Lecture Notes for

Machine Learning in Python

Professor Eric Larson

Town Hall + MLP History

Class Logistics and Agenda

- Logistics:
  - ICA on your own (back propagation)
- Multi Week Agenda:
  - Town Hall, Lab 3
  - Neural Networks History, up to 1980
  - Multi-layer Architectures
  - Programming Multi-layer training

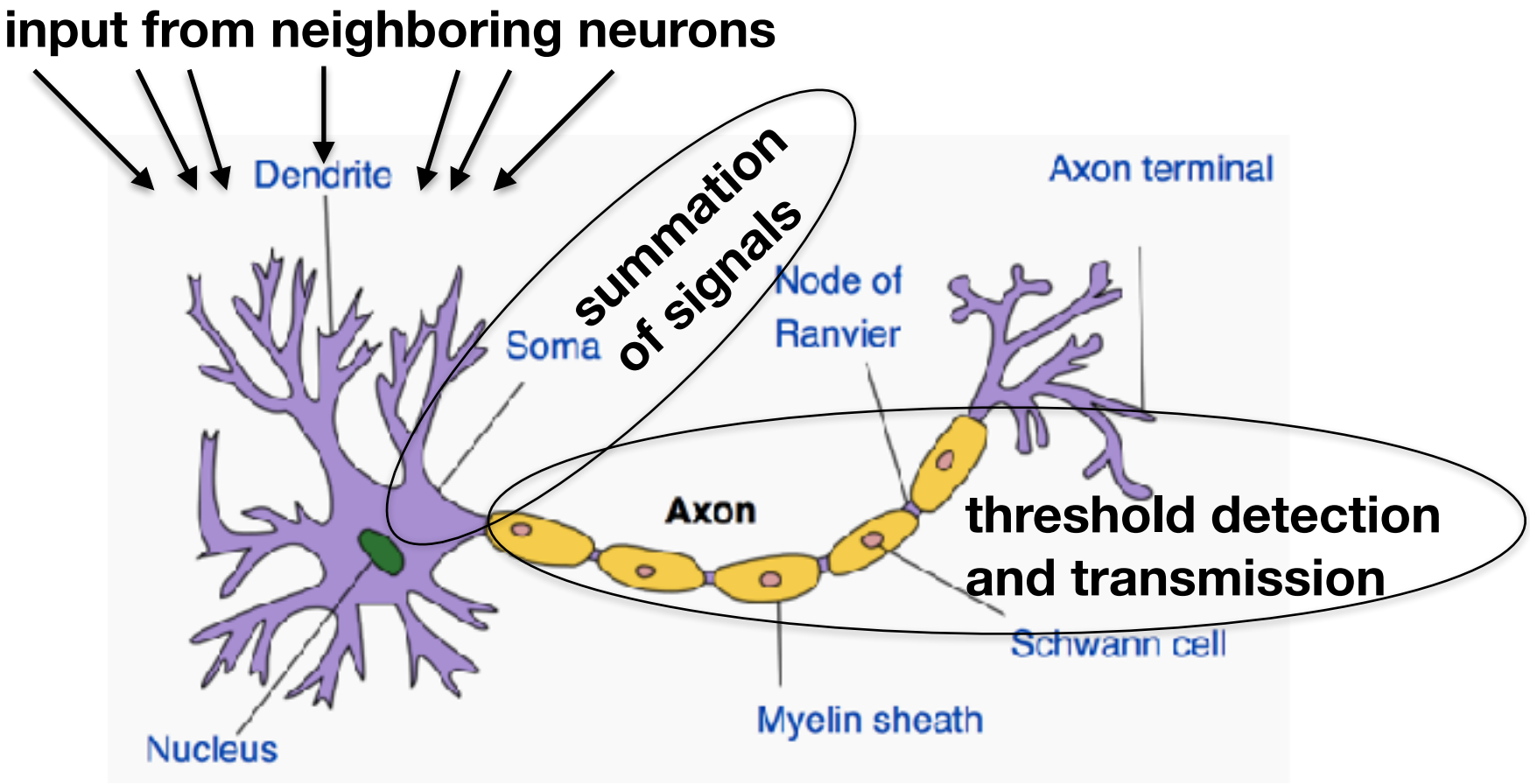
Town Hall


CAN'T FORGET A TOWN HALL
IF YOU NEVER KNEW ABOUT IT
memegenerator.net

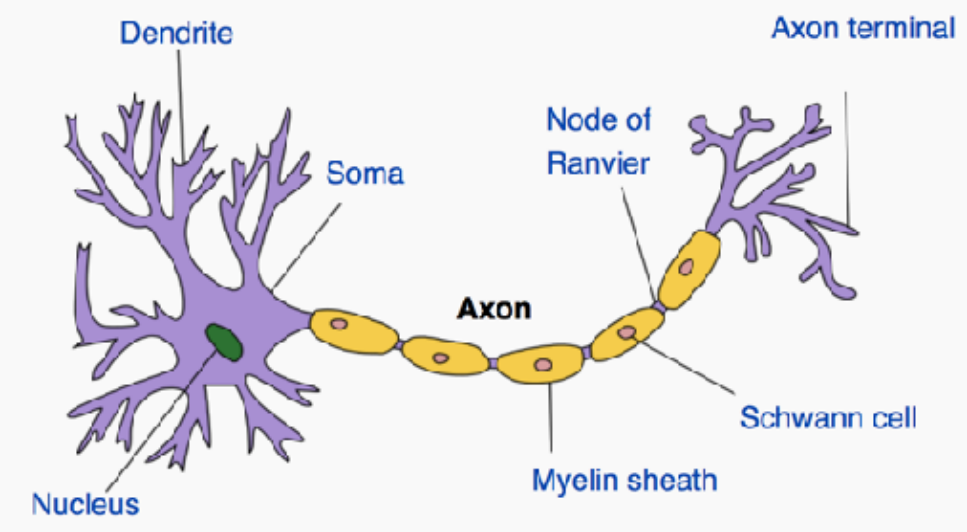
A History of Neural Networks

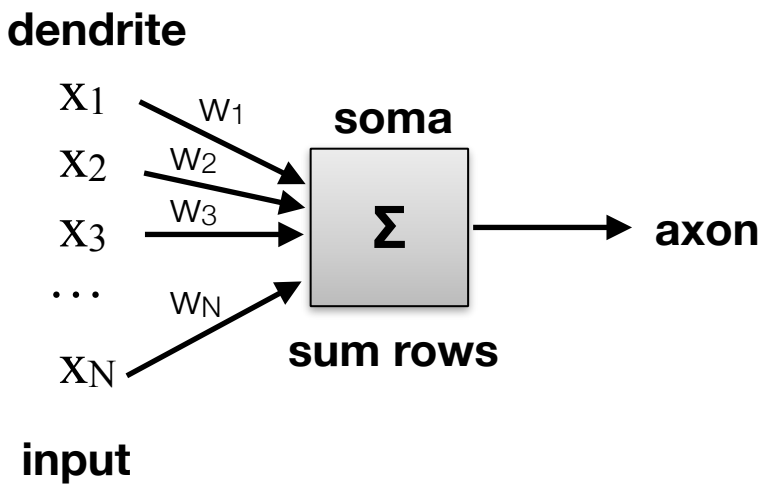
Neurons

- From biology to modeling:



McCulloch and Pitts, 1943





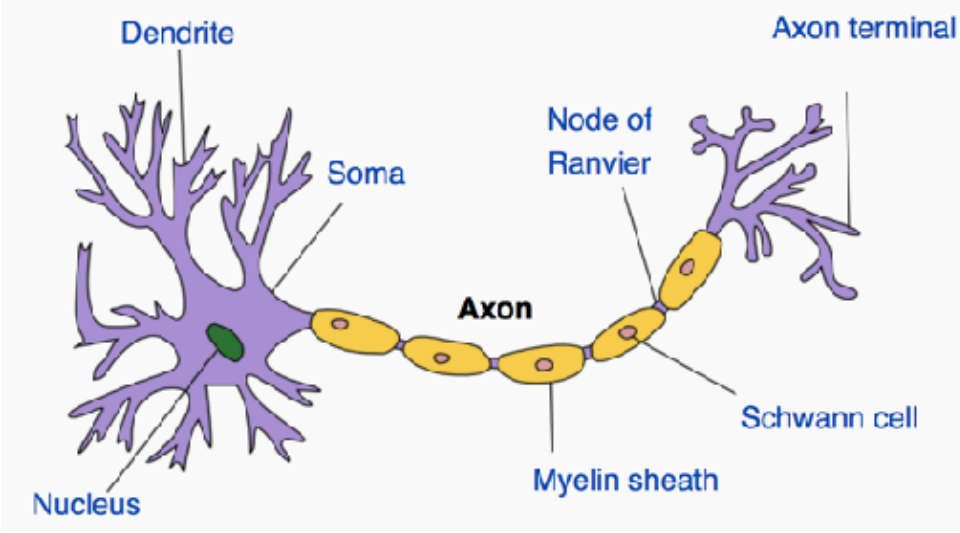
logic gates of the mind

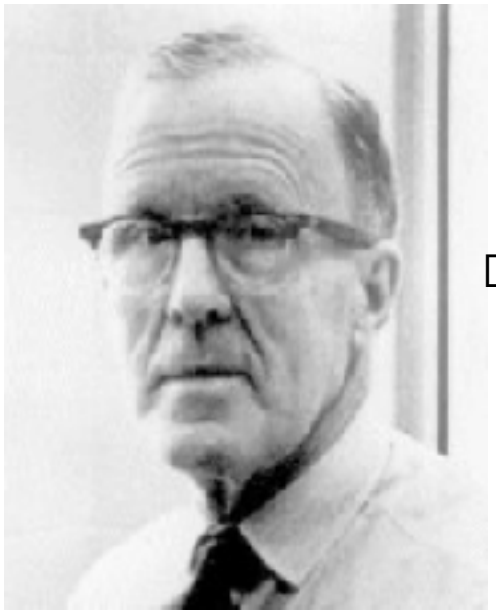
Warren McCulloch

Walter Pitts

Neurons

- McCulloch and Pitts, 1943
- Donald Hebb, 1949
  - Hebb's Law: close neurons fire together
  - neurons "learn" to couple
  - easier synaptic transmission
  - basis of neural pathways





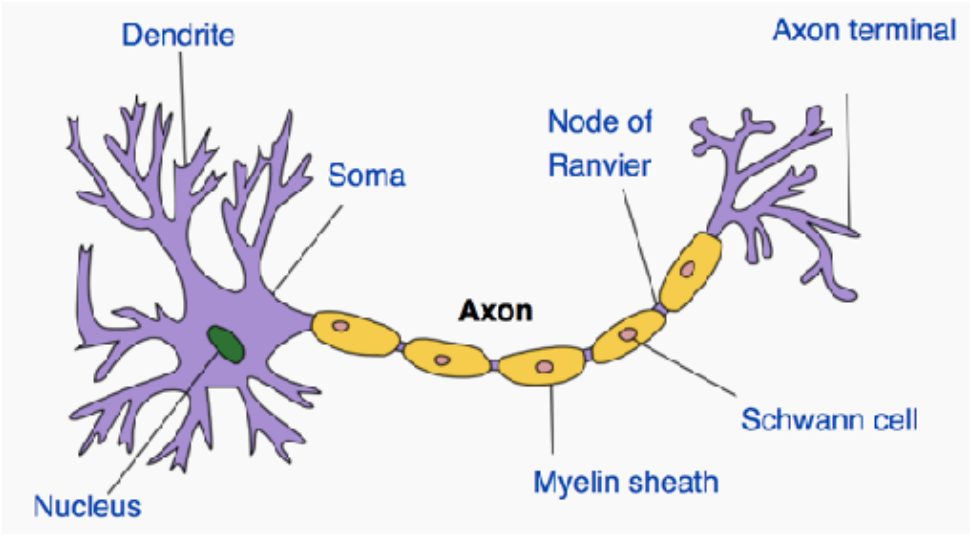
Donald O. Hebb

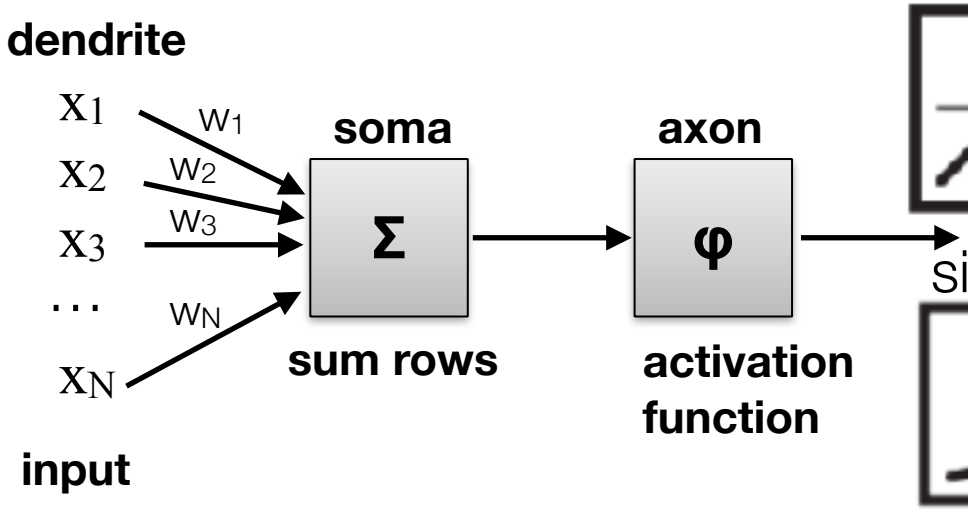
Warren McCulloch

Walter Pitts

Rosenblatt's perceptron, 1957

Frank Rosenblatt





hard limit

$a=-1 \quad z<0$

$a=1 \quad z\geq 0$

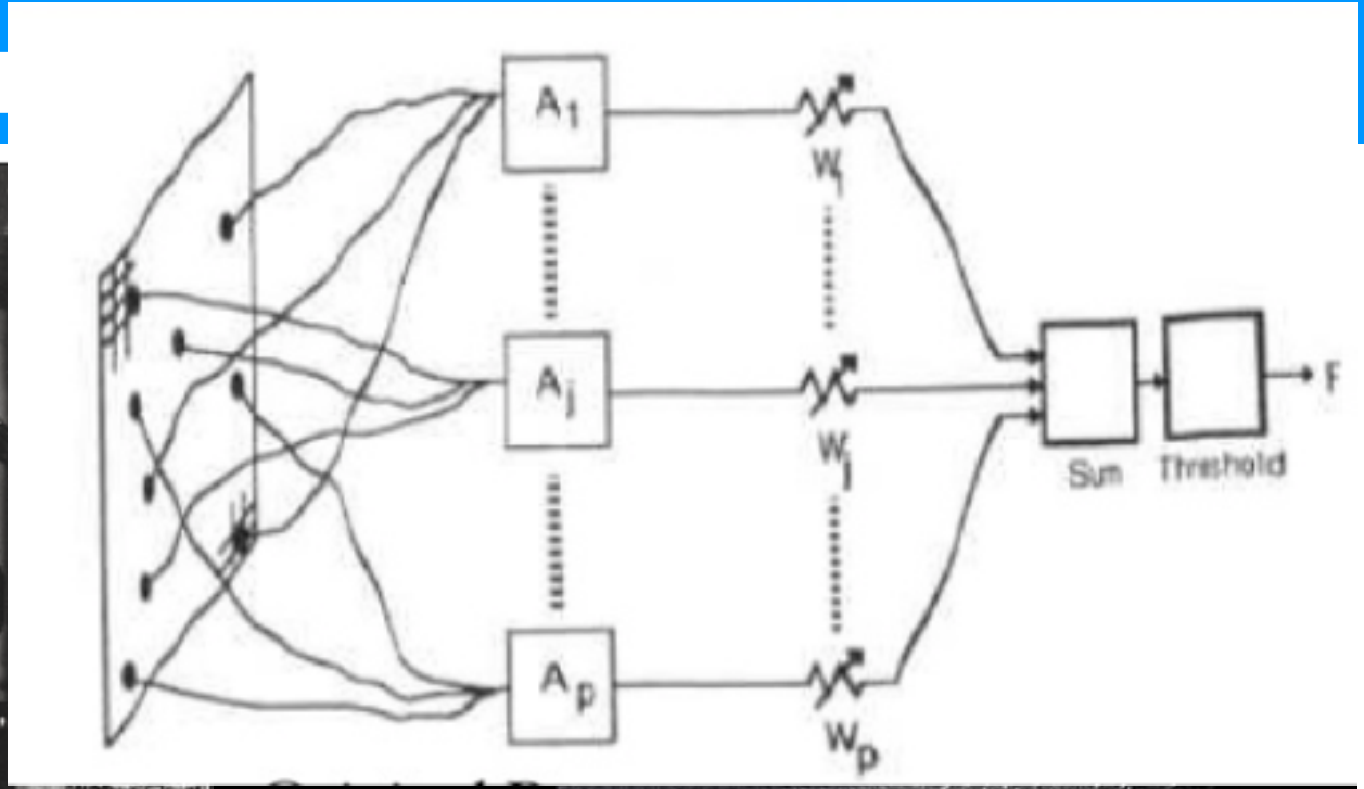
linear

$a=z$

sigmoid

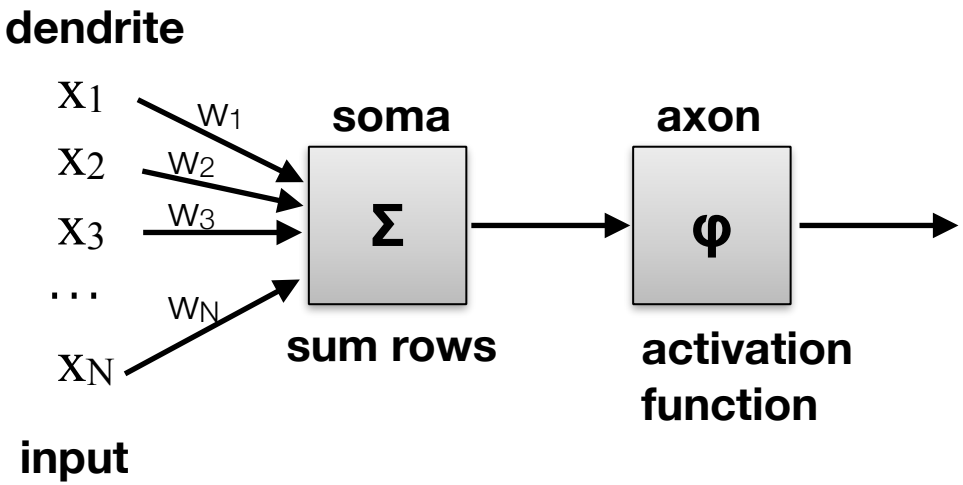
$$a=\frac{1}{1+\exp(-z)}$$

The Mark 1 P

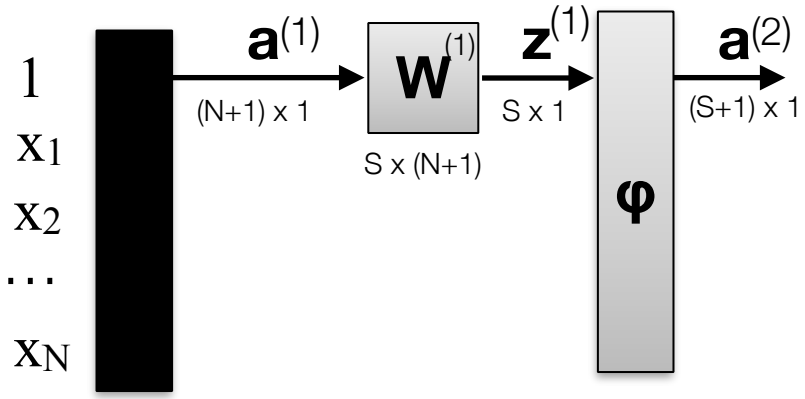


Perceptron Learning Rule:
~Stochastic Gradient Descent

Some Notation



- need bias term
- matrix representation
- multiple layers



$\mathbf{a}^{(1)}=\mathbf{x}$ + concat bias term

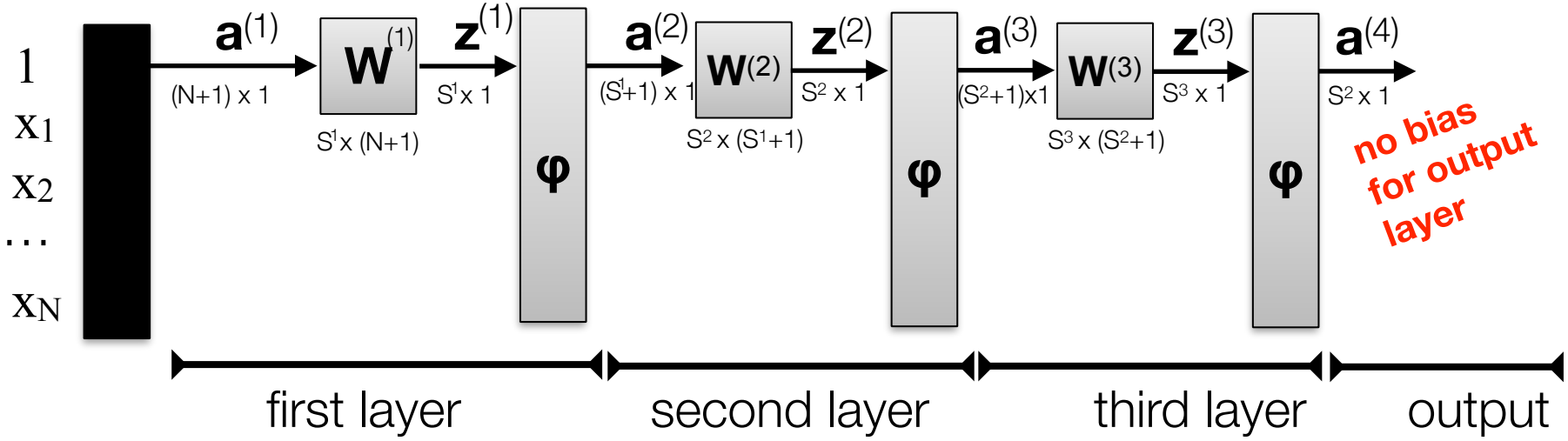
$\mathbf{z}^{(1)}=\mathbf{W}^{(1)}\mathbf{a}^{(1)}$

$$\mathbf{W}=\begin{bmatrix} w_{1,2} & w_{1,3} & w_{1,4} & \dots & w_{1,N+1} \\ & & \dots & & \\ w_{S,2} & w_{S,3} & w_{S,4} & \dots & w_{S,N+1} \end{bmatrix}$$

$\mathbf{a}^{(2)}=\boldsymbol{\phi}(\mathbf{z})$ + concat bias term

notation adapted from *Neural Network Design*, Hagan, Demuth, Beale, and De Jesus

Multiple Layers Notation



$\mathbf{a}^{(L+1)} = \boldsymbol{\phi}(\mathbf{z}^{(L)})$ + concat bias term

$\mathbf{a}^{(4)}$ rows=unique classes

$\mathbf{z}^{(L)} = \mathbf{W}^{(L)}\mathbf{a}^{(L)}$

$$\mathbf{W}^{(L)} = \begin{bmatrix} w^{(L)}_{1,1} & w^{(L)}_{1,2} & w^{(L)}_{1,3} & \dots & w^{(L)}_{1,S^{L-1}+1} \\ \dots & & & & \\ w^{(L)}_{S^L,1} & w^{(L)}_{S^L,2} & \dots & & w^{(L)}_{S^L,S^{L-1}+1} \end{bmatrix}$$

$\mathbf{z}^{(L)} = \mathbf{W}^{(L)}\boldsymbol{\phi}(\mathbf{z}^{(L-1)})$

$\mathbf{z}^{(L)} = \mathbf{W}^{(L)}\boldsymbol{\phi}(\mathbf{W}^{(L-1)}\mathbf{a}^{(L-1)})$

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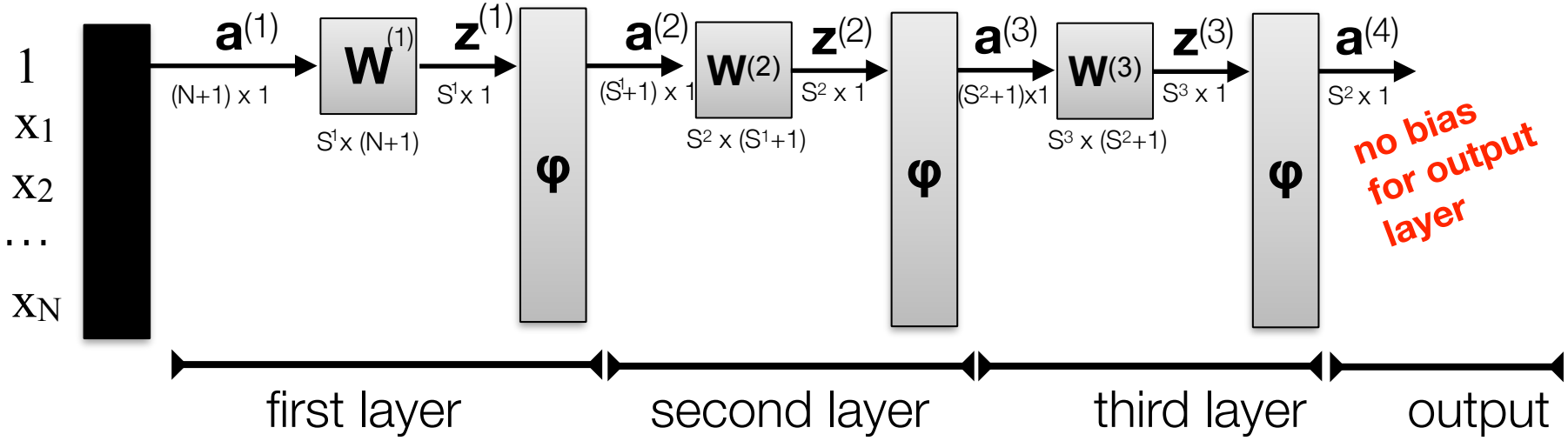
Multiple layers notation

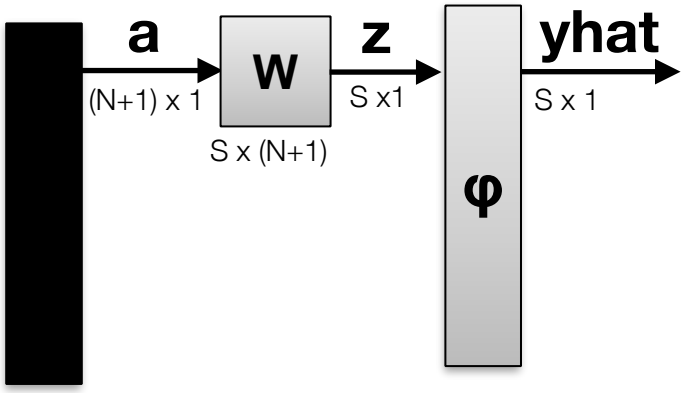


- **Self test**: How many parameters need to be trained in the above network?
  - A. $[(N+1) \times S^1] + [(S^1+1) \times S^2] + [(S^2+1) \times S^3]$
  - B. $|\mathbf{W}^{(1)}| + |\mathbf{W}^{(2)}| + |\mathbf{W}^{(3)}|$
  - C. can't determine from diagram
  - D. it depends on the sizes of intermediate variables, $\mathbf{z}^{(i)}$

notation adapted from *Neural Network Design*, Hagan, Demuth, Beale, and De Jesus

Simple Architectures

- Rosenblatt's perceptron, 1957



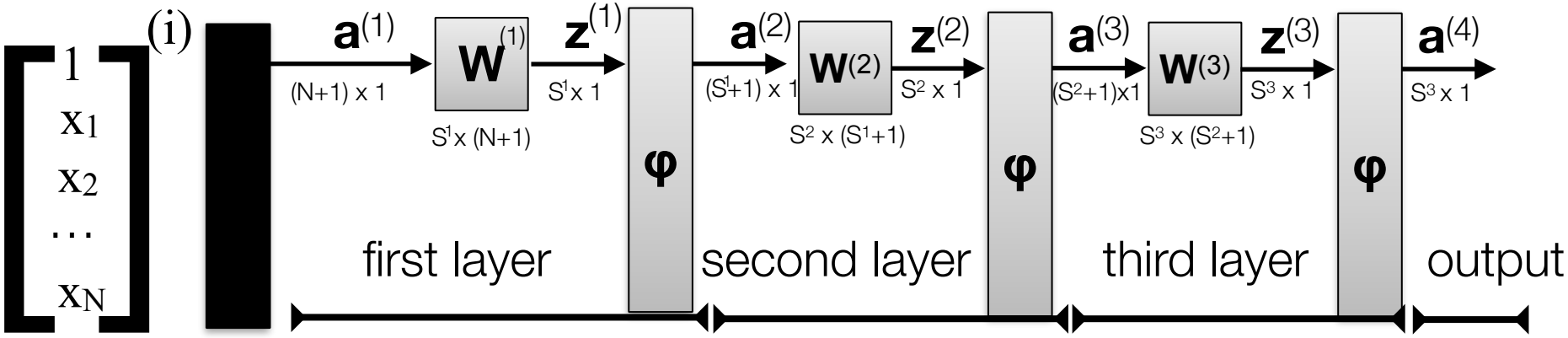
hard limit

```
a=−1    z< 0
a= 1    z>=0
```

Self Test - If this is a binary classification problem, how large is *S*?

A. Can't determine
B. 2
C. 1
D. N

Compact feedforward notation



$$\mathbf{z}^{(L)} = \mathbf{W}^{(L)}\mathbf{a}^{(L)}$$

$$[\mathbf{z}^{(L)}]^{(i)} = \mathbf{W}^{(L)}[\mathbf{a}^{(L)}]^{(i)}$$

$$\begin{bmatrix} z^{(L)}_1 \\ \dots \\ z^{(L)}_{S^L} \end{bmatrix}^{(i)} = \begin{bmatrix} w^{(L)}_{1,1} & w^{(L)}_{1,2} & w^{(L)}_{1,3} & \dots & w^{(L)}_{1,S^{L-1}+1} \\ & \dots & & & \\ w^{(L)}_{S^L,1} & w^{(L)}_{S^L,2} & \dots & & w^{(L)}_{S^L,S^{L-1}+1} \end{bmatrix} \begin{bmatrix} a^{(L)}_1 \\ \dots \\ a^{(L)}_{S^{L-1}+1} \end{bmatrix}^{(i)}$$

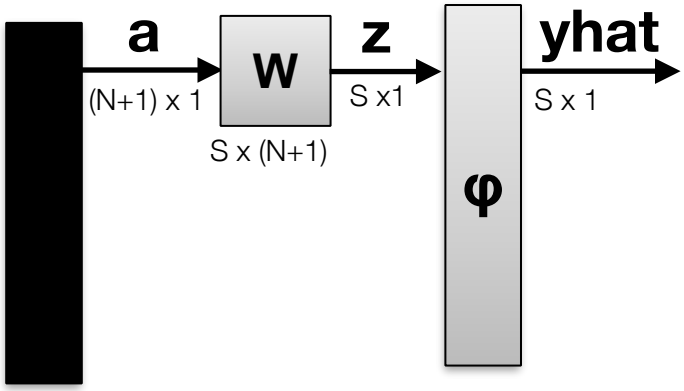
$$\begin{bmatrix} \begin{bmatrix} z^{(L)}_1 \\ \dots \\ z^{(L)}_{S^L} \end{bmatrix}^{(1)} \dots \begin{bmatrix} z^{(L)}_1 \\ \dots \\ z^{(L)}_{S^L} \end{bmatrix}^{(M)} \end{bmatrix} = \mathbf{W}^{(L)} \begin{bmatrix} \begin{bmatrix} a^{(L)}_1 \\ \dots \\ a^{(L)}_{S^{L-1}+1} \end{bmatrix}^{(1)} \dots \begin{bmatrix} a^{(L)}_1 \\ \dots \\ a^{(L)}_{S^{L-1}+1} \end{bmatrix}^{(M)} \end{bmatrix}$$

$$\mathbf{Z}^{(L)} = \mathbf{W}^{(L)}\mathbf{A}^{(L)}$$

$$\mathbf{Z}^{(L)} = \mathbf{W}^{(L)}\boldsymbol{\Phi}(\mathbf{W}^{(L-1)}\mathbf{A}^{(L-1)})$$

Training Neural Network Architectures

Rosenblatt's Perceptron, 1957



$$\sum_{i}^{M} (\mathbf{y}^{(i)} - \hat{\mathbf{y}}^{(i)})^2$$

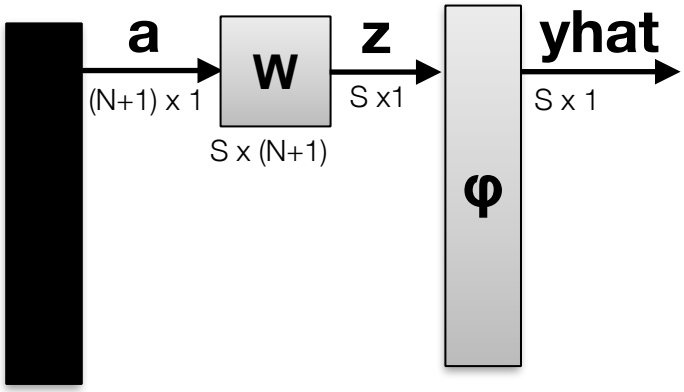
Need objective Function, minimize MSE $J(\mathbf{W}) = ||\mathbf{Y} - \hat{\mathbf{Y}}||^2$

where $\mathbf{y}^{(i)}$ is one-hot encoded!

$$\begin{bmatrix} y_1 \\ \dots \\ y_C \end{bmatrix}^{(i)} \Rightarrow \left[\begin{bmatrix} y_1 \\ \dots \\ y_C \end{bmatrix}^{(1)} \dots \begin{bmatrix} y_1 \\ \dots \\ y_C \end{bmatrix}^{(M)} \right] = \mathbf{Y}$$

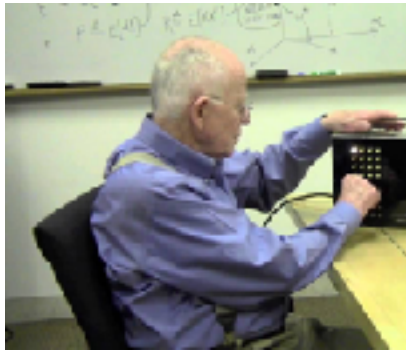
Simple Architectures

- Adaline network, Widrow and Hoff, 1960



phi

Marcian "Ted" Hoff



Bernard Widrow

Objective Function, minimize MSE $J(\mathbf{W})=||\mathbf{Y}-\hat{\mathbf{Y}}||^2$

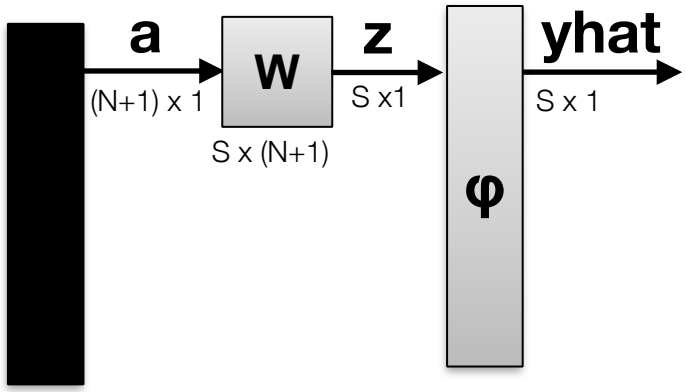
New objective function becomes: $J(\mathbf{W})=||\mathbf{Y}-\mathbf{W}\cdot\mathbf{A}||^2$

Need gradient $\nabla J(\mathbf{W})$ for update equation $\mathbf{W} \leftarrow \mathbf{W} + \eta \nabla J(\mathbf{W})$

We have been using the **Widrow-Hoff Learning Rule**

Simple Architectures

- Adaline network, Widrow and Hoff, 1960



phi

Marcian “Ted” Hoff

Bernard Widrow

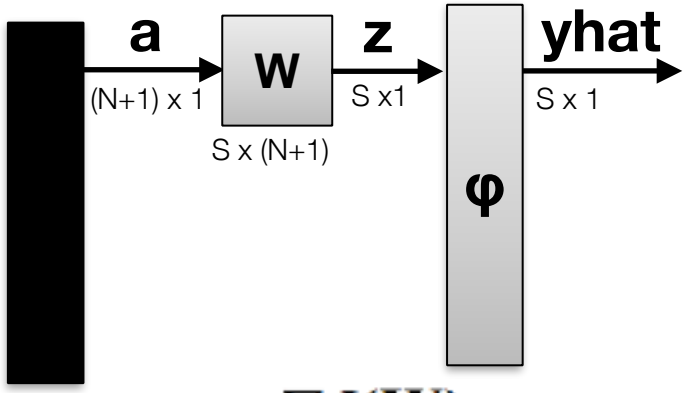
need gradient $\nabla J(\mathbf{W})$ for update equation $\mathbf{W} \leftarrow \mathbf{W} + \eta \nabla J(\mathbf{W})$

For case S=1, $\mathbf{W}$ has only one row, $\mathbf{w}$ this is just **linear regression…**

$$\mathbf{w} \leftarrow \mathbf{w} + \eta[\mathbf{X} * (\mathbf{y} - \hat{\mathbf{y}})]$$

Simple Architectures

- Modern Perceptron network



$$phi = \frac{1}{1+\exp(-z)}$$

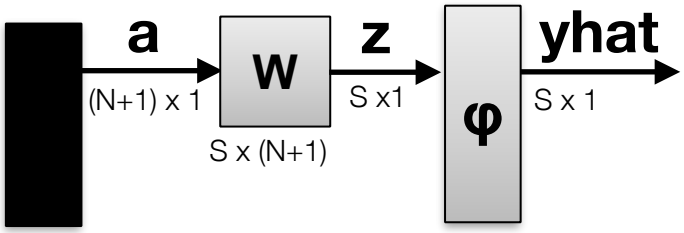
need gradient $\nabla J(\mathbf{W})$ for update equation $\mathbf{W} \leftarrow \mathbf{W} + \eta \nabla J(\mathbf{W})$

For case S=1, this is just **logistic regression…**
and **we have already solved this**!

$$\mathbf{w} \leftarrow \mathbf{w} + \eta[\mathbf{X} * (\mathbf{y} - \mathbf{g}(\mathbf{x}))]$$

What happens when S > 1 ?

What if we have more than S=1?



$$\begin{bmatrix} \begin{bmatrix} \phi(z_1) \\ \dots \\ \phi(z_S) \end{bmatrix}^{(1)} & \dots & \begin{bmatrix} \phi(z_1) \\ \dots \\ \phi(z_S) \end{bmatrix}^{(M)} \end{bmatrix} = \hat{\mathbf{Y}}$$

$$\begin{bmatrix} \begin{bmatrix} y_1 \\ \dots \\ y_S \end{bmatrix}^{(1)} & \dots & \begin{bmatrix} y_1 \\ \dots \\ y_S \end{bmatrix}^{(M)} \end{bmatrix} = \mathbf{Y}$$

$$J(\mathbf{W}) = ||\mathbf{Y} - \hat{\mathbf{Y}}||^2$$

Each target class in $\mathbf{Y}$ can be independently optimized

$$\mathbf{yhat}^{(i)} = \text{one hot} \begin{bmatrix} \varphi({}_{row=1}\mathbf{w} \cdot \mathbf{x}^{(i)}) \\ \varphi({}_{row=2}\mathbf{w} \cdot \mathbf{x}^{(i)}) \\ \dots \\ \varphi({}_{row=S}\mathbf{w} \cdot \mathbf{x}^{(i)}) \end{bmatrix}$$

which is one-versus-all!

$$J({}_1\mathbf{w}) = \sum_{i=1} [y_1{}^{(i)} - \varphi({}_1\mathbf{w} \cdot \mathbf{x}^{(i)})]^2$$

$$J({}_2\mathbf{w}) = \sum_{i=1} [y_2{}^{(i)} - \varphi({}_2\mathbf{w} \cdot \mathbf{x}^{(i)})]^2$$

$$\dots$$

$$J({}_S\mathbf{w}) = \sum_{i=1} [y_S{}^{(i)} - \varphi({}_S\mathbf{w} \cdot \mathbf{x}^{(i)})]^2$$

Simple Architectures: Summary

- Adaline network, Widrow and Hoff, 1960
  - linear regression
- Perceptron
  - *with sigmoid*: logistic regression
- One-versus-all implementation is the same as having $\mathbf{w}_{\text{class}}$ be rows of weight matrix, **W**
  - works in adaline
  - works in logistic regression

these networks were created in the 50's and 60's but were abandoned

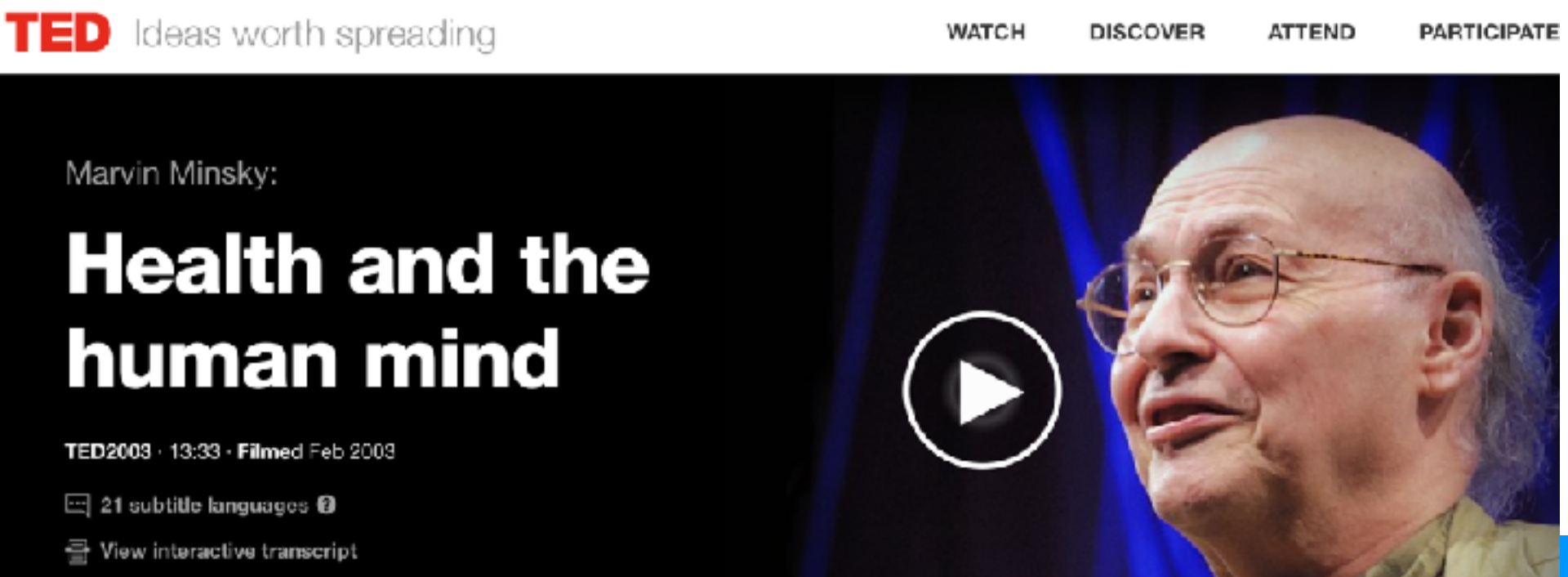
why were they not used?

The Rosenblatt-Widrow-Hoff Dilemma

- 1960's: Rosenblatt got into a public academic argument with Marvin Minsky and Seymour Papert

> "Given an elementary α-perceptron, a stimulus world W, and any classification C(W) for which a solution exists; let all stimuli in W occur in any sequence, provided that each stimulus must reoccur in finite time; then beginning from an arbitrary initial state, an error correction procedure will always yield a solution to C(W) in finite time…"

- Minsky and Papert publish limitations paper, 1969:



More Advanced Architectures: history

- 1986: *Rumelhart*, *Hinton*, and *Williams* popularize gradient calculation for multi-layer network
  - *technically* introduced by Werbos in 1982
- **difference**: Rumelhart *et al.* validated ideas with a computer
- until this point no one could train a multiple layer network consistently
- algorithm is popularly called **Back-Propagation**
- wins pattern recognition prize in 1993, becomes de-facto machine learning algorithm until: SVMs and Random Forests in ~2004
- would eventually see a resurgence for its ability to train algorithms for Deep Learning applications: **Hinton is widely considered the father of deep learning**

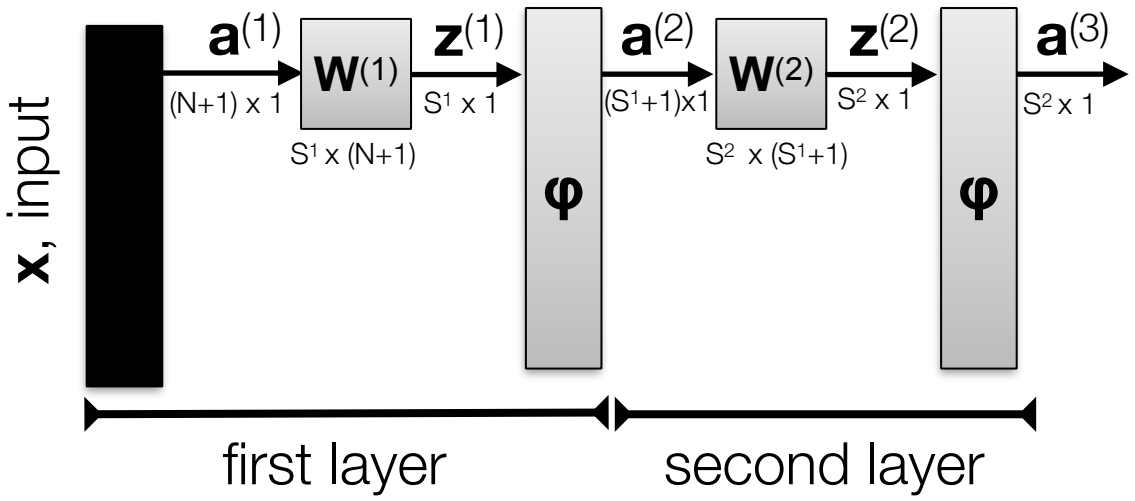
David Rumelhart

1942-2011

Geoffrey Hinton

More Advanced Architectures: MLP

- The multi-layer perceptron (MLP):
  - two layers shown, but could be arbitrarily many layers
  - algorithm is agnostic to number of layers (*kinda*)

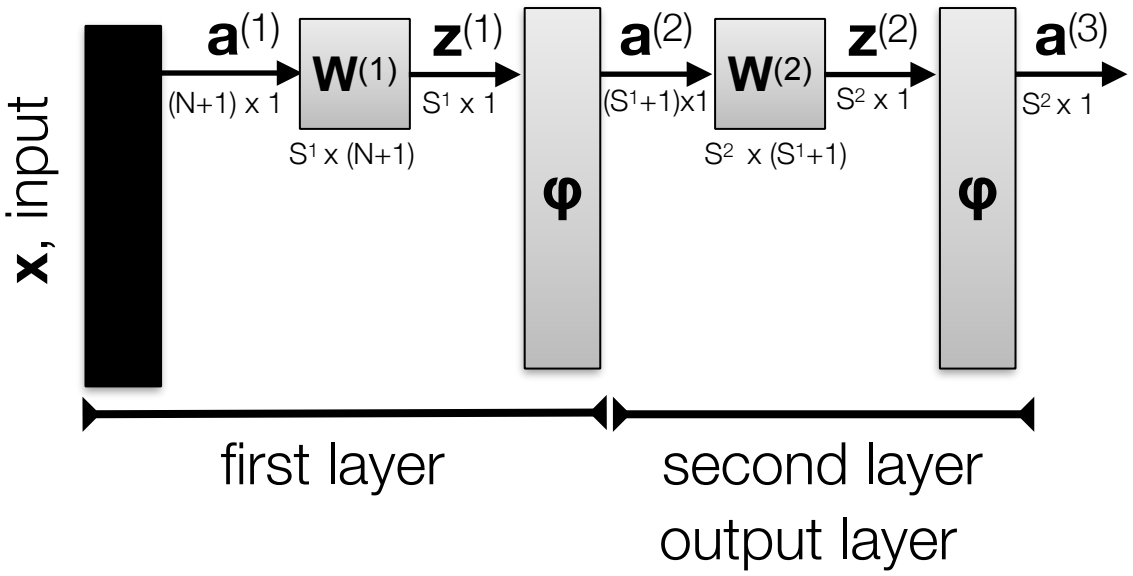


each row of **yhat** is no longer independent of the rows in **W** so we cannot optimize using one versus all!!!

$$\mathbf{yhat}^{(i)} = \text{one hot} \begin{bmatrix} \varphi(_{row=1}\mathbf{w}^{(2)} \cdot \varphi(\mathbf{W}^{(1)}\mathbf{a}^{(1)})) \\ \cdots \\ \varphi(_{row=S}\mathbf{w}^{(2)} \cdot \varphi(\mathbf{W}^{(1)}\mathbf{a}^{(1)})) \end{bmatrix}$$

Back Propagation

- Steps:
  - propagate weights forward
  - calculate gradient at final layer
  - back propagate gradient for each layer
    - via recurrence relation

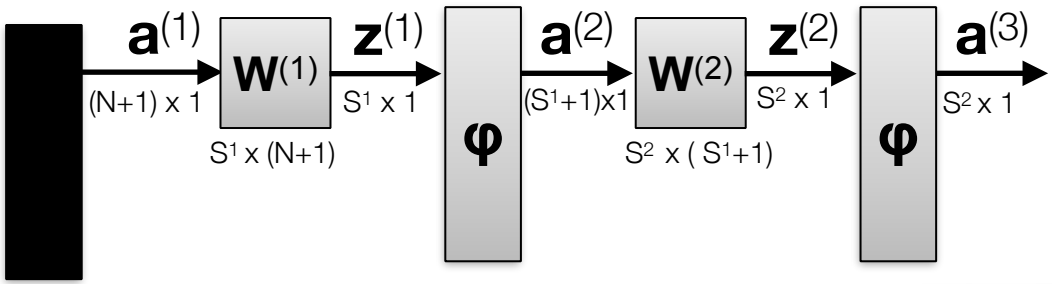


$$J(\mathbf{W}) = \sum_{k}^{M} (\mathbf{y}^{(k)} - \mathbf{a}^{(L)})^2$$

$$w_{i,j}^{(l)} \leftarrow w_{i,j}^{(l)} - \eta \frac{\partial J(\mathbf{W})}{\partial w_{i,j}^{(l)}}$$

Back propagation

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



$$w_{i,j}^{(l)} \leftarrow w_{i,j}^{(l)} - \eta \frac{\partial J(\mathbf{W})}{\partial w_{i,j}^{(l)}}$$

use chain rule:

$$\frac{\partial J(\mathbf{W})}{\partial w_{i,j}^{(l)}} = \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l)}} \frac{\partial \mathbf{z}^{(l)}}{\partial w_{i,j}^{(l)}}$$

Solve this in explainer video for next in class assignment!

End of Session

- thanks! **Next time is Flipped Assignment!!!**

More help on neural networks to prepare for next time:

Sebastian Raschka
https://github.com/rasbt/python-machine-learning-book/blob/master/code/ch12/ch12.ipynb

Martin Hagan
https://www.google.com/url?sa=t&rct=j&q=&esrc=s&source=web&cd=1&cad=rja&uact=8&ved=0ahUKEwioprvn27fPAhWMx4MKHYbwDIwQFggeMAA&url=http%3A%2F%2Fhagan.okstate.edu%2FNNDesign.pdf&usg=AFQjCNG5YbM4xSMm6K5HNsG-4Q8TvOu_Lw&sig2=bgT3k-5ZDDTPZ07Qu8Oreg

Michael Nielsen
http://neuralnetworksanddeeplearning.com

Lecture Notes for

Machine Learning in Python

Professor Eric Larson

Optimizing Neural Networks

Class Logistics and Agenda

- Logistics
- Agenda:
  - Practical Multi-layer Architectures
  - Programming Examples
- Next Time: More MLPs

Semester Summary, so far!

- Adaline network, Widrow and Hoff, 1960
  - iterative linear regression
- Perceptron
  - *with sigmoid*: logistic regression
- One-versus-all implementation is the same as having $\mathbf{w}_{\text{class}}$ be rows of weight matrix, $\mathbf{W}$
  - works in adaline
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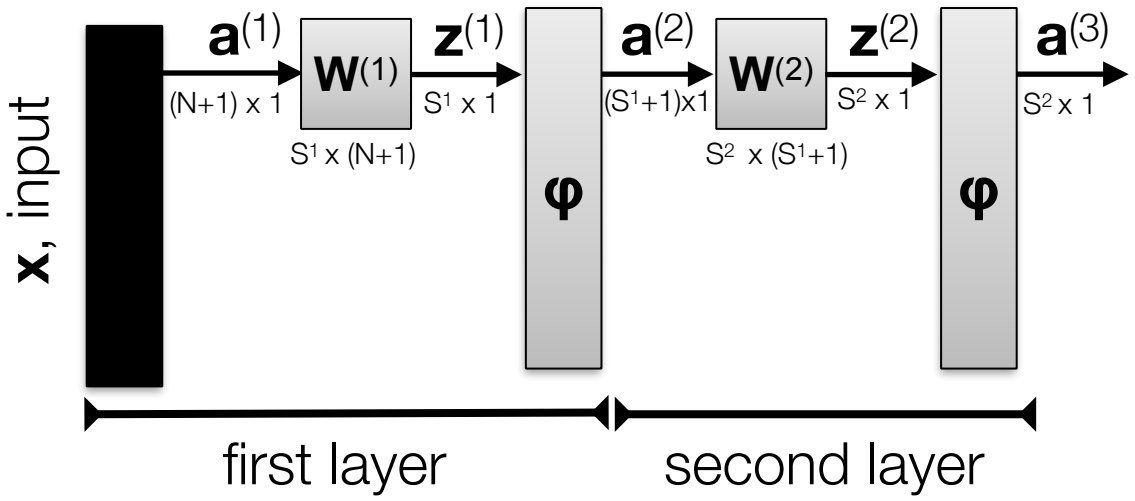

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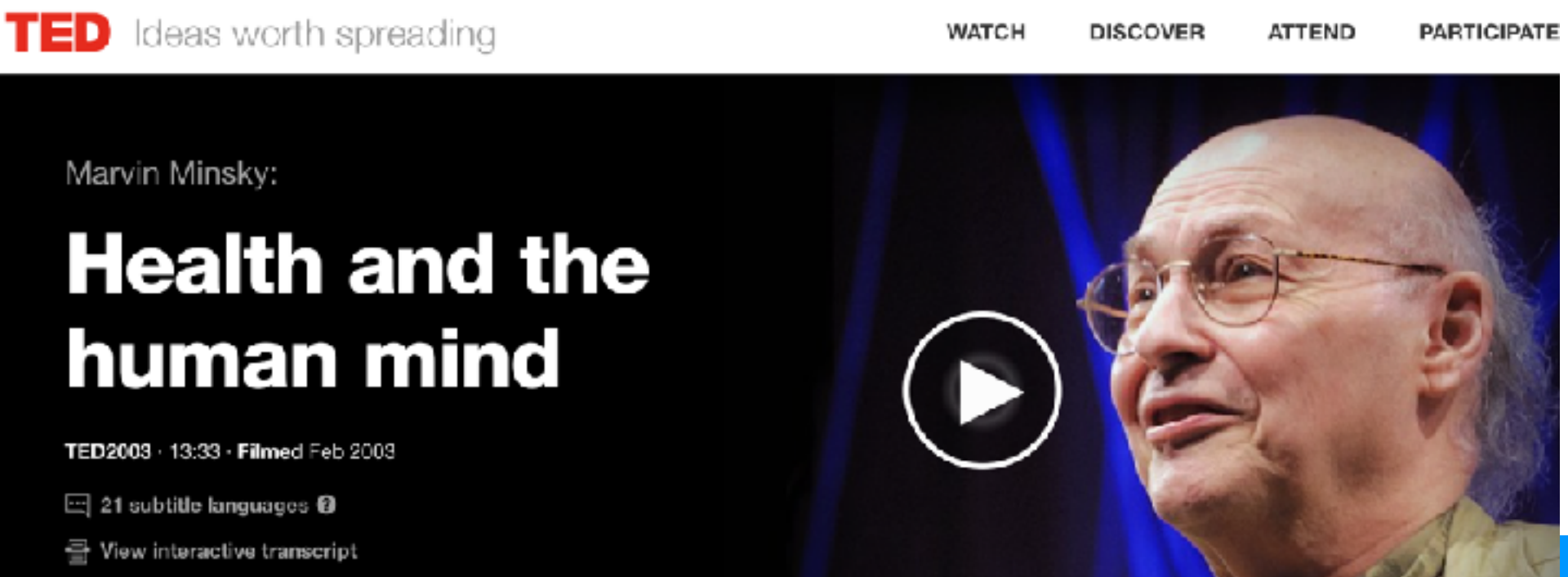


More Advanced Architectures: history

- 1986: *Rumelhart*, *Hinton*, and *Williams* popularize gradient calculation for multi-layer network
  - *actually* introduced by Werbos in 1982
- **difference**: Rumelhart *et al.* validated ideas with a computer
- until this point no one could train a multiple layer network consistently
- algorithm is popularly called **Back-Propagation**
- wins pattern recognition prize in 1993, becomes de-facto machine learning algorithm until: SVMs and Random Forests in ~2004
- would eventually see a resurgence for its ability to train algorithms for Deep Learning applications: **Hinton is widely considered the father of deep learning**

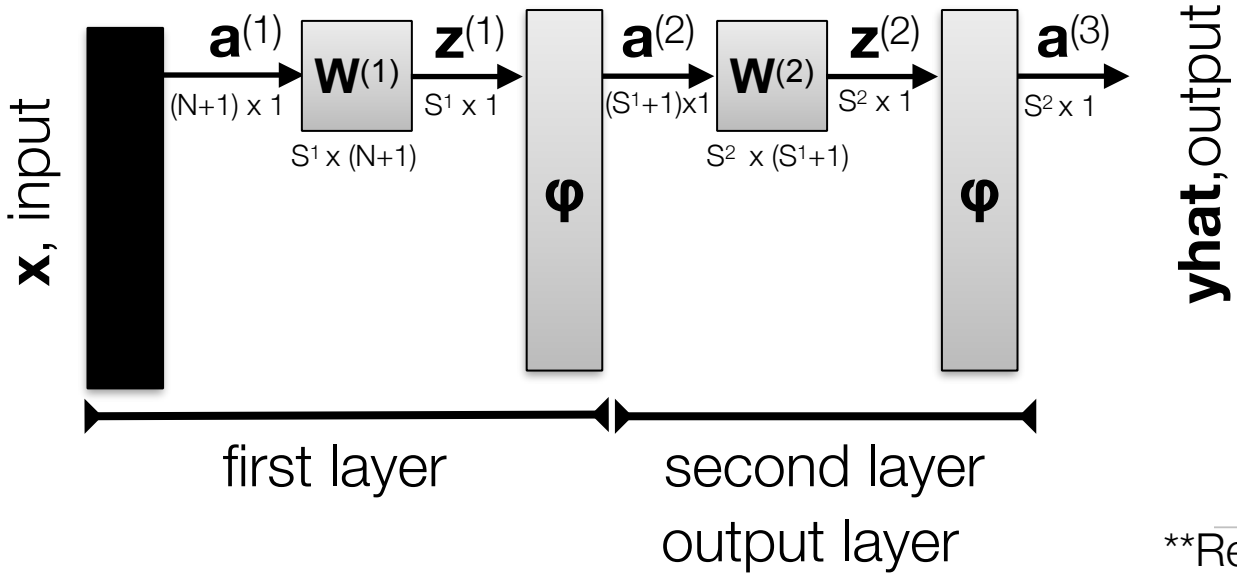
David Rumelhart

1942-2011

Geoffrey Hinton

Back propagation

- Steps:
  - propagate weights forward
  - calculate gradient at final layer
  - back propagate gradient for each layer
    - via recurrence relation

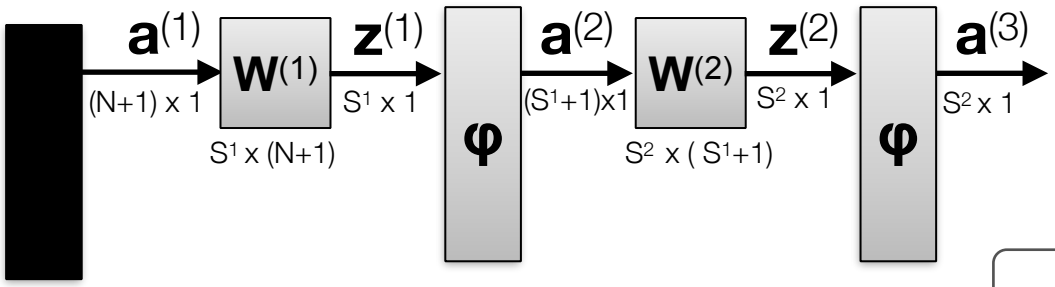


$$J(\mathbf{W}) = ||\mathbf{Y} - \hat{\mathbf{Y}}||^2$$

$$w_{i,j}^{(l)} \leftarrow w_{i,j}^{(l)} - \eta \frac{\partial J(\mathbf{W})}{\partial w_{i,j}^{(l)}}$$

**Recall from Flipped Assignment!

Back Propagation Summary



1. Forward propagate to get **Z**, **A**
2. Get final layer gradient
3. Back propagate sensitivities
4. Update each $\mathbf{W}^{(l)}$

$$\mathbf{V}^{(2)} = -2(\mathbf{Y} - \mathbf{A}^{(3)}) * \mathbf{A}^{(3)} * (1 - \mathbf{A}^{(3)})$$

$$\nabla^{(2)} = \mathbf{V}^{(2)} \cdot [\mathbf{A}^{(2)}]^T$$

$$\mathbf{V}^{(1)} = \mathbf{A}^{(2)} * (1 - \mathbf{A}^{(2)}) * [\mathbf{W}^{(2)}]^T \cdot \mathbf{V}^{(2)}$$

$$\nabla^{(1)} = \mathbf{V}^{(1)} \cdot [\mathbf{A}^{(1)}]^T$$

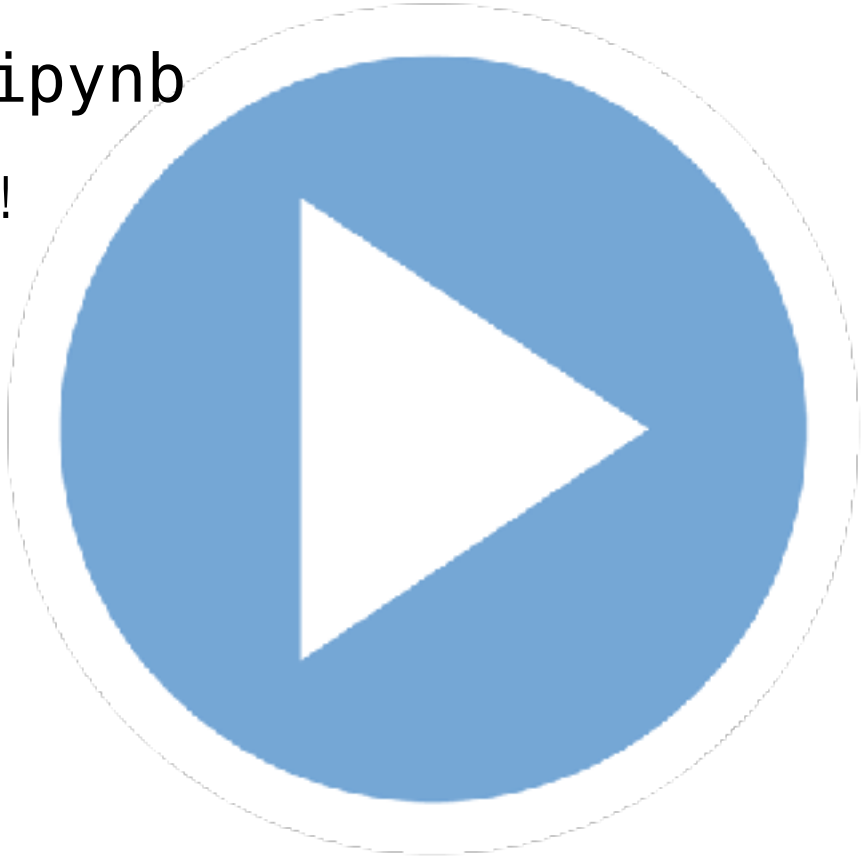
$$\mathbf{W}^{(l)} \leftarrow \mathbf{W}^{(l)} - \eta \nabla^{(l)}$$

**Recall from Flipped Assignment!

Lightning Demo

`07. MLP Neural Networks.ipynb`

same as Flipped Assignment!
with regularization
and vectorization

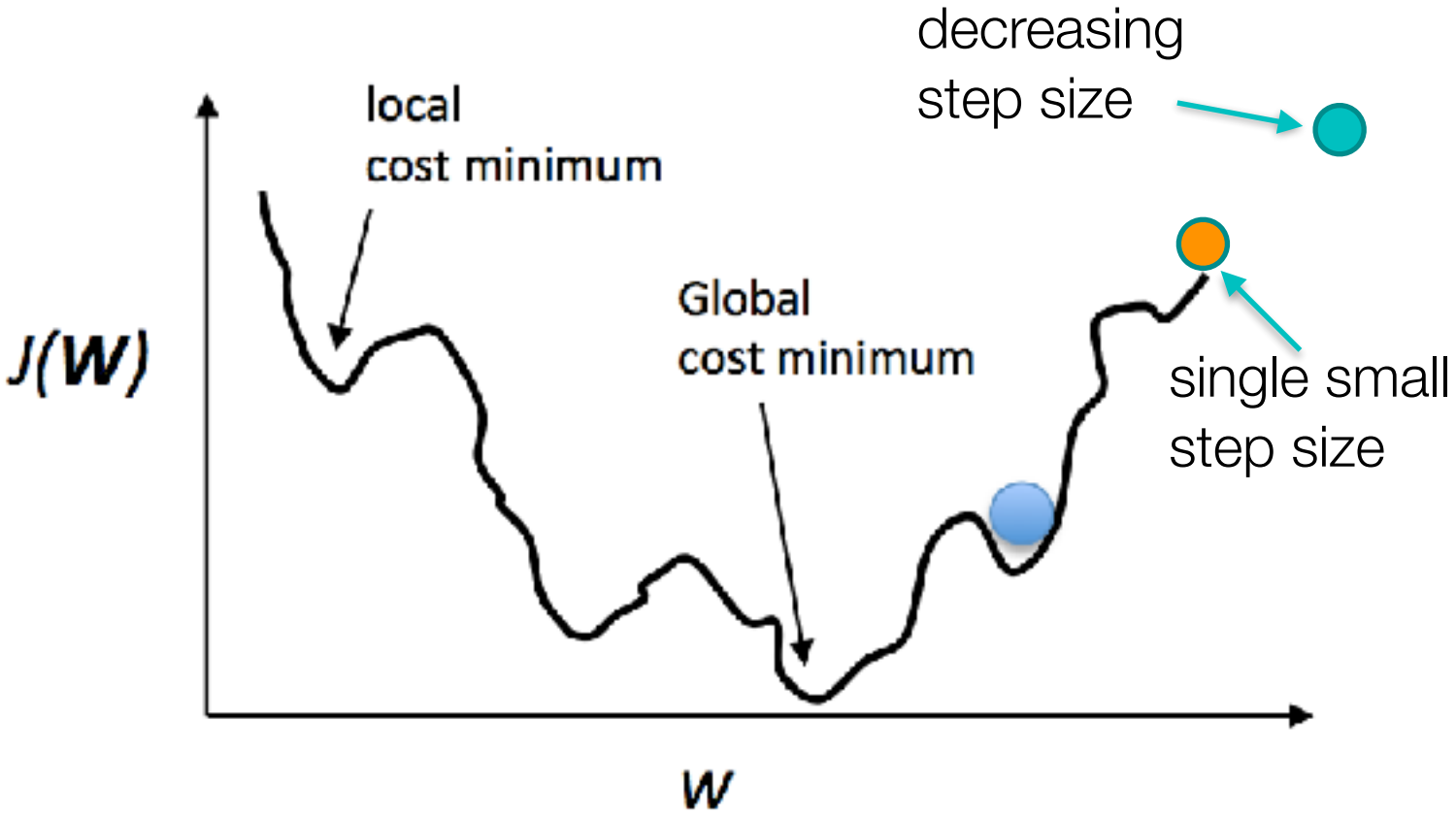


Problems with Advanced Architectures

- Numerous weights to find gradient update
  - minimize number of instances
  - **solution**: mini-batch
- **new problem**: mini-batch gradient can be erratic
  - **solution**: momentum
    - use previous update in current update

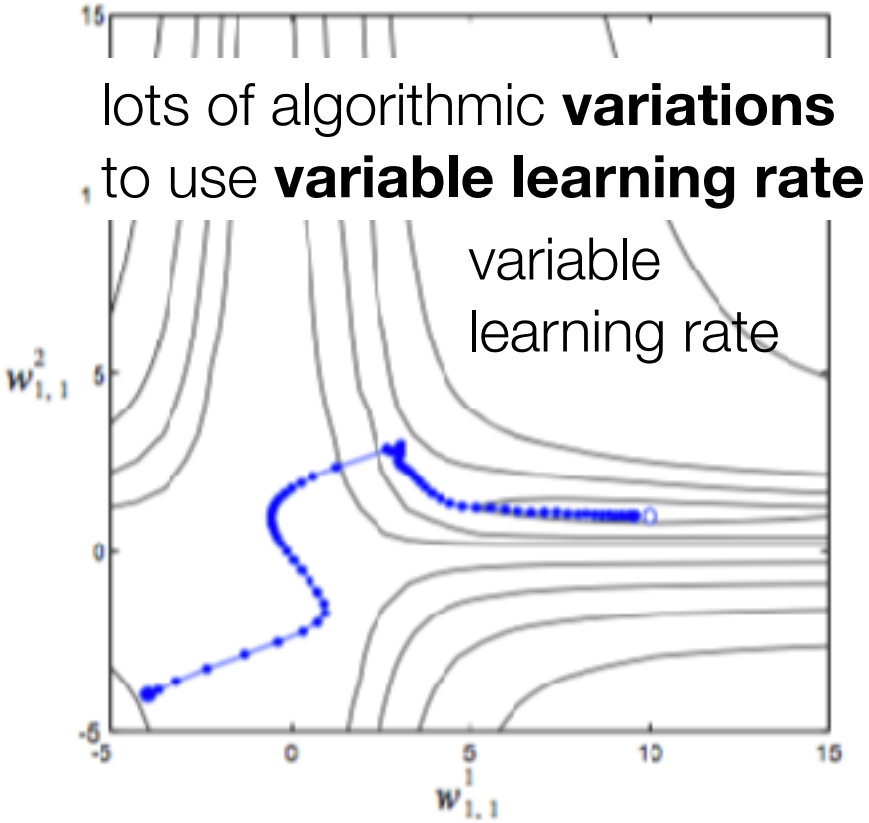
Problems with Advanced Architectures

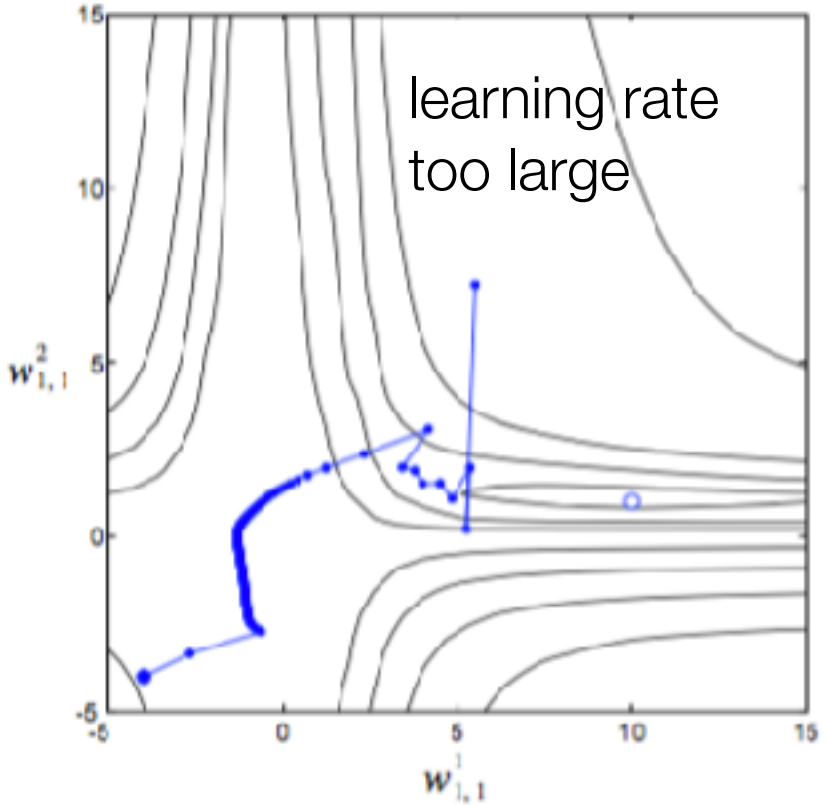
- Space is no longer convex
  - **One solution**:
    - start with large step size
    - "cool down" by decreasing step size for higher iterations



Problems with Advanced Architectures

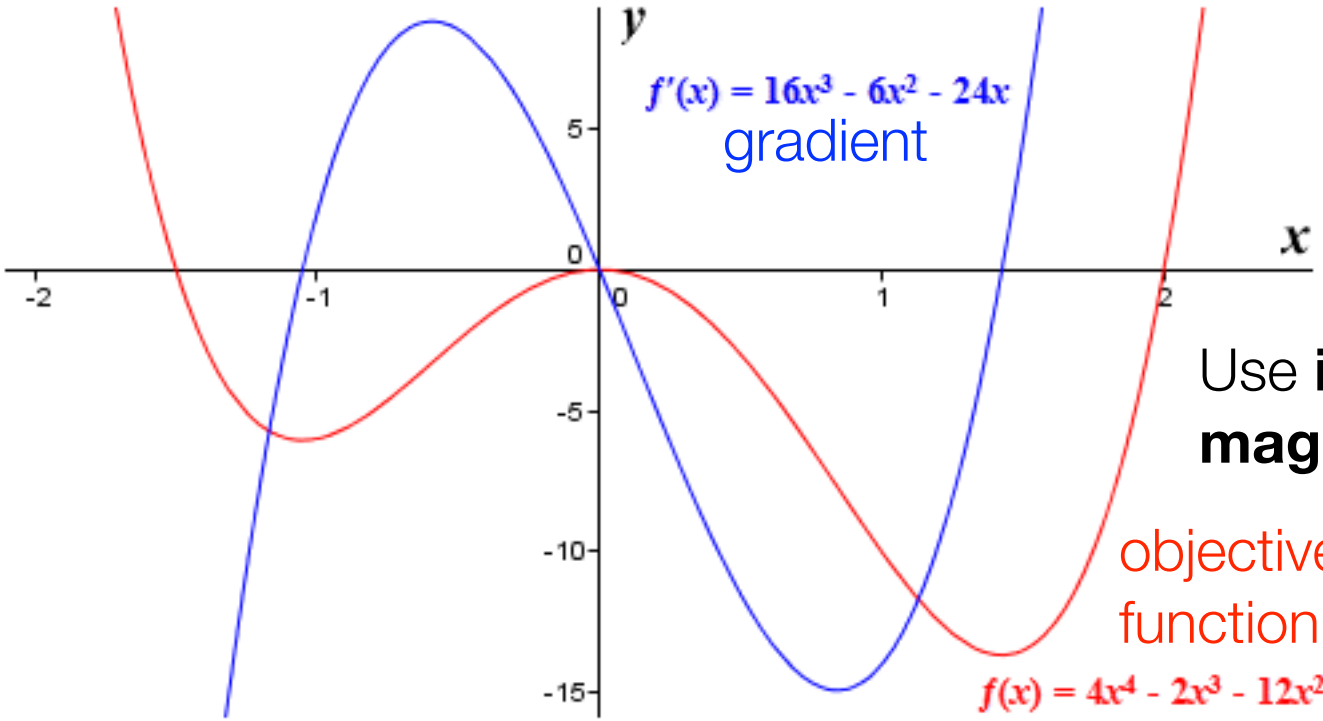
- Space is no longer convex
  - **another solution**:
    - start with arbitrary step size
    - only decrease when successive iterations do not decrease cost





Learning Rate from Gradient Magnitude?

- Deccelerate down regions that are steep
- Accelerate on plateaus



Use **inverse** of **magnitude** of **gradient**!

Also **accumulate inverse** to be robust to many **changes** in **steepness**…

http://www.technologyuk.net/mathematics/differential-calculus/higher-derivatives.shtml

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

- Momentum $\rho_k = \alpha \nabla J(\mathbf{W}_k) + \beta \nabla J(\mathbf{W}_{k-1})$
- Nesterov's Accelerated Gradient $\rho_k = \underbrace{\beta \nabla J\left(\mathbf{W}_k + \alpha \nabla J(\mathbf{W}_{k-1})\right)}_{\text{step twice}} + \alpha \nabla J(\mathbf{W}_{k-1})$
- Adagrad $\rho_k = \frac{\eta}{\sqrt{\text{trace}(G_k) + \epsilon}} * \nabla J(\mathbf{W}_k)$ where $G_k = G_{k-1} + \nabla J(\mathbf{W}_k) \cdot \nabla J(\mathbf{W}_k)^T$
- Adadelta G accumulated over a fixed time window, not all previous iterations
- RMSProp G learning rate decreases with squared gradient magnitude
- Adam G updates with decaying momentum of J and J^2
- Nadam 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**
  - **Global Optimum** == **Overfit**

Adam, a more detailed look

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

Algorithm 1: *Adam*, our proposed algorithm for stochastic optimization. See section 2 for details, and for a slightly more efficient (but less clear) order of computation. g_t^2 indicates the elementwise square $g_t \odot g_t$. Good default settings for the tested machine learning problems are $\alpha = 0.001$, $\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\epsilon = 10^{-8}$. All operations on vectors are element-wise. With β_1^t and β_2^t we denote β_1 and β_2 to the power t.

Require: α: Stepsize
Require: $\beta_1, \beta_2 \in [0, 1)$: Exponential decay rates for the moment estimates
Require: $f(\theta)$: Stochastic objective function with parameters θ
Require: θ_0: Initial parameter vector
$m_0 \leftarrow 0$ (Initialize 1st moment vector)
$v_0 \leftarrow 0$ (Initialize 2nd moment vector)
$t \leftarrow 0$ (Initialize timestep)
while θ_t not converged **do**
$t \leftarrow t + 1$
$g_t \leftarrow \nabla_\theta f_t(\theta_{t-1})$ (Get gradients w.r.t. stochastic objective at timestep t)
$m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot g_t$ (Update biased first moment estimate)
$v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 - \beta_2) \cdot g_t^2$ (Update biased second raw moment estimate)
$\hat{m}_t \leftarrow m_t / (1 - \beta_1^t)$ (Compute bias-corrected first moment estimate)
$\hat{v}_t \leftarrow v_t / (1 - \beta_2^t)$ (Compute bias-corrected second raw moment estimate)
$\theta_t \leftarrow \theta_{t-1} - \alpha \cdot \hat{m}_t / (\sqrt{\hat{v}_t} + \epsilon)$ (Update parameters)
end while
return θ_t (Resulting parameters)

get gradient

gradient momentum

squared gradient momentum

boost moments magnitudes (notice t in exponent)

update gradient, normalized by second moment

Demo

`07. MLP Neural Networks.ipynb`

comparison:

mini-batch

- momentum
- adaptive learning

L-BFGS

Lecture Notes for

Machine Learning in Python

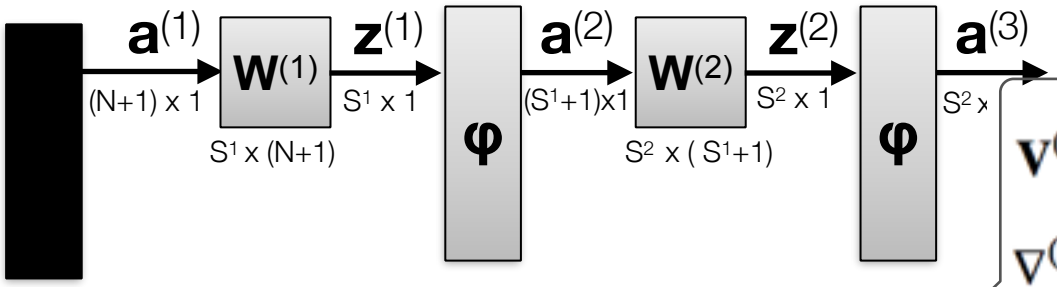
Professor Eric Larson

Neural Network Optimization and Activation

Class Logistics and Agenda

- Agenda:
  - More optimization and architectures
  - Programming Examples
  - Town Hall

Review:



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1. Forward propagate to get **Z**, **A**
2. Get final layer gradient
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4. Update each $\mathbf{W}^{(l)}$

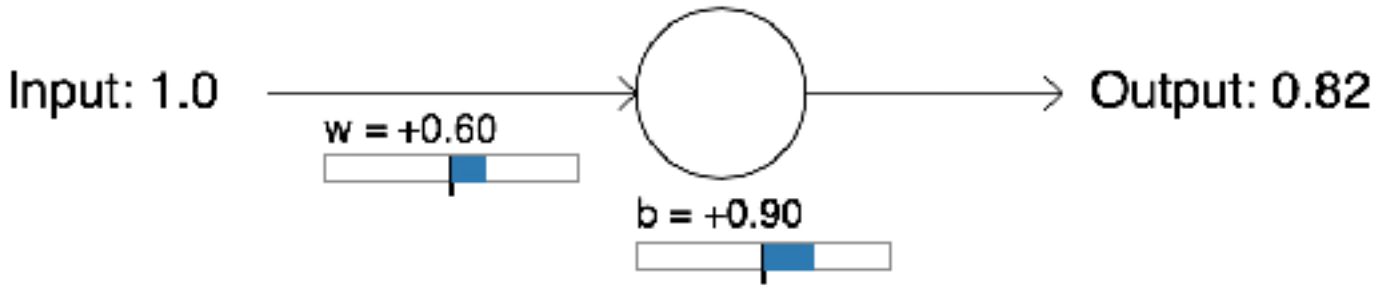
- **Self Test**:
  True or False: If we change the cost function, $J(\mathbf{W})$, we only need to update the final layer sensitivity calculation, $\mathbf{V}^{(2)}$, of the back propagation steps. The remainder of the algorithm is unchanged.
  - A. True
  - B. False

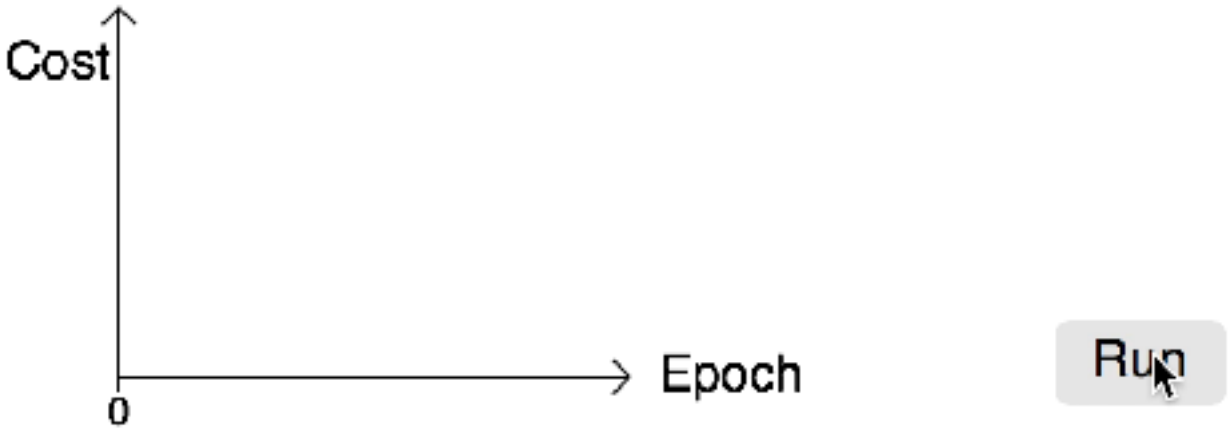
Practical Implementation of Architectures

- MSE

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

least squares objective,
tends to slow training initially





Neural Networks and Deep Learning, Michael Nielson, 2015

Practical Implementation of Architectures

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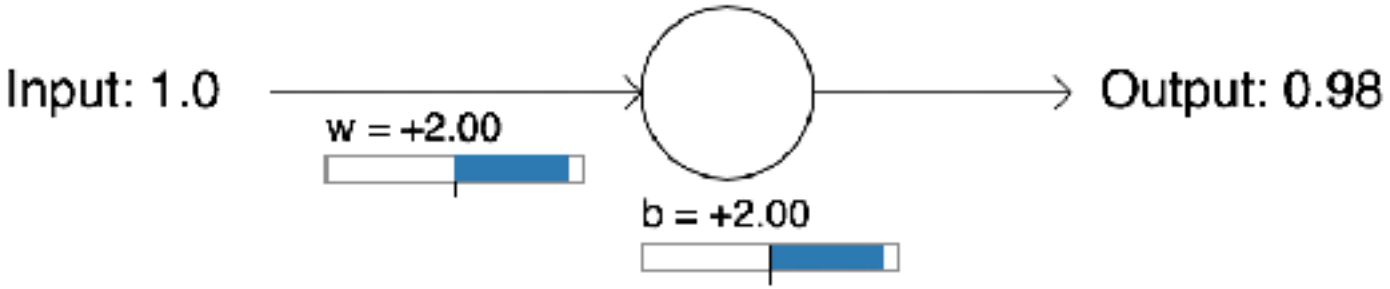
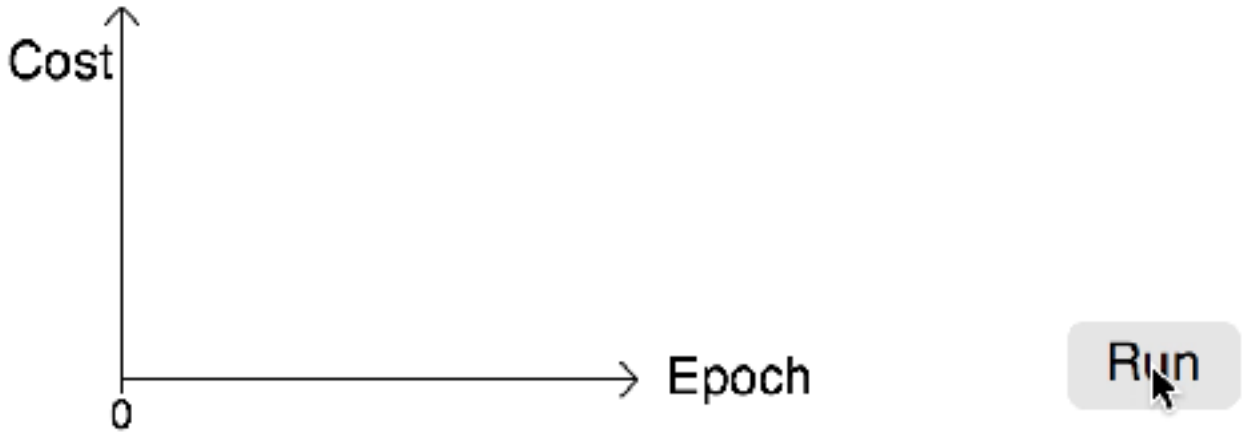




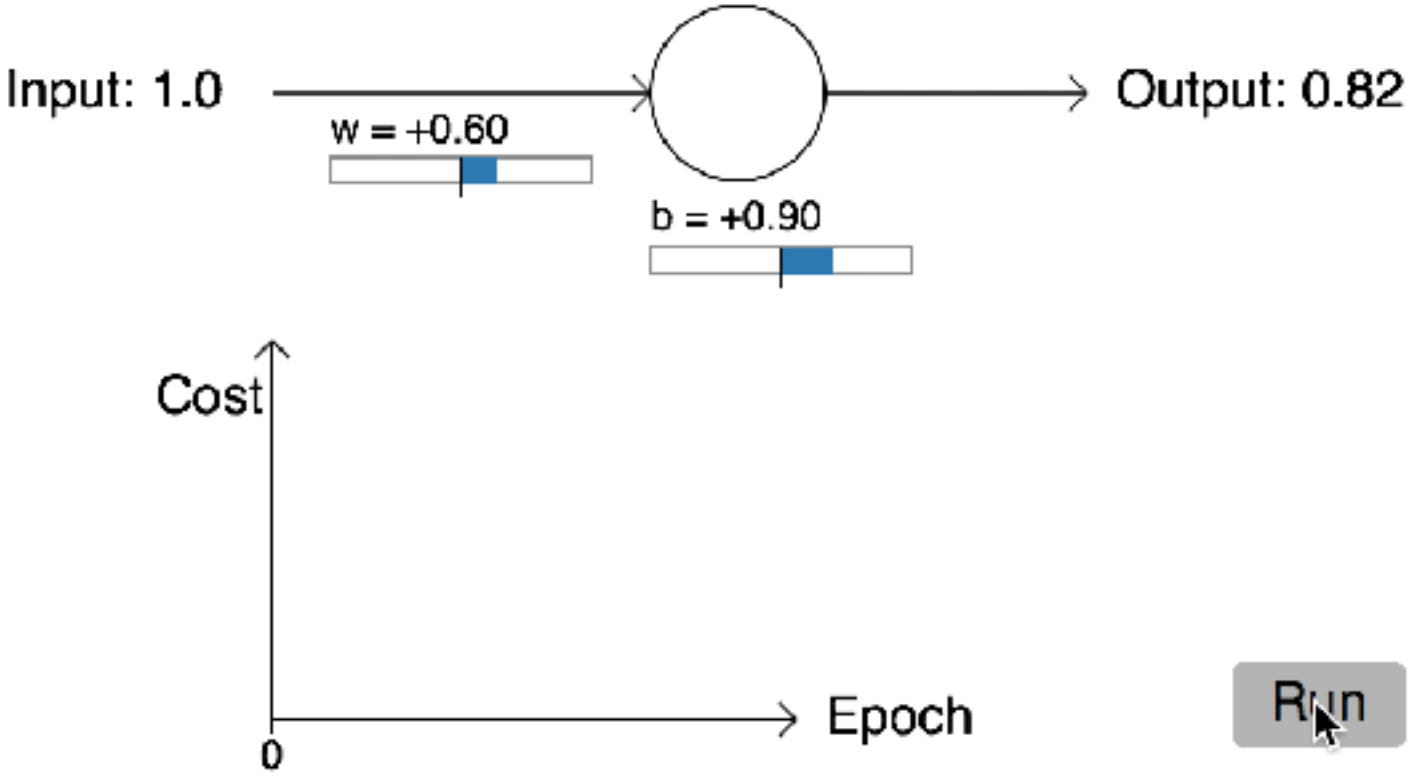
Neural Networks and Deep Learning, Michael Nielson, 2015

Practical Implementation of Architectures

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

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

speeds up initial training



Neural Networks and Deep Learning, Michael Nielson, 2015

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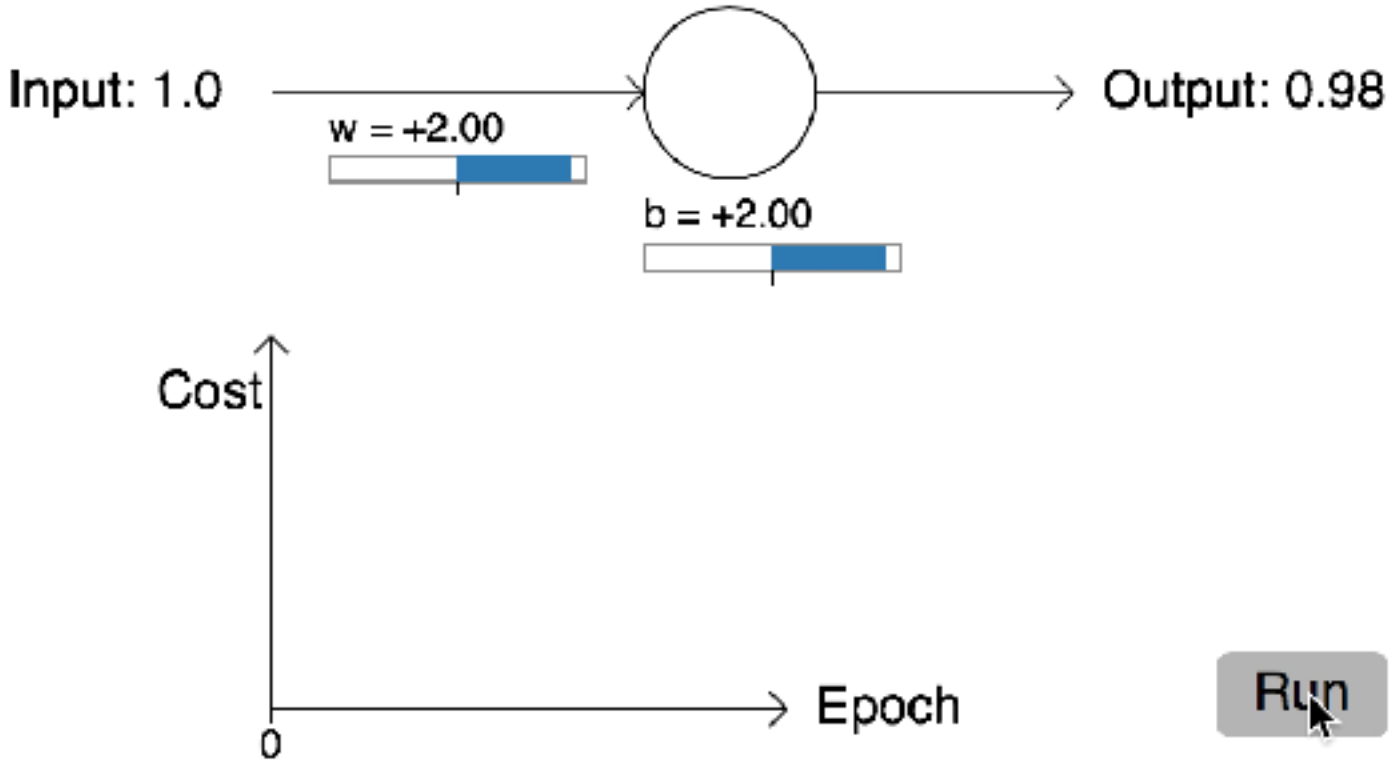

Neural Networks and Deep Learning, Michael Nielson, 2015

Practical Implementation of Architectures

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speeds up initial training

$$\left[\frac{\partial J(\mathbf{W})}{\mathbf{z}^{(L)}}\right]^{(i)}$$

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

Practical Implementation of Architectures

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

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

speeds up initial training

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

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

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

grad2 = V2 @ A2.T
grad1 = V1[1:,:] @ A1.T
```

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

new update

bp-5

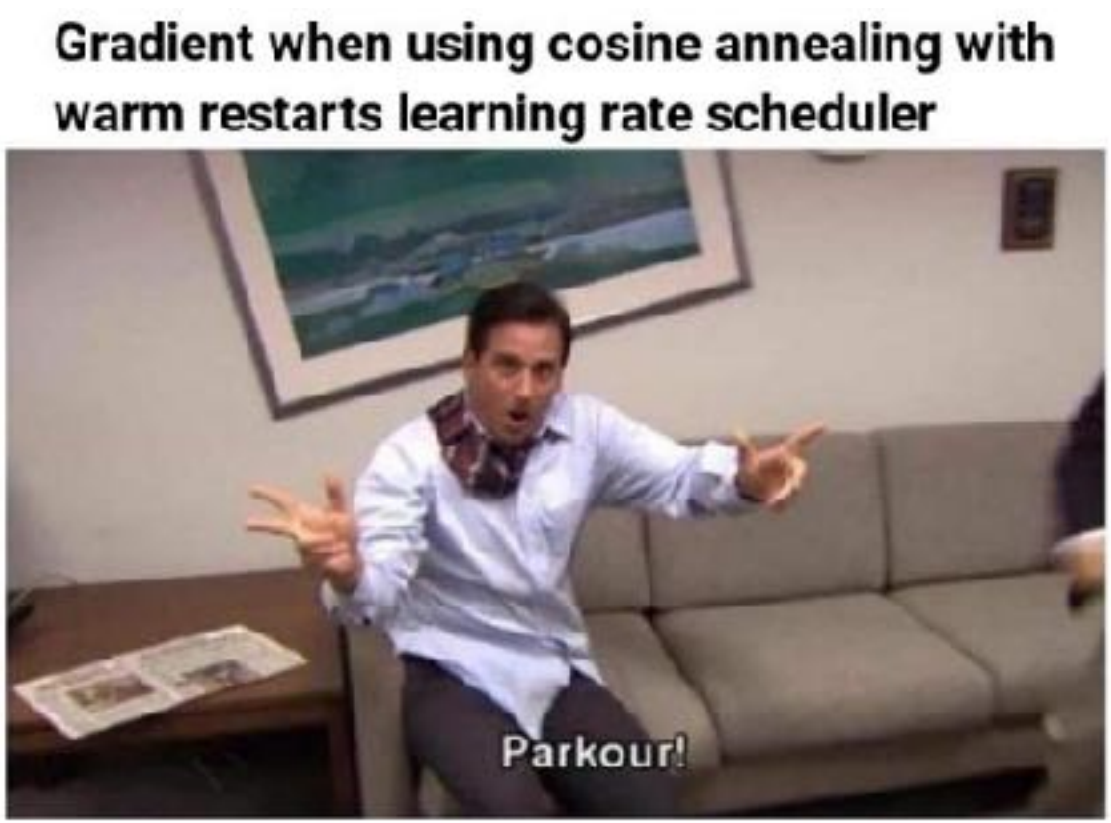
$$\mathbf{V}^{(2)} = -2(\mathbf{Y} - \mathbf{A}^{(3)}) * \mathbf{A}^{(3)} * (1 - \mathbf{A}^{(3)})$$ old update

08. Practical_NeuralNets.ipynb

Demo

cross entropy

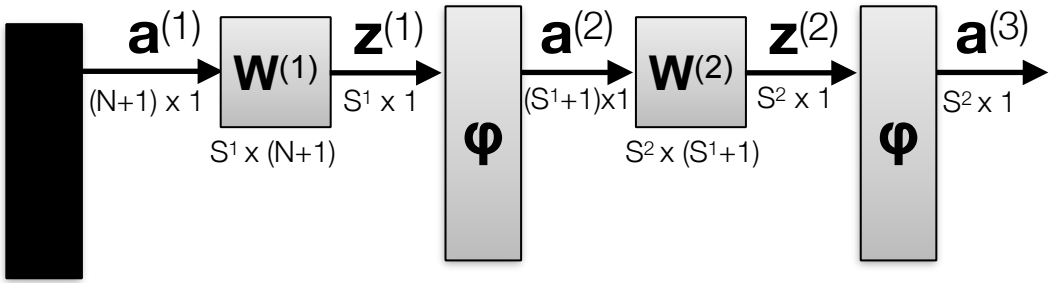
Practical Implementation of Architectures



Expansion and Dropout

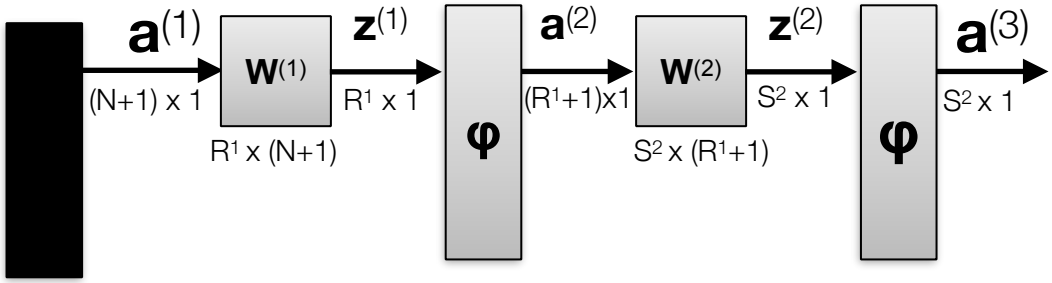
Practical Implementation of Architectures

- Dropout
  - don't train all hidden neurons at the same time



For each mini-batch,

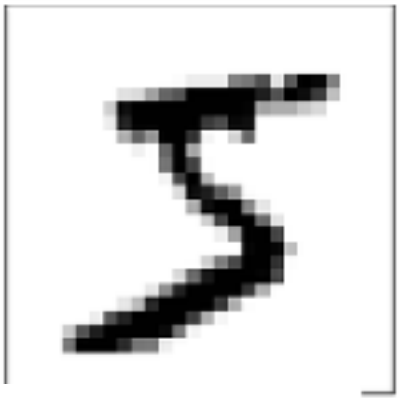
R^1 is subset of S^1

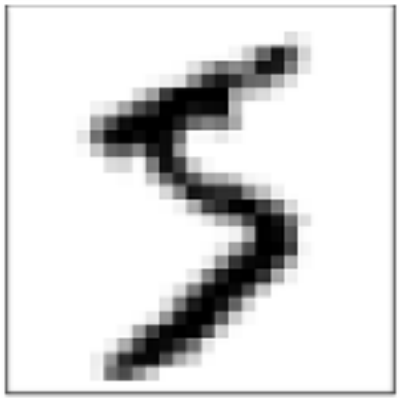


Why does this work?

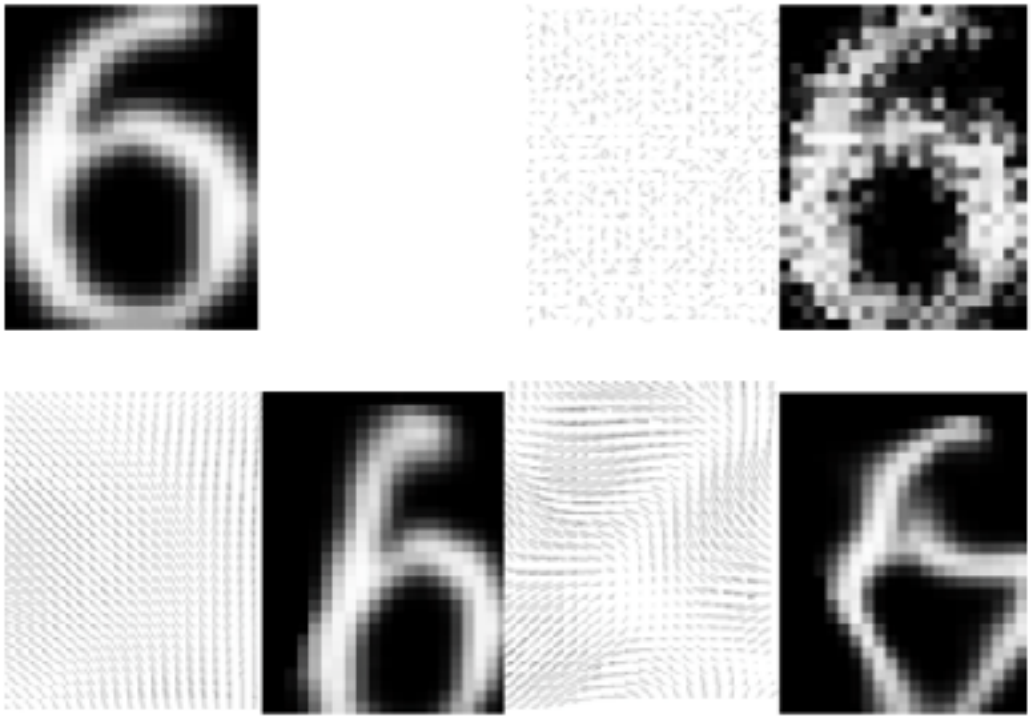
Practical Implementation of Architectures

- Expansion
  - get more data
  - perturb your data





Neural Networks and Deep Learning, Michael Nielsen, 2015



Best Practices for Convolutional Neural Networks Applied to Visual Document Analysis, by Patrice Simard, Dave Steinkraus, and John Platt (2003)

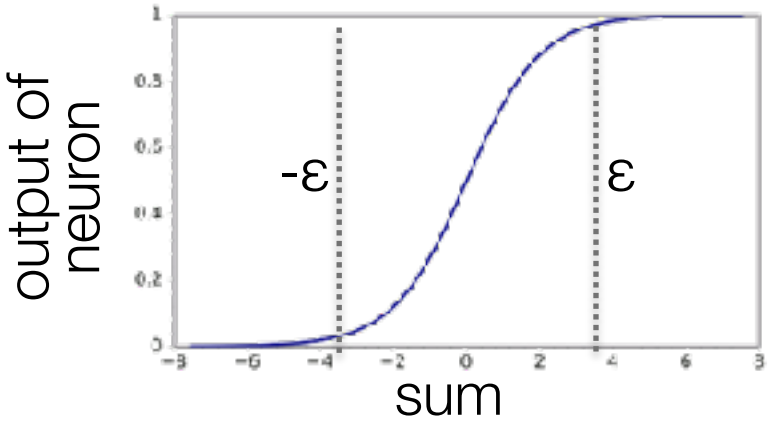
98.4%→99.3%

Practical Implementation of Architectures

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

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

each row is summed before sigmoid



want sum to be between $-\varepsilon<\Sigma<\varepsilon$ for no saturation

solution: squash initial weights magnitude

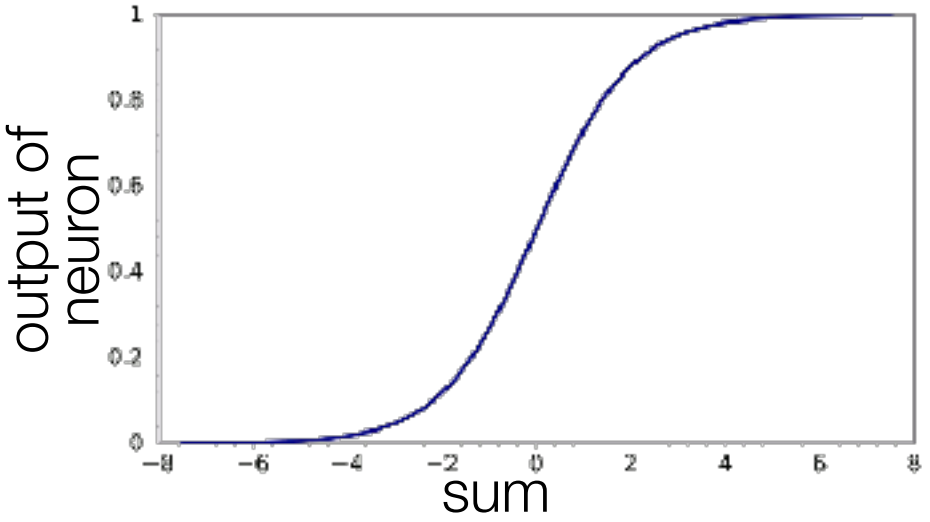
- one choice: each element of **W** selected from a Gaussian with **zero mean** and **unit standard deviation**
- for adding Gaussian distributions, variances add together:
  - make each variance $1/\mathbf{W}_{num\_elements\_in\_row}$
  - which is the same as standard deviation = $1/sqrt(\mathbf{W}_{num\_elements\_in\_row})$

Self Test

- for adding Gaussian distributions, variances add together

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

- If you initialized the weights with too large variance, you would expect the output of the neuron, ϕ, to be:
  - A. saturated to “1”
  - B. saturated to “0”
  - C. could either be saturated to “0” or “1”
  - D. would not be saturated

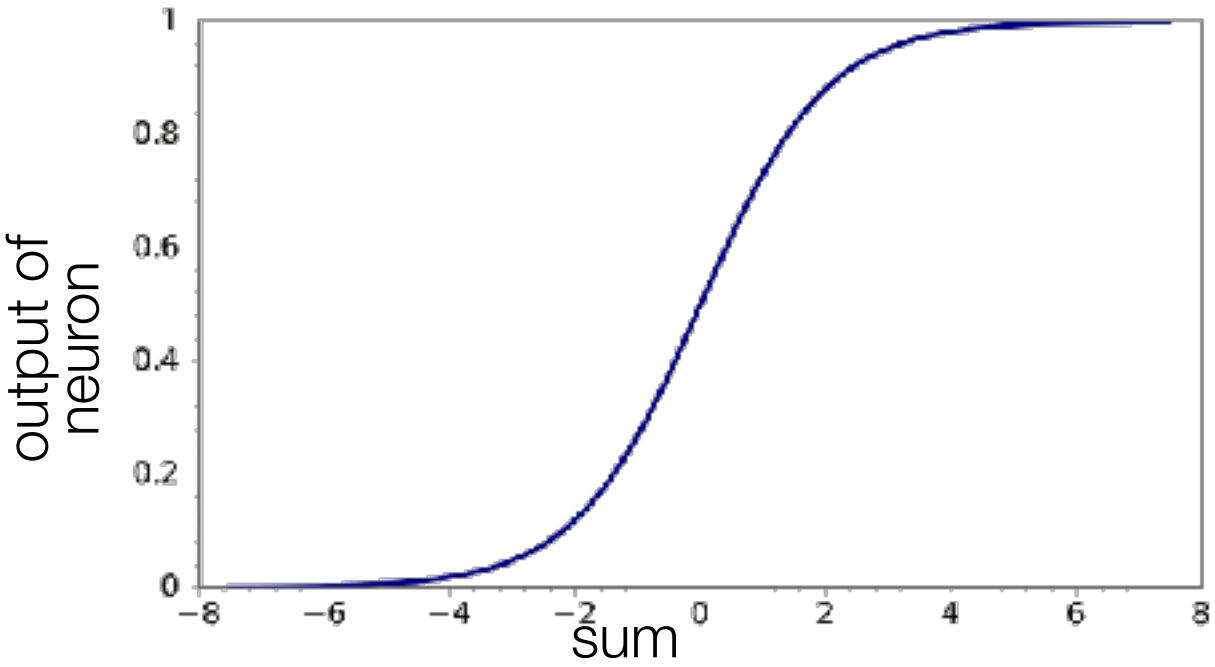


Self Test

- for adding Gaussian distributions, variances add together

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

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



More Weight Initialization

Understanding the difficulty of training deep feedforward neural networks

Xavier Glorot **Yoshua Bengio**
DIRO, Université de Montréal, Montréal, Québec, Canada

We should not saturate **feedforward** or **back propagated** variance

$$y_i = \sum_j^{n^{(L)}} w_{ij} x_j$$ break down feed forward by each multiply

$$\text{Var}[y_i] = \sum_j^{n^{(L)}} \underbrace{E[w_{ij}]^2 \text{Var}[x_j] + \text{Var}[w_{ij}] E[x_j]^2}_{\text{0, if uncorrelated}} + \text{Var}[w_{ij}]\text{Var}[x_j]$$ assume i.i.d.

$$\text{Var}[y_i] = n^{(L)} \text{Var}[w_{ij}] \text{Var}[x_j]$$

Similar for back prop.

$$\text{Var}[s_i^{(L)}] = n^{(L+1)} \text{Var}[w_{ij}] \text{Var}[s_j^{(L+1)}]$$

$$w_{ij} \approx \mathcal{N}\left(0, \sqrt{\frac{1}{n^{(L)}}}\right)$$

forward
from data

$$w_{ij} \approx \mathcal{N}\left(0, \sqrt{\frac{1}{n^{(L+1)}}}\right)$$

backward
from sensitivity.

$$w_{ij} \approx \mathcal{N}\left(0, \sqrt{\frac{2}{n^{(L)} + n^{(L+1)}}}\right)$$

compromise

More Weight Initialization

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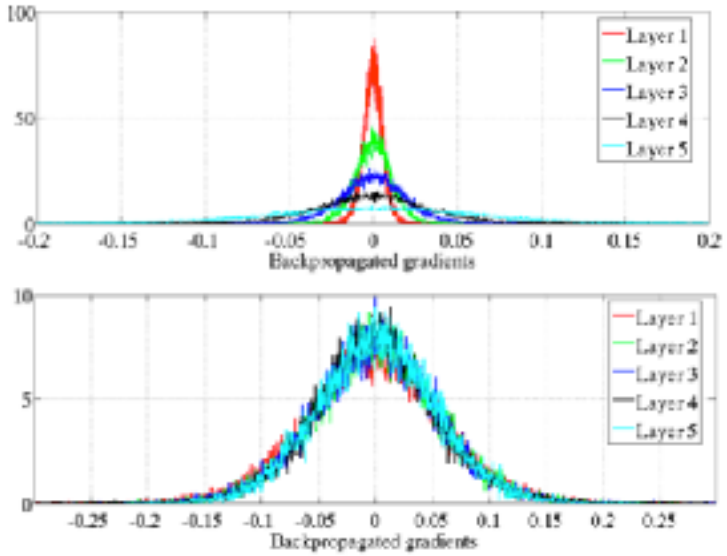


Figure 7: *Back-propagated gradients normalized histograms with hyperbolic tangent activation, with standard (top) vs normalized (bottom) initialization. Top: 0-peak decreases for higher layers.*

Starting gradient magnitudes per layer
standard normalization

Staring gradient magnitudes per layer
Glorot normalization

Glorot and He Initialization

We have solved this assuming the weights need be in the range -1 to 1 and assuming that x is distributed Gaussian ($tanh$)

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

	Uniform	Gaussian
Tanh	$\sigma = \sqrt{\frac{6}{n^{(L)} + n^{(L+1)}}}$	$\sigma = \sqrt{\frac{2}{n^{(L)} + n^{(L+1)}}}$
Sigmoid	$\sigma = 4\sqrt{\frac{6}{n^{(L)} + n^{(L+1)}}}$	$\sigma = 4\sqrt{\frac{2}{n^{(L)} + n^{(L+1)}}}$
ReLU	$\sigma = \sqrt{2}\sqrt{\frac{6}{n^{(L)} + n^{(L+1)}}}$	$\sigma = \sqrt{2}\sqrt{\frac{2}{n^{(L)} + n^{(L+1)}}}$

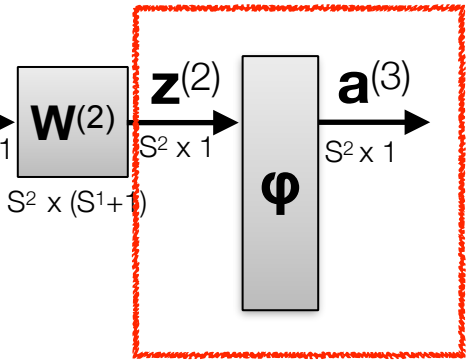
Summarized by Glorot and He

08. Practical_NeuralNets.ipynb **Demo**

Dropout
Smarter Weight Initialization

Practical Implementation of Architectures

- A new nonlinearity: **softmax**



$$a_j^{(L+1)} = \frac{\exp(z_j^{(L)})}{\sum_i \exp(z_i^{(L)})}$$

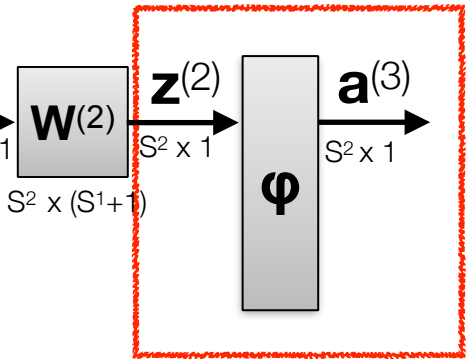
instead of final layer sigmoid!

it has many of the same properties as sigmoid mapping
but also the advantage of **interpretation as a true probability**

Update equations are **identical** to that of Cross Entropy with a sigmoid. We typically do not try to take derivative of softmax, therefore it is only used in final layer.

Practical Implementation of Architectures

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



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

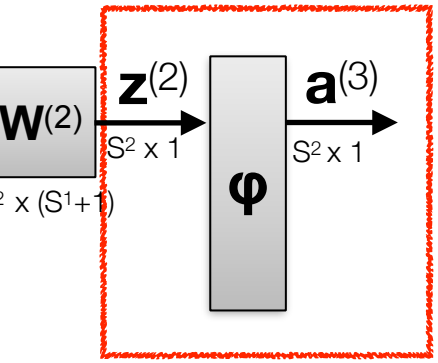
it has the advantage of **large gradients** and **extremely simple** derivative

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

08. Practical_NeuralNets.ipynb **Demo**

ReLU Nonlinearities

Other Activation Functions



- Sigmoid Weighted Linear Unit **SiLU**
  - also called Swish
- Mixing of sigmoid, σ, and ReLU

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

$$\frac{\partial \varphi(z)}{\partial z} = \varphi(z) + \sigma(z)[1 - \varphi(z)]$$

$$= a^{(l+1)} + \sigma(z^{(l)}) \cdot [1 - a^{(l+1)}]$$

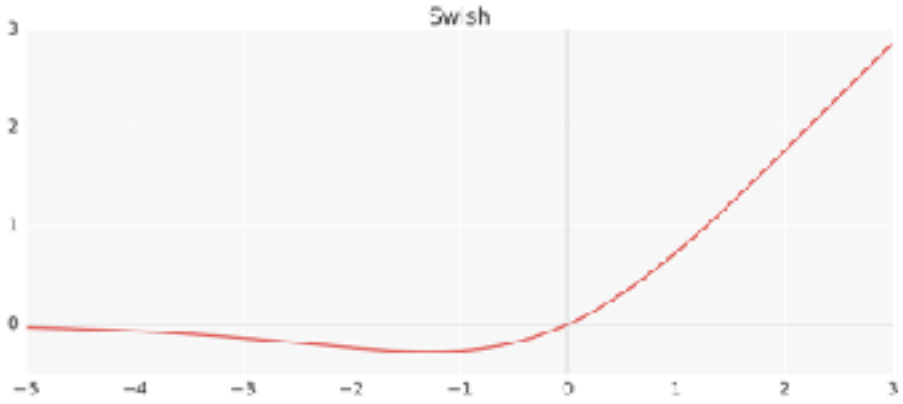


Figure 1: The Swish activation function.

Derivative Calculation:

$$= \sigma(x) + x \cdot \sigma(x)(1 - \sigma(x))$$
$$= \sigma(x) + x \cdot \sigma(x) - x \cdot \sigma(x)^2$$
$$= x \cdot \sigma(x) + \sigma(x)(1 - x \cdot \sigma(x))$$

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

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

Practical Details

- Neural networks can separate any data through multiple layers. The true realization of Rosenblatt:

> "Given an elementary α-perceptron, a stimulus world W, and any classification C(W) for which a solution exists; let all stimuli in W occur in any sequence, provided that each stimulus must reoccur in finite time; then beginning from an arbitrary initial state, an error correction procedure will always yield a solution to C(W) in finite time…"

- **Universality**: No matter what function we want to compute, we know that there is a neural network which can do the job.

- One nonlinear hidden layer with an output layer can perfectly train any problem with enough data, but might just be memorizing…
  - … it might be better to have even more layers for decreased computation and generalizability

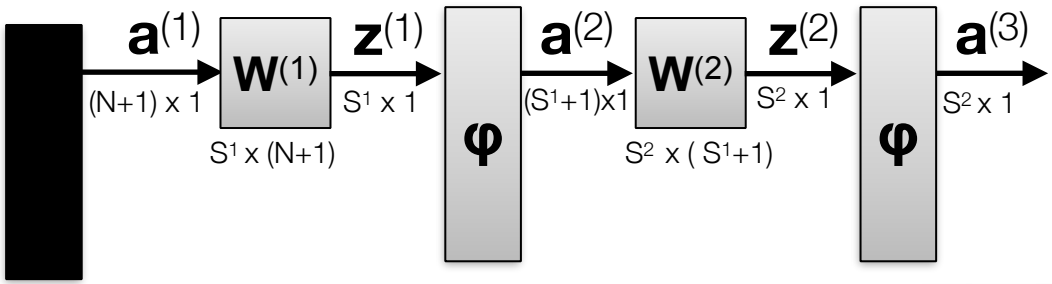
End of Session

- Next Time: Town Hall
- Next Time: Deep Learning in Keras

Back Up Slides

Back propagation

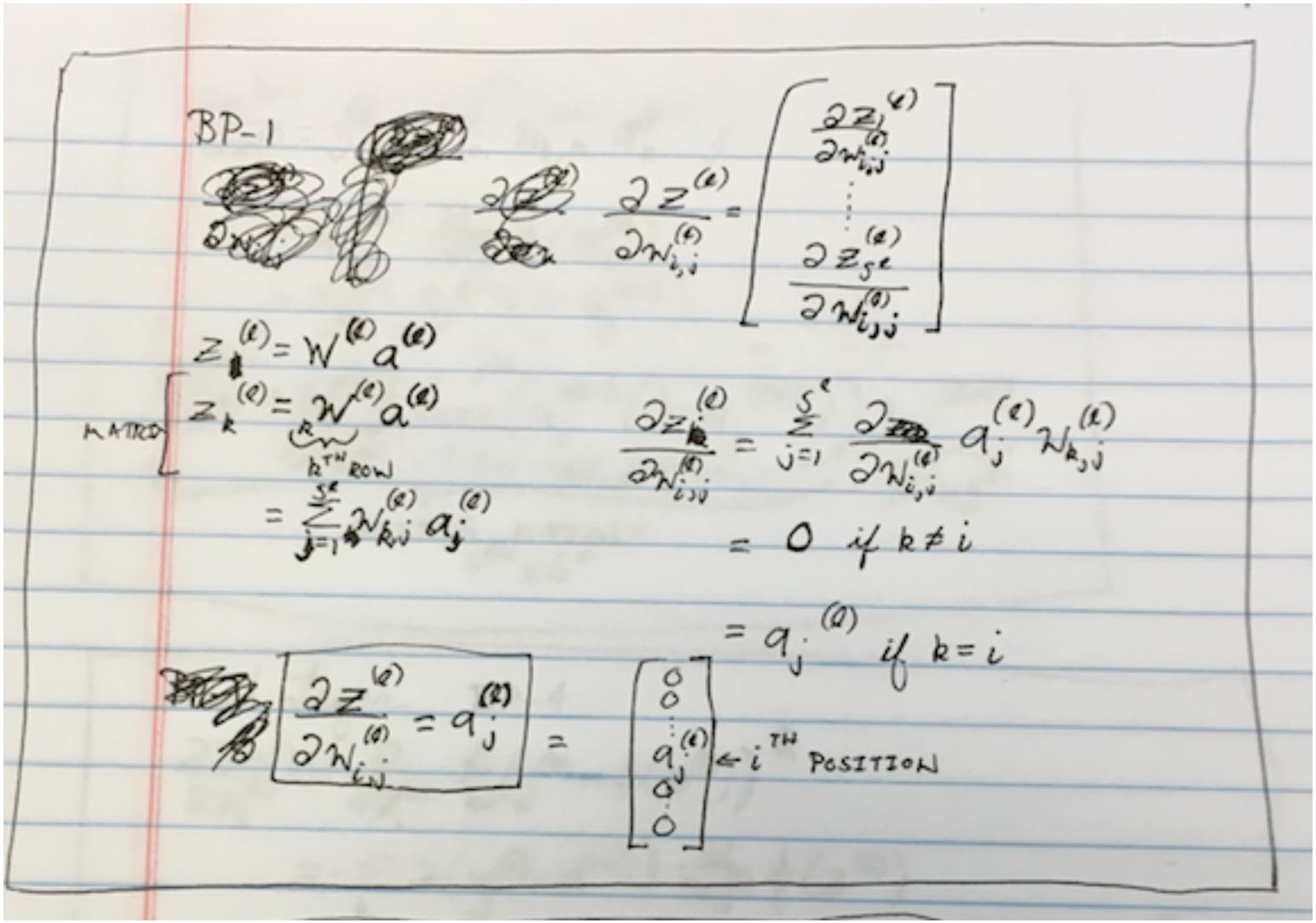
$$J(\mathbf{W}) = \sum_{k}^{M} (\mathbf{y}^{(k)} - \mathbf{a}^{(L)})^2$$



$$w_{i,j}^{(l)} \leftarrow w_{i,j}^{(l)} - \eta \frac{\partial J(\mathbf{W})}{\partial w_{i,j}^{(l)}}$$

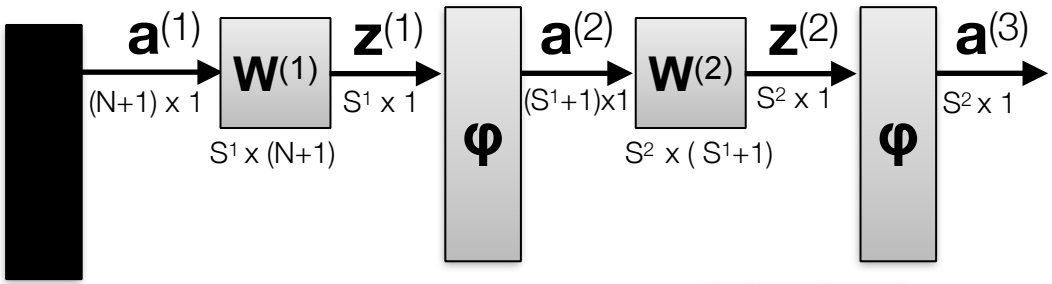
use chain rule:

$$\frac{\partial J(\mathbf{W})}{\partial w_{i,j}^{(l)}} = \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l)}} \frac{\partial \mathbf{z}^{(l)}}{\partial w_{i,j}^{(l)}}$$


BP-1
$\frac{\partial z^{(\ell)}}{\partial w_{i,j}^{(\ell)}} = \begin{bmatrix} \frac{\partial z_1^{(\ell)}}{\partial w_{i,j}^{(\ell)}} \\ \vdots \\ \frac{\partial z_{s^\ell}^{(\ell)}}{\partial w_{i,j}^{(\ell)}} \end{bmatrix}$
$z^{(\ell)} = W^{(\ell)} a^{(\ell)}$
MATRIX
$z_k^{(\ell)} = w^{(\ell)} a^{(\ell)}$
k^{TH} ROW
$= \sum_{j=1}^{s^\ell} w_{k,j}^{(\ell)} a_j^{(\ell)}$
$\frac{\partial z_k^{(\ell)}}{\partial w_{i,j}^{(\ell)}} = \sum_{j=1}^{s^\ell} \frac{\partial}{\partial w_{i,j}^{(\ell)}} a_j^{(\ell)} w_{k,j}^{(\ell)}$
$= 0$ if $k \neq i$
$= a_j^{(\ell)}$ if $k = i$
$\frac{\partial z^{(\ell)}}{\partial w_{i,j}^{(\ell)}} = a_j^{(\ell)} =$
i^{TH} POSITION

Back propagation

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

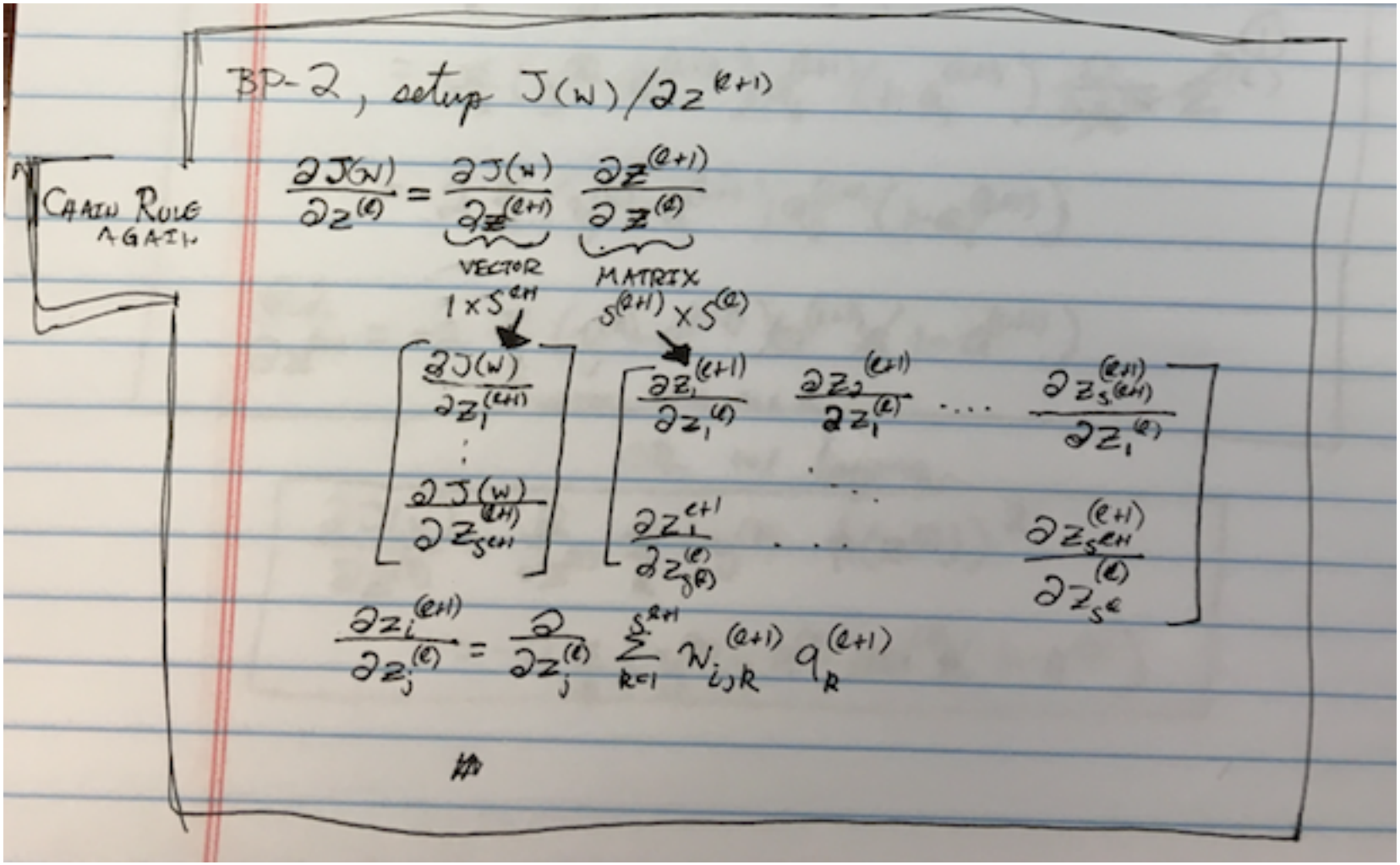


$$w_{i,j}^{(l)} \leftarrow w_{i,j}^{(l)} - \eta \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l)}} a_j^{(l)}$$

can we use chain rule again?

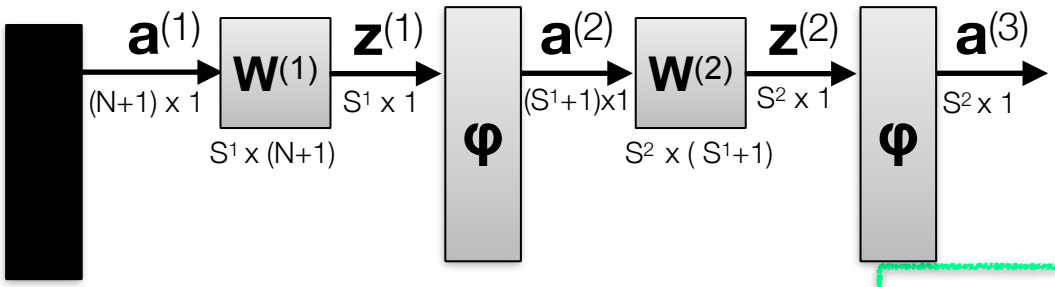
$$\frac{\partial J(\mathbf{W})}{\partial w_{i,j}^{(l)}} = \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l)}} a_j^{(l)}$$

- Steps:
  - propagate weights forward
  - calculate gradient at final layer
  - back propagate gradient for each layer
    - via recurrence relation


BP-2, setup $\frac{\partial J(W)}{\partial z^{(\ell+1)}}$
CHAIN RULE AGAIN
$\frac{\partial J(W)}{\partial z^{(\ell)}} = \frac{\partial J(W)}{\partial z^{(\ell+1)}} \frac{\partial z^{(\ell+1)}}{\partial z^{(\ell)}}$
VECTOR
$1 \times s^{(\ell+1)}$
MATRIX
$s^{(\ell+1)} \times s^{(\ell)}$
$\frac{\partial z_i^{(\ell+1)}}{\partial z_j^{(\ell)}} = \frac{\partial}{\partial z_j^{(\ell)}} \sum_{k=1}^{s^{\ell+1}} w_{i,k}^{(\ell+1)} a_k^{(\ell+1)}$

Back propagation

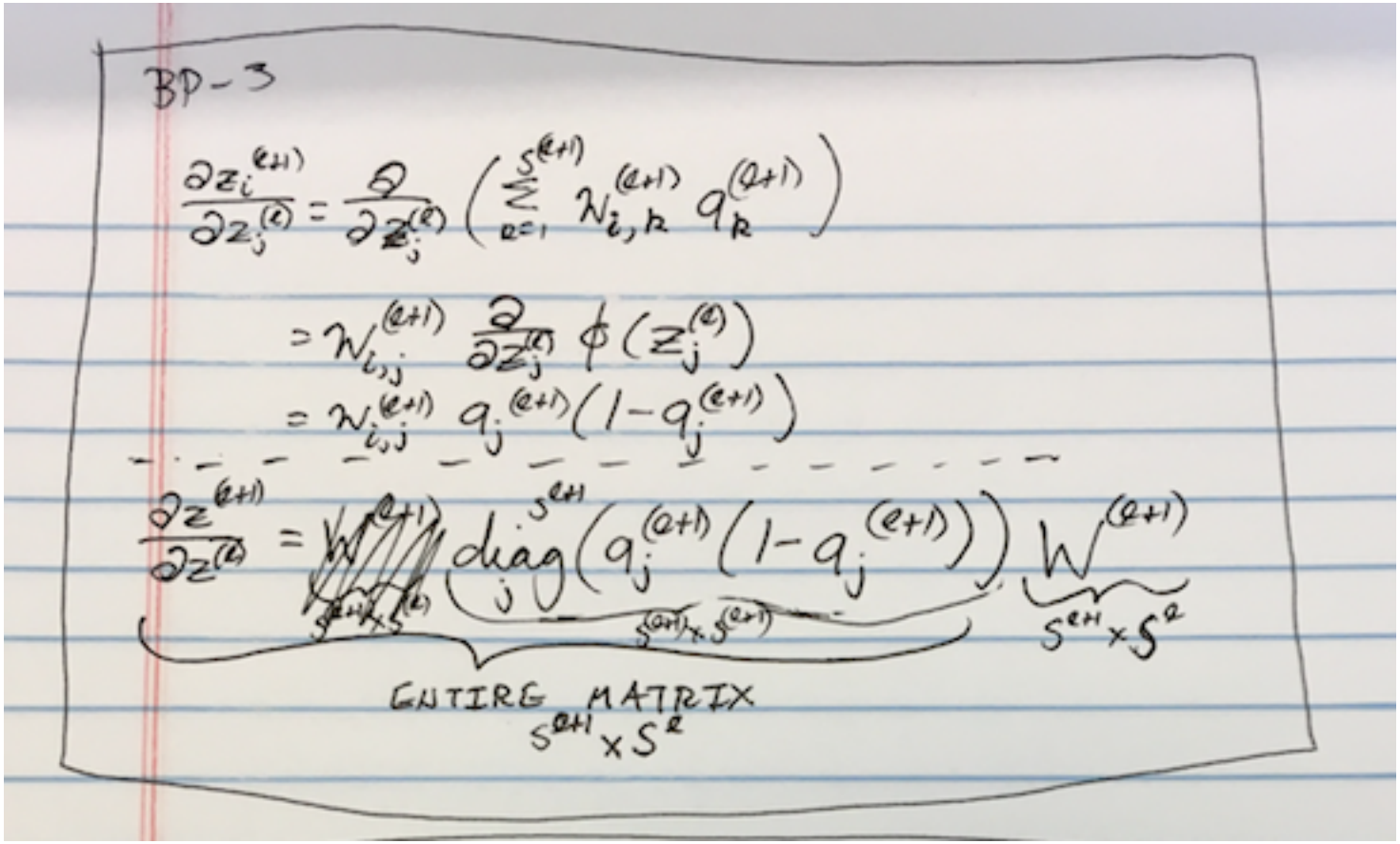
$$J(\mathbf{W}) = \sum_{k}^{M} (\mathbf{y}^{(k)} - \mathbf{a}^{(L)})^2$$



$$w_{i,j}^{(l)} \leftarrow w_{i,j}^{(l)} - \eta \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l)}} a_j^{(l)}$$

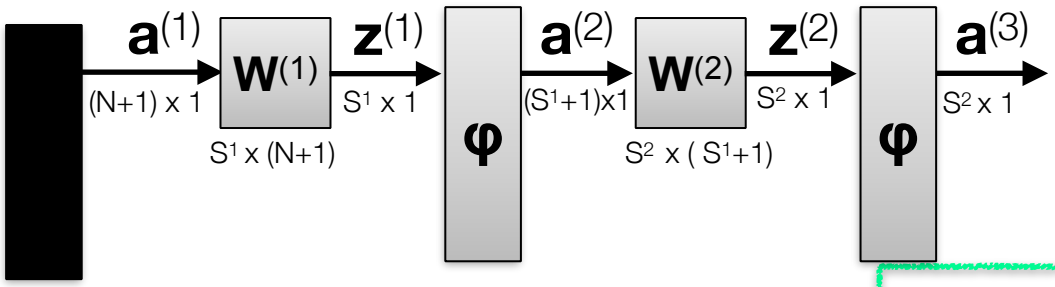
can we get this gradient?

$$\frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l)}} = \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l+1)}} \frac{\partial \mathbf{z}^{(l+1)}}{\partial \mathbf{z}^{(l)}}$$


BP-3
$\frac{\partial z_i^{(\ell+1)}}{\partial z_j^{(\ell)}} = \frac{\partial}{\partial z_j^{(\ell)}} \left(\sum_{k=1}^{S^{(\ell+1)}} w_{i,k}^{(\ell+1)} a_k^{(\ell+1)} \right)$
$= w_{i,j}^{(\ell+1)} \frac{\partial}{\partial z_j^{(\ell)}} \phi(z_j^{(\ell)})$
$= w_{i,j}^{(\ell+1)} a_j^{(\ell+1)} (1 - a_j^{(\ell+1)})$
$\frac{\partial z^{(\ell+1)}}{\partial z^{(\ell)}} = \underbrace{\underbrace{\operatorname{diag}_j \left(a_j^{(\ell+1)} (1 - a_j^{(\ell+1)}) \right)}_{S^{(\ell+1)} \times S^{(\ell+1)}} W^{(\ell+1)}}_{S^{\ell+1} \times S^{\ell}}$
ENTIRE MATRIX
$S^{\ell+1} \times S^{\ell}$

Back propagation

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



$$w_{ij}^{(l)} \leftarrow w_{ij}^{(l)} - \eta \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l)}} a_j^{(l)}$$

use chain rule: $\frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l)}} = \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l+1)}} \frac{\partial \mathbf{z}^{(l+1)}}{\partial \mathbf{z}^{(l)}}$

$$\frac{\partial \mathbf{z}^{(l+1)}}{\partial \mathbf{z}^{(l)}} = \text{diag}[\mathbf{a}^{(l+1)} * (1 - \mathbf{a}^{(l+1)})] \cdot \mathbf{W}^{(l+1)}$$

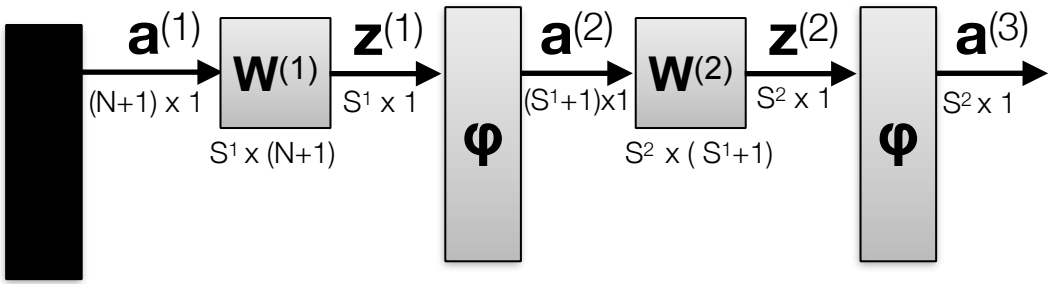
$$\frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l)}} = \text{diag}[\mathbf{a}^{(l+1)} * (1 - \mathbf{a}^{(l+1)})] \cdot \mathbf{W}^{(l+1)} \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l+1)}}$$

recurrence relation

If we know last layer, we can **back propagate** towards previous layers!

Back propagation

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



$$w_{ij}^{(l)} \leftarrow w_{ij}^{(l)} - \eta \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l)}} a_j^{(l)}$$

one more step need last layer gradient:

$$\frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(2)}} = \frac{\partial}{\partial \mathbf{z}^{(2)}} (\mathbf{y}^{(k)} - \phi(\mathbf{z}^{(2)}))^2$$

$$\frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l+1)}}$$

$$\frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(2)}} = -2(\mathbf{y}^{(k)} - \mathbf{a}^{(3)}) * \mathbf{a}^{(3)} * (1 - \mathbf{a}^{(3)})$$

Final Layer BP-4

$$\frac{\partial J(w)}{\partial z_i^{(L)}} = \frac{\partial}{\partial z_i^{(L)}} \sum_{k=1}^{M} \left(y^{(k)} - \phi(z^{(L)})\right)^2$$

$$= -\sum_k 2\left(y^{(k)} - a^{(L+1)}\right) \frac{\partial}{\partial z_i^{(L)}} \phi(z^{(L)})$$

$$= -2\sum_k \left(y^{(k)} - a^{(L+1)}\right) a_i^{(L+1)}\left(1 - a_i^{(L+1)}\right) \frac{\partial}{\partial z_i^{(L)}} z^{(L)} \quad (1)$$

$$= -2 \sum_k \left(y^{(k)} - a^{(L+1)}\right) a_i^{(L+1)}\left(1 - a_i^{(L+1)}\right)$$

$$\frac{\partial J}{\partial z^{(L)}} = -2 \sum_k \left(y^{(k)} - a^{(L+1)}\right) * a^{(L+1)} * \left(1 - a^{(L+1)}\right)$$

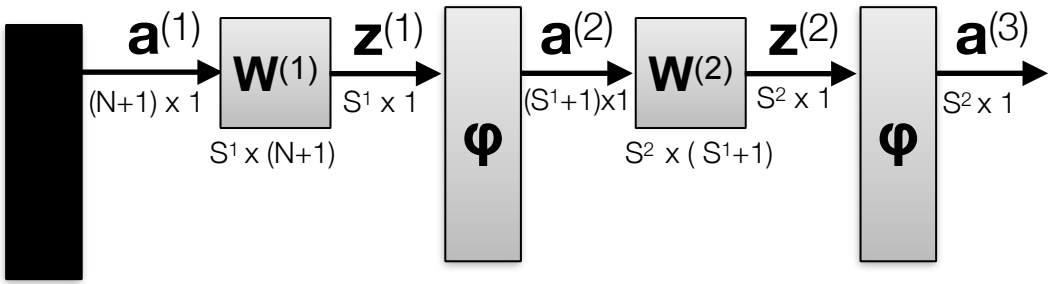
↑ ONE DIM, TAKE OUT K

OR w/ layers

$$\frac{\partial J(w)}{\partial z^{(2)}} = \frac{\partial}{\partial z^{(2)}} \sum_k \left(y^{(k)} - \phi(z^{(2)})\right)^2$$

$$= -2 \sum_k \left(y^{(k)} - a^{(3)}\right) * a^{(3)} * \left(1 - a^{(3)}\right)$$

Back propagation summary



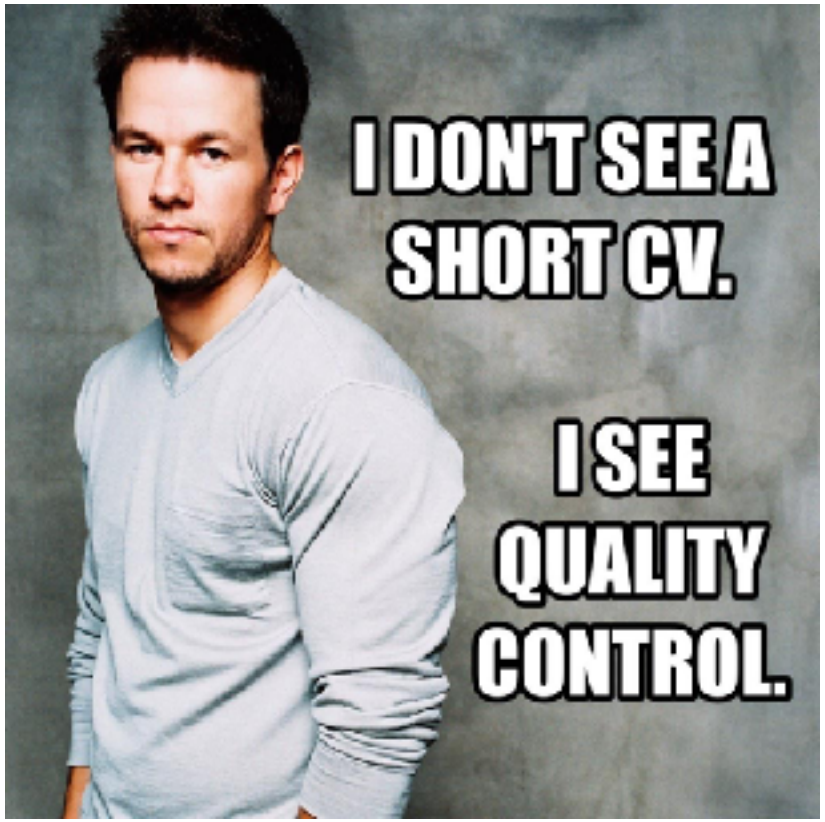
- **Self Test**:
  True or False: If we change the cost function, $J(\mathbf{W})$, we only need to update the final layer calculation of the back propagation steps. The remainder of the algorithm is unchanged.
  - A. True
  - B. False

$$\mathbf{V}^{(2)} = -2(\mathbf{Y} - \mathbf{A}^{(3)}) * \mathbf{A}^{(3)} * (1 - \mathbf{A}^{(3)})$$

$$\nabla^{(2)} = \mathbf{V}^{(2)} \cdot [\mathbf{A}^{(2)}]^T$$

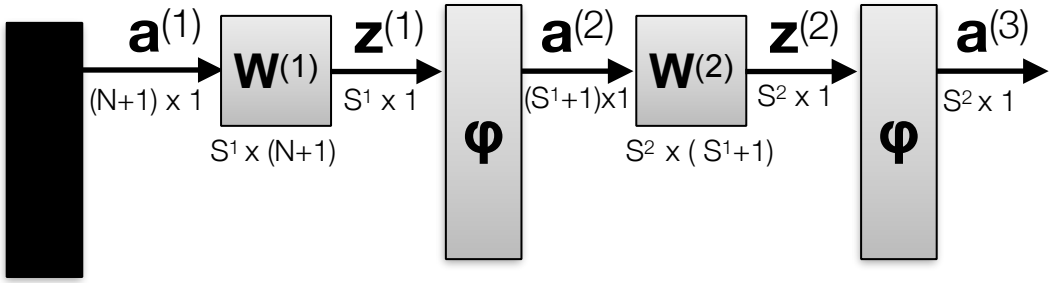
Programming Multi-layer Neural Networks

07. MLP Neural Networks.ipynb



Guided Example

Recall from the in-class asisgnment



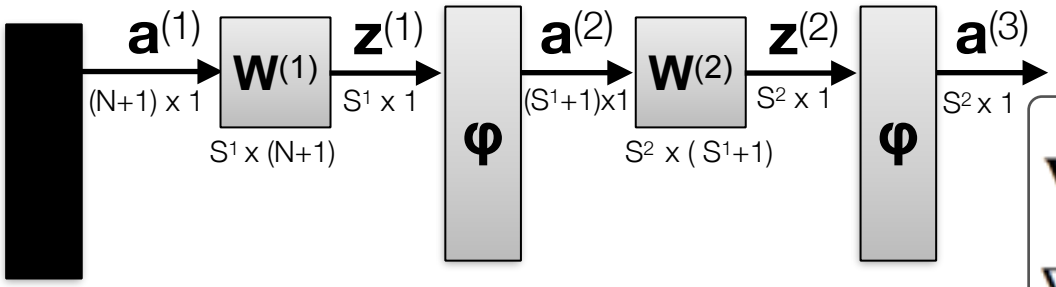
1. Forward propagate to get **Z**, **A**

```
# feedforward all instances
A1, Z1, A2, Z2, A3 = self._feedforward(X_data,self.W1,self.W2)
```

```
def _feedforward(self, X, W1, W2):
    A1 = self._add_bias_unit(X.T, how='row')
    Z1 = W1 @ A1
    A2 = self._sigmoid(Z1)
    A2 = self._add_bias_unit(A2, how='row')
    Z2 = W2 @ A2
    A3 = self._sigmoid(Z2)
    return A1, Z1, A2, Z2, A3
```

these are more than just vectors for **one instance**!
these are for **all** instances

Back propagation implementation



1. Forward propagate to get **Z**, **A**
2. Get final layer gradient
3. Back propagate sensitivities

$$\mathbf{V}^{(2)} = -2(\mathbf{Y} - \mathbf{A}^{(3)}) * \mathbf{A}^{(3)} * (1 - \mathbf{A}^{(3)})$$

$$\nabla^{(2)} = \mathbf{V}^{(2)} \cdot [\mathbf{A}^{(2)}]^T$$

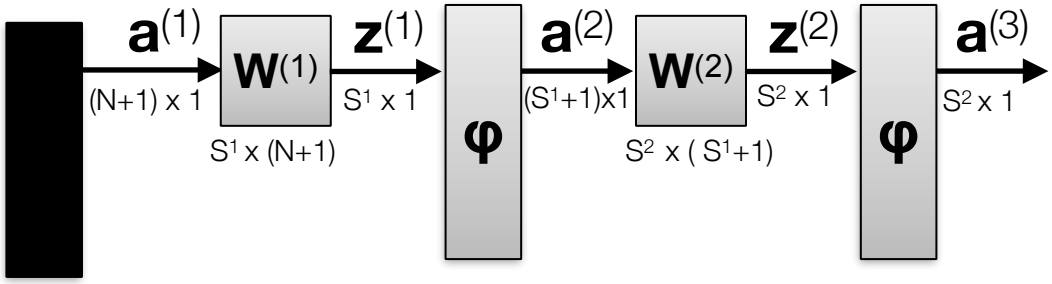
$$\mathbf{V}^{(1)} = \mathbf{A}^{(2)} * (1 - \mathbf{A}^{(2)}) * [\mathbf{W}^{(2)}]^T \cdot \mathbf{V}^{(2)}$$

$$\nabla^{(1)} = \mathbf{V}^{(1)} \cdot [\mathbf{A}^{(1)}]^T$$

```
def _get_gradient(self, A1, A2, A3, Z1, Z2, Y_enc, W1, W2):
    """ Compute gradient step using backpropagation.
    """
    # vectorized backpropagation
    V2 = -2*(Y_enc-A3)*A3*(1-A3)
    V1 = A2*(1-A2)*(W2.T @ V2)

    grad2 = V2 @ A2.T
    grad1 = V1[1:,:] @ A1.T
```

Back propagation implementation



1. Forward propagate to get **Z**, **A** for all layers
2. Get final layer gradient
3. Back propagate sensitivities
4. Update each $\mathbf{W}^{(l)}$

for each layer:

$$\mathbf{W}^{(l)} \leftarrow \mathbf{W}^{(l)} - \eta \nabla^{(l)}$$

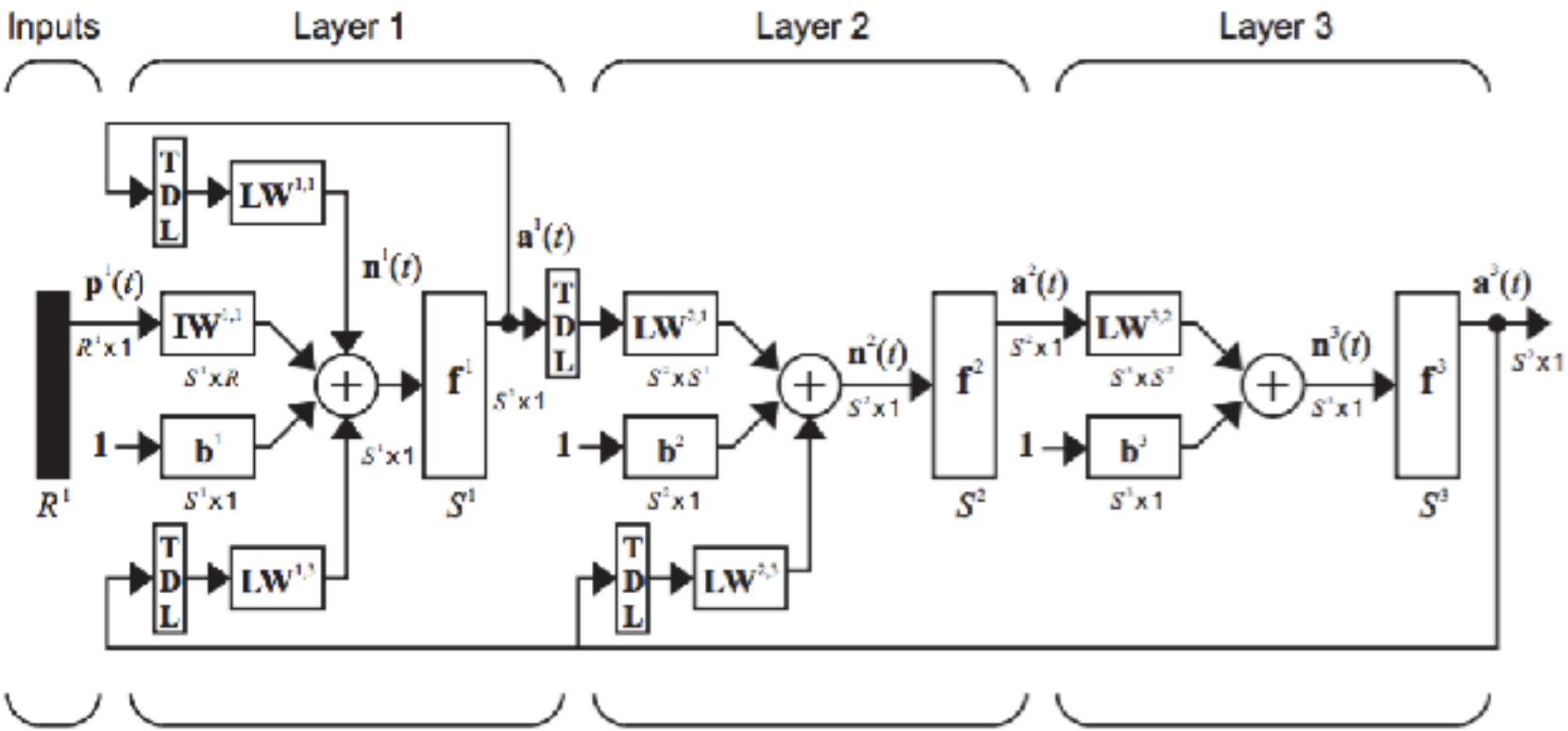
```
# feedforward all instances
A1, Z1, A2, Z2, A3 = self._feedforward(X_data,self.W1,self.W2)

# compute gradient via backpropagation
grad1, grad2 = self._get_gradient(A1=A1, A2=A2,
                                  A3=A3, Z1=Z1,
                                  Y_enc=Y_enc,
                                  W1=self.W1, W2=self.W2)

self.W1 -= self.eta * grad1
self.W2 -= self.eta * grad2
```

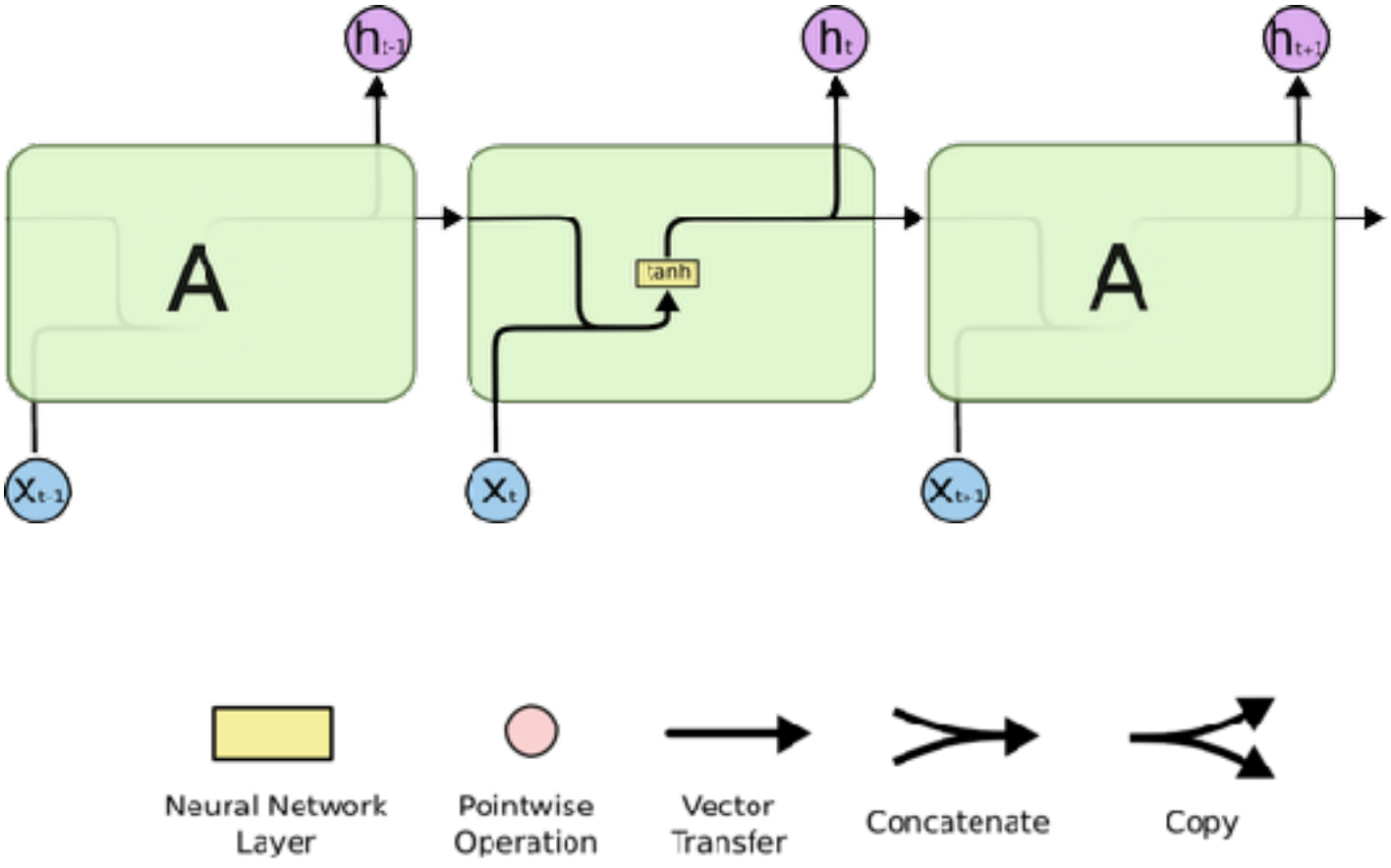
More Advanced Architectures

- Dynamic Networks (recurrent networks)
  - can use current and previous inputs, in time
  - still popular, but ultimately extremely hard to train
  - **highly successful variant**: long short term



More Advanced Architectures

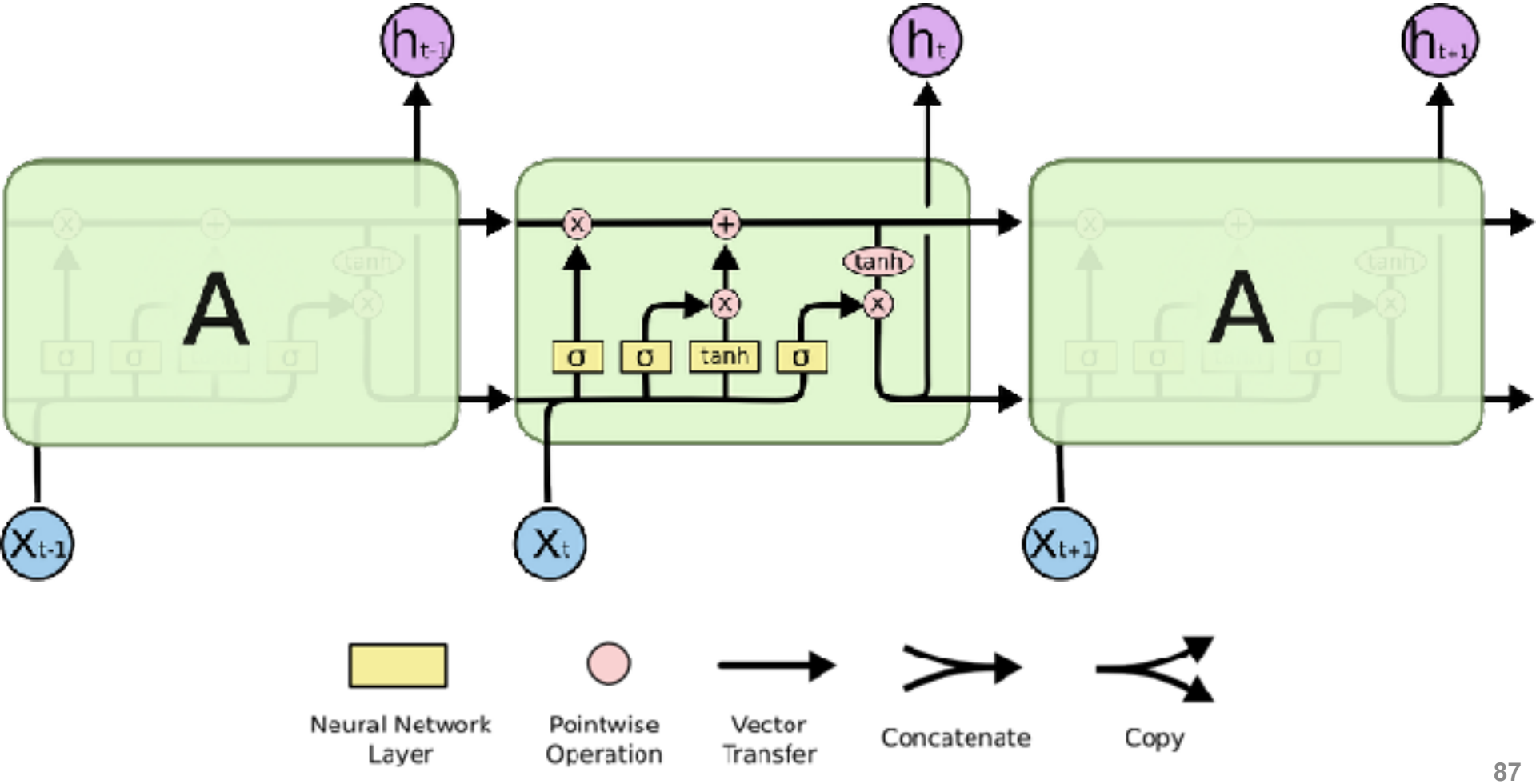
- **LSTM key idea**: limit how past data can affect output



http://colah.github.io/posts/2015-08-Understanding-LSTMs/

More Advanced Architectures

- **LSTM key idea**: limit how past data can affect output



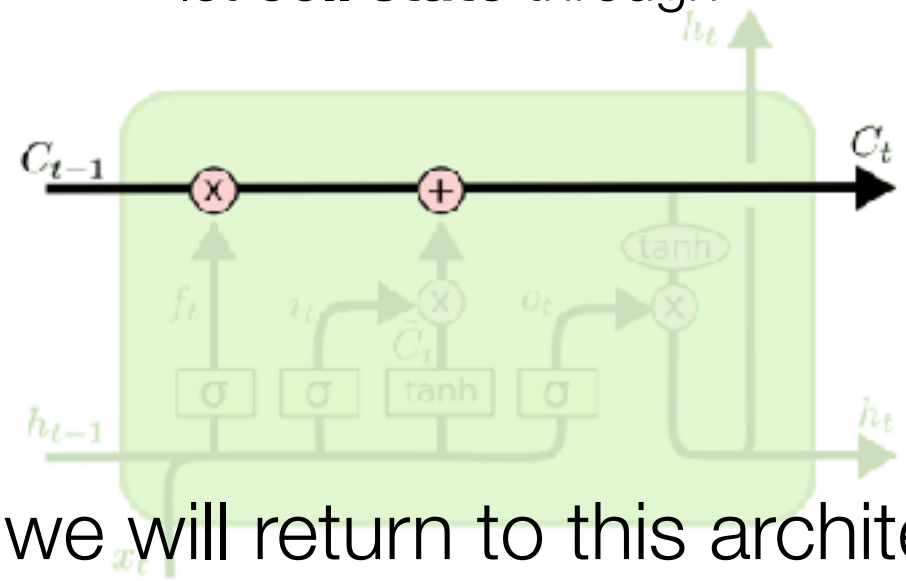
http://colah.github.io/posts/2015-08-Understanding-LSTMs/

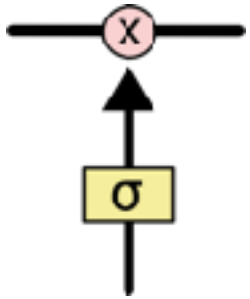
More Advanced Architectures

- **LSTM key idea**: limit how past data can affect output

let **cell state** through

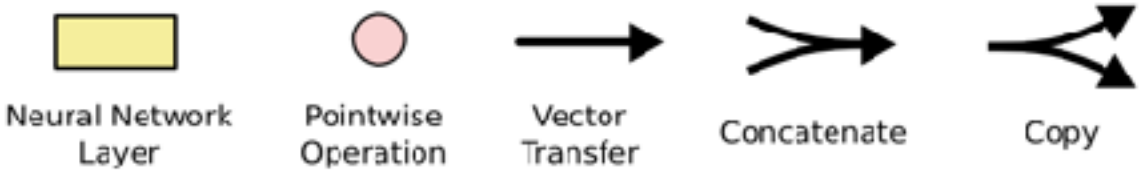
potentially **forget past** inputs via "gate" σ





we will return to this architecture later, for now:

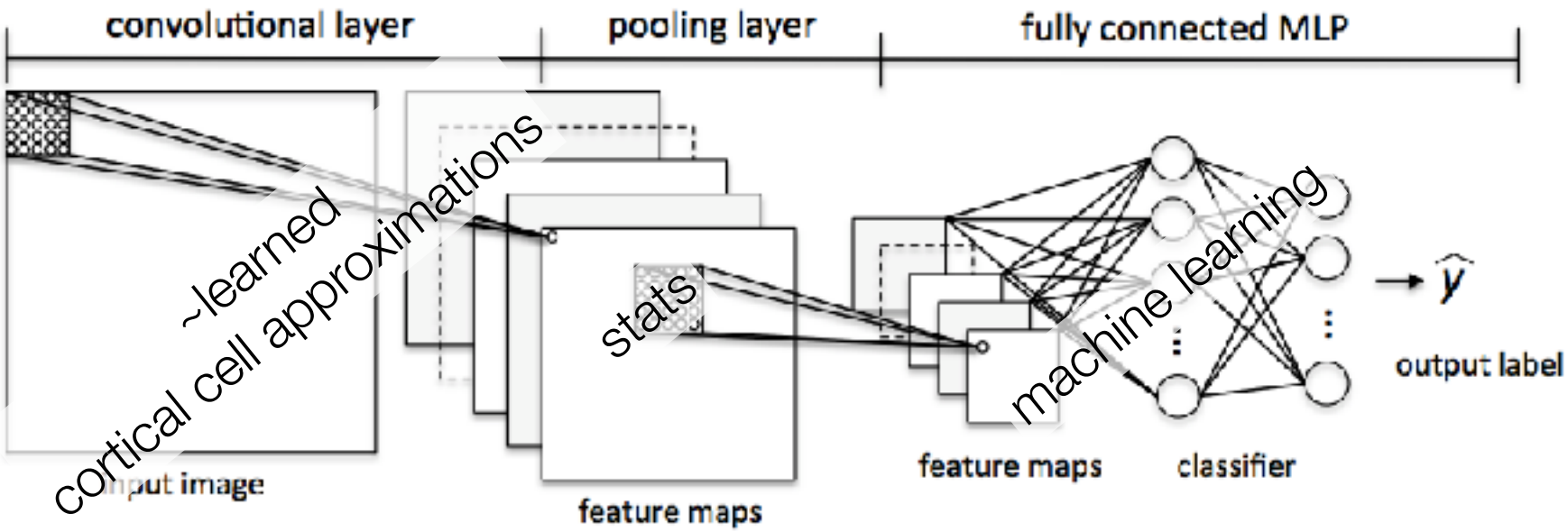
put it in long term memory 😂



http://colah.github.io/posts/2015-08-Understanding-LSTMs/

More Advanced Architectures

- Convolutional Neural Networks
  - image processing operations



we will return to this architecture later, for now:

put it in long term memory

Problems with these Advanced Architectures

- These architectures have been around for 30 years
- And solved some amazingly hard problems
- but they had **big training problems** that back propagation could not solve readily:
  - unstable gradients (vanishing/exploding)
  - **extremely** non-convex space
    - more layers==many more local optima to get stuck
  - sometimes **gradient optimization is too computational** for weight updates
    - might need better optimization strategy than SGD
- The solution to these problems came from having large amounts of training data, better setup of the optimization
  - eventually was termed **deep learning**