

# Lecture Notes for **Machine Learning in Python**



Professor Eric Larson  
**Neural Network Optimization and Activation**

# Class Logistics and Agenda

- Logistics
  - grading update
  - flipped model next time!
- Agenda:
  - More optimization techniques and programming examples
    - Momentum
    - Initialization
    - More activations: Tanh, ReLU, SiLU
    - Adaptive learning: AdaGrad, AdaM, etc.

# Class Overview, by topic

Table Data  
Visualization

Numpy, Pandas, Seaborn  
Overviews with some in-depth discussion

Dimension  
Reduction and  
Image Processing

Scikit-learn, Scikit Image,  
Intuition only, Some mathematics

Linear and  
Logistic  
Regression

Numpy, Recreate API for Scikit-learn  
Detailed mathematics for simple optimization  
intuition for advanced optimization

Neural Networks  
and Back Prop.

Numpy  
Detailed mathematics for NN operations

Wide and Deep  
Networks

Convolutional  
Networks

Recurrent  
Networks

Keras, Tensorflow  
Intuition, Detailed implement.

Ethics in  
Language Models

ConceptNet  
Case studies

## 08a. Practical\_NeuralNetsWithBias.ipynb

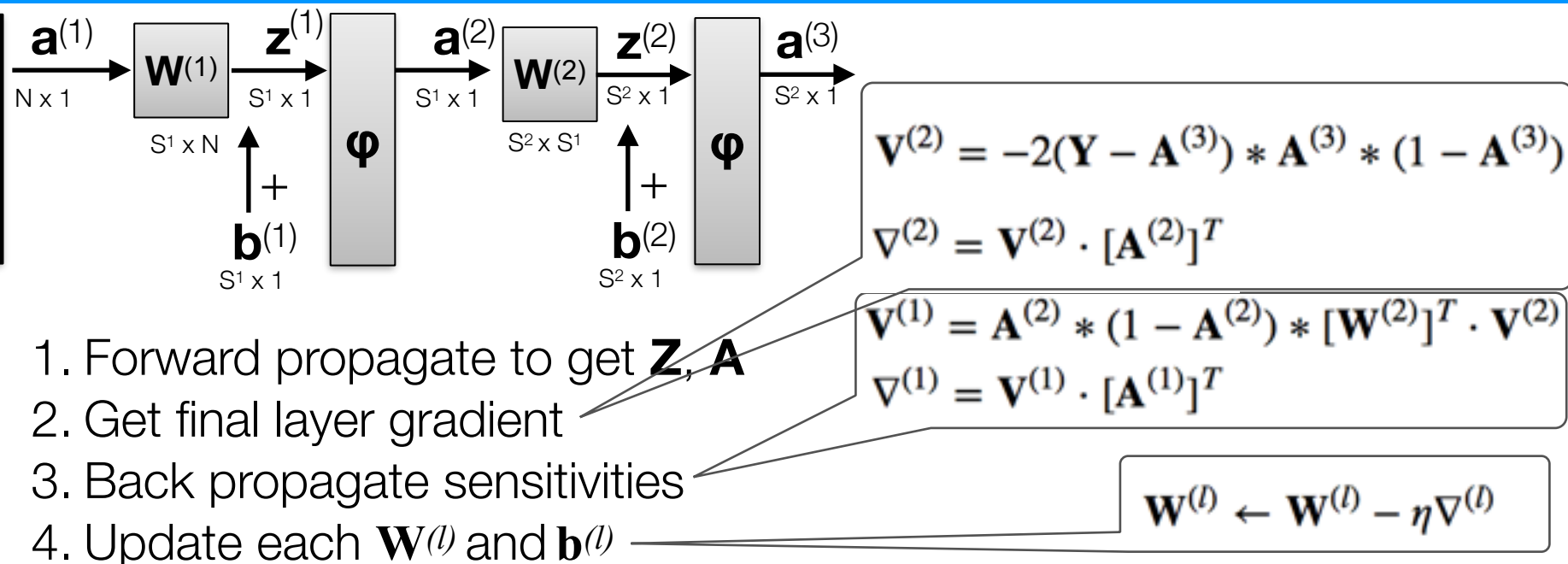
Quick Review:  
Momentum  
Cooling



# Objective Function



# Changing the Objective Function



## • Self Test:

**True or False:** If we change the cost function,  $J(\mathbf{W})$ , we only need to update the final layer sensitivity calculation,  $\mathbf{V}^{(2)}$ , of the back propagation steps. The remainder of the algorithm is unchanged.

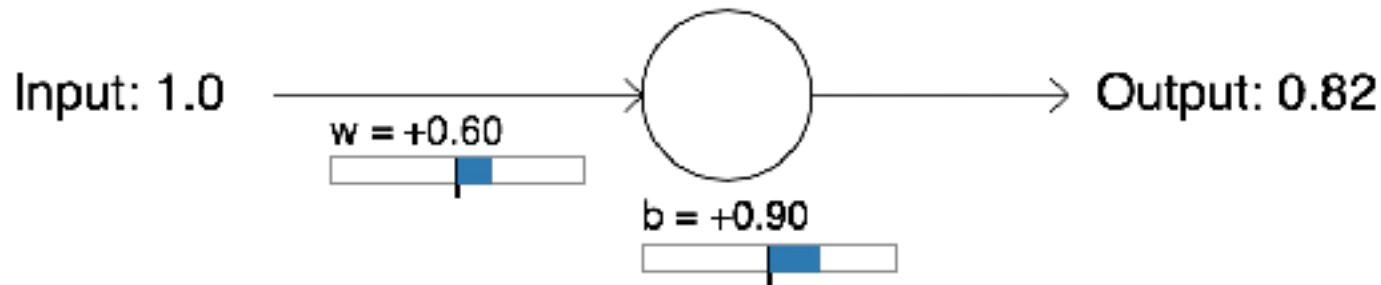
- A. True
- B. False

# Practical Implementation of Architectures

- Mean squared error:

$$J(\mathbf{W}) = \sum_k^M (\mathbf{y}^{(k)} - \mathbf{a}^{(L)})^2$$

least squares objective,  
tends to slow training initially



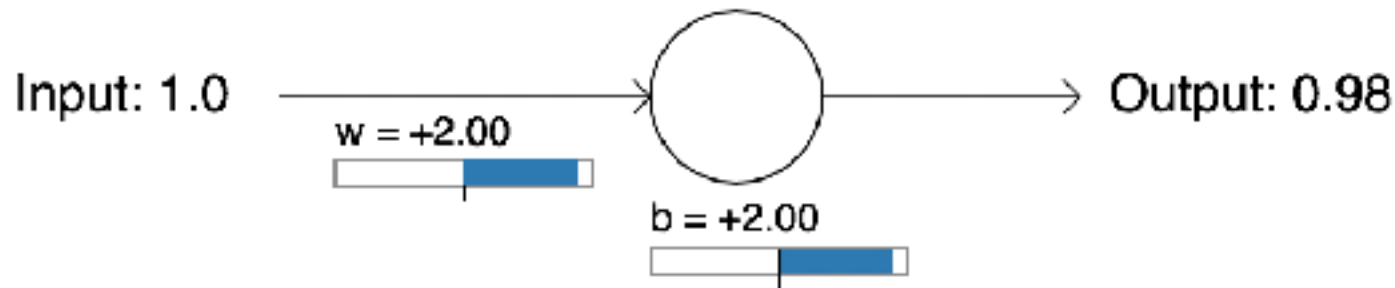
Run

# Practical Implementation of Architectures

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Run

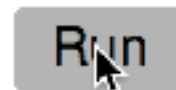
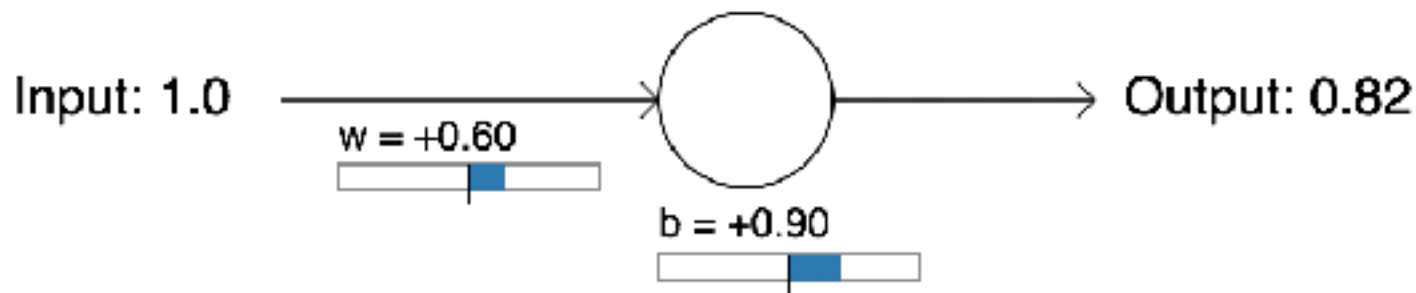


# Practical Implementation of Architectures

- Our old friend, **Binary Cross entropy**

$$J(\mathbf{W}) = - [\mathbf{y}^{(i)} \ln([\mathbf{a}^{(L+1)}]^{(i)}) + (1 - \mathbf{y}^{(i)}) \ln(1 - [\mathbf{a}^{(L+1)}]^{(i)})]$$

speeds up initial training

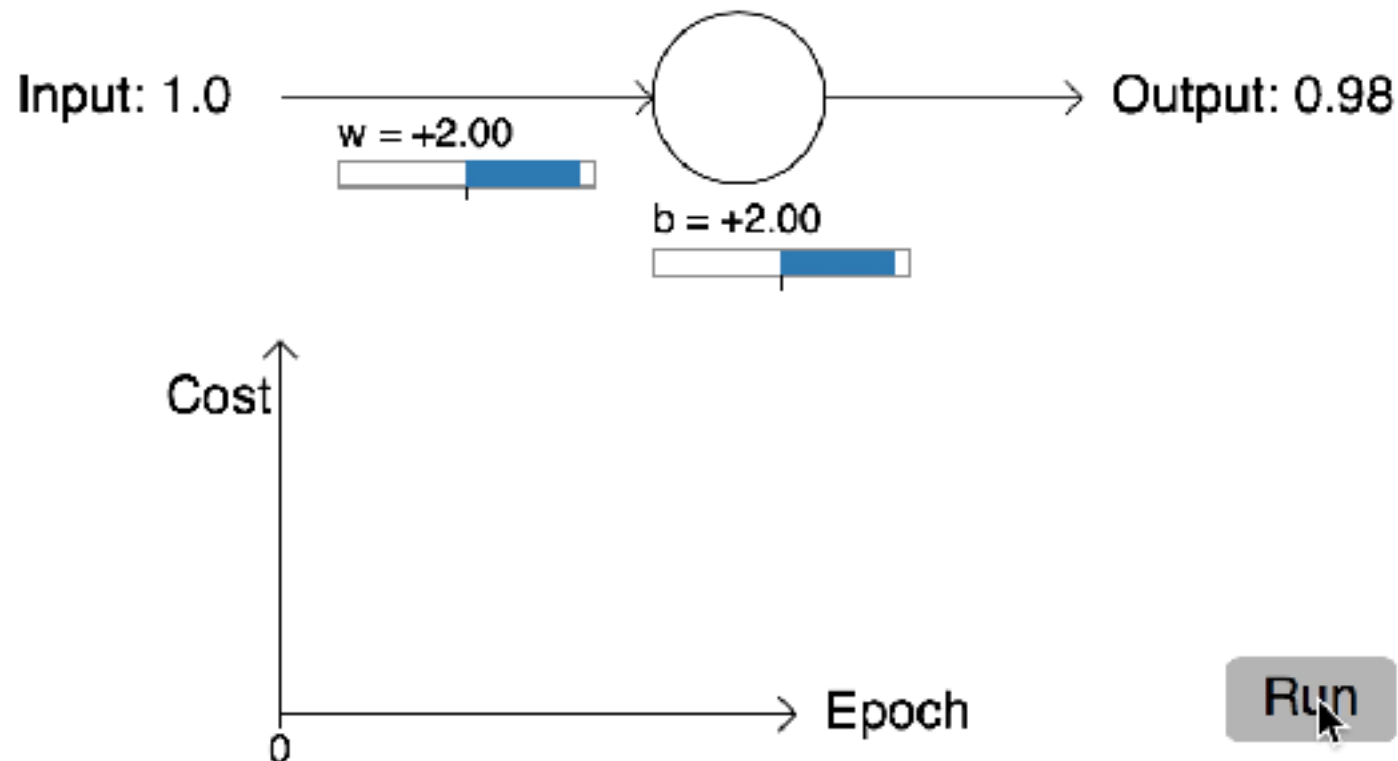


# Practical Implementation of Architectures

- Negative of MLE: **Binary Cross entropy**

$$J(\mathbf{W}) = - [\mathbf{y}^{(i)} \ln([\mathbf{a}^{(L+1)}]^{(i)}) + (1 - \mathbf{y}^{(i)}) \ln(1 - [\mathbf{a}^{(L+1)}]^{(i)})]$$

speeds up initial training



# Practical Implementation of Architectures

$$J(\mathbf{W}) = - [\mathbf{y}^{(i)} \ln([\mathbf{a}^{(L+1)}]^{(i)}) + (1 - \mathbf{y}^{(i)}) \ln(1 - [\mathbf{a}^{(L+1)}]^{(i)})]$$

likely to speed up initial training

$$\begin{aligned} \left[ \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(L)}} \right]^{(i)} &= - \frac{\partial}{\partial \mathbf{z}^{(L)}} [\mathbf{y}^{(i)} \ln([\mathbf{a}^{(L+1)}]^{(i)}) + (1 - \mathbf{y}^{(i)}) \ln(1 - [\mathbf{a}^{(L+1)}]^{(i)})] \quad \text{only } \mathbf{a} \text{ has dependence on } \mathbf{z} \\ &= - \left[ \mathbf{y}^{(i)} \frac{\partial}{\partial \mathbf{z}^{(L)}} (\ln([\mathbf{a}^{(L+1)}]^{(i)})) + (1 - \mathbf{y}^{(i)}) \frac{\partial}{\partial \mathbf{z}^{(L)}} (\ln(1 - [\mathbf{a}^{(L+1)}]^{(i)})) \right] \\ &= - \left[ \mathbf{y}^{(i)} \frac{1}{[\mathbf{a}^{(L+1)}]^{(i)}} \left( \frac{\partial}{\partial \mathbf{z}^{(L)}} [\mathbf{a}^{(L+1)}]^{(i)} \right) + \frac{(1 - \mathbf{y}^{(i)})}{1 - [\mathbf{a}^{(L+1)}]^{(i)}} \left( - \frac{\partial}{\partial \mathbf{z}^{(L)}} [\mathbf{a}^{(L+1)}]^{(i)} \right) \right] \\ &= - \left[ \mathbf{y}^{(i)} \frac{1}{[\mathbf{a}^{(L+1)}]^{(i)}} ([\mathbf{a}^{(L+1)}]^{(i)} (1 - [\mathbf{a}^{(L+1)}]^{(i)})) - \frac{(1 - \mathbf{y}^{(i)})}{1 - [\mathbf{a}^{(L+1)}]^{(i)}} ([\mathbf{a}^{(L+1)}]^{(i)} (1 - [\mathbf{a}^{(L+1)}]^{(i)})) \right] \\ &= - [\mathbf{y}^{(i)} (1 - [\mathbf{a}^{(L+1)}]^{(i)}) - (1 - \mathbf{y}^{(i)}) ([\mathbf{a}^{(L+1)}]^{(i)})] \\ &= - [\mathbf{y}^{(i)} - \mathbf{y}^{(i)} [\mathbf{a}^{(L+1)}]^{(i)} - [\mathbf{a}^{(L+1)}]^{(i)} + [\mathbf{a}^{(L+1)}]^{(i)} \mathbf{y}^{(i)}] = [\mathbf{a}^{(L+1)}]^{(i)} - \mathbf{y}^{(i)} \end{aligned}$$

$$\mathbf{V}^{(2)} = -2(\mathbf{Y} - \mathbf{A}^{(3)}) \odot \mathbf{A}^{(3)} \odot (1 - \mathbf{A}^{(3)}) \text{ old update}$$

# Practical Implementation of Architectures

- Back to our old friend: **Cross entropy**

$$J(\mathbf{W}) = - [\mathbf{y}^{(i)} \ln([\mathbf{a}^{(L+1)}]^{(i)}) + (1 - \mathbf{y}^{(i)}) \ln(1 - [\mathbf{a}^{(L+1)}]^{(i)})]$$

likely to speed up initial training

$$\left[ \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(L)}} \right]^{(i)} = [\mathbf{a}^{(L+1)}]^{(i)} - \mathbf{y}^{(i)}$$

$$\left[ \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(2)}} \right]^{(i)} = [\mathbf{a}^{(3)}]^{(i)} - \mathbf{y}^{(i)}$$

two layer network

$$\mathbf{V}^{(2)} = \mathbf{A}^{(3)} - \mathbf{Y}$$

new update

```
# vectorized backpropagation  
V2 = (A3-Y_enc) # <- this is only line t  
V1 = A2*(1-A2)*(W2.T @ V2)
```

$$\mathbf{V}^{(2)} = -2(\mathbf{Y} - \mathbf{A}^{(3)}) \odot \mathbf{A}^{(3)} \odot (1 - \mathbf{A}^{(3)}) \text{ old update}$$

bp-5

# Practical Initialization of Architectures

SQL programmers be like

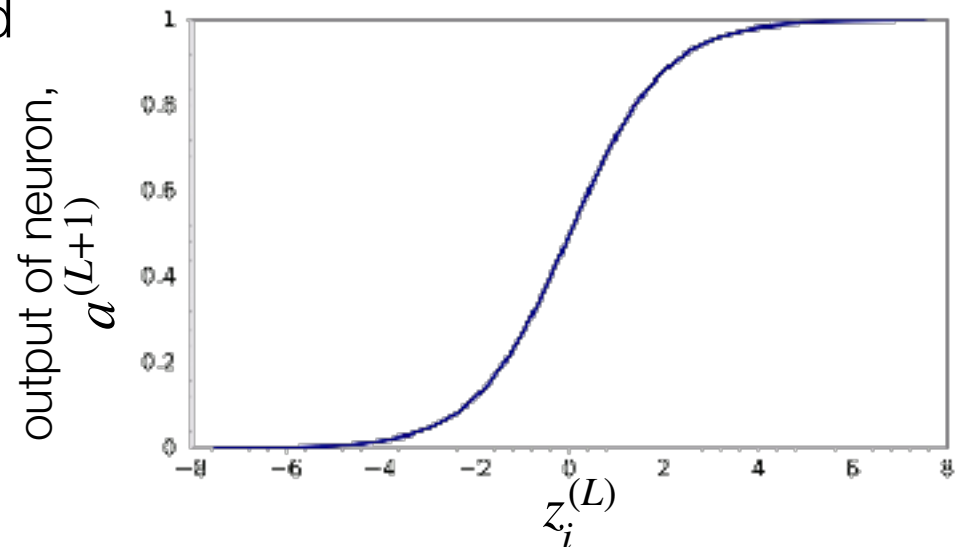


# Formative Self Test

- for adding Gaussian random variables, variances add together

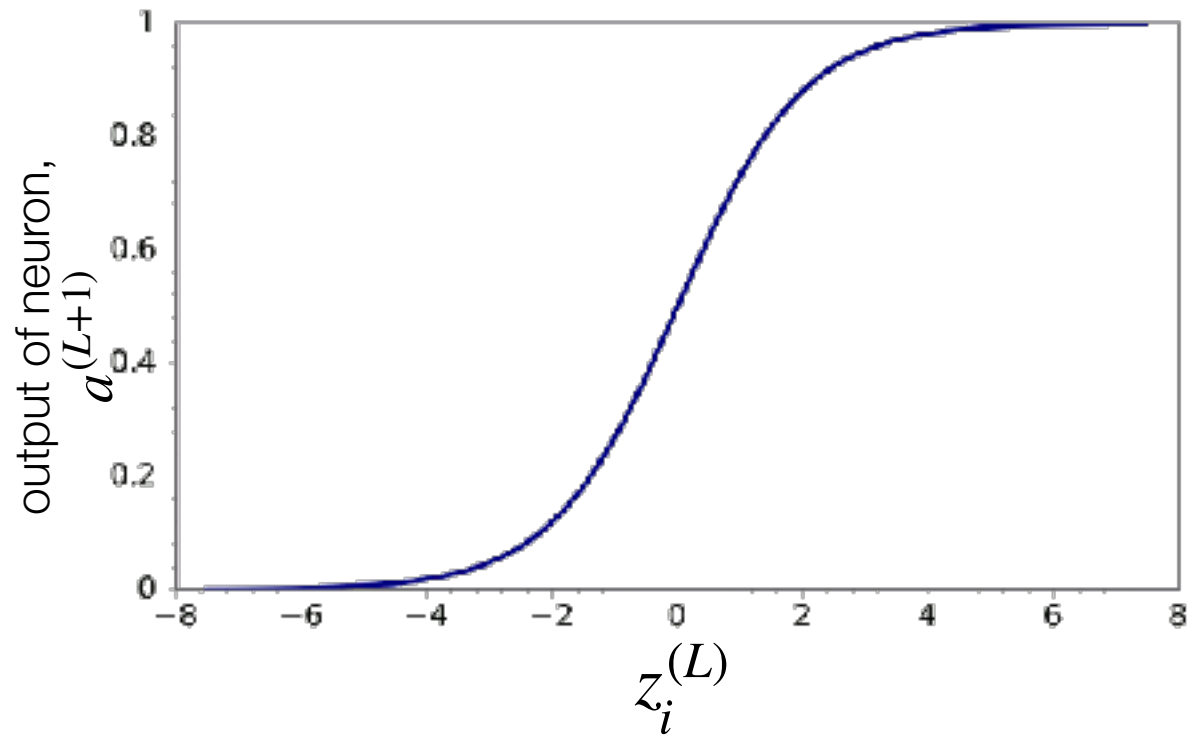
$\mathbf{a}^{(L+1)} = \phi(\mathbf{W}^{(L)}\mathbf{a}^{(L)})$  assume each element of  $\mathbf{a}^{(L)}$  is Gaussian

- If you initialized the weights,  $\mathbf{W}$ , with too large variance, you would expect the output of the neuron,  $\mathbf{a}^{(L+1)}$ , to be:
  - A. saturated to “1”
  - B. saturated to “0”
  - C. could either be saturated to “0” or “1”
  - D. would not be saturated



# Formative Self Test

- What is the derivative of a saturated sigmoid neuron?
  - A. zero
  - B. one
  - C.  $a \times (1 - a)$
  - D. it depends



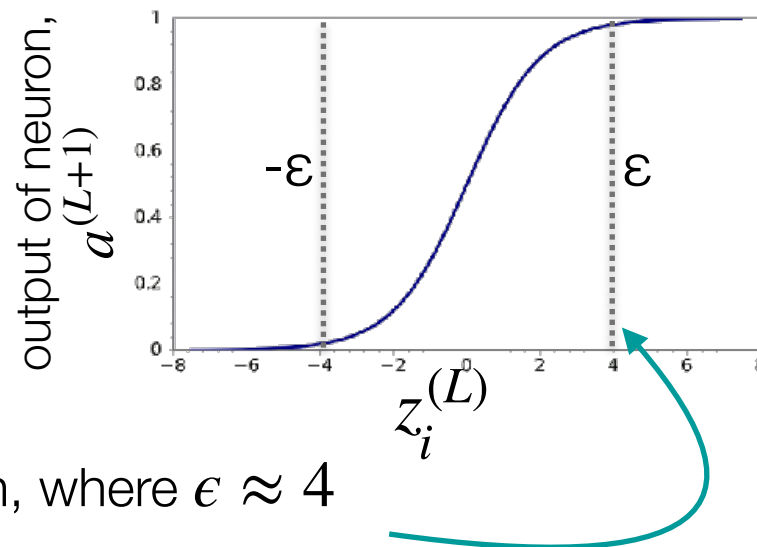
# Practical Implementation of Architectures

**Weight initialization:** try not to saturate your neurons right away!

$$\mathbf{z}^{(L)} = \mathbf{W}^{(L)} \mathbf{a}^{(L)} \quad z_i^{(L)} = \sum_j w_{ij} a_j^{(L)}$$

each row is summed before sigmoid

$$\mathbf{a}^{(L+1)} = \phi(\mathbf{z}^{(L)})$$

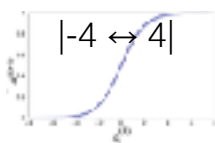


- want each  $-\epsilon < z_i^{(L)} < \epsilon$  for no saturation, where  $\epsilon \approx 4$
- want  $\text{Std}[z_i^{(L)}] \approx 4$  which means  $\text{Std}[a_i^{(L+1)}] \approx 1$ 
  - because  $\sigma(z_i^{(L)}) = a_i^{(L+1)}$ , so it will be well distributed from  $[0,1]$
- since  $z_i^{(L)} = \sum w_{ij} a_j^{(L)}$ , we should squash initial weight magnitudes,  $w_{ij}$ , such that  $\text{Std}[z_i^{(L)}] \approx 4$
- draw each  $w_{ij} \sim \mathcal{N}(0, \alpha)$  from a Gaussian with **zero mean** and **specific standard deviation** need to solve for a good  $\alpha$



**Goal:**  $\text{Std}[z_i^{(L)}] \approx 4$  in order to achieve  $\text{Std}[a_i^{(L+1)}] = 1$

Variance of each layer  $\text{Var}[z_i^{(L)}] = E[(z_i^{(L)} - E[z_i^{(L)}])^2] = E[(z_i^{(L)})^2] - E[z_i^{(L)}]^2$



try not to  
saturate

$$z_i^{(L)} = \sum_j^{n^{(L)}} w_{ij} a_j^{(L)}$$

break down feed forward by multiply in  $i^{th}$  row

$$\text{Var}[z_i^{(L)}] = \sum_j^{n^{(L)}} \underbrace{E[w_{ij}]^2 \text{Var}[a_j^{(L)}] + \text{Var}[w_{ij}] E[a_j^{(L)}]^2 + \text{Var}[w_{ij}] \text{Var}[a_j^{(L)}]}_{0, \text{ if uncorrelated}} = \sum_j^{n^{(L)}} \text{Var}[w_{ij}] \text{Var}[a_j^{(L)}]$$

$$\text{Var}[z_i^{(L)}] = n^{(L)} \underbrace{\text{Var}[w_{ij}] \text{Var}[a_j^{(L)}]}_{\approx 1} = n^{(L)} \text{Var}[w_{ij}]$$

$$\text{Std}[z_i^{(L)}] = \sqrt{n^{(L)}} \cdot \text{Std}[w_{ij}]$$

$$\text{Std}[z_i^{(L)}] = 4 = \sqrt{n^{(L)}} \cdot \text{Std}[w_{ij}]$$

$$\text{Std}[w_{ij}] = 4 \cdot \sqrt{\frac{1}{n^{(L)}}}$$

$$w_{ij}^{(L)} \sim \mathcal{N}\left(0, 4 \cdot \sqrt{\frac{1}{n^{(L)}}}\right) \quad \text{forward from sigmoid}$$

Understanding the difficulty of training deep feedforward neural networks

# Glorot Weight Initialization

$$\text{Std}[z_i^{(L)}] = 4 = \sqrt{n^{(L)}} \cdot \text{Std}[w_{ij}]$$

$$w_{ij}^{(L)} \sim \mathcal{N}\left(0, 4 \cdot \sqrt{\frac{1}{n^{(L)}}}\right) \quad \text{forward from sigmoid}$$

$$\mathbf{v}^{(L)} = \mathbf{a}^{(L)}(1 - \mathbf{a}^{(L)})\mathbf{W}^{(L)} \cdot \mathbf{v}^{(L+1)}$$

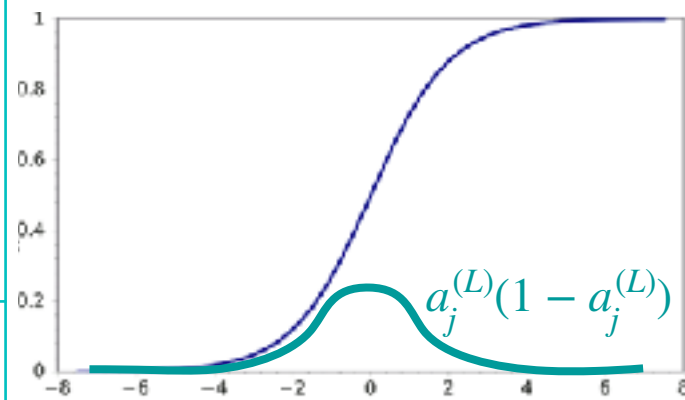
want to keep variance of  $\mathbf{v}$  stable  
magnitude  $\rightarrow$  stable gradient

Similar calculation for back prop.

$$\text{Var}[v_i^{(L)}] = n^{(L+1)}\text{Var}[w_{ij}]\text{Var}[v_j^{(L+1)} \cdot a_j^{(L)}(1 - a_j^{(L)})]$$

$$\text{Std}[v_i^{(L)}] = \sqrt{n^{(L+1)}} \cdot \text{Std}[w_{ij}] \cdot 0.25 \quad \text{want} = 1$$

$$w_{ij}^{(L)} \sim \mathcal{N}\left(0, 4 \cdot \sqrt{\frac{1}{n^{(L+1)}}}\right) \quad \text{backward from sensitivity}$$



$$w_{ij}^{(L)} \sim \mathcal{N}\left(0, 4 \cdot \sqrt{\frac{2}{n^{(L)} + n^{(L+1)}}}\right) \quad \text{compromise}$$

$$w_{ij}^{(L)} \sim U\left[\pm 4 \sqrt{\frac{6}{n^{(L)} + n^{(L+1)}}}\right] \quad \text{if drawn from uniform dist.}$$

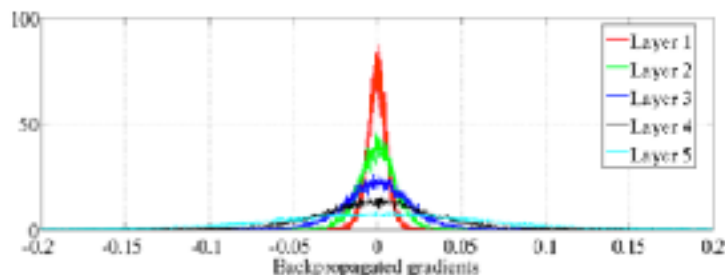
# Glorot Weight Initialization

## Understanding the difficulty of training deep feedforward neural networks

Xavier Glorot

DIRO, Université de Montréal, Montréal, Québec, Canada

Yoshua Bengio



Starting gradient histograms  
per layer  
*standard initialization*

Figure 7: *Back-propagated gradients normalized histograms with hyperbolic tangent activation, with standard (top) vs normalized (bottom) initialization. Top: 0-peak decreases for higher layers.*

## 08a. Practical\_NeuralNetsWithBias.ipynb

Momentum

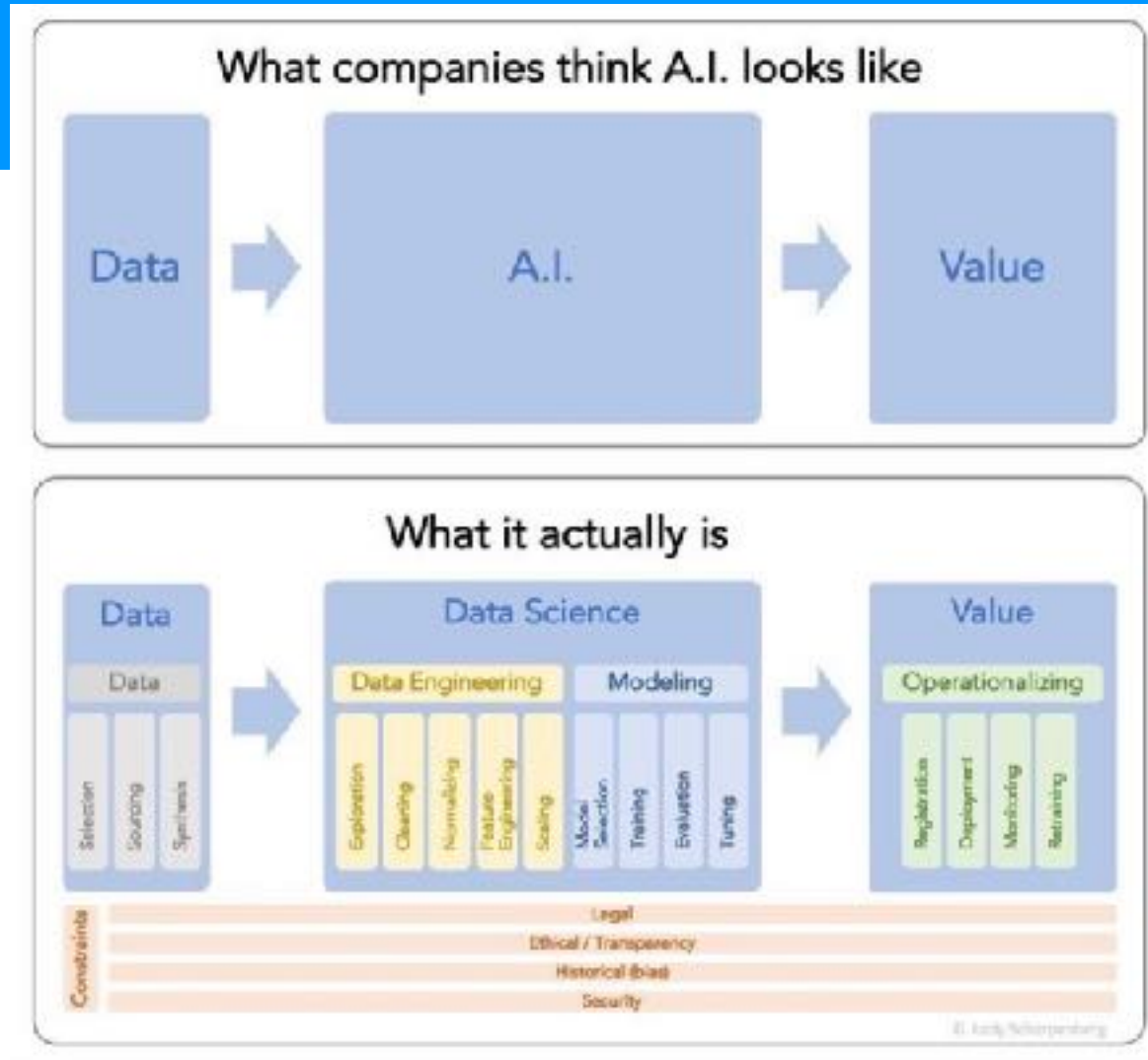
Cooling

Cross Entropy

Smarter Weight Initialization

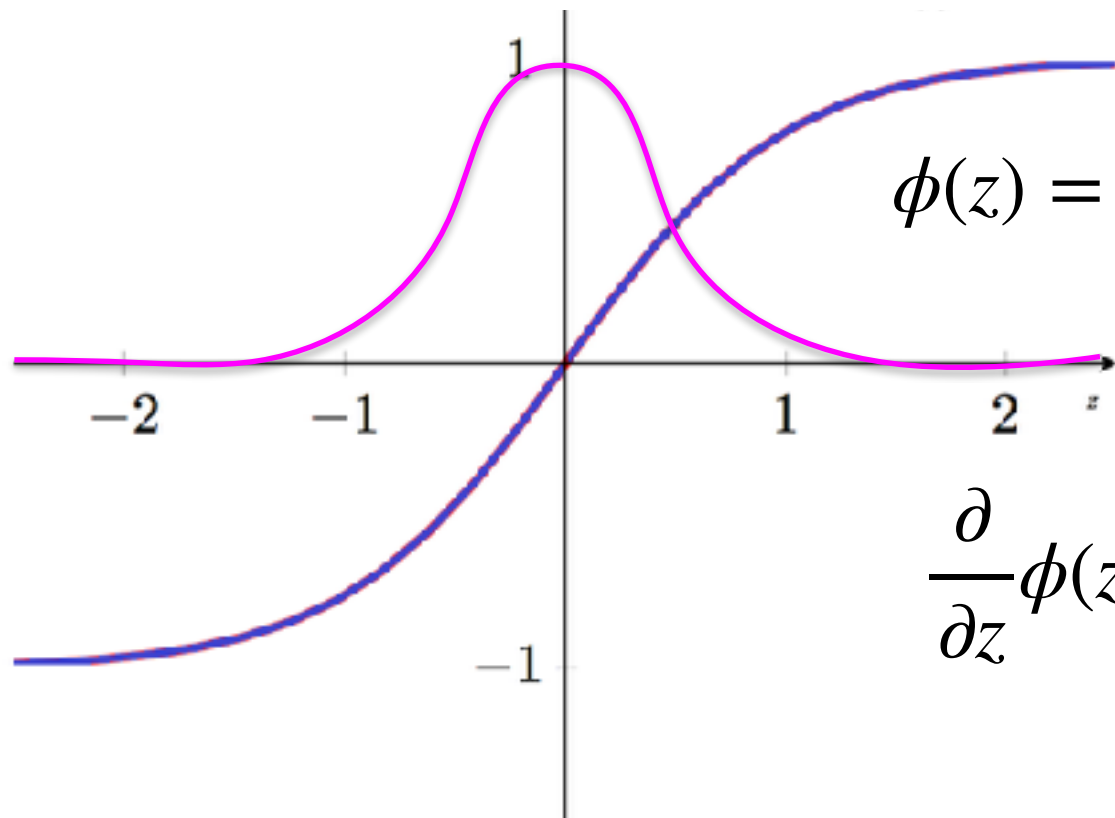


# Beyond Sigmoid: Other Activations



# New Activation: Hyperbolic Tangent

- Basically a sigmoid from -1 to 1

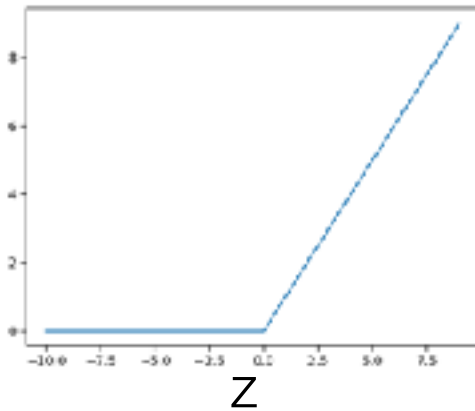


$$\phi(z) = \frac{\sinh(z)}{\cosh(z)} = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

$$\frac{\partial}{\partial z}\phi(z) = \text{sech}^2(z)$$

# New Activation: ReLU

- A new nonlinearity: **rectified linear units**



$$\phi(z) = \begin{cases} z, & \text{if } z > 0 \\ 0, & \text{else} \end{cases}$$

it has the advantage of **large gradients** and **extremely simple** derivative

$$\frac{\partial}{\partial z} \phi(z) = \begin{cases} 1, & \text{if } z > 0 \\ 0, & \text{else} \end{cases}$$

# Other Activation Functions

- Sigmoid Weighted Linear Unit **SiLU** (also called Swish)
- Mixing of sigmoid,  $\sigma$ , and ReLU

$$\phi(z) = \sigma(z) \cdot z$$

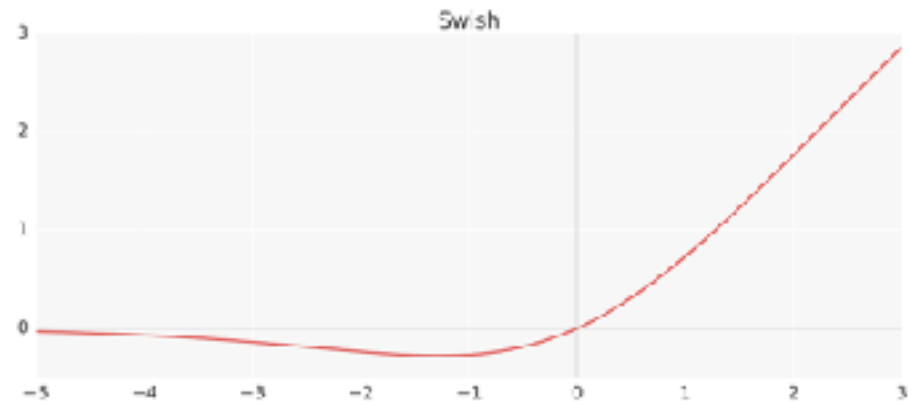


Figure 1: The Swish activation function.

$$\frac{\partial \phi(z)}{\partial z} = \frac{\partial}{\partial z} \sigma(z) \cdot z$$

$$= z \cdot \left[ \frac{\partial}{\partial z} \sigma(z) \right] + \sigma(z) \cdot \left[ \frac{\partial}{\partial z} z \right]$$

$$= z \cdot \sigma(z)(1 - \sigma(z)) + \sigma(z)$$

$$= z \cdot \sigma(z) + \sigma(z) \cdot (1 - z \cdot \sigma(z))$$

$$= \phi(z) + \sigma(z) \cdot (1 - \phi(z))$$

Elfwing, Stefan, Eiji Uchibe, and Kenji Doya. "Sigmoid-weighted linear units for neural network function approximation in reinforcement learning." *Neural Networks* (2018).

Ramachandran P, Zoph B, Le QV. Swish: a Self-Gated Activation Function. *arXiv preprint arXiv:1710.05941*. 2017 Oct 16



# Glorot and He Initialization

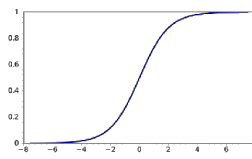
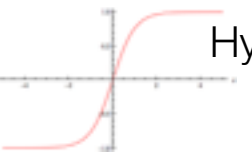
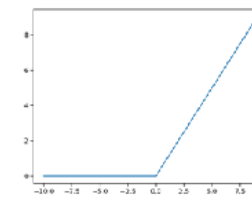
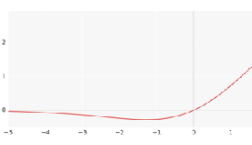
We have solved this assuming the activation output is in the range -4 to 4 (for a sigmoid) and assuming that we use Gaussian for sampling.

This range is different depending on the activation and assuming Gaussian or Uniform sampling.

	Uniform	Gaussian
Tanh	$w_{ij}^{(L)} \sim \sqrt{\frac{6}{n^{(L)} + n^{(L+1)}}}$	$w_{ij}^{(L)} \sim \sqrt{\frac{2}{n^{(L)} + n^{(L+1)}}}$
Sigmoid	$w_{ij}^{(L)} \sim 4\sqrt{\frac{6}{n^{(L)} + n^{(L+1)}}}$	$w_{ij}^{(L)} \sim 4\sqrt{\frac{2}{n^{(L)} + n^{(L+1)}}}$
ReLU SiLU	$w_{ij}^{(L)} \sim \sqrt{2}\sqrt{\frac{6}{n^{(L)} + n^{(L+1)}}}$	$w_{ij}^{(L)} \sim \sqrt{2}\sqrt{\frac{2}{n^{(L)} + n^{(L+1)}}}$

Summarized by Glorot and He

# Activations Summary

	Definition	Derivative	Weight Init (Uniform Bounds)
 <p>Sigmoid</p>	$\phi(z) = \frac{1}{1 + e^{-z}}$	$\nabla \phi(z) = a(1 - a)$	$w_{ij}^{(L)} \sim \pm 4 \sqrt{\frac{6}{n^{(L)} + n^{(L+1)}}}$
 <p>Hyperbolic Tangent</p>	$\phi(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$	$\nabla \phi(z) = \frac{4}{(e^z + e^{-z})^2}$	$w_{ij}^{(L)} \sim \pm \sqrt{\frac{6}{n^{(L)} + n^{(L+1)}}}$
 <p>ReLU</p>	$\phi(z) = \begin{cases} z, & \text{if } z > 0 \\ 0, & \text{else} \end{cases}$	$\nabla \phi(z) = \begin{cases} 1, & \text{if } z > 0 \\ 0, & \text{else} \end{cases}$	$w_{ij}^{(L)} \sim \pm \sqrt{2} \sqrt{\frac{6}{n^{(L)} + n^{(L+1)}}}$
 <p>SiLU</p>	$\phi(z) = \frac{z}{1 + e^{-z}}$	$\nabla \phi(z) = \phi(z) + \sigma(z) \cdot (1 - \phi(z))$	

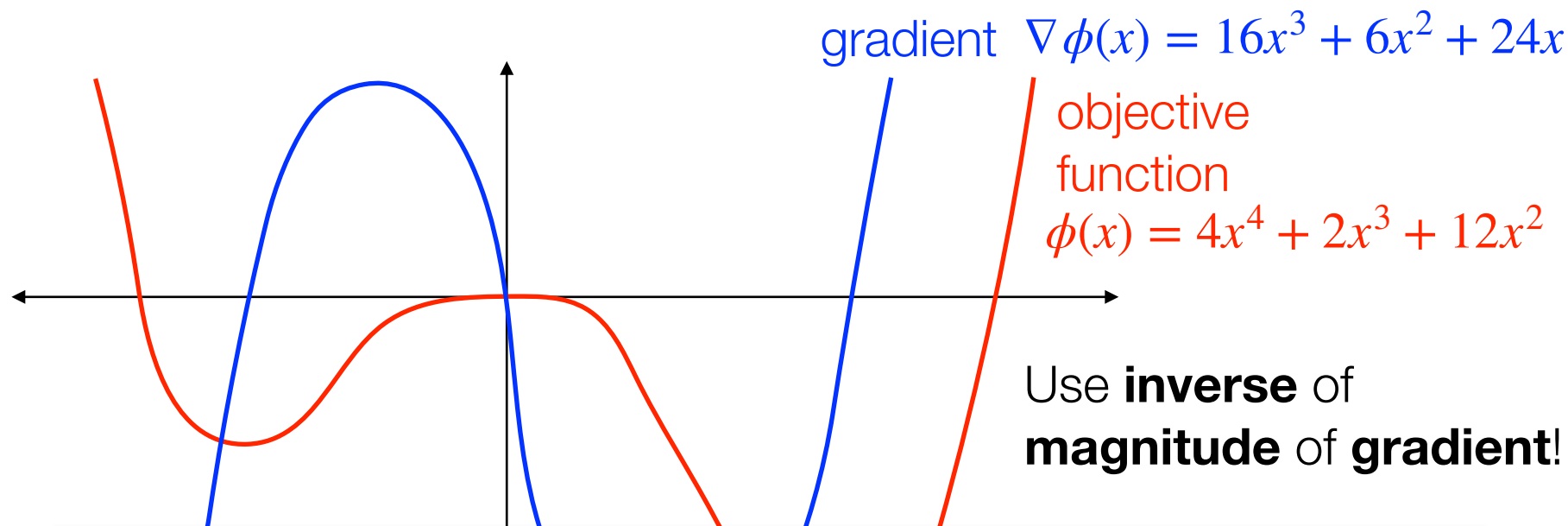
# More Adaptive Optimization



Going beyond  
changing the learning rate

# Be adaptive based on Gradient Magnitude?

- Decelerate down regions that are steep
- Accelerate on plateaus



How can we do this separately for every  $w_{ij}^{(l)}$  in every  $\mathbf{W}^{(l)}$ ?

**Momentum:** be robust to **abrupt changes** in **steepness** (accumulate inverse magnitudes)

# Be adaptive based on Gradient Magnitude?

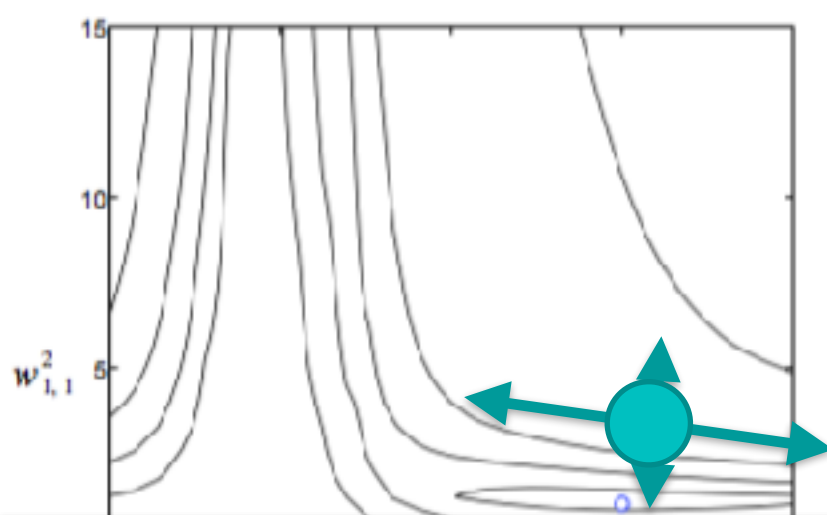
Inverse magnitude of gradient in multiple directions?

$$\mathbf{W}_{k+1} \leftarrow \mathbf{W}_k + \eta \frac{1}{\sqrt{\mathbf{G}_k + \epsilon}} \odot \nabla J(\mathbf{W}_k)$$

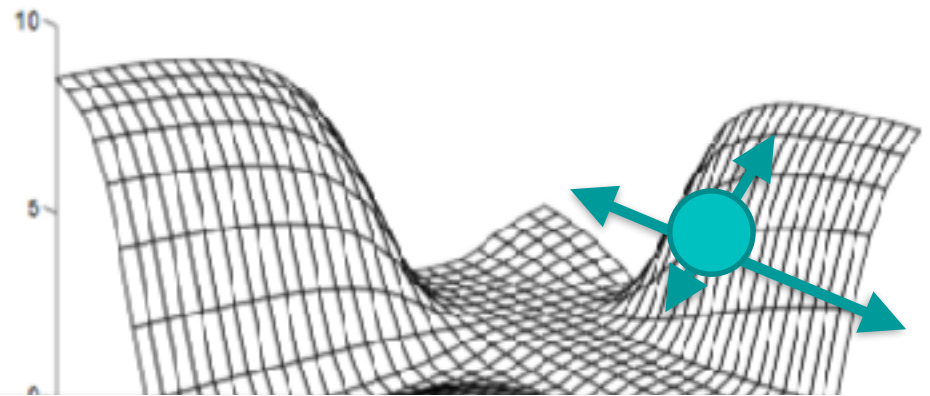
↑                      ↙  
new matrix for normalizing      gradient

$$\mathbf{G}_k = \nabla J(\mathbf{W}_k) \odot \nabla J(\mathbf{W}_k)$$

same size as  $\mathbf{W}$



```
G = gradW1 * gradW1  
W1 += eta*gradW1 / sqrt(G+eps)
```



Now we just need to add momentum to  $\mathbf{G}_k^{(l)}$

Note:  $\mathbf{G}$  exists for every layer, but we will abuse layer notation

# Common Adaptive Strategies $\mathbf{W}_{k+1} = \mathbf{W}_k - \eta \cdot \rho_k$

Adjust each element of gradient by the steepness

<ul style="list-style-type: none"><li>AdaGrad</li></ul> <p>all operations are per element</p>	$\rho_k = \frac{1}{\sqrt{\mathbf{G}_k + \epsilon}} \odot \nabla J(\mathbf{W}_k)$	where $\mathbf{G}_k = \gamma \cdot \mathbf{G}_{k-1} + \nabla J(\mathbf{W}_k) \odot \nabla J(\mathbf{W}_k)$
<ul style="list-style-type: none"><li>RMSProp</li></ul> <p>all operations are per element</p>	$\rho_k = \frac{1}{\sqrt{\mathbf{V}_k + \epsilon}} \odot \nabla J(\mathbf{W}_k)$	$\begin{aligned}\mathbf{G}_k &= \nabla J(\mathbf{W}_k) \odot \nabla J(\mathbf{W}_k) \\ \mathbf{V}_k &= \gamma \cdot \mathbf{V}_{k-1} + (1 - \gamma) \cdot \mathbf{G}_k\end{aligned}$
<ul style="list-style-type: none"><li>AdaDelta</li></ul> <p>all operations are per element</p>	$\rho_k = \frac{\mathbf{M}_k}{\sqrt{\mathbf{V}_k + \epsilon}}$	$\mathbf{M}_{k+1} = \gamma \cdot \mathbf{M}_k + (1 - \gamma) \cdot \nabla J(\mathbf{W}_k)$
<ul style="list-style-type: none"><li>AdaM</li></ul>	$\mathbf{G}$ updates with decaying momentum of $J$ and $J^2$	
<ul style="list-style-type: none"><li>NAdaM</li></ul>	same as Adam, but with nesterov's acceleration	

**None** of these are “**one-size-fits-all**” because the space of neural network **optimization varies** by problem, AdaM is **popular** but **not a panacea**

# Adaptive Momentum

All operations are element wise:

$$\beta_1 = 0.9, \beta_2 = 0.999, \eta = 0.001, \epsilon = 10^{-8}$$

$$k = 0, \mathbf{M}_0 = \mathbf{0}, \mathbf{V}_0 = \mathbf{0}$$

Published as a conference paper at ICLR 2015

ADAM: A METHOD FOR STOCHASTIC OPTIMIZATION

Diederik P. Kingma\*  
University of Amsterdam, OpenAI

Jimmy Lei Ba\*  
University of Toronto

**For each epoch:**

update iteration  $k \leftarrow k + 1$

get gradient  $\nabla J(\mathbf{W}_k)$

accumulated gradient  $\mathbf{M}_k \leftarrow \beta_1 \cdot \mathbf{M}_{k-1} + (1 - \beta_1) \cdot \nabla J(\mathbf{W}_k)$

accumulated squared gradient  $\mathbf{V}_k \leftarrow \beta_2 \cdot \mathbf{V}_{k-1} + (1 - \beta_2) \cdot \nabla J(\mathbf{W}_k) \odot \nabla J(\mathbf{W}_k)$

boost moments magnitudes  
(notice  $k$  in exponent)  $\hat{\mathbf{M}}_k \leftarrow \frac{\mathbf{M}_k}{(1 - [\beta_1]^k)} \quad \hat{\mathbf{V}}_k \leftarrow \frac{\mathbf{V}_k}{(1 - [\beta_2]^k)}$

update gradient, normalized  
by second moment  
similar to AdaDelta  $\mathbf{W}_k \leftarrow \mathbf{W}_{k-1} - \eta \cdot \frac{\hat{\mathbf{M}}_k}{\sqrt{\hat{\mathbf{V}}_k + \epsilon}}$

gradient with momentum  
squared magnitude normalizer

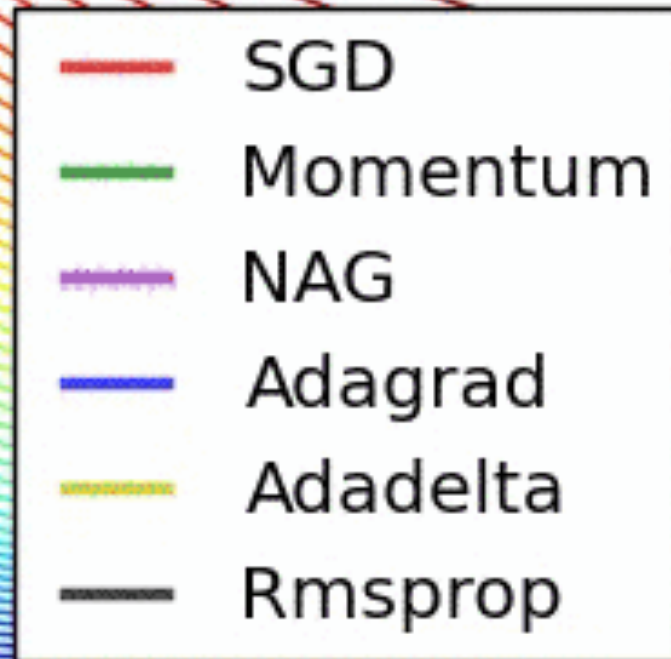


# Visualization of Optimization

<https://ruder.io/optimizing-gradient-descent/>

## Takeaways:

1. **SGD** slows tremendously on plateau
2. **Momentum** and **Nesterov** drastically overshoot
3. Adaptive strategies are similar





## 08a. Practical\_NeuralNetsWithBias.ipynb

Momentum

Cooling

~~Cross Entropy~~

~~Smarter Weight Initialization~~

ReLU Nonlinearities

Adaptive training with AdaGrad

