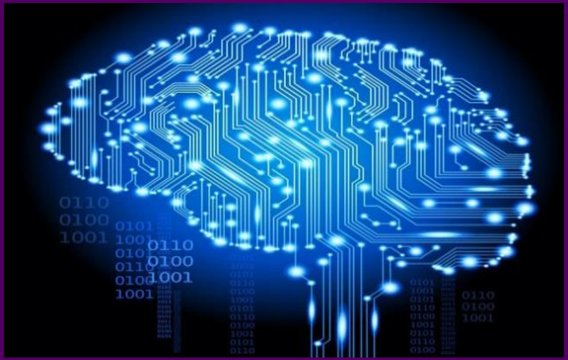
Deep Learning
MSiA 490-30



Theory and Applications

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Feedback: News and Ideas

~5-10 min to share ideas/news

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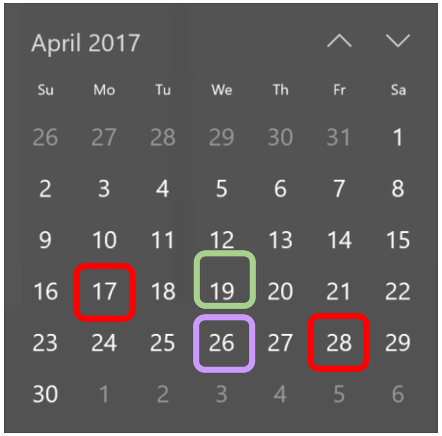
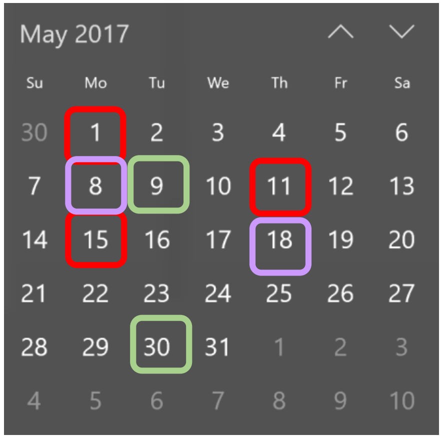
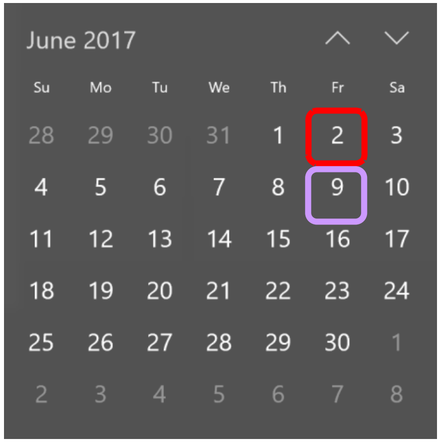
Assignment schedule

- Assignment 1: Due April 26th
  - Basic NN concepts
  - Optimization
  - Discuss with 1 partner, submit individually
- Assignment 2 (Group): Due May 18th
  - Computer Vision
  - Preparation for project
- Mini Quiz 1: May 8th: Basic NN, optimization and generalization multiple choice
- Mini Quiz 2: June 9th (2nd half): Generative, recurrent and applications multiple choice







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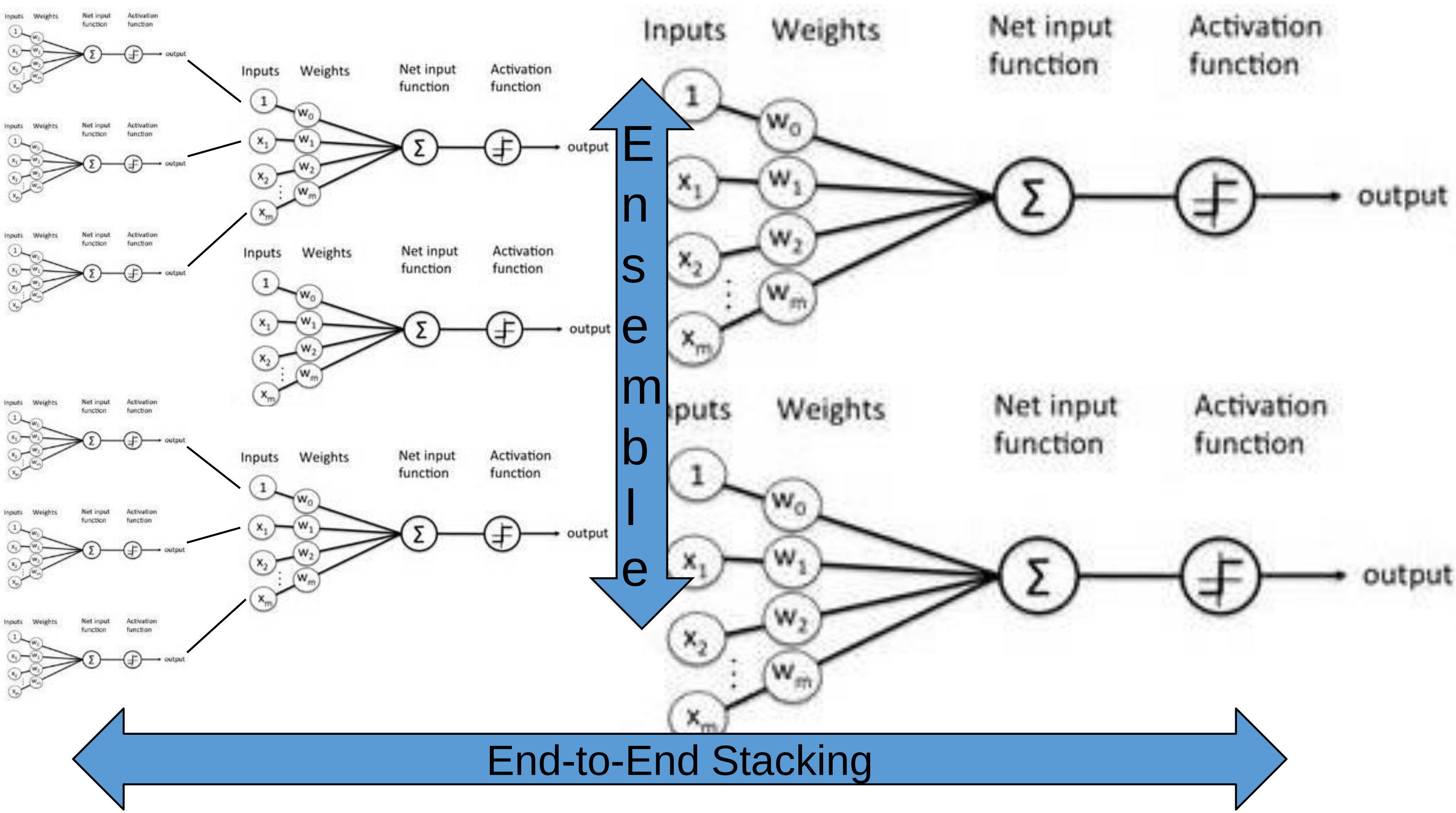
Last time

- Introduced multilayer nets
  - Apply optimization rules in layers
- This time
  - Why Optimization may slow down/fail
  - Some simple workarounds
  - Advanced optimization methods

“Layered” Logistic Regression



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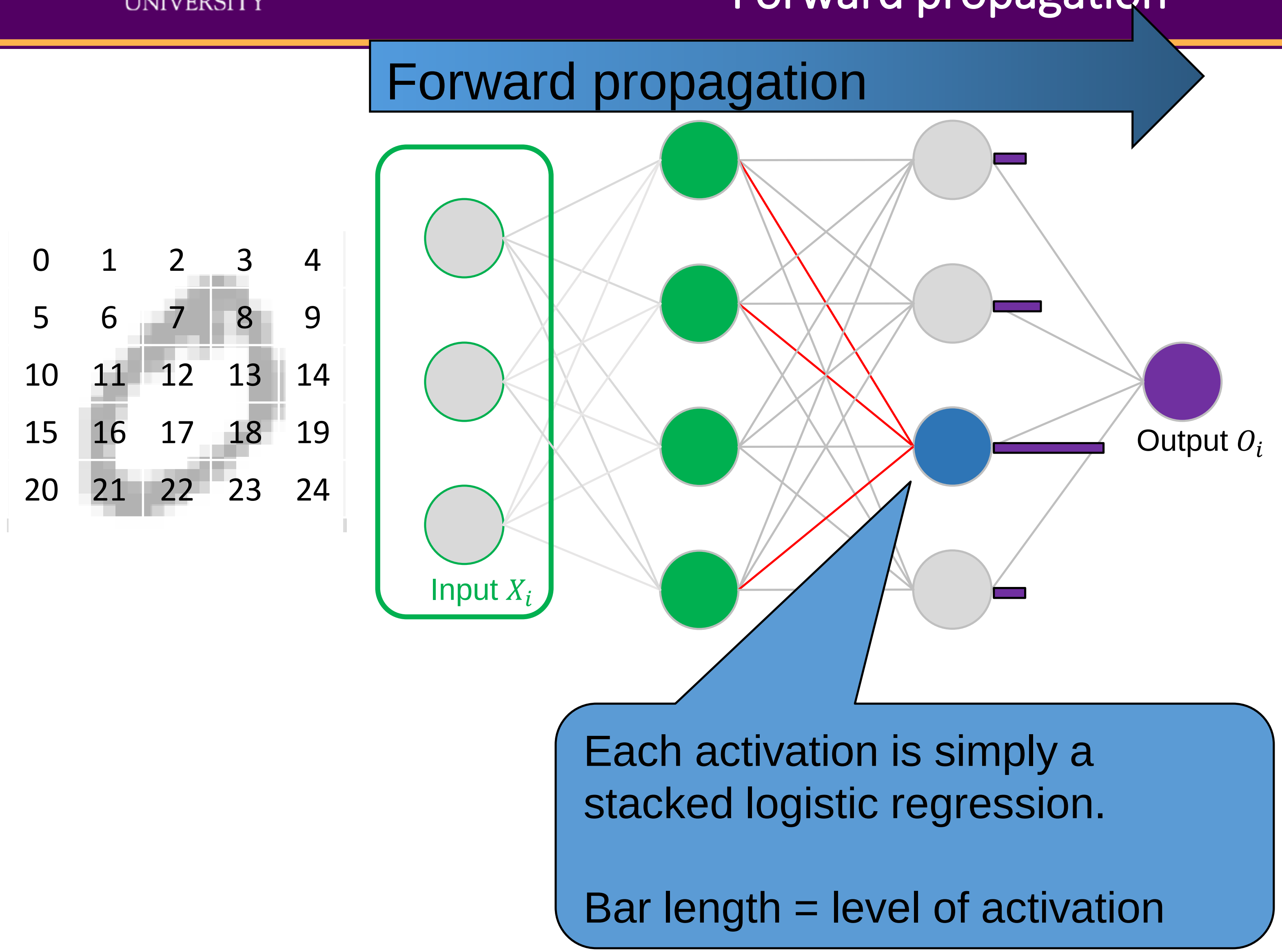
Forward propagation



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Backpropagation

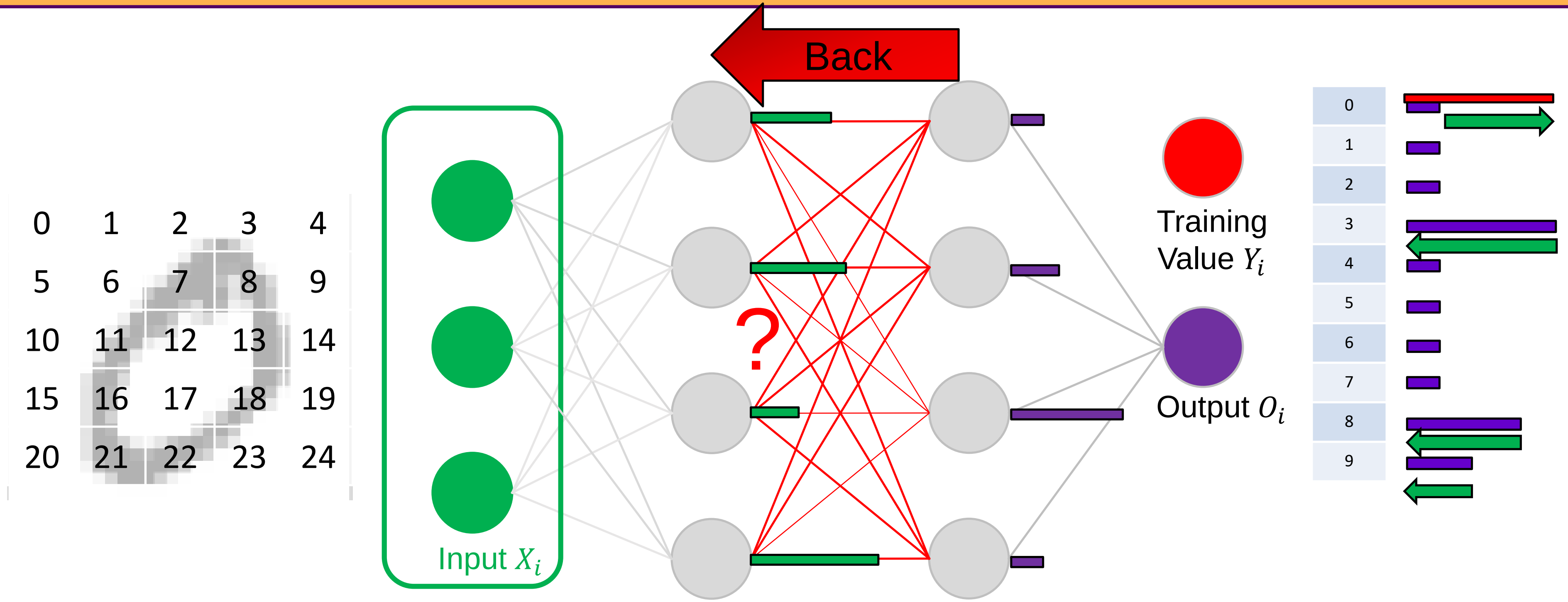

Figure out how to adjust input(green) weights(red) to match target activations(purple)

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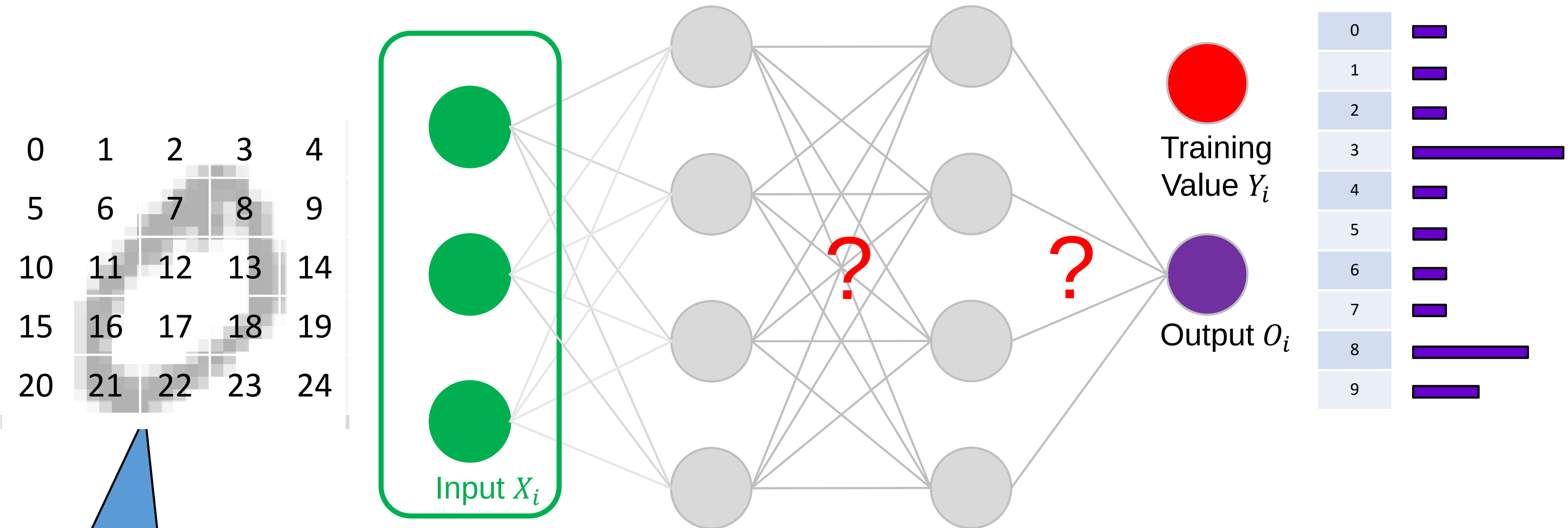
Feedforward networks



Input is
28x28=784
60,000 Ex

Flatten image to 784 dim x 60k

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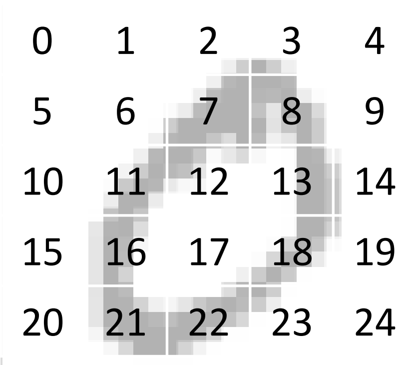
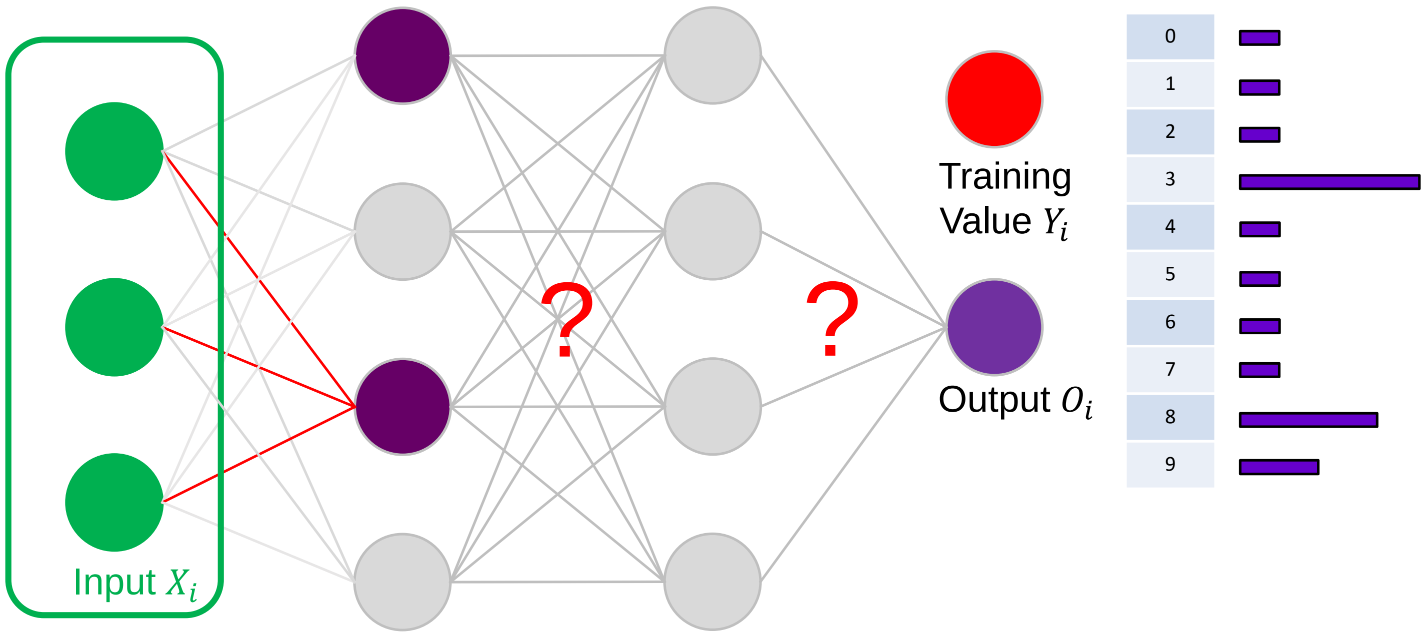
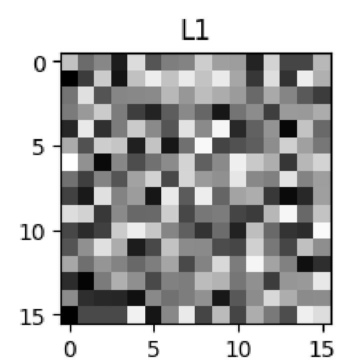
Visualizing NN





L1 = sigmoid(W1.dot(X))

Layer 1 is 256 units: 16x16 (60k) visualization



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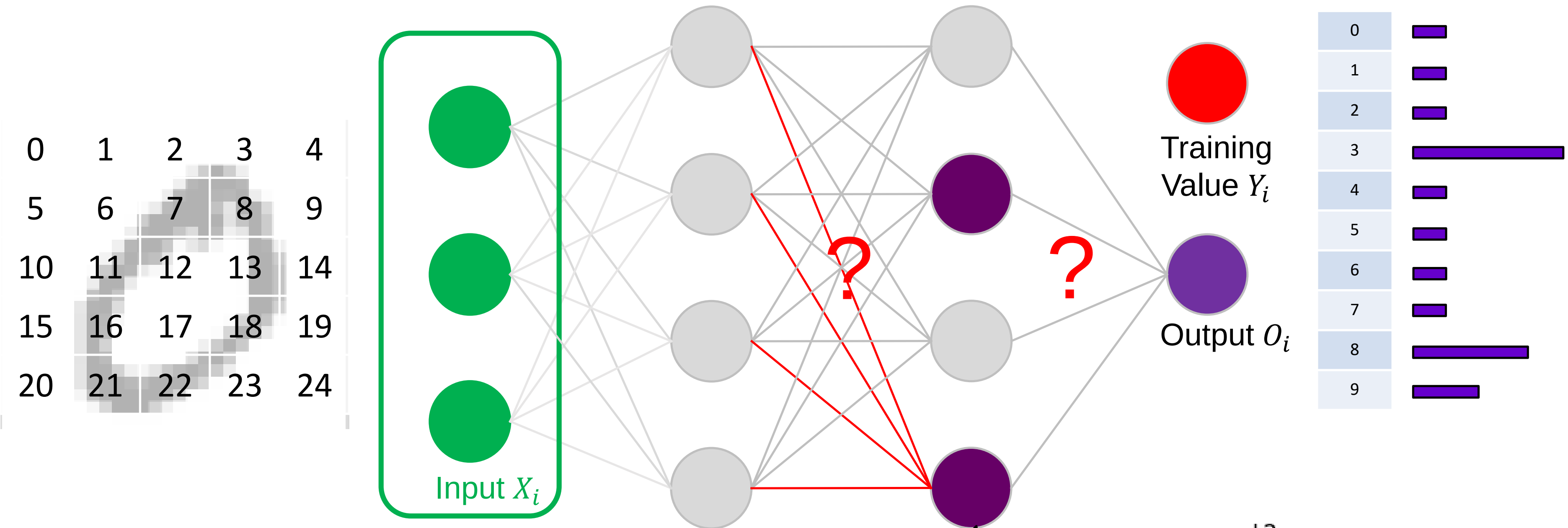
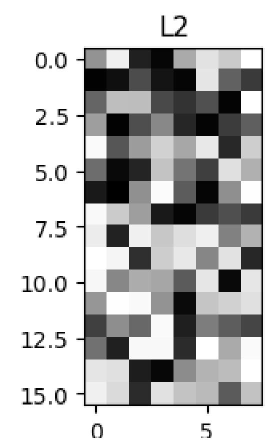
Visualizing NN

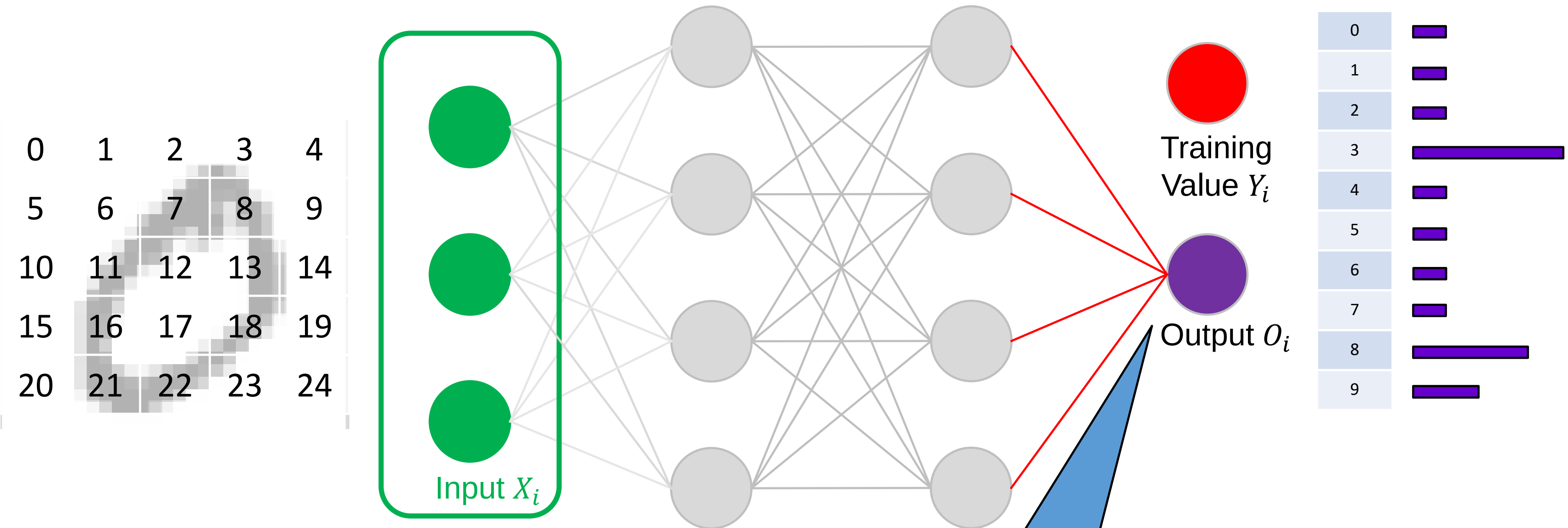


L1 = sigmoid(W1.dot(X))
L2 = sigmoid(W2.dot(L1))

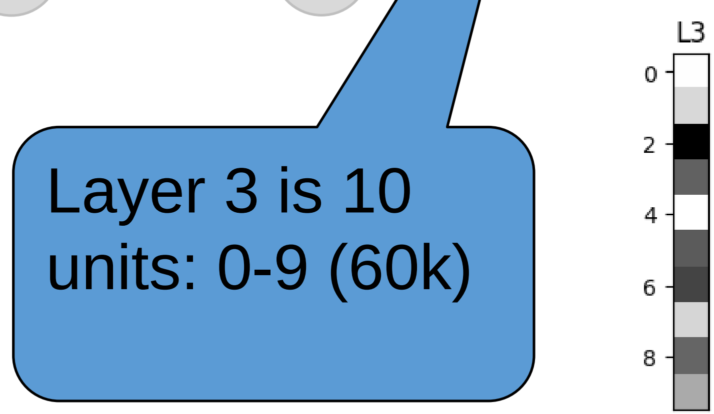
Layer 2 is 128 units: 16x8 (60k) visualization



Visualizing NN



L1 = sigmoid(W1.dot(X))
L2 = sigmoid(W2.dot(L1))
L3 = sigmoid(W3.dot(L2))



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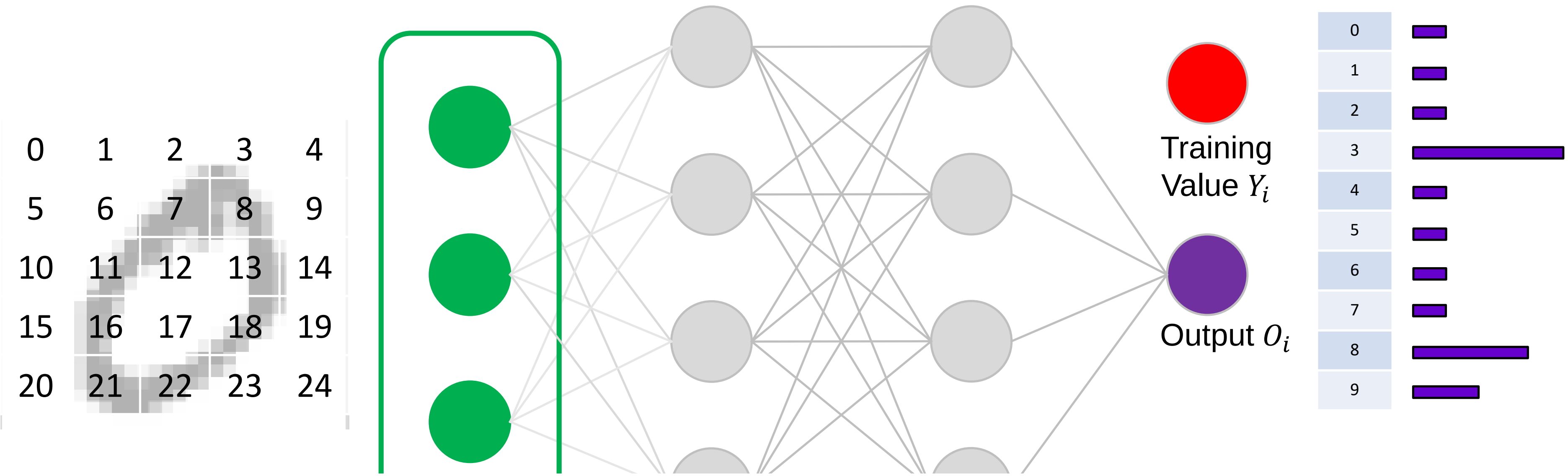
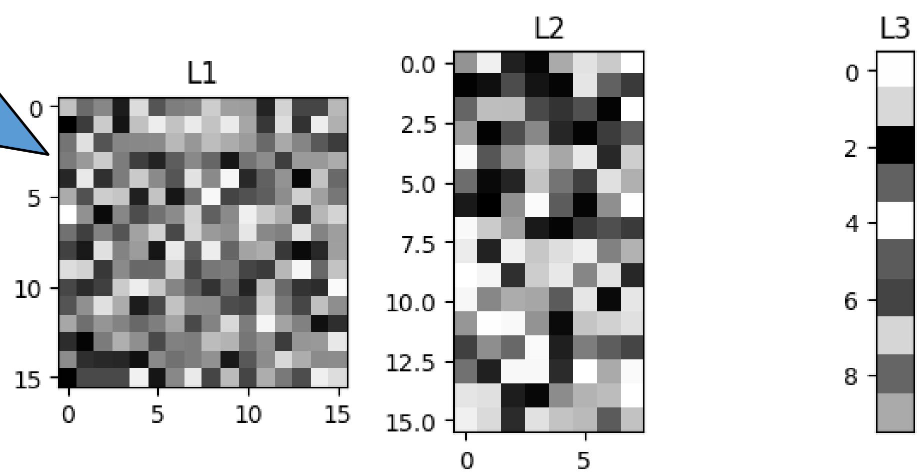


Mean activations over 60k images



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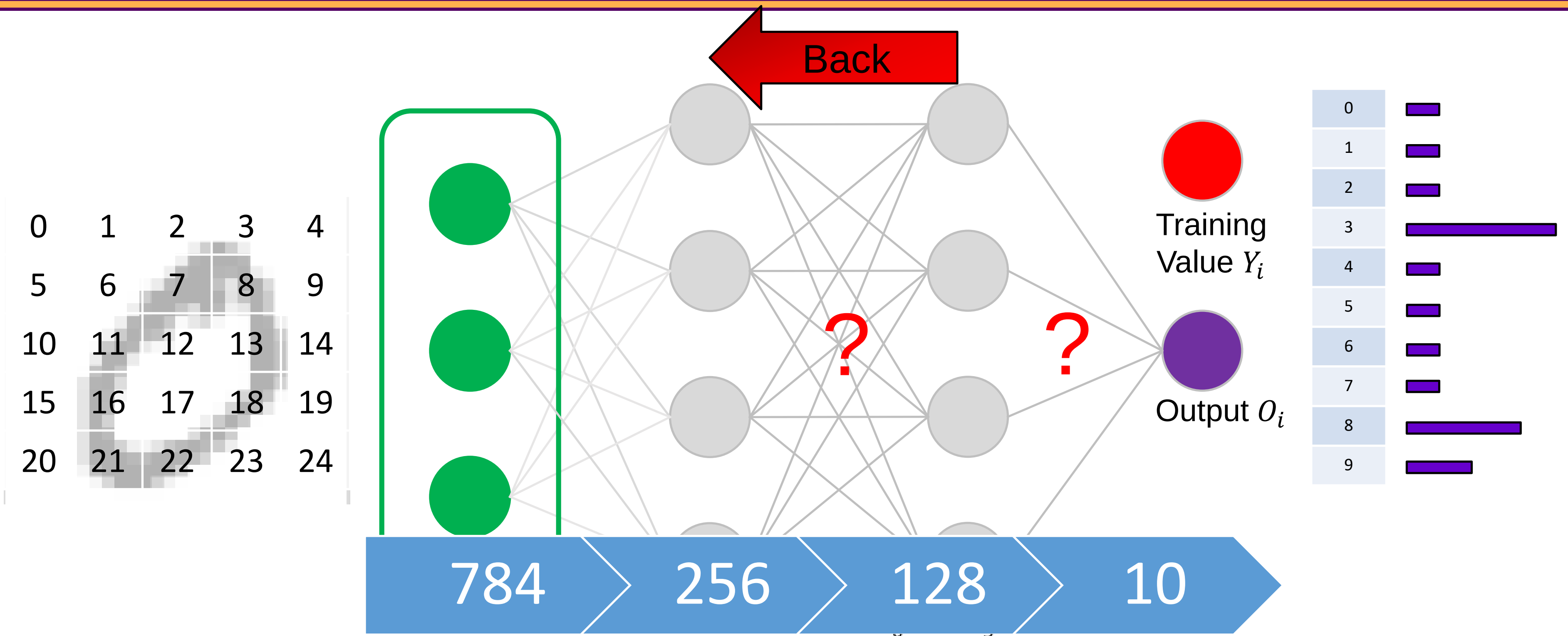
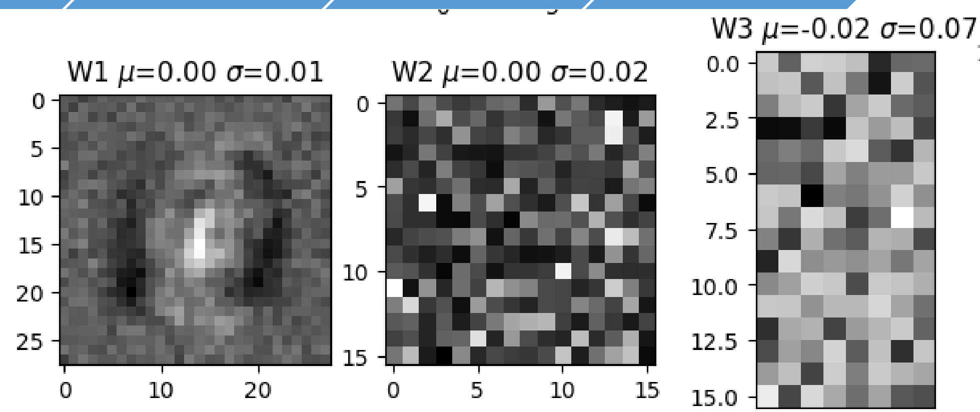
Visualizing NN



Mean weights over 60k images. Remember: $w_i x_i$ means input and weights share same shape



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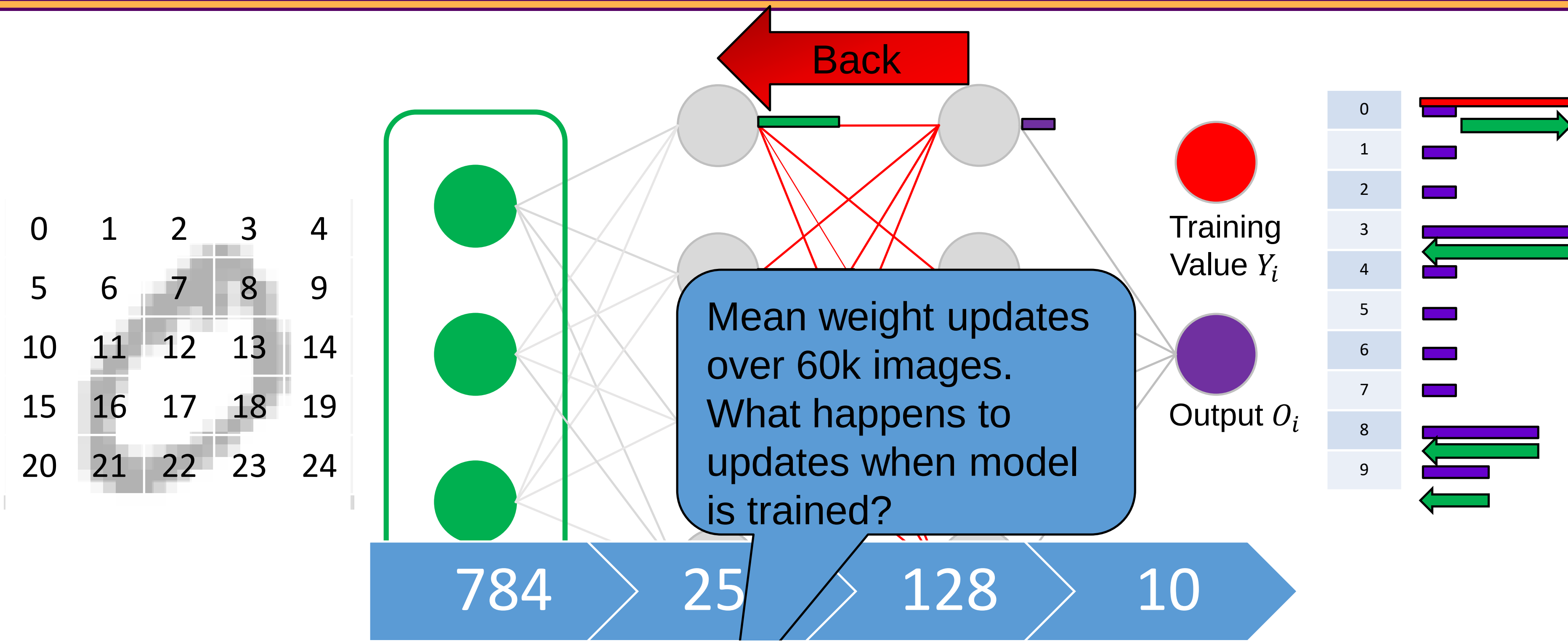
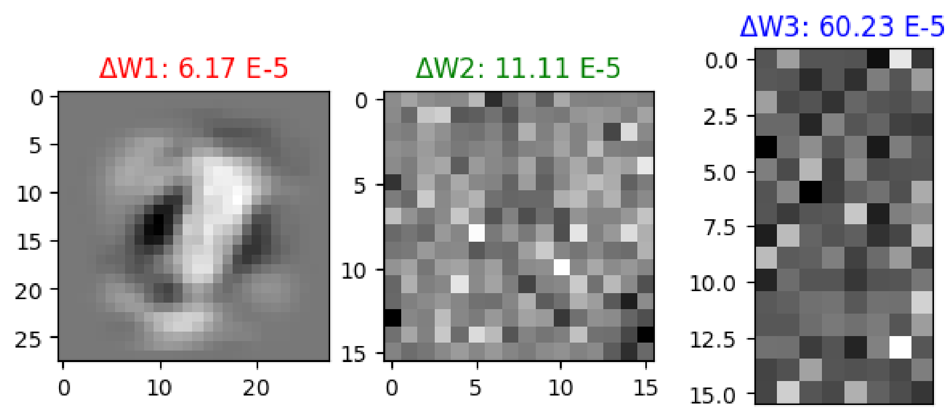
Visualizing NN



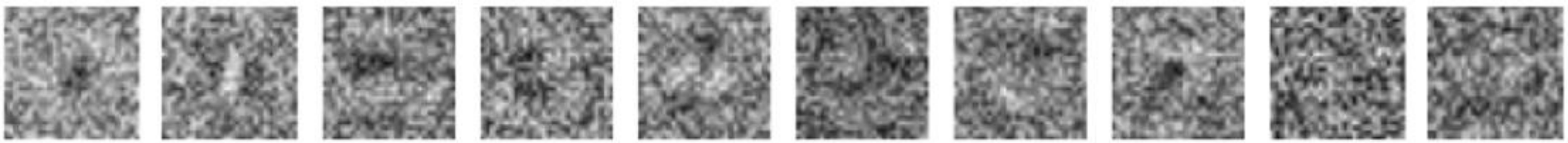

```
# Backward pass
dW3 = (L3 - T) * L3*(1 - L3)
dW2 = W3.T.dot(dW3)*(L2*(1-L2))
dW1 = W2.T.dot(dW2)*(L1*(1-L1))
# Update
W3 -= lr*np.dot(dW3, L2.T)
W2 -= lr*np.dot(dW2, L1.T)
W1 -= lr*np.dot(dW1, X.T)
```



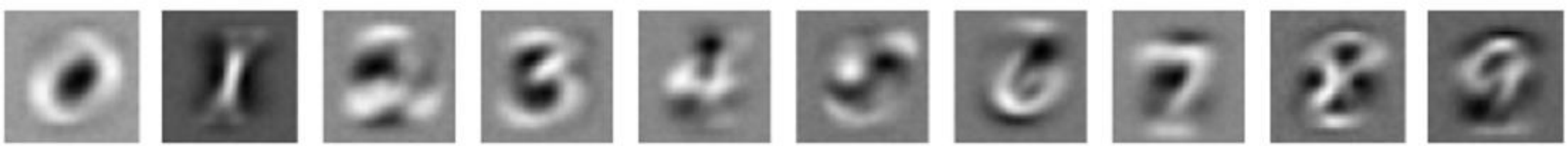
Effects of Regularization

- L1 regularization encourages stronger feature learning

No regularization



L1 regularization



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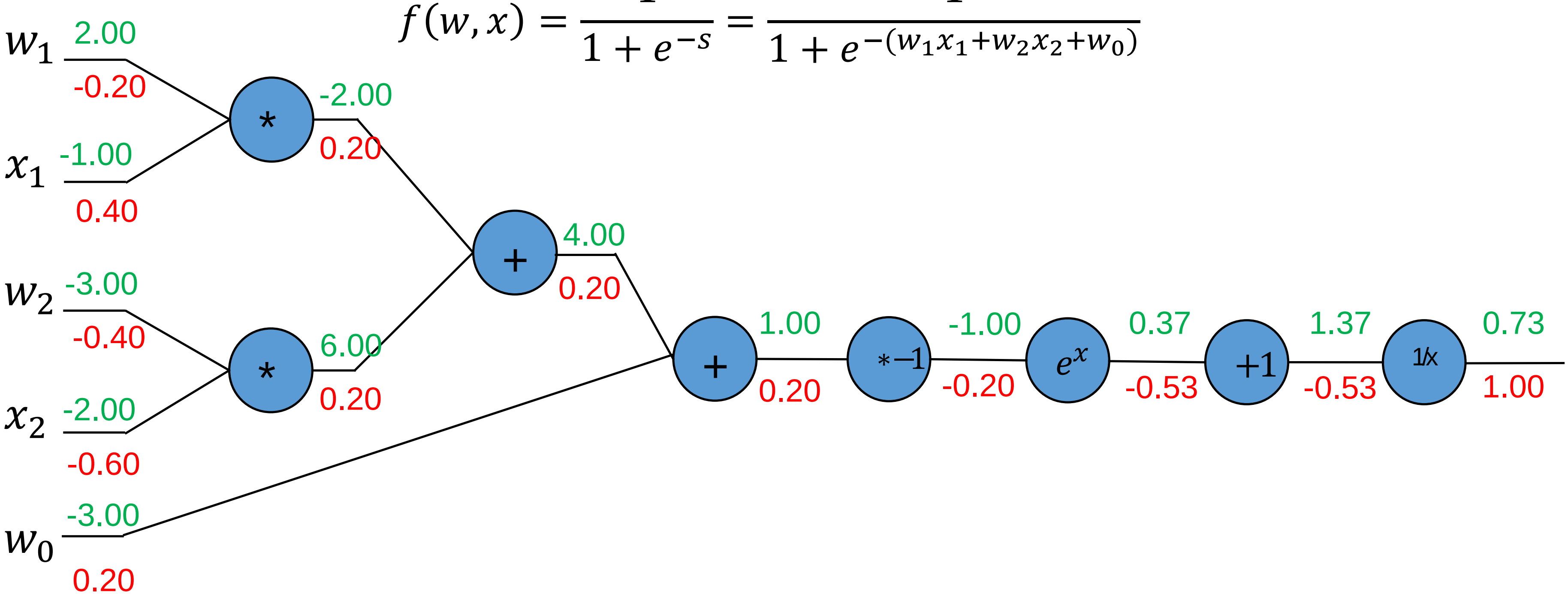
Backprop in “depth”

$$f(w,x) = \frac{1}{1+e^{-s}} = \frac{1}{1+e^{-(w_1x_1+w_2x_2+w_0)}}$$



$f(x) = e^x$	$\rightarrow$ $\frac{\partial f}{\partial x} = e^x$	$f(x) = \frac{1}{x}$	$\rightarrow$ $\frac{\partial f}{\partial x} = \frac{-1}{x^2}$
$f_a(x) = ax$	$\rightarrow$ $\frac{\partial f}{\partial x} = a$	$f_c(x) = c + x$	$\rightarrow$ $\frac{\partial f}{\partial x} = 1$

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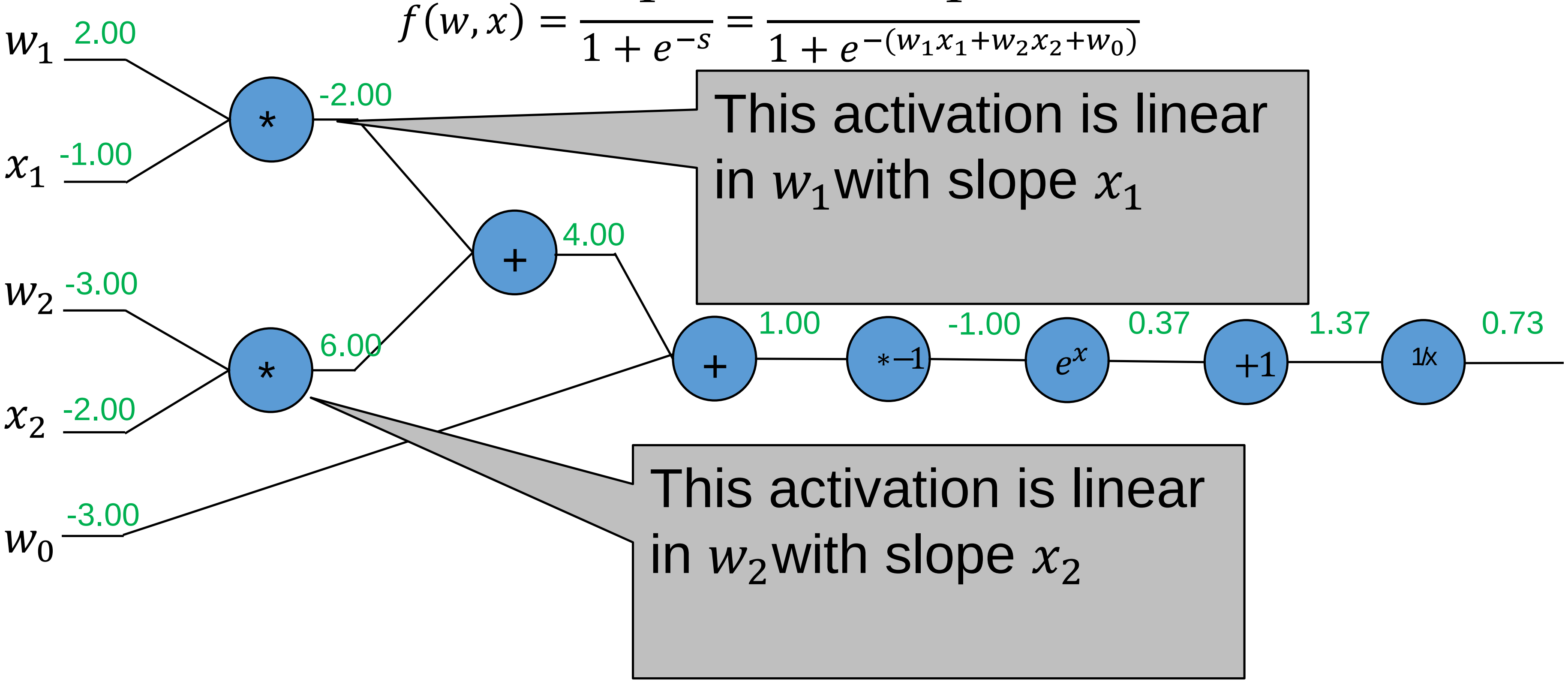
Backprop in "depth": Forward pass

$$f(w,x) = \frac{1}{1+e^{-s}} = \frac{1}{1+e^{-(w_1x_1+w_2x_2+w_0)}}$$



$f(x) = e^x$	$\rightarrow$	$\frac{\partial f}{\partial x} = e^x$	$f(x) = \frac{1}{x}$	$\rightarrow$	$\frac{\partial f}{\partial x} = \frac{-1}{x^2}$
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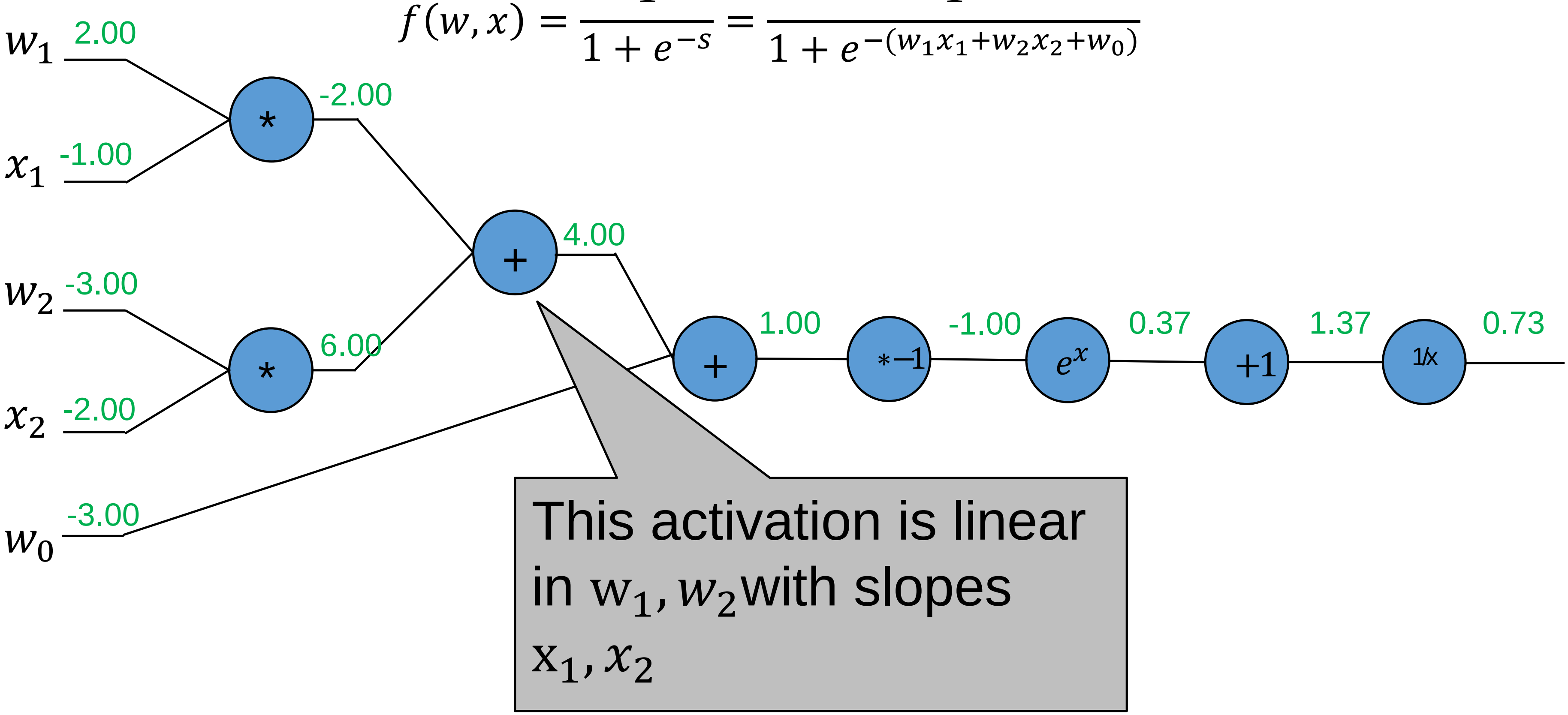

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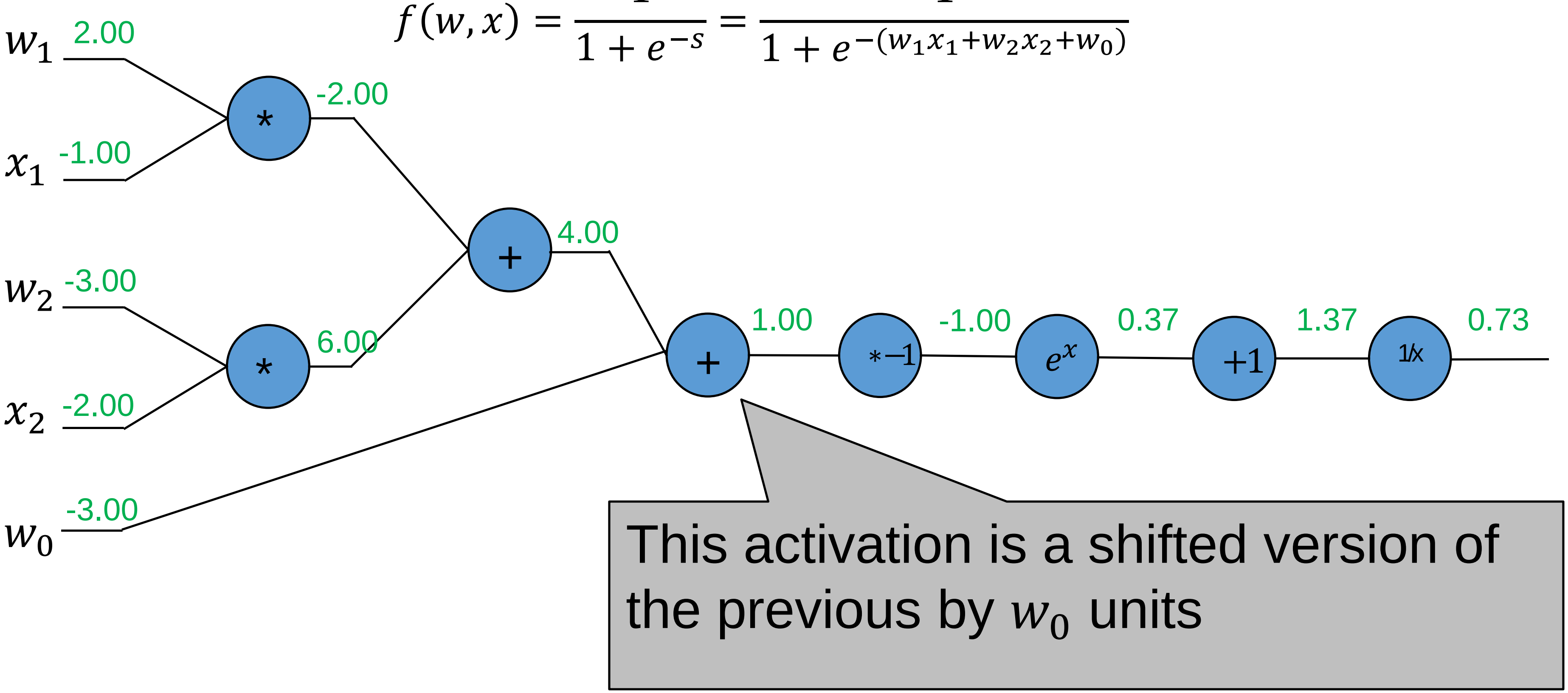

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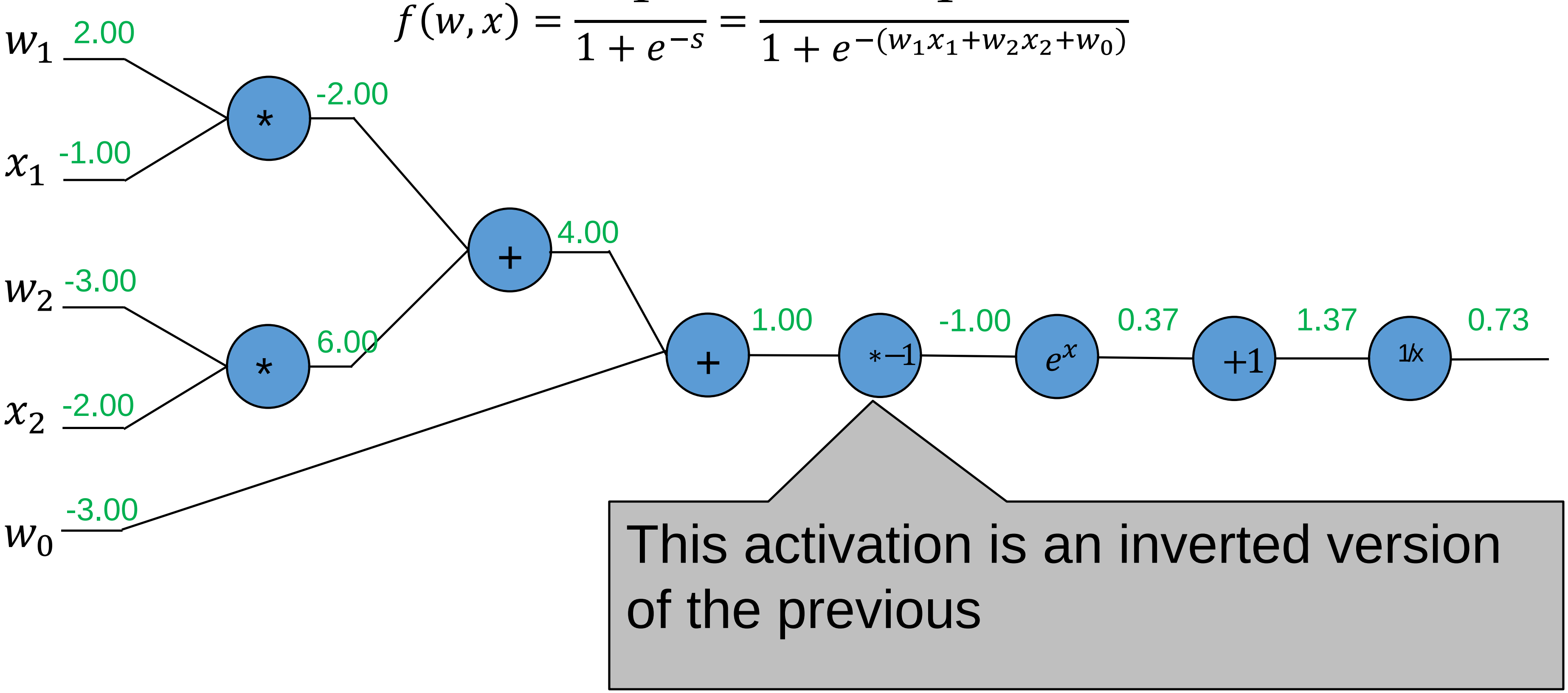

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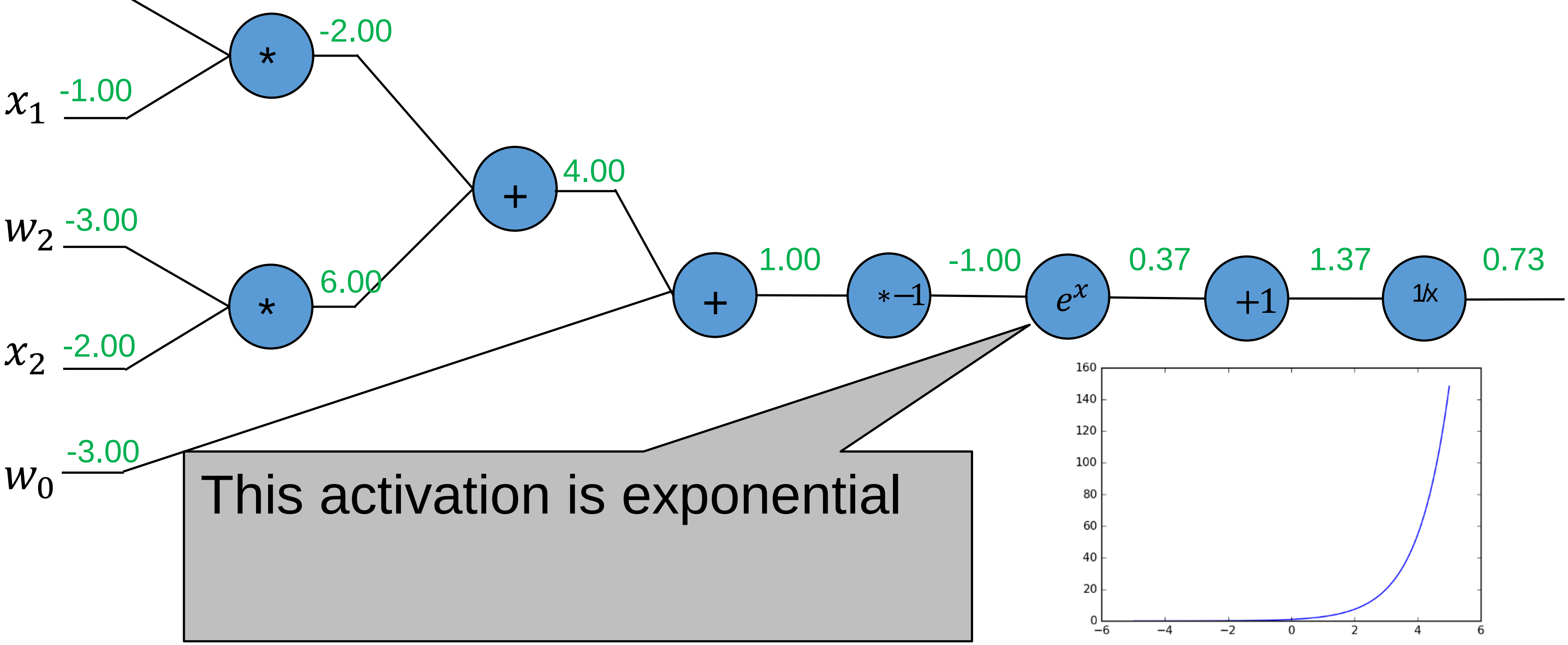

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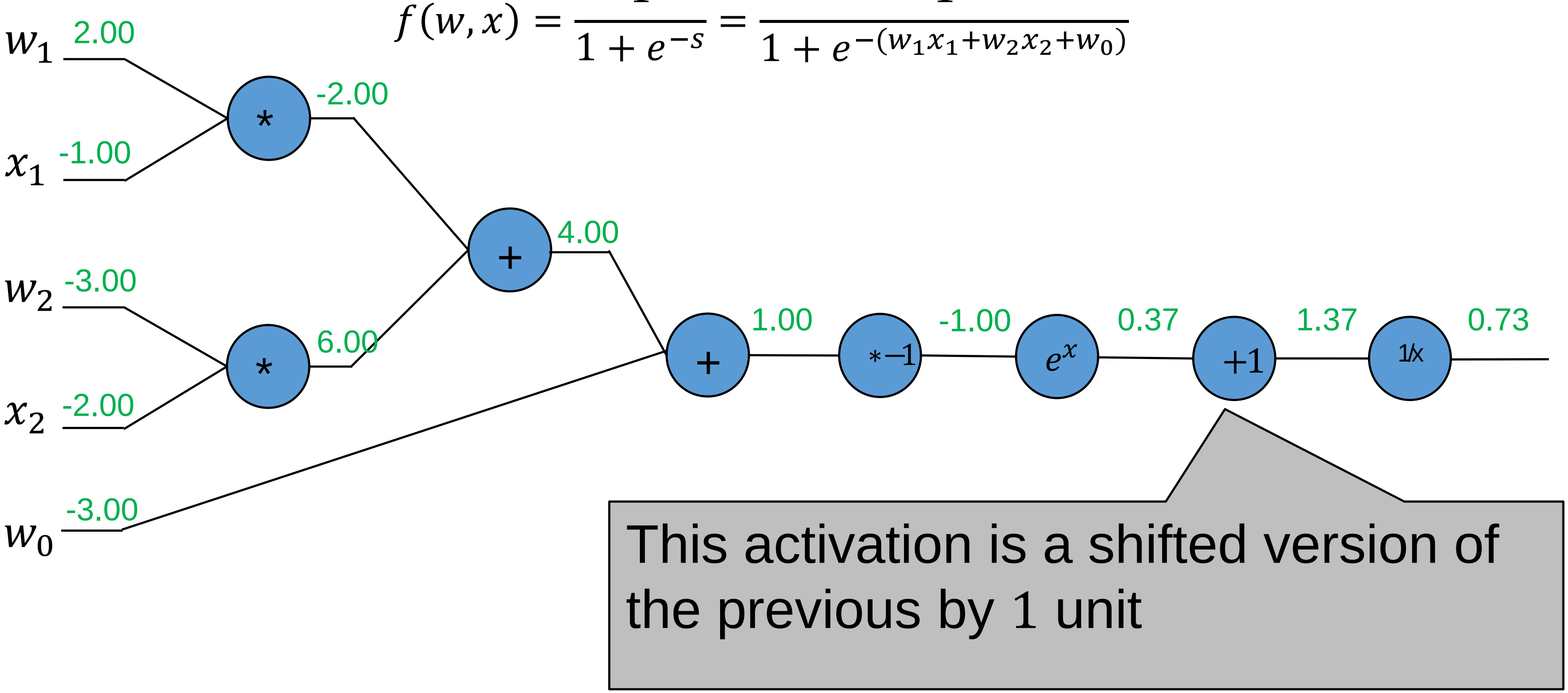

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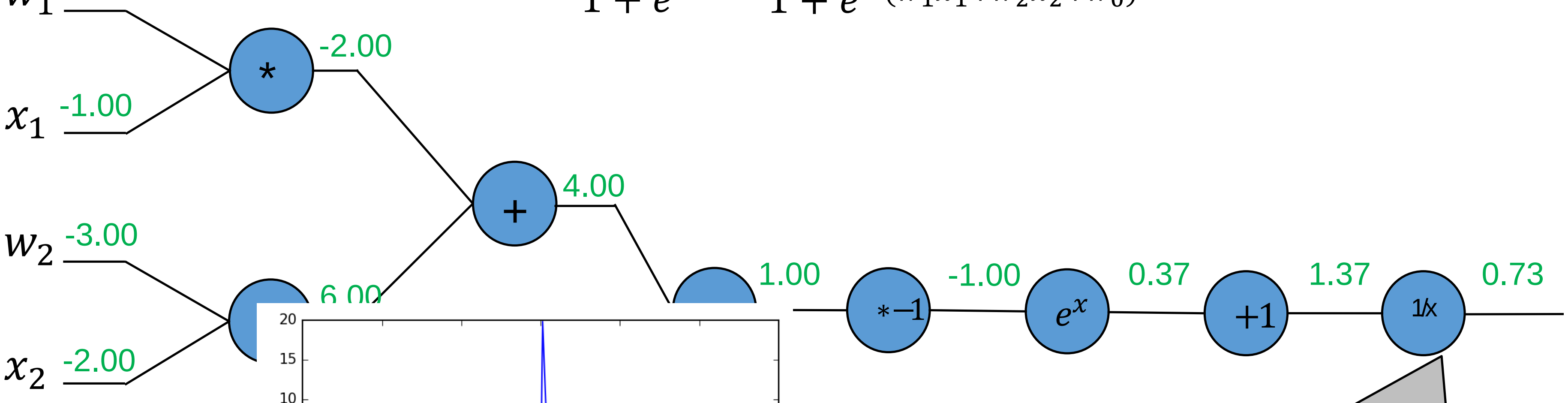

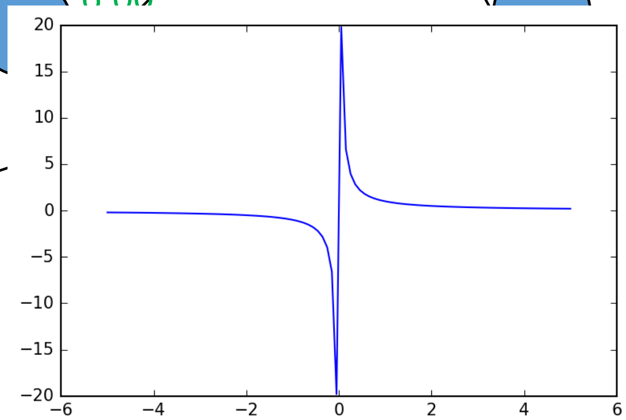

This activation is hyperbolic

$f(x) = e^x \quad \rightarrow \quad \frac{\partial f}{\partial x} = e^x$	$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{\partial f}{\partial x} = \frac{-1}{x^2}$
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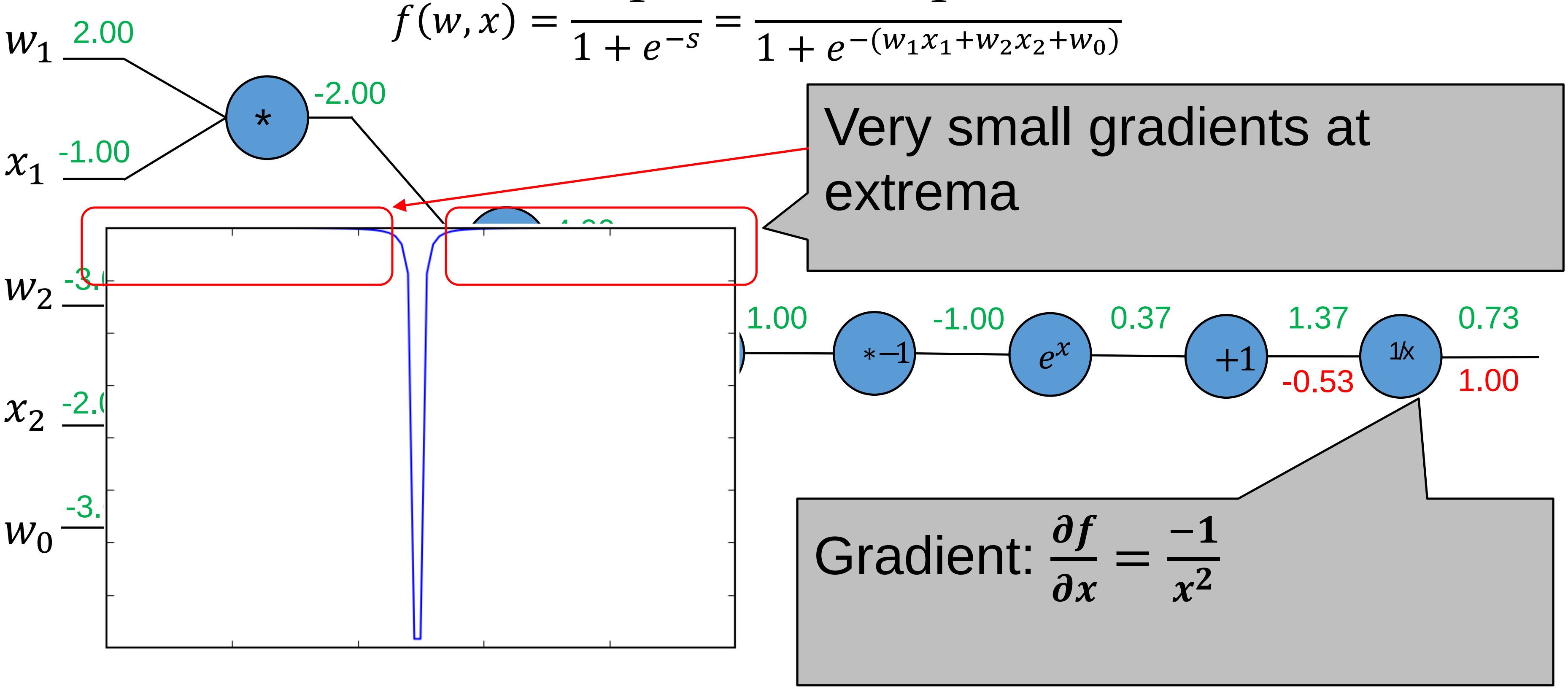
Backprop in “depth”: Backward pass

$$f(w,x) = \frac{1}{1+e^{-s}} = \frac{1}{1+e^{-(w_1x_1+w_2x_2+w_0)}}$$



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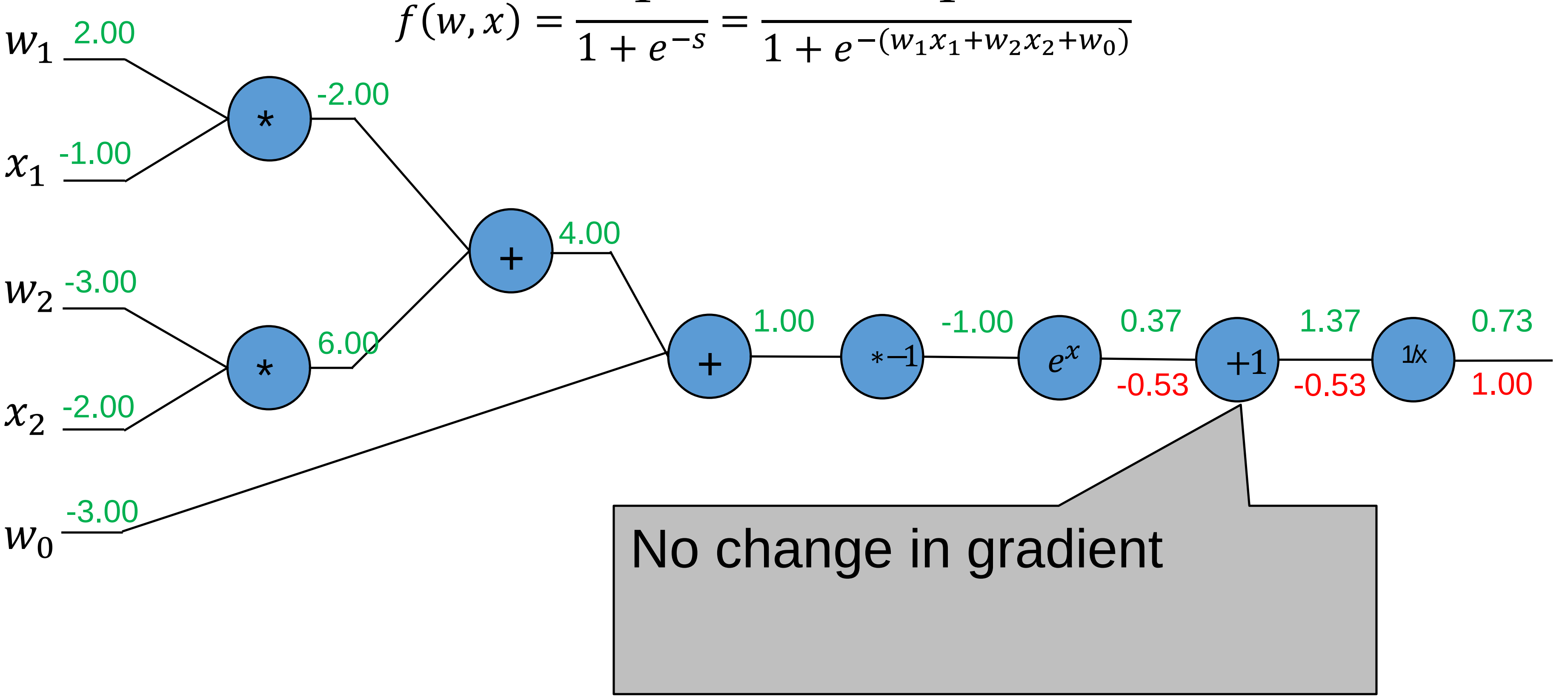
Backprop in "depth": Backward pass

$$f(w,x) = \frac{1}{1+e^{-s}} = \frac{1}{1+e^{-(w_1x_1+w_2x_2+w_0)}}$$



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Backprop in “depth”: Backward pass

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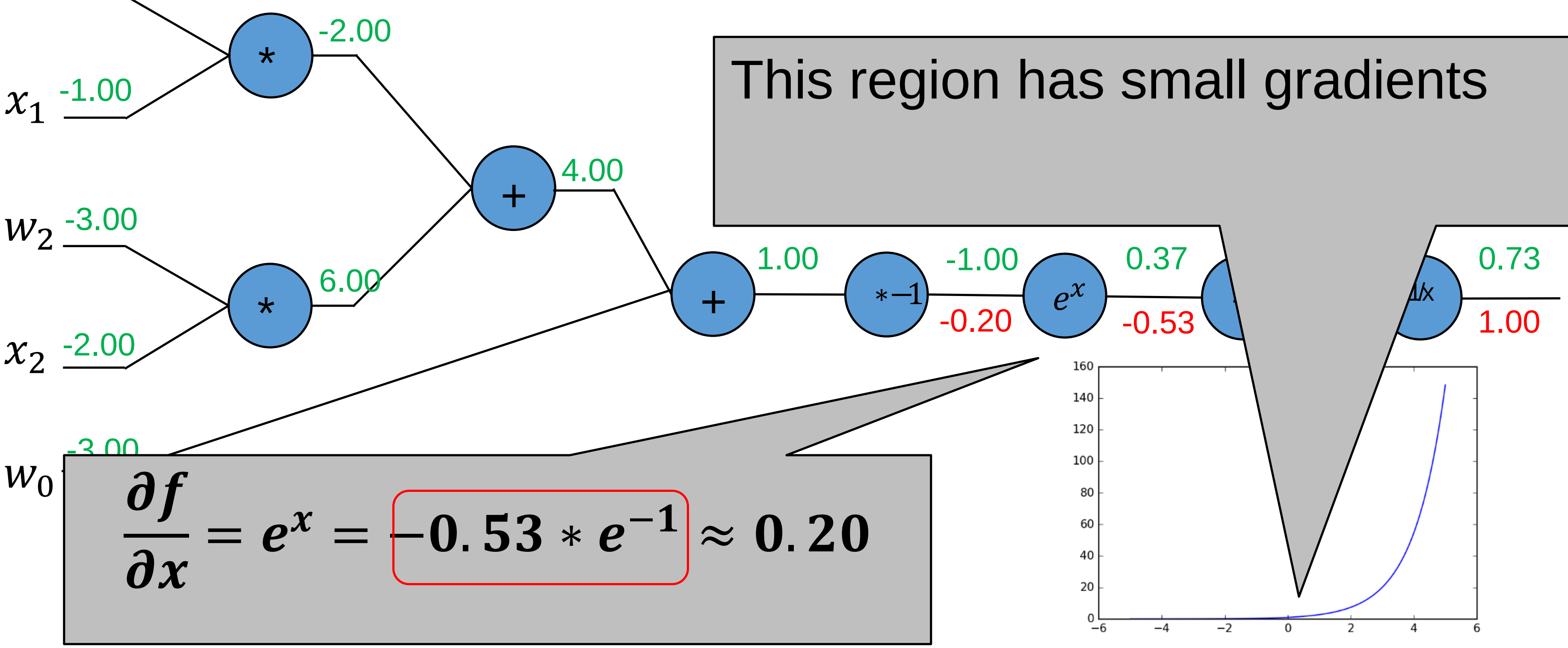

$$\frac{\partial f}{\partial x} = e^x = \boxed{-0.53 * e^{-1}} \approx 0.20$$

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Backprop in "depth": Backward pass

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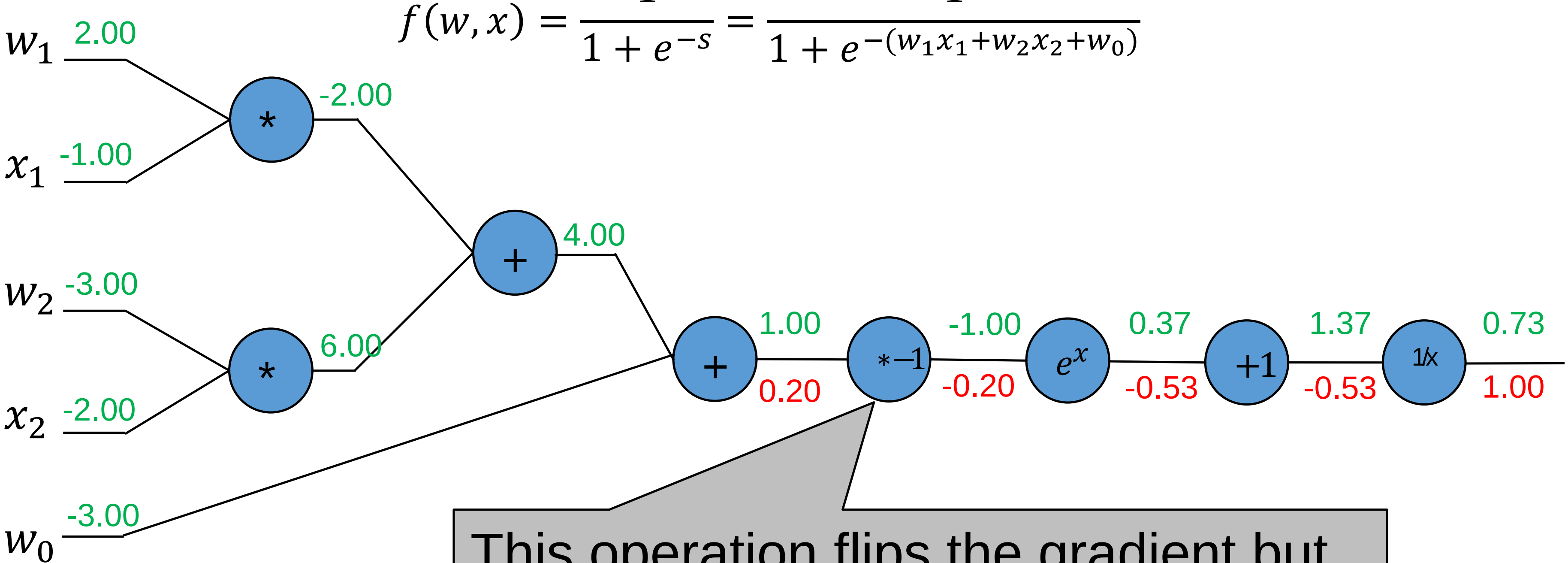

This operation flips the gradient but preserves magnitude

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Backprop in "depth": Backward pass

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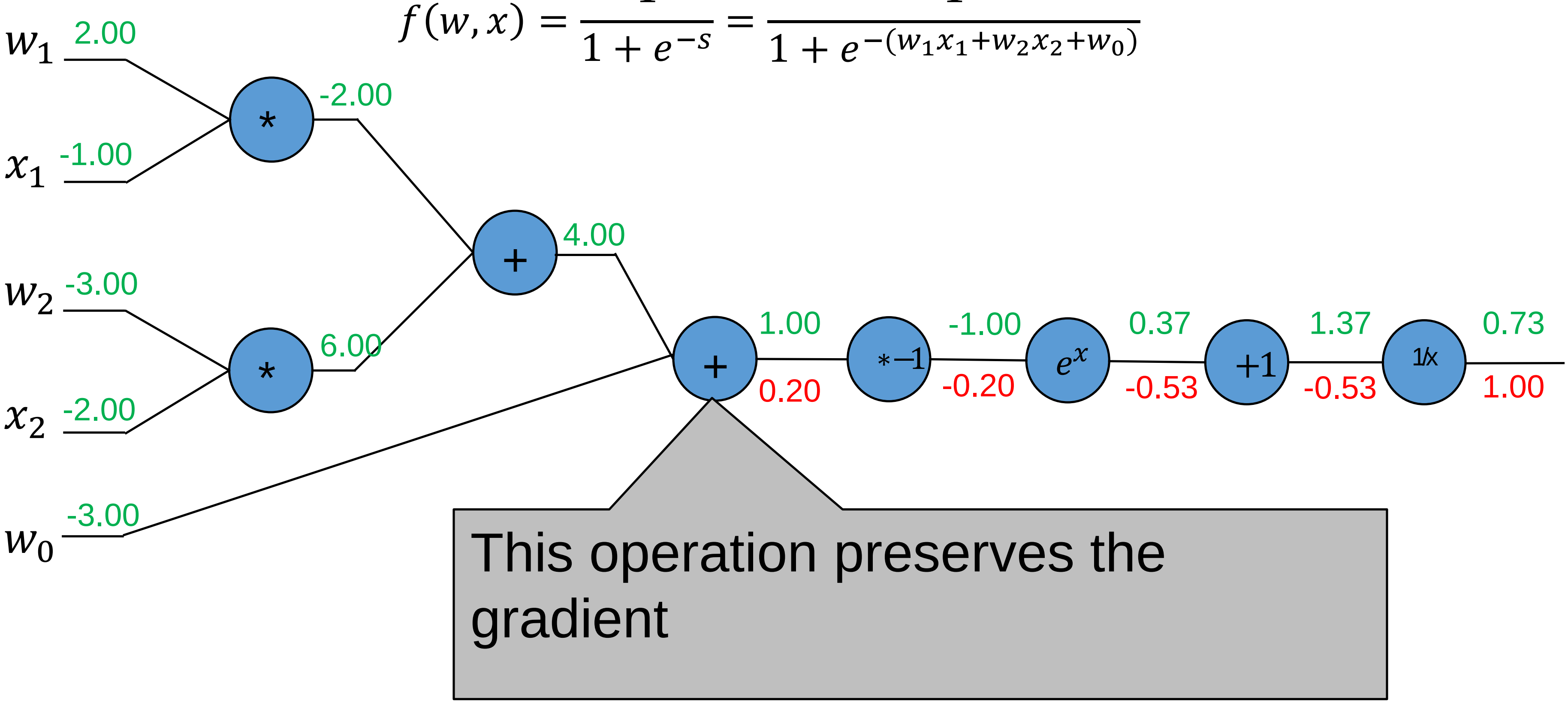

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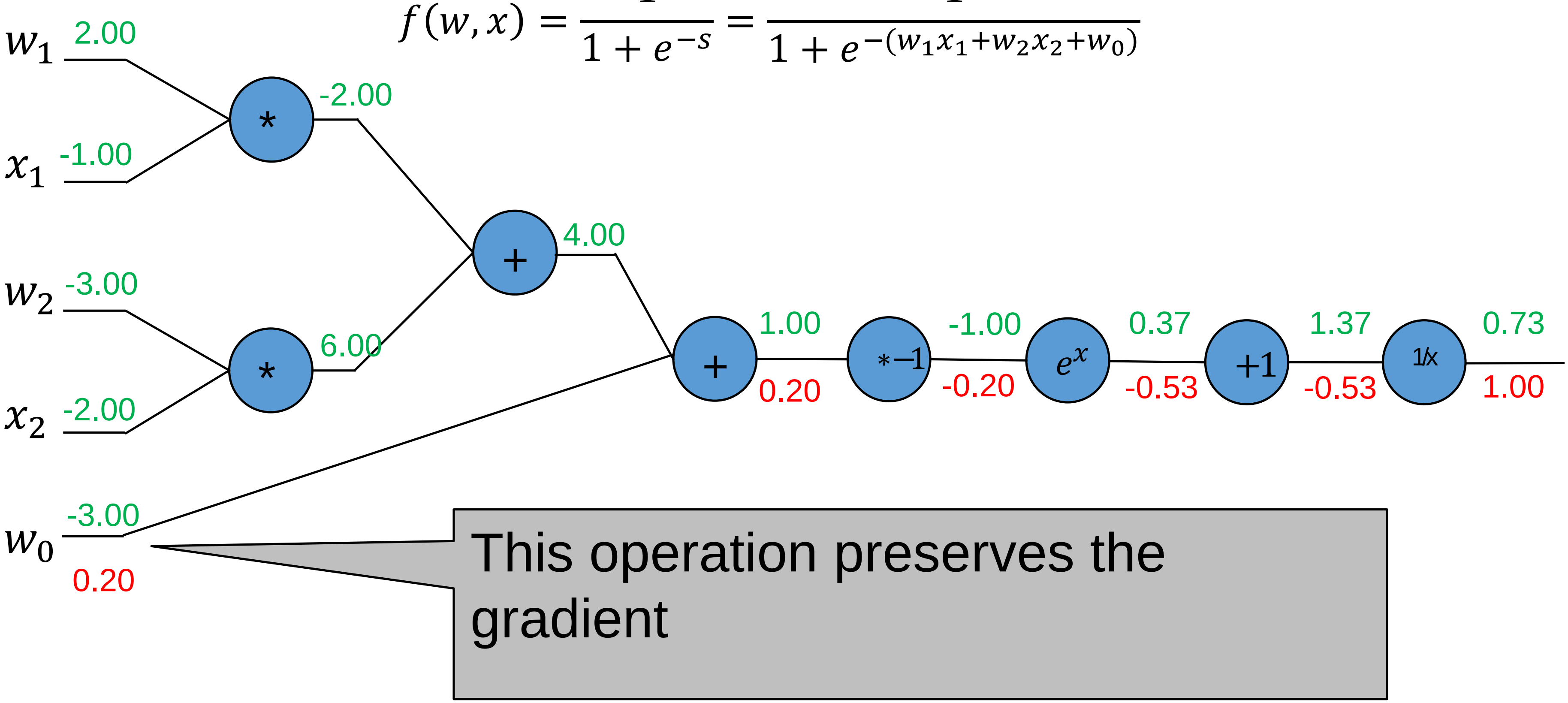

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Backprop in “depth”: Backward pass

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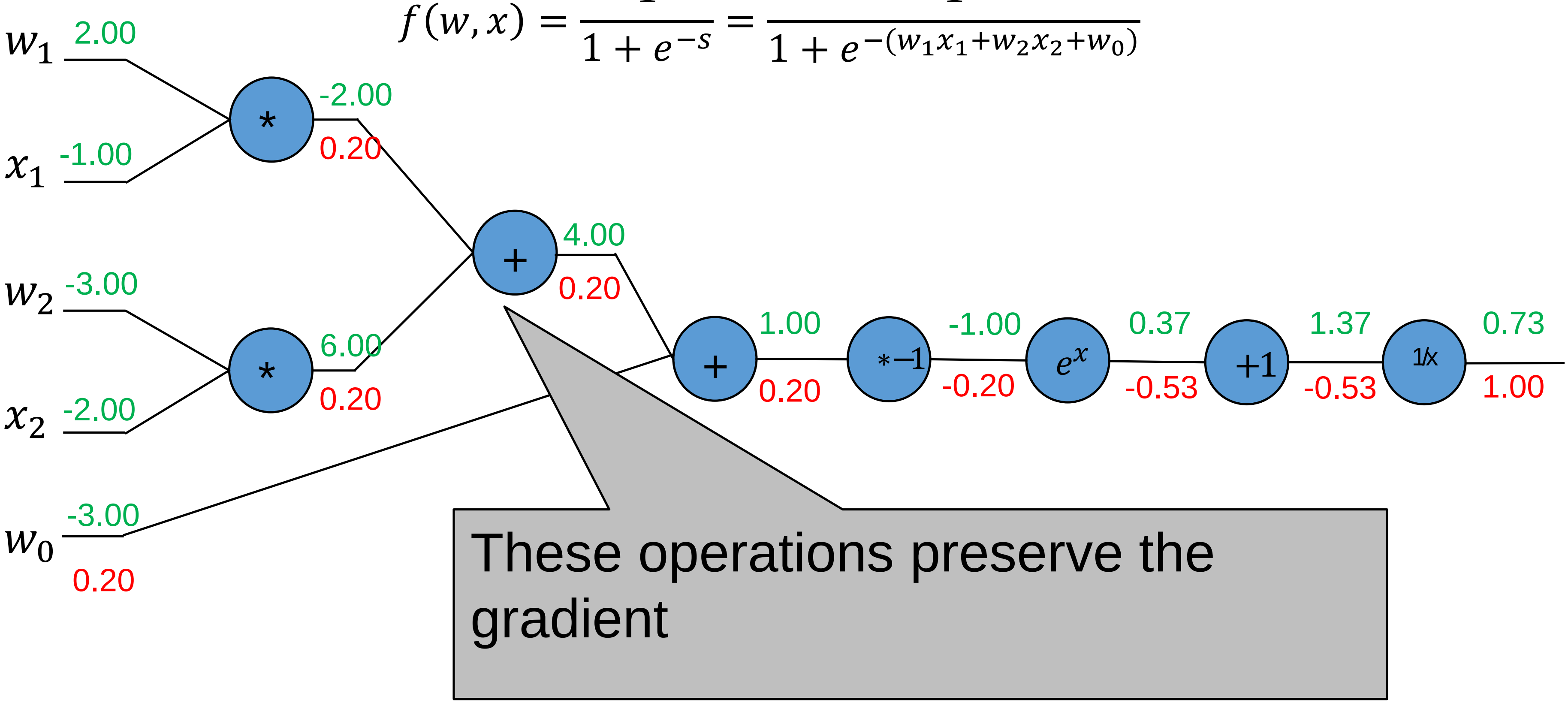

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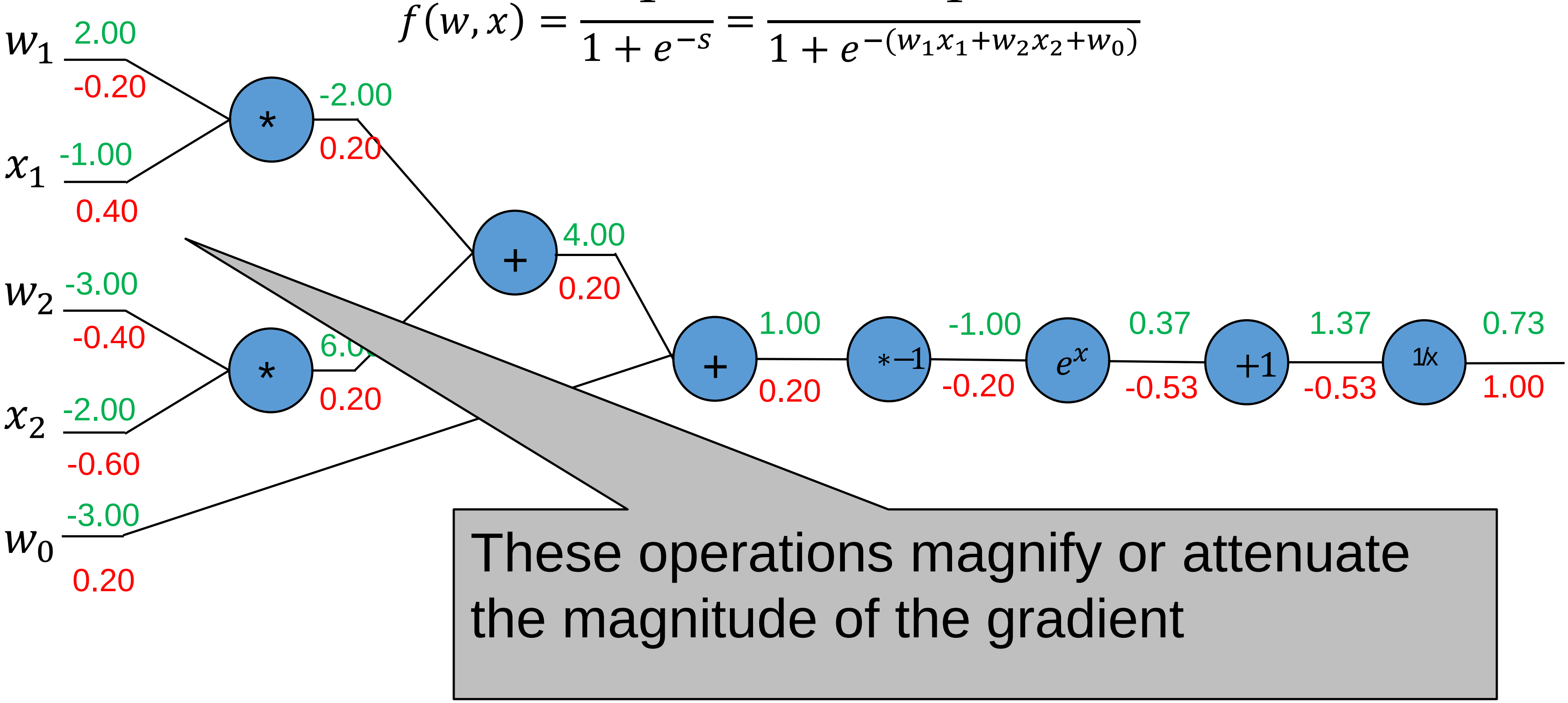
Backprop in "depth": Backward pass

$$f(w,x) = \frac{1}{1+e^{-s}} = \frac{1}{1+e^{-(w_1x_1+w_2x_2+w_0)}}$$



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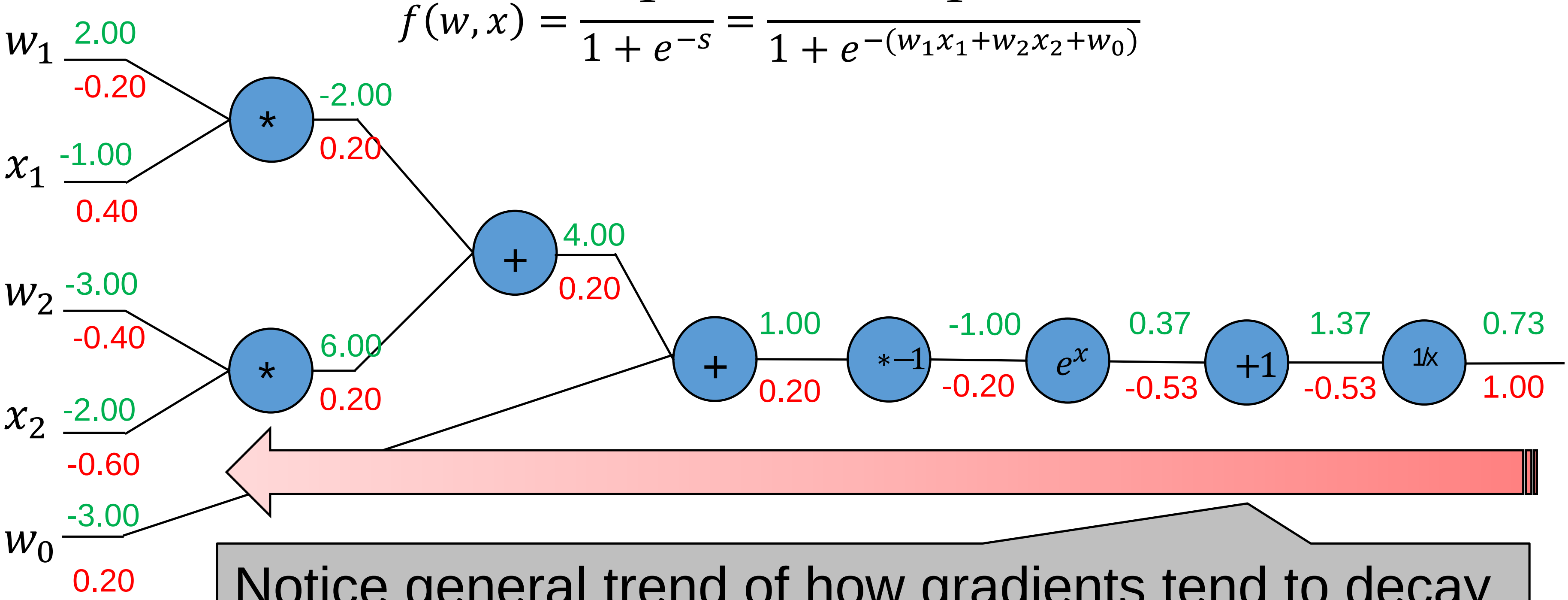
Backprop in “depth”: Backward pass

$$f(w,x) = \frac{1}{1+e^{-s}} = \frac{1}{1+e^{-(w_1x_1+w_2x_2+w_0)}}$$



Notice general trend of how gradients tend to decay in magnitude through layers of backprop… why?

$f(x) = e^x \quad \rightarrow$	$\frac{\partial f}{\partial x} = e^x$	$f(x) = \frac{1}{x} \quad \rightarrow$	$\frac{\partial f}{\partial x} = \frac{-1}{x^2}$
$f_a(x) = ax \quad \rightarrow$	$\frac{\partial f}{\partial x} = a$	$f_c(x) = c + x \quad \rightarrow$	$\frac{\partial f}{\partial x} = 1$

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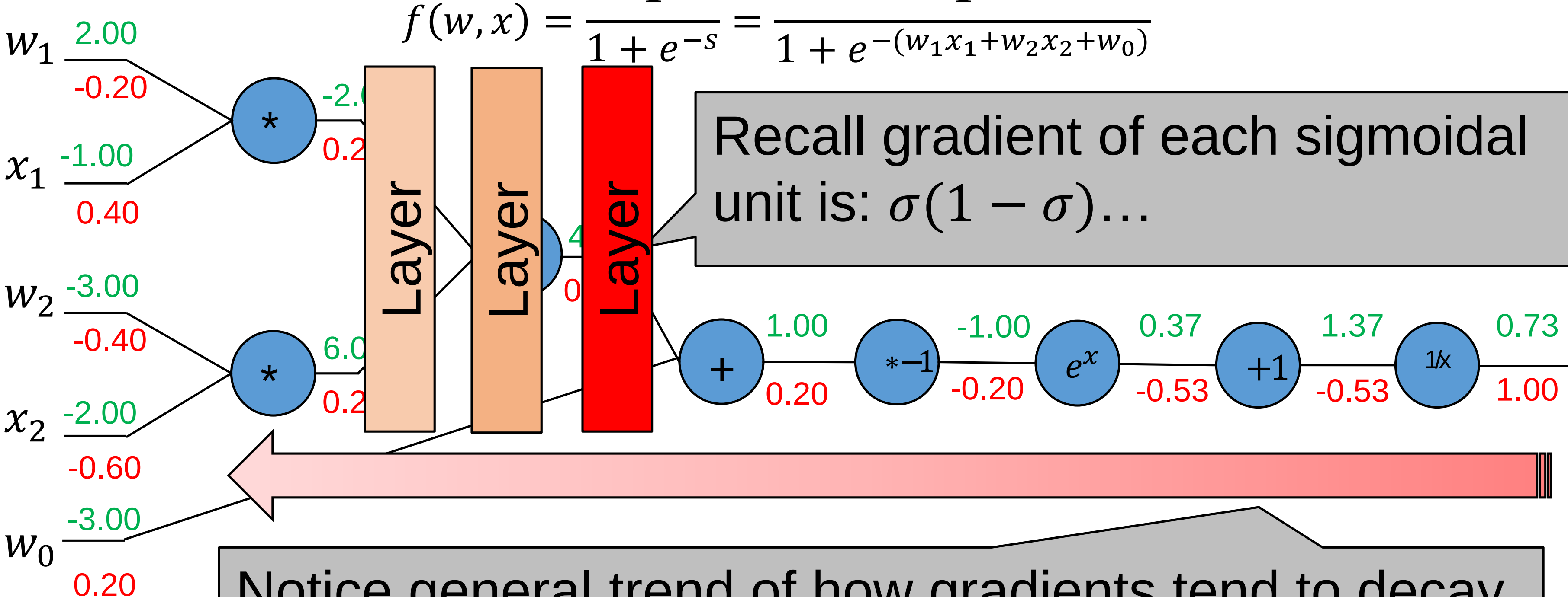

Recall gradient of each sigmoidal unit is: $\sigma(1-\sigma)$…

Notice general trend of how gradients tend to decay in magnitude through layers of backprop… why?

$f(x) = e^x \quad \rightarrow \quad \frac{\partial f}{\partial x} = e^x$	$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{\partial f}{\partial x} = \frac{-1}{x^2}$
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Backprop in "depth": Backward pass

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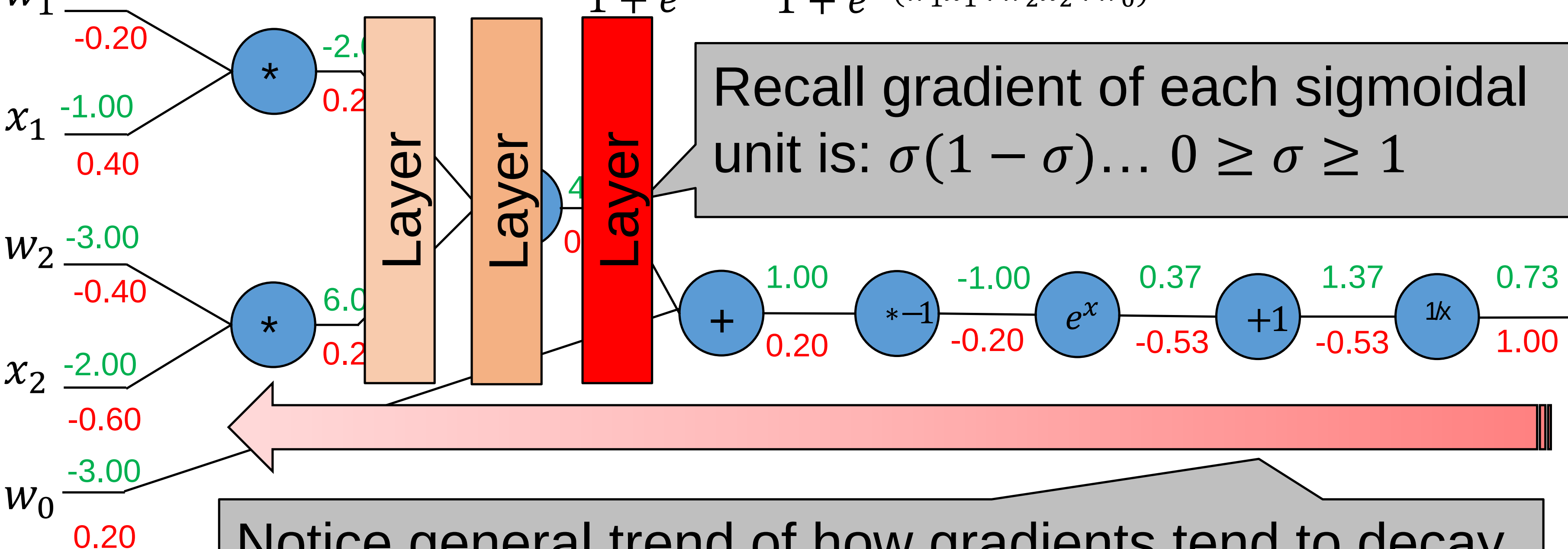

Recall gradient of each sigmoidal unit is: $\sigma(1-\sigma)\ldots\ 0 \geq \sigma \geq 1$

Notice general trend of how gradients tend to decay in magnitude through layers of backprop… why?

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Backprop in “depth”: Backward pass

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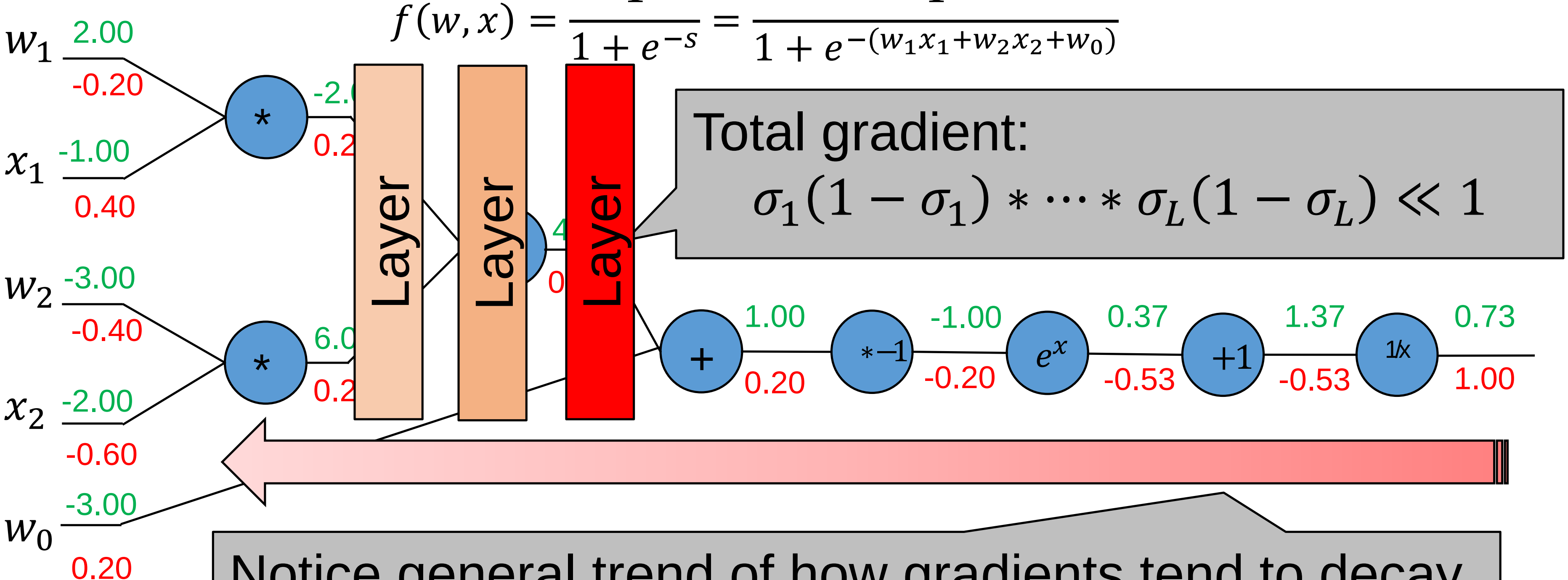

Total gradient:

$$\sigma_1(1-\sigma_1) * \cdots * \sigma_L(1-\sigma_L) \ll 1$$

Notice general trend of how gradients tend to decay in magnitude through layers of backprop… why?

$f(x) = e^x$	$\rightarrow$	$\frac{\partial f}{\partial x} = e^x$	$f(x) = \frac{1}{x}$	$\rightarrow$	$\frac{\partial f}{\partial x} = \frac{-1}{x^2}$
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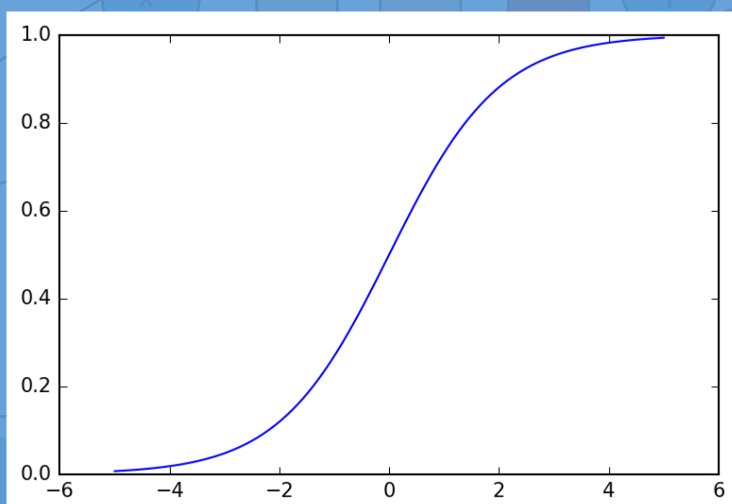
Backprop in "depth": Backward pass

$$f(w,x) = \frac{1}{1+e^{-s}} = \frac{1}{1+e^{-(w_1x_1+w_2x_2+w_0)}}$$

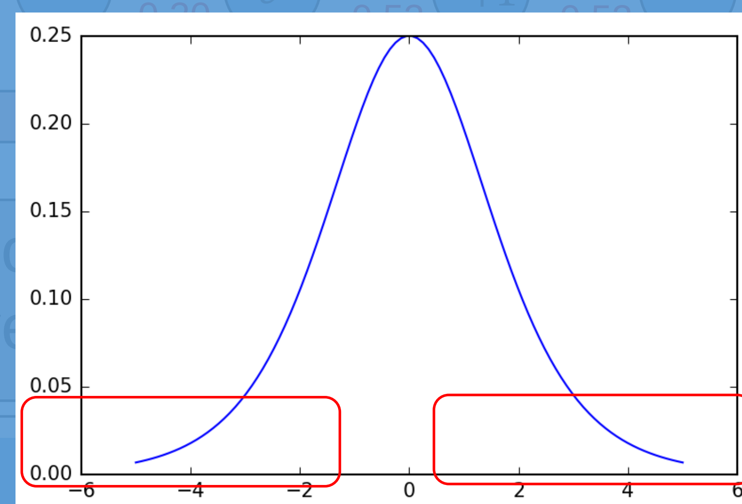
The overall effect is that gradients decay with each layer of sigmoidal activations.

→ Training slows down a lot at extrema

$\sigma(s)$



$\sigma'(s) = \sigma(s)(1-\sigma(s))$



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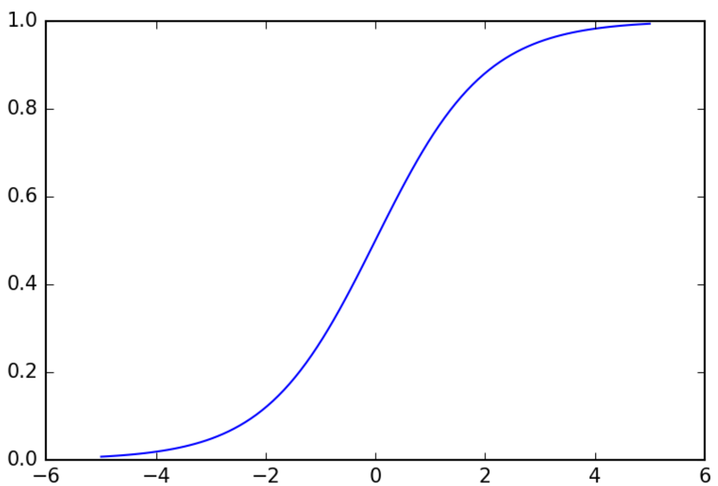
Active regions of Sigmoids

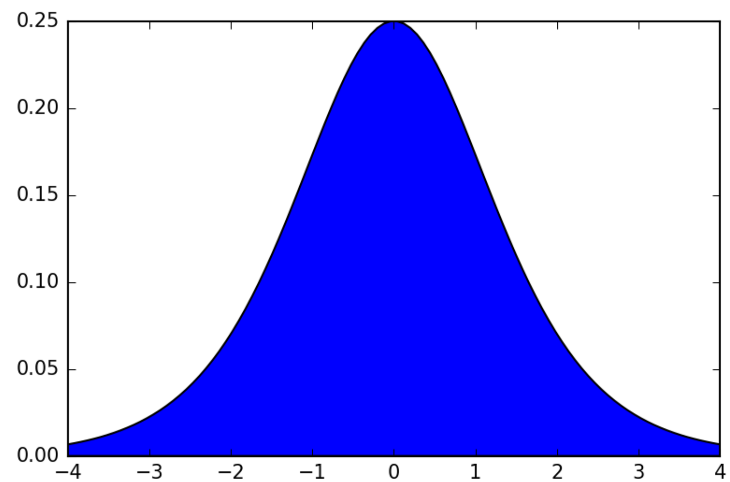
- Sigmoids are relatively effective in active region
- > 95% of gradient density in $\sigma'(s)$ is in [-4,4]

→ Idea: keep sigmoid activations in this active region

$$\sigma(s)$$



$$\sigma'(s) = \sigma(s)(1 - \sigma(s))$$



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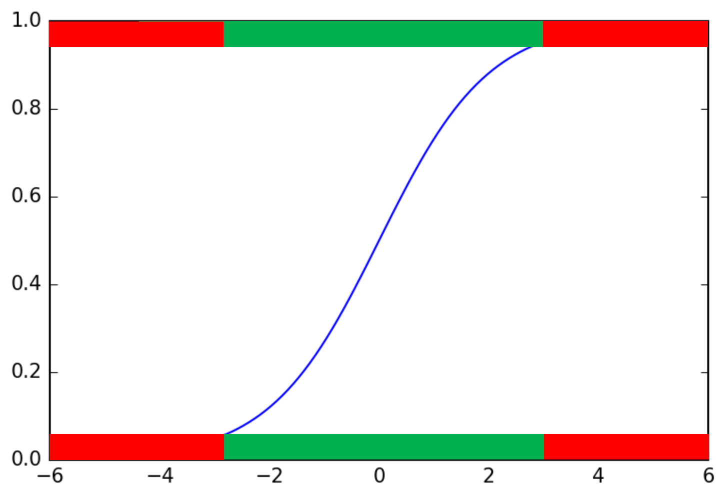
Active regions of Sigmoids

- Idea: keep sigmoid activations in this active region

$$f(w,x) = \frac{1}{1+e^{-s}} = \frac{1}{1+e^{-(w_1x_1+w_2x_2+w_0)}}$$

This means that: $-3 \leq w_1x_1 + w_2x_2 + w_0 \leq 3$

$\sigma(s)$



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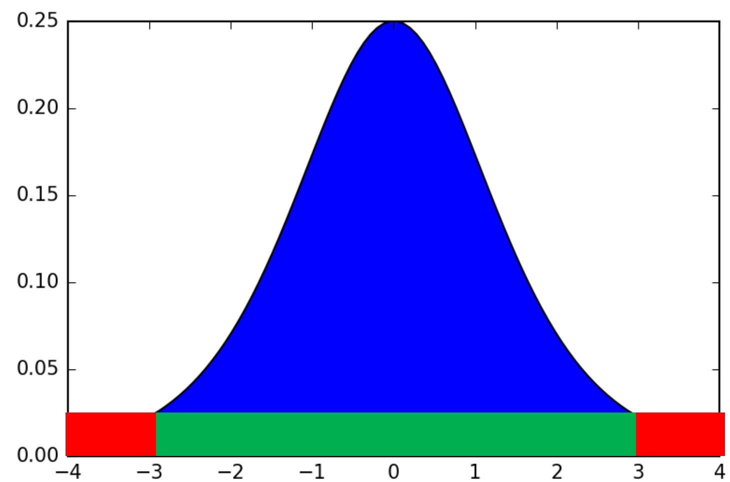

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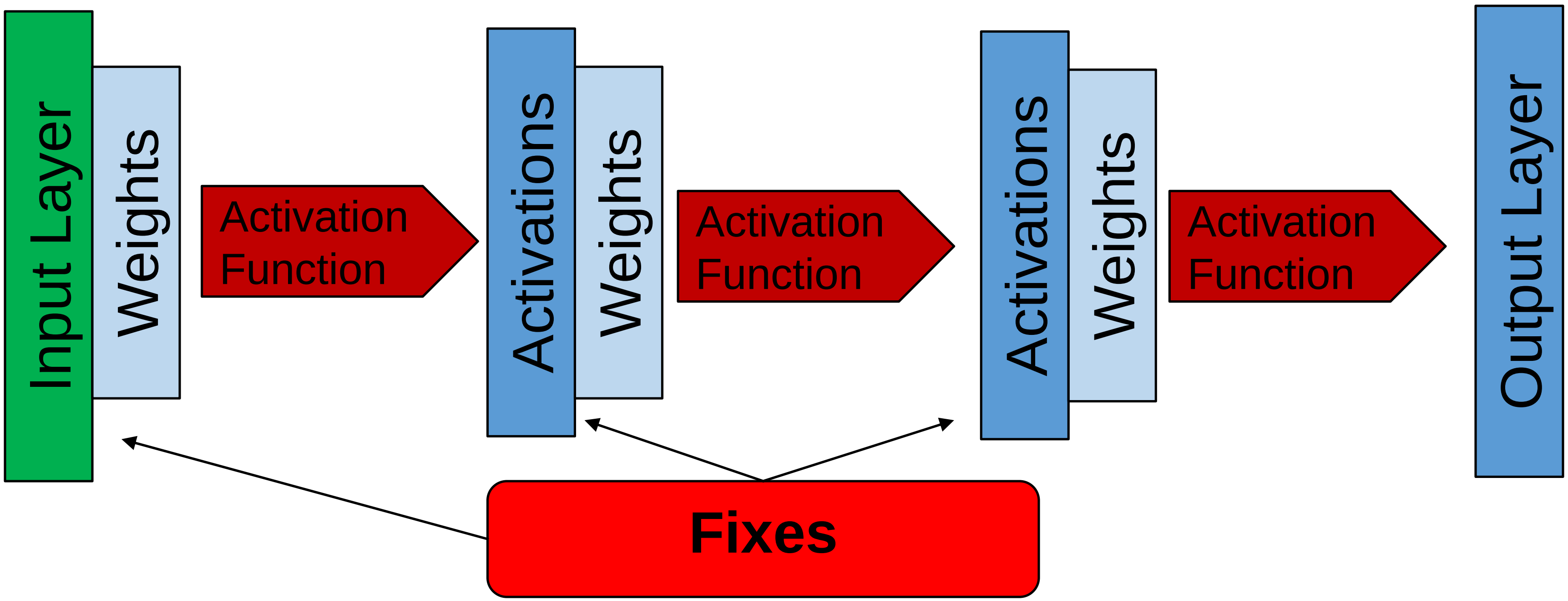
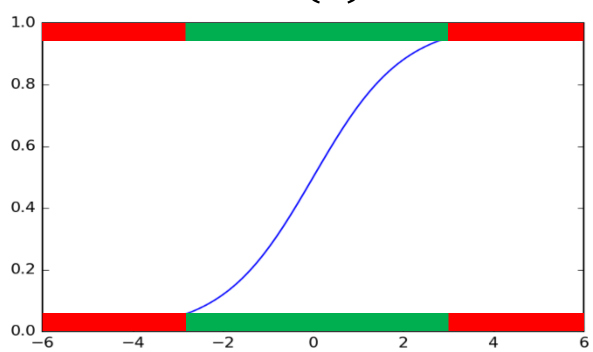
Keeping Sigmoids in active region



$\sigma(s)$



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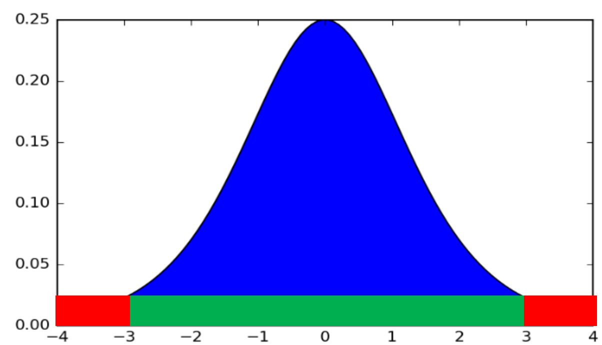


Simple fix: Clip gradients

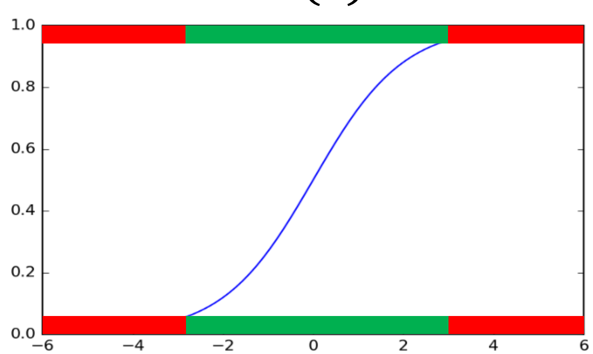
Very simple fix:
If $\sigma'(s)$ < 0.01 → $\sigma'(s) = 0.01$
We can set this limit arbitrarily

→ This ensures that there will always be a non-saturated gradient

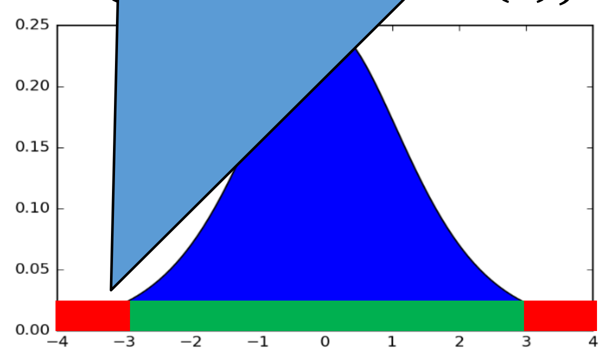
Class: Are there any cons to this approach?

Fixes

$\sigma(s)$



$\sigma'($ … $- \sigma(s))$

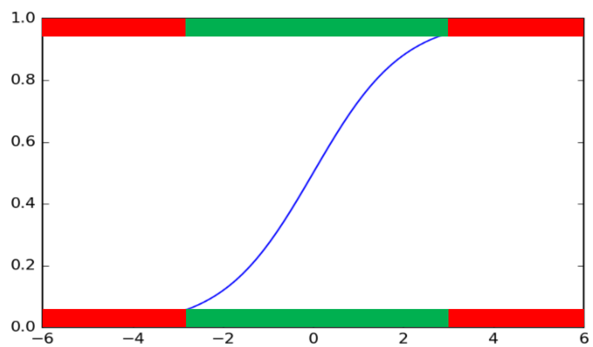


Simple fix: Clip gradients

Class: Are there any cons to this approach?

- If the threshold is set too low, we recover the original sigmoid with the vanishing gradients
- If the threshold is set too high, we get only the linear region and lose the benefit of a nonlinearity,
    - E.g. The matrices can be multiplied out into a single linear layer, thus losing effective depth

$\sigma(s)$



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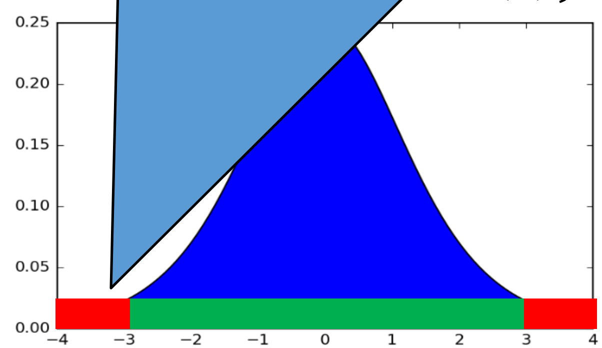
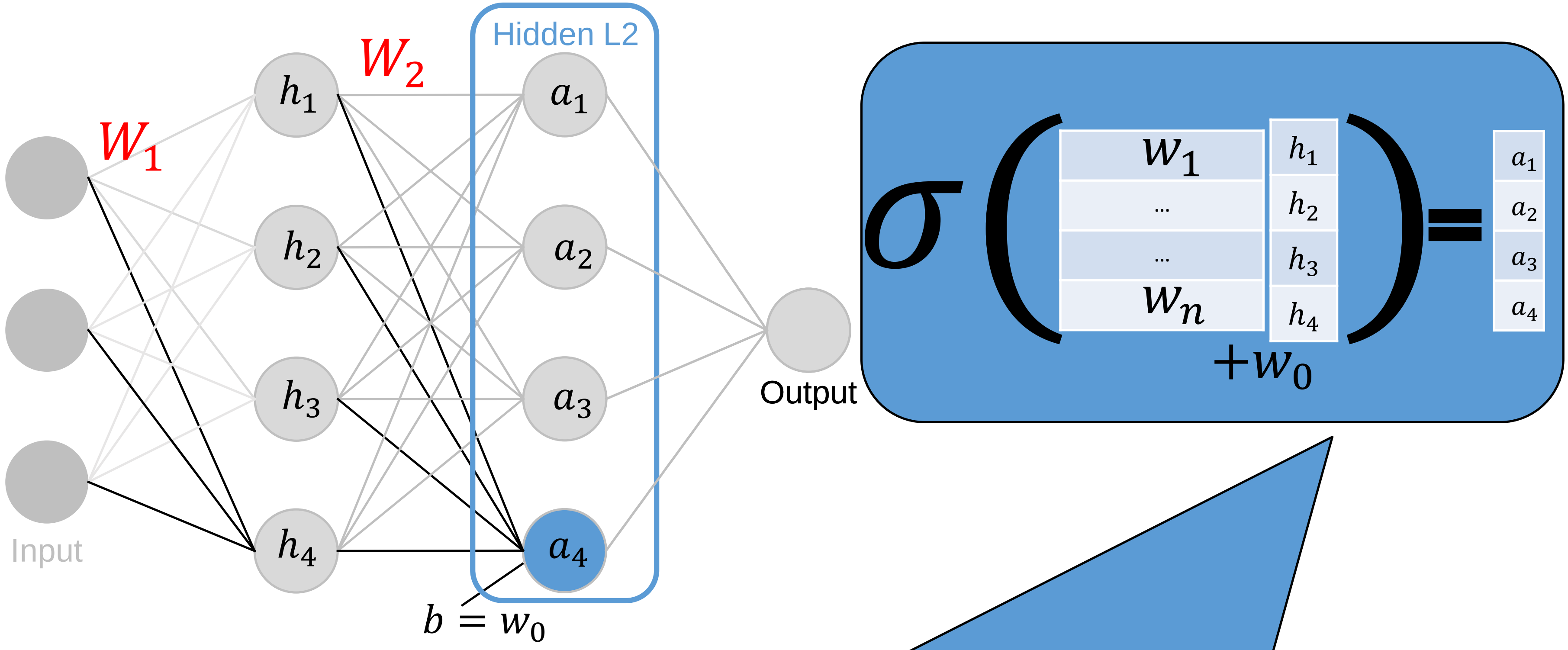


Weight constraints



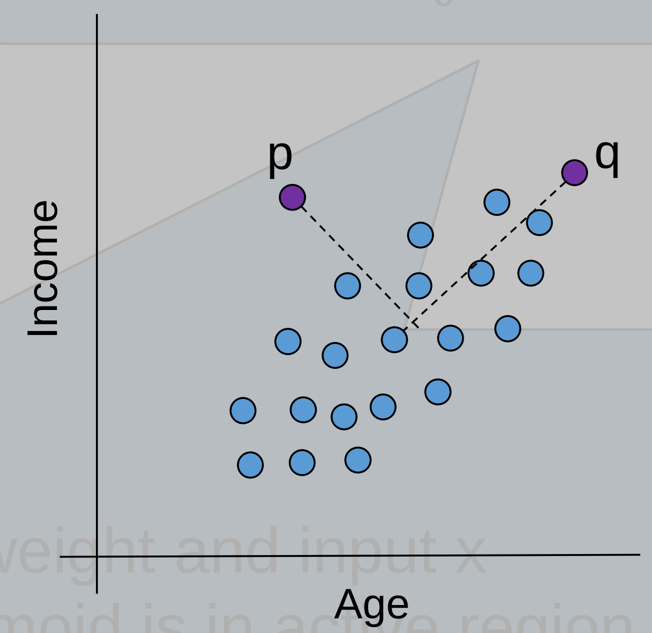
Recall:

- Weights are row vectors
- Each activation is a dot product of weight and input x
- We want $-3 \leq w \cdot x \leq 3$ so that sigmoid is in active region

Bases of a weight matrix

Some insight:

- Weights (rows) of matrix act as a set of basis vectors
- Multiplying ***x*** by the matrix stretches it according to the basis vectors of the matrix



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Eigenvectors of W

Some insight:

- Weights (rows) of matrix act as a set of basis vectors
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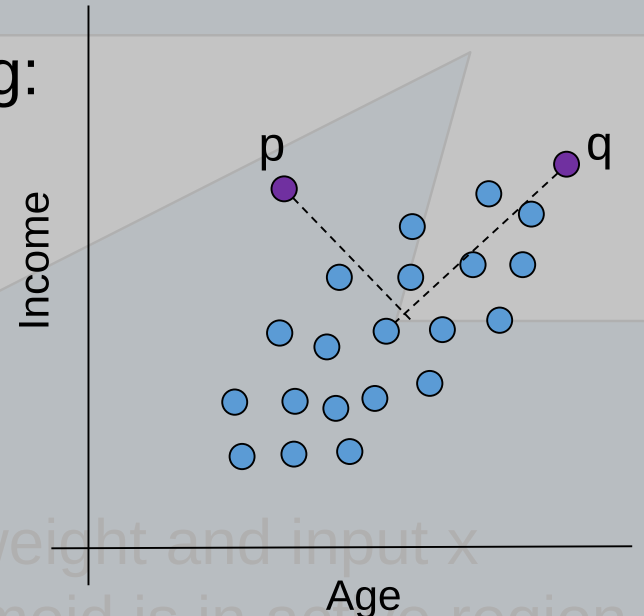
- We can find these bases by solving:

$Ax = \lambda x$



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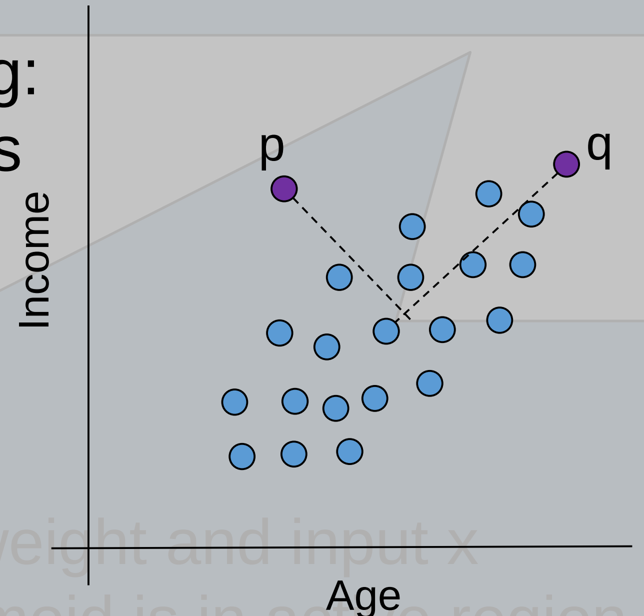
$Ax = \lambda x$ → Eigenvalues, eigenvectors

v_1
…
…
v_n

λ_1			
	λ_2		
		…	
			λ_n



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$$\begin{bmatrix} v_1 \\ \cdots \\ \cdots \\ v_n \end{bmatrix} \quad \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \cdots & \\ & & & \lambda_n \end{bmatrix}$$

Each λ_i acts as a stretch factor. If $\lambda_i < 1$ or $\lambda_i > 1$, then resulting vector shrinks or grows.

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Eigenvectors of W

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Each λ_i acts as a stretch factor. If $\lambda_i < 1$ or $\lambda_i > 1$, then resulting vector shrinks or grows. We want $\lambda_i \approx 1$!

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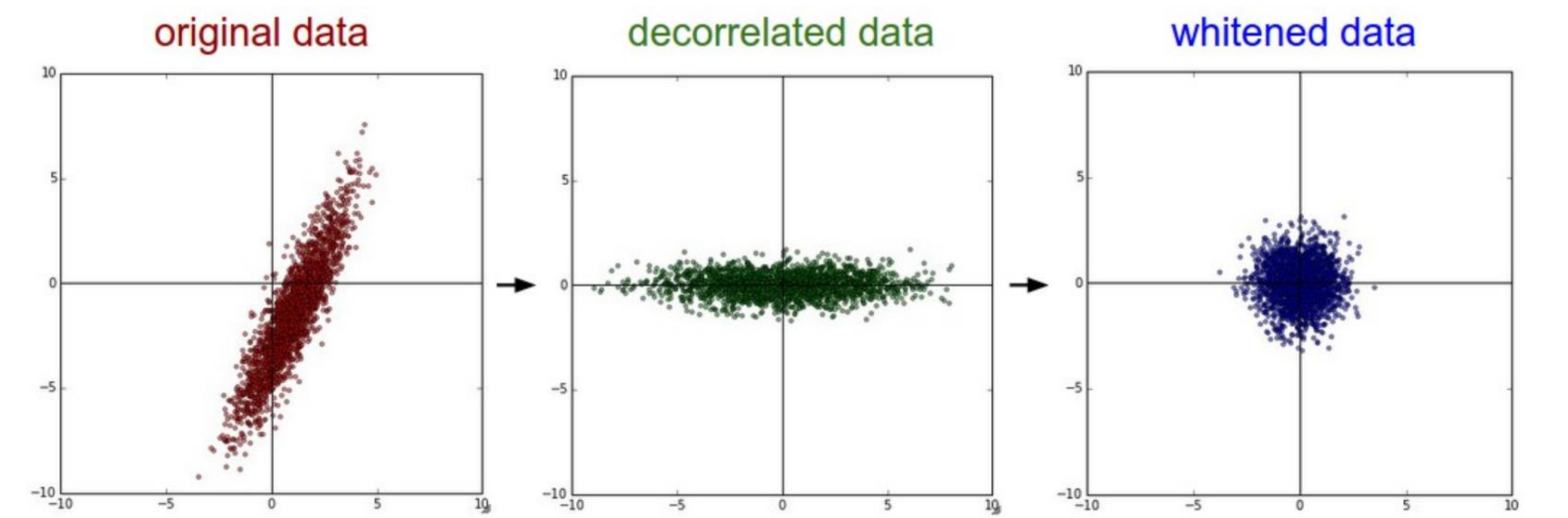
Keeping sigmoids in active region



(data has diagonal covariance matrix)

(covariance matrix is the identity matrix)

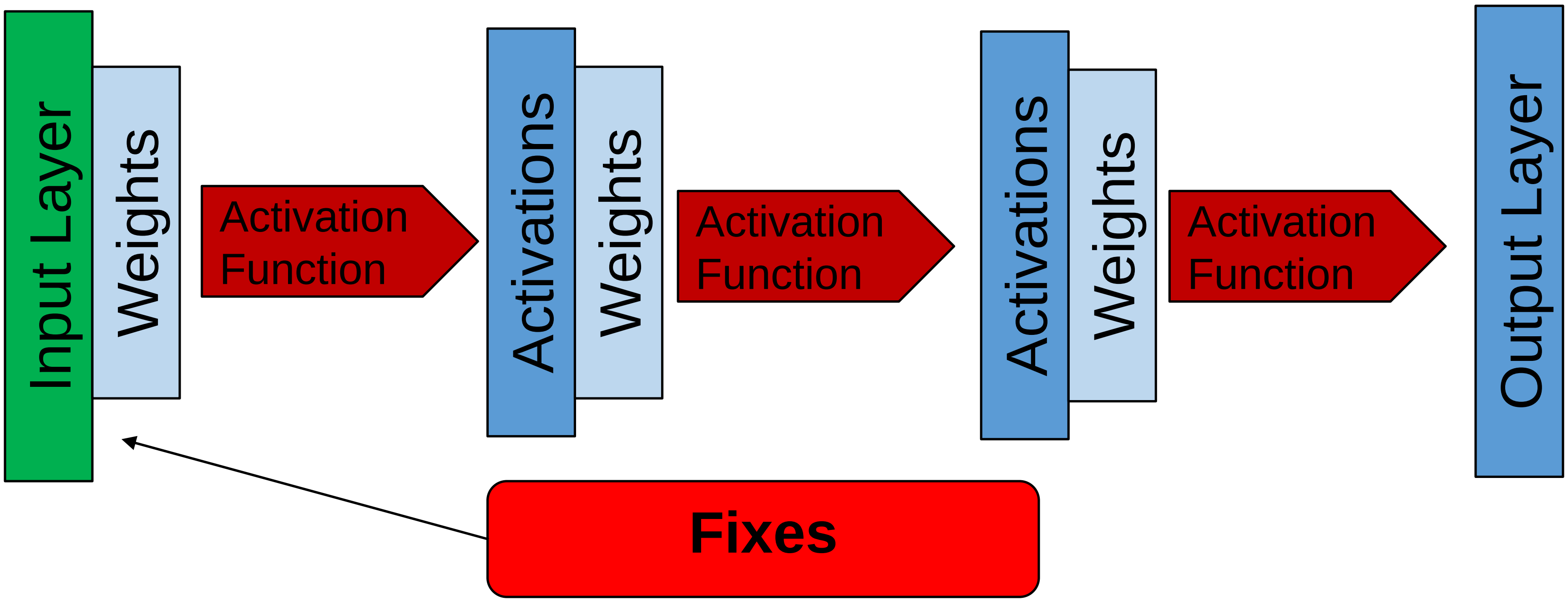
Practical tip:

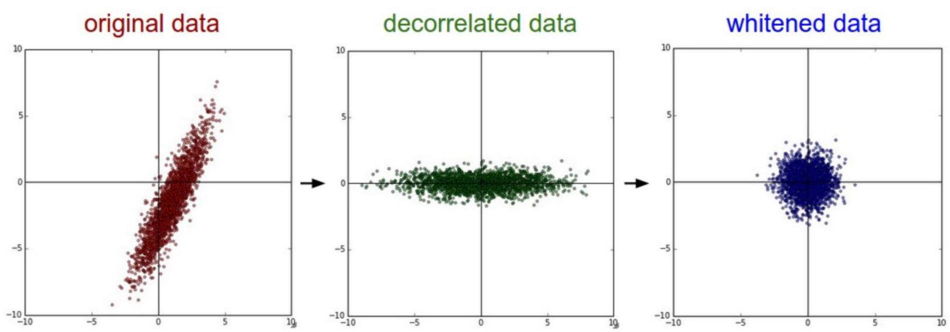
- Subtract data mean(bias=0), Divide by standard deviation
- Whiten data (PCA/ZCA) if possible

See: http://ufldl.stanford.edu/wiki/index.php/Exercise:PCA_and_Whitening

- Keeps activations at each layer in an active region

Keeping sigmoids in active region





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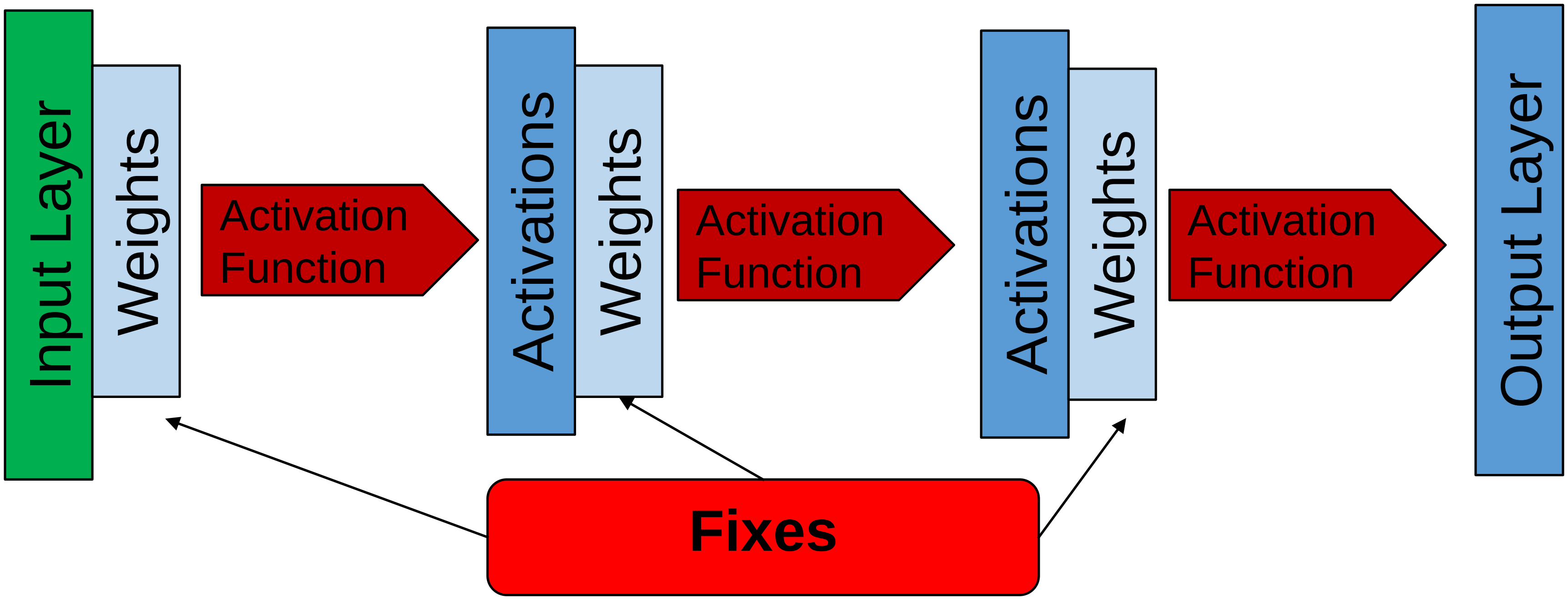
Keeping sigmoids in active region



- What about weights?
- Weights are usually initialized randomly
- Poor initialization can lead to small/large eigenvalues and shrinkage/explosion of gradients
- **Practical fix:** Initialize weights with $\mu = 0, \sigma \ll 1$

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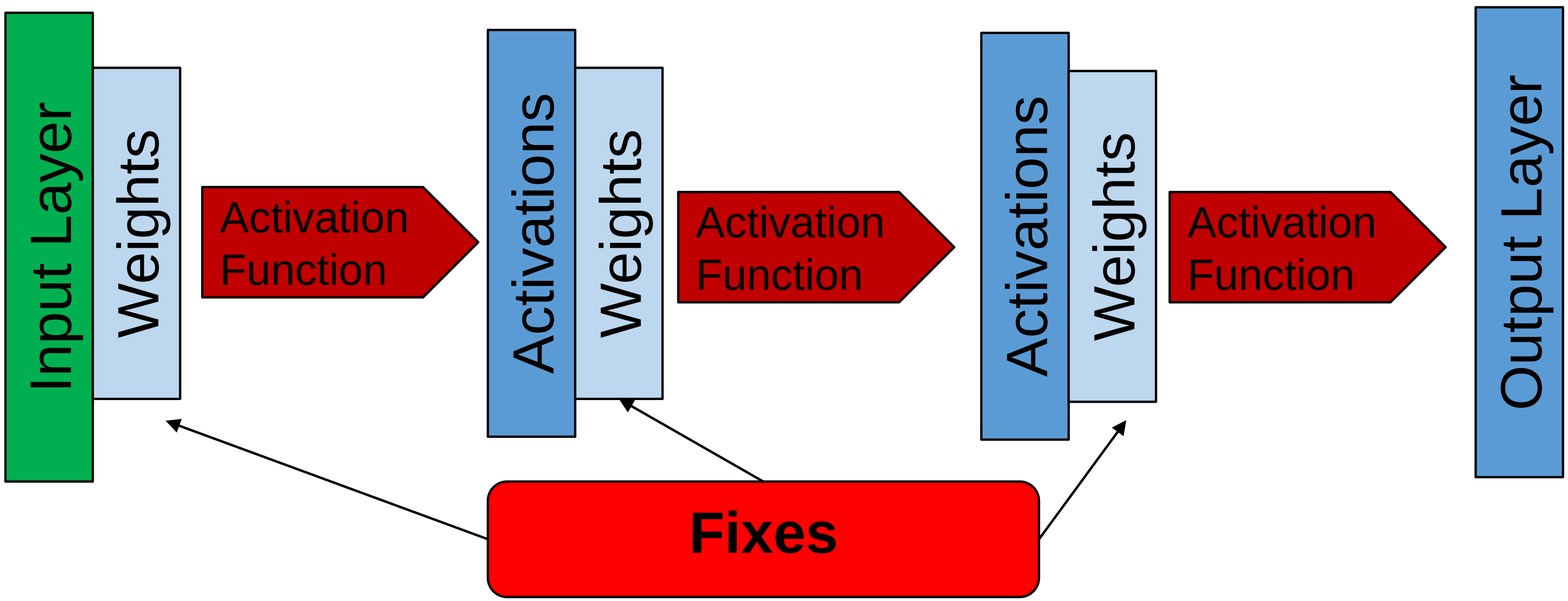
Keeping sigmoids in active region



- $f(w,x) = \sum_i w_i x_i$. Scale of output is determined by fan-in. Suppose $w_i x_i$ is Gaussian distributed with μ_i, σ_i. $\sigma^2 = \sum_{i=1}^{n} \sigma_i^2 = n\sigma^2$. We overshot by $\sqrt(n)$.
- **Theory:** Normalize inputs by fan-in $\sigma_i/\sqrt(n)$ to maintain unit variance in output.

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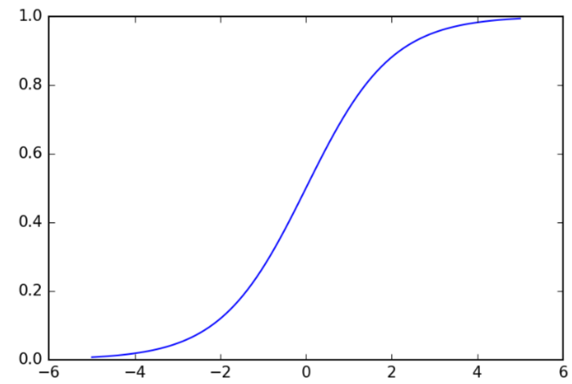
Nature of the logistic activation

- $0 \leq \sigma(\sum_i w_i x_i) \leq 1$

$\sigma(s)$



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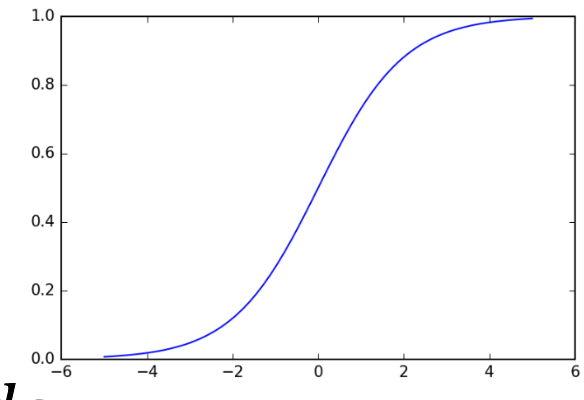
Nature of the logistic activation

- $0 \leq \sigma(\sum_i w_i x_i) \leq 1$
- Inputs at next layer are always positive
- How does that constrain the gradients? $\sigma'(s) = \sigma(s)\big(1 - \sigma(s)\big)ds$

$\sigma(s)$



Nature of the logistic activation

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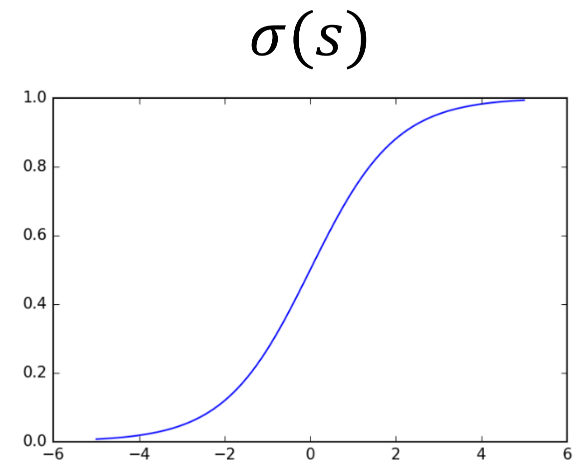
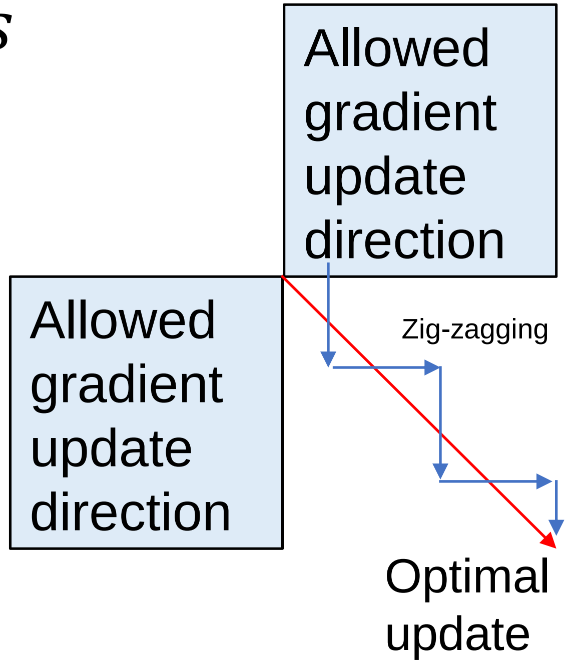
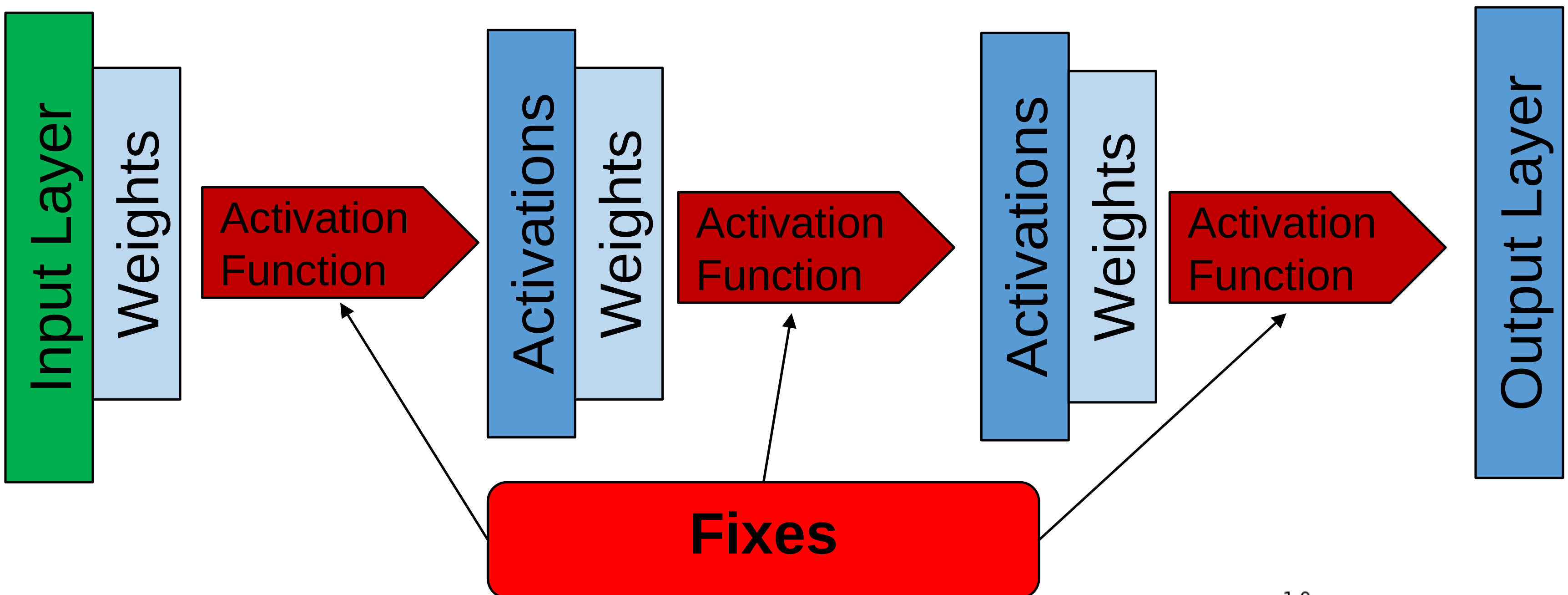
- Inputs at next layer are always positive
- How does that constrain the gradients? $\sigma'(s) = \sigma(s)\big(1 - \sigma(s)\big)ds$
- Depending on the sign of ds, gradients are always all positive or all negative





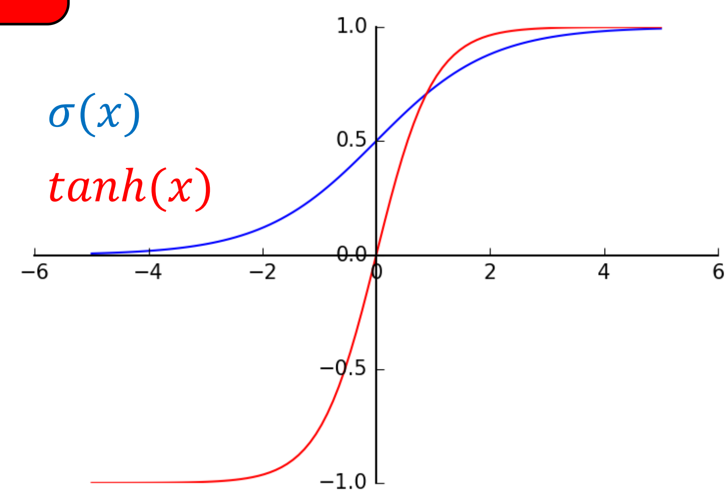
Tanh(x)



Advice: Choose a mean-centered Activation function

$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = 2\sigma(2x) - 1$$

- Addresses data centering issue (if input is zero mean)
- Addresses zigzag issue (activation can be negative)
- Does not address vanishing gradients



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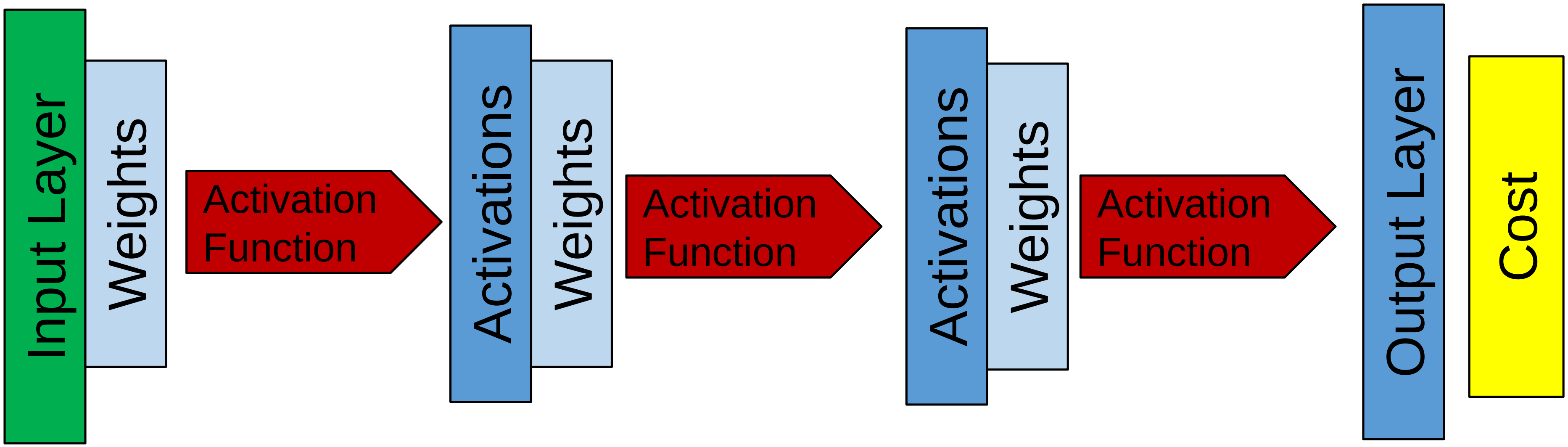
Cost function



- What about the cost function?
- We’ve been using $MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - t_i)^2$
- Derivative of MSE: $2(y_i - t_i)\ dy$

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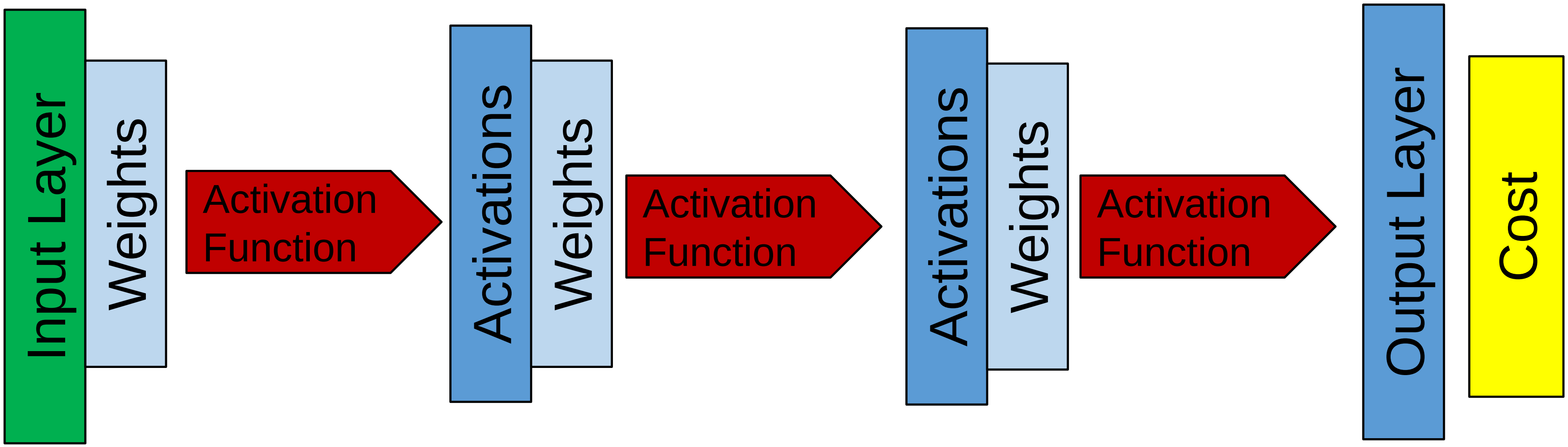
Cost function



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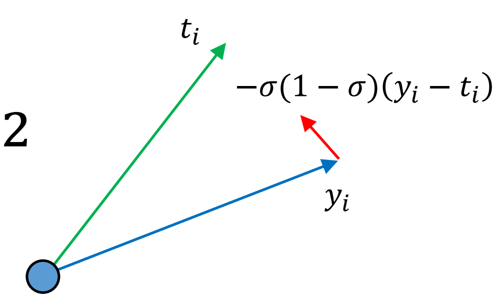

Measure of disagreement between prediction y and target t

$dy = \sigma(1-\sigma)$
Derivative of activation function. Remember that this is **SLOW**.

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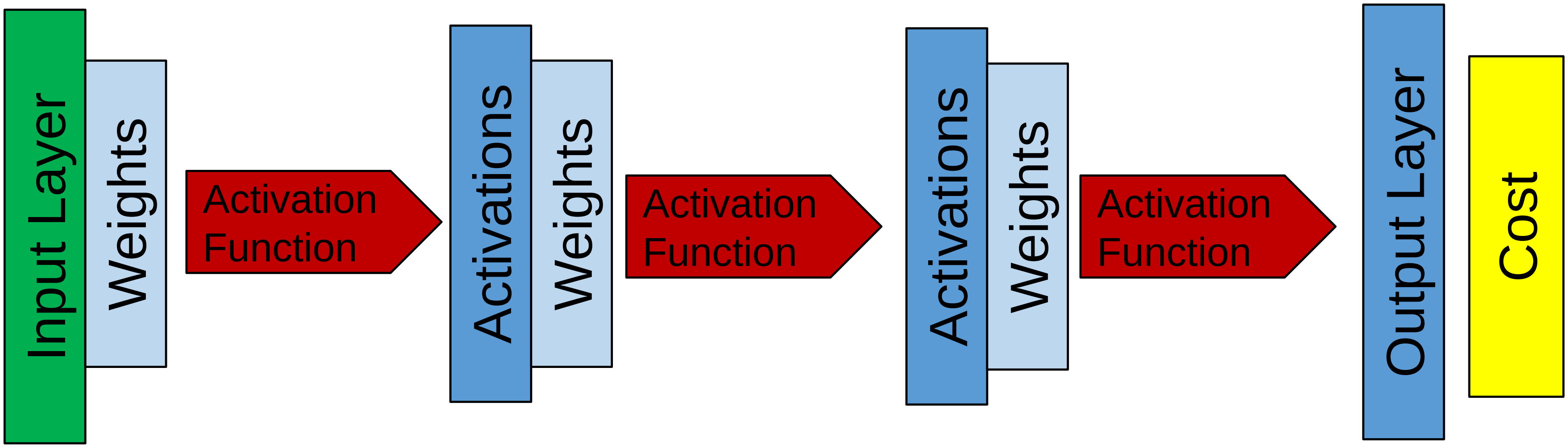
Cost function



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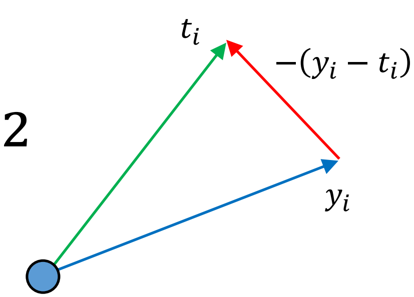
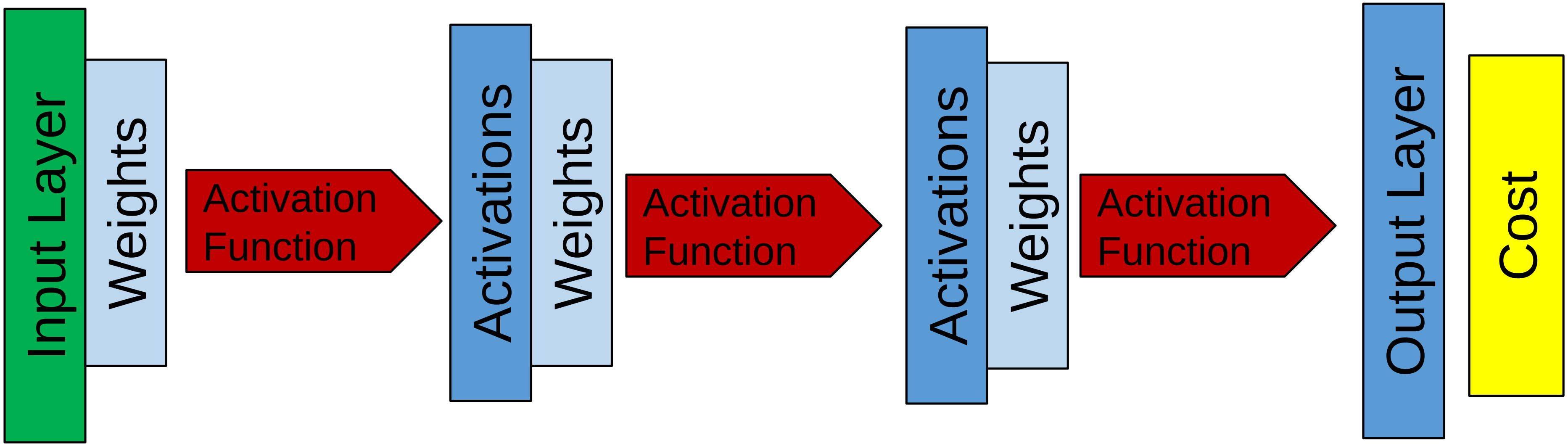


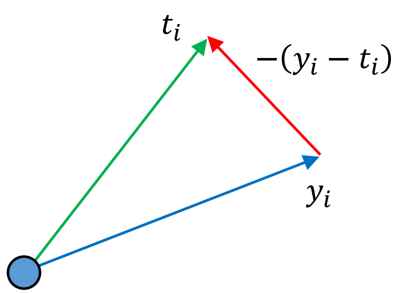
Measure of disagreement between prediction y and target t. Let's KEEP this.

And find a way to eliminate or at least speed up this…

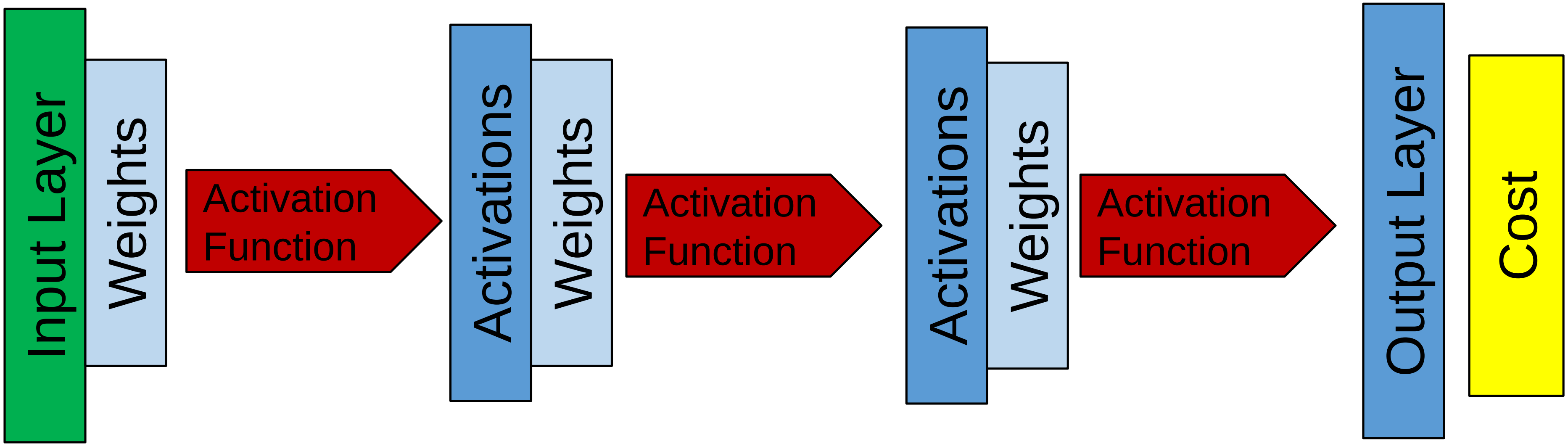
Keeping sigmoids in active region



- Desired gradient: $\partial E = y - t$



Keeping sigmoids in active region



- Desired gradient: $\partial E = y - t$
- Cross entropy cost: $E = -t \ln y \, - (1 - t)\ln(1 - y)$

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Cross entropy in depth

- $E = -\frac{1}{n}\sum_x t \ln \sigma(z) + (1-t)\ln(1-\sigma(z))$
- $\frac{\partial E}{\partial w_j} = -\frac{1}{n}\sum_x \left(\frac{t}{\sigma(z)} - \frac{1-t}{1-\sigma(z)}\right)\sigma'(z)x_j$
- $= -\frac{1}{n}\sum_x \left(\frac{t(1-\sigma(z))-(1-t)\sigma(z)}{\sigma(z)(1-\sigma(z))}\right)\sigma(z)(1-\sigma(z))x_j$
- $= -\frac{1}{n}\sum_x \left(\frac{t \cancel{-t\sigma(z)} - \sigma(z) + \cancel{t\sigma(z)}}{\cancel{\sigma(z)(1-\sigma(z))}}\right)\cancel{\sigma(z)(1-\sigma(z))}x_j$
- $= \frac{1}{n}\sum_x(\sigma(z)-t)x_j$
- → Slow $\sigma'(z)$ cancels out!
- See Nielsen Ch 3 for details: http://neuralnetworksanddeeplearning.com/chap3.html
- Also read Nielsen Ch 3 to learn where cross entropy comes from

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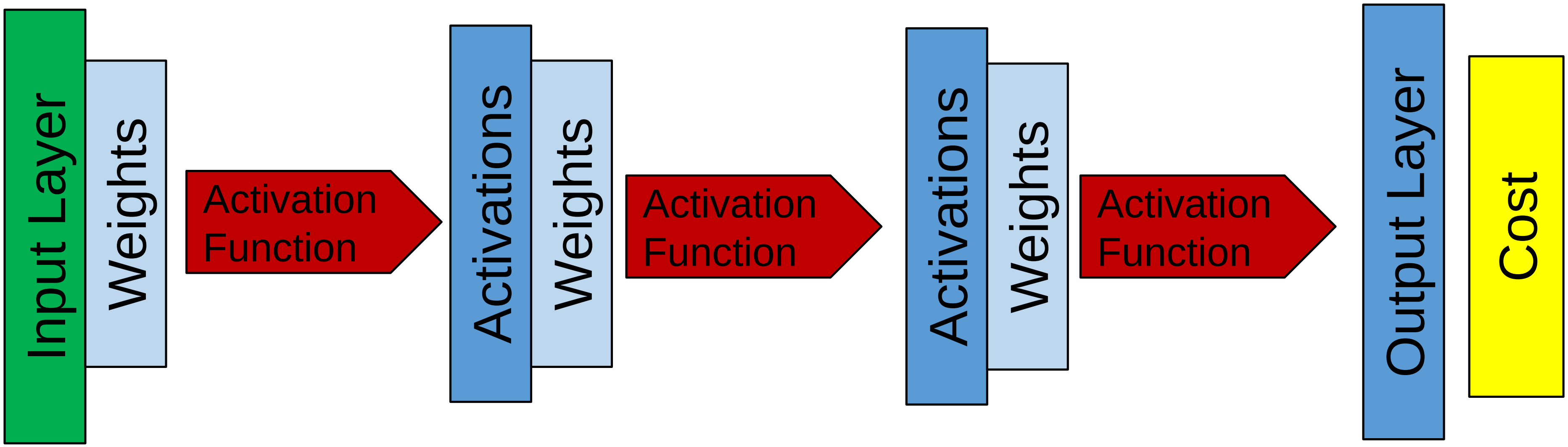
Keeping sigmoids in active region



- Cross entropy cost: $E = -t \ln y - (1-t)\ln(1-y)$
- Cross entropy gradient: $\partial E = y - t$

  MSE gradient: $\partial E = (y-t)\boxed{dy}$

  $dy = \sigma(1-\sigma)$
  Derivative of activation function
- Gradient is proportional to difference
- No learning slowdown due to sigmoid gradients

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But how did we get cross entropy?

- Using $\sigma'(z) = \sigma(z)\big(1 - \sigma(z)\big) = a(1 - a)$
- We'd like the $a(1 - a)$ to cancel out of the cost, so
- $\frac{\partial E}{\partial a} = \frac{a-y}{a(1-a)}$

a-y is just the discrepancy between the prediction y and actual value t. a(1-a) cancels out with the derivative.

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But how did we get cross entropy?

- Using $\sigma'(z) = \sigma(z)\big(1-\sigma(z)\big) = a(1-a)$
- We'd like the $a(1-a)$ to cancel out of the cost to get the gradient to be $a-t$, so
- $\frac{\partial E}{\partial a} = \frac{a-t}{a(1-a)} = \frac{a+at-at-t}{a(1-a)} = \frac{a(1-t)-t(1-a)}{a(1-a)} = \frac{1-t}{1-a} - \frac{t}{a}$
- $\int \frac{\partial E}{\partial a} da = \int \frac{a-t}{a(1-a)} da = \int \frac{1-t}{1-a} da - \int \frac{t}{a} da$

$= -t \ln a - (1-t)\ln(1-a)$

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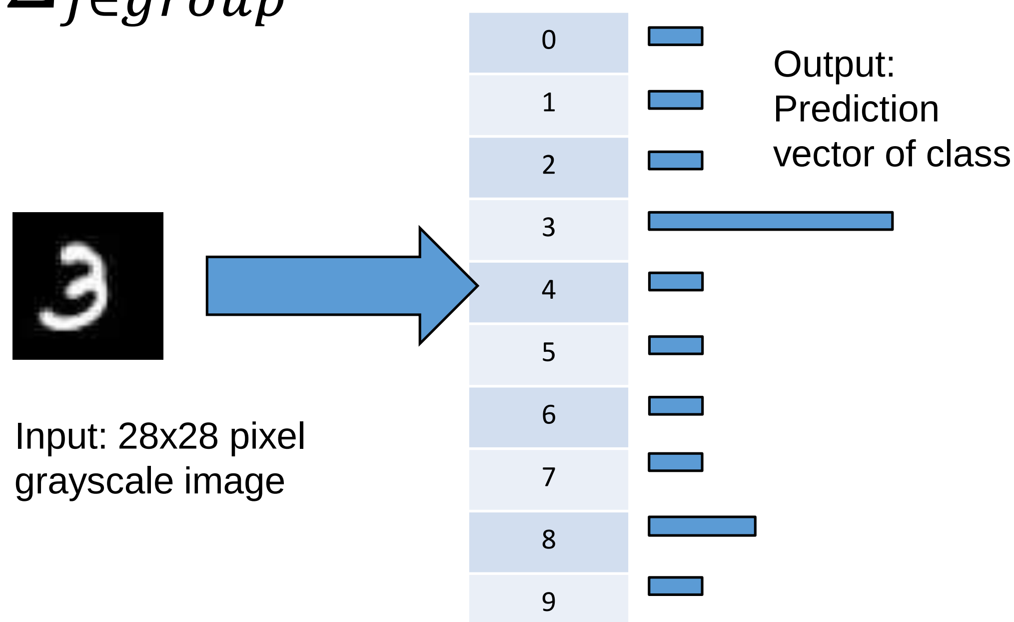
Softmax

- Recall sigmoid function: $\sigma(z) = \frac{1}{1+e^{-z}}$
- Softmax is a generalization of the sigmoid:

$$y_i = \frac{e^{z_i}}{\sum_{j \in group} e^{z_j}}$$

- Softmax generalizes 2-class logistic regression/sigmoids to n classes
- Suitable for mutually exclusive classes



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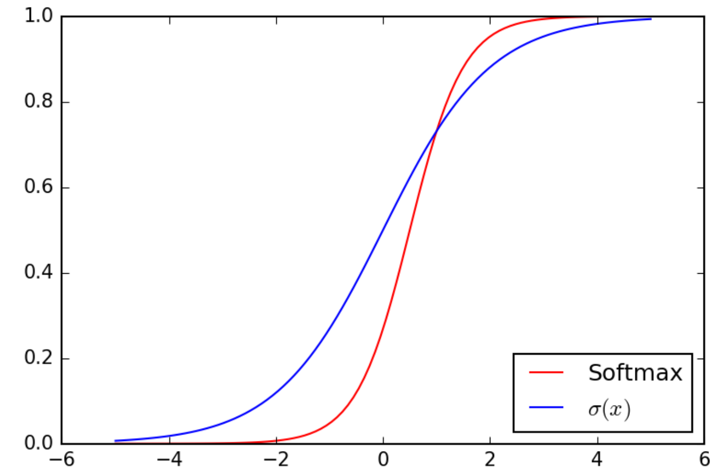

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- With $\hat{z} = (z+1)/2$, we recover the

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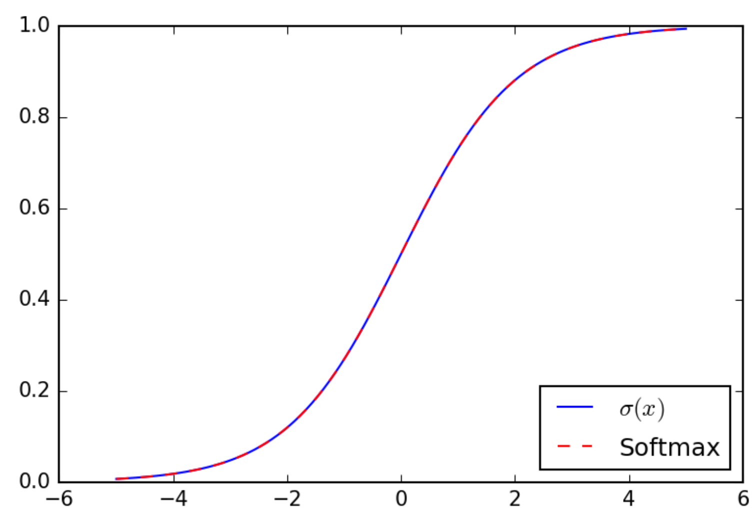

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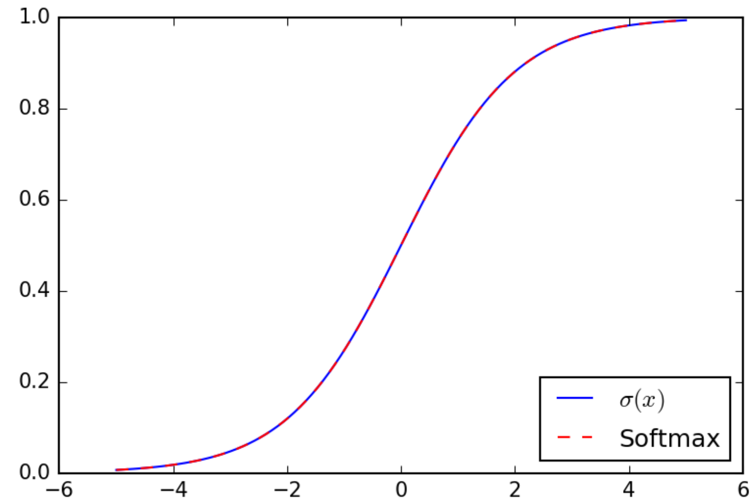
$$y_i' = y_i(1 - y_i)$$



Softmax

Cross entropy is the "best" cost function to use for the softmax:

$$C_j = -\sum_j t_j \ln y_j$$

For the familiar two-class case:

$$C = \boxed{-t_j \ln y_j} - \boxed{(1-t)\ln(1-y)}$$

Class 1

Class 2 = 1 - Class 1

Sigmoid function.

- As we found with the sigmoid,

$$y_i' = y_i(1-y_i)$$

- Recall sigmoid function: $\sigma(z) = \frac{1}{1+e^{-z}}$
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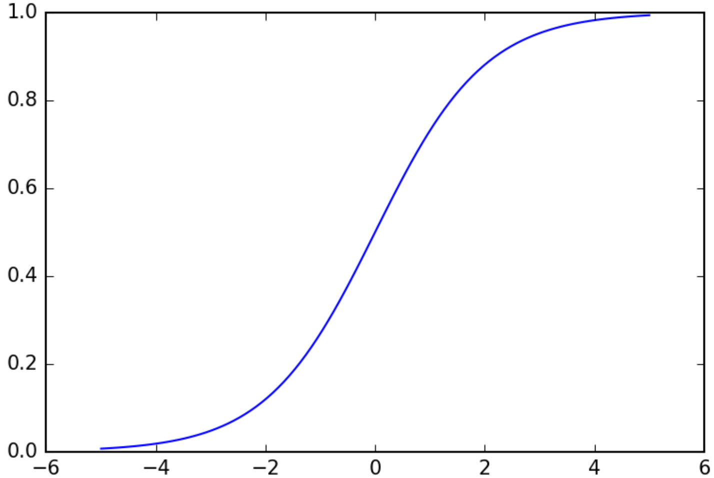
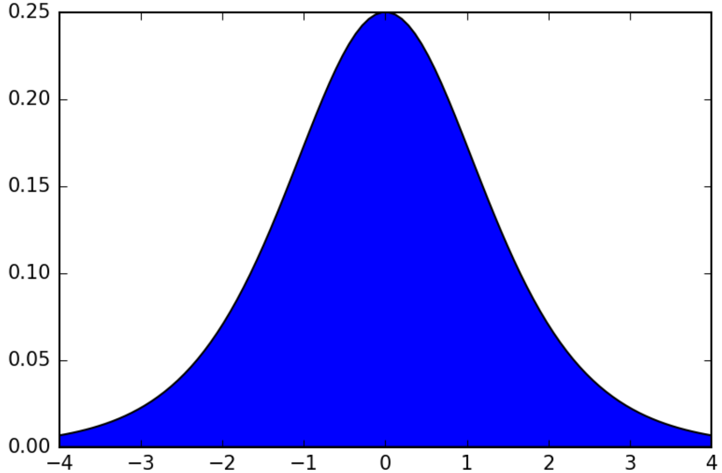
Recall: Trouble in Sigmoid land

- Sigmoids are relatively effective in active region

$$\sigma(s)$$



$$\sigma'(s) = \sigma(s)(1 - \sigma(s))$$



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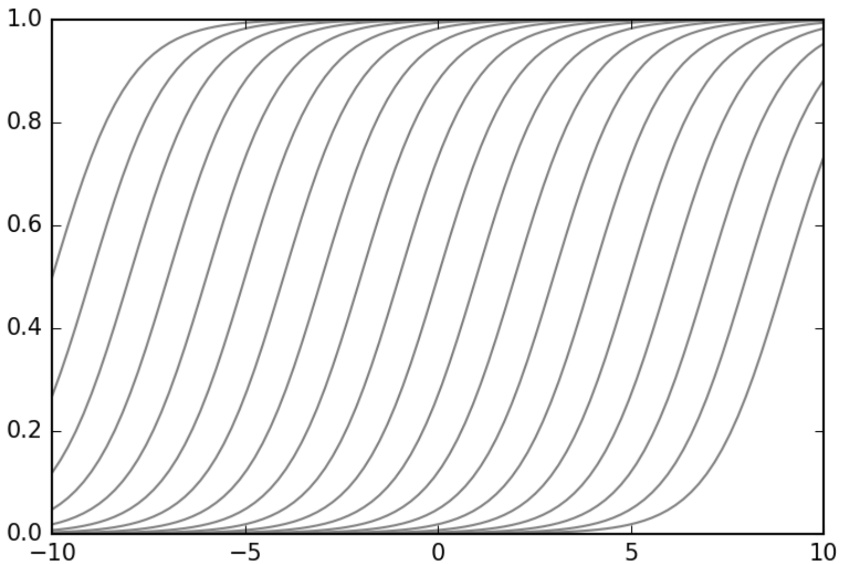
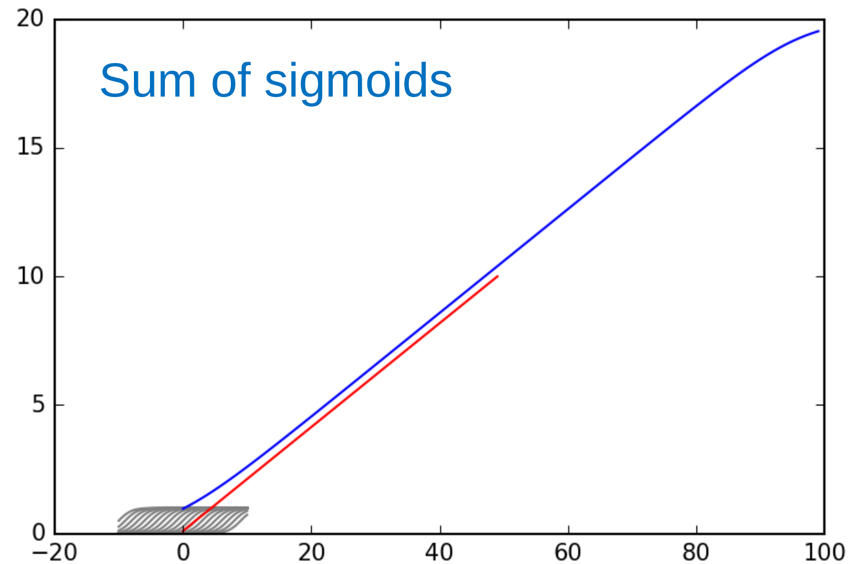
Recall: Trouble in Sigmoid land

- Sigmoids are relatively effective in active region
- What if we replicate the sigmoids with different biases?

$$\sigma(s) + \sigma(s-1) + \sigma(s-i) + \cdots + \sigma(s-n)$$

- And share their weights w_i?





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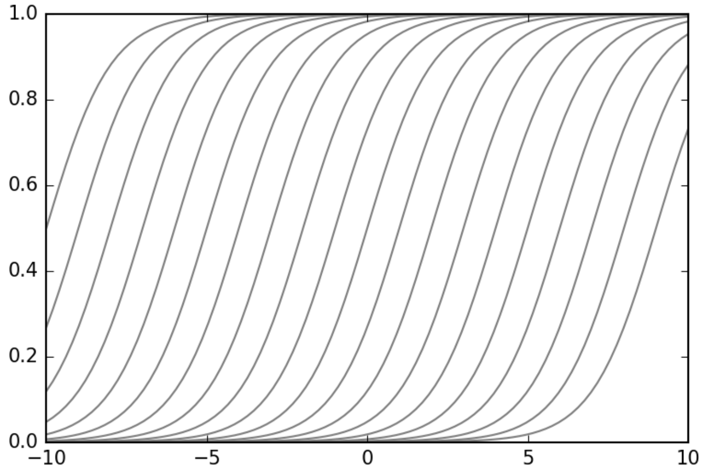
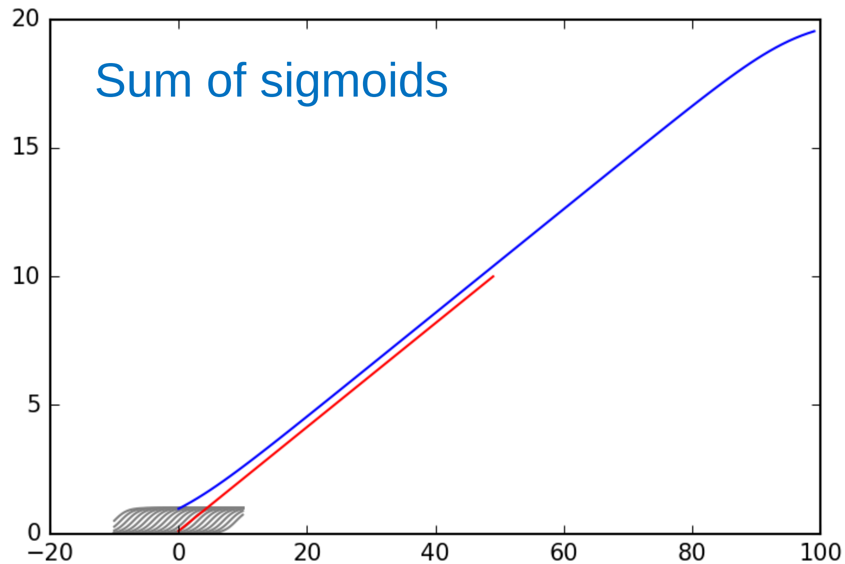
Recall: Trouble in Sigmoid land

- What if we replicate the sigmoids with different biases?

$$\sum_{i=1}^{\infty} \sigma(s + 0.5 - i) \approx \log(1 + e^{s}) \approx \max(0, s + noise)$$

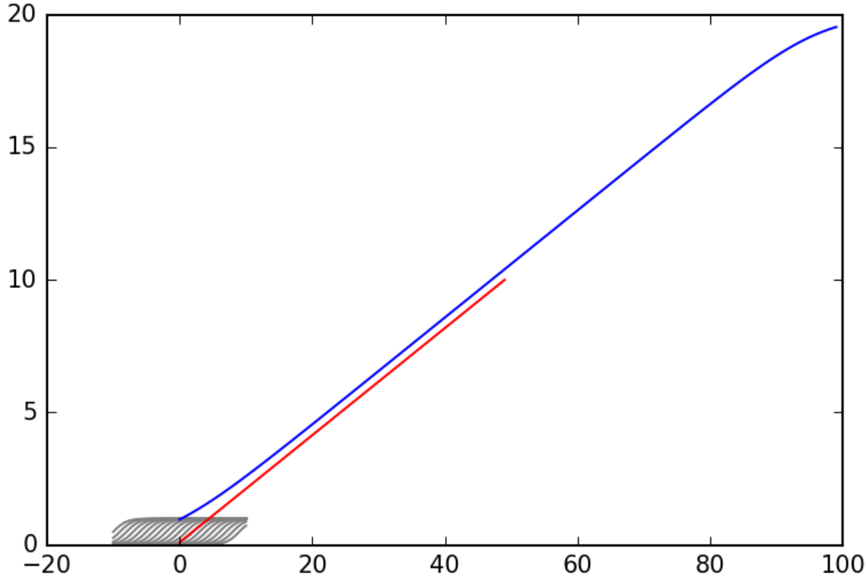
- Called rectified linear unit: ReLU
- Easy to approximate





Nice try, but….

- $f(s) = \max(0, s)$
- $\frac{\partial}{\partial s} f = \begin{cases} 0, & s \leq 0 \\ 1 * ds, & s > 0 \end{cases}$



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- $f(s) = \max(0, s)$
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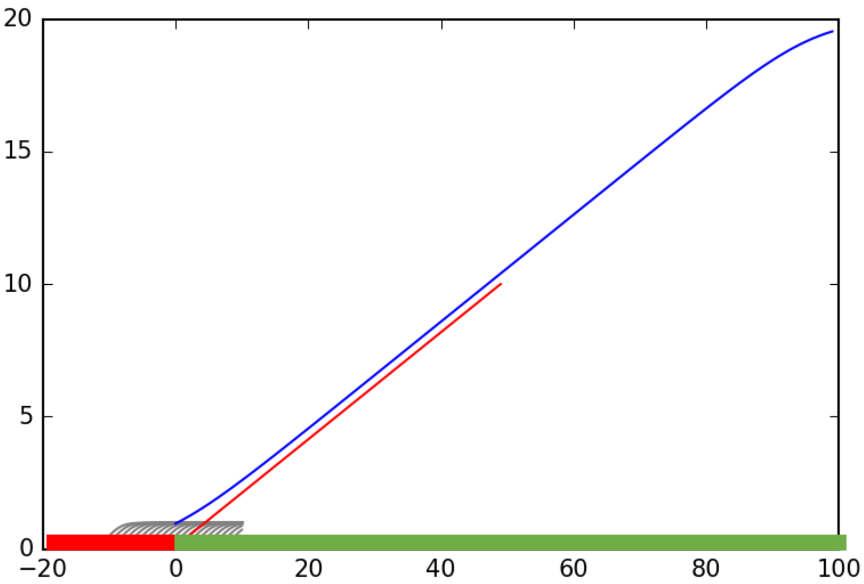
- ReLU neurons also suffer from vanishing gradients
- Neurons can "die" if they get a negative activation and never recover



Nice try, but....

- $f(s) = \max(0, s)$
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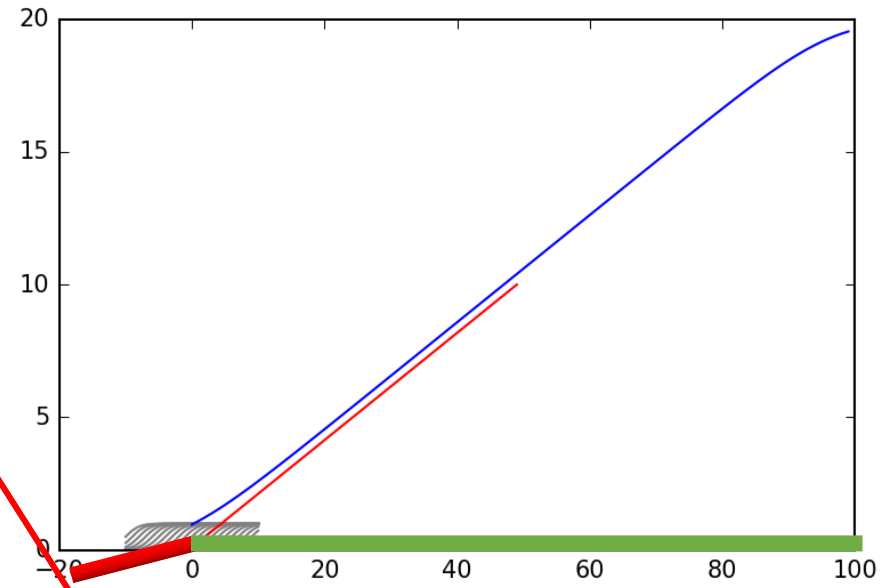

Fix:
Clip 0 gradient to something small so neuron can "recover"
Called: Leaky ReLU

Delving Deep into rectifiers. Kaiming He, MSR 2015

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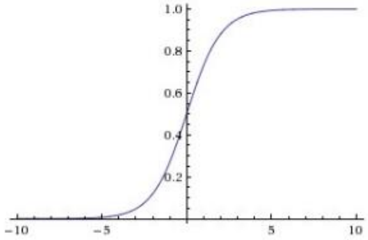
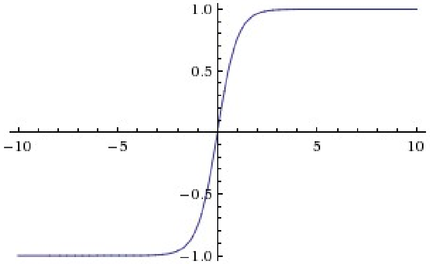
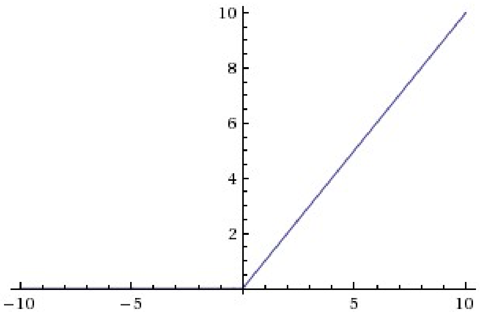
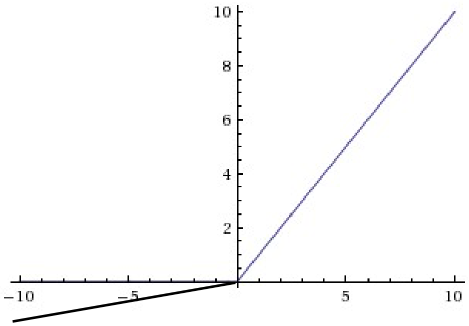
Activation Functions

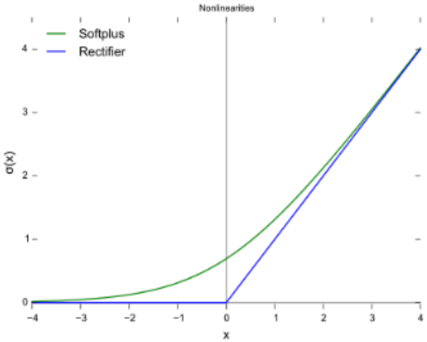
- Sigmoid
- Hyperbolic tangent
- ReLU = max(0,x)
  - Leaky ReLU
  - Soft ReLU – $\ln(1 + e^{x})$











[Mark's paper] Activation ensembles: https://arxiv.org/abs/1702.07790

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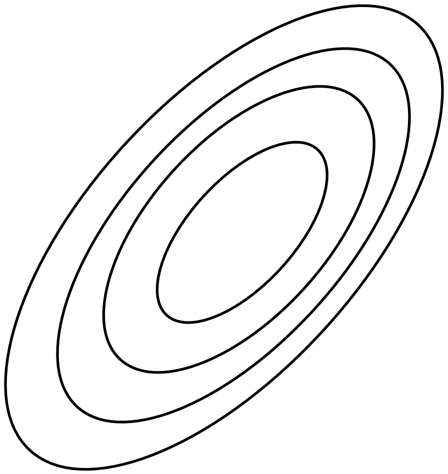
Optimization Visualized

- To find the best weights, we minimize the cost function using optimization



Cost function is usually MSE or cross entropy

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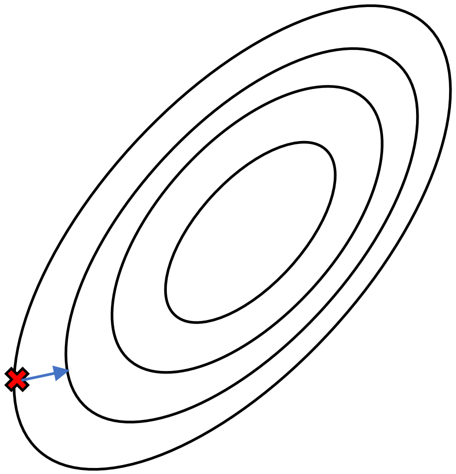
Optimization Visualized

- To find the best weights, we minimize the cost function using optimization
- Optimization starts from an initial point



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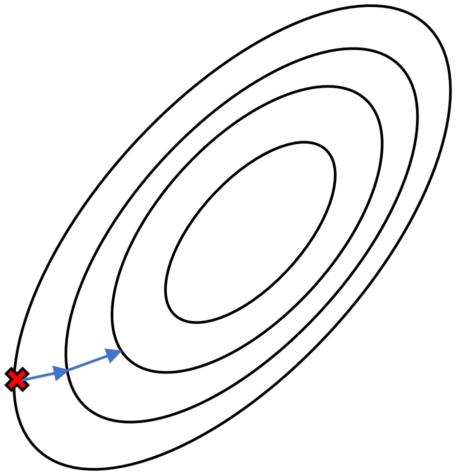

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- To find the best weights, we minimize the cost function using optimization
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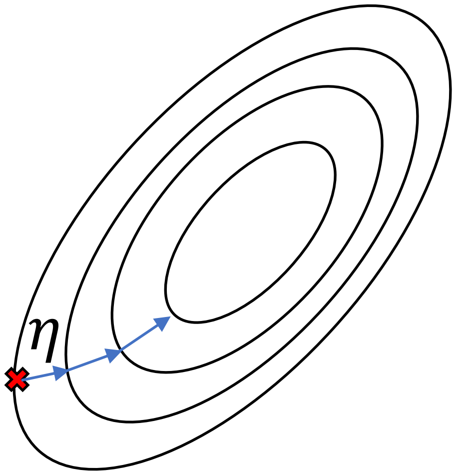
- Usually the fastest way is to take a step η in the direction of the steepest descent, called the gradient



η is known as the learning rate

$$w_{i+1} = w_i - \eta \nabla w_i$$

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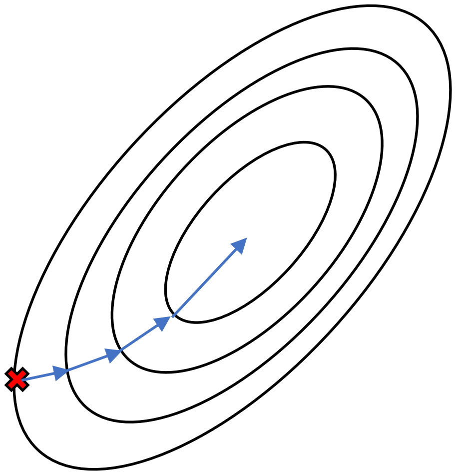

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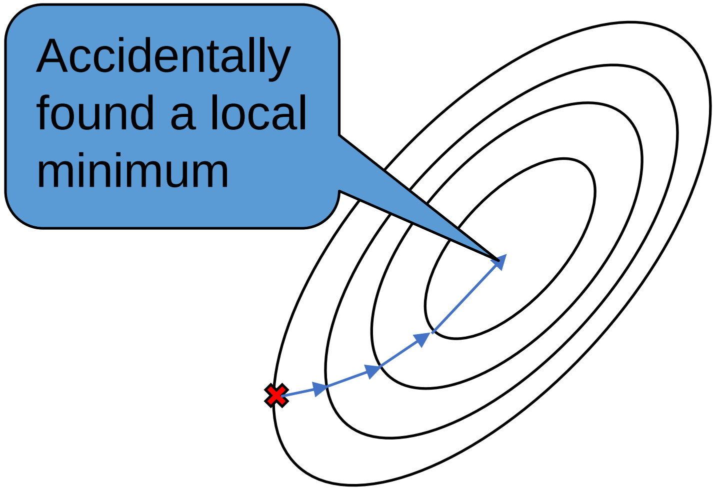
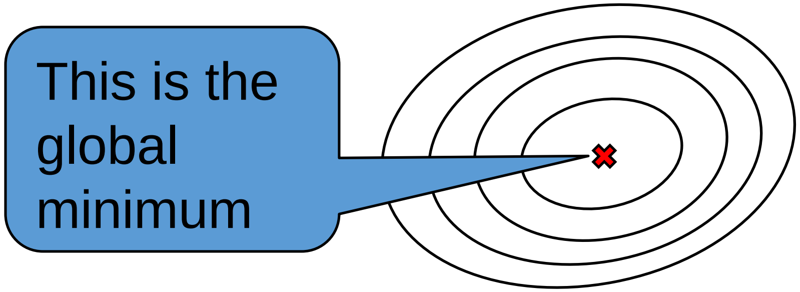
  - Local minima





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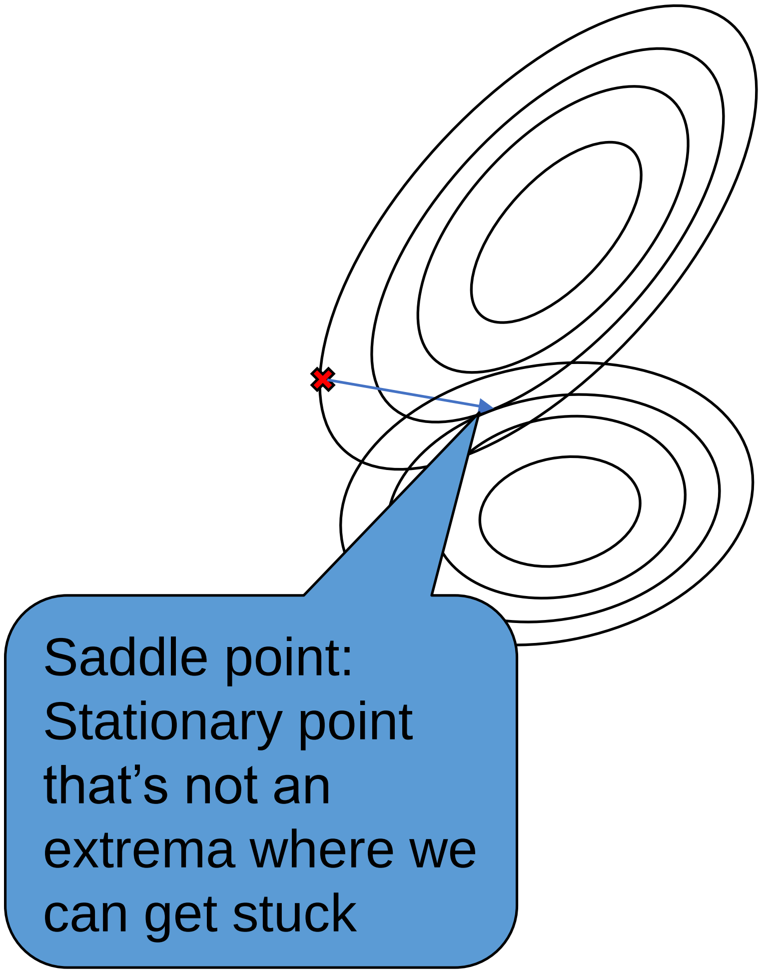

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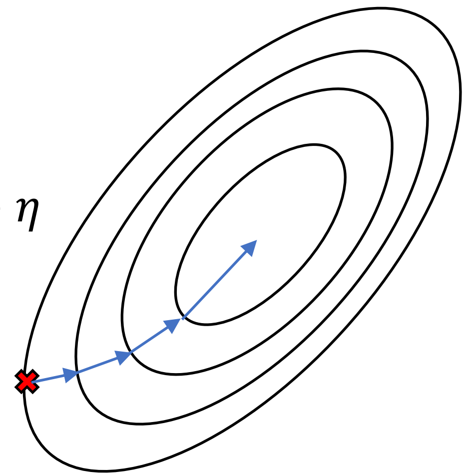
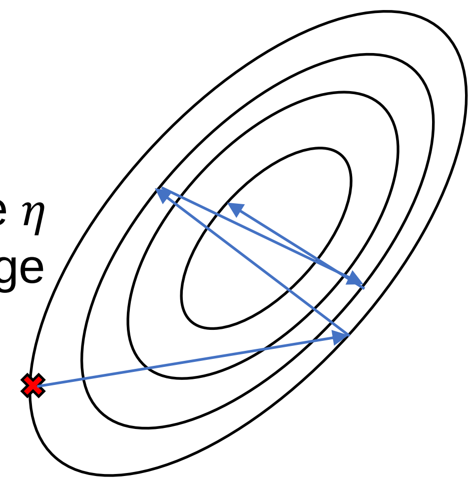
  - Local minima
  - Saddle points
  - Bad learning rates η

Step size η is good



Step size η is too large



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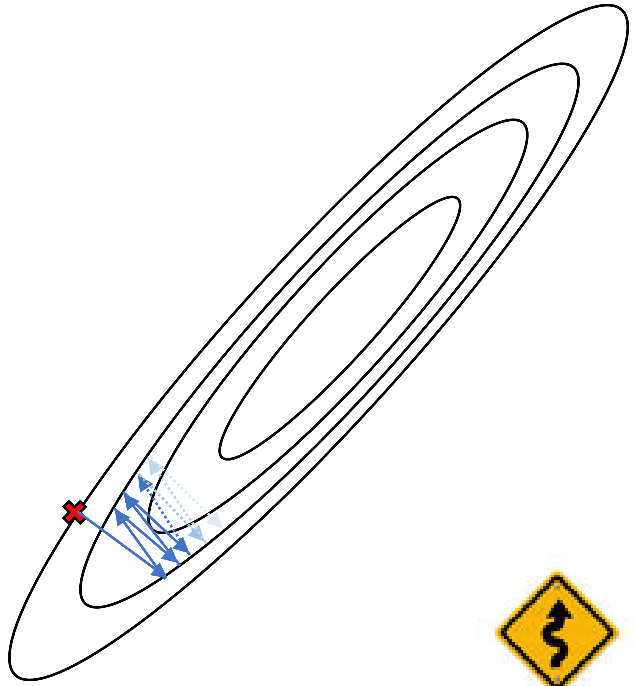

If you forget to normalize your data, weights or activations ;)

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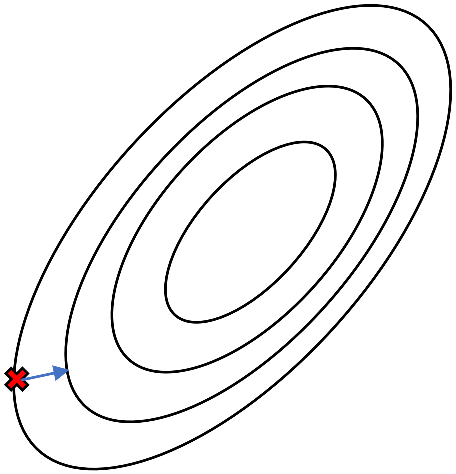
Estimating gradients

- At each step, the optimizer computes the location of the next point estimate: direction ∇w and step size η



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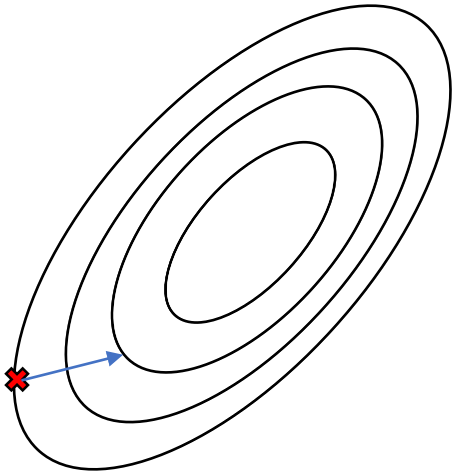
Estimating gradients

- At each step, the optimizer computes the location of the next point estimate: direction ∇w and step size η
- This can be done several ways:
  - Full batch



- Full batch means running through all the training data
  - For MNIST, this mean 60,000 samples
  - For some datasets, this could mean terabytes or petabytes of data
  - … if we do that, perhaps we should take a larger step η to justify the cost of computing over all the data
  - Full gradient does the best job in finding the true gradient

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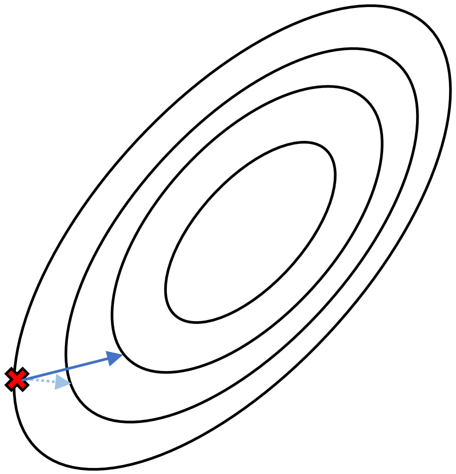
Estimating gradients

- At each step, the optimizer computes the location of the next point estimate: direction ∇w and step size η
- This can be done several ways:
  - Full batch
  - Mini-batch



- Mini batch means running through a smaller batch of the training data
  - This is much cheaper than running through all the data. Each batch is called an epoch.
  - However, the gradient estimate is more noisy, so it makes sense to take a smaller step η
  - Depending on the conditioning of the problem, the added cost of small step sizes may outweigh the savings of running a small sample

NB: Statisticians often take a smaller sample of the data to build a model. Doing a mini-batch is similar.

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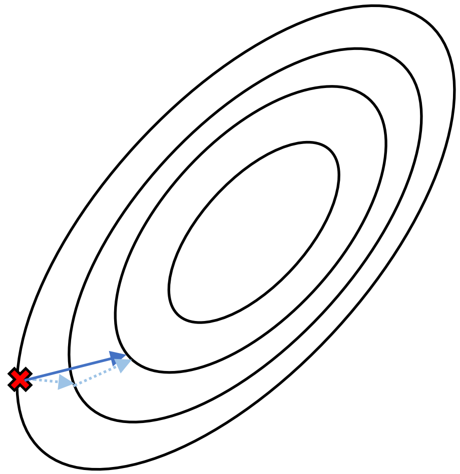

NB: Statisticians often take a smaller sample of the data to build a model. Doing a mini-batch is similar.

Also, we could take several mini-batches and average over them to get a better estimate

Batch size can make a difference, so choose judiciously

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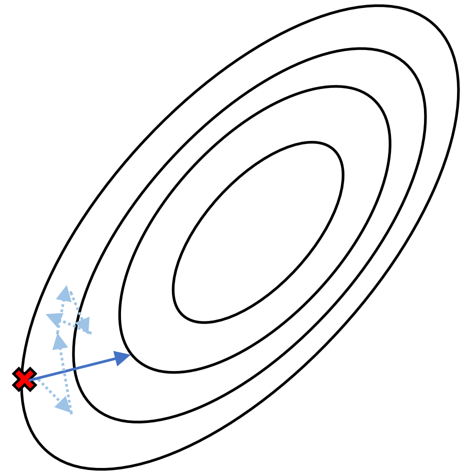
Estimating gradients

- At each step, the optimizer computes the location of the next point estimate: direction ∇w and step size η
- This can be done several ways:
  - Full batch
  - Mini-batch
  - Online



- Online methods update after each training case
  - The gradient can be very noisy due to the lack of averaging
  - Smaller steps are advised
  - This could work well for streaming data sets where it's impractical to store the incoming data

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Estimating gradients

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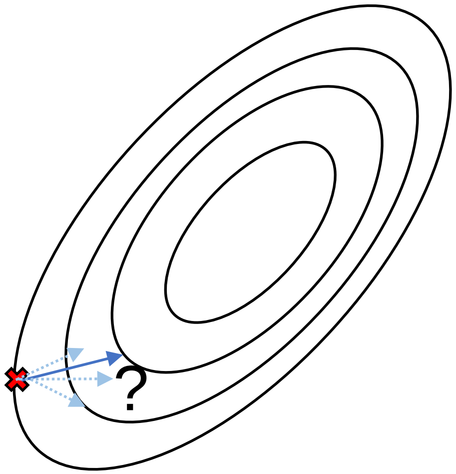

- How big should the step size η be?

Estimating gradients

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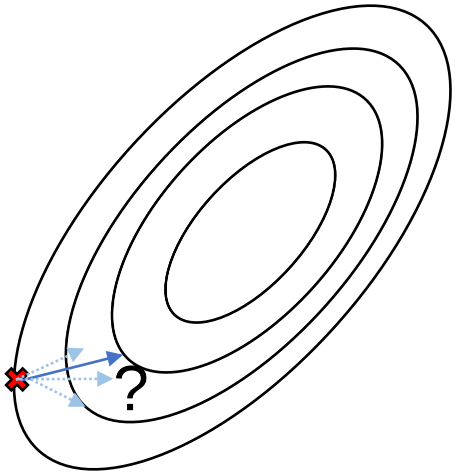

- How big should the step size η be?
  - Fixed global learning rate?
  - Adaptive global learning rate?
  - Learning rate per direction?

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Estimating gradients

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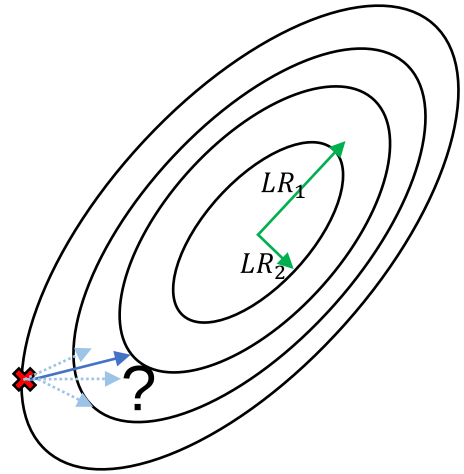

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Estimating gradients

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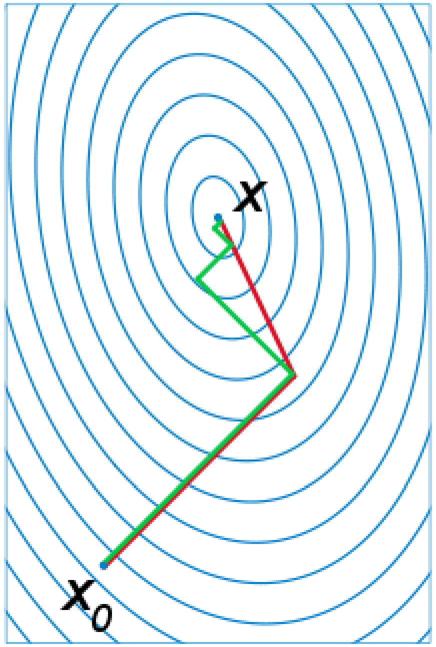
  - Full batch
  - Mini-batch
  - Online
- How big should the step size η be?
  - Fixed global learning rate?
  - Adaptive global learning rate?
  - Learning rate per direction?
  - Using something other than steepest descent?
    - E.g. Conjugate gradient



Conjugate gradient [Wikipedia]
Green – gradient descent
Red - Conjugate gradient

Conjugate gradient means choosing a new direction that's conjugate to the previous directions to not "mess up" the work of previous iterations.

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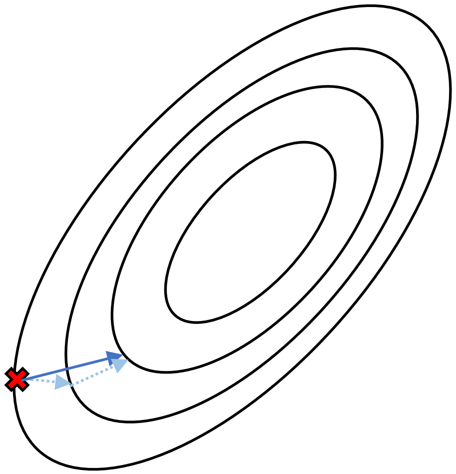
Speeding up mini batches

- Each mini-batch epoch estimates gradient ∇w and step size η using a random subset of the data
- Since the gradient is noisy, it's usually necessary to take smaller steps



Various ways to slice data for minibatching

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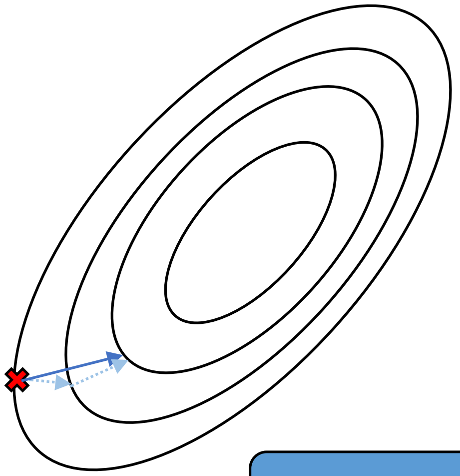
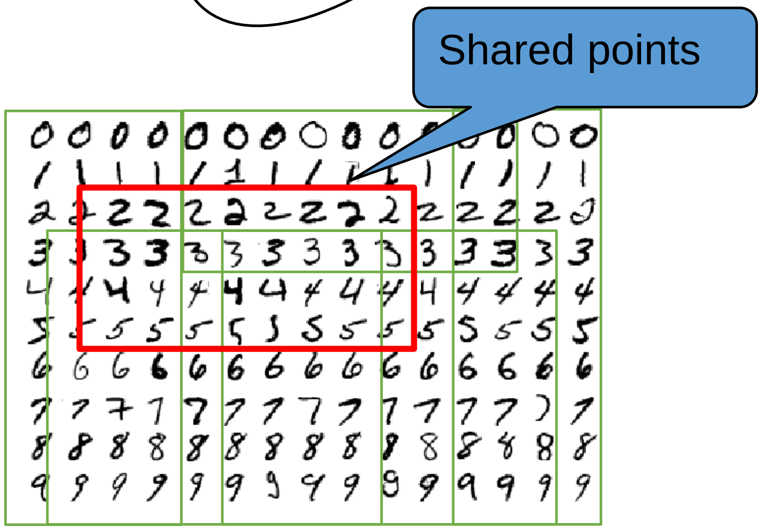
Speeding up mini batches

- Each mini-batch epoch estimates gradient ∇w and step size η using a random subset of the data
- Since the gradient is noisy, it's usually necessary to take smaller steps
- However, some of the minibatches share training examples, and hence share some part of their gradient





Various ways to slice data for minibatching

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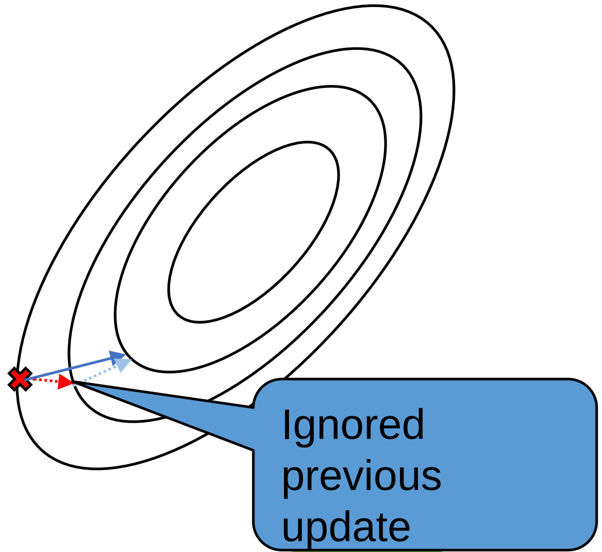

Various ways to slice data for minibatching

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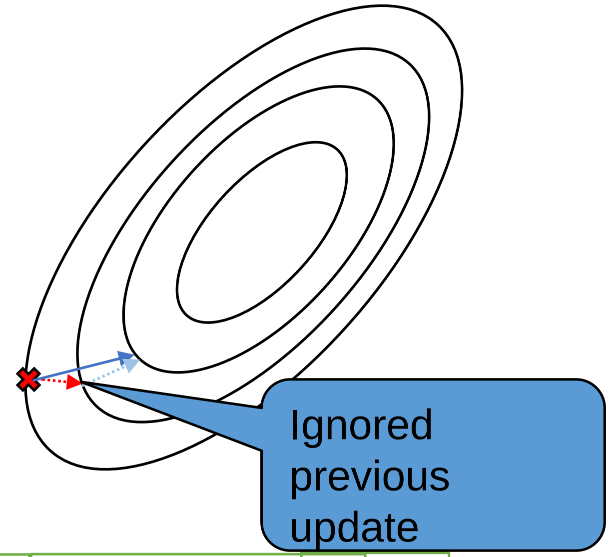
Speeding up mini batches

- Each mini-batch epoch estimates gradient ∇w and step size η using a random subset of the data
- Since the gradient is noisy, it's usually necessary to take smaller steps
- However, some of the minibatches share training examples, and hence share some part of their gradient
- Also, information about previous directions of travel are ignored…
- We can exploit these properties to speed up mini-batches by making a better estimate of the gradient to take larger steps with more confidence

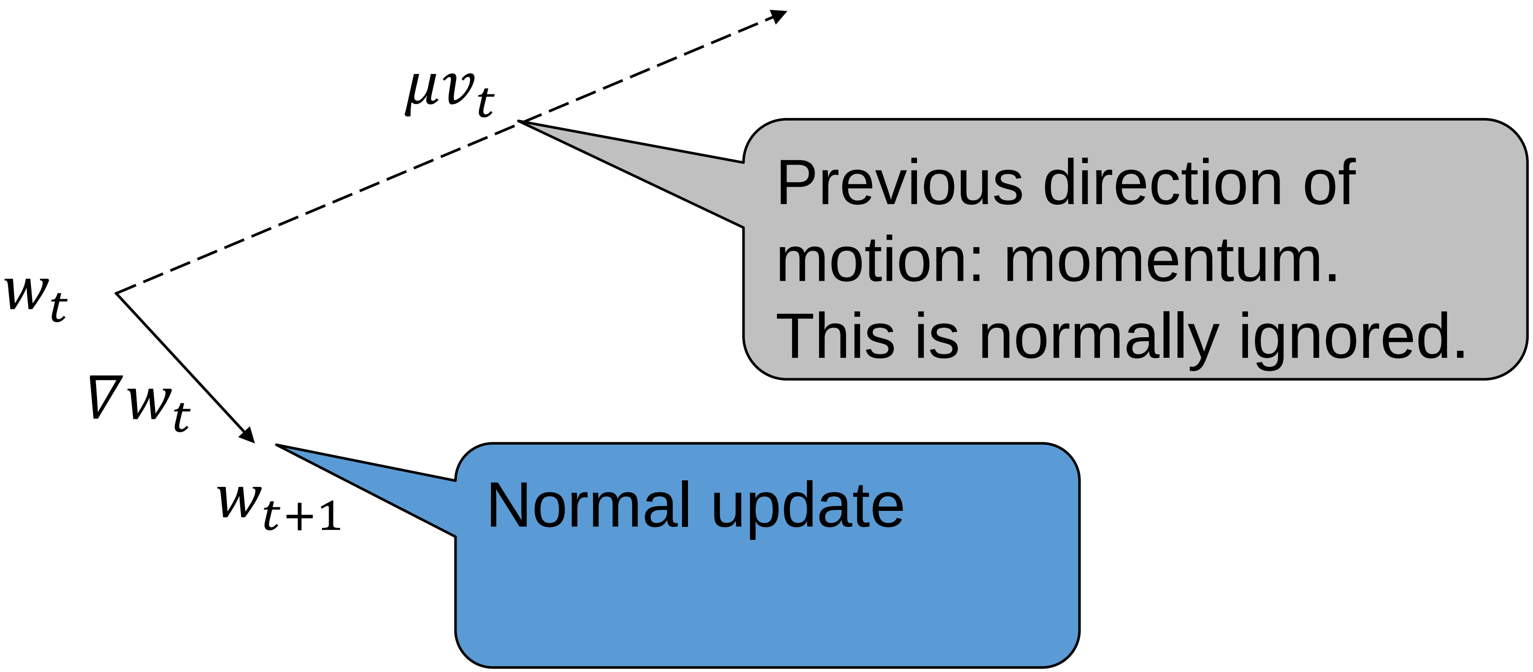


Various ways to slice data for minibatching

Momentum

Momentum

$$v_{t+1} = \mu v_t - \eta \nabla w_t$$
$$w_{t+1} = w_t + v_{t+1}$$



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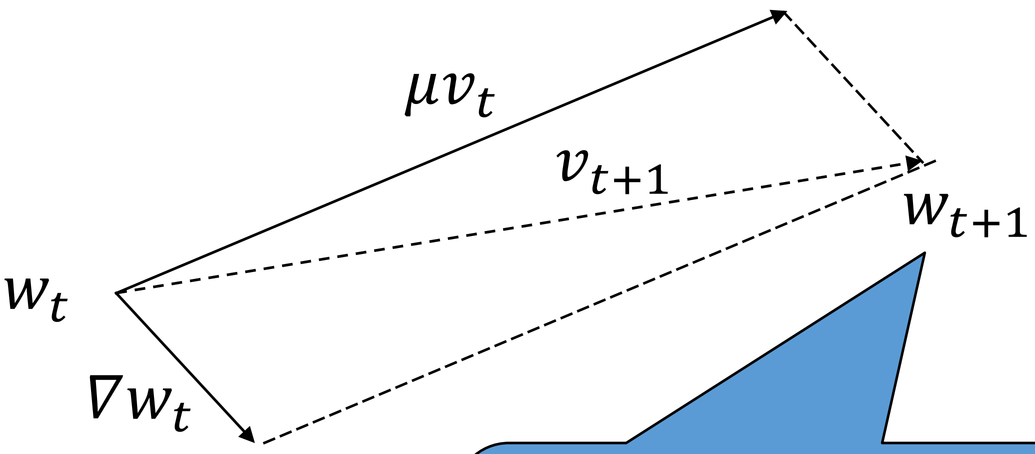
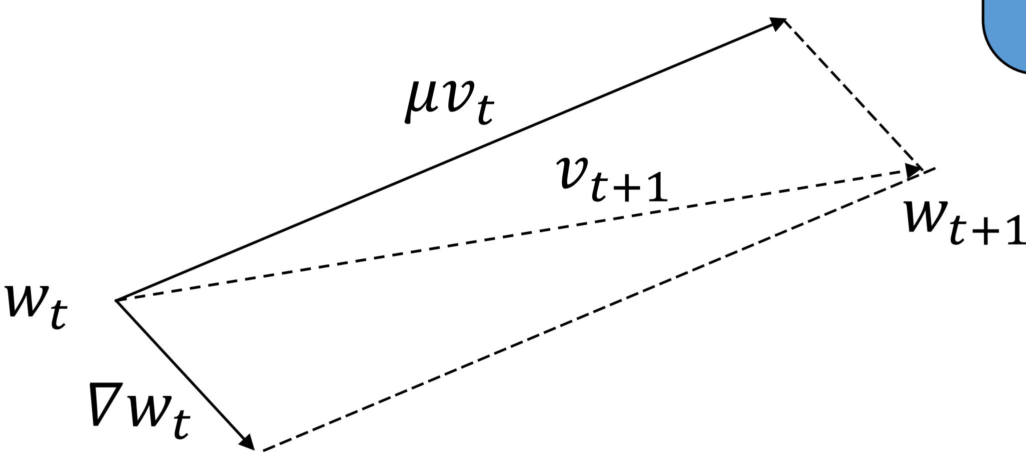


Momentum-adjusted update. Note how momentum is favored over noisy gradient estimate.

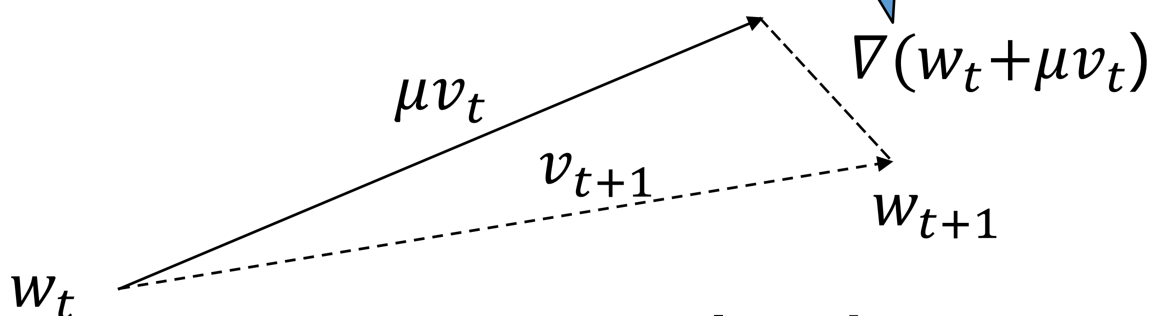
Momentum and acceleration

Momentum

$$v_{t+1} = \mu v_t - \eta \nabla w_t$$
$$w_{t+1} = w_t + v_{t+1}$$



Acceleration (2nd derivative) is now accounted for



Nesterov Acceleration

Sutskever, ICML 2013

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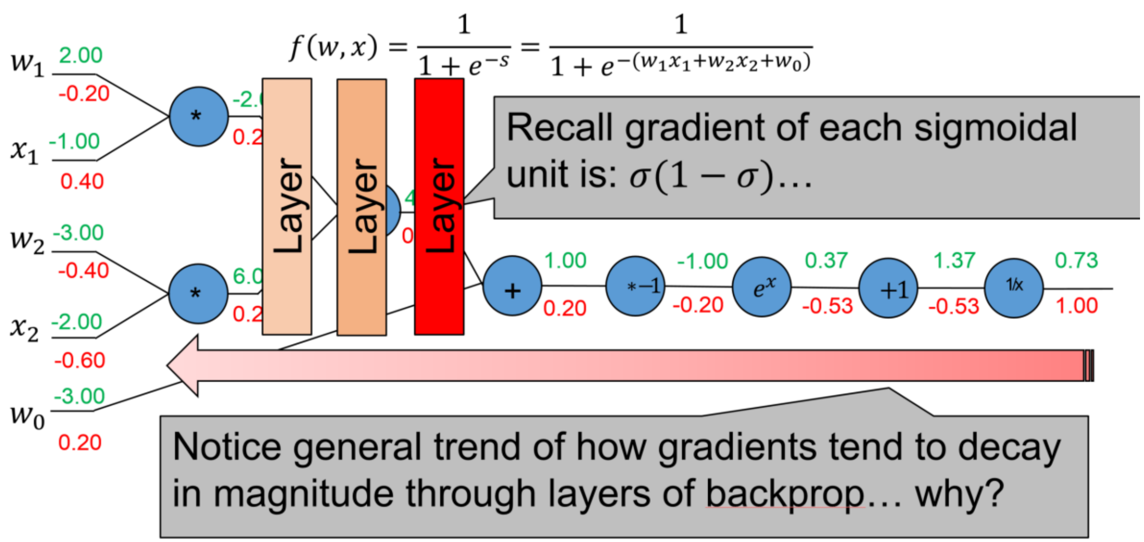
Other ways to speed up mini batches

- Adaptive learning rates
  - Remember that earlier layers tend to have smaller gradients



  - Use an adaptive multiplier to boost/attenuate gradients for each layer/weight
  - RMSprop: Keep a moving average of the squared gradient of each weight, divide gradient by this to normalize

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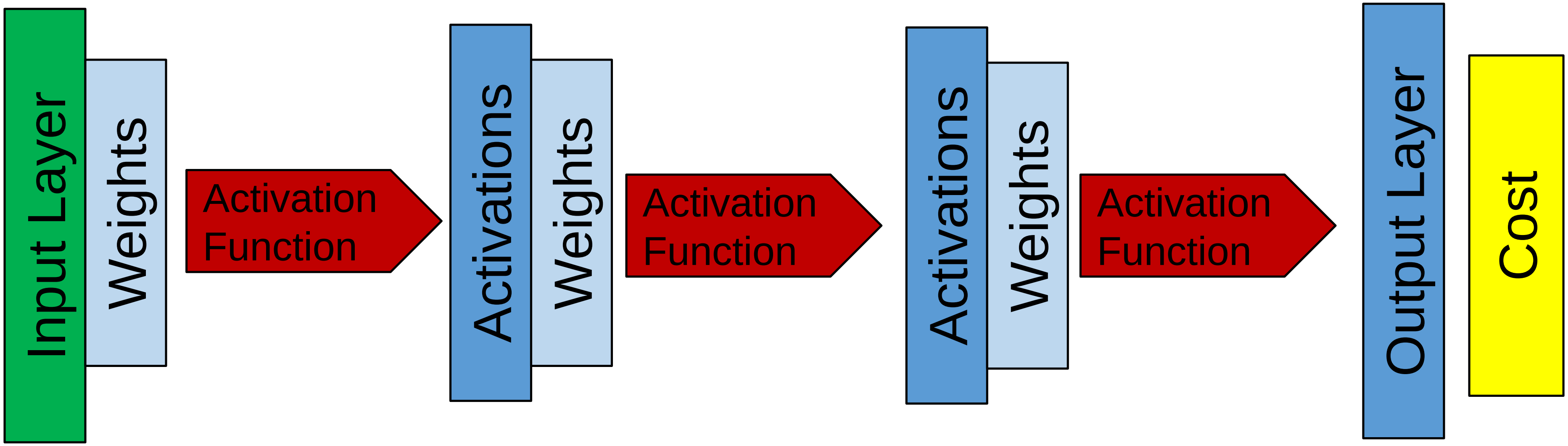
Brute force



- Brute force methods

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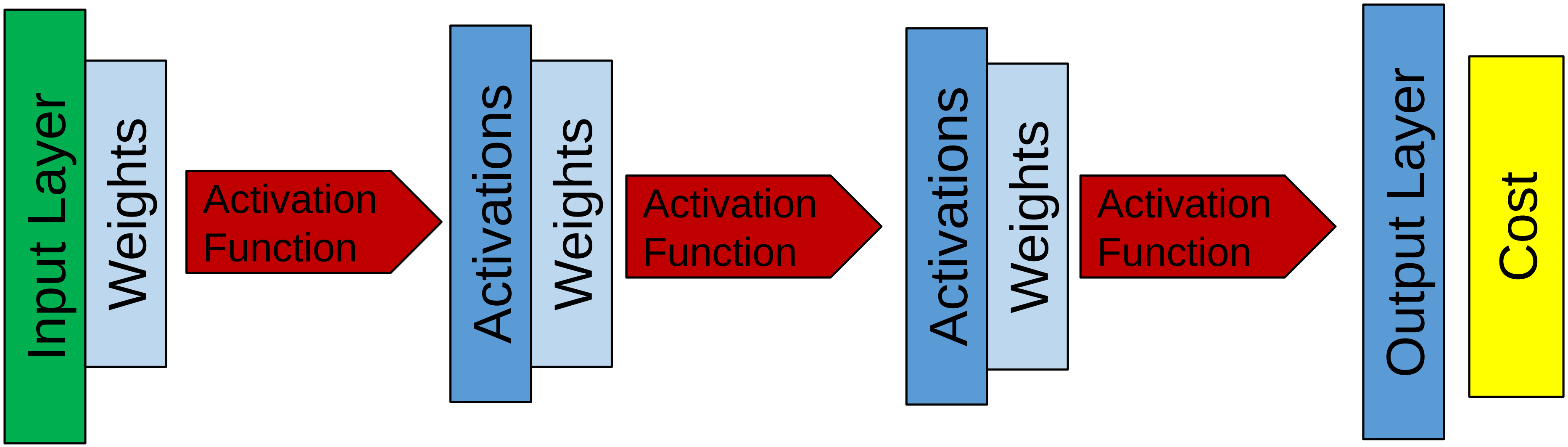
Brute force



- Brute force methods
- Commercial networks can have billions of parameters, > 30 levels, can take weeks to months to train
- MSR: 152 layers
  - http://www.wired.com/2016/01/microsoft-neural-net-shows-deep-learning-can-get-way-deeper/

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GPUs for Deep Learning

NVIDIA Digits
Devbox ~$10k

Four TITAN X GPUs with 7 TFlops of single precision, 336.5 GB/s of memory bandwidth, and 12 GB of memory per board.

VGG net takes ~2-3 weeks to train on 4 GPUs

~$1k per Titan X

Source: NVIDIA

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GPUs

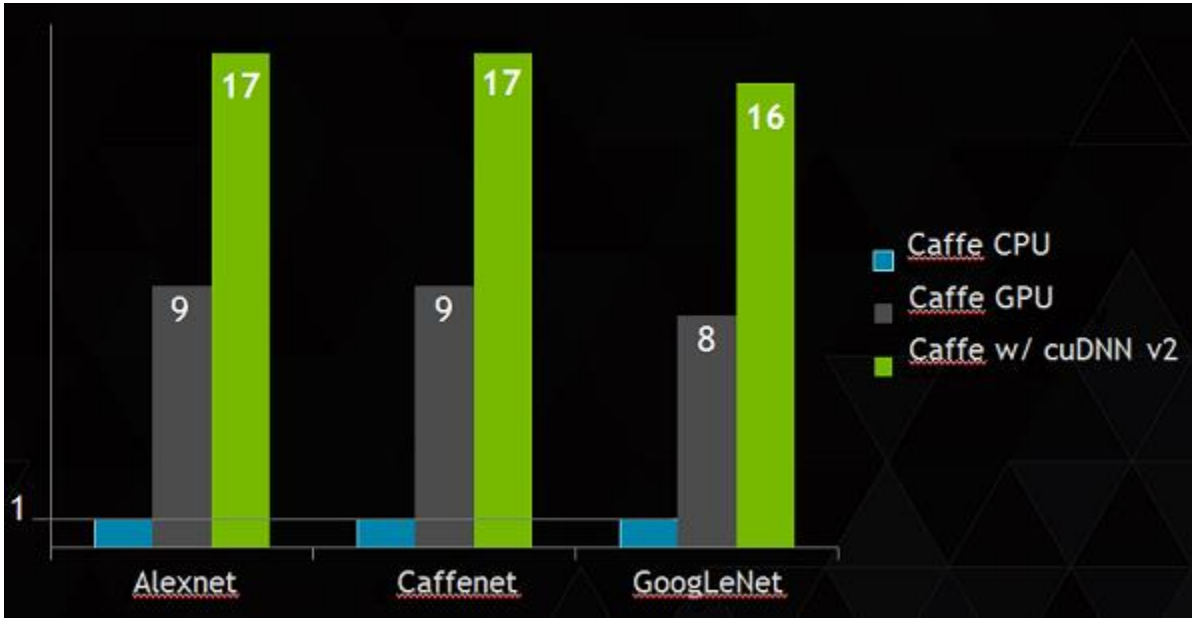
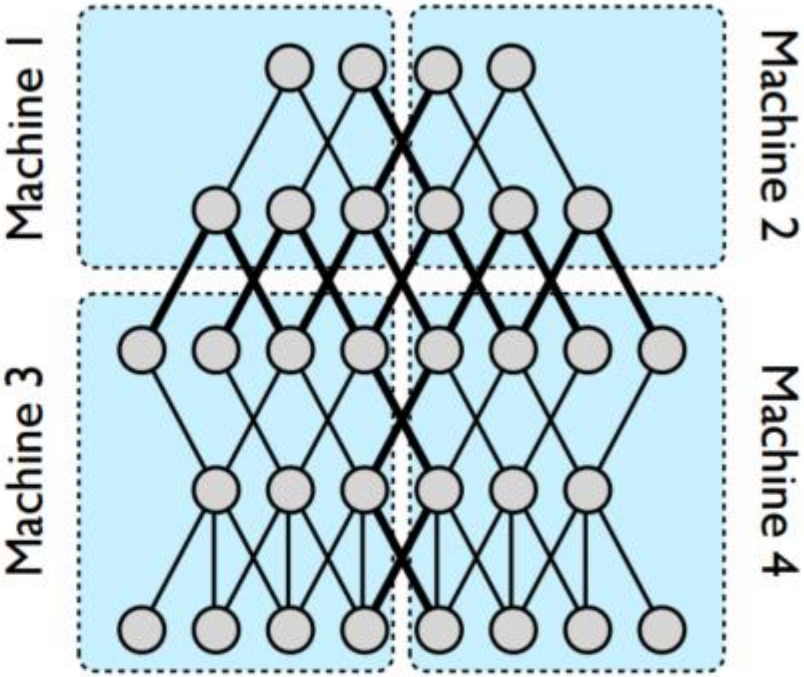
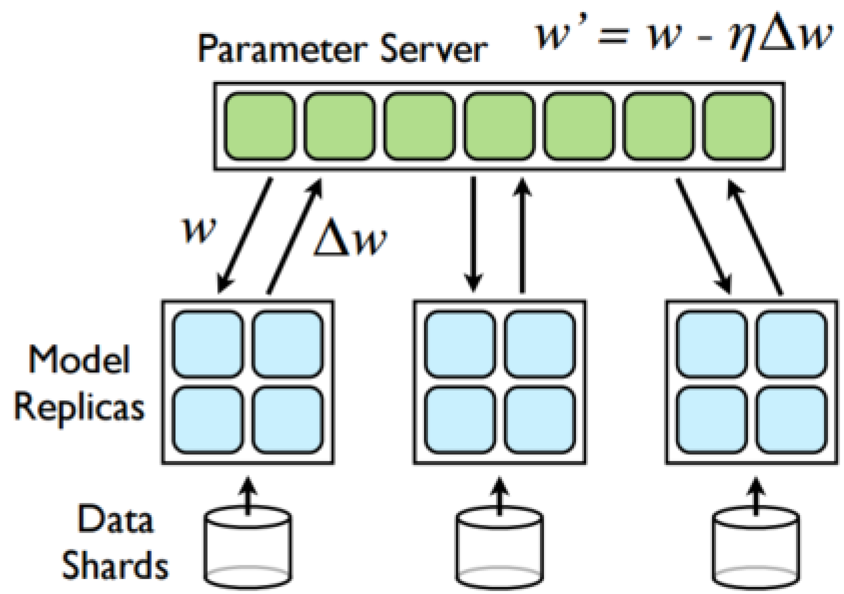


Figure 1: cuDNN performance comparison with CAFFE, using several well known networks. CPU is 16-core Intel Haswell E5-2698 2.3 GHz with 3.6 GHz Turbo. GPU is NVIDIA GeForce GTX TITAN X.

Source: NVIDIA https://devblogs.nvidia.com/parallelforall/cudnn-v2-higher-performance-deep-learning-gpus/

Deep learning parallelized



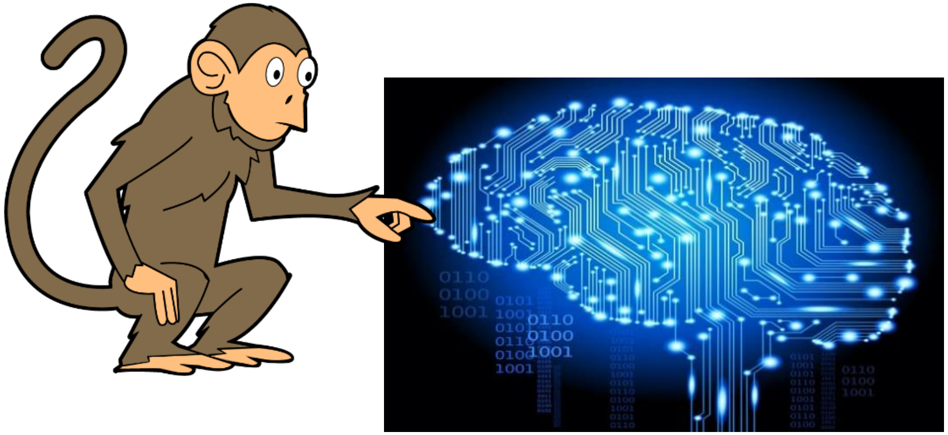


- Divide model across machines
- Sync model periodically
- Out of sync states act as noise → SGD can handle this

Large Scale Distributed Deep Networks. Dean, 2012.

In practice (for this class)

- Training models takes a lot of GPU/CPU and memory
- Luckily, for students like us, there's:
  - A set of pretrained Keras/Tensorflow models we can play with



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Summary

- **Data prep:**
  - Remember to clean data by subtracting the mean and normalizing inputs
  - If possible, try to decorrelate inputs

- **Network architecture:**
  - Use ReLU activations instead of sigmoid or tanh
  - Use softmax or cross entropy if modeling mutually exclusive classes: e.g. digits
- **Training:**
  - Try using minibatch training with momentum
  - Be careful about learning rates

Assignment

- Assignment
- Quizzes
- Project

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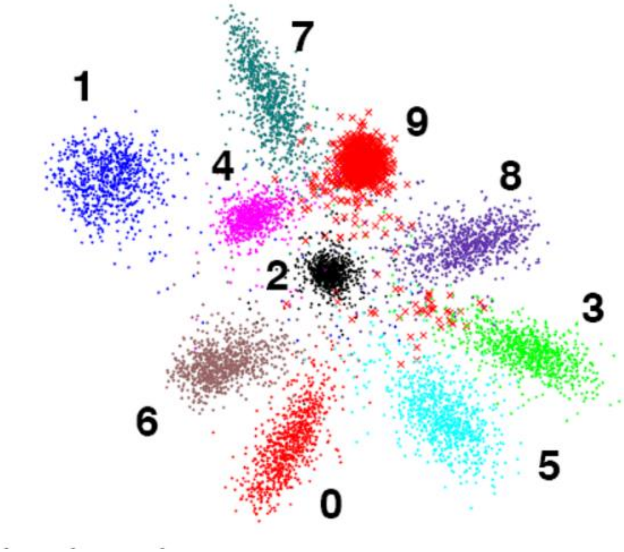
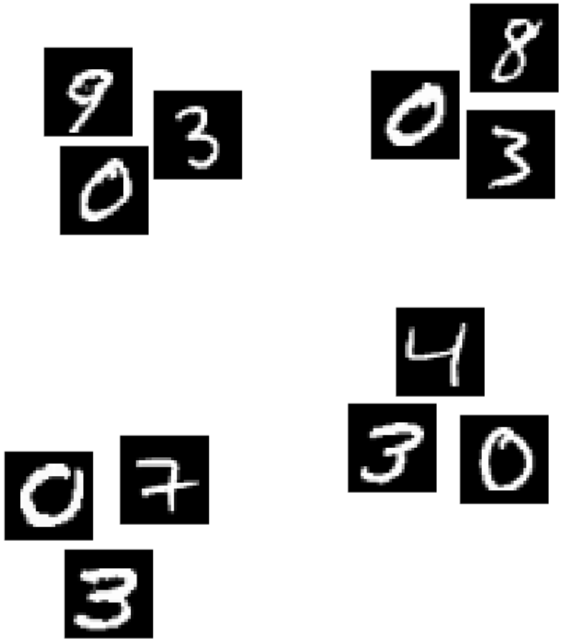
Assignment

- Discuss assignment
- Random labels & NN capacity

Random labels





Non-random labels

Show some spatial consistency in high dimensional space (clustering)

Random labels

Show no spatial consistency in high dimensional space. Relies on model overfitting.

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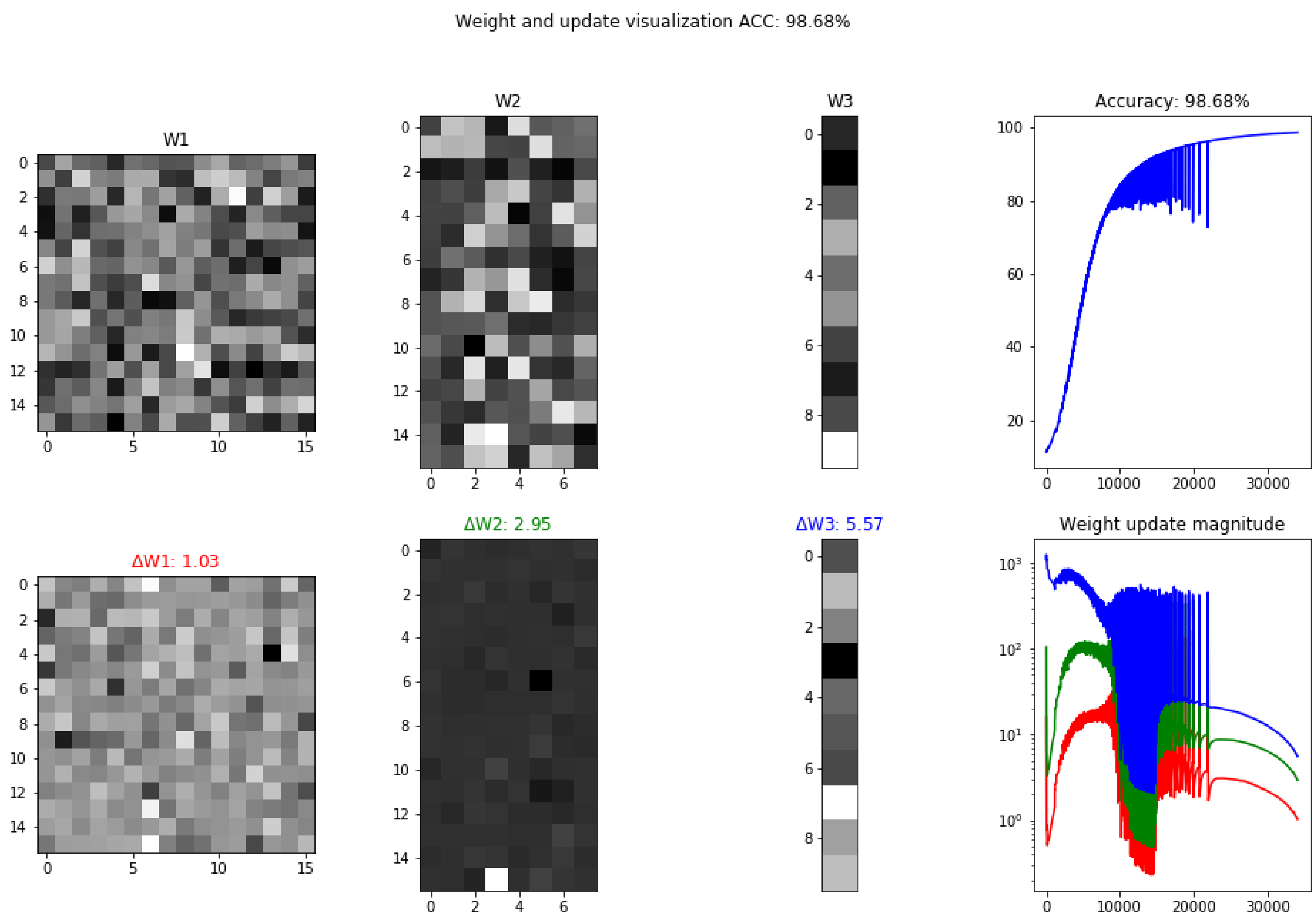
Random labels



Further reading

- Batch Normalization: http://arxiv.org/pdf/1502.03167.pdf
- 1-bit gradient updates: http://arxiv.org/pdf/1602.02830v1.pdf
- Drop-in for training deep nets: http://arxiv.org/pdf/1511.06951v1.pdf
- Weight normalization
- https://arxiv.org/abs/1602.07868

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Optional Reading

- Learning to learn gradient descent by gradient descent: https://arxiv.org/abs/1606.04474
- Synthetic gradient: https://arxiv.org/abs/1608.05343
- Learning to reinforcement learn: https://arxiv.org/abs/1611.05763
- Batch Normalization: https://arxiv.org/pdf/1502.03167.pdf
- Data-dependent init: https://arxiv.org/pdf/1511.06856.pdf

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Optional Reading

- Continuum of activations: http://uaf46365.ddns.uark.edu/continuum.pdf
- Designing NN using RL: https://arxiv.org/abs/1611.02167
- Neural arch search using RL: https://openreview.net/forum?id=r1Ue8Hcxg
- Sacred metaoptimizer: https://github.com/IDSIA/sacred
- What is softmax? http://www.kdnuggets.com/2016/07/softmax-regression-related-logistic-regression.html
- Overcoming forgetting: https://arxiv.org/abs/1612.00796
- Local minima: https://arxiv.org/abs/1611.06310

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Optional Reading

- Hyperopt:
  - https://github.com/hyperopt/hyperopt-sklearn
  - http://optunity.readthedocs.io/en/latest/
- Tanh paper: [2010] http://jmlr.org/proceedings/papers/v9/glorot10a/glorot10a.pdf - ReLU invented in 2011 (Wikipedia)
- Overview of gradient descent algs: http://sebastianruder.com/optimizing-gradient-descent/

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Optional Reading

- More on training and tanh: http://jmlr.org/proceedings/papers/v9/glorot10a/glorot10a.pdf
- More on ReLU: http://www.jmlr.org/proceedings/papers/v15/glorot11a/glorot11a.pdf