Deep Learning

Week - 4

Announcement

- CLab-1 Due 23:59 this Friday
- CLab-2 will be released by early Monday next week.
- Move our lectures to Melville Hall in Weak 5.
- Regarding the high pitch noisy: LSSG team will look into this.

Announcement

- Pass on the following info to students if they are using Safari to play the recordings:

  "This message is to let you know that LSSG has recently received user reports about a loading issue of Echo recording in Safari.

  - Issue description:
  Users may experience lag, stuttering, or whitescreen during playback on products using iOS (such as iPhones and iPads) and some desktop devices running the Safari browser.

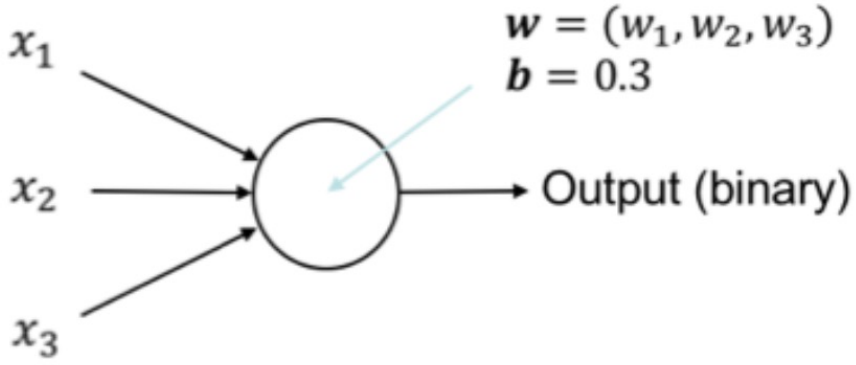
  - Current status:
  The issue has been acknowledged by Echo, and they are actively working on a solution.

  Workaround:
  - While awaiting a fix, we recommend using the Firefox browser when attempting to view and load Echo recordings

Fundamentals for Artificial Intelligence network

Recall: Perceptron as linear classifier

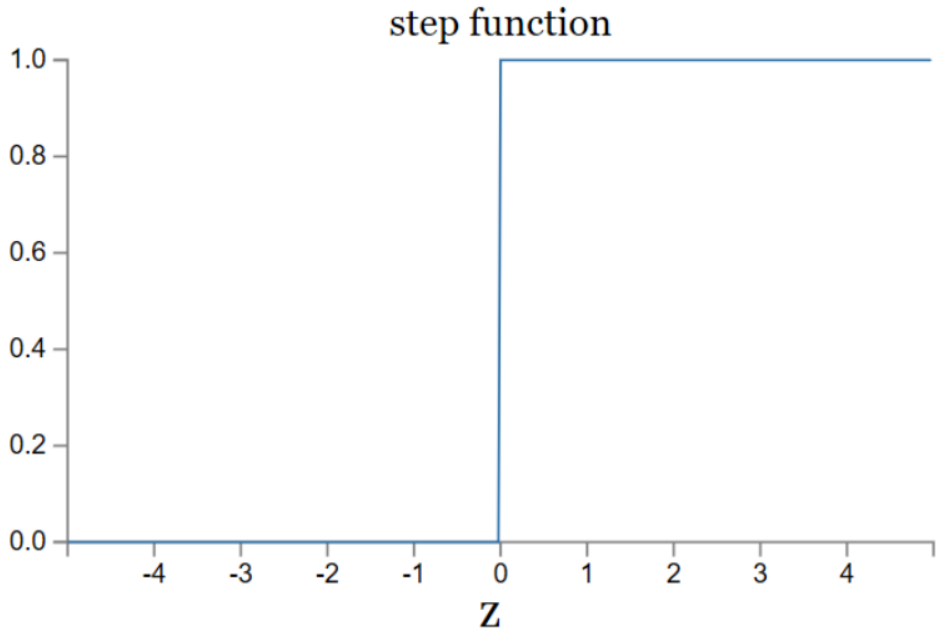
- Basic building block for composition is **perceptron** (Rosenblatt c.1960)
- Linear neuron classifier – vector of weights *w* and a 'bias' *b*



$$\text{output} = \begin{cases} 0 & \text{if } w \cdot x + b \leq 0 \\ 1 & \text{if } w \cdot x + b > 0 \end{cases} \qquad w \cdot x \equiv \sum_j w_j x_j$$

Perceptron’s activation function

$$\text{output} = \begin{cases} 0 & \text{if } w \cdot x + b \leq 0 \\ 1 & \text{if } w \cdot x + b > 0 \end{cases}$$

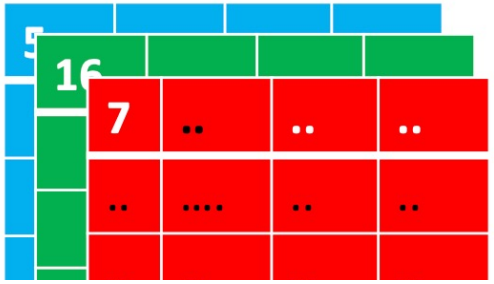


In the context of neural networks, a perceptron is an artificial neuron using the step function as the activation function.

Binary Classification Example

- Is it a Kangaroo?

{0,1}
1 – kangaroo
0 – not a kangaroo



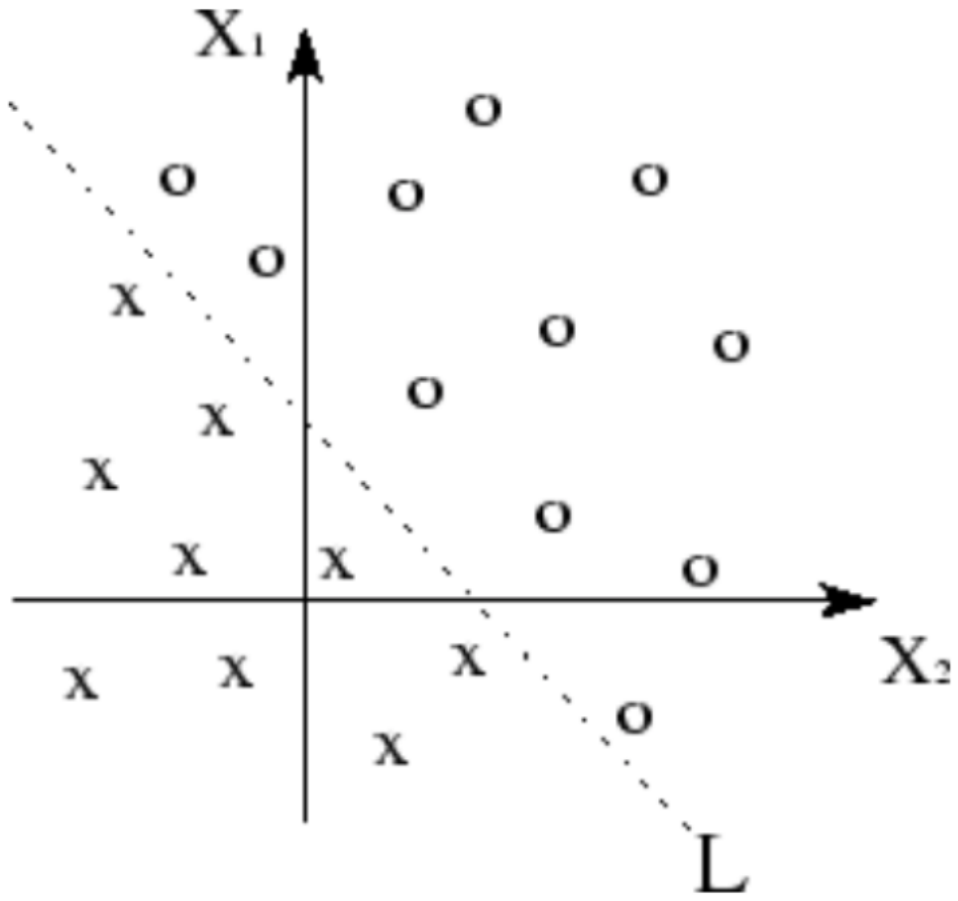
$$X = \begin{bmatrix} 5 \\ .. \\ .. \\ 16 \\ .. \\ .. \\ 7 \\ .. \end{bmatrix}$$

X Dim is n_x x m x 3
N_x is num features

Y dim is 1
X -> Y

Credit: Nick Barnes

Linear Classifier



Logistic Regression

- Logistic regression (LR) is actually a classification method.
- LR introduces an extra non-linearity over a linear classifier,

$$f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$$

by using a non-linear function $\sigma(\cdot)$

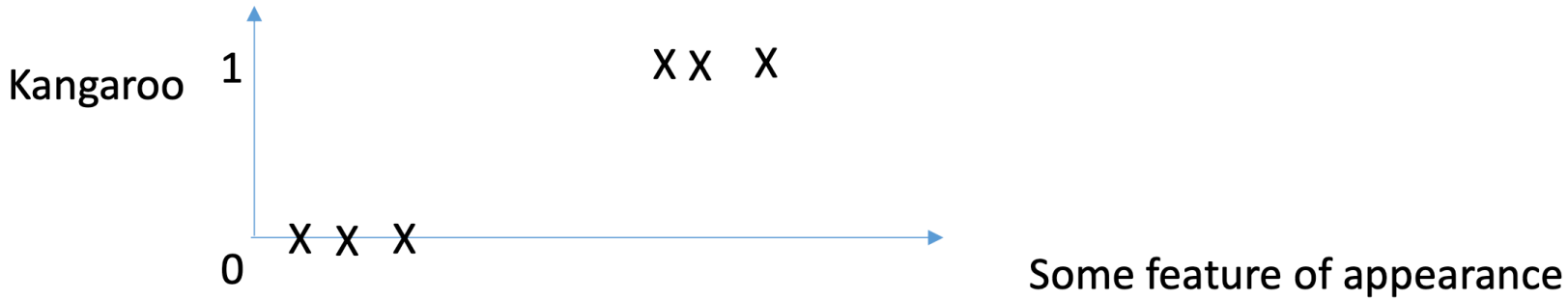
- The LR classifier is defined as

$$\sigma\left(f\left(\mathbf{x}_i\right)\right)\begin{cases}\geq 0.5 & y_i = +1\\ < 0.5 & y_i = -1\end{cases}$$

where $\sigma(f(\mathbf{x})) = \dfrac{1}{1+e^{-f(\mathbf{x})}}$

Linear Regression Vs Logistic Regression

- In 1 dimension

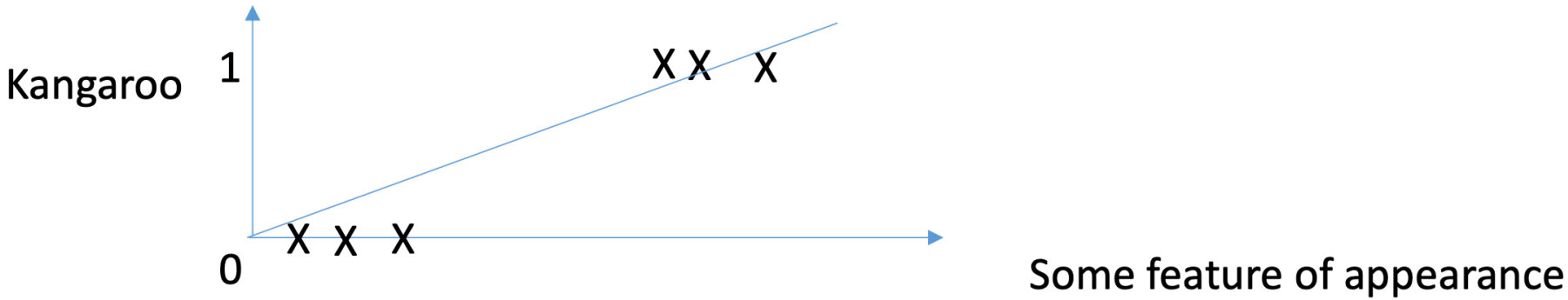


Threshold of classification is 0.5

Credit: Nick Barnes

Linear Regression Vs Logistic Regression

- In 1 dimension

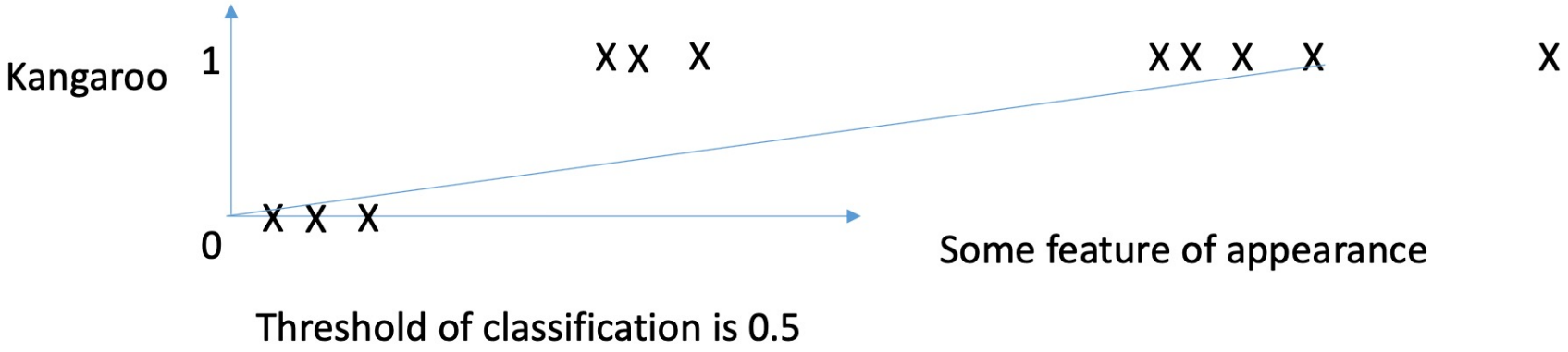


Threshold of classification is 0.5

Credits: Nick Barnes

Linear Regression Vs Logistic Regression

- But what about



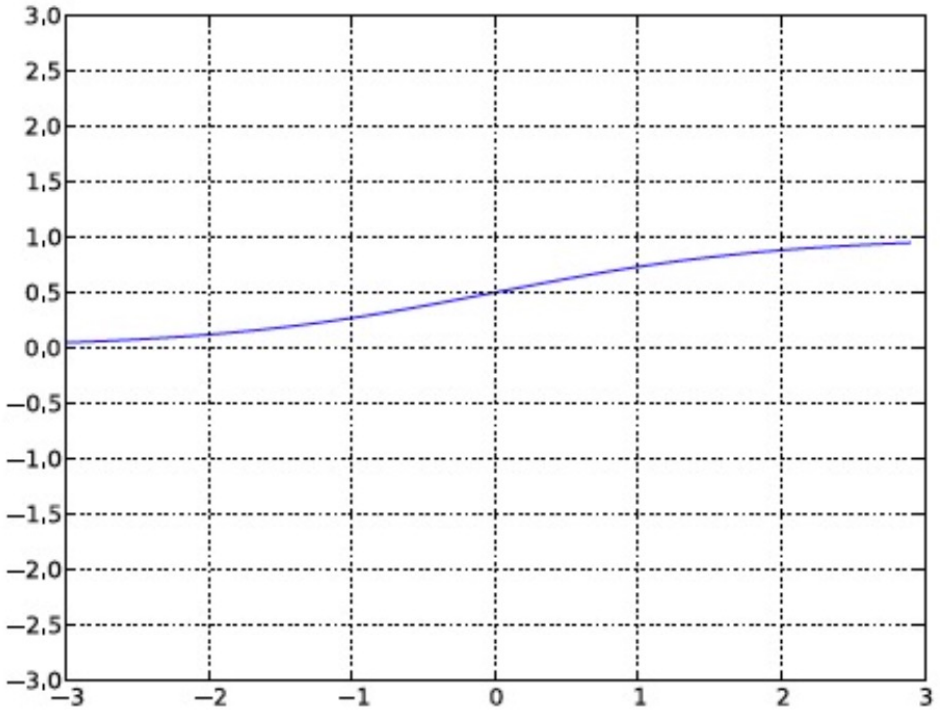
- Its not really what we want
- The decision boundary is being dominated by distant points.
- We want a function that is mostly zero below 0.5 and mostly 1 above 0.5.

Credits: Nick Barnes

Logistic Regression

- Sigmoid function
  - Squashes the curve between 0 and 1
  - Always positive
  - Bounded
  - Strictly increasing
  - Continuous
  - Differentiable

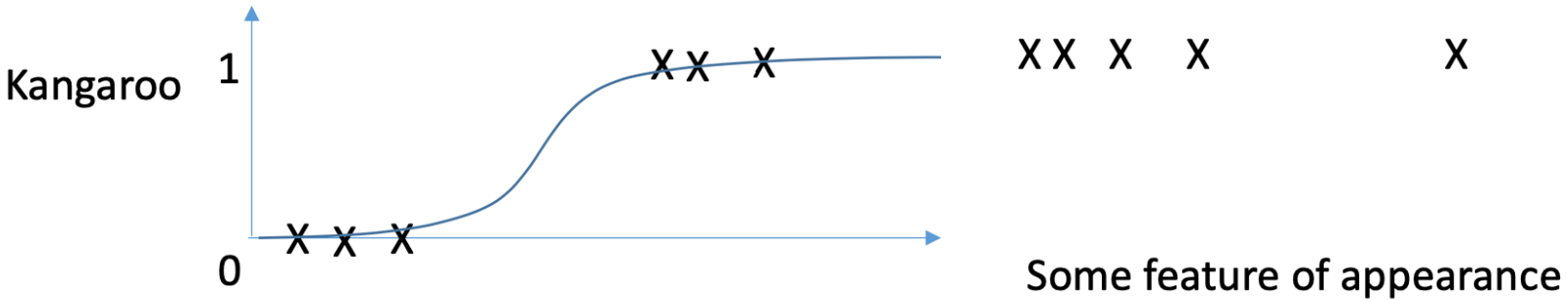
$$g(a) = \text{sigm}(a) = \frac{1}{1+\exp(-a)}$$



Credits: Nick Barnes

Logistic Regression

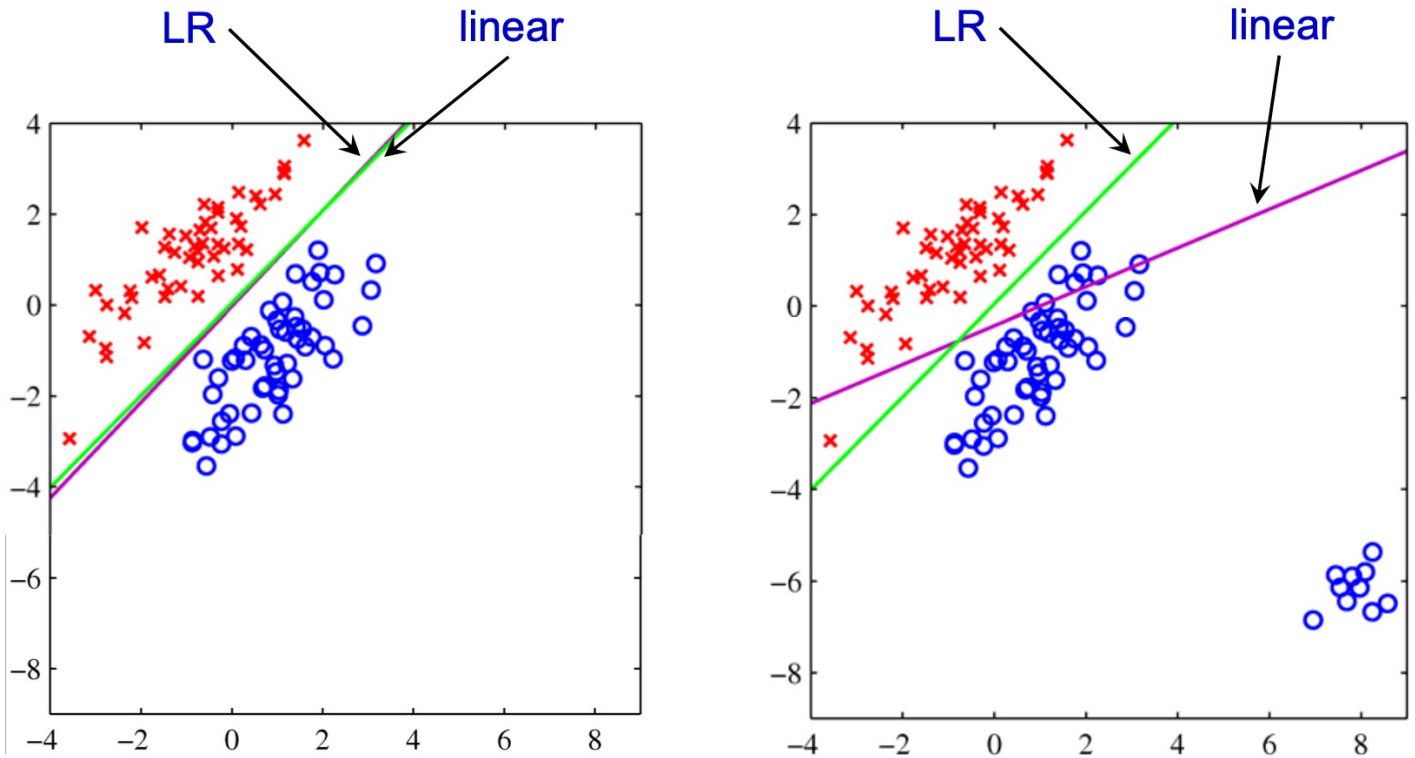
- Predict y = 1 if f(x) >= 0.5, otherwise predict y=0 if f(x)<0.5



$$g(a) = \text{sigm}(a) = \frac{1}{1+\exp(-a)}$$

Model is a sigmoid function (or a logistic function)

Logistic Regression



$\sigma(w_1x_1 + w_2x_2 + b)$ fit, vs $w_1x_1 + w_2x_2 + b$

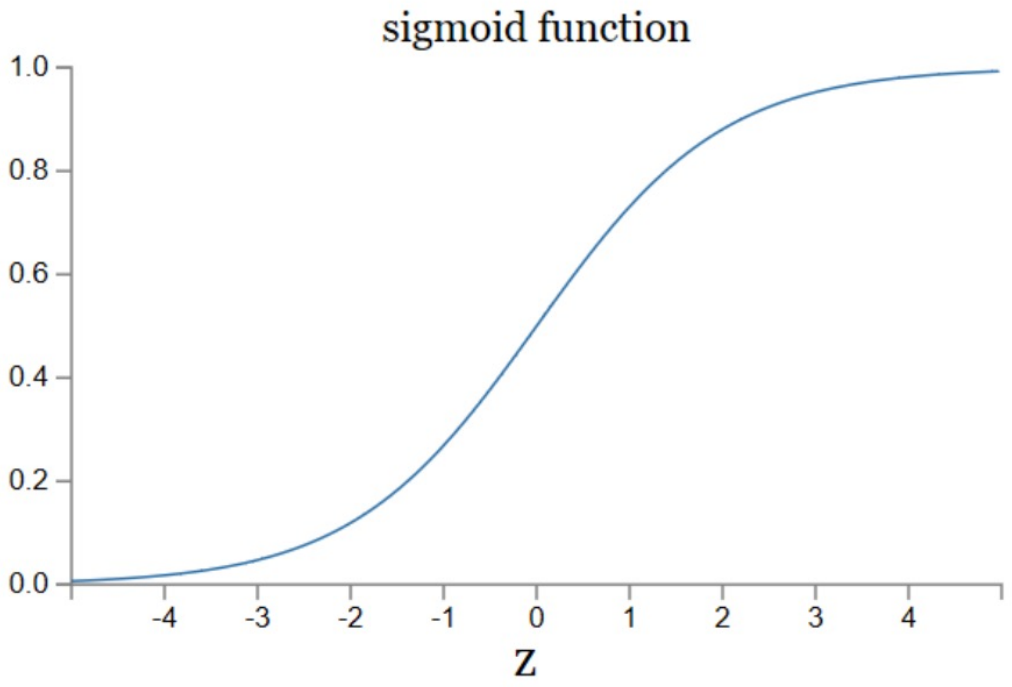
Credit: A. Zisserman

Sigmoid non-linear activation

Sigmoid, non-linear function, is used to transform features.

$$\sigma(w \cdot x + b)$$

$$\sigma(z) \equiv \frac{1}{1 + e^{-z}}.$$

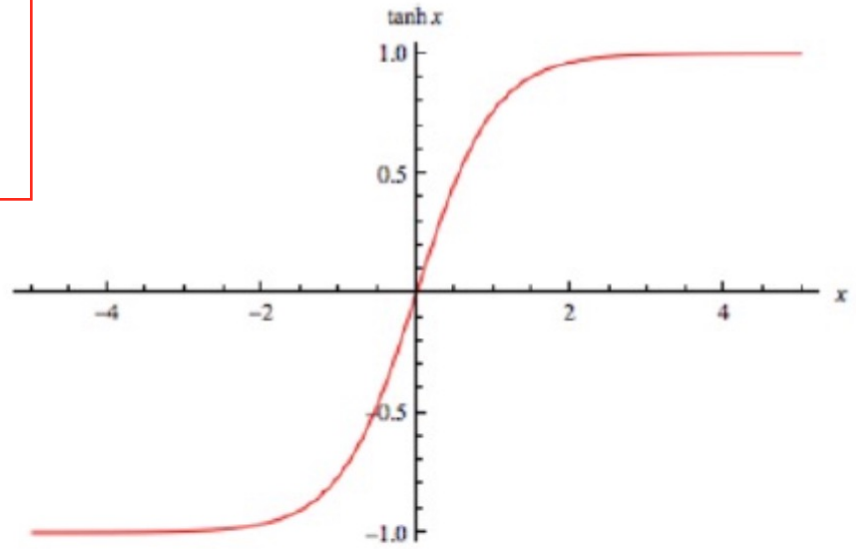


Nielsen

Activation Functions

1. Sigmoid function.
2. Hyperbolic tangent.
   - Squash between -1 and 1
   - Positive or negative
   - Bounded
   - Strictly increasing

$$\tanh(x) = \frac{\exp(x) - \exp(-x)}{\exp(x) + \exp(-x)}$$

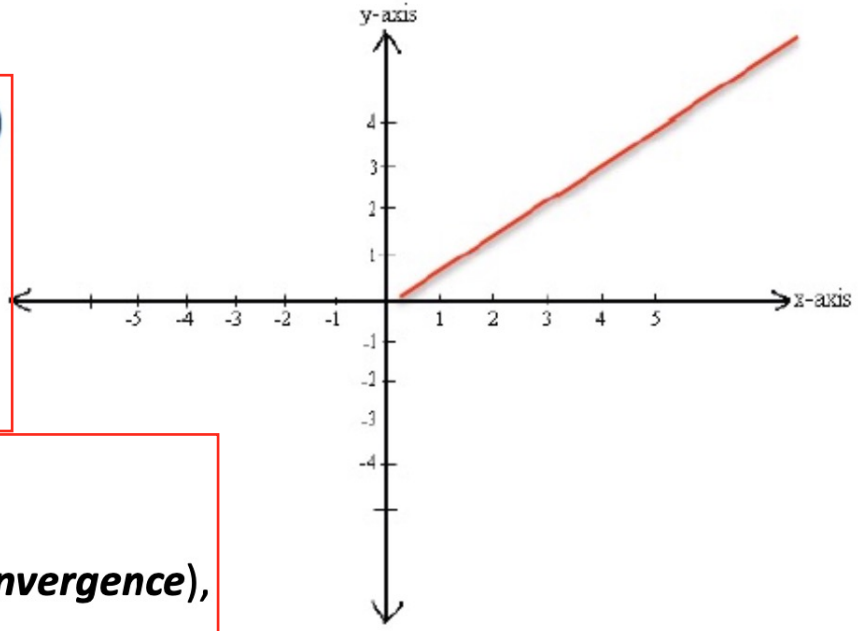


Credit: Nick Barnes

Activation Functions

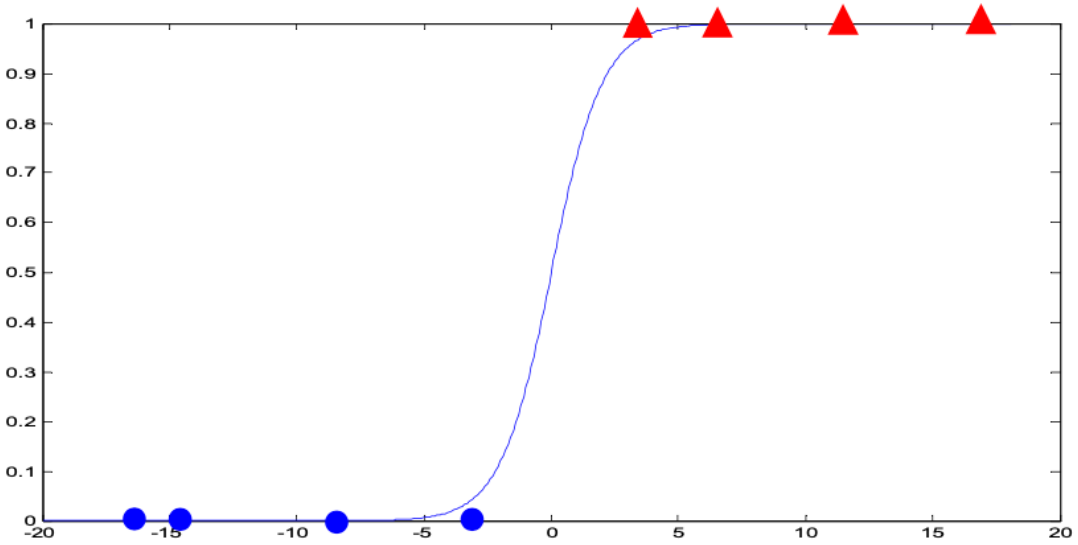
1. Sigmoid function.
2. Hyperbolic tangent.
3. Linear Rectifier (ReLU)
   - Bounded below by 0
   - Not upper bounded
   - Strictly increasing
   - Sparse neurons

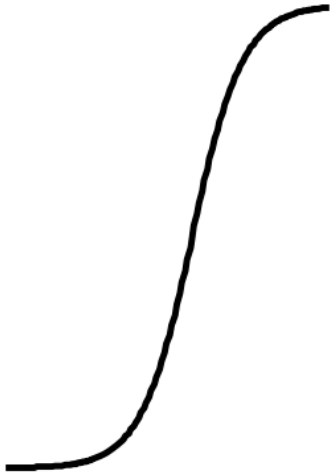
$$\text{rectifier}(x) = \max(0, x)$$

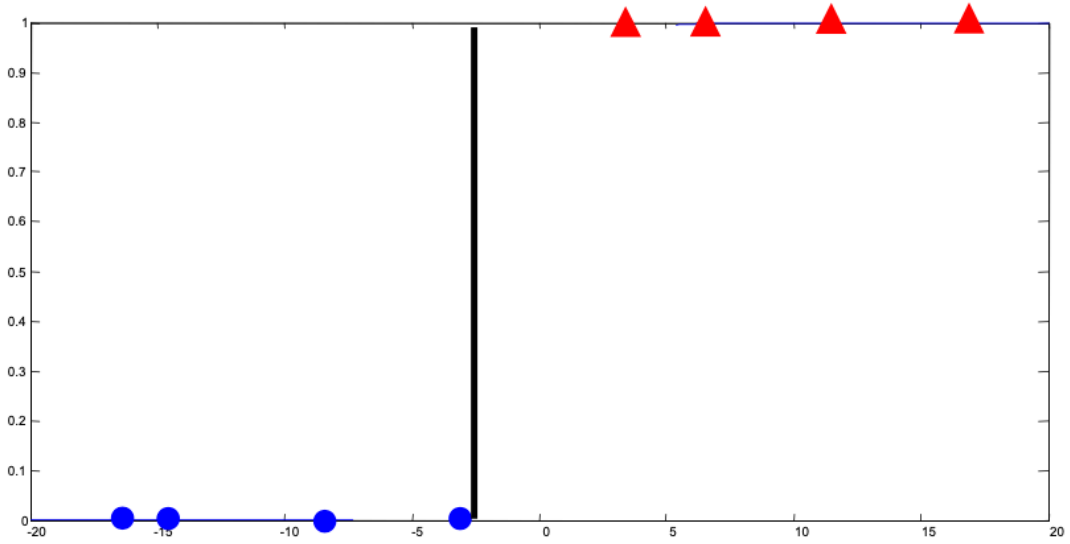


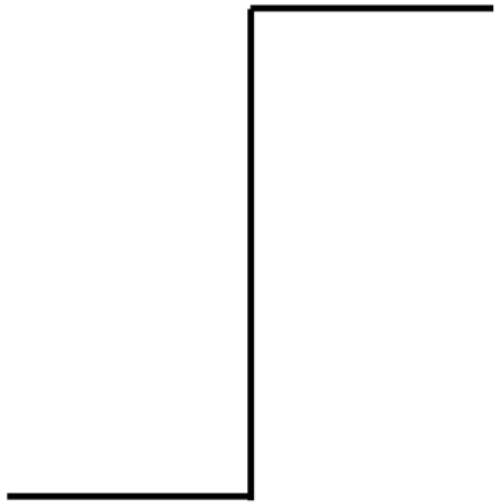
Does not saturate (>0)
Very computationally efficient (no exp)
Converges much faster (***e.g. 6x faster convergence***),

AlexNet [Krizhevsky et al., 2012]
Used it.
Glorot, 2011 introduced to deep nets
Deep Sparse Rectifier Neural Network









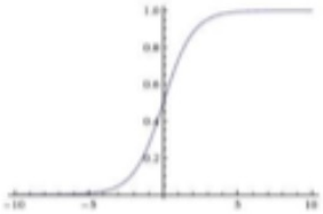
- A sigmoid favours a larger margin compared with a step classifier.

Types of activation function

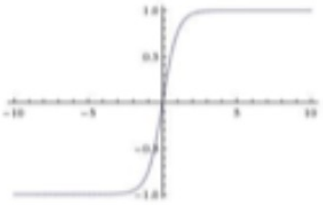
Activation Functions

Sigmoid

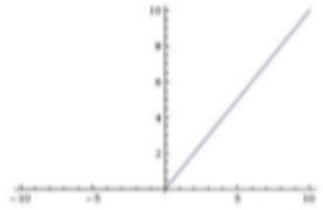
$$\sigma(x) = 1/(1+e^{-x})$$



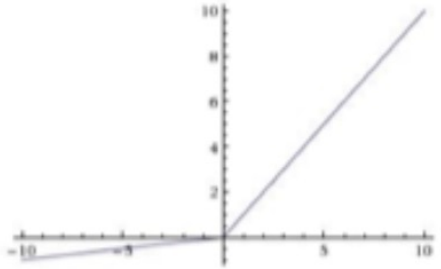
tanh tanh(x)



ReLU max(0,x)



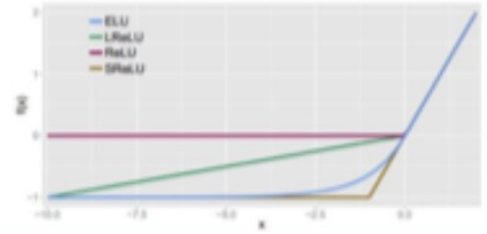
Leaky ReLU
max(0.1x, x)



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

ELU

$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha\,(\exp(x) - 1) & \text{if } x \le 0 \end{cases}$$

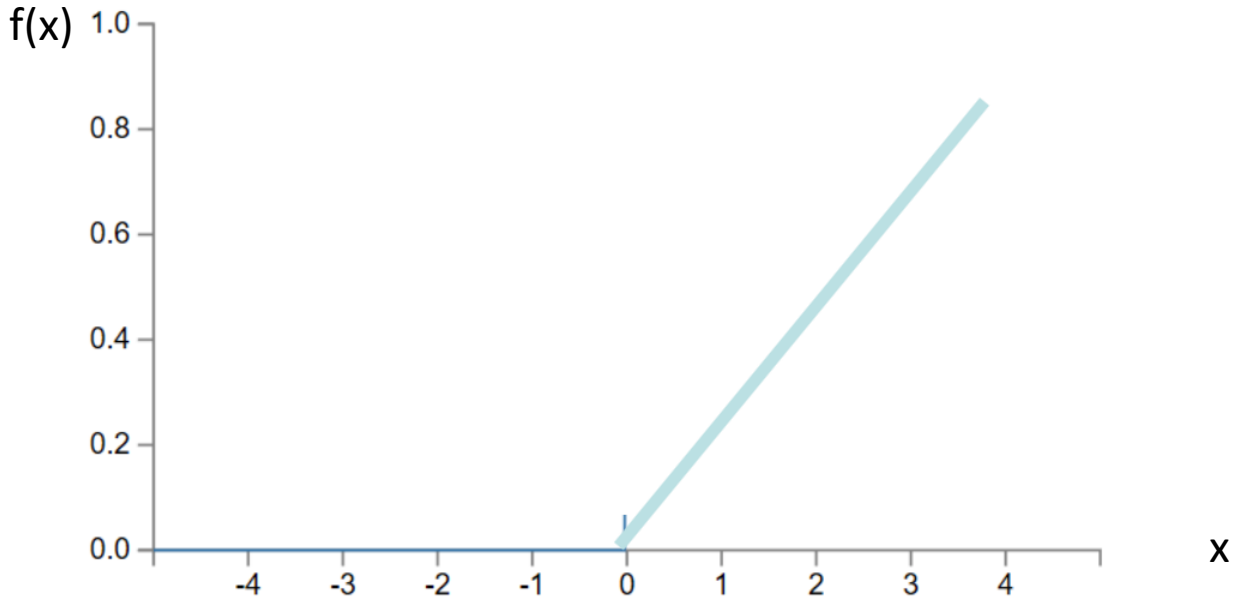


Slide from CS231n: stanford

Another non-linear activation function: Rectified Linear Unit (ReLU)

- ReLU

$$f(x) = \max(0, x)$$



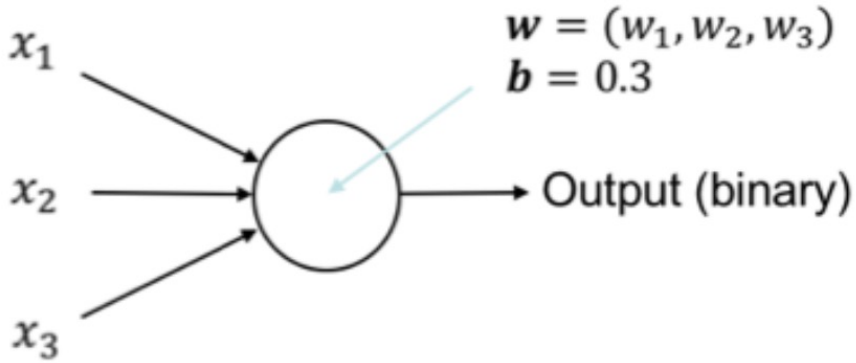
Recall: Binary Classifying an image

- Each pixel of the image would be an input.
- So, for a 28 x 28 image, we vectorize.
- **x** = 1 x 784

- **w** is a vector of weights for each pixel, 784 x 1
- b is a scalar bias per perceptron

- result = **xw** + b -> (1x784) x (784x1) + b = (1x1)+b

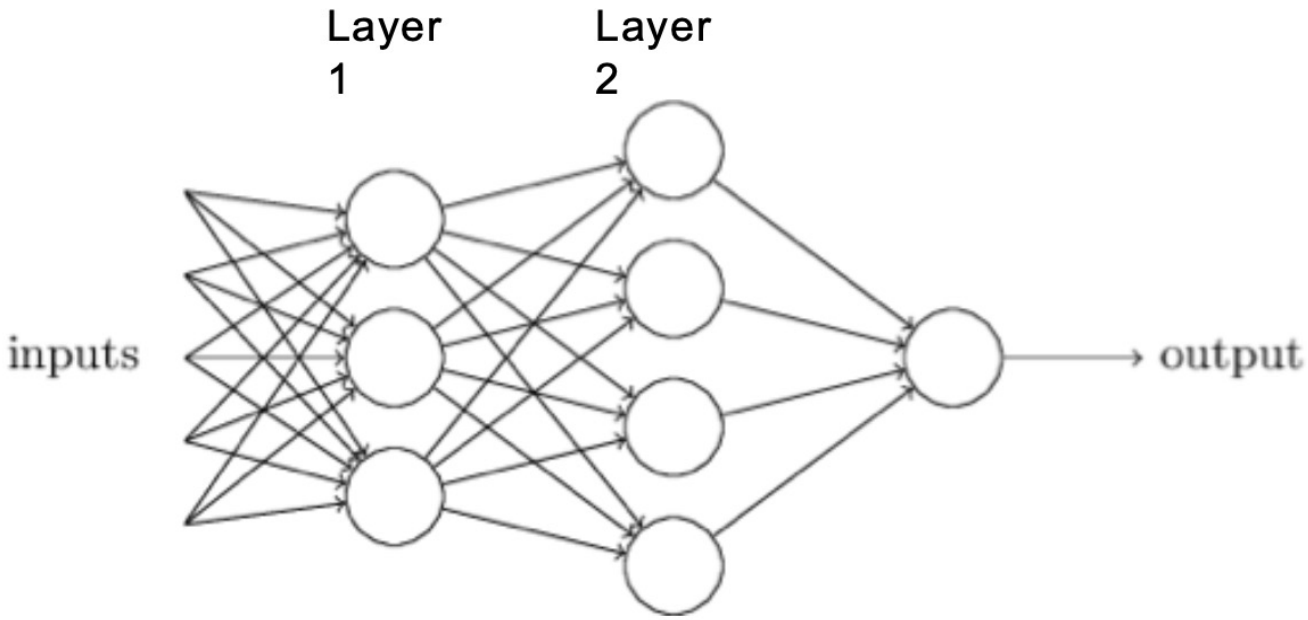
linear classifier



$$\text{output} = \begin{cases} 0 & \text{if } w \cdot x + b \leq 0 \\ 1 & \text{if } w \cdot x + b > 0 \end{cases}$$

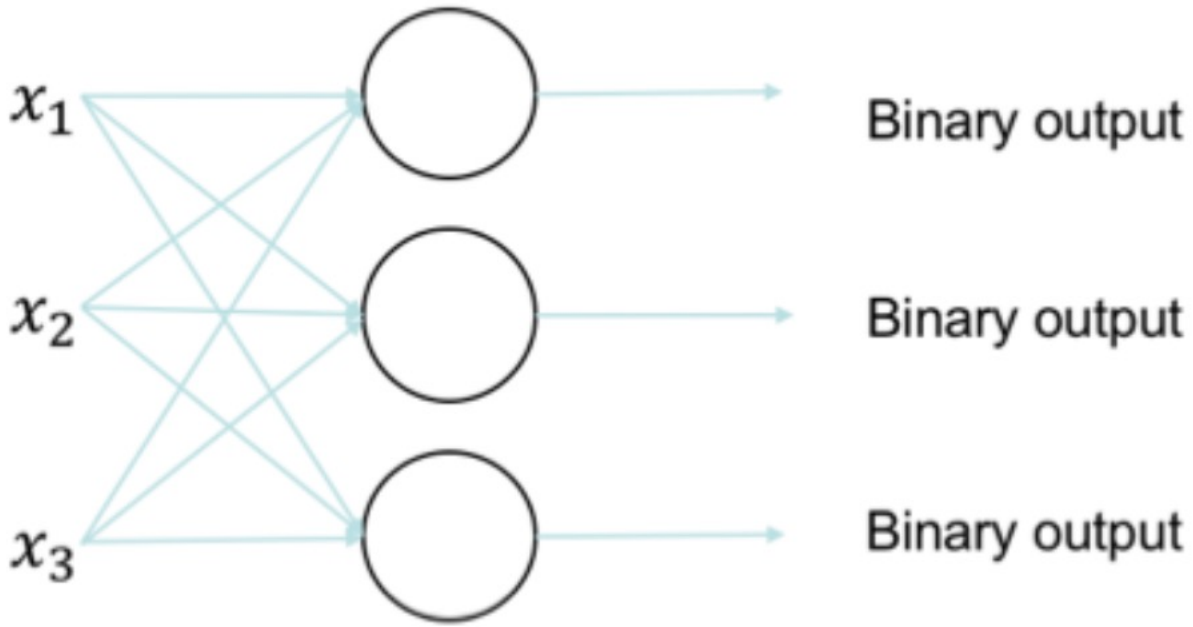
$$w \cdot x \equiv \sum_j w_j x_j$$

Composition



Sets of layers and the connections (weights) between them define the *network architecture.*

Add more neurons -> Multiclass neural networks



Recall: Multi-class classification

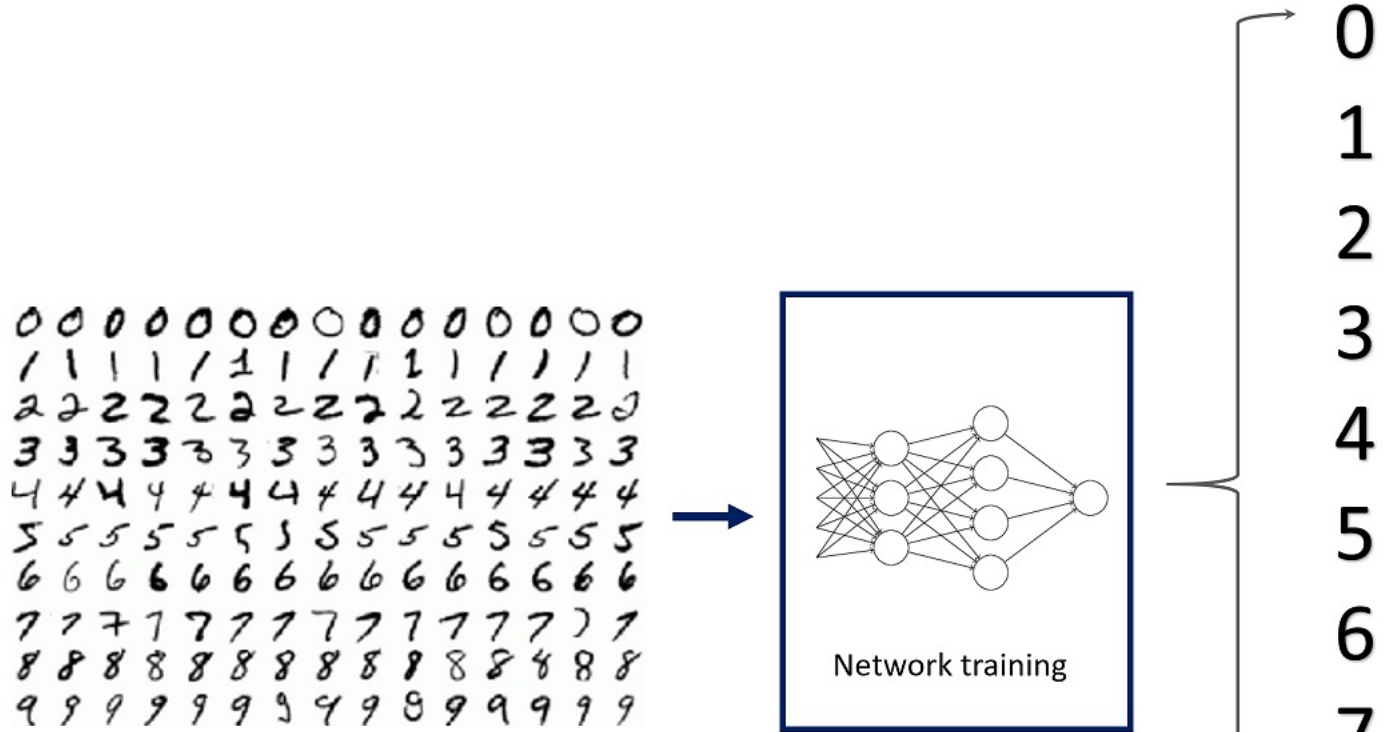
- Each pixel of the image would be an input node.
- So, for a 28x28 image, we vectorize the input image as a **x**=1x784 for

#(classes) = e.g., 10 ,in MNIST digit recognition

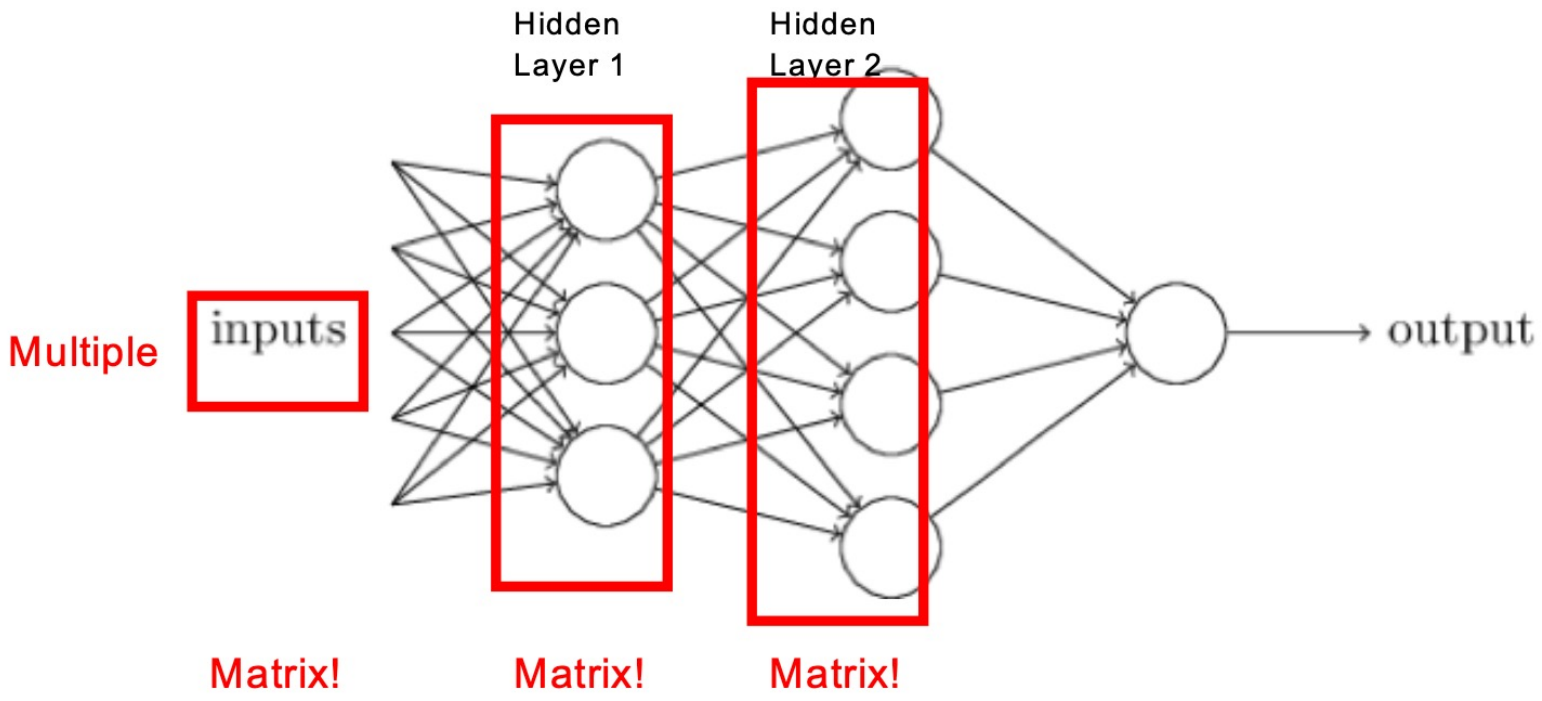
- **W** is a matrix of weights for each pixel/each perceptron – **W** = 784 x 10 (10-class classification)
- **b** is a bias *per perceptron* (vector of biases); (1 x 10)
- result **Z**=**xW**+**b** ->(1x784)x(784x10)+**b** -> (1 x 10) + (1 x 10) = 10-D output vector
- Activation function: softmax:

$$\sigma(\mathbf{z})_i = \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}} \quad \text{for } i = 1, \ldots, K \text{ and } \mathbf{z} = (z_1, \ldots, z_K) \in \mathbb{R}^K$$

Application: Multi-class classification



Parallel computation

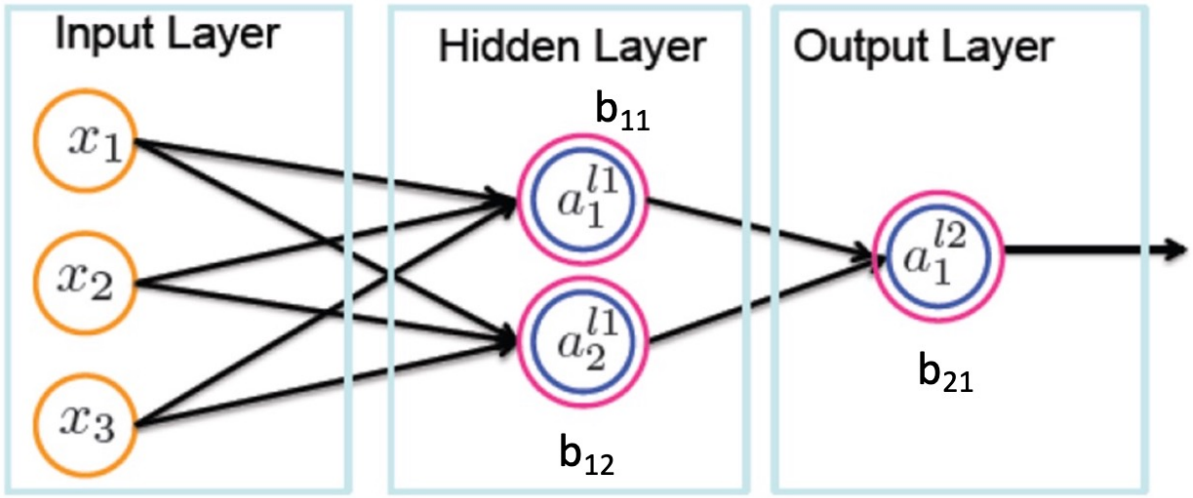


It's all just matrix-vector multiplications !

GPUs -> special hardware for fast/large matrix multiplication.

Nielsen

Single Hidden Layer Example



$$a_1^{l1} = w_{11}^{l0}\, x_1 + w_{21}^{l0}\, x_2 + w_{31}^{l0}\, x_3 + b_{11}$$

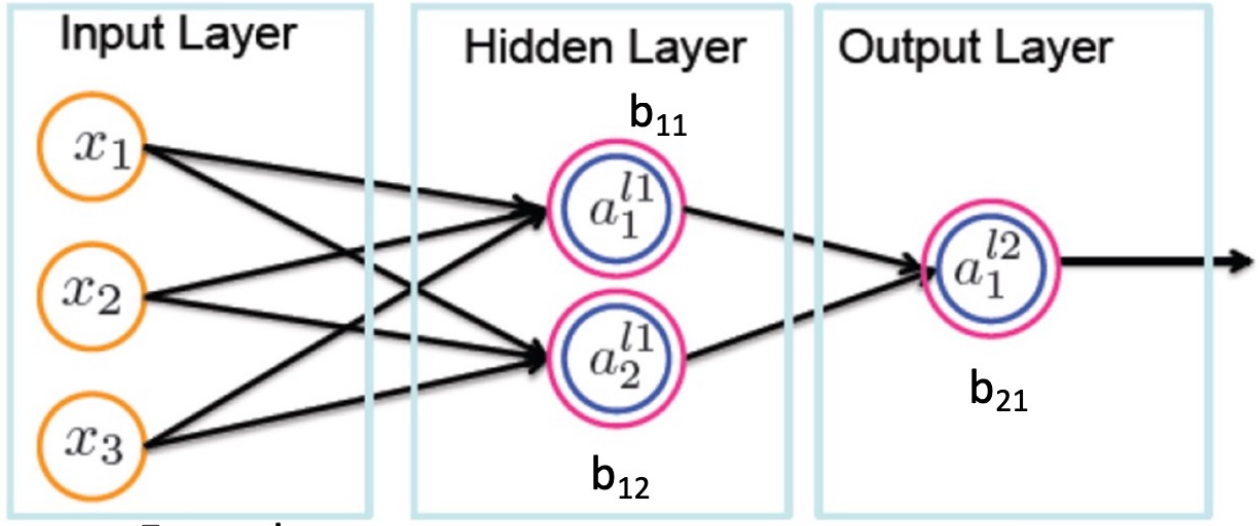
$$o_1^{l1} = g\left(a_1^{l1}\right)$$

$$o_1^{l1} = g\left(w_{11}^{l0}\, x_1 + w_{21}^{l0}\, x_2 + w_{31}^{l0}\, x_3 + b_{11}\right) \Rightarrow o_1^{l2} = g\left(w_{11}^{l1} o_1^{l1} + w_{12}^{l1} o_2^{l1} + b_{21}\right)$$

$$o_2^{l1} = g\left(w_{12}^{l0}\, x_1 + w_{22}^{l0}\, x_2 + w_{32}^{l0}\, x_3 + b_{12}\right)$$

Output Layer: $o_1^{l2} = g\left(\boldsymbol{w}^{l1}\, g\left(\boldsymbol{w}^{l0}\boldsymbol{x}\right)\right)$

Single Hidden Layer Example



Example, suppose:

X = {0.4, 0.2, 0.2}

$w_{1.}^{l0}$= {1.0, 0.5}

$w_{2.}^{l0}$ = {0.2, 1.2}

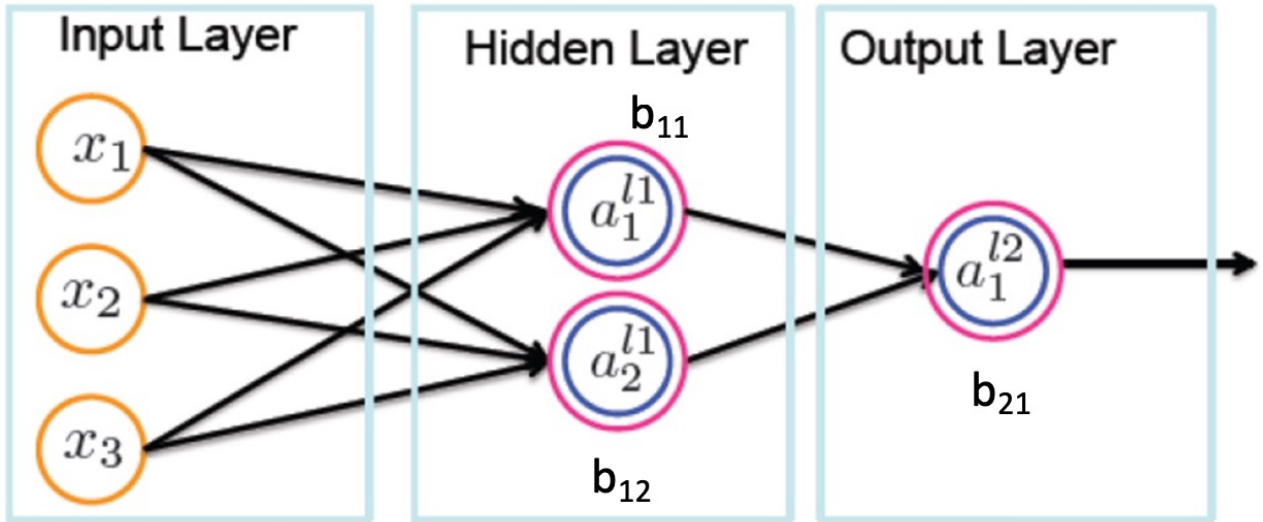
$w_{3.}^{l0}$ ={1.2,0.1}

$w_{1.}^{l1}$ = {0.3,0.9}

B_{11} = 0.1

B_{12} = 0.2

B_{21} = 0.3



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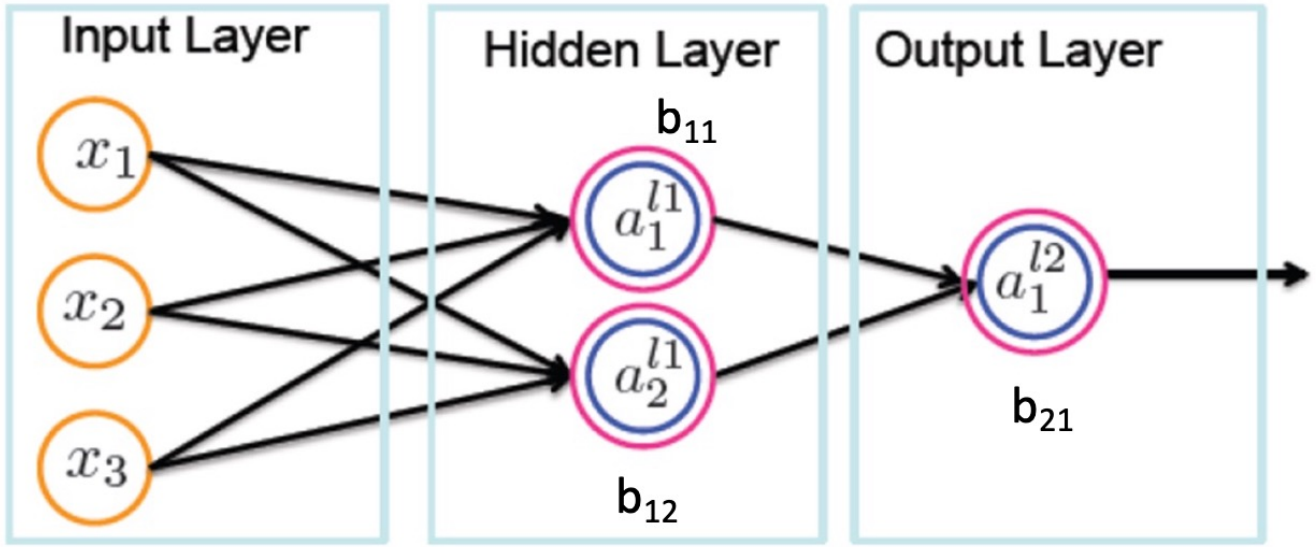
$$o_1^{l1} = g\left(w_{11}^{l0}\, x_1 + w_{21}^{l0}\, x_2 + w_{31}^{l0}\, x_3 + b_{11}\right)$$

$$= g(1.0 * 0.4 + 0.2 * 0.2 + 1.2 * 0.2 + 0.1)$$

Single Hidden Layer Example



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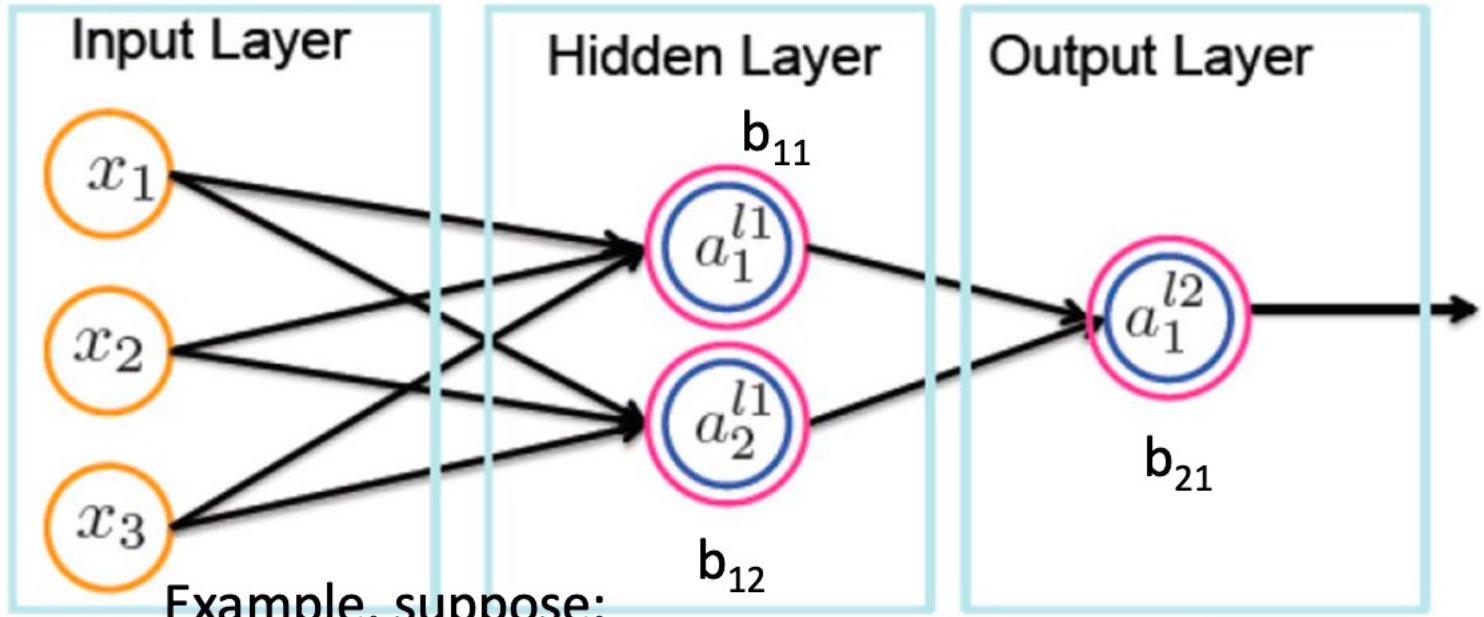
$$o_1^{l1} = g\left(w_{11}^{l0}\, x_1 + w_{21}^{l0}\, x_2 + w_{31}^{l0}\, x_3 + b_{11}\right)$$

$$= g(1.0 * 0.4 + 0.2 * 0.2 + 1.2 * 0.2 + 0.1)$$

= g(0.4+ 0.04 + 0.24 + 0.1)

= g(0.78)

=1/(1+exp(0.78))



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B_{12} = 0.2

B_{21} = 0.3

$$o_2^{l1} = g\left(w_{12}^{l0}\, x_1 + w_{22}^{l0}\, x_2 + w_{32}^{l0}\, x_3 + b_{12}\right)$$

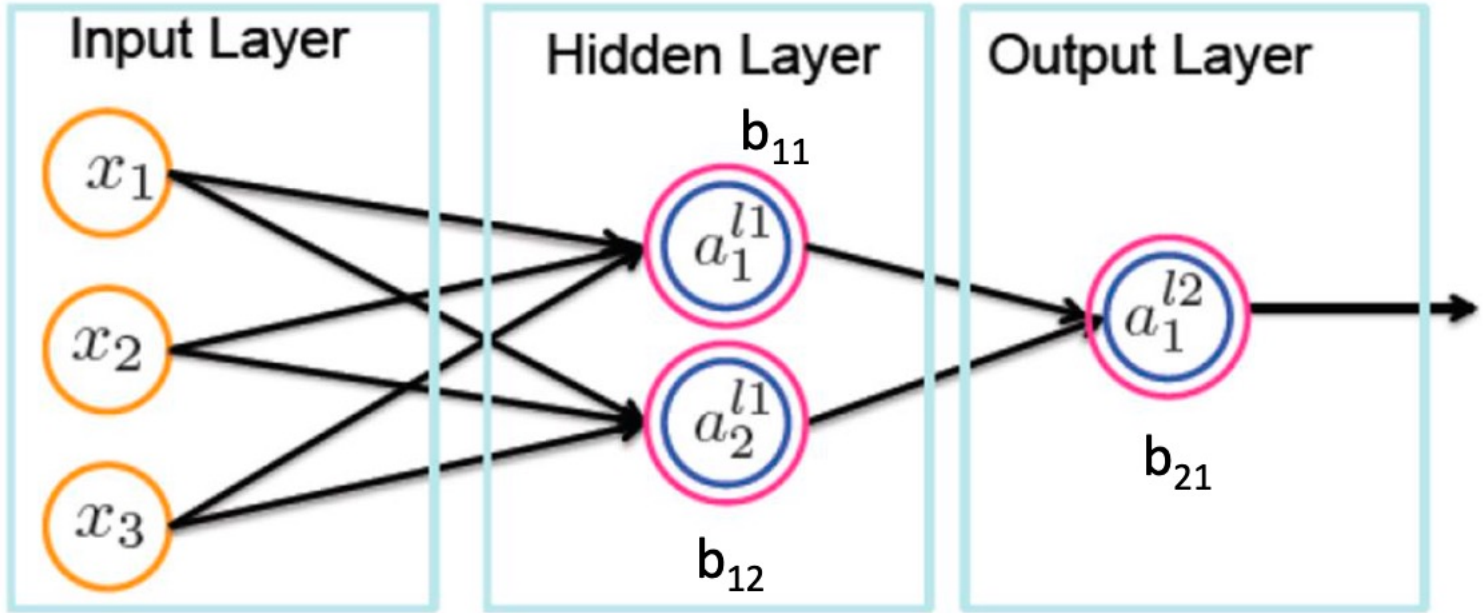
$$= g(0.5 * 0.4 + 1.2 * 0.2 + 0.1 * 0.2 + 0.2)$$

= g(0.2+ 0.24 + 0.03 + 0.2)

=g(0.49)

= 1 / (1 + exp(-0.49)

=0.62..



Note that the computation of the activations at layer 1 are vector computations, and so can be parallelized in a GPU!
Many computations are like this so GPU's greatly decrease computation time (but not order).

Example, suppose:

X = {0.4, 0.2, 0.2}

$w_{1.}^{l1}$ = {1.0, 0.5}

$w_{2.}^{l1}$ = {0.2, 1.2}

$w_{3.}^{l1}$ ={1.2,0.1}

$w_{1.}^{l2}$ = {0.3,0.9}

B_{11} = 0.1

B_{12} = 0.2

B_{21} = 0.3

$$o_1^{l2} = g\left(w_{11}^{l1} o_1^{l1} + w_{12}^{l1} o_2^{l1} + b_{21}\right)$$

$$= g(0.3 * 0.68 + 0.9 * 0.62 + 0.3)$$

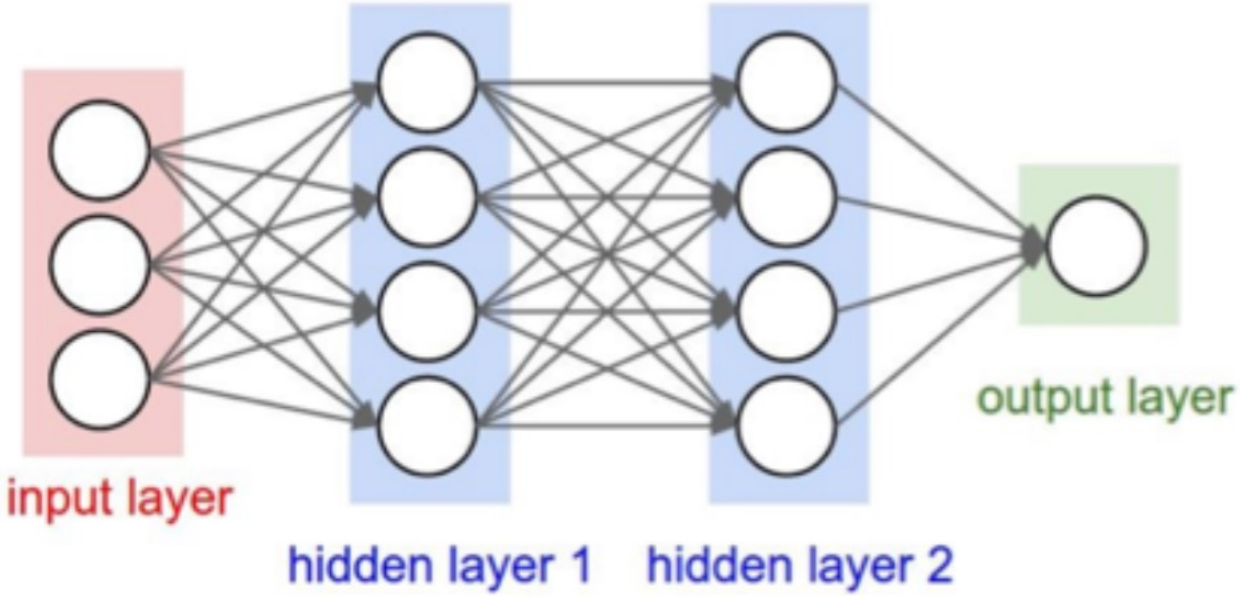
= g(0.204+ 0.558 + 0.3)

=g(1.062)

= 1 / (1 + exp(-1.062)

=0.74..

Parallel Computation



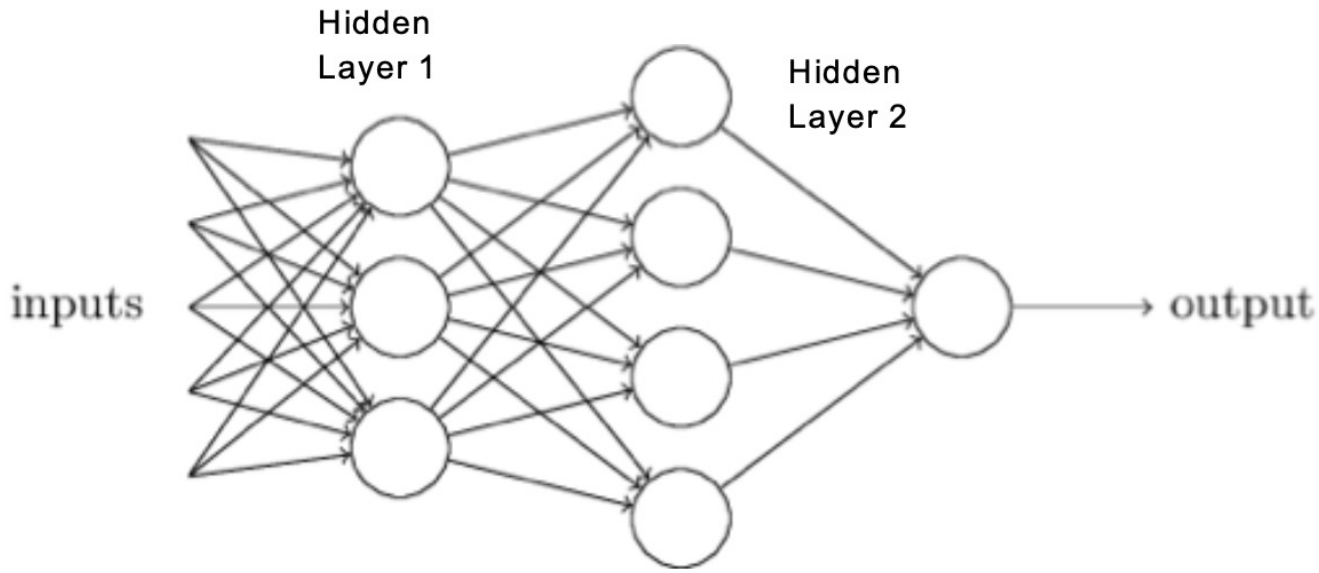

```
# forward-pass of a 3-layer neural network:
f = lambda x: 1.0/(1.0 + np.exp(-x)) # activation function (use sigmoid)
x = np.random.randn(3, 1) # random input vector of three numbers (3x1)
h1 = f(np.dot(W1, x) + b1) # calculate first hidden layer activations (4x1)
h2 = f(np.dot(W2, h1) + b2) # calculate second hidden layer activations (4x1)
out = np.dot(W3, h2) + b3 # output neuron (1x1)
```

Problems with using all-linear functions in the hidden layers

- We have formed multiple layers or chains of linear functions.
- We know that linear function of linear functions is a linear function, i.e. they can be reduced:
  - $g = f(h(x))$
  - Eg. $O_1 = xw_1+b_1$; $O_2 = o_1w_2+b_2$; $=>O_2 = (xw_1+b_1)w_2+b_2=xw_1w_2+(b_1w_2+b_2)$

Our multi-layer composition of functions is really just a single linear function!!!!

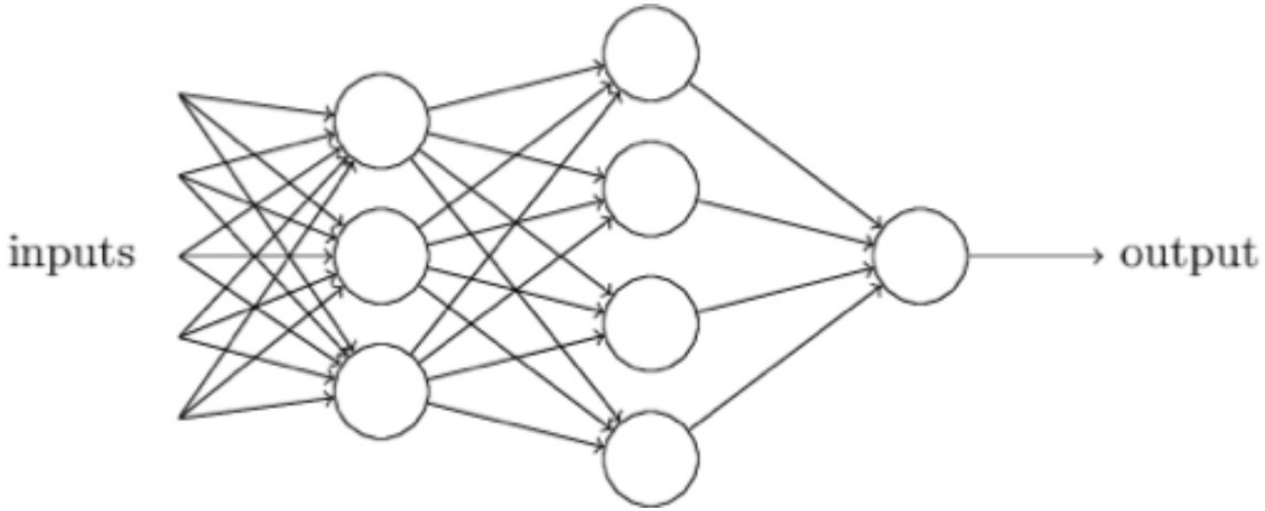
Multi-Layer Perceptron (MLP)



- Attempt to represent complex functions as compositions of smaller functions.
- Outputs from one perception are fed into inputs of another perceptron.
- Layers that are in between the input and the output are called *hidden layers*, because we are going to *learn* their weights via an optimization process.

Multi-Layer Perceptron (MLP)

- …is a '*fully connected*' neural network with non-linear activation functions.



- '*Feed-forward*' neural network

Nielson

Mathematical Theorem for MLP

- The application of MLP is grounded in theory.

– **Universal Approximation Theorem.**

With three (or more) layers and enough parameters, MLP can approximate any function.

Proof(Michael Nielson):

http://neuralnetworksanddeeplearning.com/chap4.html

If a 3-layer network can approximate any function …given enough parameters … then why should we need to go deeper ?

– Intuitively, composition is efficient because it allows the *reuse* of layer of neurons.

– Empirically, deeper networks do a better job than shallow networks at learning certain hierarchies of knowledge.

Why go **deeper** ?

- *A three-layer network is already a "universal approximator",*
  - *Only if the number of neurons in the hidden layer is sufficiently many.*
  - *The identification of the weights is troublesome (possible convergence to wrong local minima)*
- Deep neural networks
  - Have many levels of non-linearity
  - Compactly represent highly non-linear functions
  - Layered structure facilitates convergence to a good optimum
  - **There are many local optima of approximately the same (and good) quality**

Interpretation

Question: What does a hidden unit do?

Answer: It can be thought of as a classifier or feature detector.

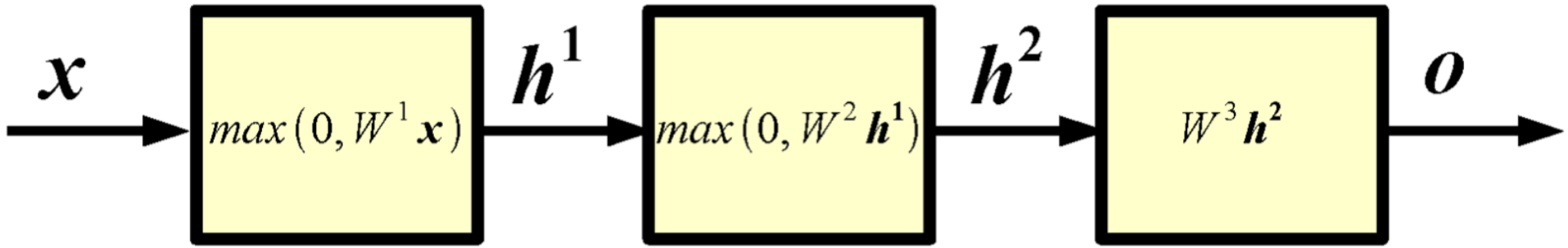
Question: How many layers? How many hidden units?

Answer: Cross-validation or hyper-parameter search methods are the answer. In general, the wider and the deeper the network the more complicated the mapping.

Question: How do I set the weight matrices?

Answer: Weight matrices and biases are learned.
First, we need to define a measure of quality of the current mapping.
Then, we need to define a procedure to adjust the parameters.

Neural Networks: example



x input

h^1 1-st layer hidden units

h^2 2-nd layer hidden units

o output

Example of a 2 hidden layer neural network (or 4 layer network, counting also input and output).

Supervised Learning

$\{(\boldsymbol{x}^i, y^i), i = 1 \dots P\}$ training dataset

$\boldsymbol{x}^i$ i-th input training example

y^i i-th target label

P number of training examples

Goal: predict the target label of unseen inputs.

Supervised Learning Example

Classification

“dog”

classification

Denoising

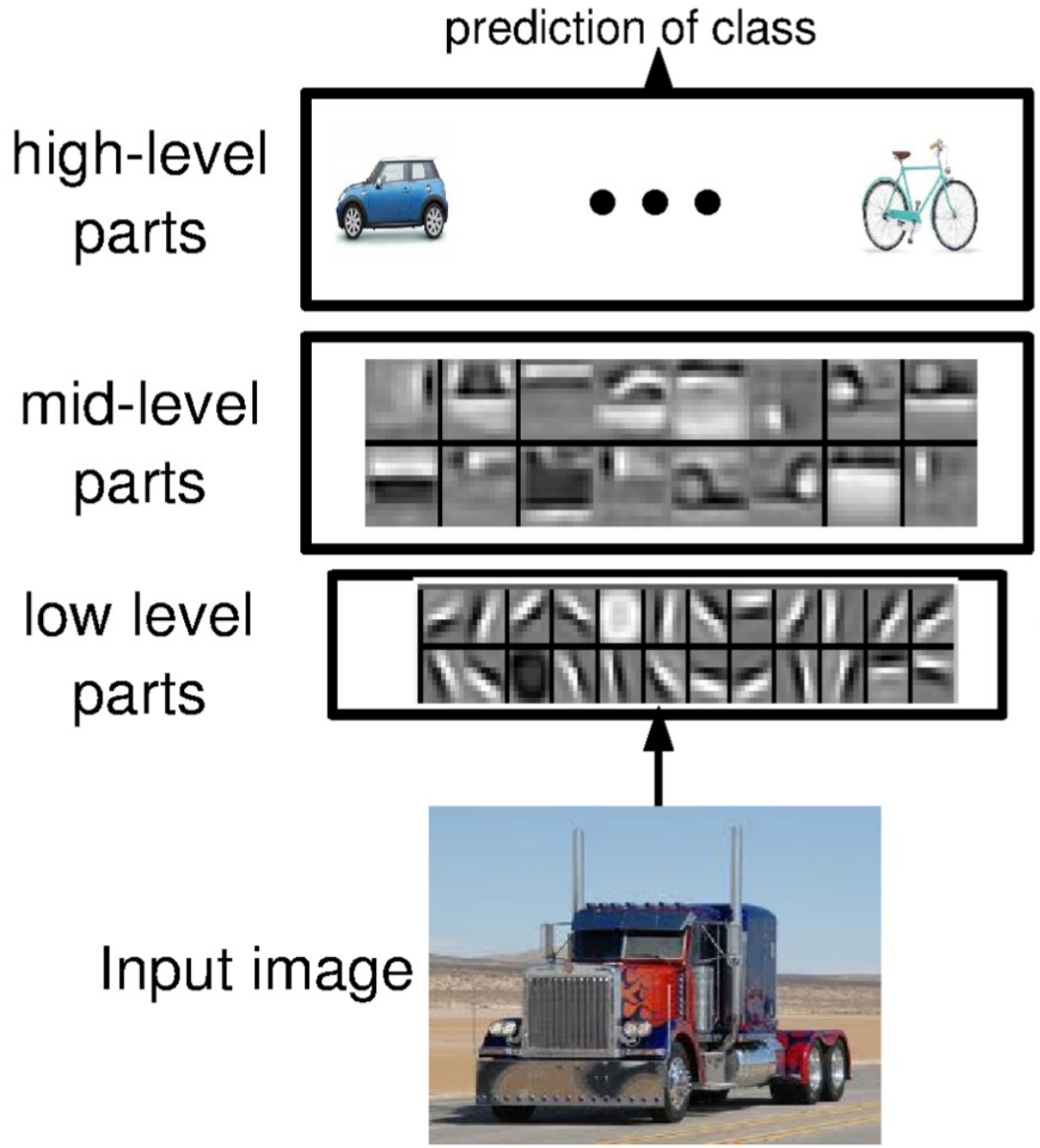
regression

OCR

“2 3 4 5”

structured prediction

Interpretation

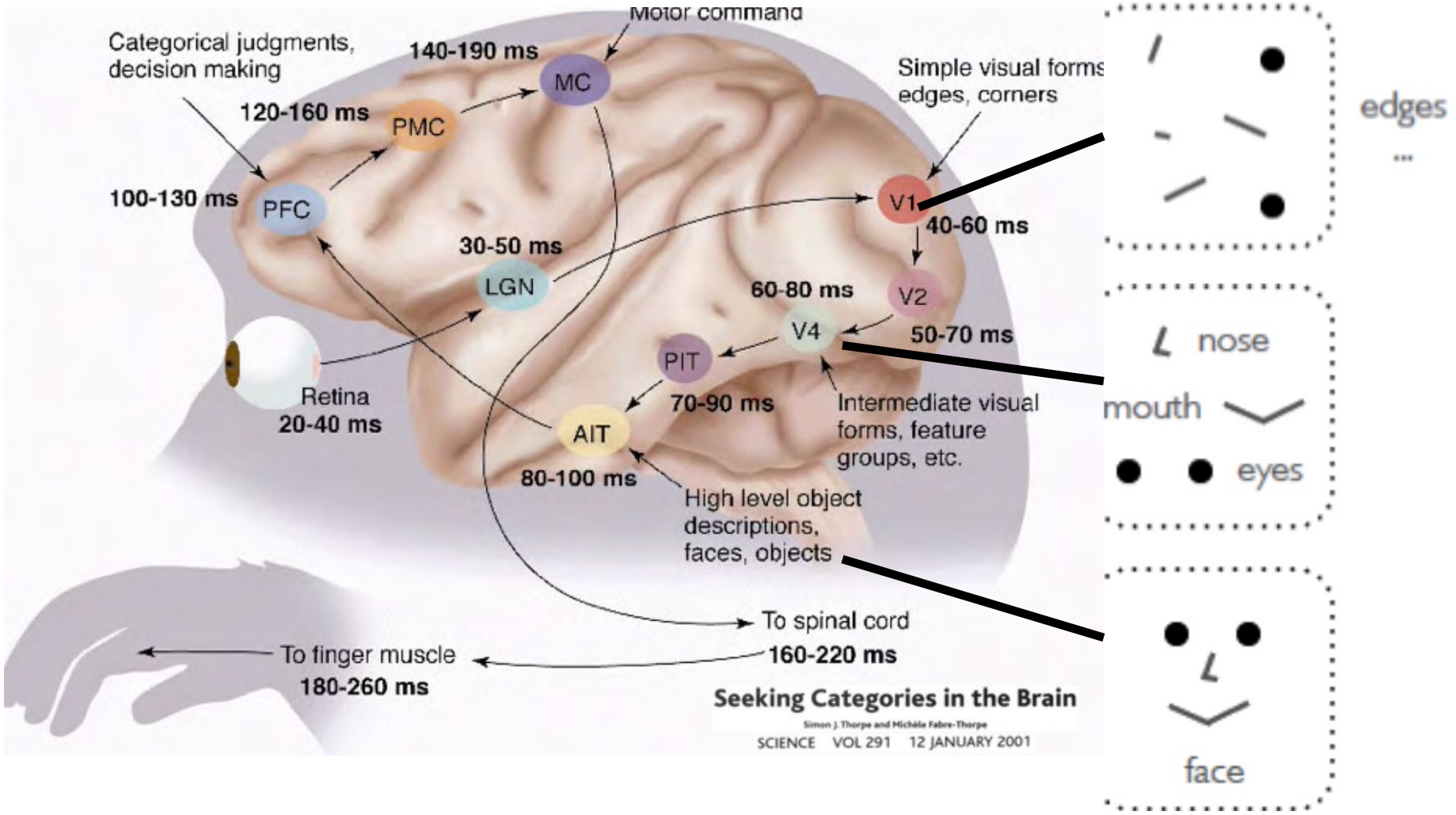


- distributed representations
- feature sharing
- compositionality

NOTE: Not actually the weights; a demonstrative visualization!

Lee et al. "Convolutional DBN's ..." ICML 2009

Biological inspiration: Human Neural Systems

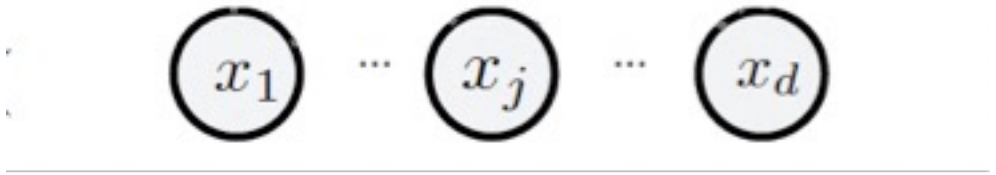


Multilayer Neural Networks

Forward Computation

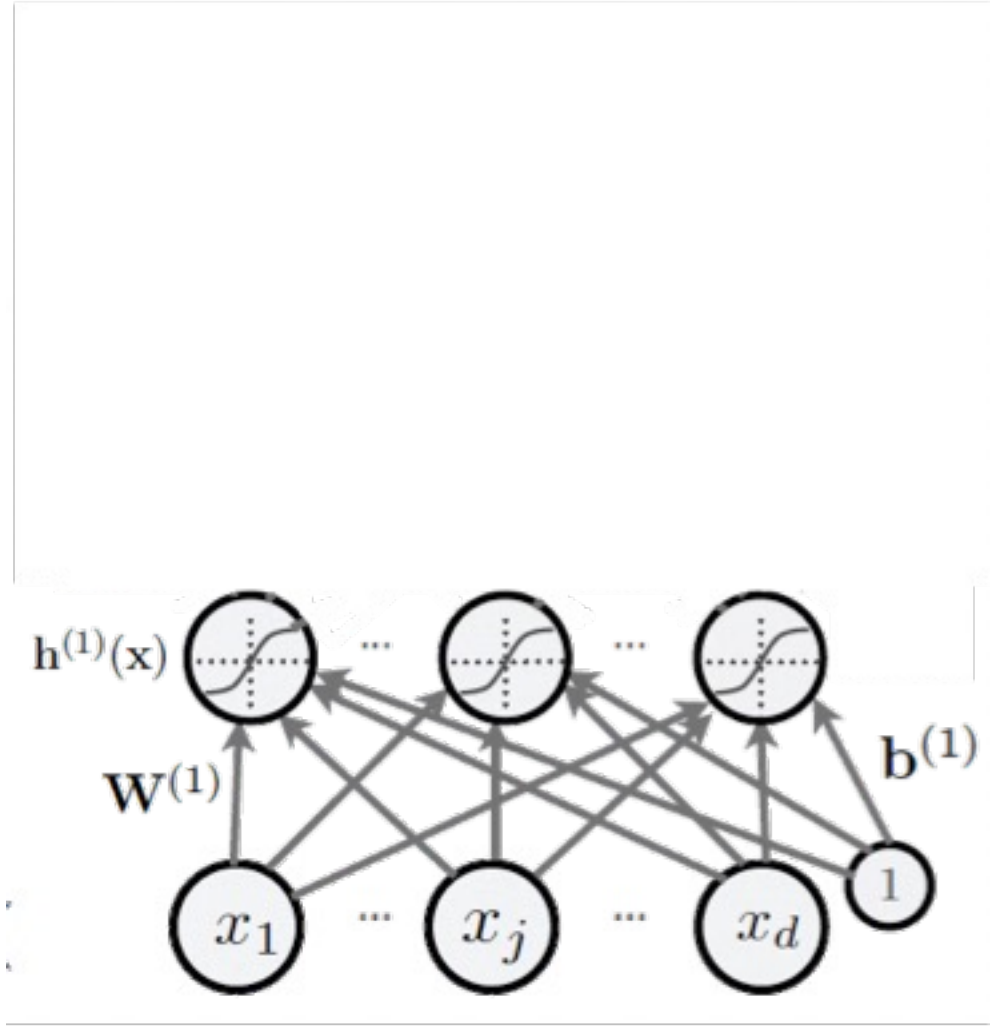
Multilayer Neural Network

- Forward



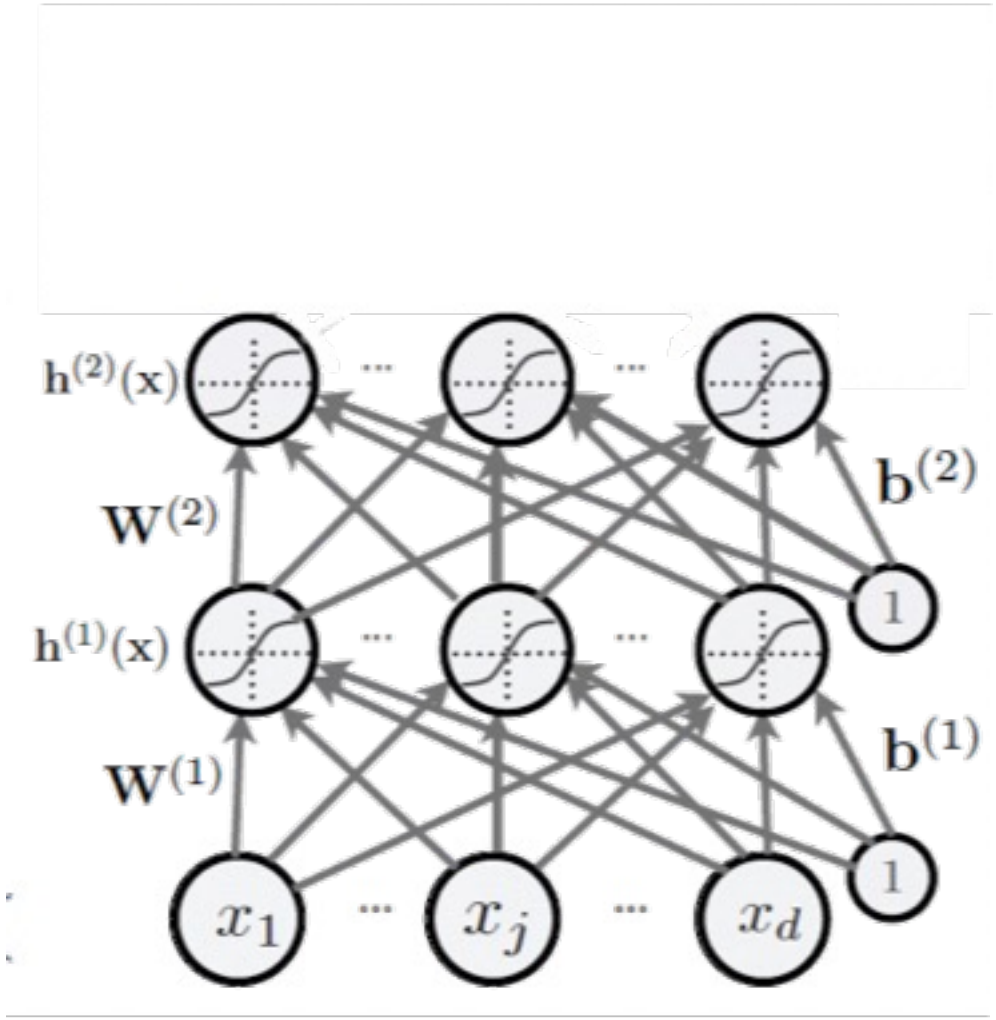
Multilayer Neural Network

- Forward



Multilayer Neural Network

- Forward



Multilayer Neural Network

- Could have *L* hidden layers:
  - Layer pre-activation for k>0:

$$\mathbf{a}^{(k)}(\mathbf{x}) = \mathbf{b}^{(k)} + \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}(\mathbf{x})$$

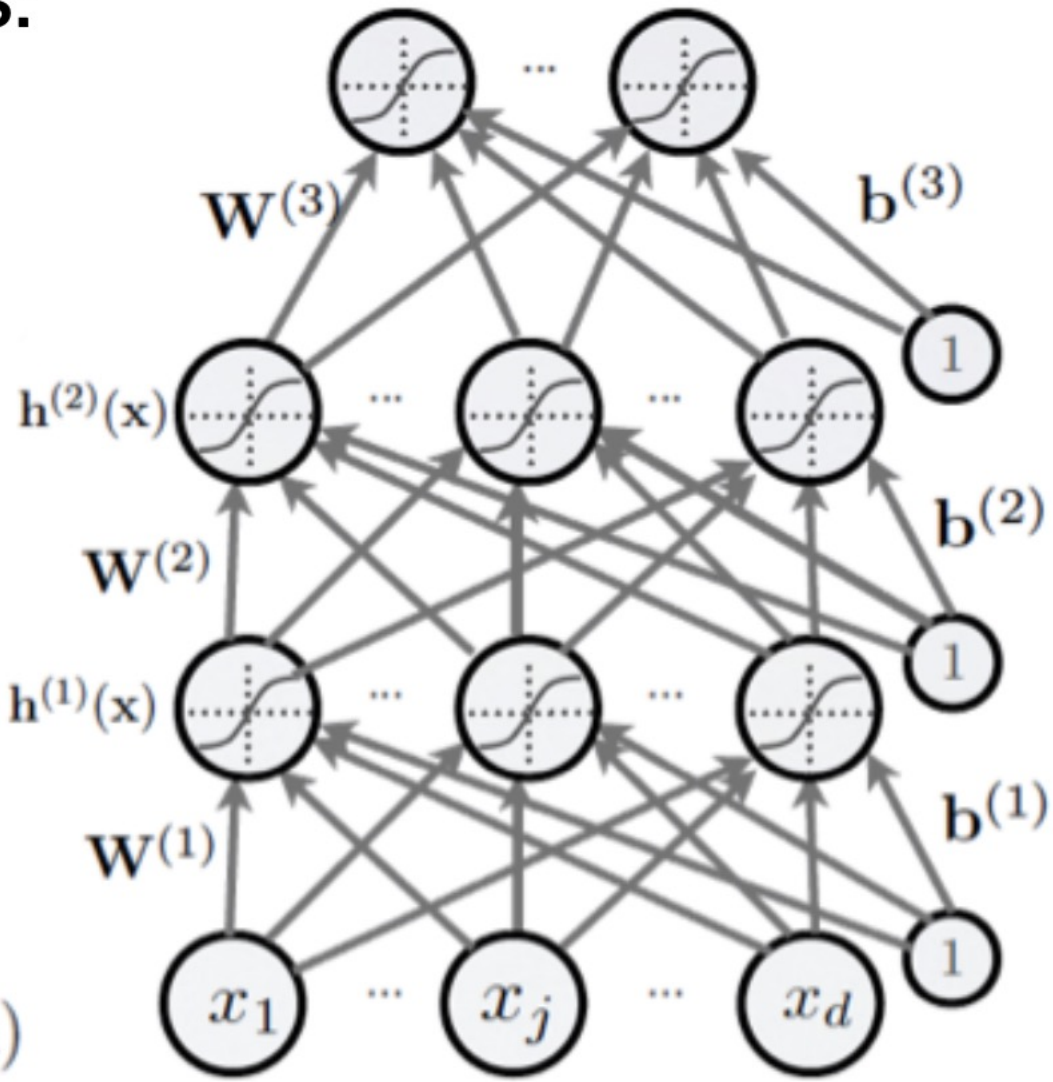
$$(\mathbf{h}^{(0)}(\mathbf{x}) = \mathbf{x})$$

  - Hidden layer activation (*k* from 1 to *L*):

$$\mathbf{h}^{(k)}(\mathbf{x}) = \mathbf{g}(\mathbf{a}^{(k)}(\mathbf{x}))$$

  - Output layer activation (*k*=*L*+1):

$$\mathbf{h}^{(L+1)}(\mathbf{x}) = \mathbf{o}(\mathbf{a}^{(L+1)}(\mathbf{x})) = \mathbf{f}(\mathbf{x})$$



Multilayer Neural Network

- Multilayer neural network models a function $f(x,\{w_i, b_i\})$ by multiple layers of neurons.
- *The goal of using neural network is to model the data by solving the weight parameters, $\{w_i, b_i\}$* , of the neural network through an *optimization process* which is defined via the backpropagation.

Machine Learning?

- In our case, this means:
  - Need to find a way to identify good values for our network's weights
  - Need to do this by relying on training examples (past experiences)
  - Need to do this by employing some sort of performance measure

→ Loss function:
mathematical minimization!

Empirical risk minimization

- Framework to design learning algorithms

$$\arg\min_{\boldsymbol{\theta}} \frac{1}{T} \sum_{t} l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)}) + \lambda \Omega(\boldsymbol{\theta})$$

  - $l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$ = loss function
  - $\Omega(\boldsymbol{\theta})$ = regularizer (penalizes certain values of $\boldsymbol{\theta}$)

- Learning is cast as mathemetical optimization
  - Ideally, we optimize classification errors, but it's not smooth
  - Loss function is a surrogate for what we truly should optimize (e.g. upper bound)

Classification error is non-smooth and non-convex

$$\hat{f}^{\mathrm{erm}} = \operatorname*{argmin}_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}\left(Y_i \neq f\left(X_i\right)\right).$$

The following is an example of convex surrogates of loss functions.

- Hinge loss: $\ell(y) = \max(0, 1 - t \cdot y)$

Recipe for design a Machine Learning system

1. Given training data:

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^{N}$$

2. Choose each of these:

- Decision function

$$\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

- Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

3. Define Goal state:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{N} \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

4. Train with BP in SGD:

(take small steps opposite the gradient)

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

Loss function for classification

- Neural network estimates $f(\mathbf{x})_c = p(y = c|\mathbf{x})$
  - We could maximize the probabilities of $y^{(t)}$ given $\mathbf{x}^{(t)}$ in the training set

- To frame as minimization, we minimize the negative log-likelihood

Natural log (ln)

$$l(\mathbf{f}(\mathbf{x}), y) = -\sum_c 1_{(y=c)} \log f(\mathbf{x})_c = -\log f(\mathbf{x})_y$$

  - We take the log to simplify for numerical stability and math simplicity
  - Sometimes referred to as cross-entropy

Regularization

- L2-regularization $\Omega(\boldsymbol{\theta}) = \sum_k \sum_i \sum_j \left(W_{i,j}^{(k)}\right)^2 = \sum_k ||\mathbf{W}^{(k)}||_F^2$
  - Only applied on weights, not on biases (weight decay)
  - Can be interpreted as having a Gaussian prior on weights
- L1-regularization $\Omega(\boldsymbol{\theta}) = \sum_k \sum_i \sum_j |W_{i,j}^{(k)}|$
  - Again, only applied on weights
  - Unlike L2, L1 will push certain weights to be exactly 0
  - Can be interpreted as having a Laplacian prior on weights

Learning Algorithm

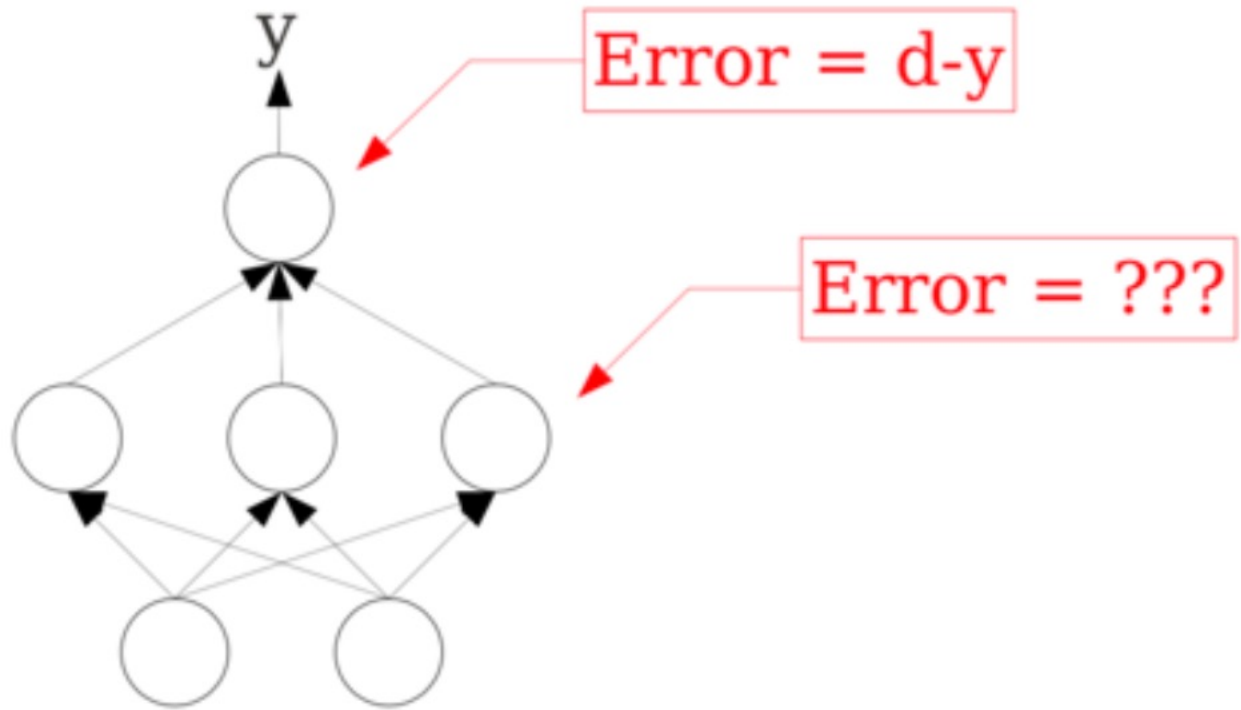
- Algorithm that performs updates after input each data:

θ ($\theta \equiv \{\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \ldots, \mathbf{W}^{(L+1)}, \mathbf{b}^{(L+1)}\}$)

- Initialize $(\mathbf{x}^{(t)}, y^{(t)})$
- For N iterations: $\theta \leftarrow \theta + \alpha \Delta$
  - iterate through each training example

Training epoch
=
Iteration over all examples

How Do We Train A Multi-Layer Network?



$$\arg\min_{\boldsymbol{\theta}} \frac{1}{T} \sum_{t} l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)}) + \lambda \Omega(\boldsymbol{\theta})$$

Review Gradient Descent

Gradient descent

- Based on observation that
  - If multi-variate function $f(\boldsymbol{\theta})$ defined and differentiable in neighborhood of a point $\boldsymbol{\theta}_0$
  - Then $f(\boldsymbol{\theta})$ decreases fastest if one goes from $\boldsymbol{\theta}_0$ in the direction of the negative gradient of $f(\boldsymbol{\theta})$ at $\boldsymbol{\theta}_0$
  - The gradient of $f(\boldsymbol{\theta})$ in $\boldsymbol{\theta}_0$ is denoted $\nabla f(\boldsymbol{\theta}_0)$
  - It follows that, for small enough γ

$$\boldsymbol{\theta}_1 = \boldsymbol{\theta}_0 - \gamma \cdot \nabla f(\boldsymbol{\theta}_0)$$

we have $f(\boldsymbol{\theta}_1) < f(\boldsymbol{\theta}_0)$

  - If executing $\boldsymbol{\theta}_{n+1} = \boldsymbol{\theta}_n - \gamma \cdot \nabla f(\boldsymbol{\theta}_n)$

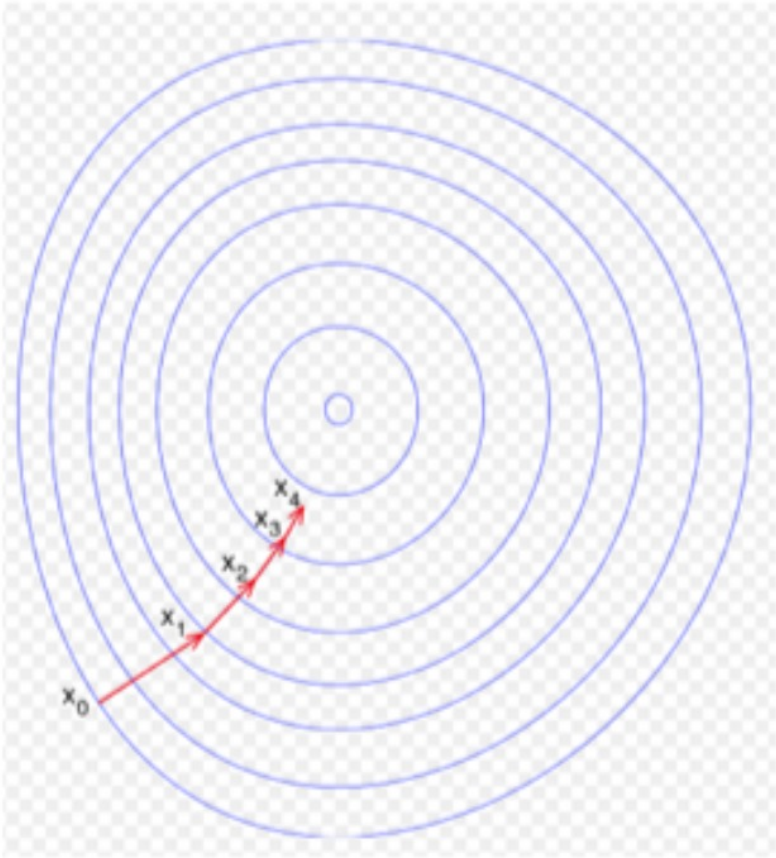
we obtain $f(\boldsymbol{\theta}_n) < f(\boldsymbol{\theta}_{n-1}) < \cdots f(\boldsymbol{\theta}_2) < f(\boldsymbol{\theta}_1) < f(\boldsymbol{\theta}_0)$

Note: here the notation *f* (.) is a general objective function to be minimised.

Gradient descent

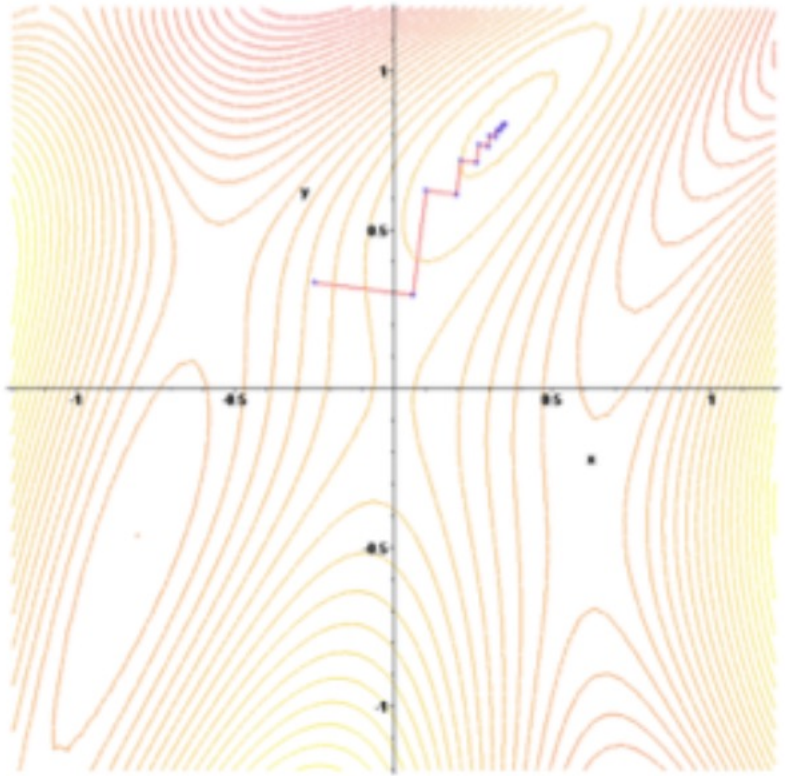
- With properly chosen γ in each iteration
  - Convergence to local minimum!
  - γ can be adapted between iterations

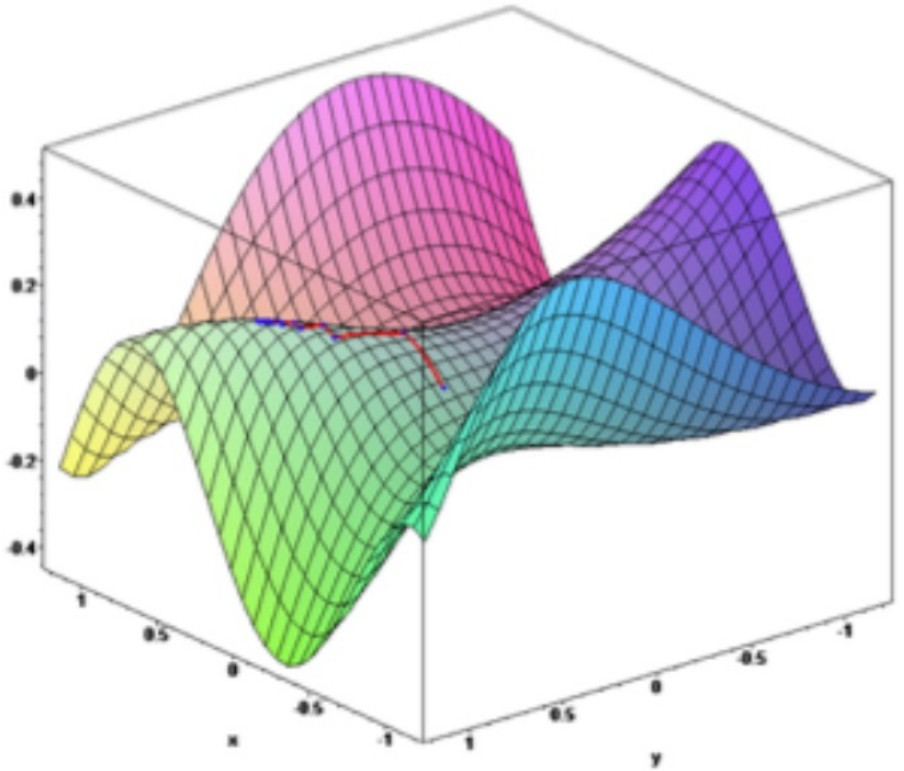
    or
  - We can iterate over γ inside individual iterations
    - Example: line-search



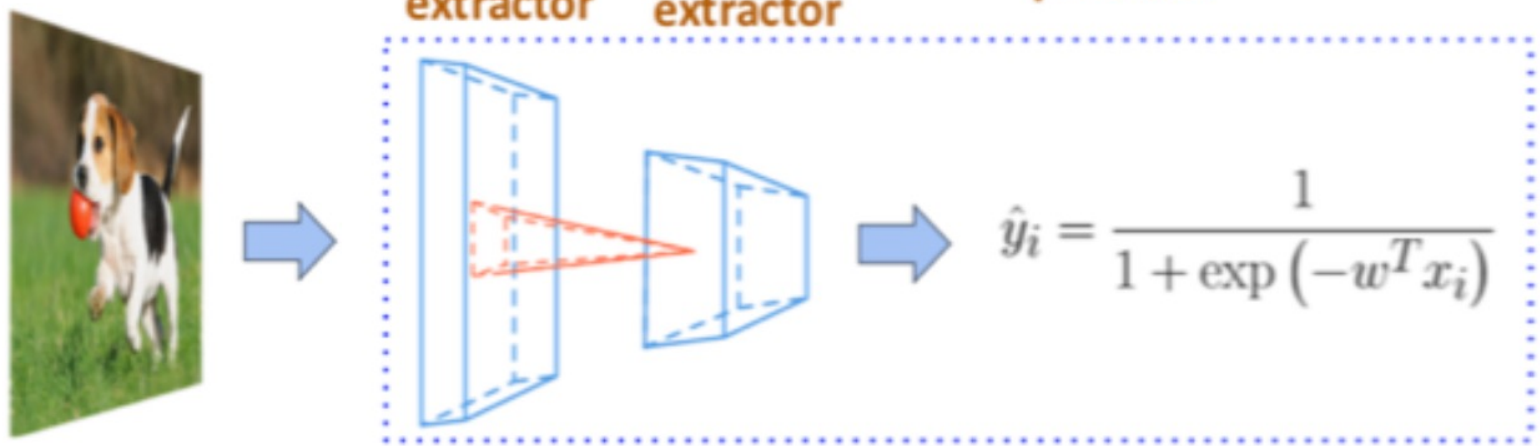
Gradient descent

- Works in arbitrary dimensions





Model Training Overview



Objective

$$L(w) = \sum_{i=1}^{n} l(y_i, \hat{y}_i) + \lambda \|w\|^2$$

Training

$$w \leftarrow w - \eta \nabla_w L(w)$$

Learning Algorithm

- Initialize $\boldsymbol{\theta}$ ($\boldsymbol{\theta} \equiv \{\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \ldots, \mathbf{W}^{(L+1)}, \mathbf{b}^{(L+1)}\}$)
- For N iterations:
  - For each training example $(\mathbf{x}^{(t)}, y^{(t)})$
  - $\Delta = -\nabla_{\boldsymbol{\theta}} l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)}) - \lambda \nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$
  - $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha \Delta$

Training epoch = Iteration over all examples

- To apply this algorithm to neural network training, we need
  - The loss function $l(\mathbf{f}(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$
  - Procedure to compute parameter gradients $\nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$
  - The regularizer $\Omega(\boldsymbol{\theta})$ (and the gradient $\nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$)
  - Initialization method

Back-propagation learning

Training deep neural networks

- Outlook:
  - Computing gradients is hard (many parameters)
    → Back-propagation!

- Network represents a chain of function calls (one per layer):

$$\boldsymbol{f}(\mathbf{x}) = \boldsymbol{f}_{L+1} \circ \boldsymbol{f}_L \circ \cdots \circ \boldsymbol{f}_1(\mathbf{x})$$

$$= \boldsymbol{f}_{L+1}(\boldsymbol{f}_L(\ldots \boldsymbol{f}_1(\mathbf{x})))$$

- Gradients: Chain rule can be applied!

$$\frac{\partial \boldsymbol{f}(\mathbf{x})}{\partial \boldsymbol{\theta}} = \frac{\partial \boldsymbol{f}_{L+1}}{\partial \boldsymbol{f}_L} \cdot \frac{\partial \boldsymbol{f}_L}{\partial \boldsymbol{f}_{L-1}} \cdot \ldots \cdot \frac{\partial \boldsymbol{f}_1}{\partial \boldsymbol{\theta}}$$

How to compute gradient?

Symbolic Differentiation

- Input formulae is a symbolic expression tree (computation graph).
- Implement differentiation rules, e.g., sum rule, product rule, chain rule

$$\frac{d(f+g)}{dx} = \frac{df}{dx} + \frac{dg}{dx} \qquad \frac{d(fg)}{dx} = \frac{df}{dx}g + f\frac{dg}{dx} \qquad \frac{d(h(x))}{dx} = \frac{df(g(x))}{dx} \cdot \frac{dg(x)}{x}$$

✗ For complicated functions, the resultant expression can be exponentially large.

✗ Wasteful to keep around intermediate symbolic expressions if we only need a numeric value of the gradient in the end

✗ Prone to error

How to compute gradient?

Numerical Differentiation

- We can approximate the gradient using

$$\frac{\partial f(\boldsymbol{x})}{\partial x_i} \approx \lim_{h \to 0} \frac{f(\boldsymbol{x} + h\boldsymbol{e_i}) - f(\boldsymbol{x})}{h}$$

$$f(W, x) = W \cdot x$$

$$[-0.8 \quad 0.3] \cdot \begin{bmatrix} 0.5 \\ -0.2 \end{bmatrix}$$

How to compute gradient?

Numerical Differentiation

- We can approximate the gradient using

$$\frac{\partial f(\boldsymbol{x})}{\partial x_i} \approx \lim_{h \to 0} \frac{f(\boldsymbol{x} + h\boldsymbol{e_i}) - f(\boldsymbol{x})}{h}$$

$$f(W, x) = W \cdot x \qquad f(W, x) = W \cdot x$$

$$[-0.8 \quad 0.3] \cdot \begin{bmatrix} 0.5 \\ -0.2 \end{bmatrix} \qquad [-0.8 + \varepsilon \quad 0.3] \cdot \begin{bmatrix} 0.5 \\ -0.2 \end{bmatrix}$$

How to compute gradient?

Numerical Differentiation

- We can approximate the gradient using

$$\frac{\partial f(\boldsymbol{x})}{\partial x_i} \approx \lim_{h \to 0} \frac{f(\boldsymbol{x} + h\boldsymbol{e_i}) - f(\boldsymbol{x})}{h}$$

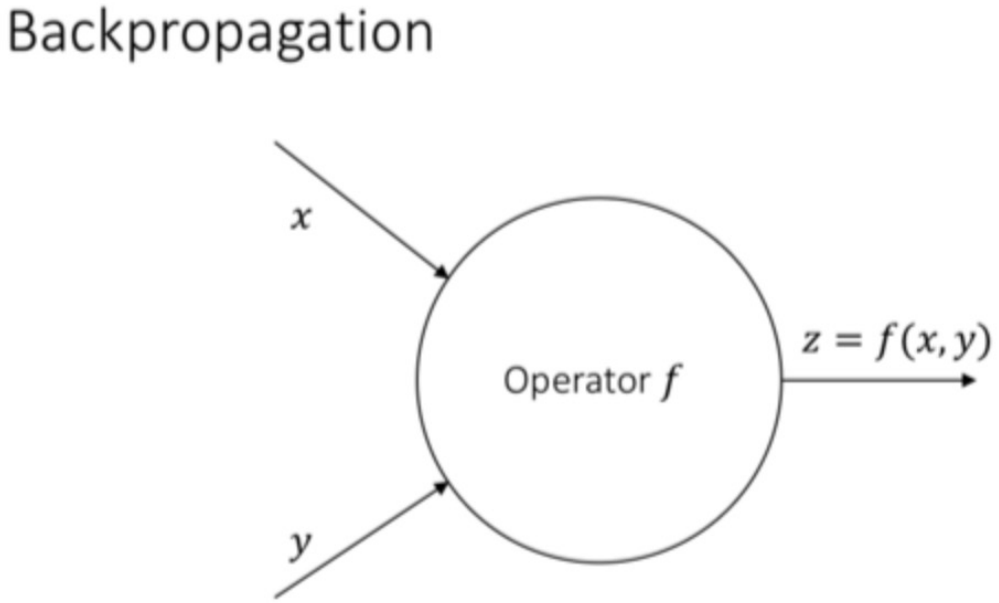
- Reduce the truncation error by using center difference

$$\frac{\partial f(\boldsymbol{x})}{\partial x_i} \approx \lim_{h \to 0} \frac{f(\boldsymbol{x} + h\boldsymbol{e_i}) - f(\boldsymbol{x} - h\boldsymbol{e_i})}{2h}$$

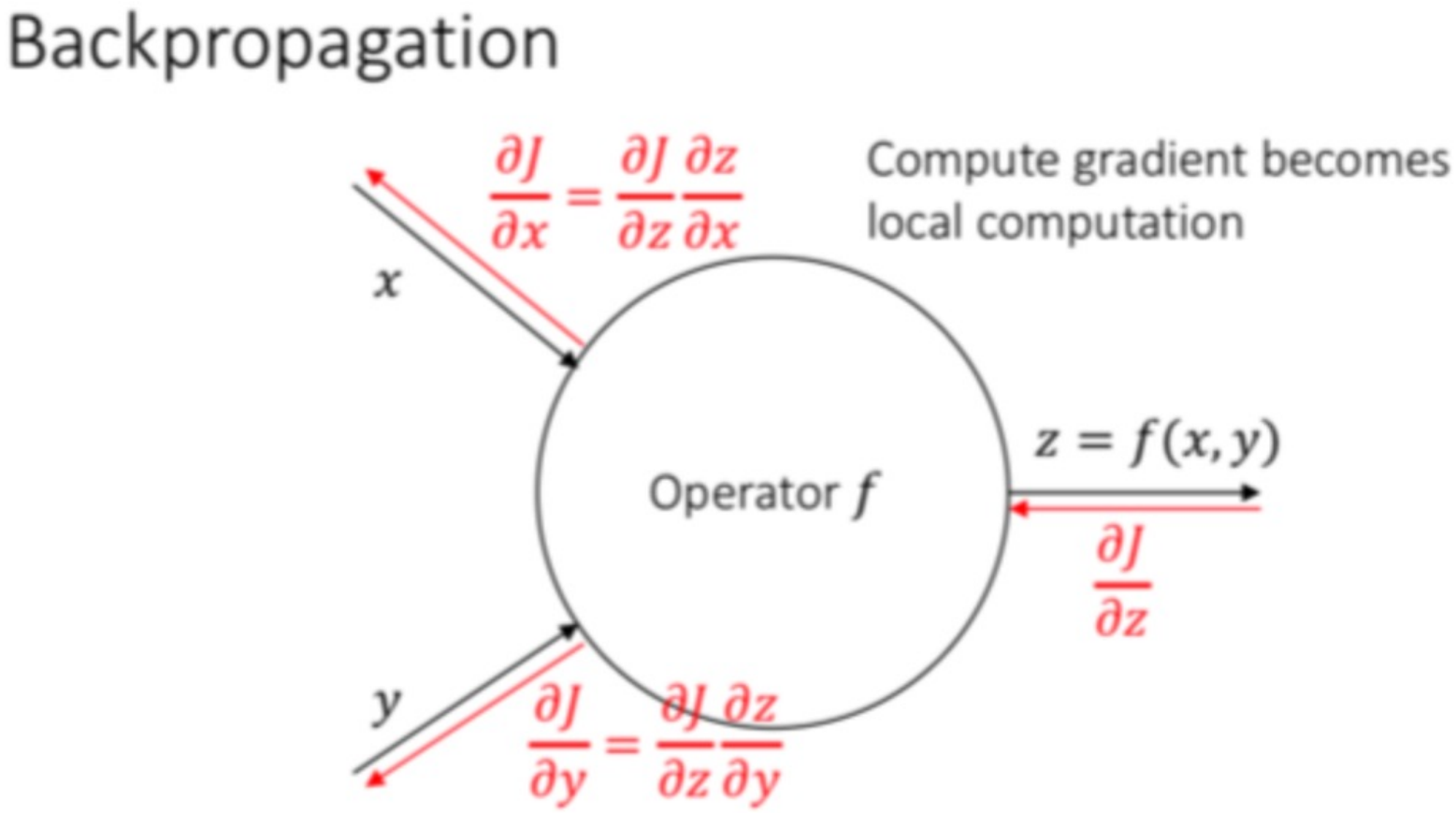
✗ Bad: rounding error, and slow to compute

✓ A powerful tool to check the correctness of implementation, usually use h = 1e-6.

Back Propagation for computing differentiation



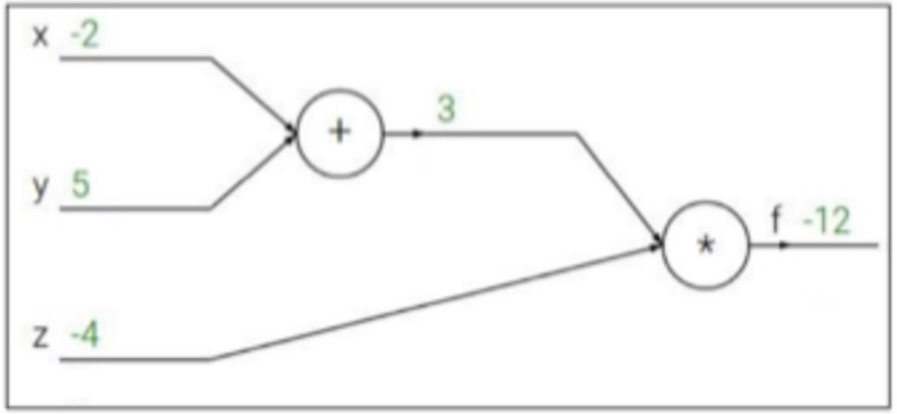
Back Propagation for computing differentiation



Example: Back-Prop

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

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



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

- slide source: Stanford CS231n lecture note.

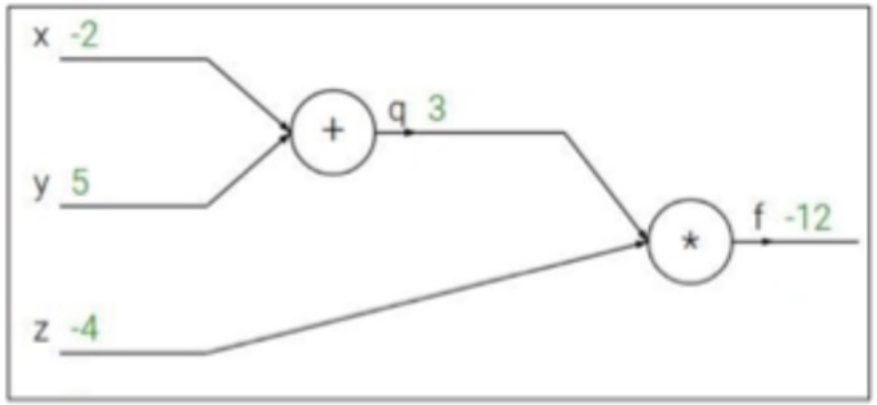
Example: Back-Prop

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

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

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

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



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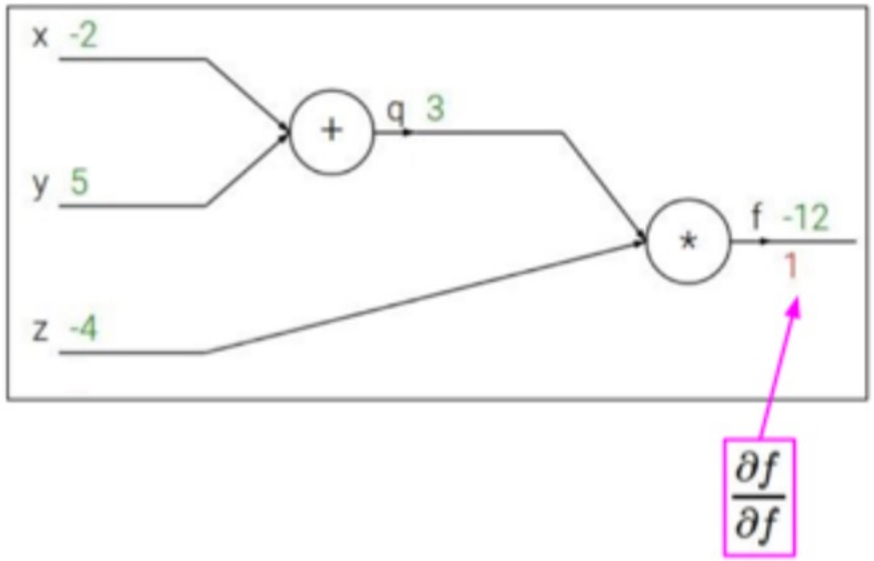

Example: Back-Prop

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

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

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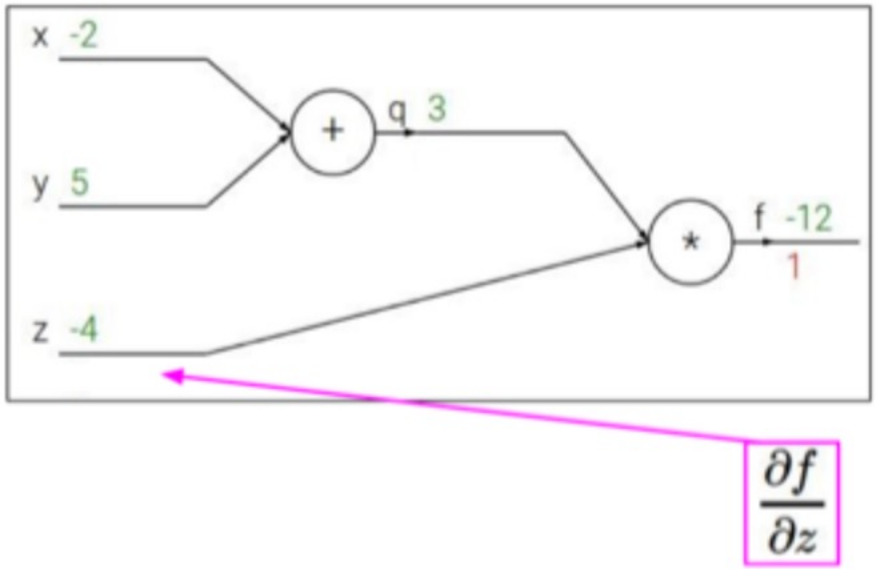

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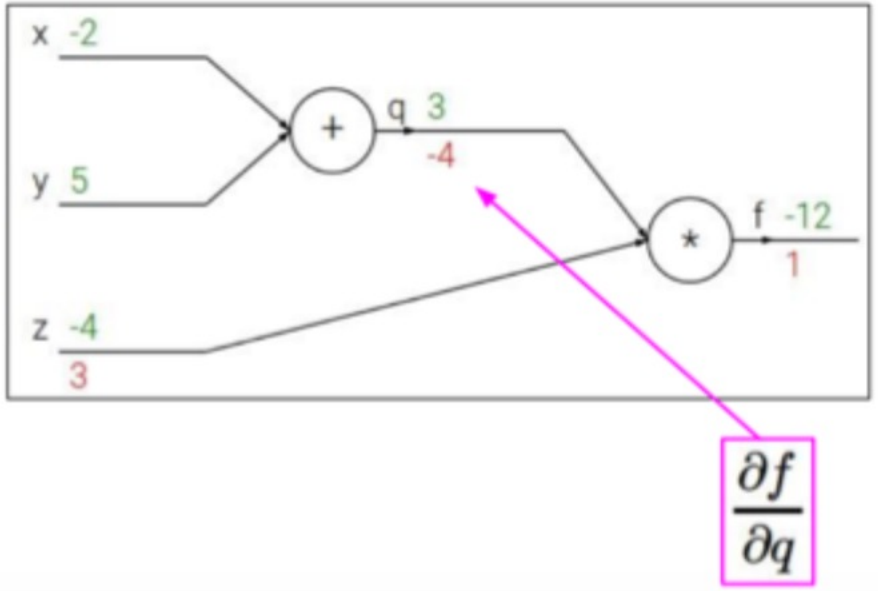

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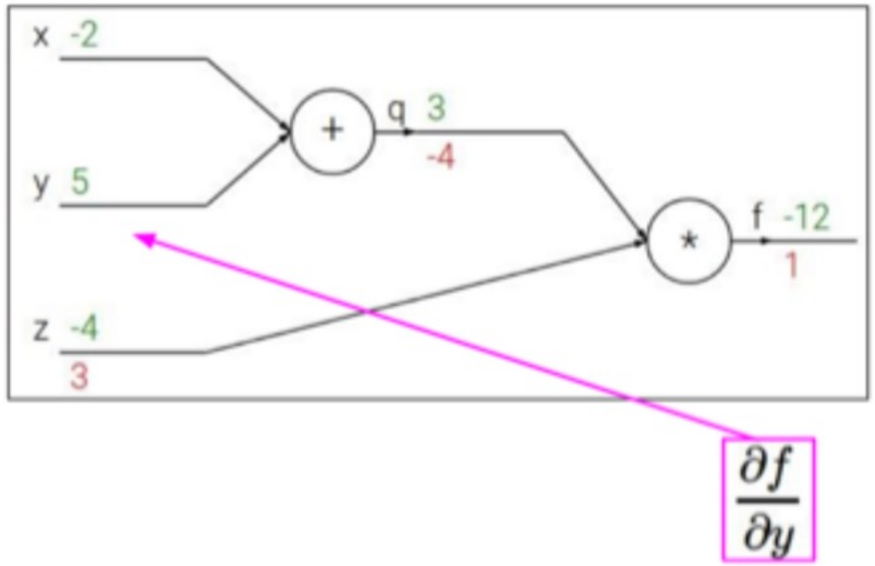

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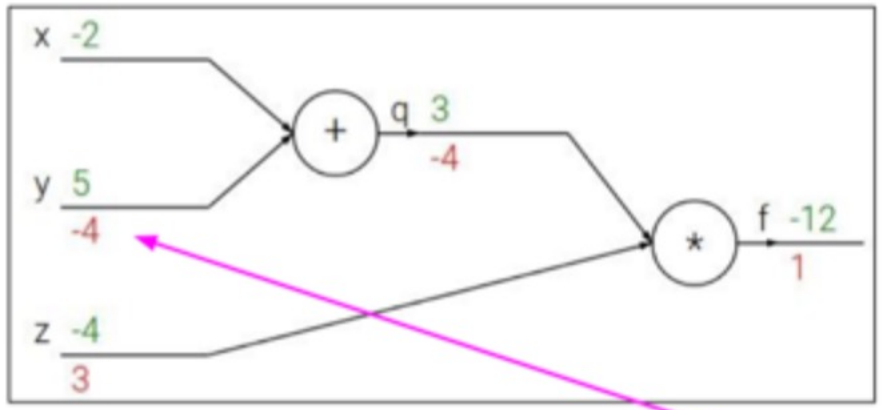

$\frac{\partial f}{\partial y}$

Chain rule:

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

Upstream Gradient

Local Gradient

Example: Back-Prop

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

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

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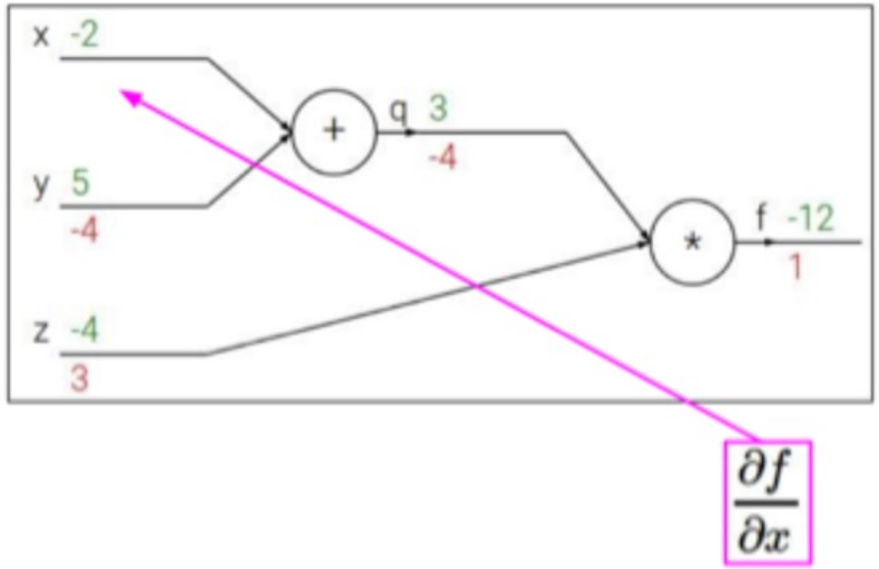
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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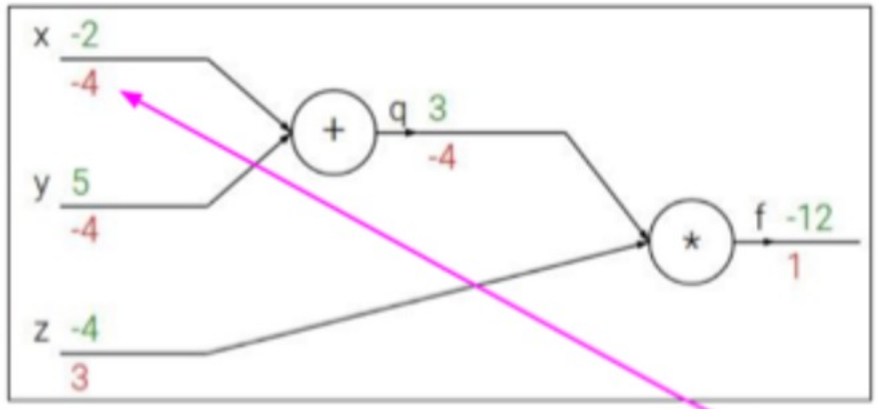

$\frac{\partial f}{\partial x}$

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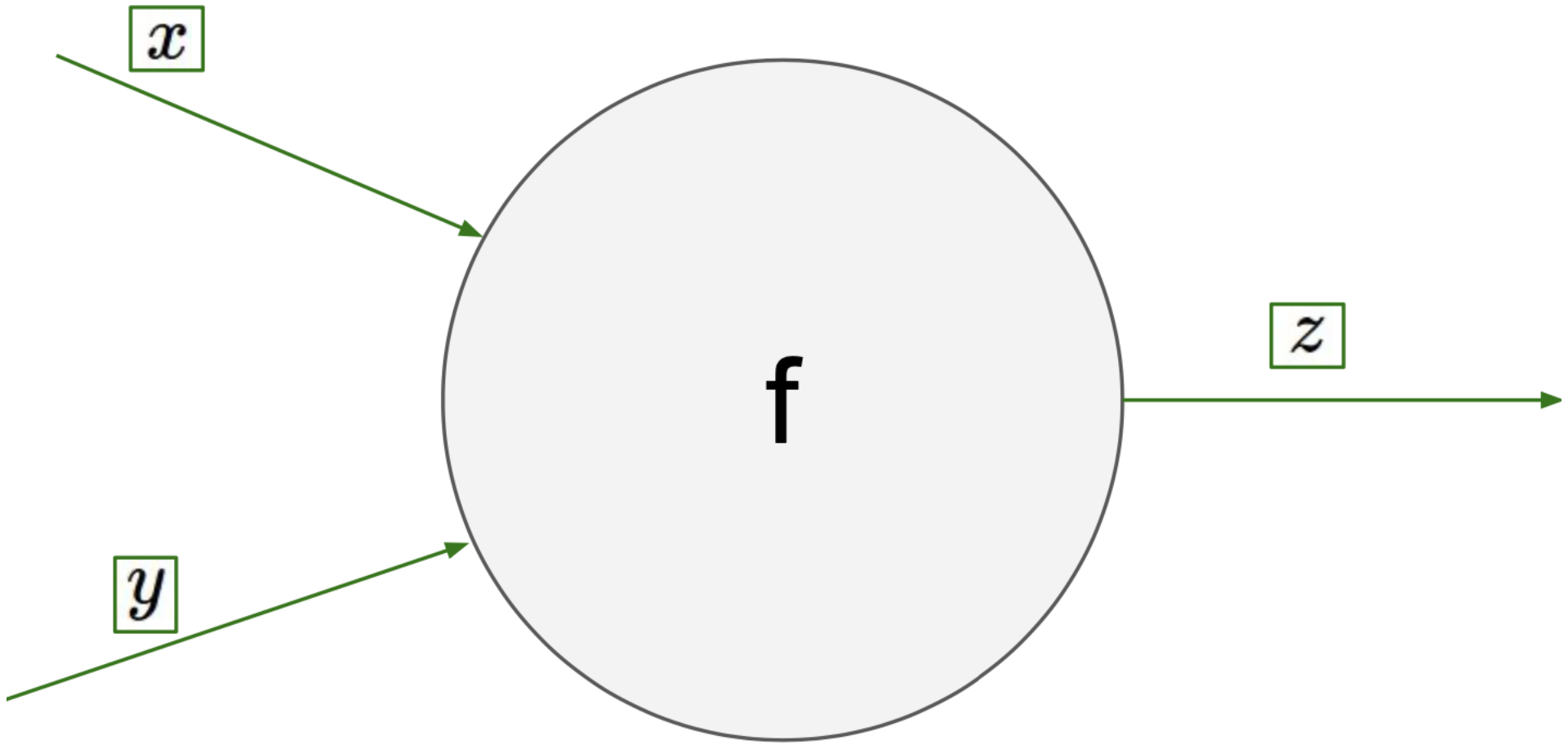
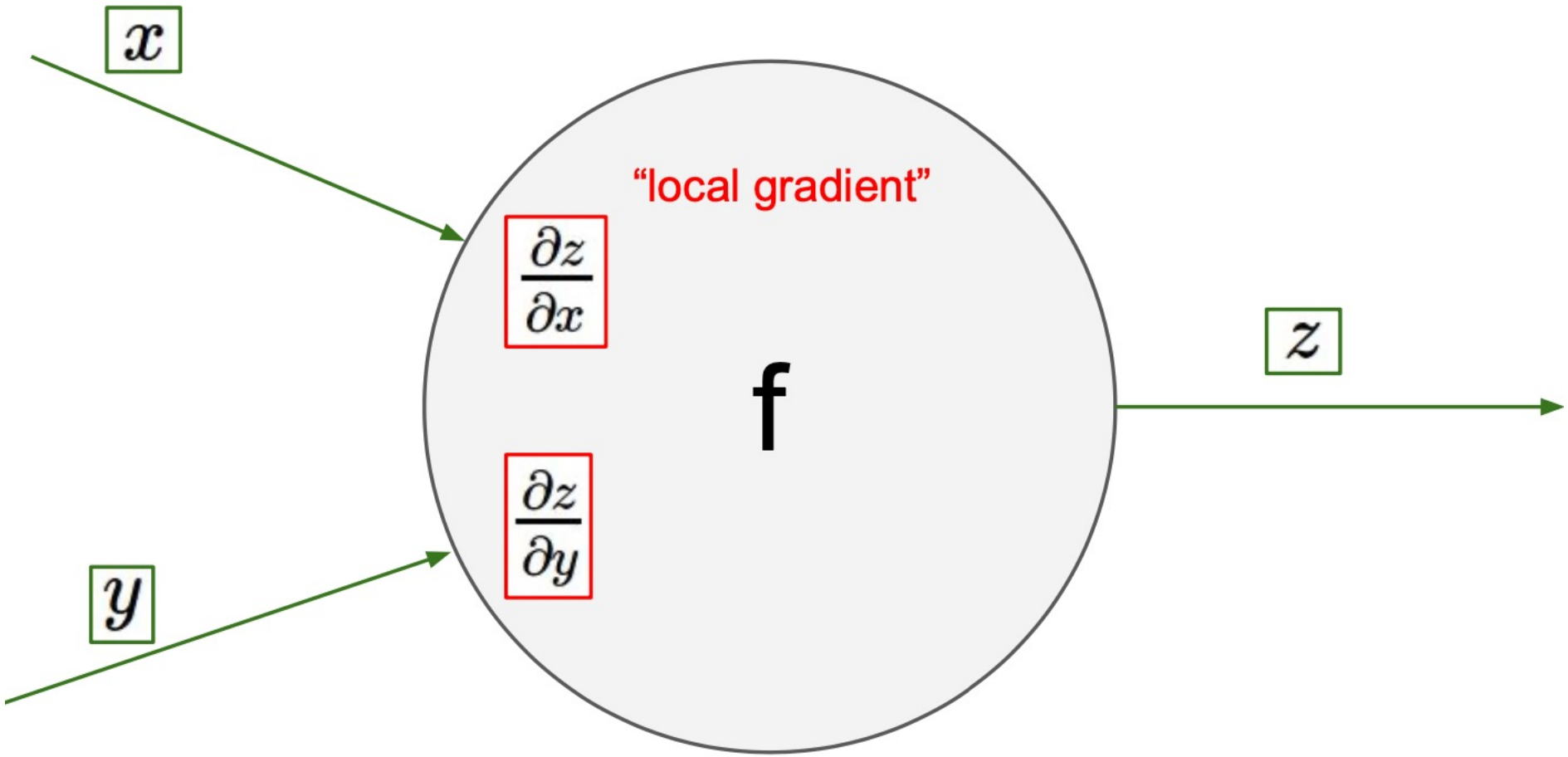
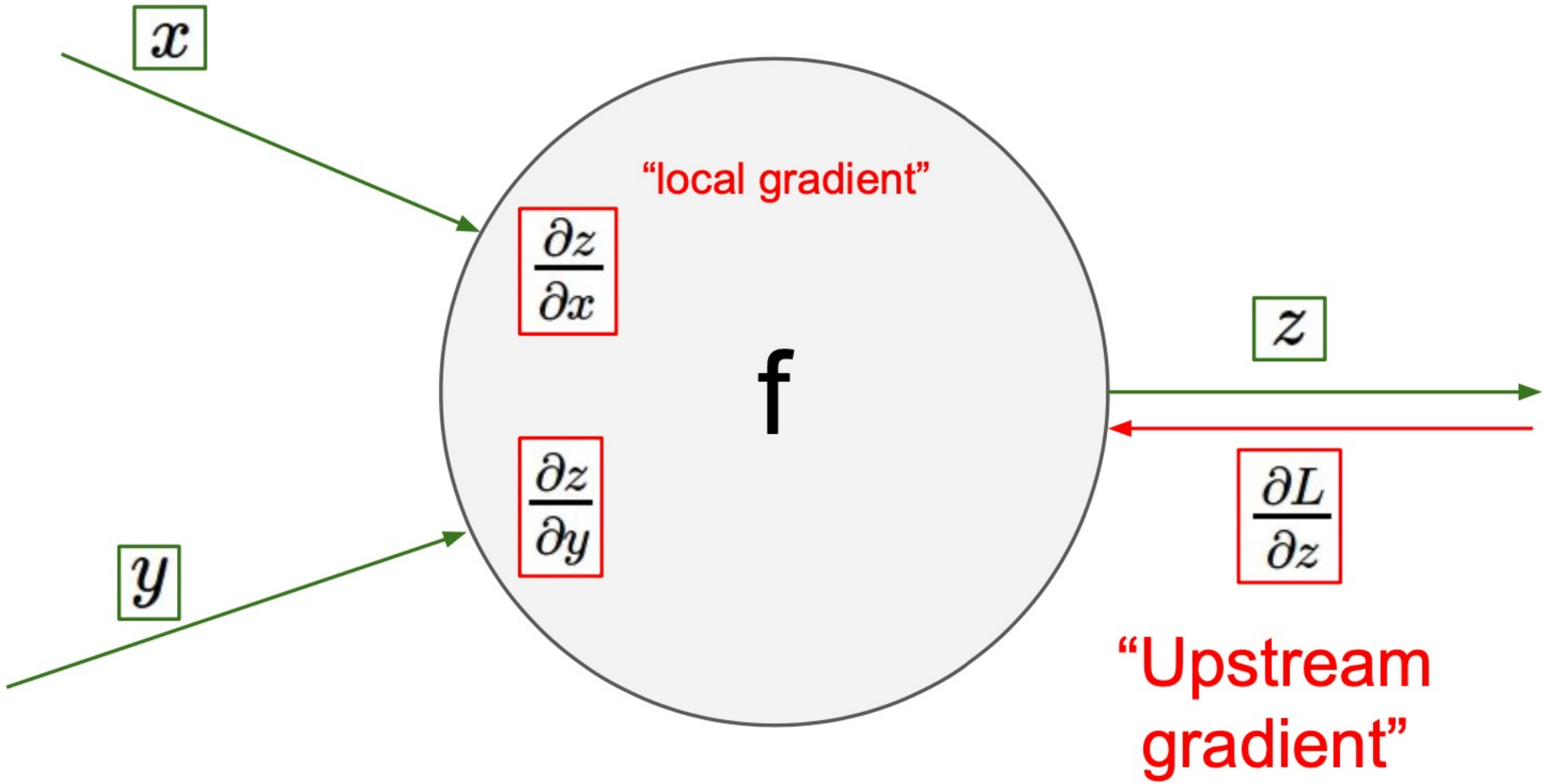
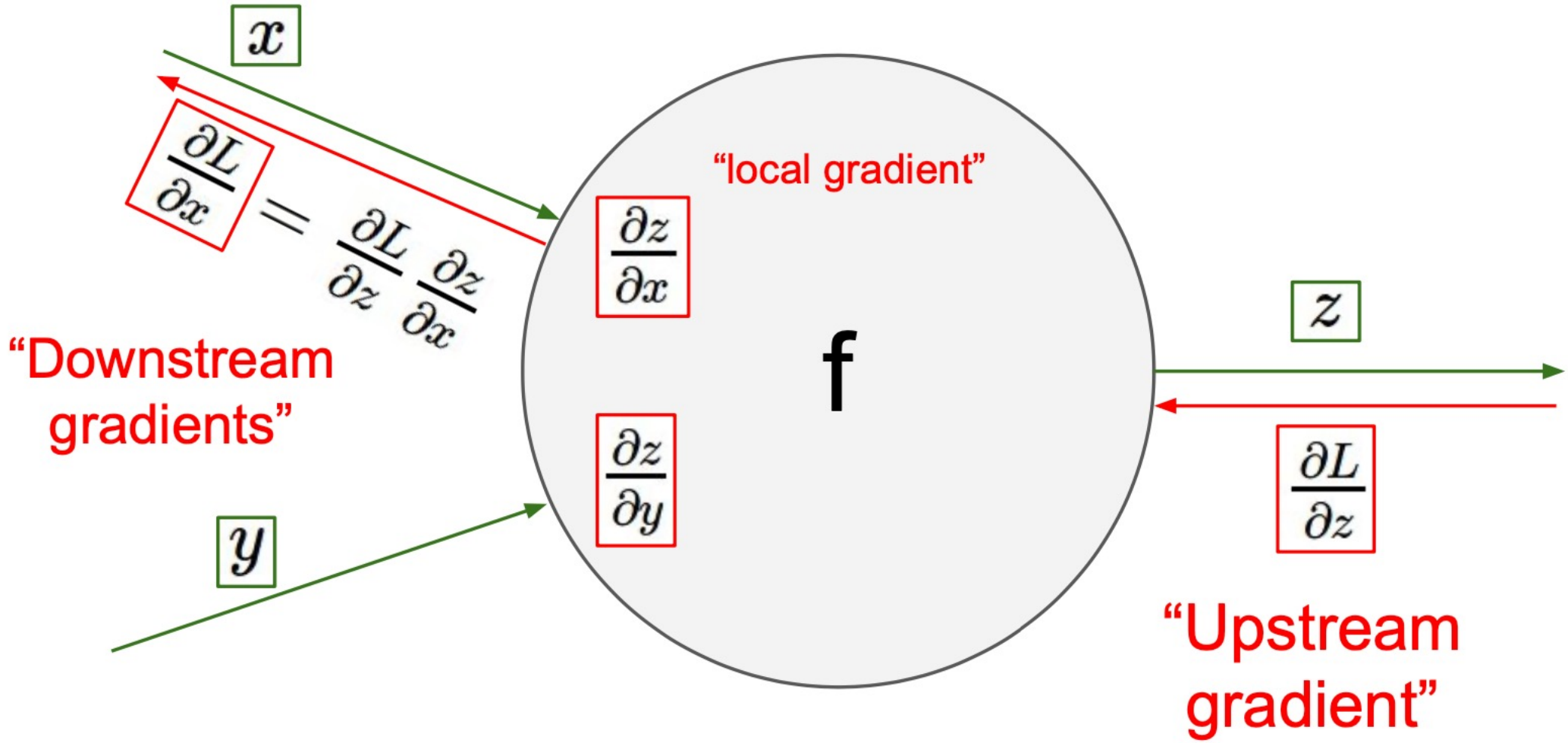
Upstream Gradient

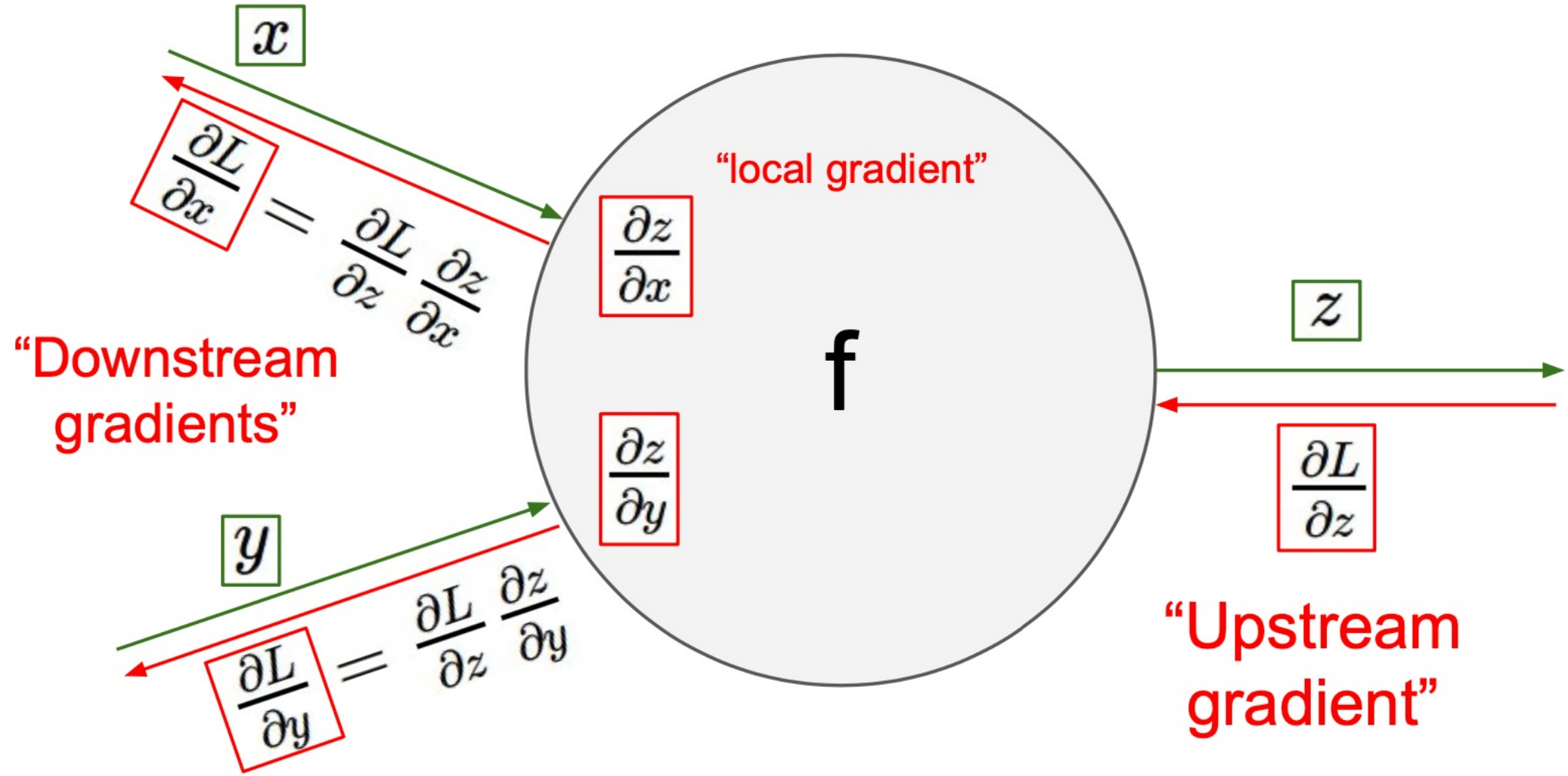
Local Gradient

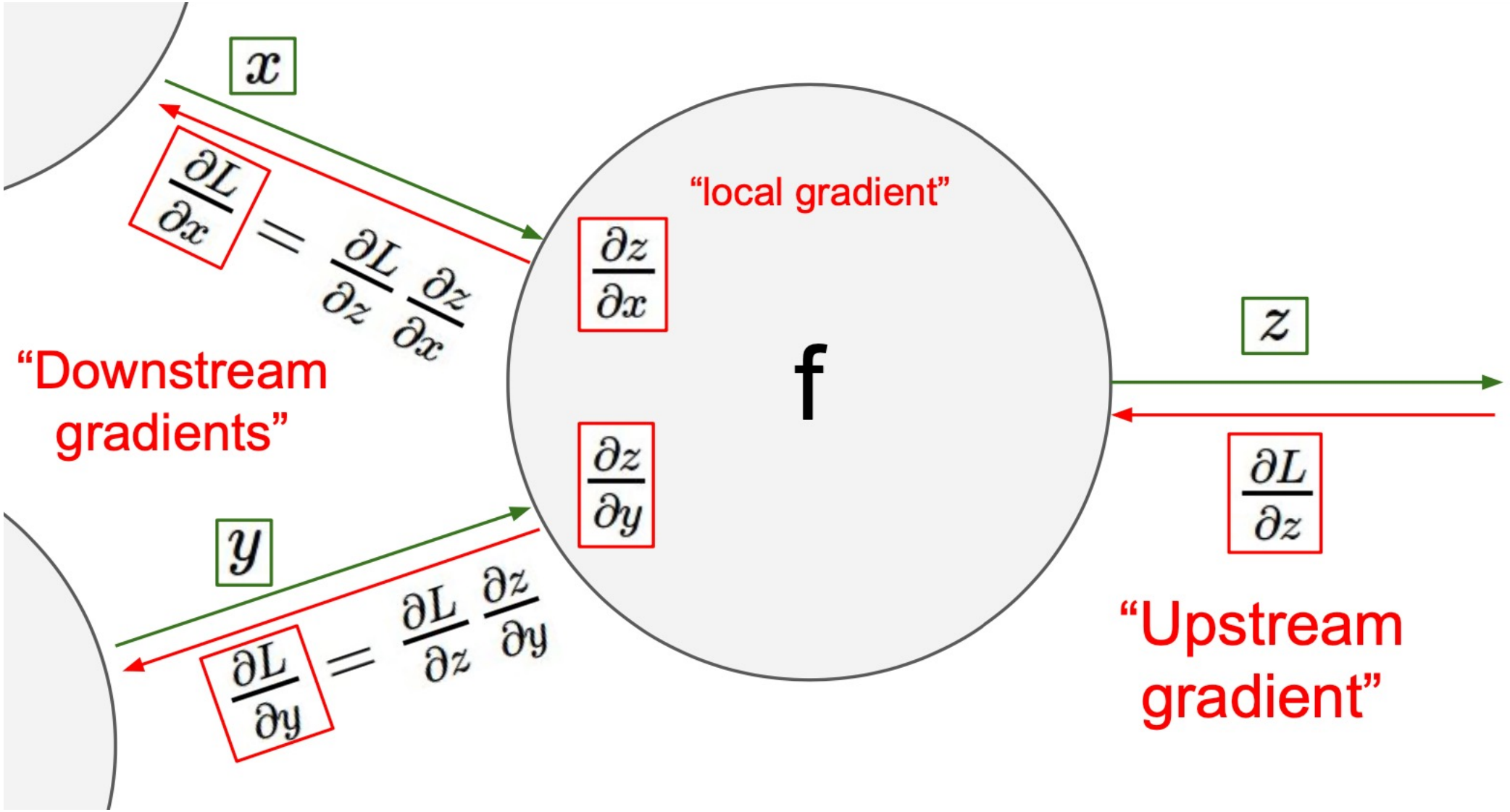

x
y
f
z


x
"local gradient"
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial z}{\partial y}$
y


x
"local gradient"
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial z}{\partial y}$
$\frac{\partial L}{\partial z}$
y
"Upstream gradient"


x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"Downstream gradients"
y
"local gradient"
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
z
$\frac{\partial L}{\partial z}$
"Upstream gradient"


x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"Downstream gradients"
y
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
"local gradient"
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
z
$\frac{\partial L}{\partial z}$
"Upstream gradient"


x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"Downstream gradients"
y
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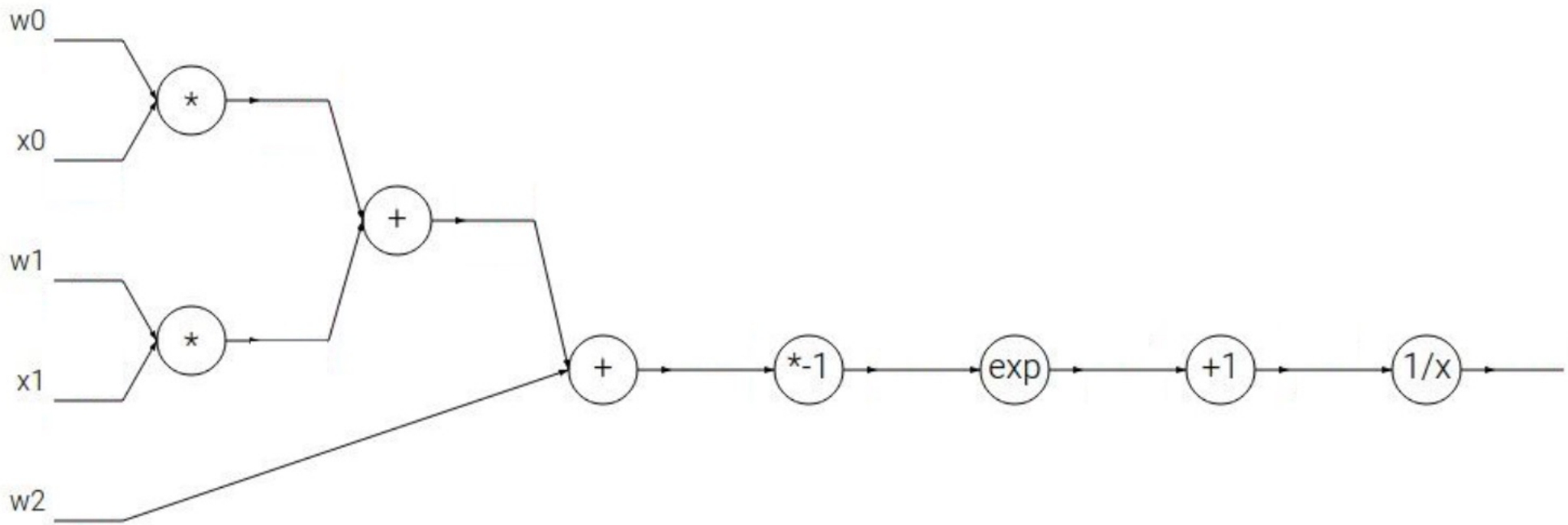
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
z
$\frac{\partial L}{\partial z}$
"Upstream gradient"

Another example: $$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



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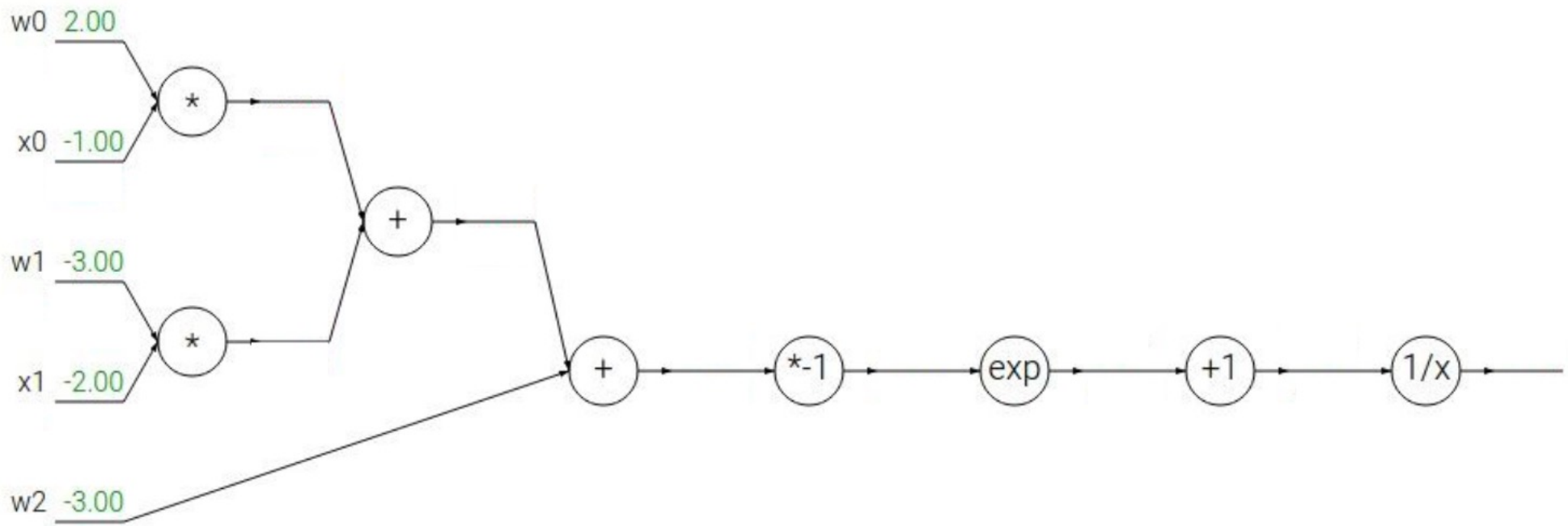

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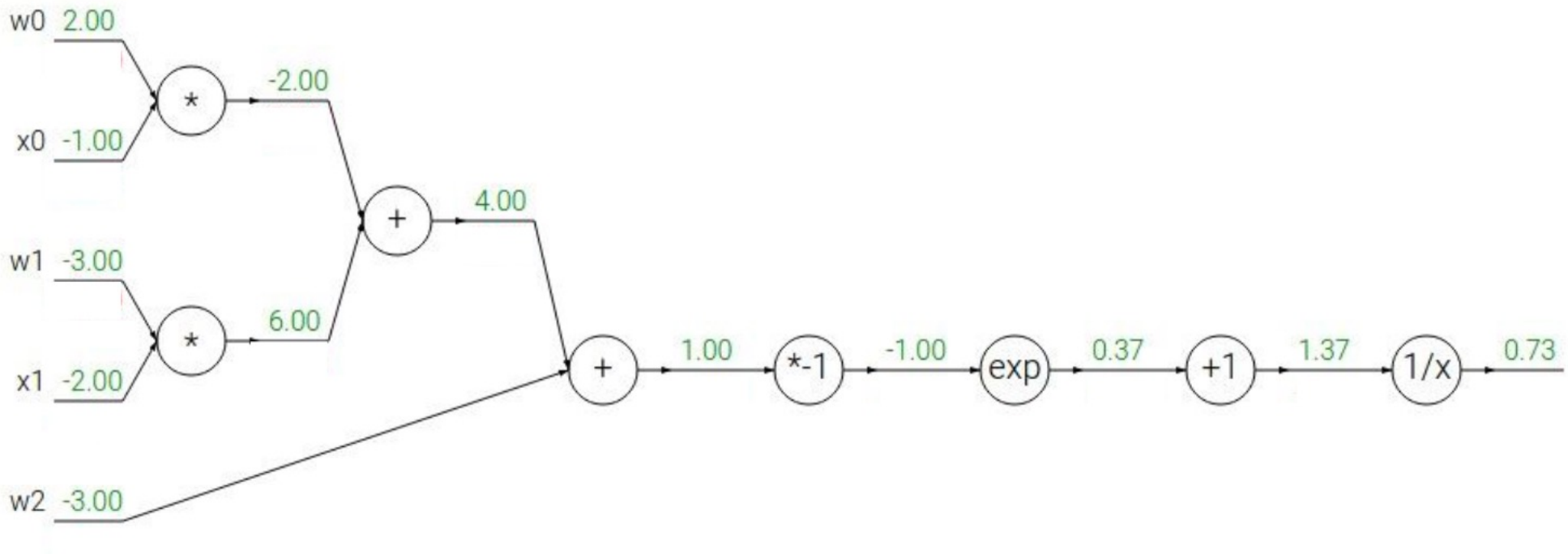

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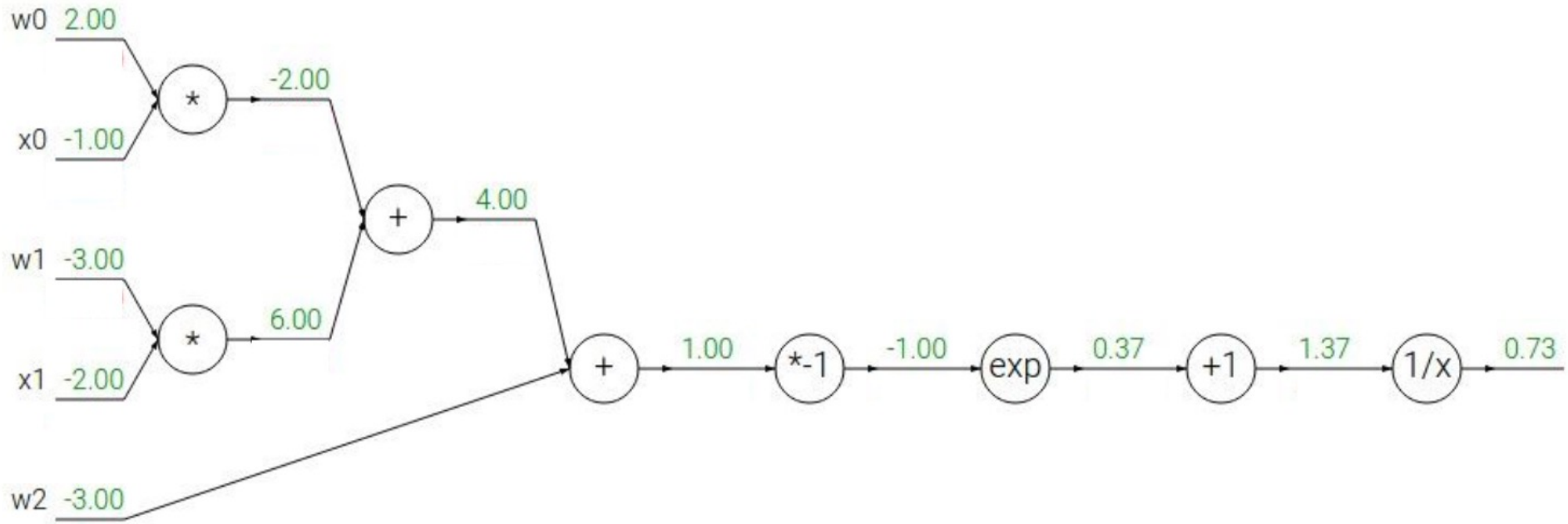

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

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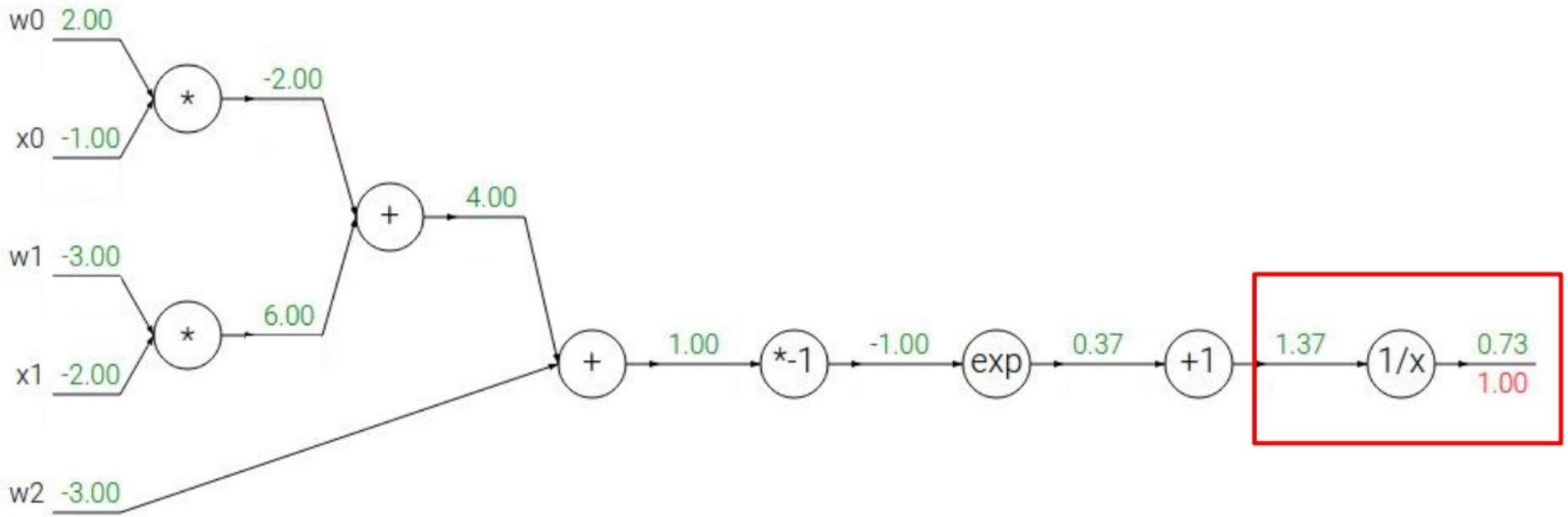

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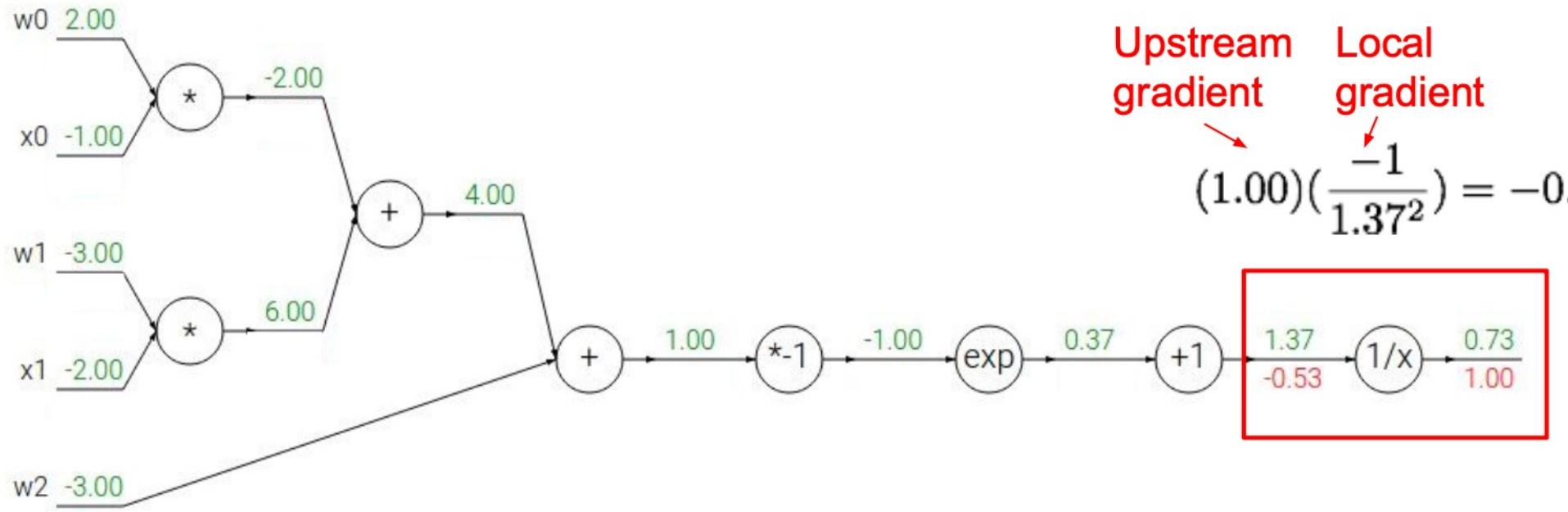

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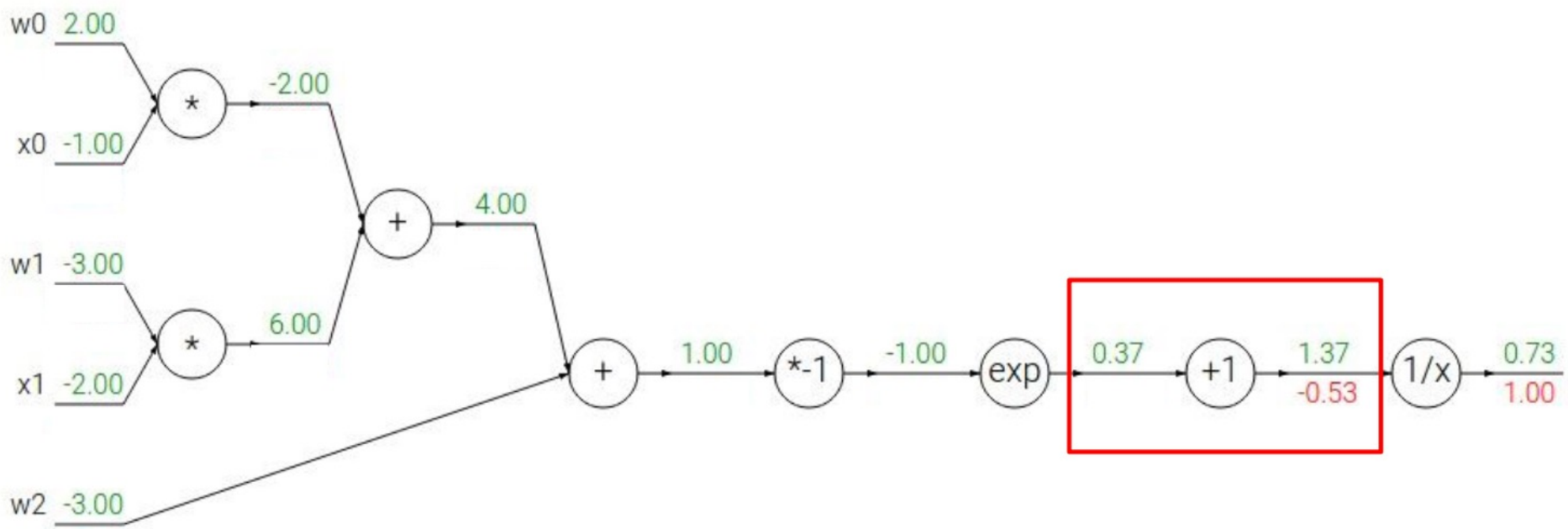

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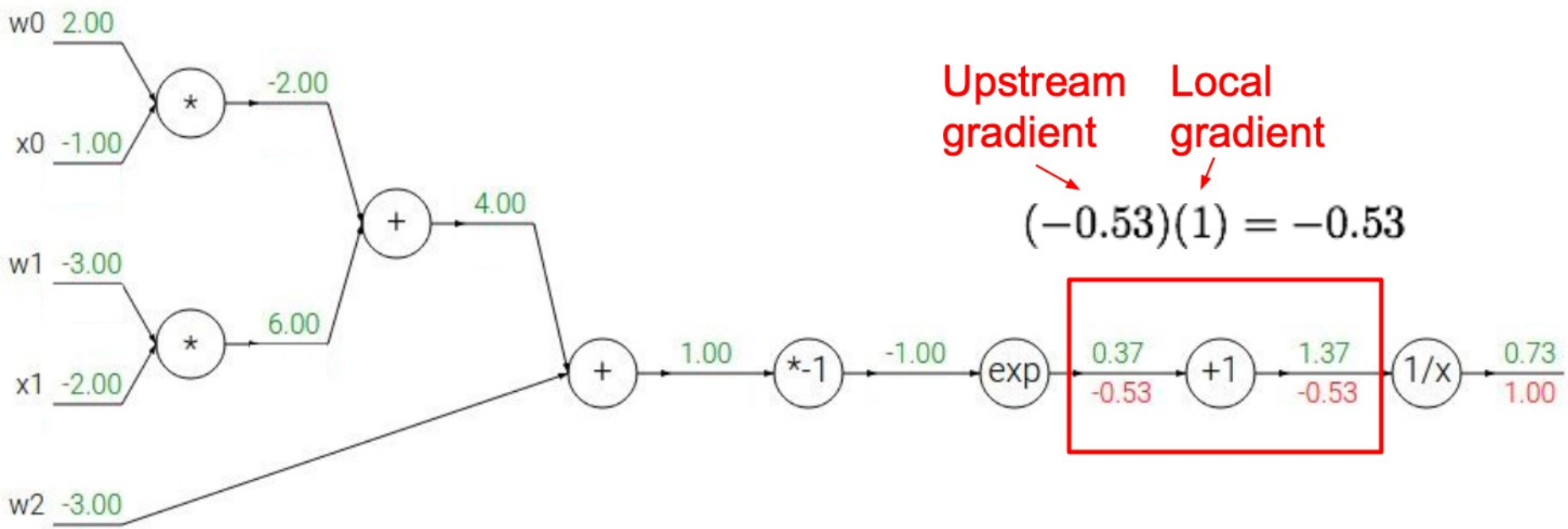

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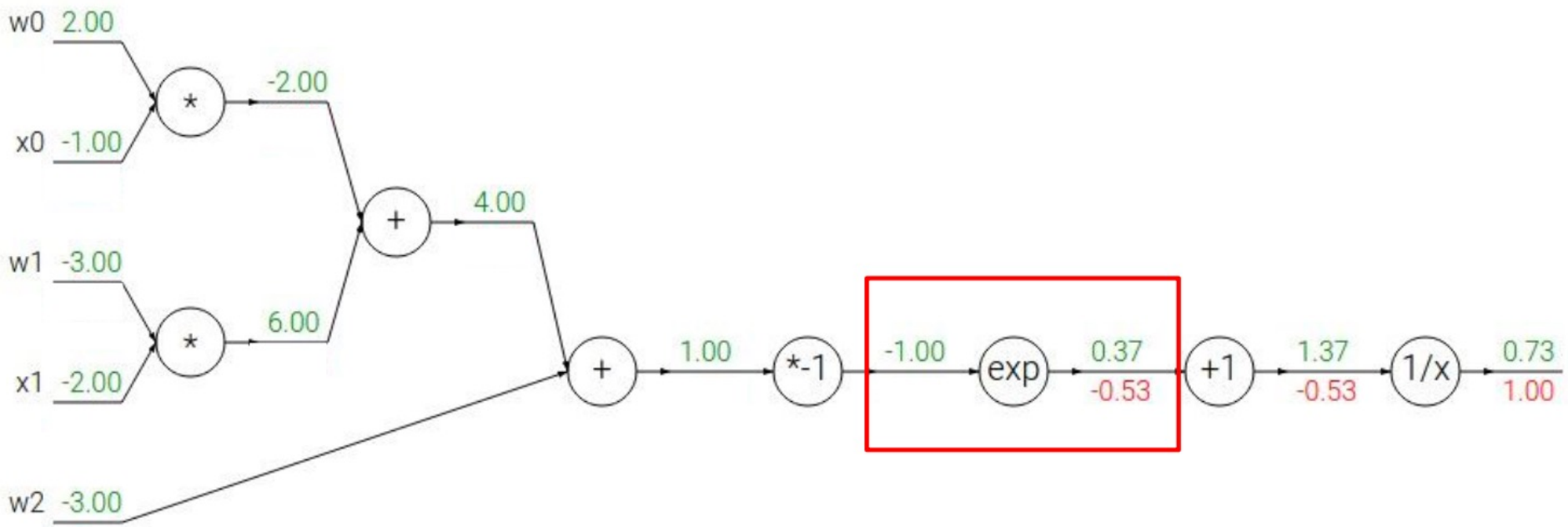

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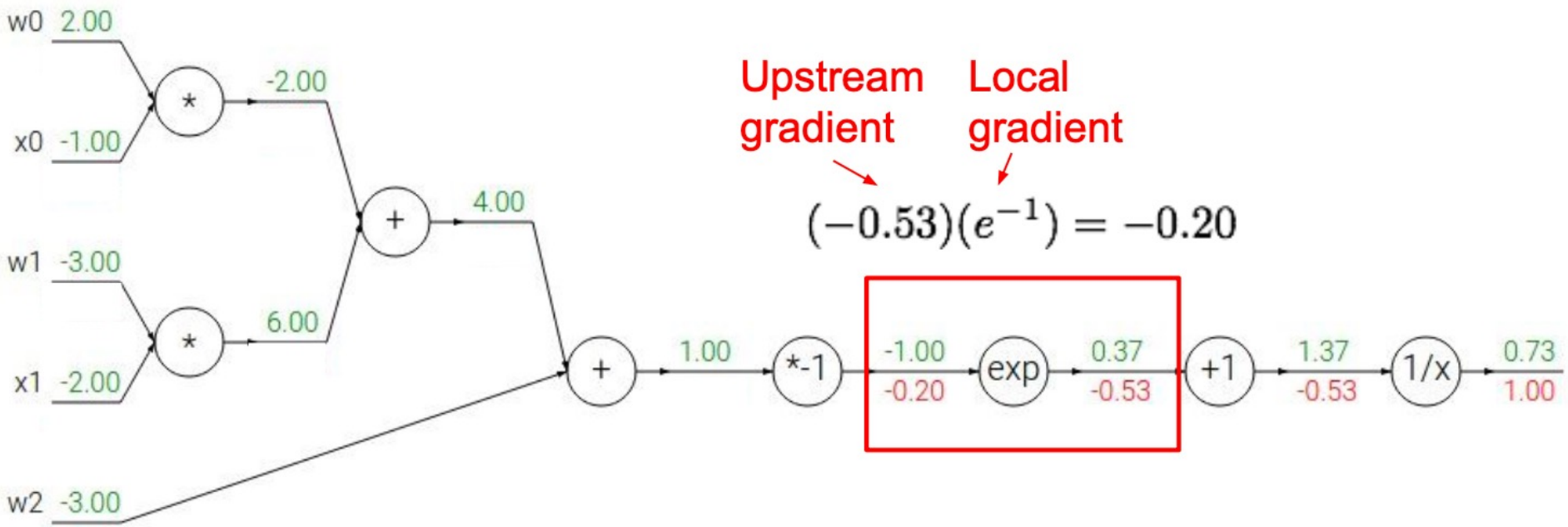

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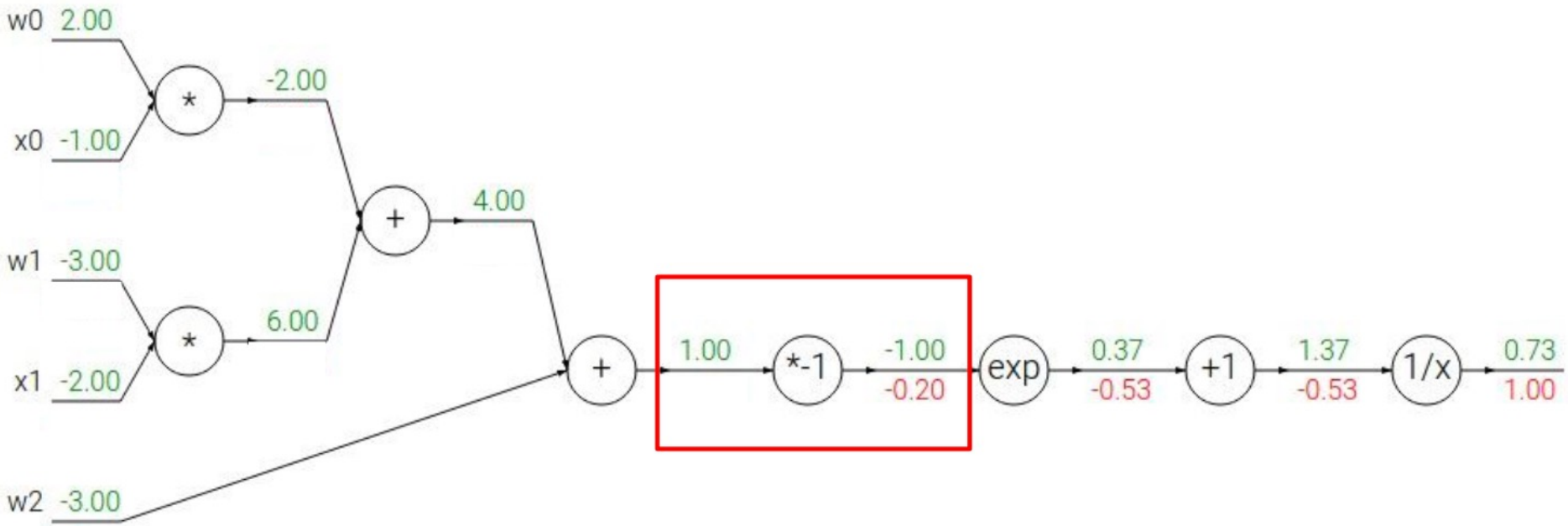

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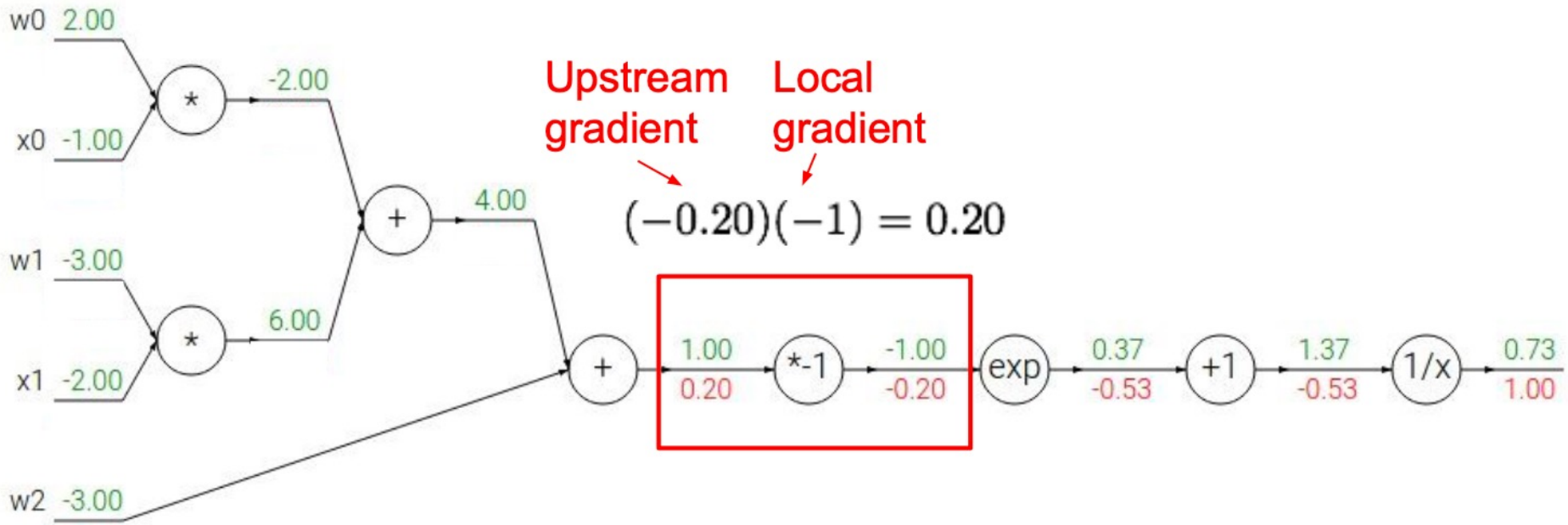

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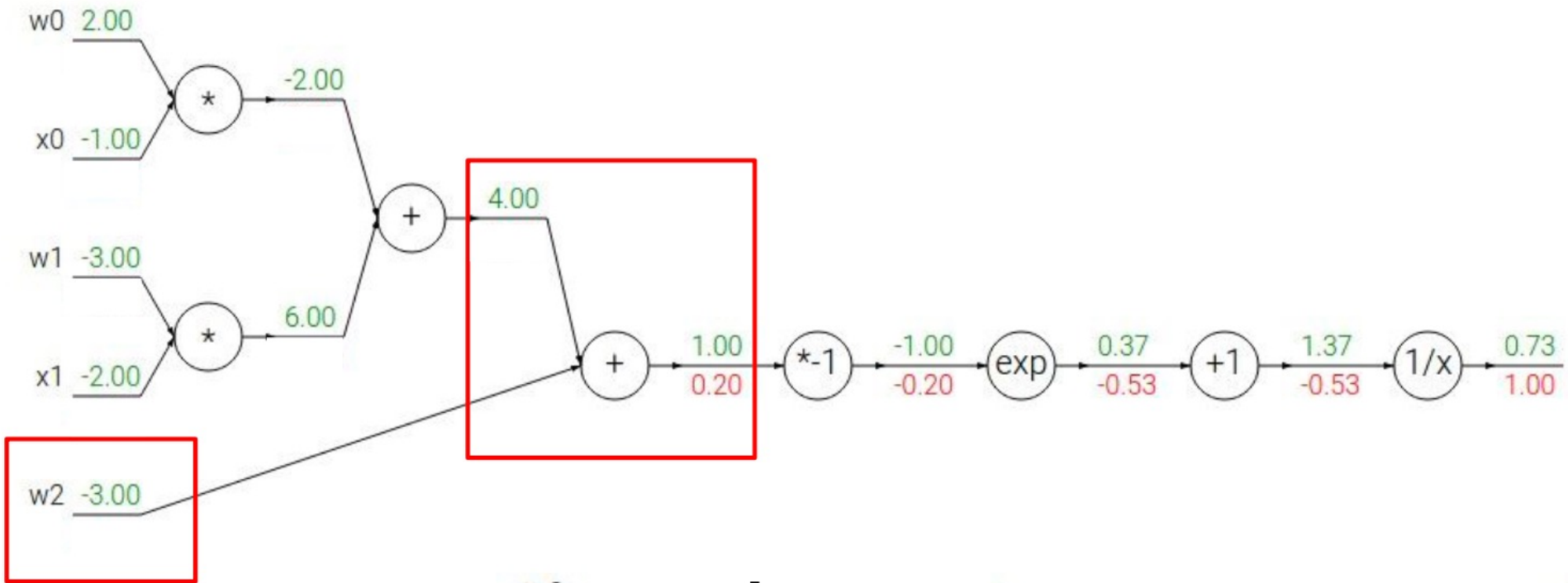

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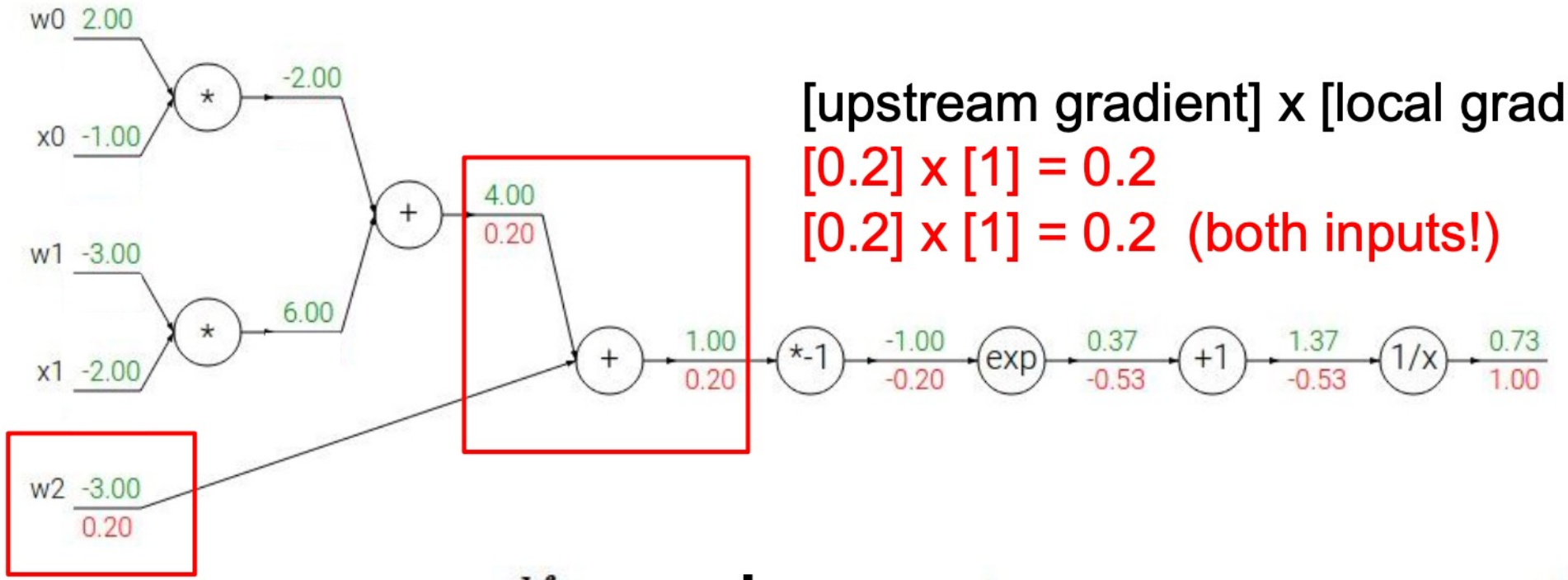

[upstream gradient] x [local gradient]

[0.2] x [1] = 0.2

[0.2] x [1] = 0.2 (both inputs!)

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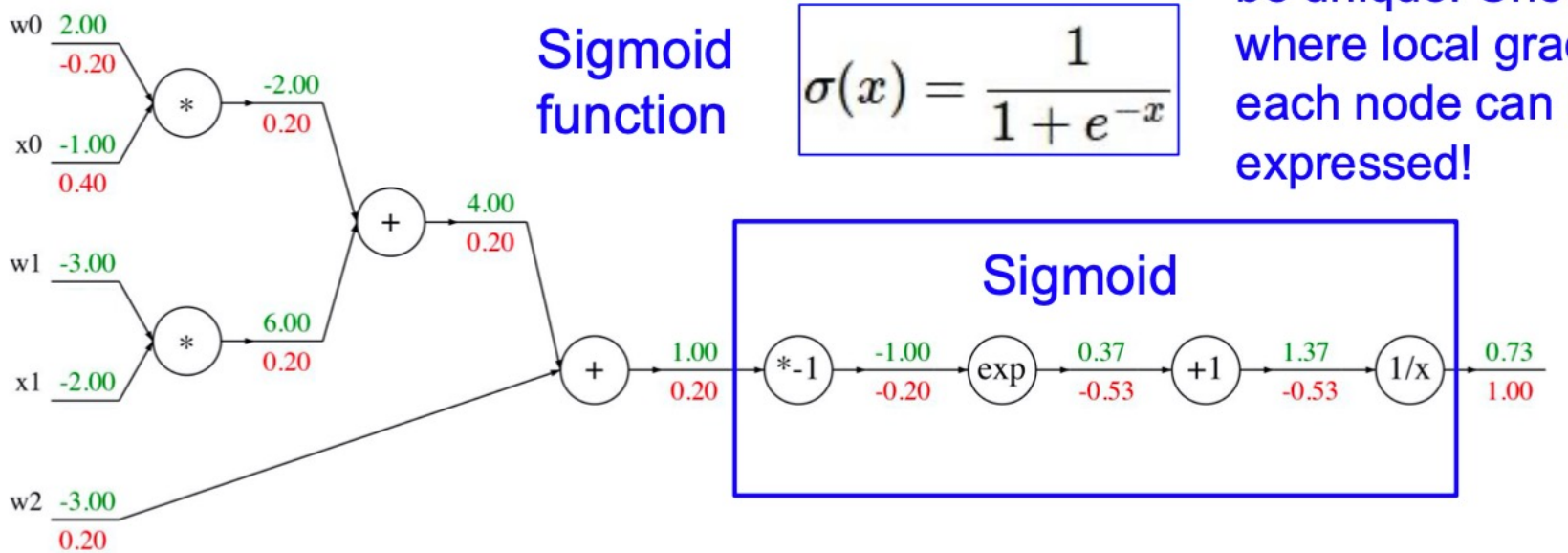

Sigmoid function

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

Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!

Another example:

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

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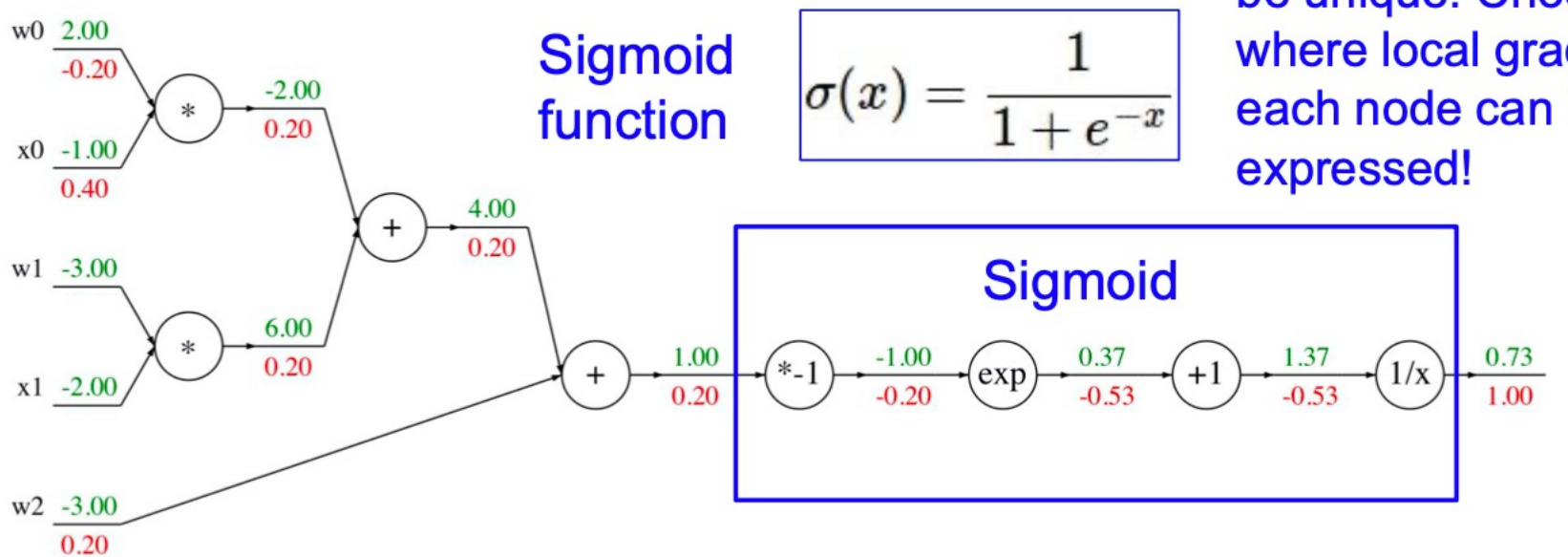

Sigmoid function

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Sigmoid local gradient:

$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$

Another example:

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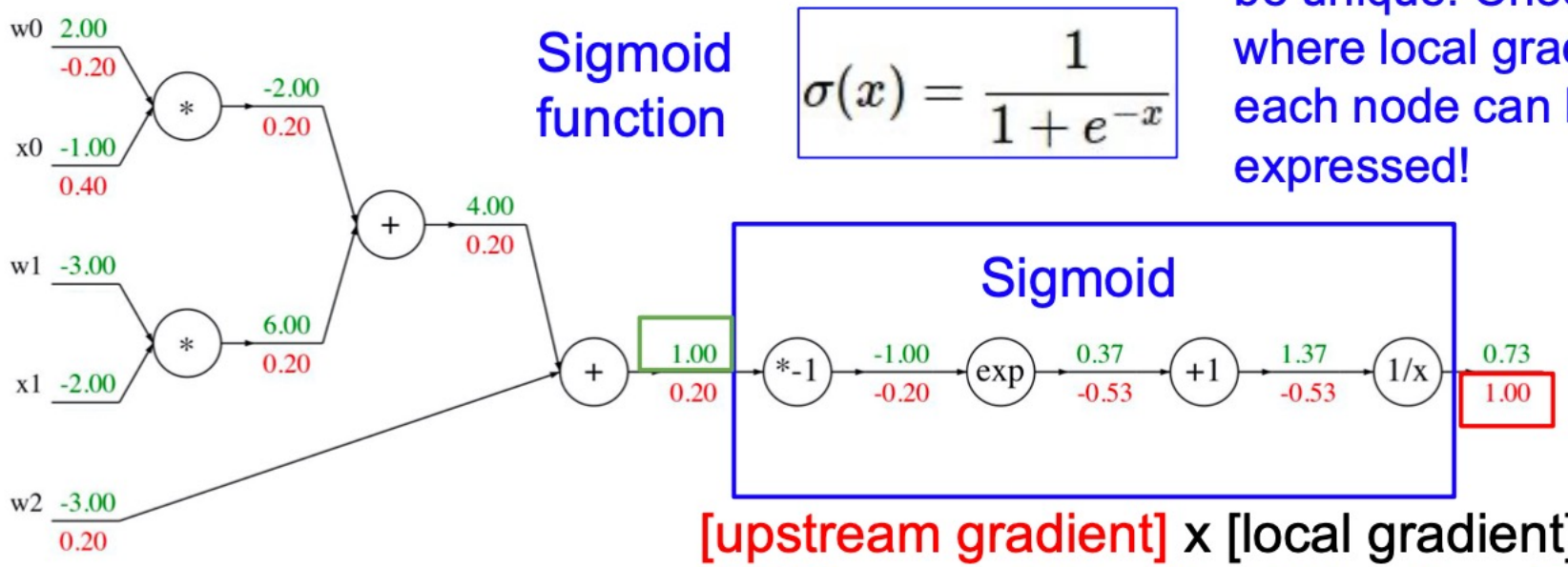
Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!



Sigmoid function

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

[upstream gradient] x [local gradient]

[1.00] x [(1 - 1/(1+e^1)) (1/(1+e^1))] = 0.2

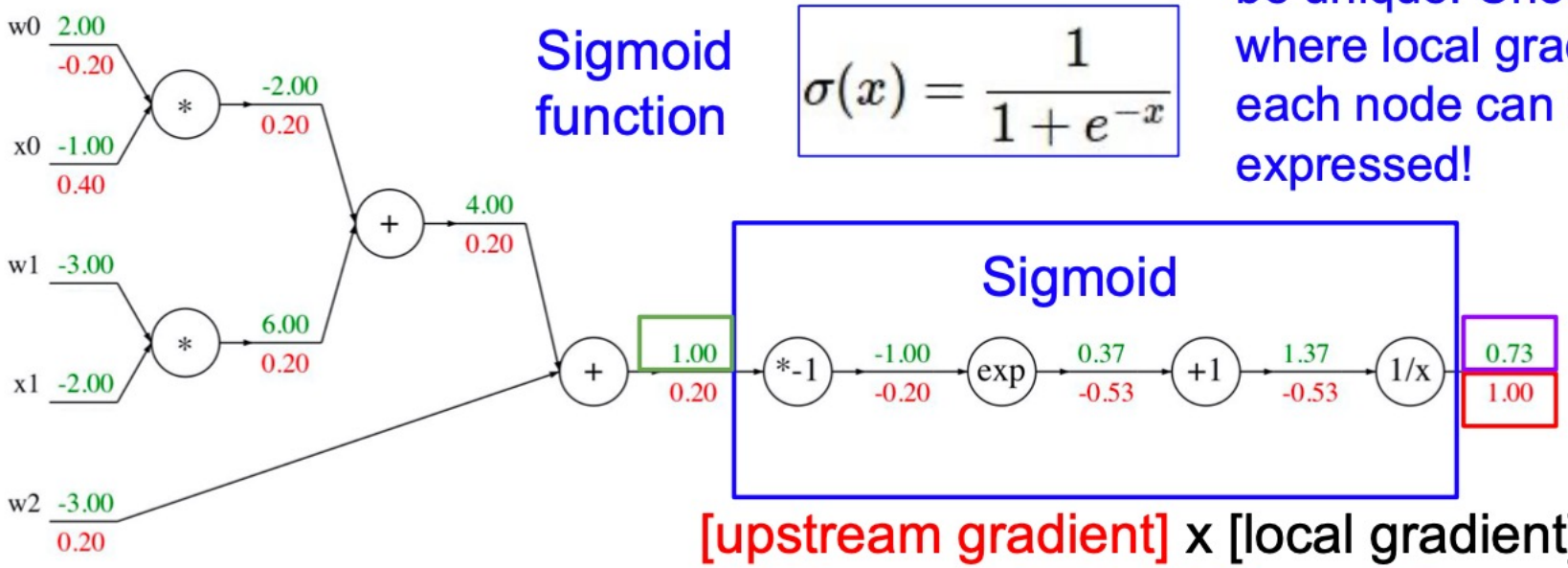
Sigmoid local gradient:

$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$

Another example:

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!



Sigmoid function

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

[upstream gradient] x [local gradient]

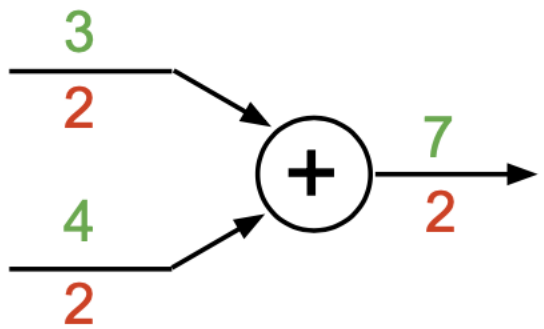
[1.00] x [(1 - 0.73) (0.73)] = 0.2

Sigmoid local gradient:

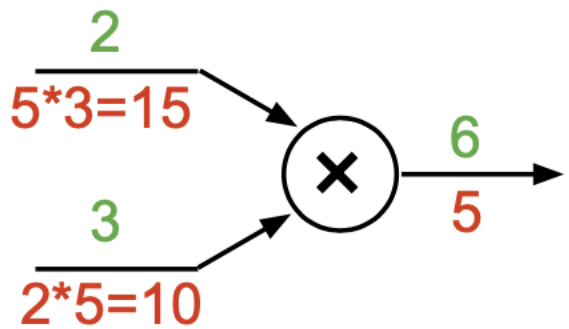
$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$

Patterns in gradient flow

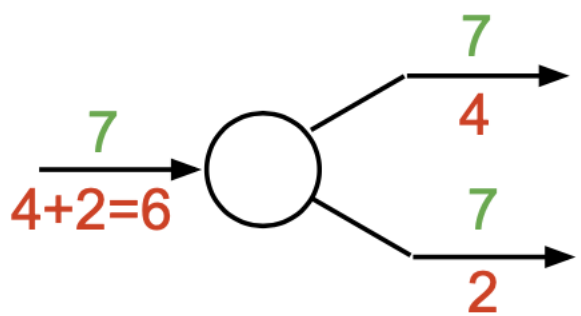
add gate: gradient distributor



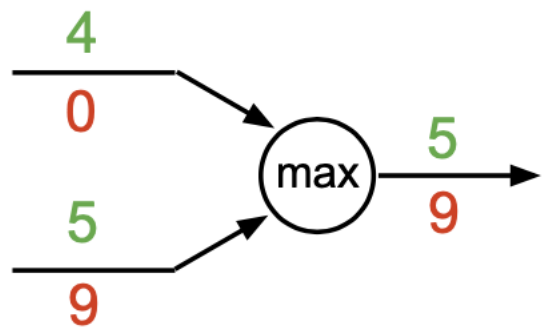
mul gate: “swap multiplier”



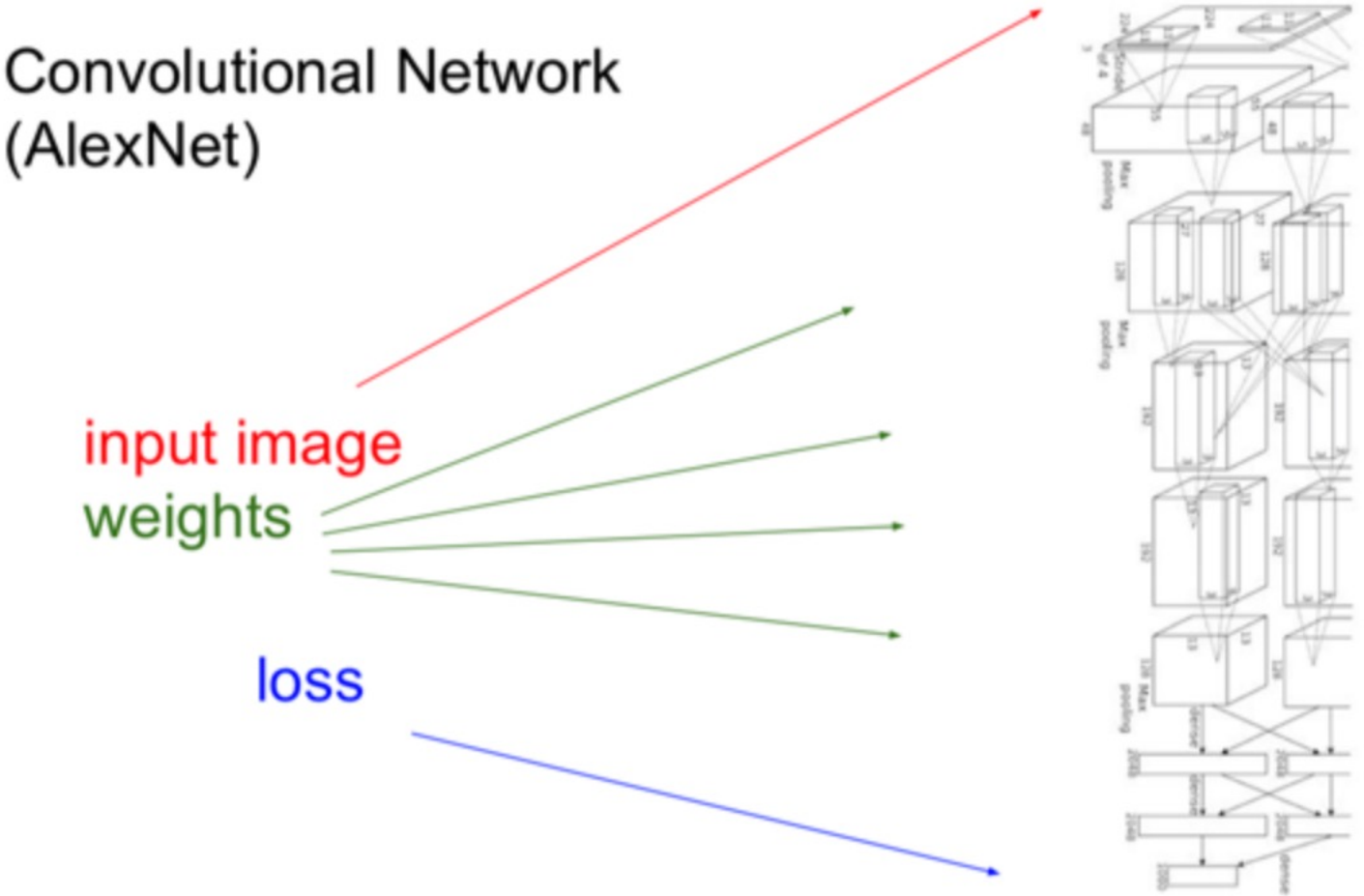
copy gate: gradient adder



max gate: gradient router



Can be applied to arbitrarily complex deep networks



Overall Steps of BP

After choosing the weights of the network randomly, the backpropagation algorithm is used to compute the necessary corrections. The algorithm can be decomposed in the following four steps:

i) Feed-forward computation

ii) Backpropagation to the output layer

iii) Backpropagation to the hidden layer

iv) Weight updates

The algorithm is stopped when the value of the error function has become sufficiently small.

Multilayer Neural Networks

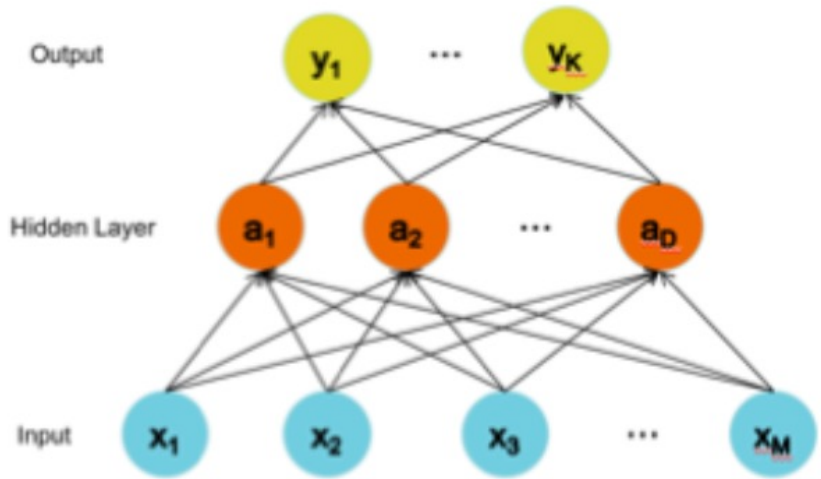
Network Design

Neural Network Architectures

- Even for a basic Multilayer Neural Network, there are many design decisions to make:

1) Number of hidden layers (depth of the network)
2) Number of neurons per hidden layer (width)
3) Type of activation functions
4) Form of objective functions

Example: Neural Network with sigmoid activation functions



(F) Loss
$J = \frac{1}{2}(y - y^*)^2$

(E) Output (sigmoid)
$y = \frac{1}{1+\exp(-b)}$

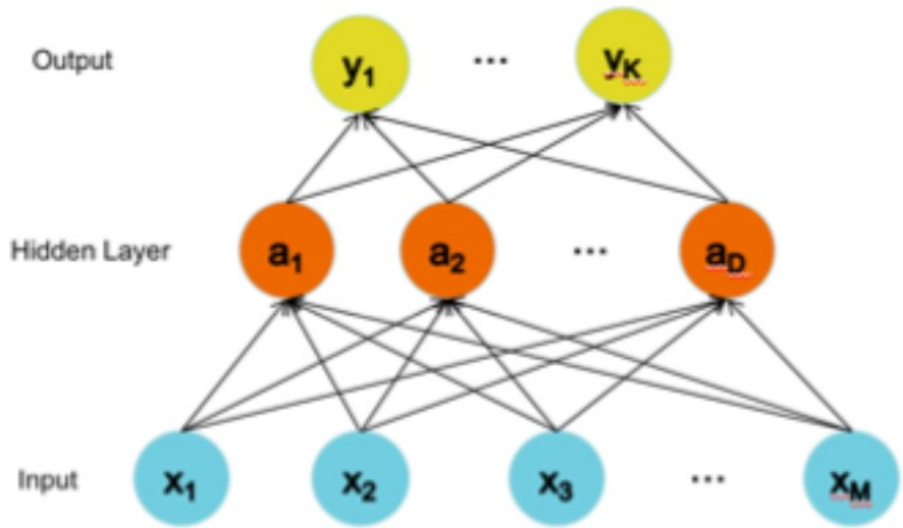
(D) Output (linear)
$b = \sum_{j=0}^{D} \beta_j z_j$

(C) Hidden (sigmoid)
$z_j = \frac{1}{1+\exp(-a_j)}, \ \forall j$

(B) Hidden (linear)
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$

(A) Input
Given $x_i, \ \forall i$

Neural Network with arbitrary nonlinear activation functions



(F) **Loss**
$J = \frac{1}{2}(y - y^*)^2$

(E) **Output (nonlinear)**
$y = \sigma(b)$

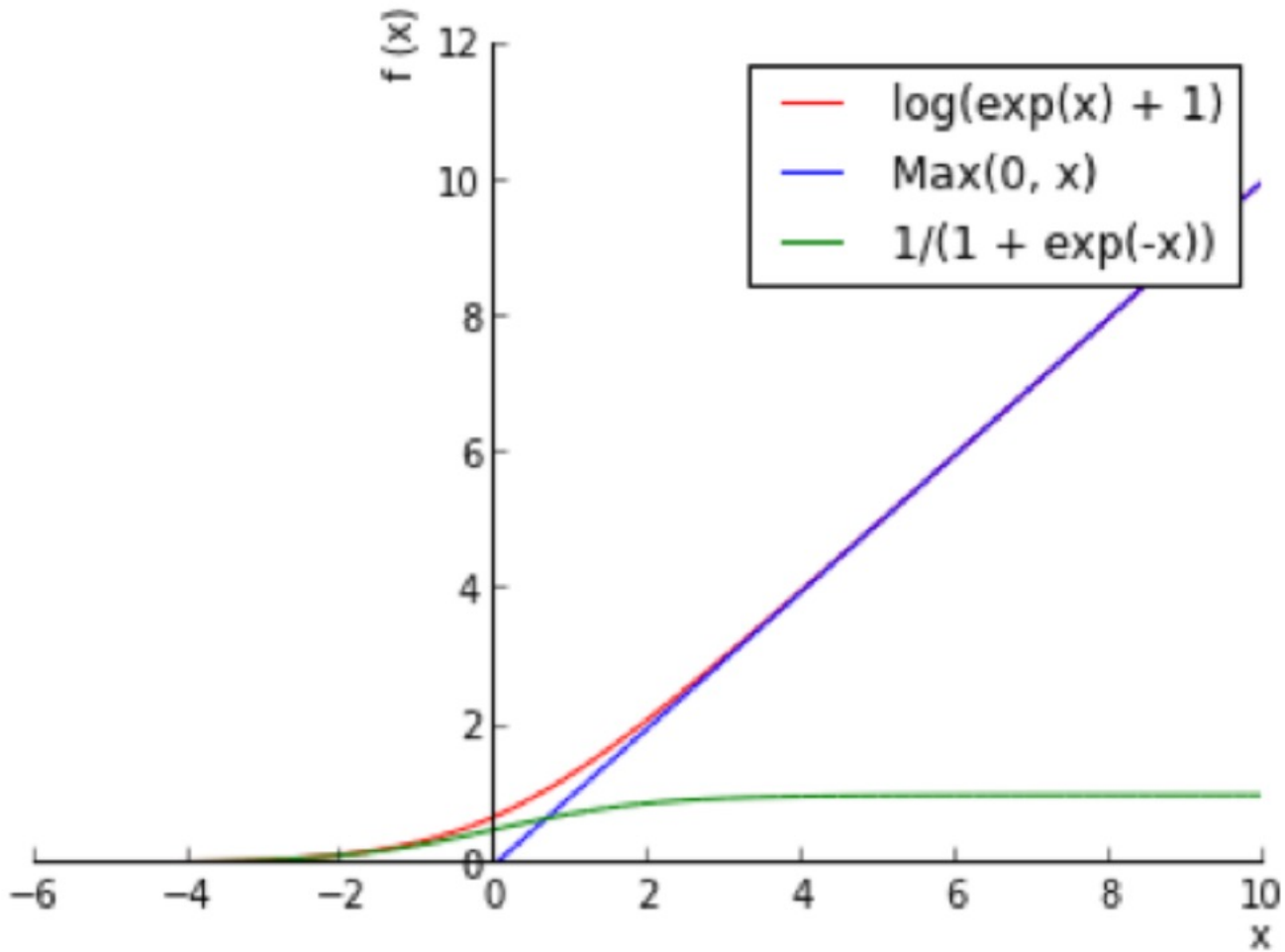
(D) **Output (linear)**
$b = \sum_{j=0}^{D} \beta_j z_j$

(C) **Hidden (nonlinear)**
$z_j = \sigma(a_j), \ \forall j$

(B) **Hidden (linear)**
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$

(A) **Input**
Given $x_i, \ \forall i$

ReLU often used in computer vision tasks



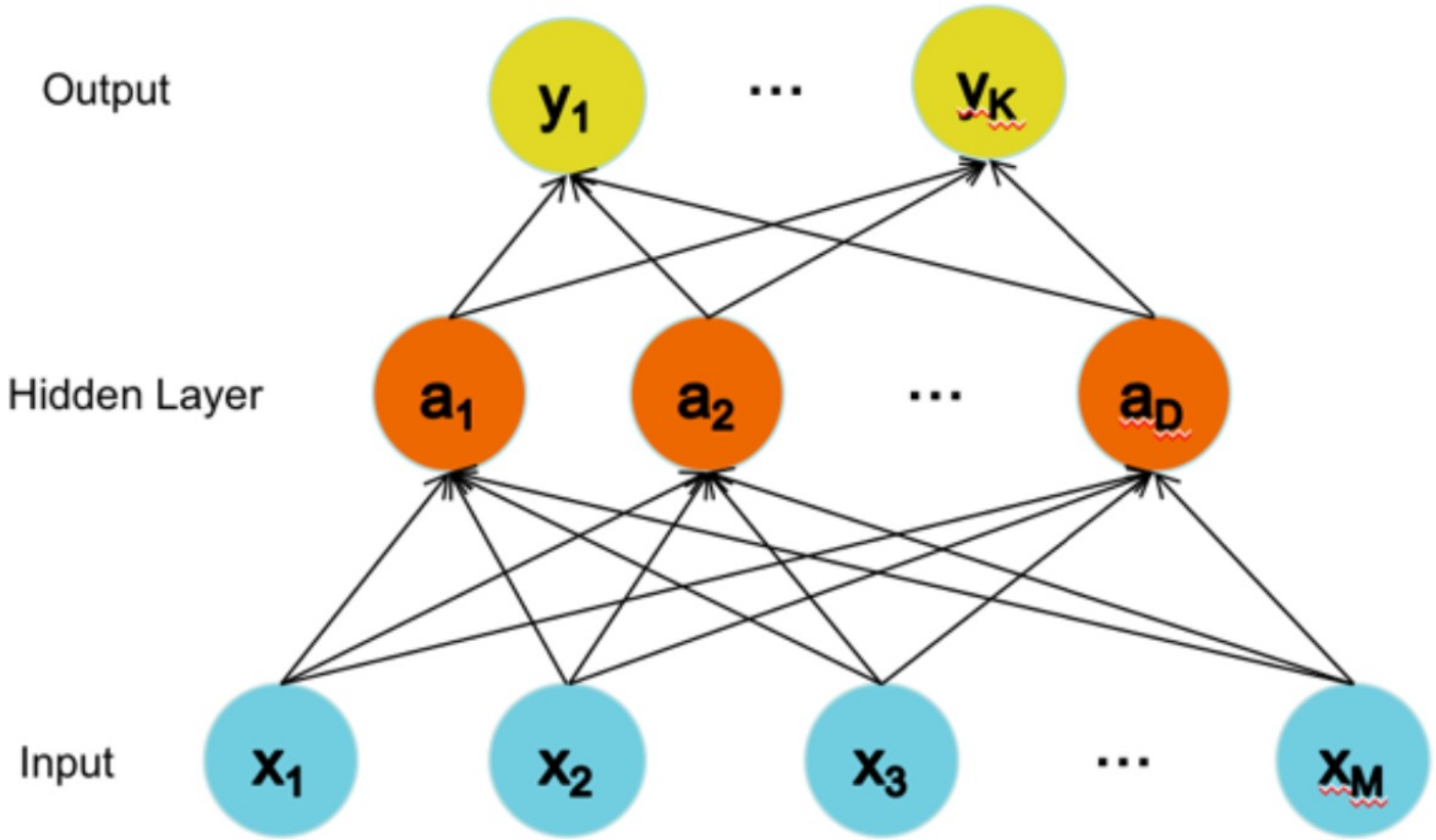
Loss Functions for NN

- Regression:
  - Use the same objective as Linear Regression
  - Quadratic loss (i.e. mean squared error)

- Classification:
  - Use the same objective as Logistic Regression
  - Cross-entropy (i.e. negative log likelihood)
  - This requires probabilities, so we add an additional "softmax" layer at the end of our network

	Forward	Backward
Quadratic	$J = \frac{1}{2}(y - y^*)^2$	$\frac{dJ}{dy} = y - y^*$
Cross Entropy	$J = y^* \log(y) + (1 - y^*) \log(1 - y)$	$\frac{dJ}{dy} = y^* \frac{1}{y} + (1 - y^*) \frac{1}{y - 1}$

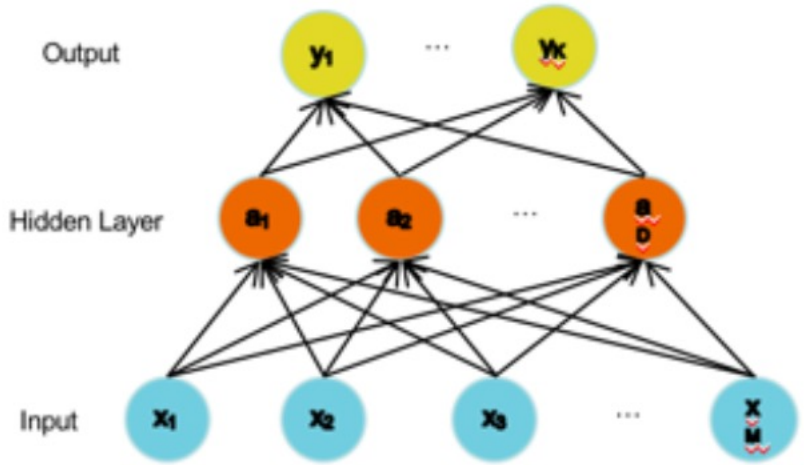
Multi-class Output

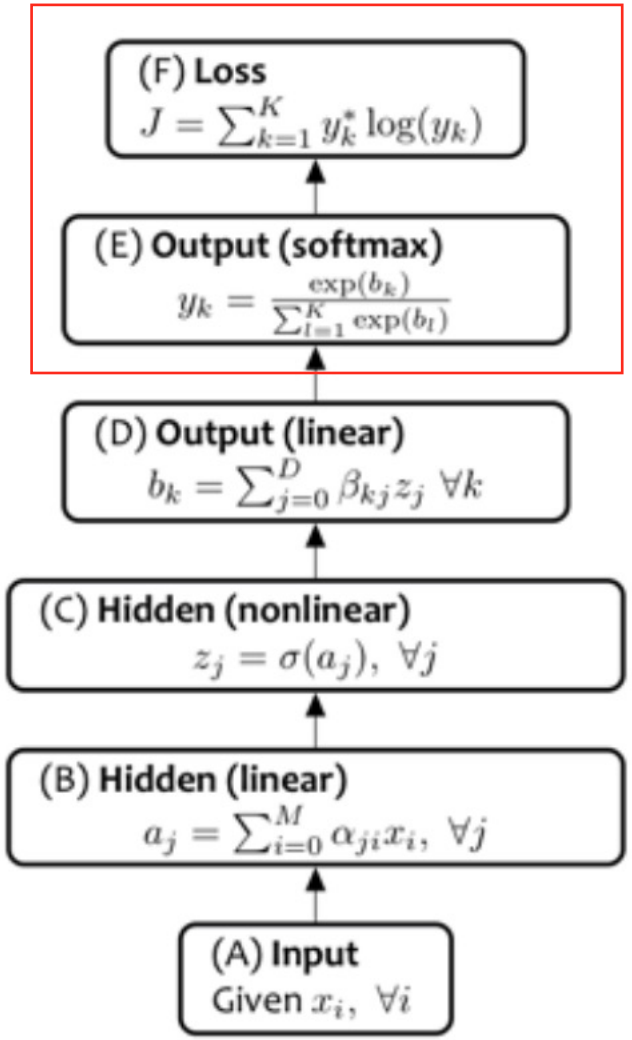


Multi-class Output

Softmax:

$$y_k = \frac{\exp(b_k)}{\sum_{l=1}^{K} \exp(b_l)}$$





Reference

- Chapter 6 Deep feedforward networks, Deep Learning, https://www.deeplearningbook.org/