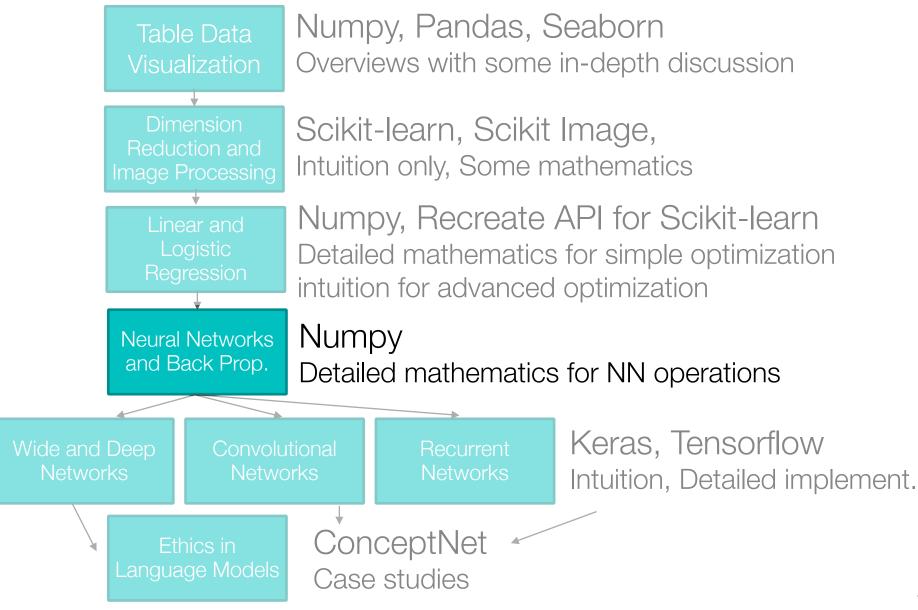
Lecture Notes for **Machine Learning in Python**

Professor Eric Larson Adaptive Neural Network Optimization

Class Logistics and Agenda

- Agenda:
 - More optimization techniques
 - Review
 - Adaptive Learning Strategies
 - Town Hall for MLP

Class Overview, by topic



Review

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

Cross entropy

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

new final layer update

Momentum

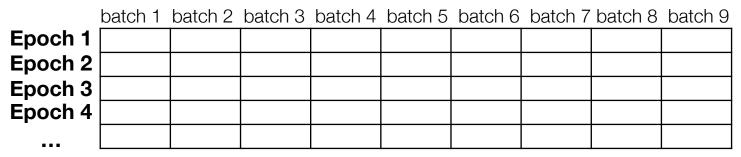
$$\rho_k = \alpha \nabla J(\mathbf{W}_k) + \beta \nabla J(\mathbf{W}_{k-1})$$

Nesterov's Accelerated Gradient

$$\rho_k = \beta \nabla J \left(\mathbf{W}_k + \alpha \nabla J(\mathbf{W}_{k-1}) \right) + \alpha \nabla J(\mathbf{W}_{k-1})$$
step twice

Mini-batching

←all data→



shuffle ordering each epoch and update W's after each batch

Learning rate adaptation (eta)

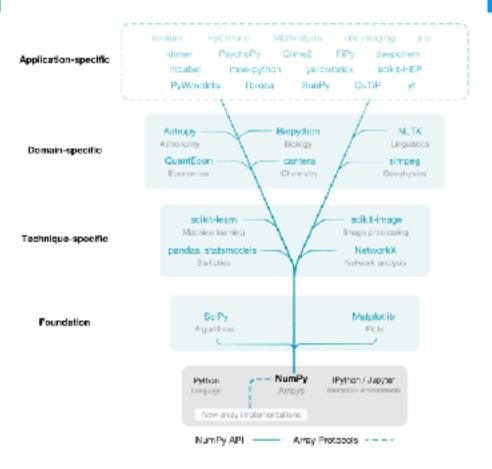
$$\eta_e = \eta_0^{(1+e\cdot\epsilon)}$$

Review: Activations Summary

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

Fig. 2: NumPy is the base of the scientific Python ecosystem.

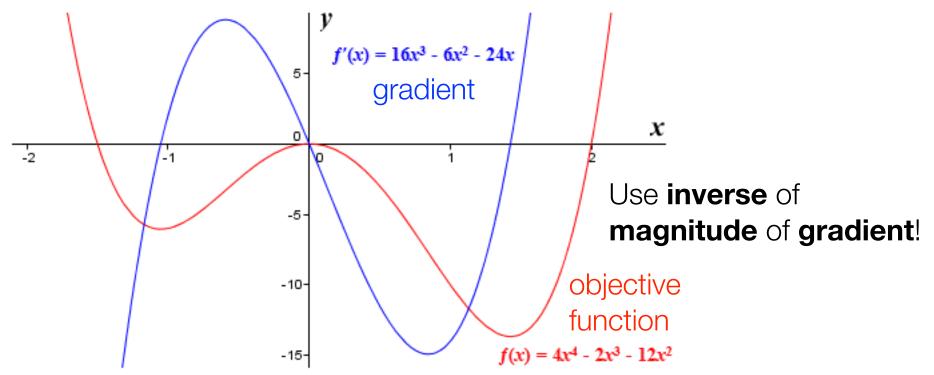
From: Array programming with NumPy



More Adaptive Optimization

Be adaptive based on Gradient Magnitude?

- Decelerate down regions that are steep
- Accelerate on plateaus



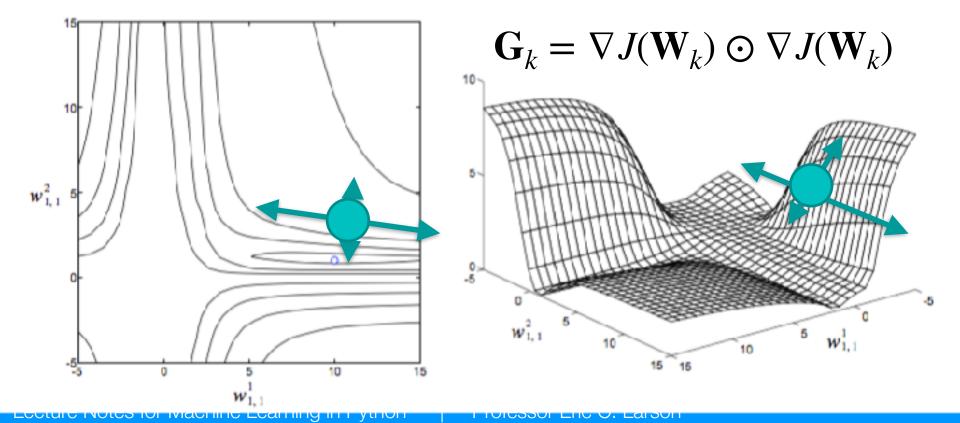
Also accumulate inverse to be robust to abrupt changes in steepness... momentum!!

http://www.technologyuk.net/mathematics/differential-calculus/higher-derivatives.shtml 77

Be adaptive based on Gradient Magnitude?

Inverse magnitude of gradient in multiple directions?

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



Common Adaptive Strategies $W_{k+1} = W_k - \eta \cdot \rho_k$

Adjust each element of gradient by the steepness

$$\text{AdaGrad} \\ \rho_k = \frac{1}{\sqrt{\mathbf{G}_k + \epsilon}} \odot \nabla J(\mathbf{W}_k) \quad \mathbf{G}_k = \mathbf{G}_{k-1} + \nabla J(\mathbf{W}_k) \odot \nabla J(\mathbf{W}_k)$$
 all operations are per element

RMSProp

$$\rho_k = \frac{1}{\sqrt{V_k + \epsilon}} \odot \nabla J(\mathbf{W}_k) \qquad \mathbf{G}_k = \nabla J(\mathbf{W}_k) \odot \nabla J(\mathbf{W}_k) \\ \mathbf{V}_k = \gamma \cdot \mathbf{V}_{k-1} + (1 - \gamma) \cdot \mathbf{G}_k$$
 all operations are per element

AdaDelta

$$\rho_k = \frac{\mathbf{M}_k}{\sqrt{\mathbf{V}_k + \epsilon}}$$

$$\mathbf{M}_{k+1} = \gamma \cdot \mathbf{M}_k + (1-\gamma) \cdot \nabla J(\mathbf{W}_k)$$

all operations are per element

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

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

For each epoch:

Diederik P. Kingma* University of Amsterdam, OpenAI

Jimmy Lei Ba" University of Toronto

update epoch
$$k \leftarrow k+1$$

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
$$V_k \leftarrow \beta_2 \cdot V_{k-1} + (1-\beta_2) \cdot \nabla J(W_k) \odot \nabla J(W_k)$$

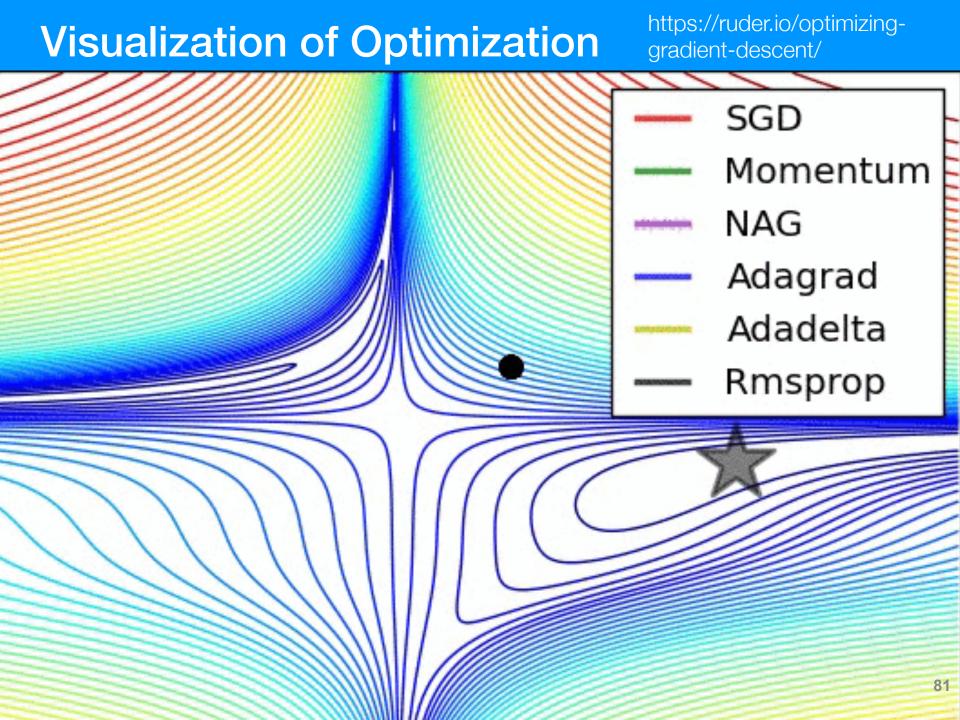
boost moments magnitudes (notice k in exponent)

$$\hat{\mathbf{M}}_k \leftarrow \frac{\mathbf{M}_k}{(1 - [\beta_1]^k)} \qquad \hat{\mathbf{V}}_k \leftarrow \frac{\mathbf{V}_k}{(1 - [\beta_2]^k)}$$

$$\hat{\mathbf{V}}_k \leftarrow \frac{\mathbf{V}_k}{(1 - [\beta_2]^k)}$$

update gradient, normalized by second moment similar to AdaDelta

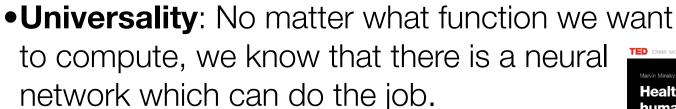
$$\mathbf{W}_k \leftarrow \mathbf{W}_{k-1} - \eta \cdot \frac{\hat{\mathbf{M}}_k}{\sqrt{\hat{\mathbf{V}}_k + \epsilon}}$$



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..."





- 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

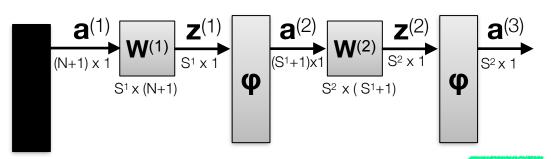
End of Session

- Next Time: Final Flipped Module!
- Then: Deep Learning in Keras

Town Hall



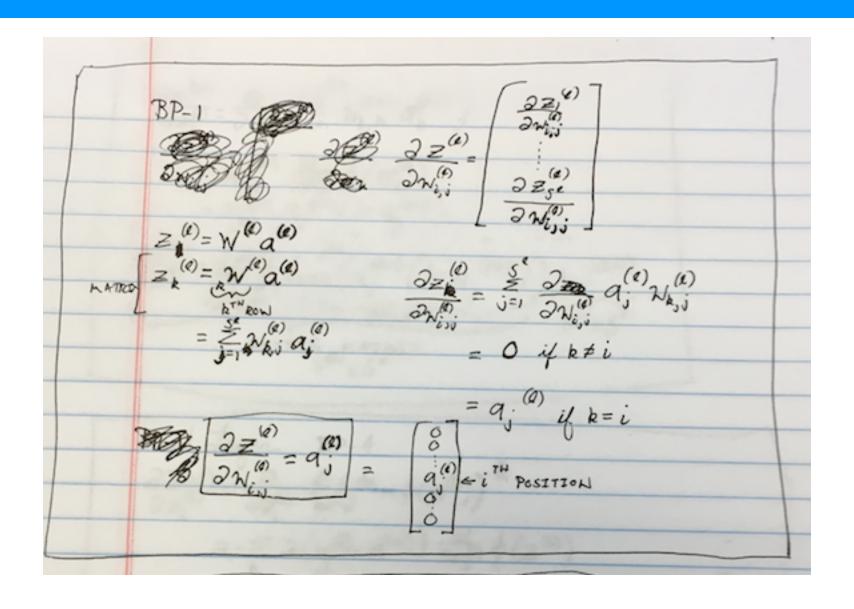
Back Up Slides



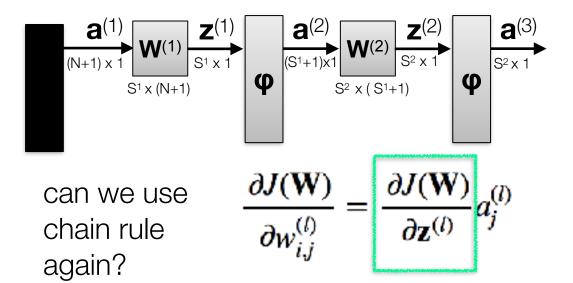
use chain rule:
$$\frac{\partial J(\mathbf{W})}{\partial w_{i,j}^{(l)}} = \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(l)}} \frac{\partial \mathbf{z}^{(l)}}{\partial w_{i,j}^{(l)}}$$

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

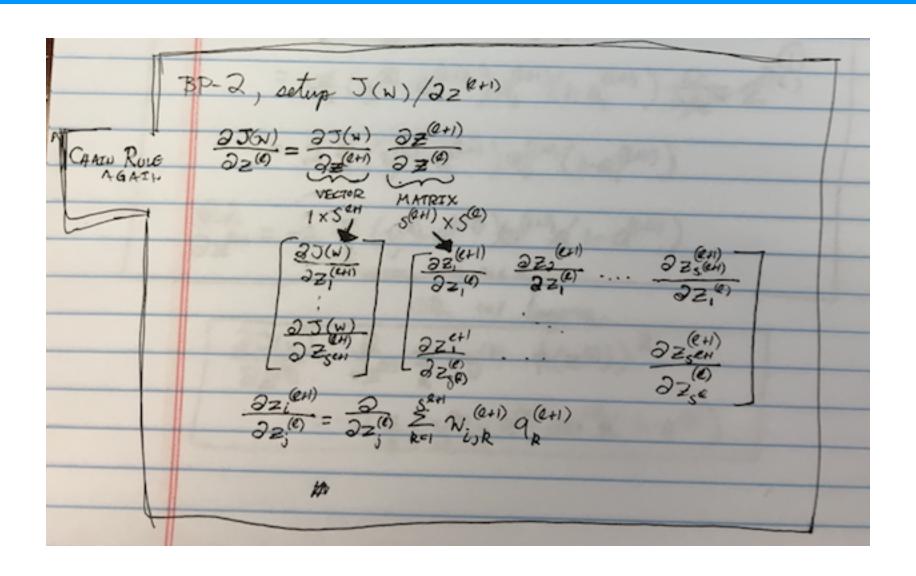
$$w_{i,j}^{(l)} \leftarrow w_{i,j}^{(l)} - \eta \frac{\partial J(\mathbf{W})}{\partial w_{i,j}^{(l)}}$$

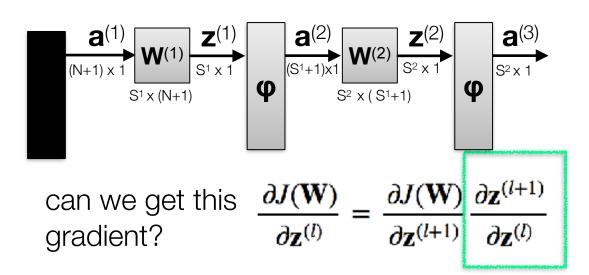


$$J(\mathbf{W}) = \sum_{k}^{M} (\mathbf{y}^{(k)} - \mathbf{a}^{(L)})^2$$



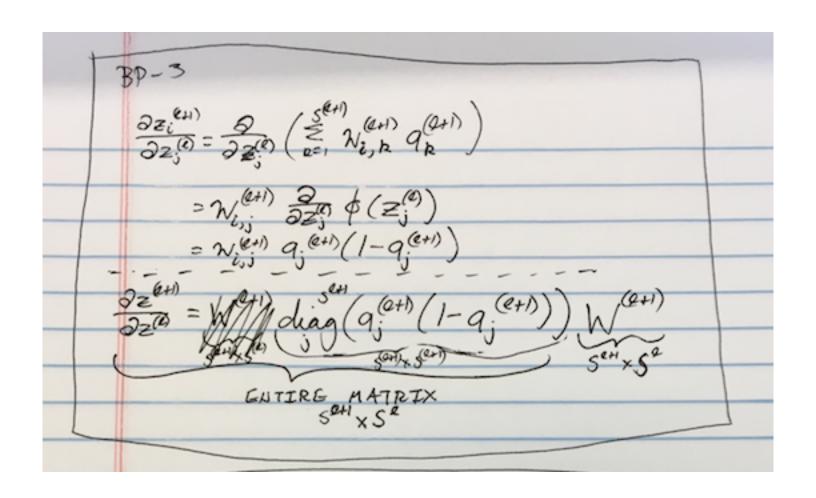
- Steps:
 - propagate weights forward
 - calculate gradient at final layer
 - back propagate gradient for each layer
 - via recurrence relation

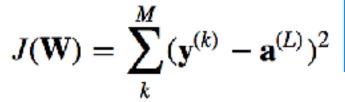


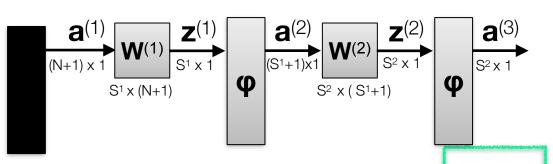


$$J(\mathbf{W}) = \sum_{k}^{M} (\mathbf{y}^{(k)} - \mathbf{a}^{(L)})^2$$

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







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

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

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

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

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

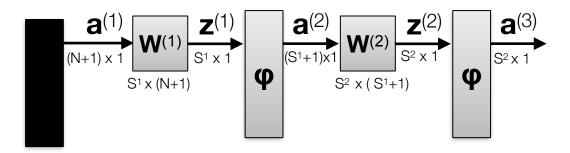
$$\frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(2)}} = \frac{\partial}{\partial \mathbf{z}^{(2)}} (\mathbf{y}^{(k)} - \phi(\mathbf{z}^{(2)}))^2$$

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

Final Layer BP-4

$$2J(w) = \frac{2}{2} \stackrel{\mathcal{E}}{\underset{k=1}{(k)}} (y^{(k)} - \phi(z^{(k)}))^{\frac{2}{3}}$$
 $= -\frac{2}{2} (y^{(k)} - a^{(k+1)}) \frac{2}{2} (y^{(k)} - a^{(k+1)}) \frac{2}{2} (y^{(k)} - a^{(k+1)})^{\frac{2}{3}} \frac{2}{2} (y^{(k)} - a^{(k)})^{\frac{2}{3}} \frac{2}{2} (y^{(k$

Back propagation summary



Self Test:

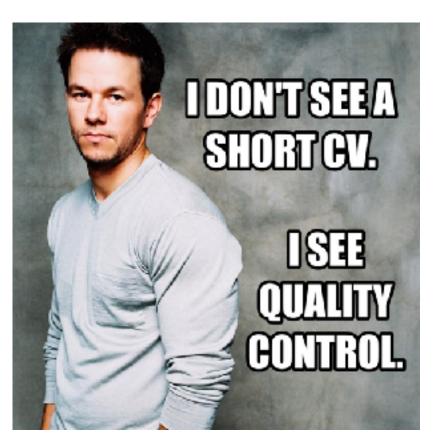
True or False: If we change the cost function, J(W), we only need to update the final layer calculation of the back propagation steps. The remainder of the algorithm is unchanged.

- A. True
- B. False

$$\mathbf{V}^{(2)} = -2(\mathbf{Y} - \mathbf{A}^{(3)}) * \mathbf{A}^{(3)} * (1 - \mathbf{A}^{(3)})$$
$$\nabla^{(2)} = \mathbf{V}^{(2)} \cdot [\mathbf{A}^{(2)}]^{T}$$

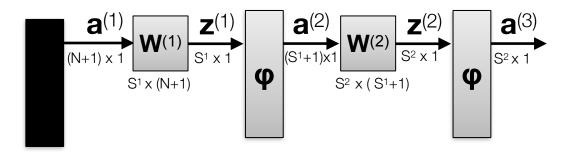
Programming Multi-layer Neural Networks

07. MLP Neural Networks.ipynb





Recall from the in-class asisgnment



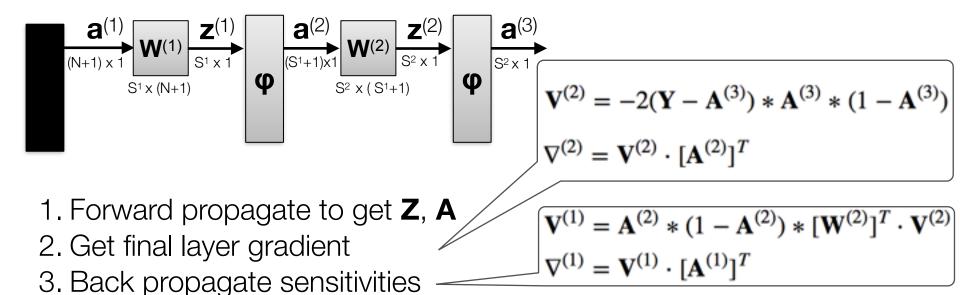
1. Forward propagate to get **Z**, **A**

```
# 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

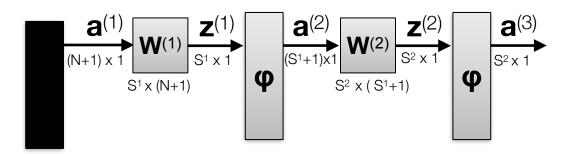


```
def _get_gradient(self, A1, A2, A3, Z1, Z2, Y_enc, W1, W2):
    """ Compute gradient step using backpropagation.
    """

# 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



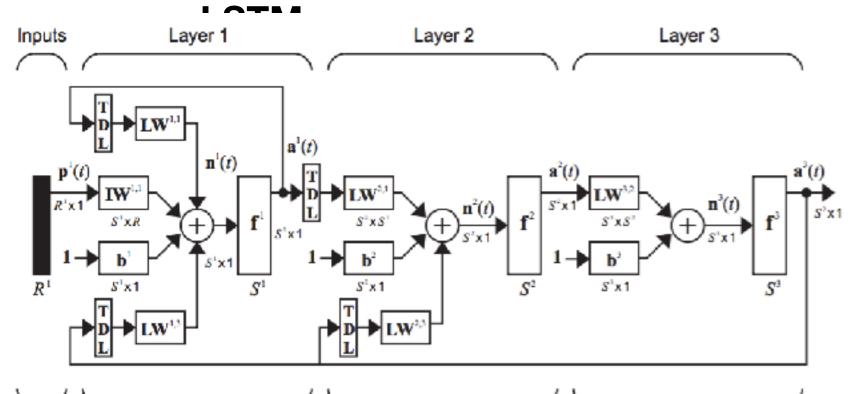
- 1. Forward propagate to get **Z**, **A** for all layers
- 2. Get final layer gradient
- 3. Back propagate sensitivities
- 4. Update each **W**⁽¹⁾

for each layer:

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

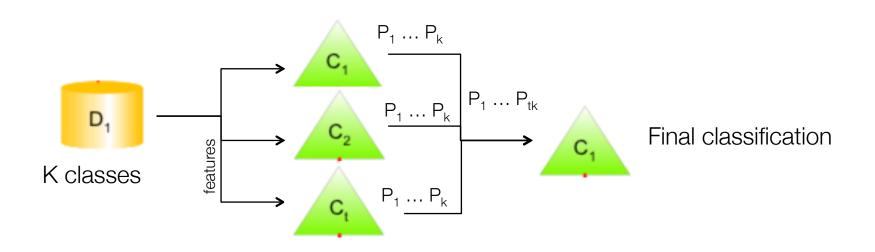
More Advanced Architectures

- 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



Stacking and Cascading ensembles

- Train an initial classifier (or ensemble)
- Use the output probabilities of each class (from each classifier, if ensemble), as features for another classifier
- Train final classifier on inferences from previous classes



Self test

- How many features (attributes) does scikit-learn use in each iteration of bagging for a random forest?
- Which best completes this statement: In scikit, the number of features considered changes
 - a: once for each tree in the forest
 - b: once for each split in each tree

each iteration!!!

max_features=sqrt(n_features)

- Linear SVMs
 - Architecture identical to logistic regression, except:
 - maximize margin
 - constrained optimization
 - Self Test: What are the trained parameters for the linear SVM?
 - A: Coefficients of w
 - B: Intercept
 - C: Slack Variables
 - D: Support Vector locations

$$\min_{w,b,\zeta} \frac{1}{2} w^T w + C \sum_{i=1}^n \zeta_i$$

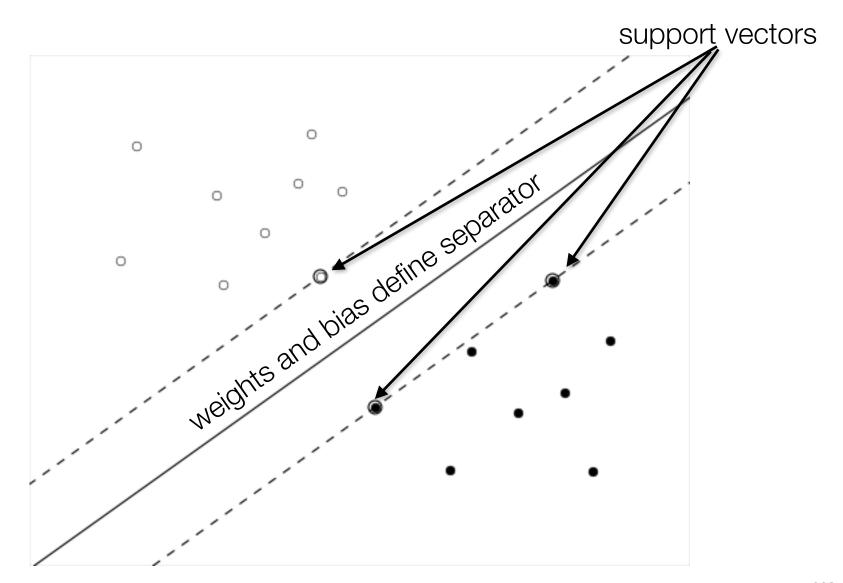
to
$$y_i(w^T \phi(x_i) + b) \ge 1 - \zeta_i$$
,
 $\zeta_i \ge 0, i = 1, ..., n$

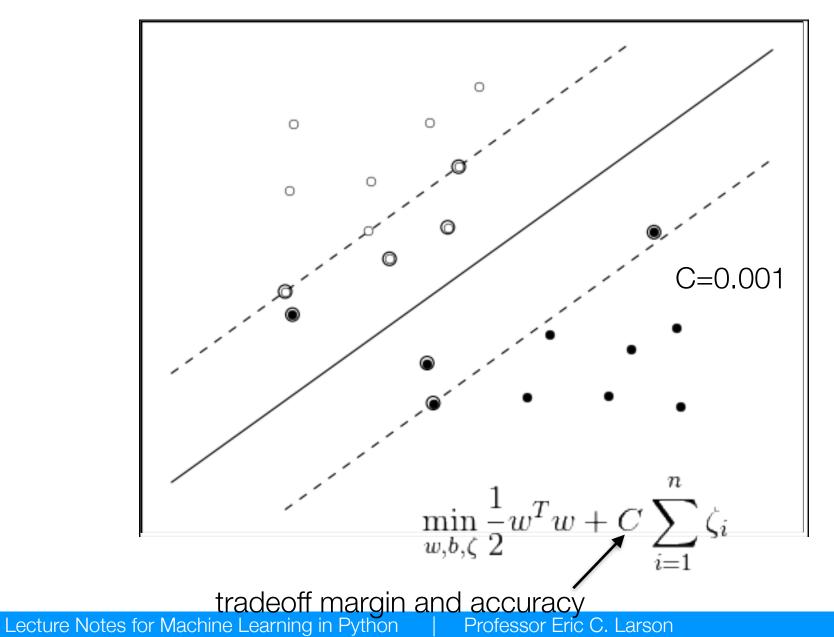
- Linear SVMs
 - Architecture near identical to logistic regression, except:
 - maximize margin
 - constrained optimization

$$\min_{w,b,\zeta} \frac{1}{2} w^T w + C \sum_{i=1}^n \zeta_i$$

to
$$y_i(w^T \phi(x_i) + b) \ge 1 - \zeta_i$$
,
 $\zeta_i \ge 0, i = 1, ..., n$

- Trained Parameters:
 - intercept and weights for each class
 - support vectors chosen for margin calculation
 - slack variables only needed during training





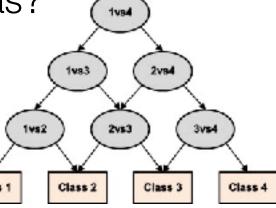
SVMs Summary: non-linear

- Non-linear SVMs
 - Architecture not like logistic regression
 - kernels == high dimensional dot-product
 - impossible to store weights
 - use kernel trick so no need to store them!
 - Trained Parameters
 - biases? how many?

selected support vectors? alphas?

slack variables?

parameters specific to kernels?



SVMs Summary: non-linear

- Popular Kernels
 - polynomial

gamma coef0 degree
$$(\gamma\langle x,x'\rangle+r)^d$$

gamma

radial basis function

$$\exp(-\gamma |x - x'|^2)$$

sigmoid

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

SVM parameterization

Demo

svm_gui.py

