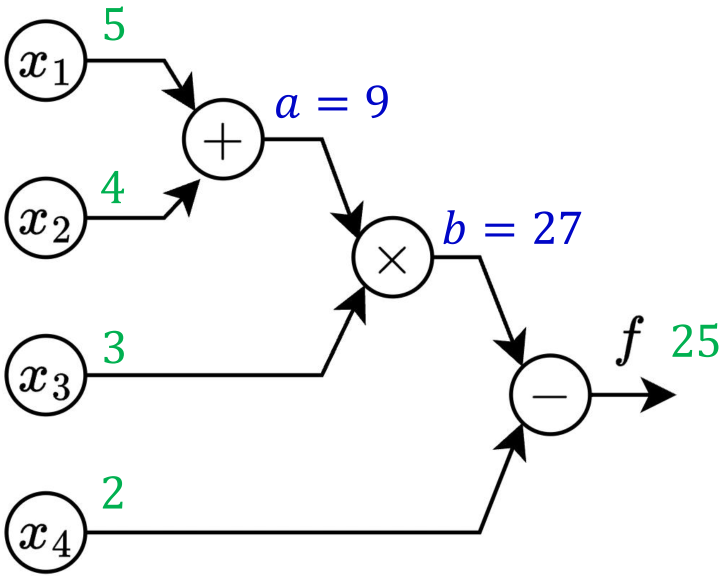
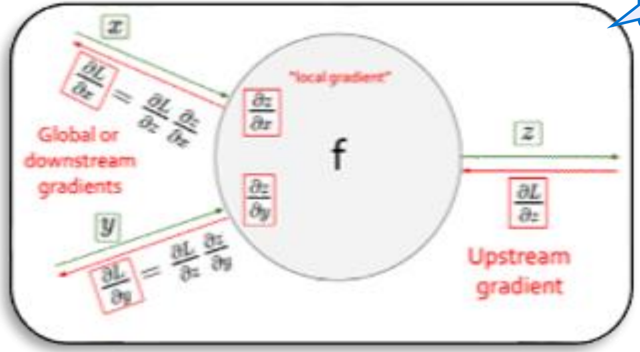




Introduce intermediate variable names

Remember this!



U: Upstream grad
L: Local grad

Graph: An Example

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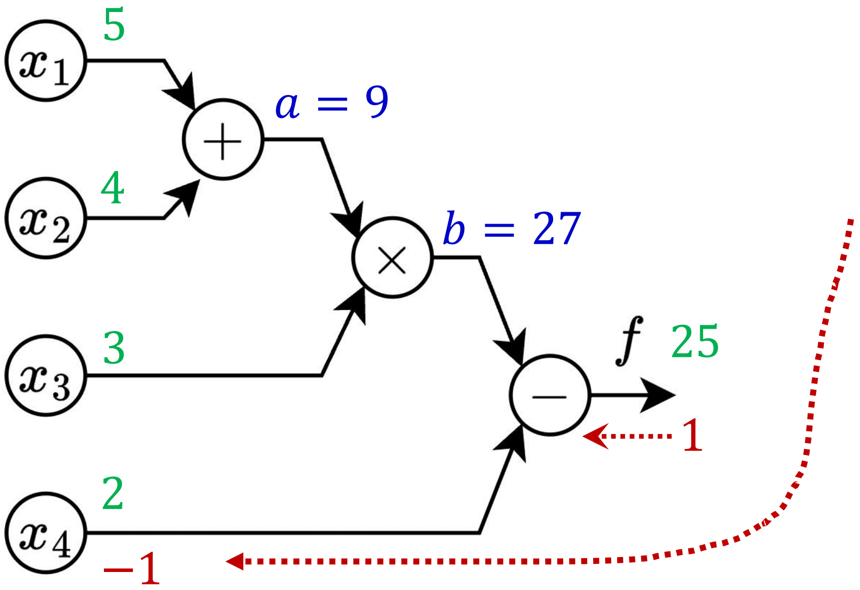
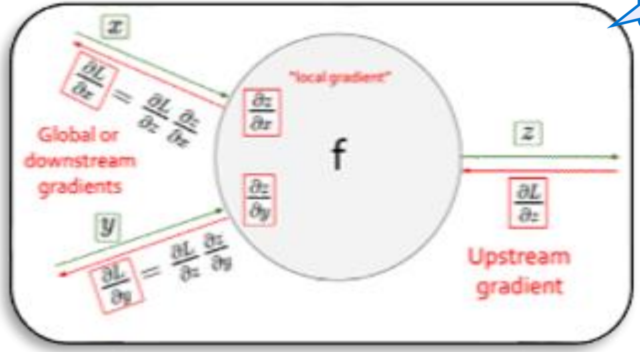


$$f = b - x_4$$

$$\frac{\partial f}{\partial x_4} = \overbrace{\frac{\partial f}{\partial x_4}}^{\text{L}} \times \overbrace{\frac{\partial f}{\partial f}}^{\text{U}} = (-1) \times 1 = -1$$

Remember this!



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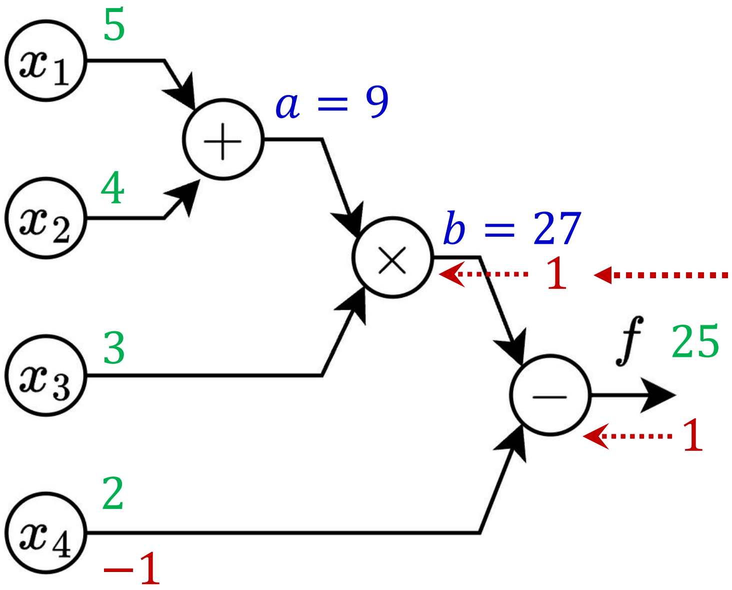

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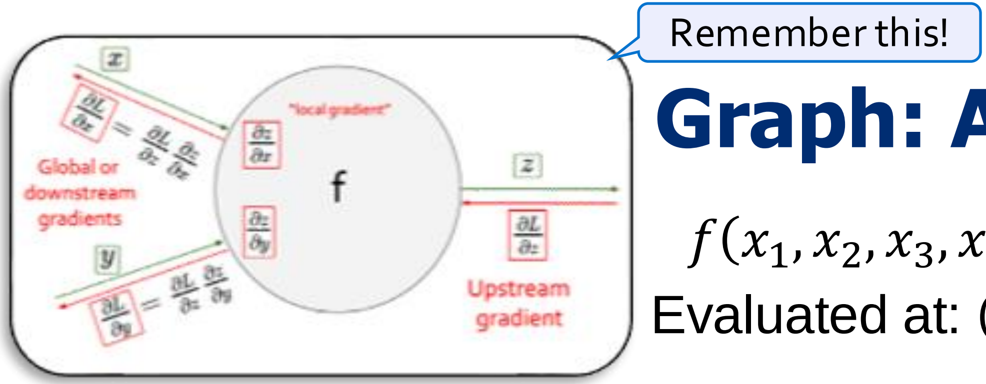

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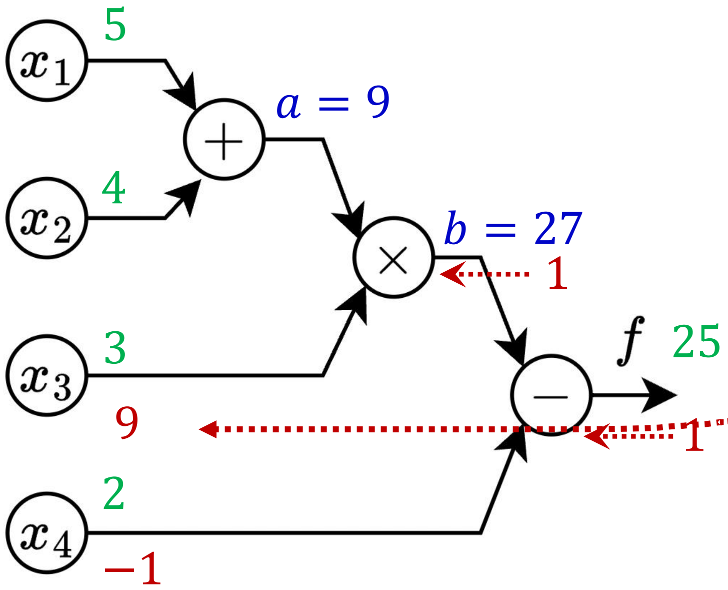

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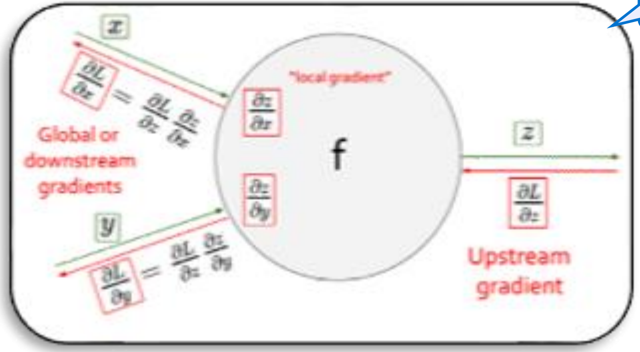

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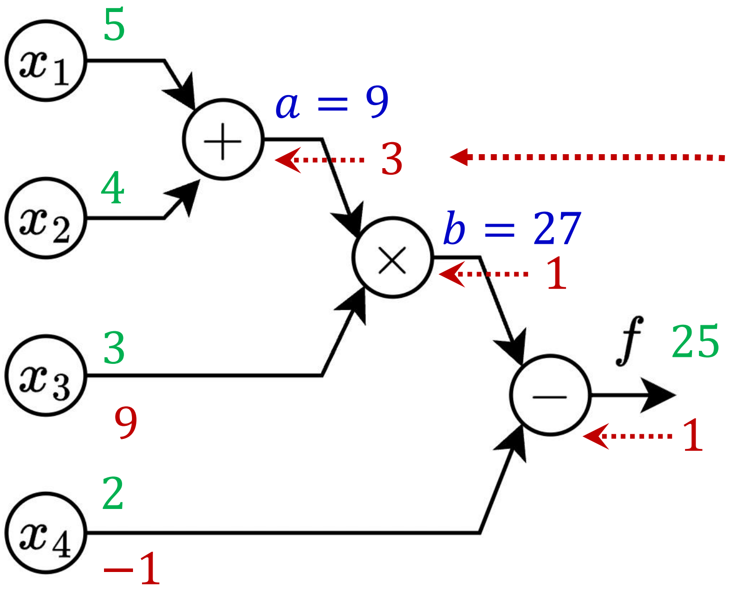

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$$\frac{\partial f}{\partial a} = \overbrace{\frac{\partial b}{\partial a}}^{\text{L}} \times \overbrace{\frac{\partial f}{\partial b}}^{\text{U}} = x_3 \times 1 = 3$$

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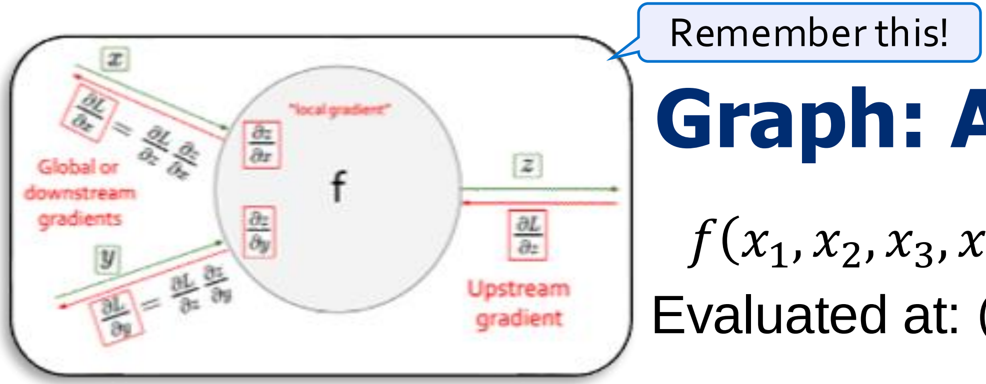
Graph: An Example



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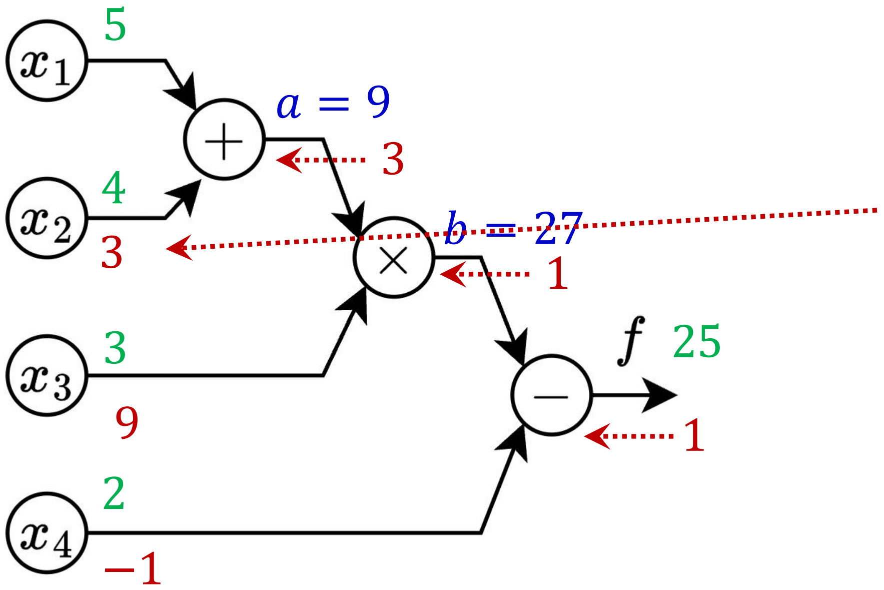

$$a = x_1 + x_2$$

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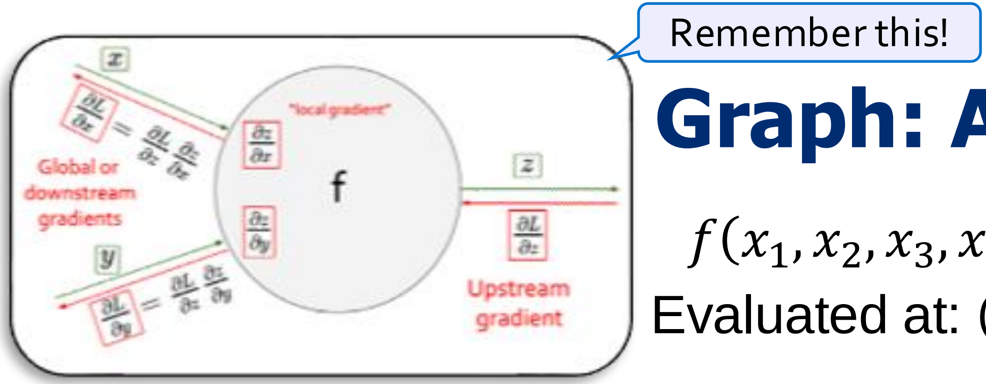

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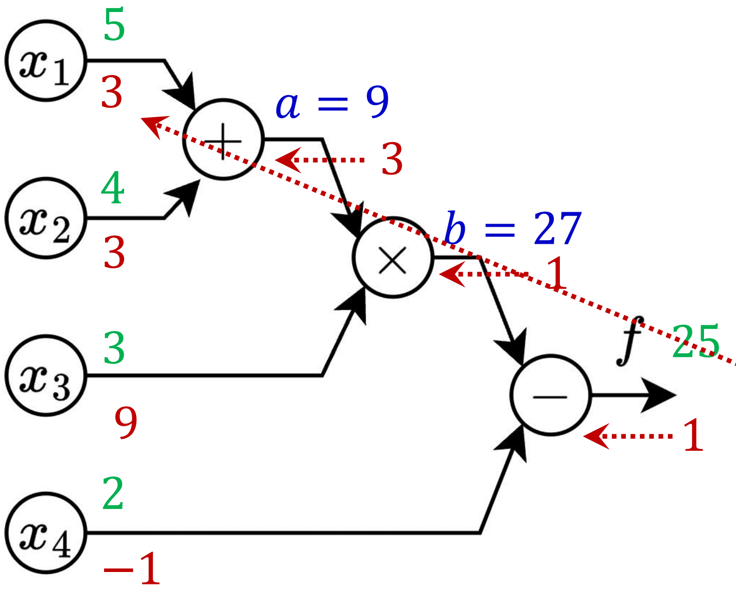

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Backprop via Computation Graph

- What if the network does not have a regular structure? Same idea!

1. Sort the nodes in topological order (what depends on what)
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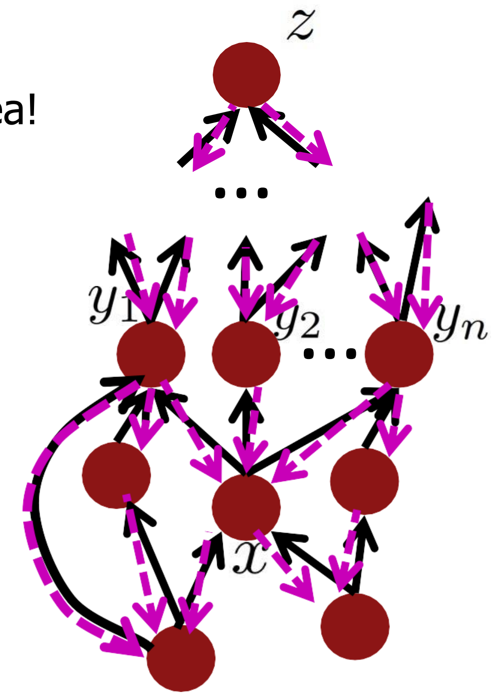


Summary

- **Computation graphs:** directed graph where the nodes correspond to mathematical operations.
  - A way of expressing mathematical operations.

- This allows general-purpose implementation of Backprop to any form of networks (not just multilayer perceptron).
  - This is why n practice you don’t need to worry about implementing Backprop!! 

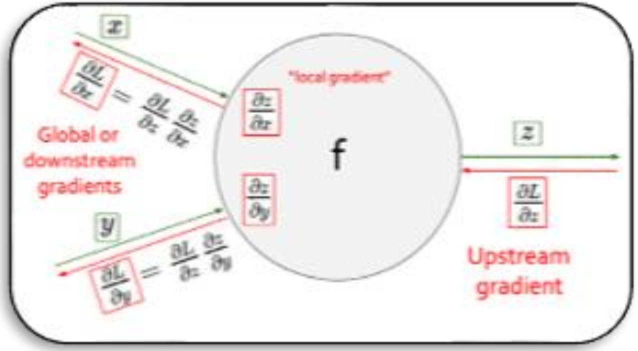
- **Next:** Implementing Backprop yourself + industrial software libraries.

Backprop via Automatic Differentiation

How Should We Implement BackProp?

- The computation graph makes it easy to backpropagate all the way
- We need to implement:
  - The nodes are the values (tensors)
  - Edges define how the values (tensors) get propagated.
- Let's think about how this is implemented!

Remember this!



The Nodes

- The nodes are the values (tensors)
  - They store value, gradients and references to the functions that created them.

```
class Tensor:
    def __init__(self, value, requires_grad=False):
        self.value = value  # Store the value of the tensor
        self.grad = 0  # Gradient initialized to zero
        self.requires_grad = requires_grad
        self._backward = lambda: None  # Function to compute gradient
        self._prev = set()  # Track previous nodes for backpropagation
```

The Nodes

```python
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    def __init__(self, value, requires_grad=False):
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```

```python
# Creating tensors
x = Tensor(3.0, requires_grad=True)
y = Tensor(2.0, requires_grad=True)
```

Now you can define tensors!!

What we actually want to run

```
# Creating tensors
x = Tensor(3.0, requires_grad=True)
y = Tensor(2.0, requires_grad=True)

# Forward pass
z = multiply(x, y)  # z = x * y
w = add(z, y)       # w = z + y
o = relu(w)         # o = ReLU(w)

# Backpropagation
o.backward()

# Print gradients
print(f"x.grad: {x.grad}")  # Should be y.value if ReLU is active
print(f"y.grad: {y.grad}")  # Should be x.value + 1 (from addition)
```

What portion of this is defined so far?

```python
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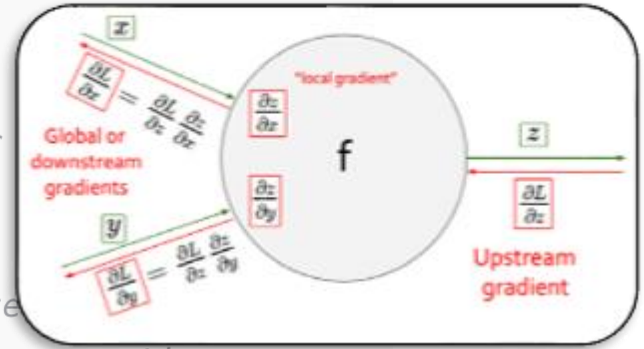


We also need to define the backward step!

```python
  def backward(self):
      """Computes gradients using reverse-mode automatic differentiation."""
      # Initialize gradient to 1 if this is the final output node
      if self.grad == 0:
          self.grad = 1

      # Topological ordering of nodes using depth-first search
      topo_order = []
      visited = set()
```

```python
def backward(self):
    """Computes gradients using reverse-mode automatic differentiation."""
    # Initialize gradient to 1 if this is the final output node
    if self.grad == 0:
        self.grad = 1

    # Topological ordering of nodes using depth-first search
    topo_order = []
    visited = set()

    def build_topo(node):
        if node not in visited:
            visited.add(node)
            for parent in node._prev:
                build_topo(parent)
            topo_order.append(node)

    build_topo(self)

    # Reverse iterate for backpropagation
    for node in reversed(topo_order):
        node._backward()
```

Defining Operation Nodes

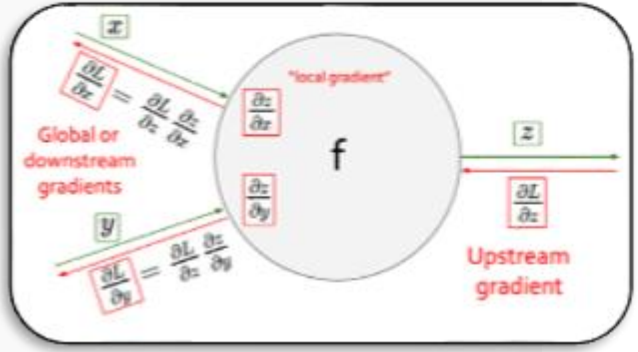
```python
def multiply(a, b):
    """Multiplication operation."""
    out = Tensor(a.value * b.value, requires_grad=(a.requires_grad or b.requires_grad))

    def _backward():
        if a.requires_grad:
            a.grad += b.value * out.grad
        if b.requires_grad:
            b.grad += a.value * out.grad

    out._backward = _backward
    out._prev = {a, b}
    return out
```

Local grad

Upstream



Defining Operation Nodes

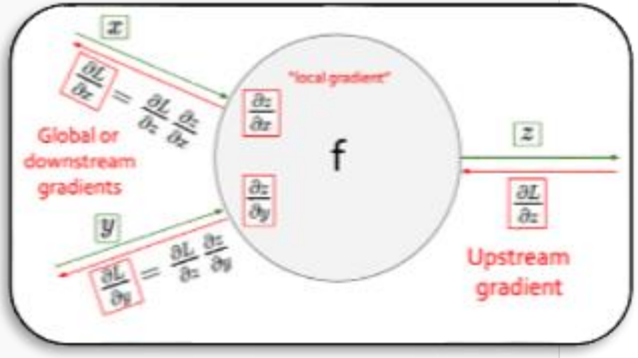
```python
def add(a, b):
    """Addition operation."""
    out = Tensor(a.value + b.value, requires_grad=(a.requires_grad or b.requires_grad))

    def _backward():
        if a.requires_grad:
            a.grad += out.grad
        if b.requires_grad:
            b.grad += out.grad

    out._backward = _backward
    out._prev = {a, b}
    return out
```

Upstream

Where is the local grad? 🤔



Defining Operation Nodes

- Operations (define how it propagates forward/backward) are also nodes!

```python
def relu(x):
    """ReLU activation function."""
    out = Tensor(max(0, x.value), requires_grad=x.requires_grad)

    def _backward():
        if x.requires_grad:
            x.grad += (out.value > 0) * out.grad  # Gradient is 1 if x > 0, else 0

    out._backward = _backward
    out._prev = {x}
    return out
```

Upstream

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Let’s run Backprop!!

```
# Creating tensors
x = Tensor(3.0, requires_grad=True)
y = Tensor(2.0, requires_grad=True)

# Forward pass
z = multiply(x, y)  # z = x * y
w = add(z, y)       # w = z + y
o = relu(w)         # o = ReLU(w)

# Backpropagation
o.backward()

# Print gradients
print(f"x.grad: {x.grad}")  # Should be y.value if ReLU is active
print(f"y.grad: {y.grad}")  # Should be x.value + 1 (from addition)
```

Question: draw the computation graph of this program!

Question: explain how “backward()” gets executed!

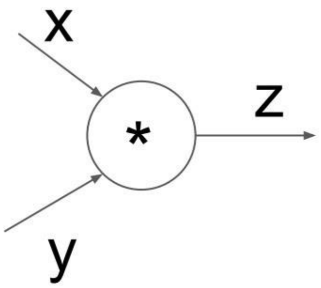
Question: At what point is the topological sort triggered?

Question: how can you further extend this program?

Auto-diff in PyTorch

PyTorch's Implementation: Forward/Backward API

- PyTorch has implementation of forward/backward operations for various operators.
- Example: multiplication operator




```python
class Multiply(torch.autograd.Function):
  @staticmethod
  def forward(ctx, x, y):
    ctx.save_for_backward(x, y)
    z = x * y
    return z
  @staticmethod
  def backward(ctx, grad_z):
    x, y = ctx.saved_tensors
    grad_x = y * grad_z   # dz/dx * dL/dz
    grad_y = x * grad_z   # dz/dy * dL/dz
    return grad_x, grad_y
```

Need to cash some values for use in backward

Upstream gradient

Multiply upstream and local gradients

PyTorch Operators

- PyTorch’s lower-level functions translate activities to graphics processor via libraries like OpenGL.

- PyTorch's autograd engine is implemented in C++ for performance but exposed in Python.

mul_scalar_.glsl	[vulkan] Add image format qualifier to glsl files (#69330)	last year
nchw_to_image.glsl	[vulkan] Enable 2D texture types (#86971)	2 months ago
nchw_to_image2d.glsl	[vulkan] Enable 2D texture types (#86971)	2 months ago
nchw_to_image_int32.glsl	[Vulkan] Enable copying QInt8 and QInt32 tensors from cpu to vulkan. (#...	last month
nchw_to_image_int8.glsl	[Vulkan] Enable copying QInt8 and QInt32 tensors from cpu to vulkan. (#...	last month
nchw_to_image_uint8.glsl	[Vulkan] Enable copying QInt8 and QInt32 tensors from cpu to vulkan. (#...	last month
permute_4d.glsl	[vulkan] Add image format qualifier to glsl files (#69330)	last year
quantize_per_tensor_qint32.glsl	[Vulkan] Enable QInt8 and QInt32 quantization (#89788)	last month
quantize_per_tensor_qint8.glsl	[Vulkan] Enable QInt8 and QInt32 quantization (#89788)	last month
quantize_per_tensor_quint8.glsl	[Vulkan] Enable QInt8 and QInt32 quantization (#89788)	last month
quantized_add.glsl	[Vulkan][TCC] Fix quantized shaders (#89456)	last month
quantized_conv2d.glsl	[Vulkan][TCC] Fix quantized shaders (#89456)	last month
quantized_conv2d_dw.glsl	[Vulkan][TCC] Fix quantized shaders (#89456)	last month
quantized_conv2d_pw_2x2.glsl	[Vulkan][TCC] Fix quantized shaders (#89456)	last month
quantized_div.glsl	[Vulkan][TCC] Fix quantized shaders (#89456)	last month
quantized_mul.glsl	[Vulkan][TCC] Fix quantized shaders (#89456)	last month
quantized_sub.glsl	[Vulkan][TCC] Fix quantized shaders (#89456)	last month
quantized_upsample_nearest2d.glsl	[Vulkan][TCC] Fix quantized shaders (#89456)	last month
reflection_pad2d.glsl	[vulkan] Add image format qualifier to glsl files (#69330)	last year
replication_pad2d.glsl	[vulkan] replication_pad2d.glsl: use clamp() instead of min(max()) (#...	7 months ago
select_depth.glsl	[Vulkan] Implement select.int operator (#81771)	5 months ago
sigmoid.glsl	[vulkan] Add image format qualifier to glsl files (#69330)	last year
sigmoid_.glsl	[vulkan] Add image format qualifier to glsl files (#69330)	last year
slice_4d.glsl	[vulkan] Add image format qualifier to glsl files (#69330)	last year
softmax.glsl	[vulkan] Add image format qualifier to glsl files (#69330)	last year
stack_feature.glsl	[Vulkan] Implement Stack operator (#81064)	5 months ago
sub.glsl	[Vulkan] Implement arithmetic ops where one of the arguments is a ten...	5 months ago
sub_.glsl	[Vulkan] Implement arithmetic ops where one of the arguments is a ten...	5 months ago
tanh.glsl	[vulkan] Clamp tanh activation op input to preserve numerical stabili...	10 months ago
tanh_.glsl	[vulkan] Clamp tanh activation op input to preserve numerical stabili...	10 months ago
threshold.glsl	[vulkan] fix some broken tests in vulkan_api_test (#80962)	6 months ago
upsample_nearest2d.glsl	[vulkan] Add image format qualifier to glsl files (#69330)	last year

Example Activation Functions

master · pytorch / aten / src / ATen / native / vulkan / glsl / **tanh.glsl**

SS-JIA [vulkan] Clamp tanh activation op input to preserve numerical stabili... ...

2 contributors

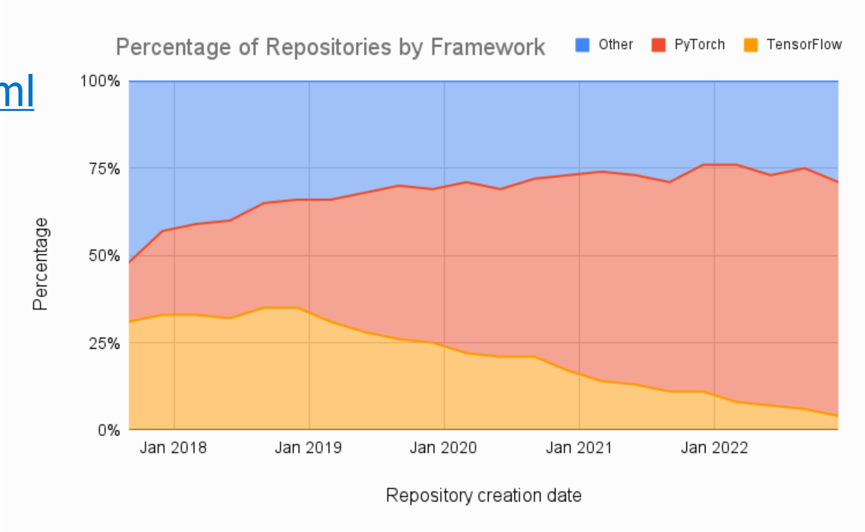
27 lines (21 sloc) | 777 Bytes

```
#version 450 core
#define PRECISION $precision
#define FORMAT    $format

layout(std430) buffer;

/* Qualifiers: layout - storage - precision - memory */

layout(set = 0, binding = 0, FORMAT) uniform PRECISION restrict writeonly image3D   uOutput;
layout(set = 0, binding = 1)         uniform PRECISION                    sampler3D uInput;
layout(set = 0, binding = 2)         uniform PRECISION restrict           Block {
  ivec4 size;
} uBlock;

layout(local_size_x_id = 0, local_size_y_id = 1, local_size_z_id = 2) in;

void main() {
  const ivec3 pos = ivec3(gl_GlobalInvocationID);

  if (all(lessThan(pos, uBlock.size.xyz))) {
    const vec4 intex = texelFetch(uInput, pos, 0);
    imageStore(
        uOutput,
        pos,
        tanh(clamp(intex, -15.0, 15.0)));
  }
}
```

Check out PyTorch Documentations

- This is the main library the vast majority of the community uses.
- It contains hundreds of mathematical operations with “backward()” function to allow automatic gradient computation on computation graph.

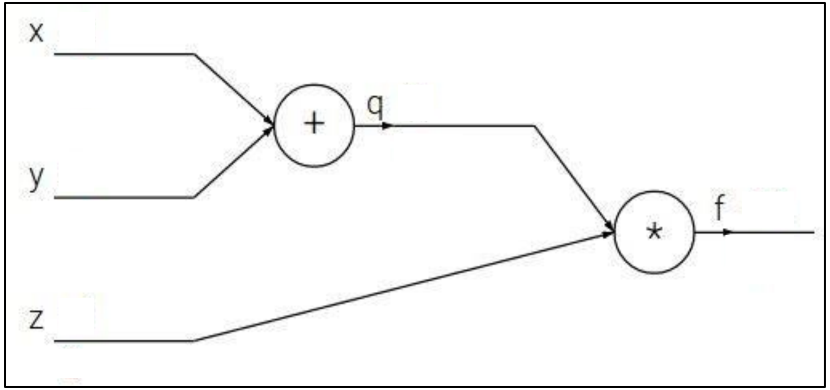
- See: https://pytorch.org/docs/stable/index.html



Backprop in PyTorch

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

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




```
import torch

# Define tensors with requires_grad=True to track gradients
x = torch.tensor(-2.0, requires_grad=True)
y = torch.tensor(5.0, requires_grad=True)
z = torch.tensor(-4.0, requires_grad=True)

# Define the computation graph
f = (x + y) * z  # f = ( -2 + 5 ) * (-4)

# Perform backpropagation
f.backward()
```

Why Learn All These Details About Backprop?

- **Modern deep learning frameworks compute gradients for you!**
- But why take a class on compilers or systems when they are implemented for you?
  - Understanding what is going on under the hood is useful!
- Backpropagation doesn't always work perfectly out of the box
  - Understanding why is crucial for debugging and improving models

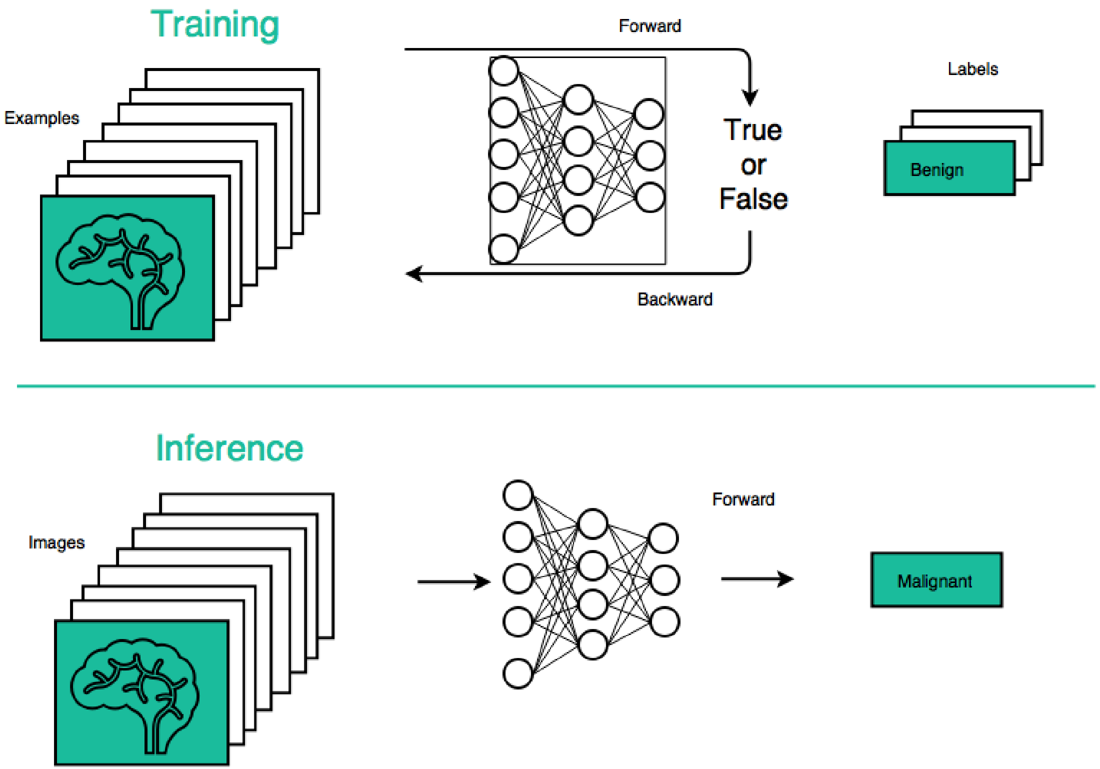
Summary

- Modern deep learning libraries such as PyTorch implement a vast library of operations to allow automatic and efficient Backprop.
- We will make extensive use of PyTorch in this class (yay!)
- Next: We will discuss a few practical considerations regarding training NNs.

Practical considerations for training neural nets

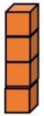
Batching

- GPUs are fast with Tensor operations
- Rather than visiting instances in sequentially , batch them together for faster training and inference.

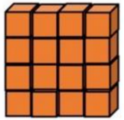


Batches of Data: Example

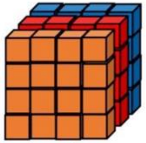
- The case of natural language:
  - Each word is mapped to a vector $\mathbb{R}^{d}$



  - Then, each sentence of length is mapped to a matrix $\mathbb{R}^{\ell \times d}$



  - A batch of sentences (size b) is mapped to a tensor $\mathbb{R}^{\ell \times d \times b}$



Data of any dimension in PyTorch

- PyTorch makes it easy to batch data.
  - All its functionalities are designed around batched process.
  - For example, you can create any tensor of **any** dimension.

TORCH.RAND

```
torch.rand(*size, *, generator=None, out=None, dtype=None, layout=torch.strided, device=None,
requires_grad=False, pin_memory=False) → Tensor
```

Returns a tensor filled with random numbers from a uniform distribution on the interval $[0, 1)$

The shape of the tensor is defined by the variable argument `size`.

Parameters

- **size** (*int*...) – a sequence of integers defining the shape of the output tensor. Can be a variable number of arguments or a collection like a list or tuple.

You can define tensors of any dimension

https://pytorch.org/docs/stable/generated/torch.rand.html

Batches of Data, In Practice

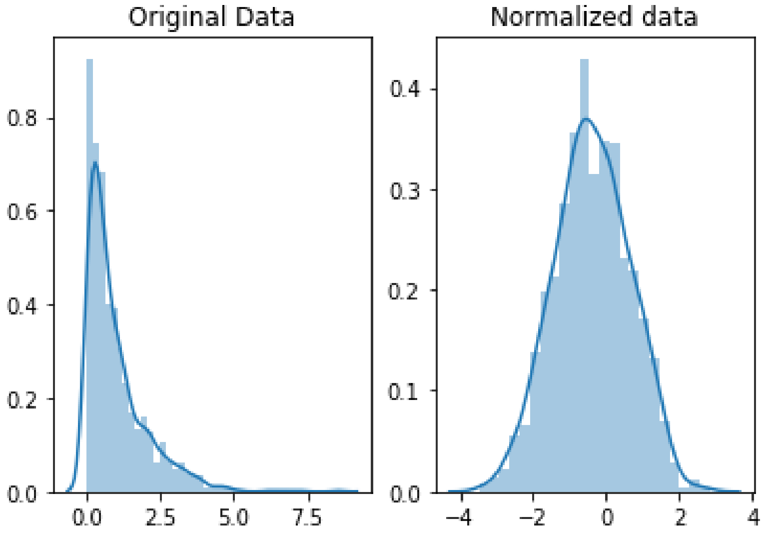
- Avoid loops, use tensors.

```python
import torch

def matmul(A, B):
  C = torch.zeros_like(A)
  for i in range(A.size(0)):
    for j in range(B.size(1)):
      for k in range(A.size(1)):
        C[i, j] += A[i, k] * B[k, j]
  return C

# Example usage:
A = torch.randn(10, 10)
B = torch.randn(10, 10)
C = matmul(A, B)
```

```python
import torch

# Example usage:
A = torch.randn(10, 10)
B = torch.randn(10, 10)
C = torch.matmul(A, B)
```

Normalize Your Data!

- We do not like very large numbers.
  - Large numbers lead to numerical problems (e.g., overflow) and lead to NaNs 😭
- We prefer if our data is distributed around zero.



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Normalize Your Data!

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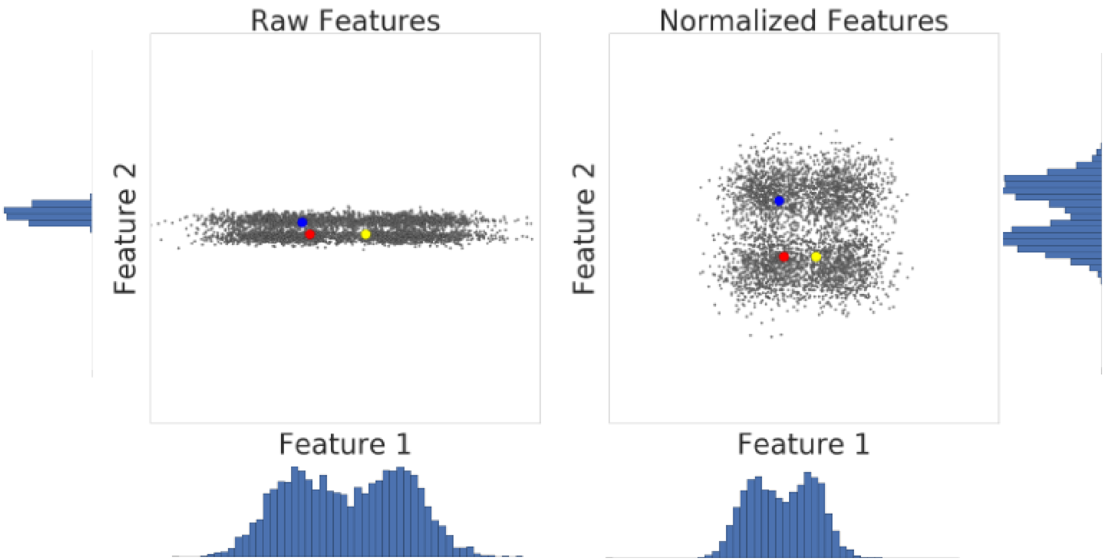
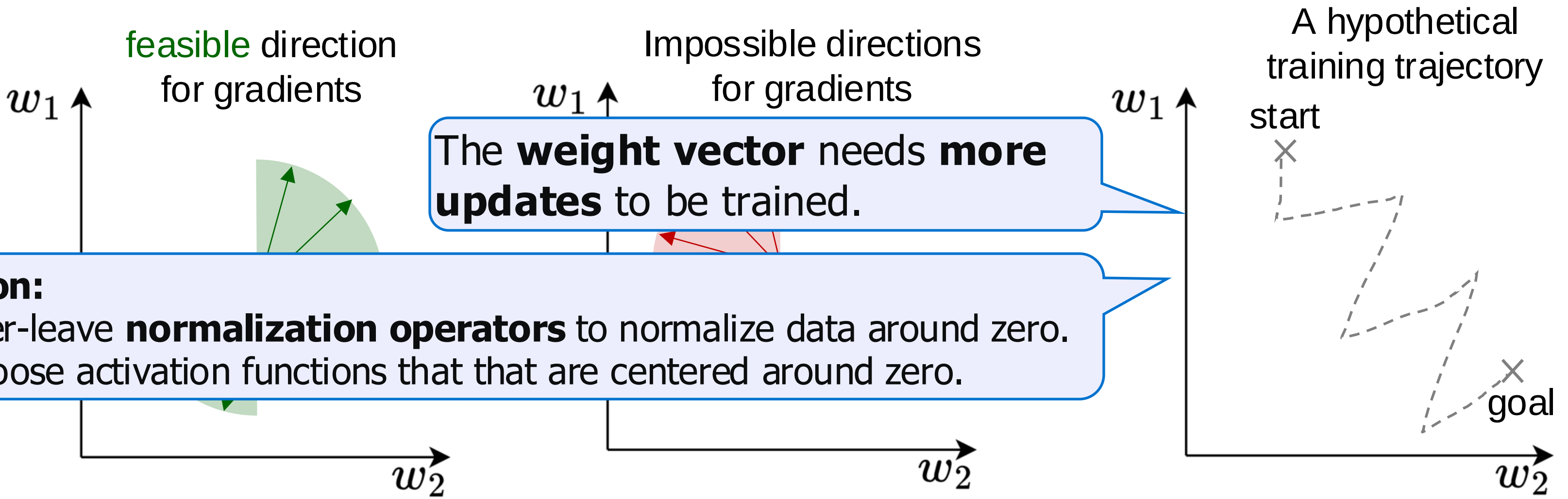


https://developers.google.com/machine-learning/clustering/prepare-data

Non-Zero-Centered Data

$$f = \boldsymbol{w}^\top \boldsymbol{x} + \boldsymbol{b} \quad \Rightarrow \frac{\partial \mathcal{L}}{\partial w_i} = \frac{\partial \mathcal{L}}{\partial f}\frac{\partial f}{\partial w_i} = \text{upstream} \times x_i$$

- If data is always positive (i.e., $\forall i$: $x_i > 0$), all the dimensions of $\nabla_{\boldsymbol{w}}\mathcal{L}$ would have the same sign (all positive or all negative, same sign as upstream).



The **weight vector** needs **more updates** to be trained.

Solution:
(i) Inter-leave **normalization operators** to normalize data around zero.
(ii) Choose activation functions that that are centered around zero.

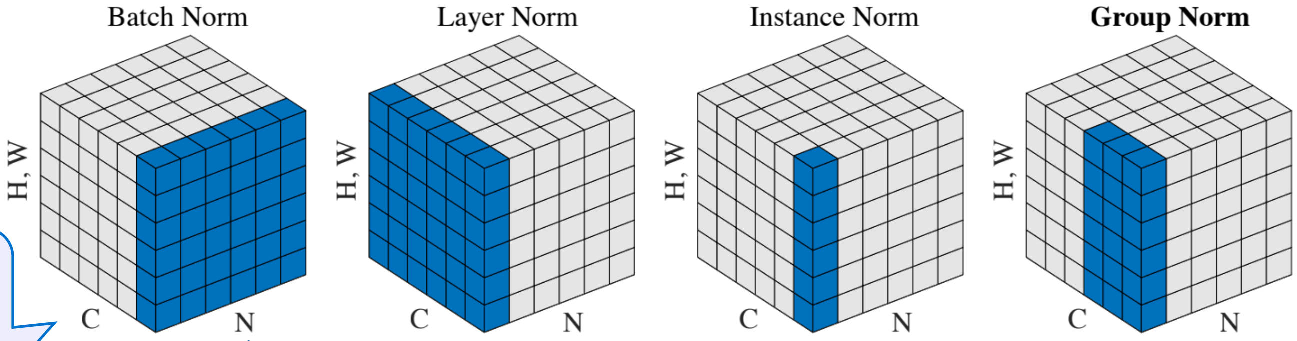
Normalization

$$y = \frac{x - \mathrm{E}[x]}{\sqrt{\mathrm{Var}[x] + \epsilon}} * \gamma + \beta$$

- Normalization of values standardizes the ranges of values
- Prevents value disparities
- Stabilizes + speeds up training

Scenario	Recommended Normalization
CNNs (Image Classification, Object Detection, Segmentation)	BatchNorm (BN), GroupNorm (GN)
NLP & Transformers (BERT, GPT, RNNs, LSTMs)	LayerNorm (LN)
Style Transfer & GANs	InstanceNorm (IN)
Small Batch Training (Medical Imaging, Object Detection)	GroupNorm (GN)

H, W: height and width of images; in language, different words in your sentence.

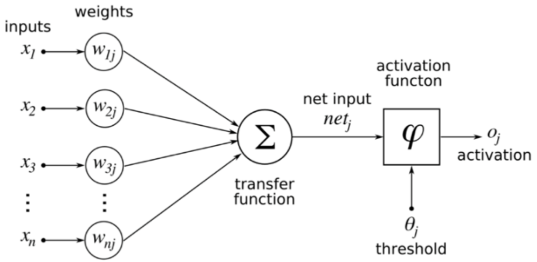


C: channels of each RGB pixel; in language, dimensions of each word vector

N: batch size

See PyTorch documentations: https://pytorch.org/docs/stable/nn.html#normalization-layers

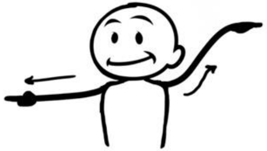
Activation Functions

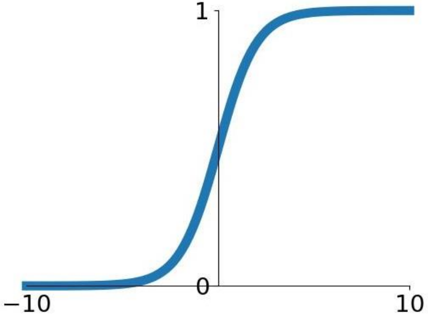


- How do you choose what activation function to use?
- In general, it is problem-specific and might require trial-and-error.
- Here are some tips about popular action functions.

Activation Functions : Sigmoid

- Squashes numbers to range [0,1]
- Historically popular, interpretation as "firing rate" of a neuron

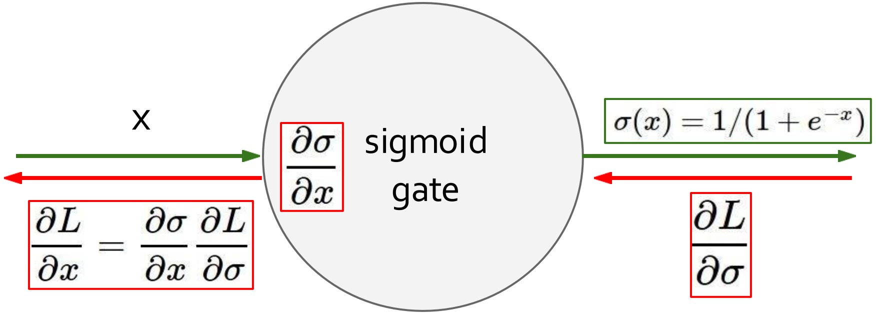




$$\sigma(x) = 1/(1+e^{-x})$$

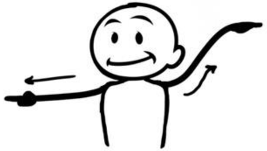
- Limitation 1: Saturated neurons "kill" the gradients
  - Whenever |x| > 5, the gradients are basically zero.
- Limitation 2: Not centered around zero.

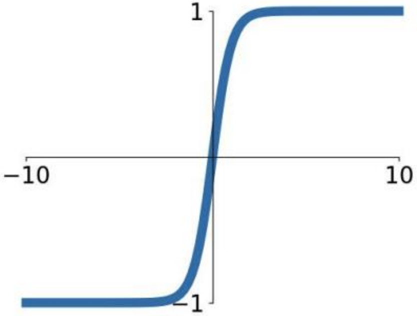
If all the gradients flowing back will be zero and weights will never change.



[dance figure: https://www.imaginary.org/gallery/maths-dance-moves]

Activation Functions : Tanh





tanh(x)

[LeCun et al., 1991]

- Symmetric around [-1, 1]
- Still saturates |x| > 3 and "kill" the gradients
- Zero-centered — faster optimization (why?)

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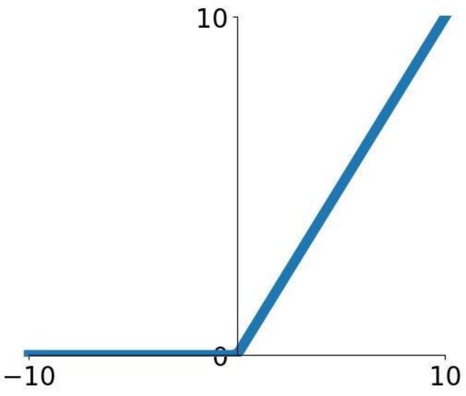
[dance figure: https://www.imaginary.org/gallery/maths-dance-moves]

Activation Functions : ReLU

- Computationally efficient
- In practice, converges faster than sigmoid/tanh in practice
- Does not saturate (in +region) — will die less!

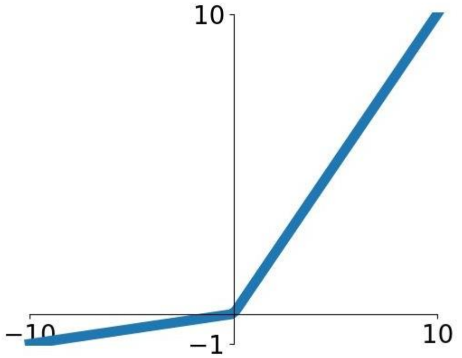


ReLU
(Rectified Linear Unit)

[Krizhevsky et al., 2012]

[dance figure: https://www.imaginary.org/gallery/maths-dance-moves]

Activation Functions : Leaky ReLU



$$f(x) = \max(0.01x, x)$$

- Does not saturate — will not die.
- Computationally efficient
- In practice it converges faster than sigmoid/tanh in practice

- Other parametrized variants:
  - Parametric Rectifier (PReLU): $f(x) = \max(\alpha x, x)$ [He et al., 2015]
  - Maxout: $\max(w_1^T x + b_1, w_2^T x + b_2)$ [Goodfellow et al., 2013]

- Provide more flexibility, though at the cost of more learnable parameters.
  - For example, Maxout doubles the number of parameters.

[dance figure: https://www.imaginary.org/gallery/maths-dance-moves]

Choose Activations: In Practice

- Other activations: ELU, Swish, GELU, Softplus, ….

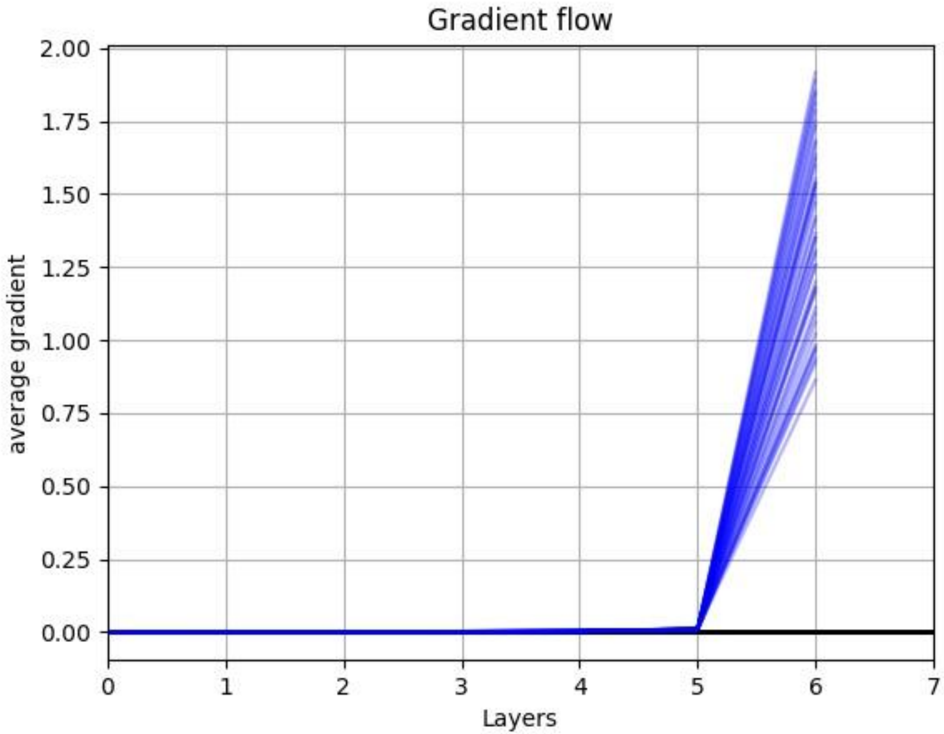
- In general, it is problem-specific and might require trial-and-error.

- A useful recipe:
  1. Generally, ReLU is a good activation to start with.
  2. Time/compute permitting, you can try other activations to squeeze out more performance.

Exploding/Vanishing Gradients

- If many numbers |x| > 1 get multip
- NaN gradients --> no learning!

- If many numbers |x| < 1 get multip
- Zero gradients -> no learning!

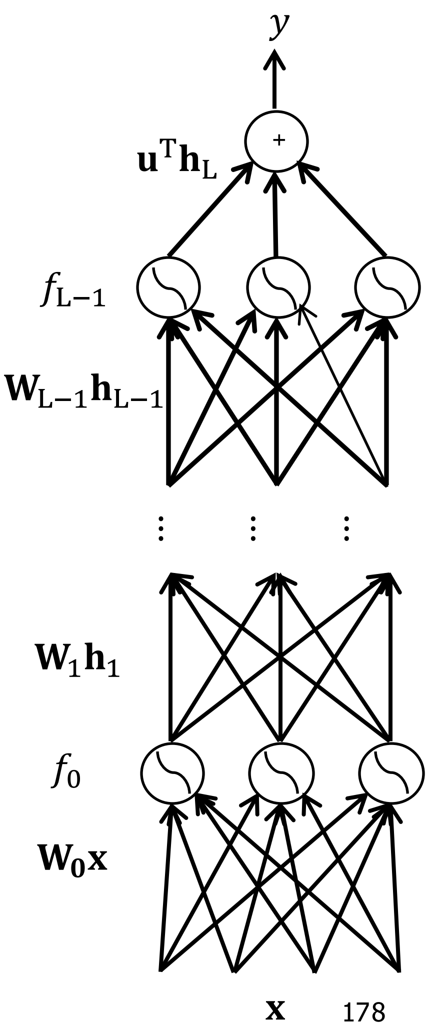


Exploding/Vanishing Gradients

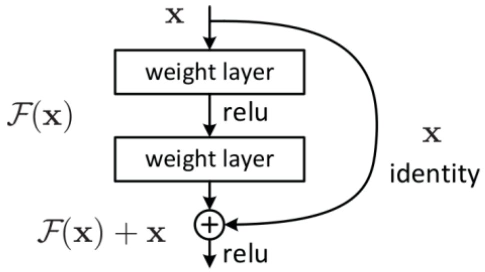
- Remember gradient computation at layer $L - k$:

$$\nabla_{\mathcal{L}}(\mathbf{W}_{L-k}) = \underbrace{\left(\mathbf{J}_\ell(\mathrm{y})\ \mathbf{J}_y(\mathbf{h}_\mathrm{L})\ \mathbf{J}_{\mathbf{h}_\mathrm{L}}(\mathbf{h}_{\mathrm{L}-1})\ \mathbf{J}_{\mathbf{h}_{\mathrm{L}-1}}(\mathbf{W}_{\mathrm{L}-2})\ \dots\ \mathbf{J}_{\mathbf{h}_{L-k+1}}(\mathbf{W}_{L-k})\right)^\mathrm{T}}_{\text{O(k)-many matrix multiplication}}$$

- This matrix multiplication could quickly approach
  - ∞, if the matrix elements are a large — exploding gradients.
  - 0, if the matrix elements are small — vanishing gradients.
  - $\infty/0$ gradients would kill learning (no flow of information).

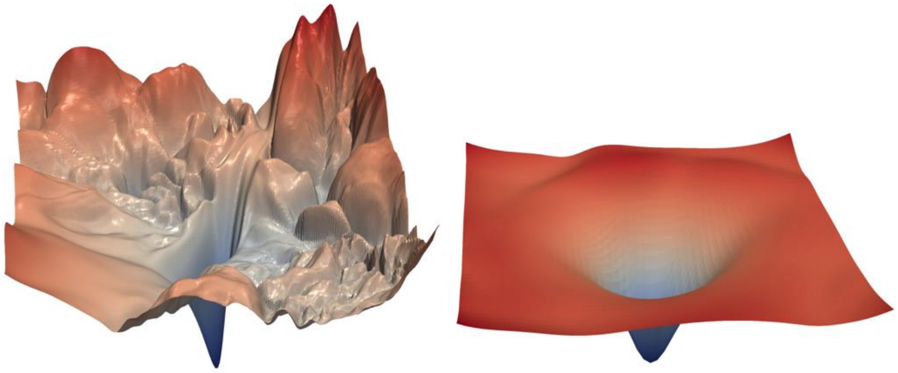


Residual Connections/Blocks



- Create direct "information highways" between layers.
- Shown to diminish vanishing/exploding gradients
- Early in the training, there are fewer layers to propagate through.
  - The network would restore the skipped layers, as it learns richer features.
  - It is also shown to make the optimization objective smoother.

[Fun fact: the paper (He et al. 2015) introducing residual layers is the most cited paper of century!!]

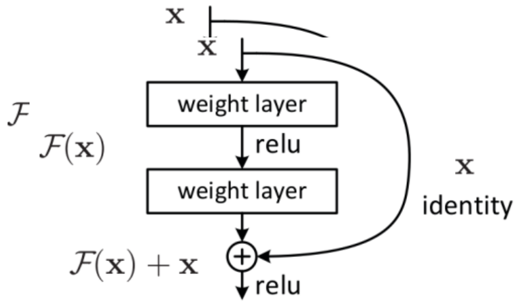


(a) without skip connections (b) with skip connections

[Li et al. "Visualizing the Loss Landscape of Neural Nets"]

Residual Connections/Blocks

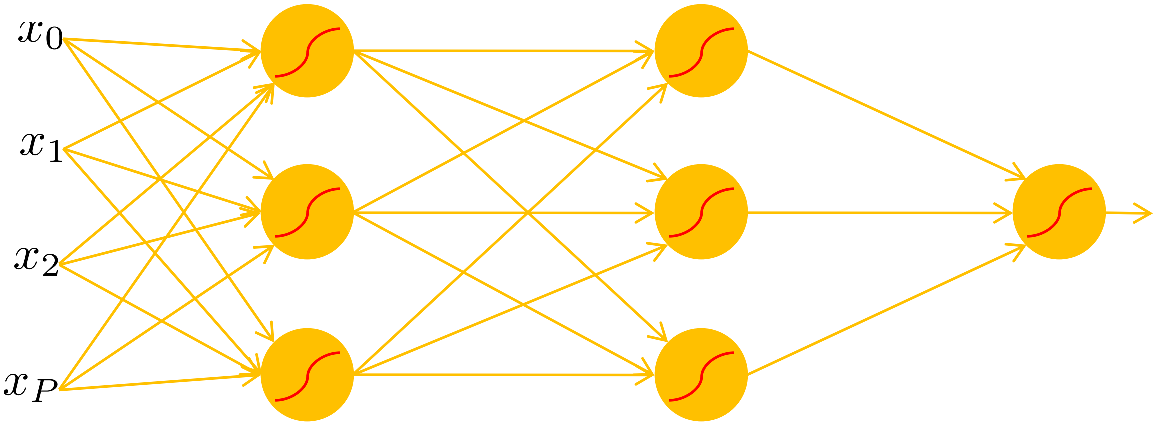
```python
# Define a simple residual block with a skip connection
class SimpleResidualBlock(nn.Module):
    def __init__(self, input_dim):
        super().__init__()
        self.linear1 = nn.Linear(input_dim, input_dim)
        self.relu = nn.ReLU()
        self.linear2 = nn.Linear(input_dim, input_dim)

    def forward(self, x):
        identity = x  # Skip connection (input is added back)
        out = self.linear1(x)
        out = self.relu(out)
        out = self.linear2(out)
        out += identity  # Residual connection
        out = self.relu(out)
        return out
```



Question: identify residual connections here

Weight Initialization

- Initializing all weights with a fixed constant (e.g., 0’s) is a very bad idea! (why?)



- If the neurons start with the same weights, then all the neurons will follow the same gradient, and will always end up doing the same thing as one another.
- Effective initialization is one that breaks such ”symmetries” in the weight space.

Weight Initialization

- Better idea: initialize weights with random Gaussian noise.

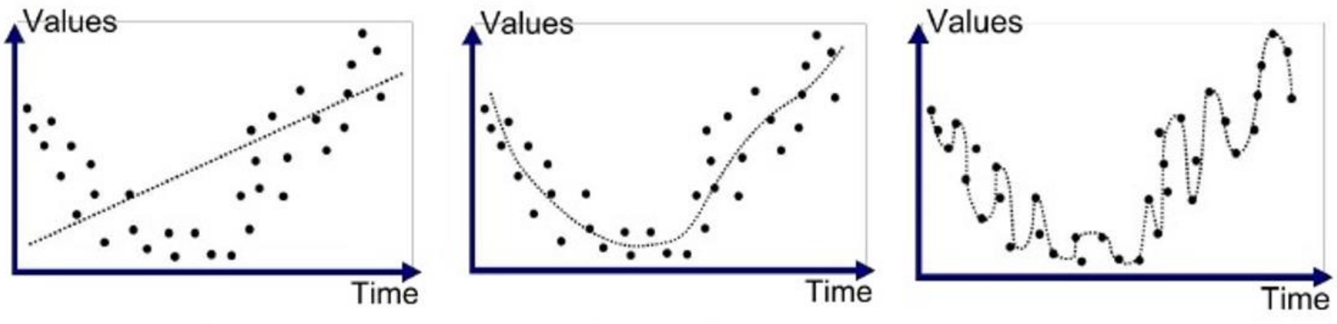
```
x = torch.tensor.empty(3, 5)
nn.init.normal_(w)
```

- There are fancier initializations (Xavier, Kaiming, etc.) that we won't get into.

[read more here: https://pytorch.org/docs/stable/nn.init.html]

Over-training/-fitting Prevention

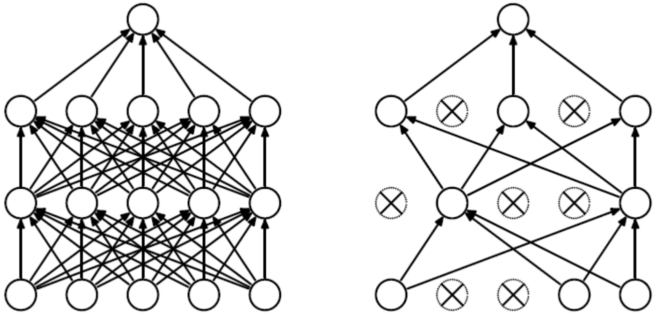
- Running too many epochs and/or a NN with many hidden layers may lead to an overfit network
- Keep a held-out validation set and evaluate accuracy after every epoch
- Early stopping: maintain weights for best performing network on the validation set and return it when performance decreases significantly beyond that.



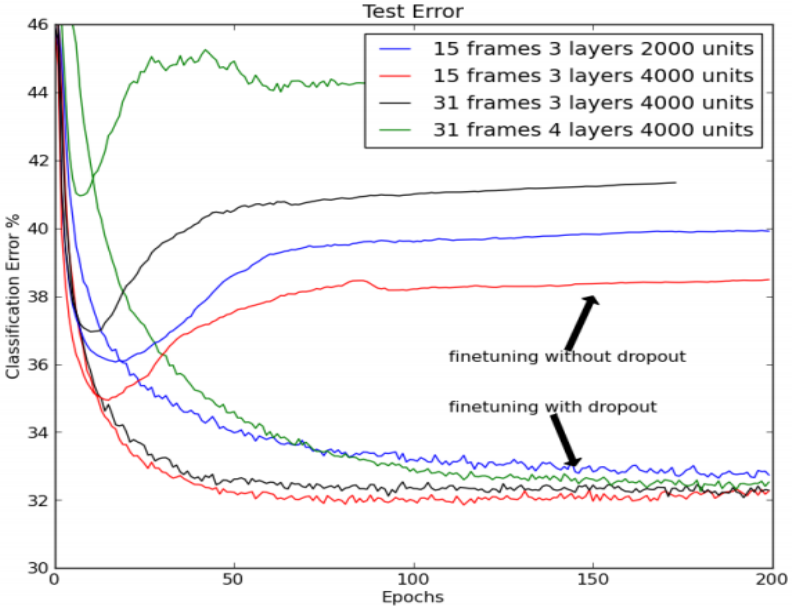
Underfitted | Good Fit/Robust | Overfitted

Dropout Training

- In each forward pass, randomly set some neurons to zero
- Probability of dropping is a hyperparameter; 0.5 is common
- Dropout is implicitly an ensemble (average) of many models that share parameters.
  - Each binary mask is one model
  - For example, a layer with 4096 units has $2^{4096} \sim 10^{1233}$ possible masks!
  - Only ~ 10^{82} atoms in the universe ...

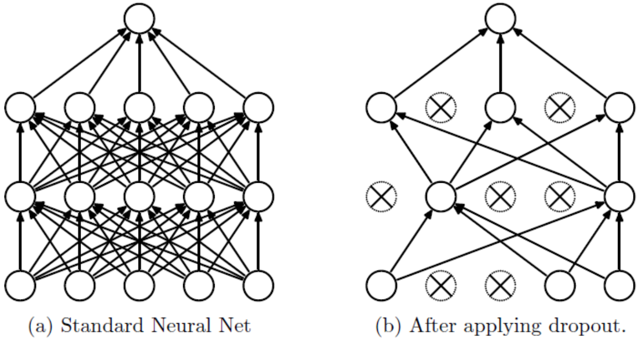


(a) Standard Neural Net (b) After applying dropout.



[Hinton et al, 2012; Srivastava et al, "Dropout: A simple way to prevent neural networks from overfitting", JMLR 2014]

Dropout During Test Time



- The issue for the test time:
  - Dropout adds randomization. ☹
  - Each dropout mask would lead to a slightly different outcome.
- Without dropout, the input values to each neuron would be higher than what was seen during the training (mismatch between train/test).
- In ideal world, we would like to "average out" the outcome across all the possible random masks.
  - Not feasible since there are many possible networks.

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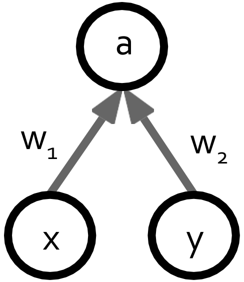
Dropout During Test Time: Example



- Consider the following network: $w_1 x_1 + w_2 x_2$
- Suppose we apply dropout (p=0.5) to the following model.
- How should we use this model at the inference time?
- Think about training output:

$$E[a] = \frac{1}{4}(w_1 x_1 + w_2 x_2) + \frac{1}{4}(0 + 0) + \frac{1}{4}(0 + w_2 x_2) + \frac{1}{4}(w_1 x_1 + 0) = \frac{1}{2}(w_1 x_1 + w_2 x_2)$$

- If we do not apply dropout: $E[a] = w_1 x_1 + w_2 x_2$
- **Solution:** scale the values proportional to dropout probability.
  - Can be applied in either testing (scaling down) or training (scaling up).
  - A very common interview question! ☺

Dropout in Practice

Just call the PyTorch function!

```
dropout = nn.Dropout(p=0.2)
x = torch.randn(20, 16)
y = dropout(x)
```

It automatically

- activates the dropout for training.

```
# training step
...
model.train()
...
```

- deactivatives it during evaluations and scales the values according to its parameter.

```
# evaluate model:
...
model.eval()
...
```

See PyTorch documentations https://pytorch.org/docs/stable/generated/torch.nn.Dropout.html

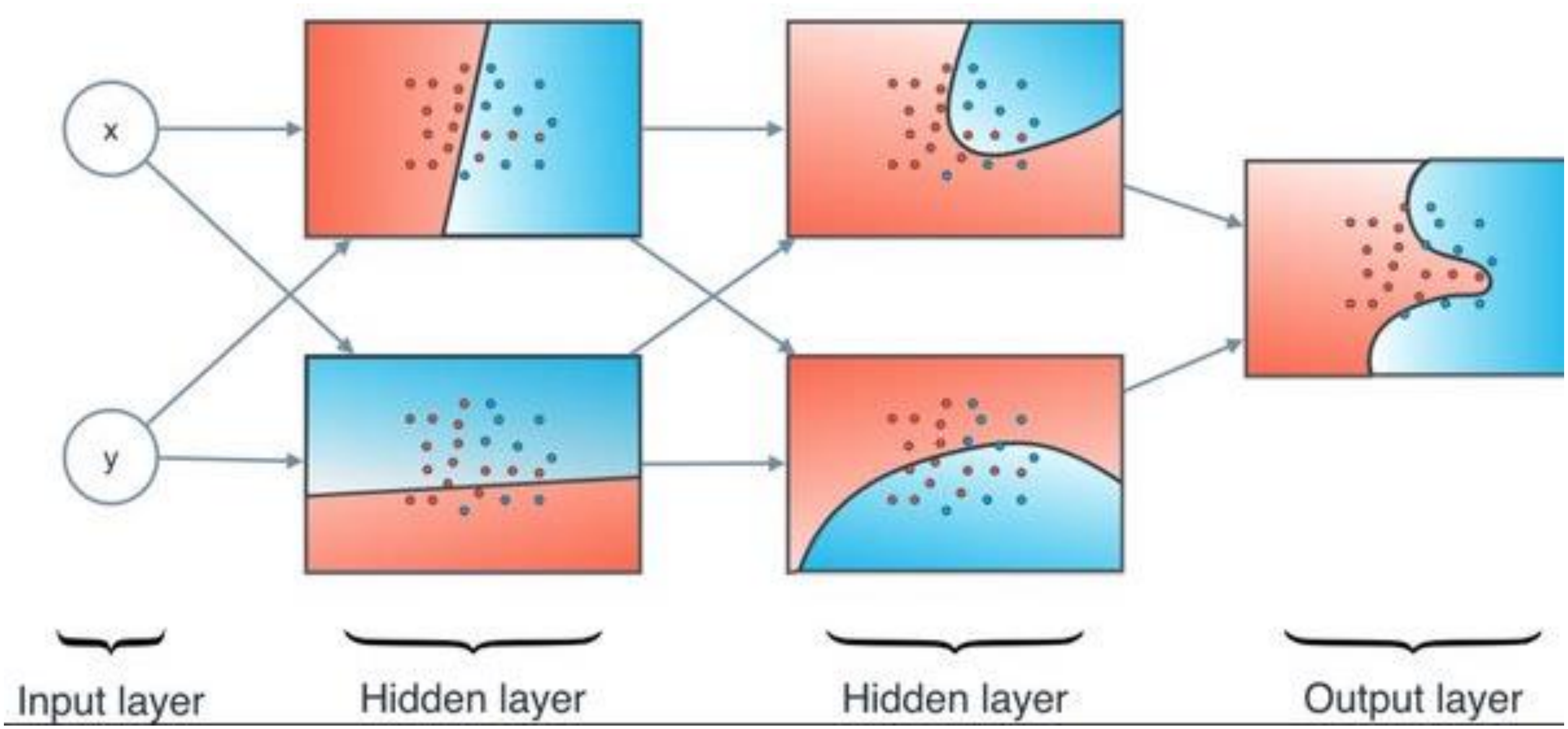
The Only Time You Want to Overfit: The First Tryout

- A model with buggy implementation (e.g., incorrect gradient calculations or updates) cannot learn anything.
- Therefore, a good and easy sanity check is to see if you can overfit few examples.
  - This is really the first test you should do, before any hyperparameter tuning.
- Try to train to 100% training accuracy/performance on a small sample (<30) of training data and monitor the **training** loss trends.
  - Does it down? If not, something must be wrong.
  - Try checking the learning rate or modifying the initialization.
  - If those don't help, check the gradients.
    - If they're NaN or Inf, might indicate exploding gradients.
    - If they're zeros, might indicate vanishing gradients.

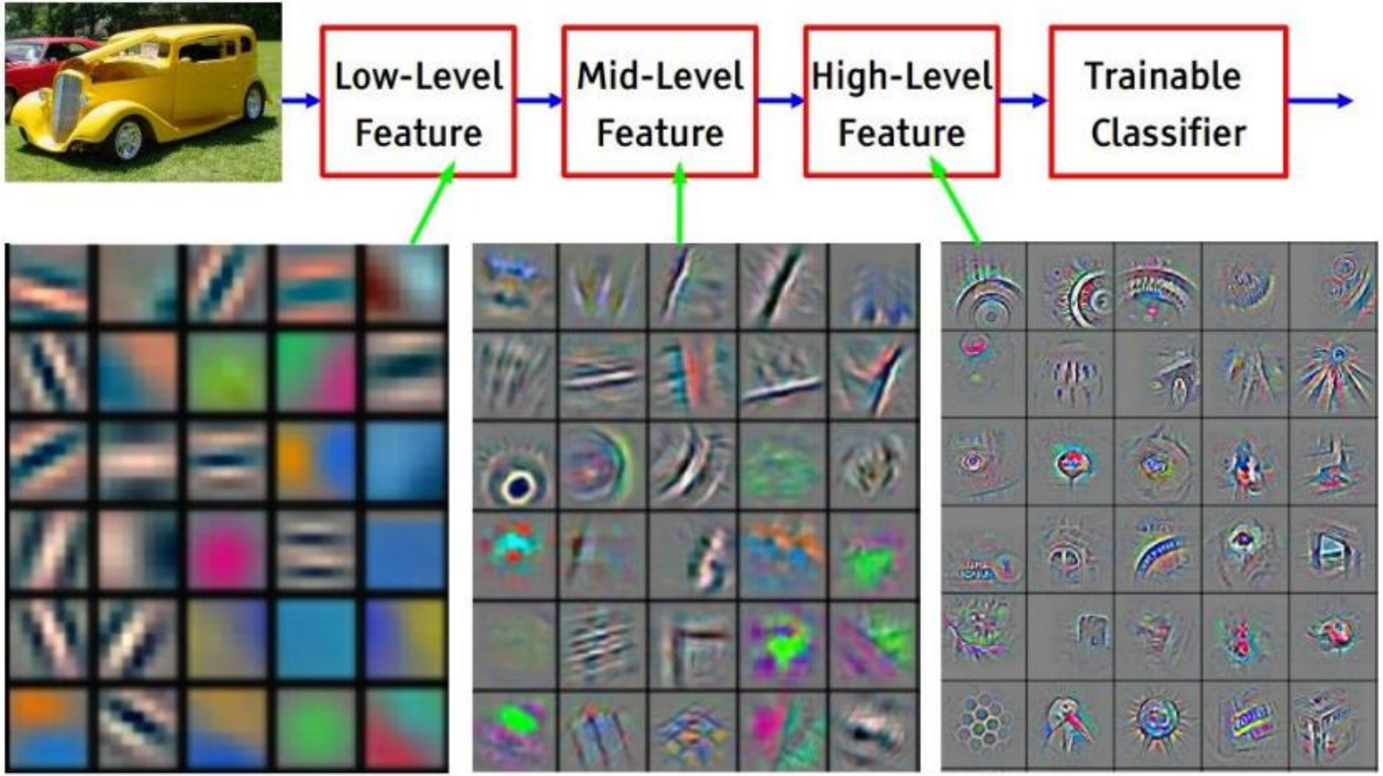
Additional Comments on Training

- No guarantee of convergence; neural networks form non-convex functions with multiple local minima
- In practice, many large networks can be trained on large data.
- Many steps (tens of thousands) may be needed for adequate training.
- May be tricky to set learning rate or number of hidden units/layers.
- To avoid local minima: several trials with different random initial weights with majority or voting techniques

Intuition about Neural Net Representations

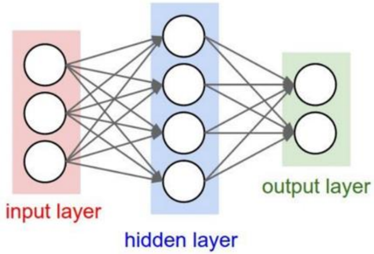


Intuition about Neural Net Representations



[Zeiler & Fergus 2013; Yosinski et al. 2015]

Summary



- Feed-forward network architecture
  - But many of the concepts here hold for any architecture.

- We learned Backprop, a general-purpose algorithm for efficient training of NNs.
  - Recursively (and hence efficiently) apply the chain-rule along computation graph.
  - The most important algorithm in neural networks! 🎉

- Lots of empirical tricks for training neural networks:
  - Things to be careful about: over-fitting, activations, exploding/vanishing gradients, …