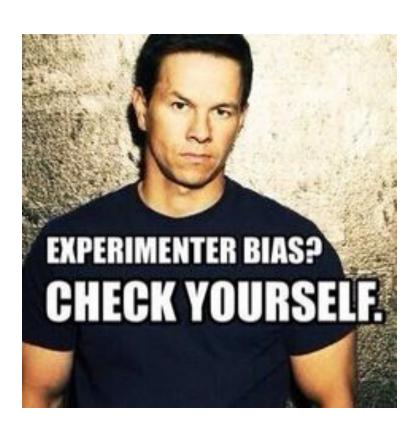
Lecture Notes for Machine Learning in Python

Professor Eric Larson Week Seven A

Class Logistics and Agenda

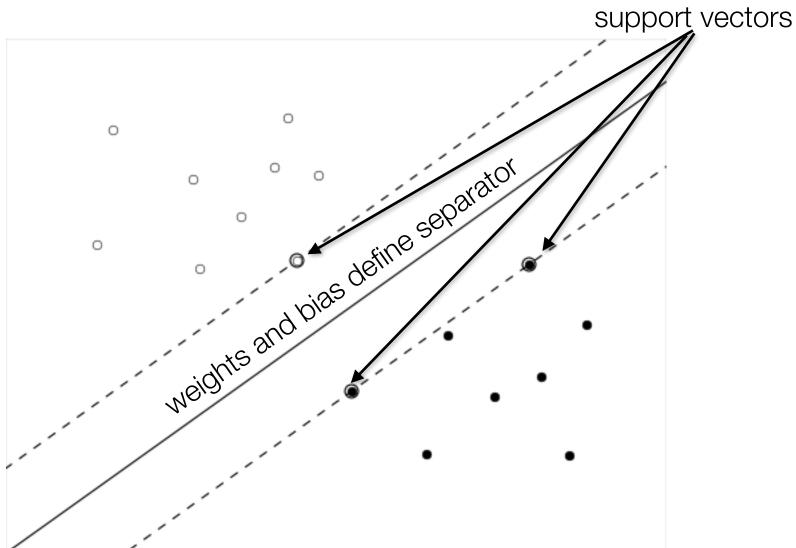
- Grades Coming Soon
- A2 will be about using linear classifiers to perform classifications tasks
 - extending?
- Two Week Agenda:
 - SVM Review
 - Neural Networks History
 - Multi-layer Architectures
 - Programming Multi-layer training

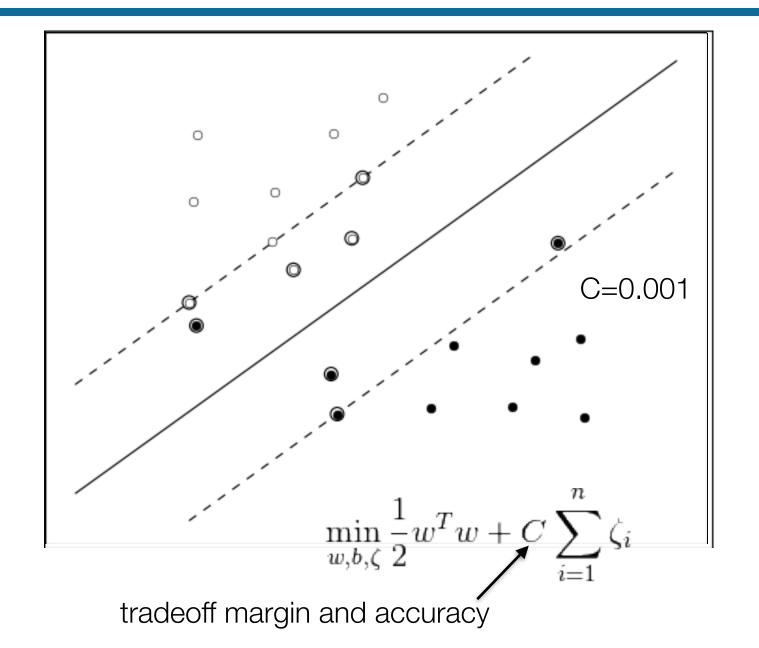
Support Vector Machine Review



- Linear SVMs
 - Architecture near identical to logistic regression, except: $\min_{w,b,\zeta} \frac{1}{2} w^T w + C \sum_{i=1}^{\infty} \zeta_i$
 - maximize margin
 - constrained optimization to $y_i(w^T\phi(x_i) + b) \ge 1 \zeta_i$,
 - **Self Test**: What are the trained $\zeta_i \geq 0, i = 1, ..., n$ parameters for the linear SVM?
 - A: Coefficients of w
 - B: Bias terms
 - C: Slack Variables
 - D: Support Vector locations

- Linear SVMs
 - Architecture near identical to logistic regression, except: $\min_{w,b,\zeta} \frac{1}{2} w^T w + C \sum_{i=1}^{N} \zeta_i$
 - maximize margin
 - constrained optimization to $y_i(w^T\phi(x_i) + b) \ge 1 \zeta_i$, $\zeta_i \geq 0, i = 1, ..., n$
 - Trained Parameters:
 - bias and weights for each class
 - support vectors chosen for margin calculation
 - slack variables for inseparable cases



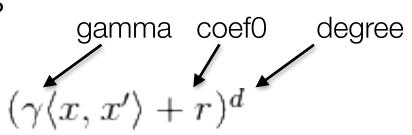


SVMs Summary: non-linear

- Non-linear SVMs
 - Architecture not like logistic regression
 - kernels == high dimensional dot-product
 - impossible to store weights
 - use kernel trick to no need to store them!
 - Parameters
 - biases
 - selected support vectors
 - slack variables
 - parameters specific to kernels

SVMs Summary: non-linear

- Popular Kernels
 - polynomial



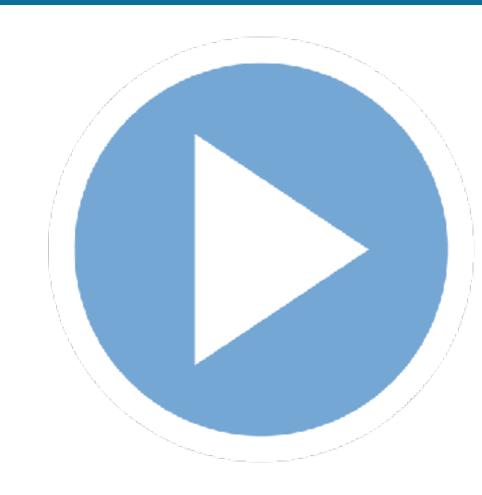
- radial basis function $\exp(-\gamma|x-x'|^2)$
- sigmoid

gamma coef0
$$\tanh(\gamma\langle x,x'\rangle+r)$$

Demo

SVM parameterization

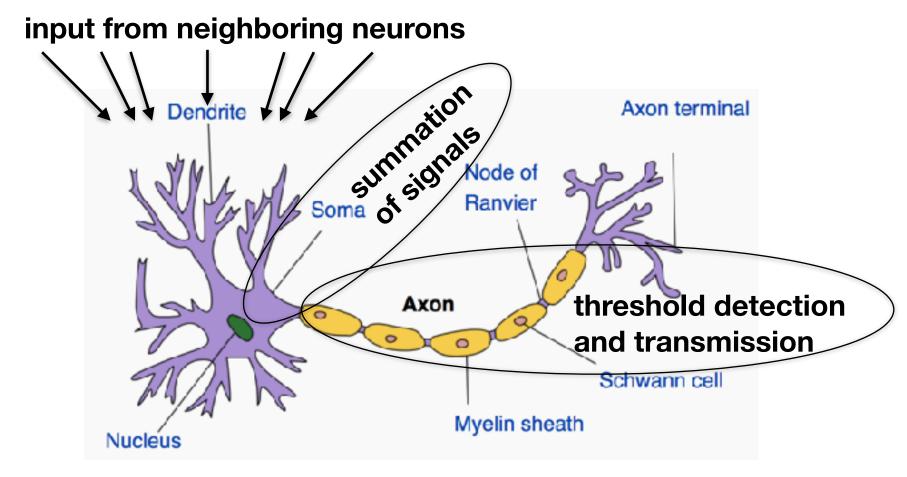
svm_gui.py



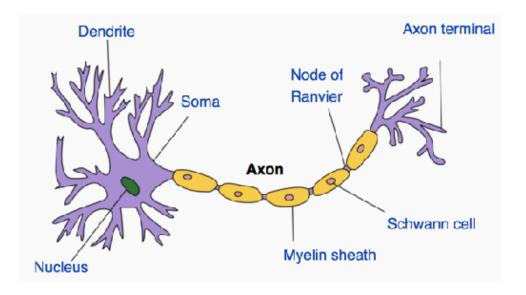
A history of Neural Networks



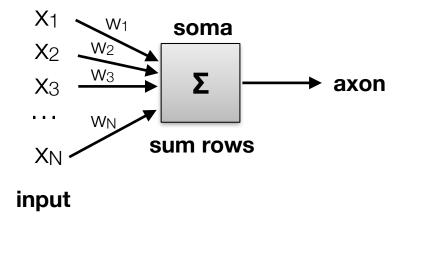
From biology to modeling:



McCulloch and Pitts, 1943



dendrite



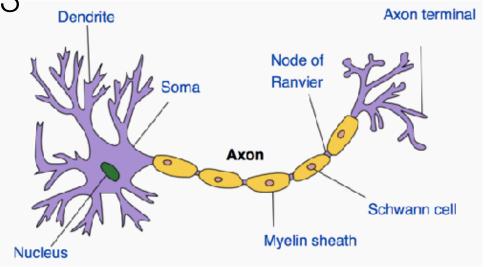


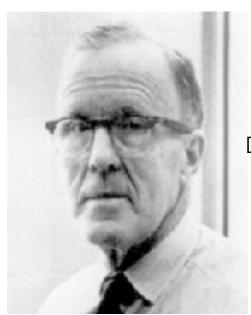
Warren McCulloch



Walter Pitts

- McCulloch and Pitts, 1943
- Donald Hebb, 1949
 - close neurons fire together
 - basis of memory
 - and neural pathways





Donald O. Hebb

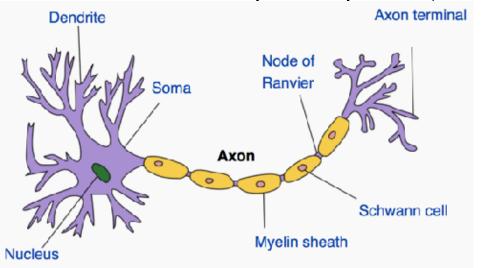


Warren McCulloch



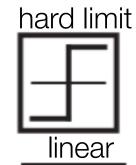
Walter Pitts

Rosenblatt's perceptron, 1957

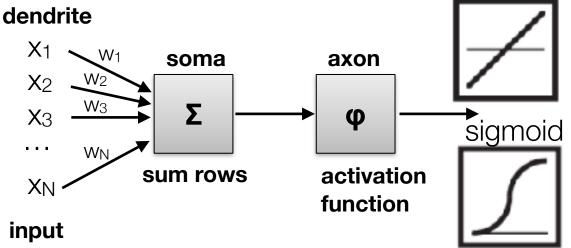




Frank Rosenblatt

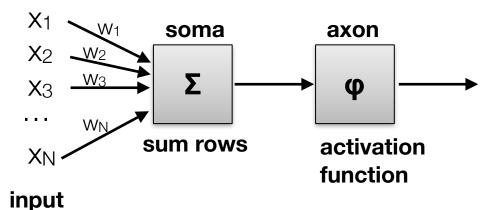


$$a = -1$$
 $z < 0$
 $a = 1$ $z > = 0$



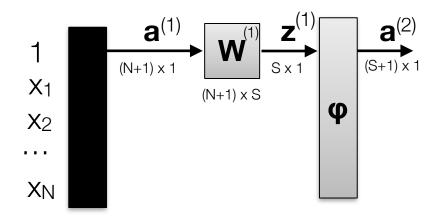
$$a = \frac{1}{1 + \exp(-z)}$$

dendrite



Some notation

- need bias term
- matrix representation
- multiple layers

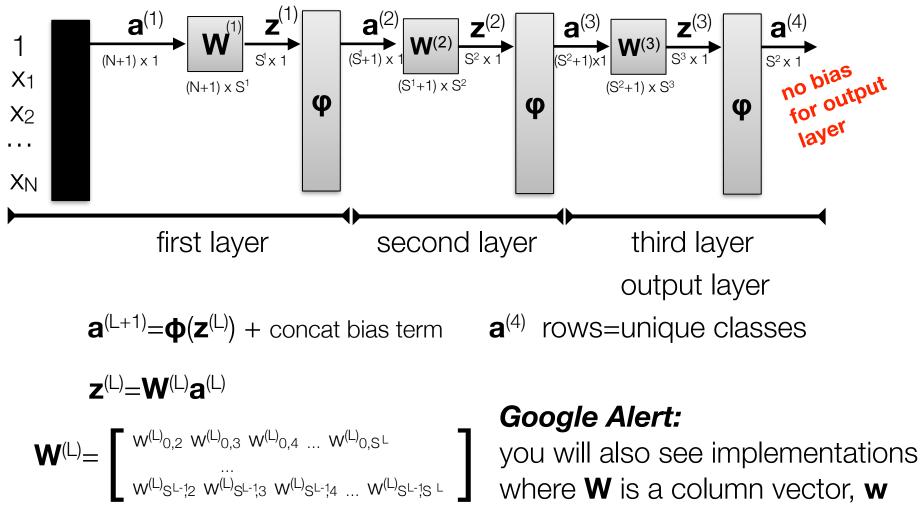


$$\mathbf{a}^{(1)} = \mathbf{X} + \text{concat bias term}$$

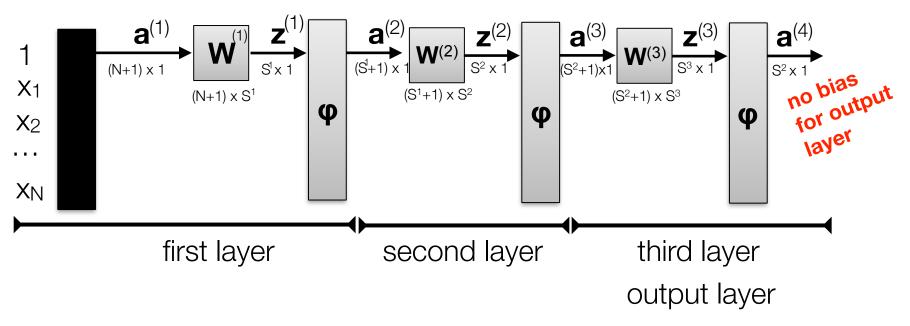
$$z = Wa^{(1)}$$

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

Multiple layers notation

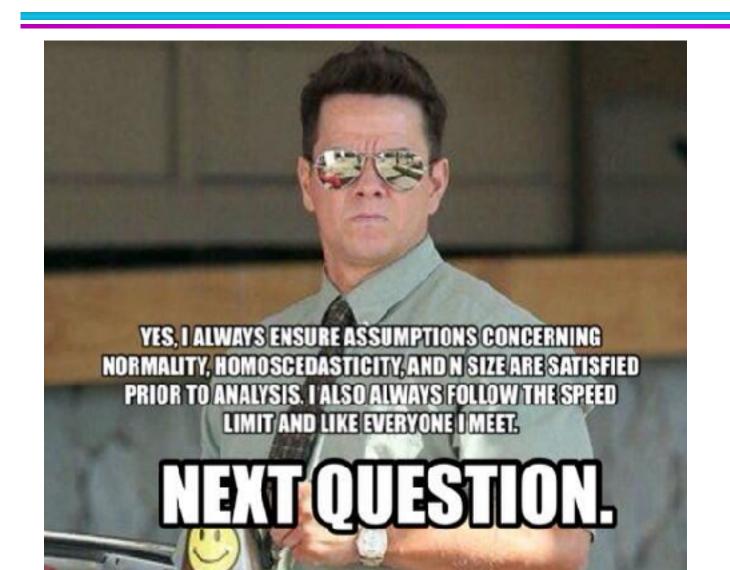


Multiple layers notation

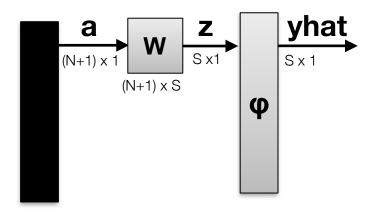


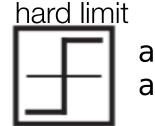
- Self test: How many parameters need to be trained in the above network?
 - A. $(N+1) \times S^1 + (S^1+1) \times S^2 + (S^2+1) \times S^3$
 - B. $|\mathbf{W}^{(1)}| + |\mathbf{W}^{(2)}| + |\mathbf{W}^{(3)}|$
 - C. can't determine from diagram
 - D. it depends on the sizes of intermediate variables,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

Training Neural Network Architectures



Rosenblatt's perceptron, 1957





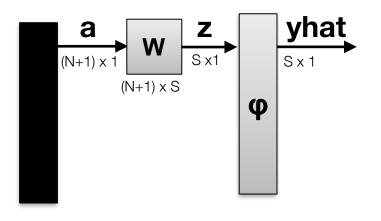


a=-1 z< 0 a= 1 z>=0

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

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

Rosenblatt's perceptron, 1957





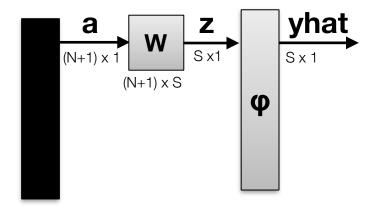


Need objective Function, minimize MSE

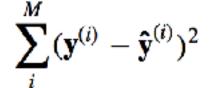
$$\sum_{i}^{M} (\mathbf{y}^{(i)} - \hat{\mathbf{y}}^{(i)})^{2} \qquad J(W) = \sum_{i}^{M} (\mathbf{y}^{(i)} - \phi(\mathbf{W} \cdot \mathbf{x}^{(i)}))^{2}$$

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

Adaline network, Widrow and Hoff, 1960



linear a=z





Marcian "Ted" Hoff



Bernard Widrow

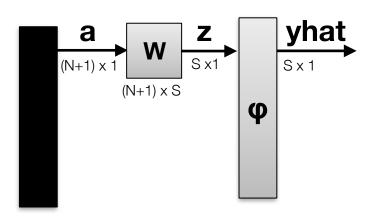
Objective Function, minimize MSE

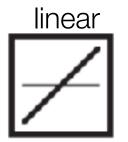
new objective function becomes: $J(W) = \sum_{i=0}^{M} (\mathbf{y}^{(i)} - \mathbf{W} \cdot \mathbf{x}^{(i)})^2$

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

Adaline network, Widrow and Hoff, 1960





a=z

Marcian "Ted" Hoff



Bernard Widrow

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

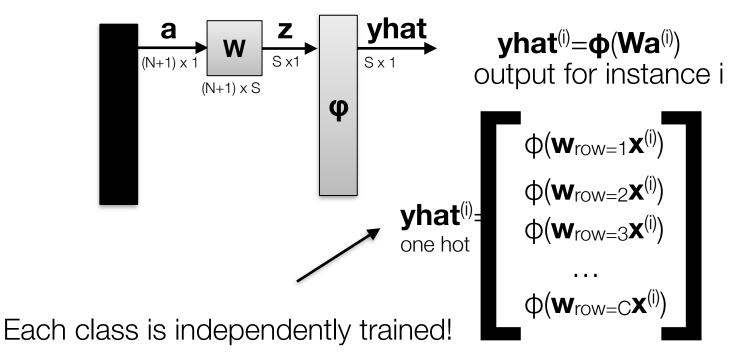
For case S=1, this is just solving **linear regression**

and we have already solved this!

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

for **W**, each row can be solved independently!





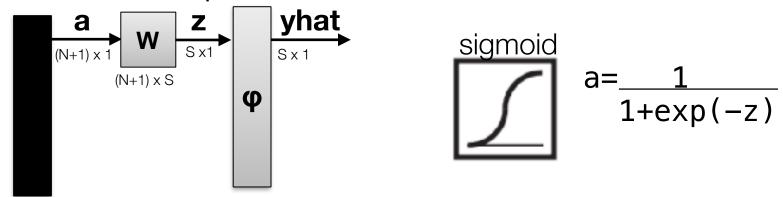
$$\mathbf{w} \leftarrow \mathbf{w} + \eta [\mathbf{X} * (\mathbf{y} - \mathbf{\hat{y}})]$$

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

which is one-versus-all! we have already solved this!



Modern Perceptron network



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 solving **logistic regression** and **we have already solved this**!

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

for **W**, each row can be solved independently!

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

which is one-versus-all!

Simple Architectures: summary

- Adaline network, Widrow and Hoff, 1960
 - linear regression with classifier
- Perceptron
 - with sigmoid activation: logistic regression
- One-versus-all implementation is the same as having w_{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:



TED Ideas worth spreading

DISCOVER

Marvin Minsky:

Health and the human mind

TED2003 · 13:33 · Filmed Feb 2003.







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

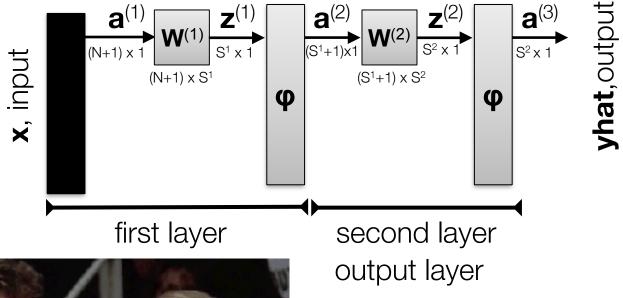


Geoffrey Hinton



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)



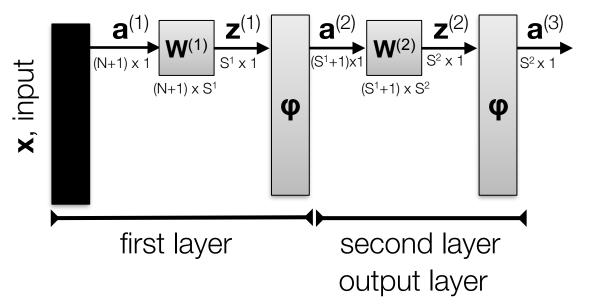


each row of **yhat** is no longer independent of the rows in **W**

Back propagation

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

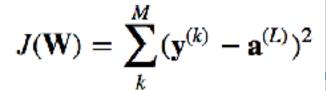


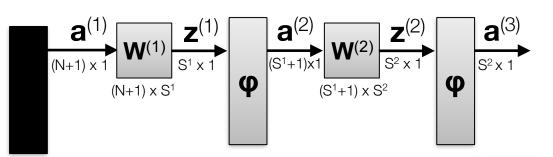


$$\sum_{k}^{\infty} J(\mathbf{W}) = \sum_{k}^{M} (\mathbf{y}^{(k)} - \mathbf{a}^{(L)})^2$$

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

Back propagation





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

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 next time!

End of Session

thanks!

More help on neural networks:

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=0ahUKEwioprvn 27fPAhWMx4MKHYbwDlwQFggeMAA&url=http%3A%2F%2Fhagan.okstate.edu% 2FNNDesign.pdf&usg=AFQjCNG5YbM4xSMm6K5HNsG-4Q8TvOu_Lw&sig2=bgT3 k-5ZDDTPZ07Qu8Oreg

Michael Nielsen

http://neuralnetworksanddeeplearning.com

Lecture Notes for Machine Learning in Python

Professor Eric Larson Week Seven B

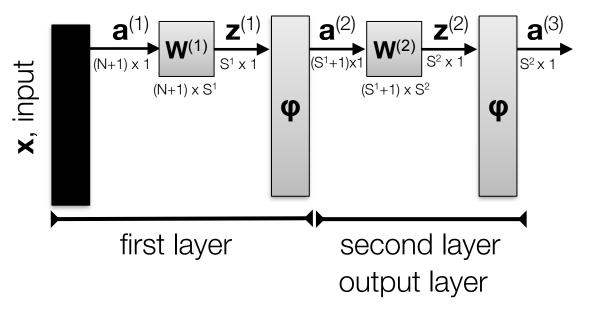
Class Logistics and Agenda

- Grades Coming Soon, but slowly
- A2 posted, schedule revised
- Two Week Agenda:
 - SVM Review
 - Neural Networks History
 - Multi-layer Architectures
 - Programming Multi-layer training
- Next Time: fall break

Back propagation

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

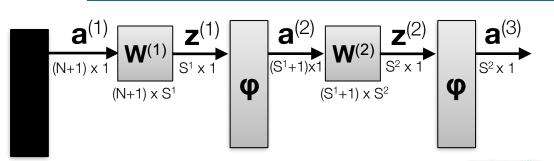




$$\sum_{k}^{M} J(\mathbf{W}) = \sum_{k}^{M} (\mathbf{y}^{(k)} - \mathbf{a}^{(L)})^2$$

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

Back propagation

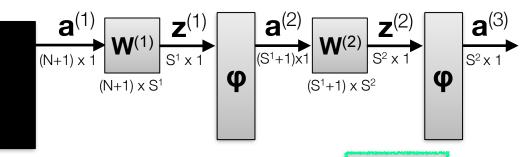


use chain rule:
$$\frac{\partial J(\mathbf{W})}{\partial w_{i,j}^{(l)}} = \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l)}} \frac{\partial \mathbf{z}^{(l)}}{\partial w_{i,j}^{(l)}}$$

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

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

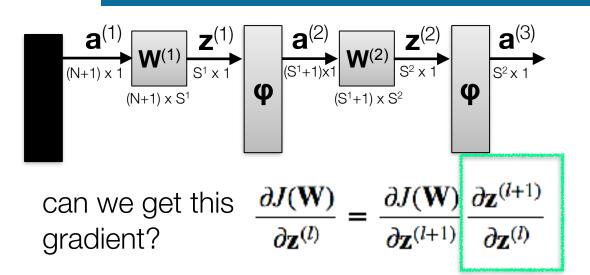
$$J(\mathbf{W}) = \sum_{k}^{M} (\mathbf{y}^{(k)} - \mathbf{a}^{(L)})^2$$



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

can we use chain rule again?

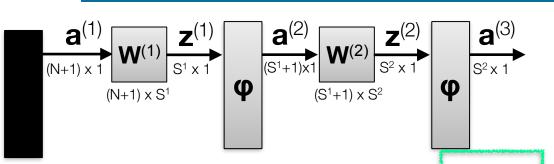
$$\frac{\partial J(\mathbf{W})}{\partial w_{i,j}^{(l)}} = \boxed{\frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l)}}} a_j^{(l)}$$



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

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

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



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

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

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

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

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

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

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

one more step

need last layer gradient:

$$\frac{\partial J(\mathbf{W})}{\partial J(\mathbf{W})}$$

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

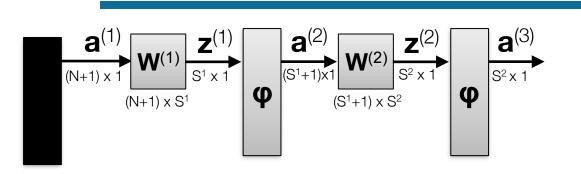
$$\frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(2)}} = -2(\mathbf{y}^{(k)} - \mathbf{a}^{(3)}) * \mathbf{a}^{(3)} * (1 - \mathbf{a}^{(3)})$$

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

40 bp-4

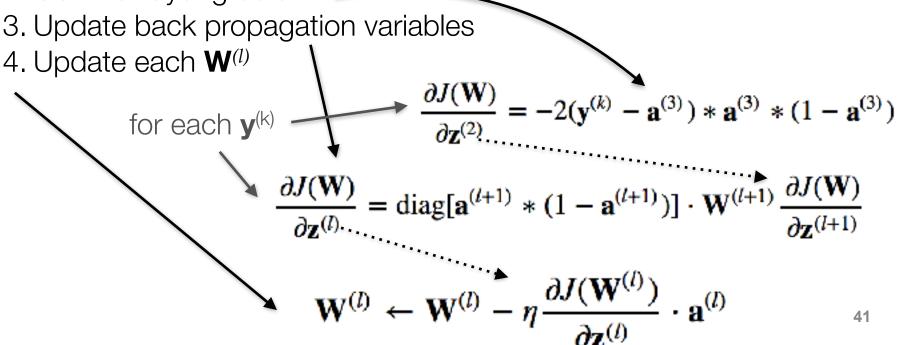
Back propagation summary

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



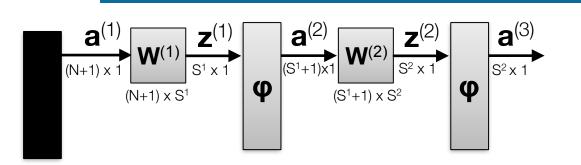
$$w_{i,j}^{(l)} \leftarrow w_{i,j}^{(l)} - \eta \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l)}} a_j^{(l)}$$

- 1. Forward propagate to get **z**, **a** for all layers
- 2. Get final layer gradient
- 3. Update back propagation variables



Back propagation summary

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



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

• Self Test:

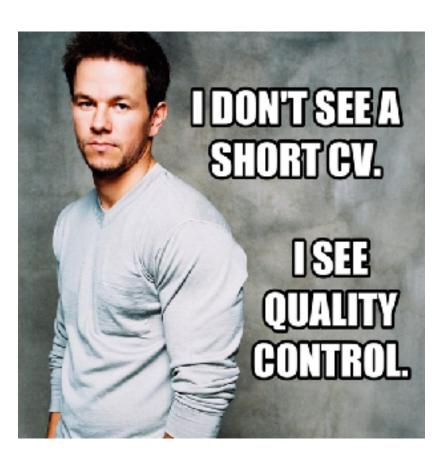
True or False: If we change the cost function, $J(\mathbf{W})$, we only need to update the final layer calculation of the back propagation steps. The remainder of the algorithm is unchanged. $\frac{\partial J(\mathbf{W})}{\partial z(\mathbf{x})} = -2(\mathbf{y}^{(k)} - \mathbf{a}^{(3)}) * \mathbf{a}^{(3)} * (1 - \mathbf{a}^{(3)})$

- A. True
- B. False

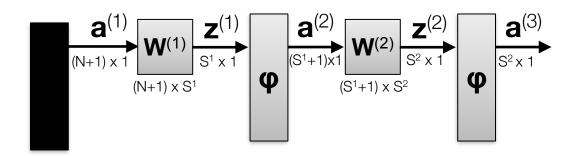
$$\frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l)}} = \operatorname{diag}[\mathbf{a}^{(l+1)} * (1 - \mathbf{a}^{(l+1)})] \cdot \mathbf{W}^{(l+1)} \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l+1)}}$$

$$\mathbf{W}^{(l)} \leftarrow \mathbf{W}^{(l)} - \eta \frac{\partial J(\mathbf{W}^{(l)})}{\partial \mathbf{z}^{(l)}} \cdot \mathbf{a}^{(l)}$$

Programming Multi-layer Neural Networks

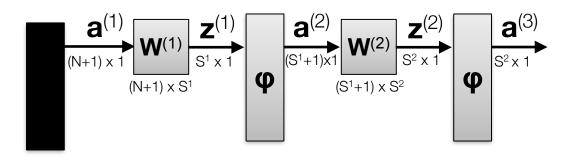






1. Forward propagate to get **z**, **a** for all layers

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



1. Forward propagate to get **z**, **a** for all layers

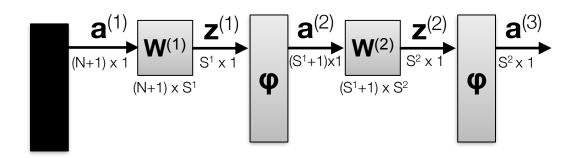
for each **y**^(k)

2. Get final layer gradient
3. Update back propagation variables
$$\frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(2)}} = -2(\mathbf{y}^{(k)} - \mathbf{a}^{(3)}) * \mathbf{a}^{(3)} * (1 - \mathbf{a}^{(3)})$$

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

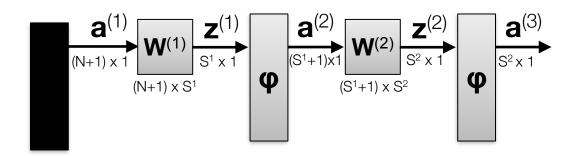
separate activations for **each** instance

```
# for each instance's activations
for (a1,a2,a3,y) in zip(A1,A2.T,A3.T,Y_enc.T):
   dJ dz2 = -2*(y - a3)*a3*(1-a3)
   dJ dz1 = dJ dz2 @ W2 @ np.diag(a2*(1-a2))
```



- 1. Forward propagate to get **z**, **a** for all layers
- 2. Get final layer gradient
- 2. Get final layer gradient 3. Update back propagation variables $\mathbf{W}^{(l)} \leftarrow \mathbf{W}^{(l)} \eta \frac{\partial J(\mathbf{W}^{(l)})}{\partial J(\mathbf{W}^{(l)})}$

```
grad1 = np.zeros(W1.shape)
grad2 = np.zeros(W2.shape)
# for each instance's activations
for (a1,a2,a3,y) in zip(A1,A2.T,A3.T,Y enc.T):
    dJ dz2 = -2*(y - a3)*a3*(1-a3)
    dJ dz1 = dJ dz2 @ W2 @ np.diag(a2*(1-a2))
    grad2 += dJ_dz2[:,np.newaxis] @ a2[np.newaxis,:]
    gradl += dJ dzl[l:,np.newaxis] @ al[np.newaxis,:] # don't incorporate bias
```



- 1. Forward propagate to get **z**, **a** for all layers
- 2. Get final layer gradient
- 2. Get final layer gradient 3. Update back propagation variables $\mathbf{W}^{(l)} \leftarrow \mathbf{W}^{(l)} \eta \frac{\partial J(\mathbf{W}^{(l)})}{\partial z^{(l)}} \cdot \mathbf{a}^{(l)}$

4. Update each **W**^(l)

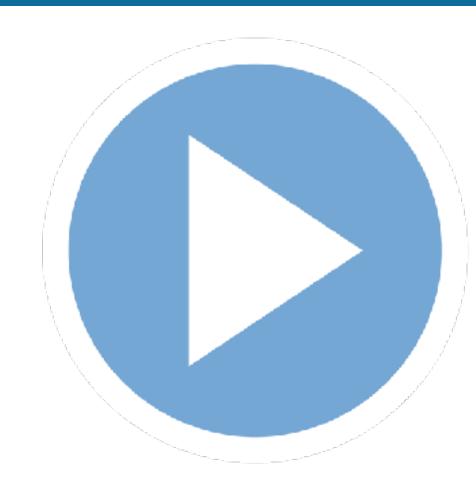
```
# feedforward all instances
A1, Z1, A2, Z2, A3 = self._feedforward(X_data,self.W1,self.W2)
# compute gradient via backpropagation
grad1, grad2 = self. get_gradient(A1=A1, A2=A2,
                                  A3=A3, Z1=Z1,
                                  Y enc=Y enc,
                                  W1=self.W1, W2=self.W2)
self.W1 -= self.eta * grad1
self.W2 -= self.eta * grad2
```

all together outting it

Demo

Two Layer Perceptron

with regularization vectorization



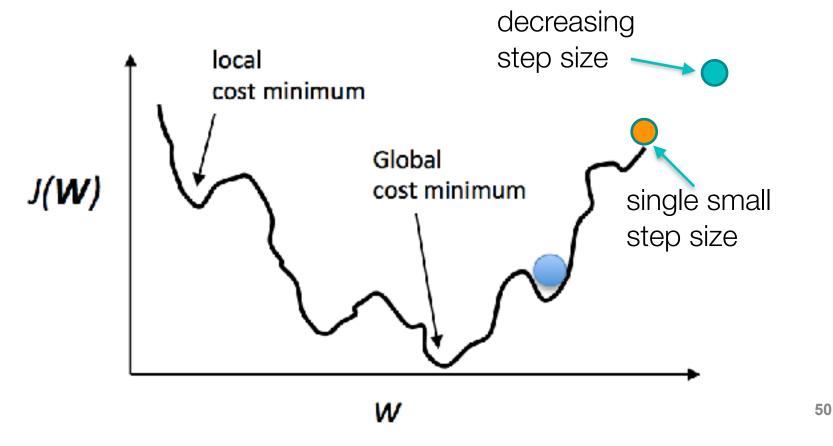
Problems with Advanced Architectures

- 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

Self Test:

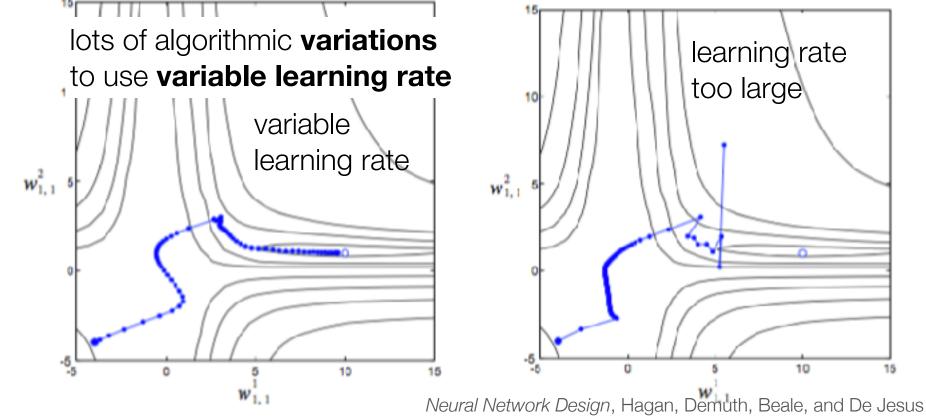
Problems with Advanced Architectures

- 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



Demo

Two Layer Perceptron

comparison:

mini-batch momentum decreased learning L-BFGS

