Lecture Notes for **Machine Learning in Python**



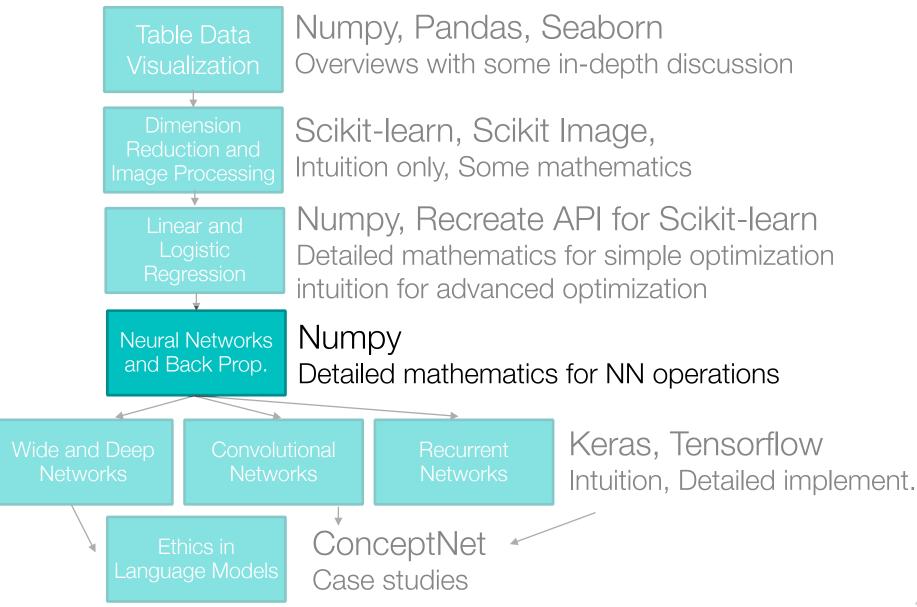
Professor Eric Larson

Neural Network Optimization and Activation

Class Logistics and Agenda

- Agenda:
 - More optimization techniques and programming examples
 - Momentum
 - Initialization
 - More activations: Tanh, ReLU, SiLU
 - Adaptive learning: AdaGrad, AdaM, etc.

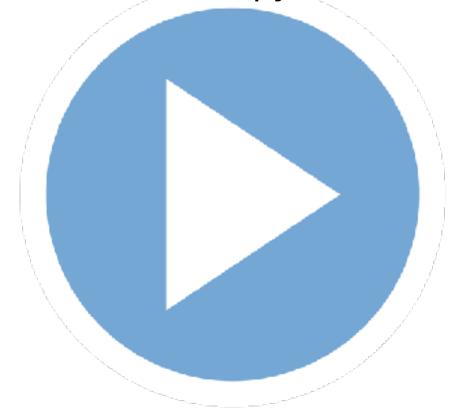
Class Overview, by topic



Demo

08a. Practical_NeuralNetsWithBias.ipynb

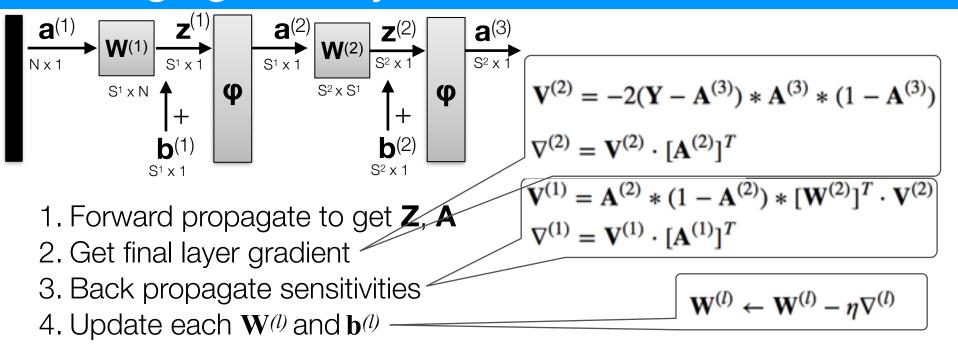
Quick Review: Momentum Cooling





Objective Function

Changing the Objective Function

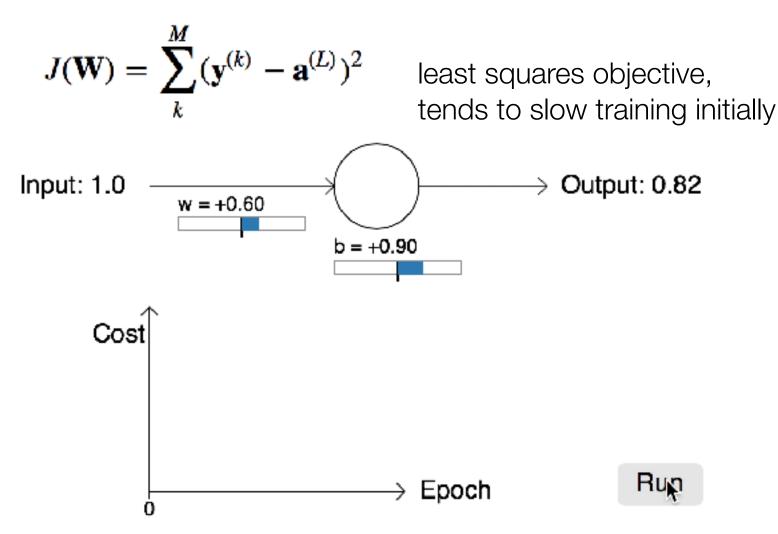


• Self Test:

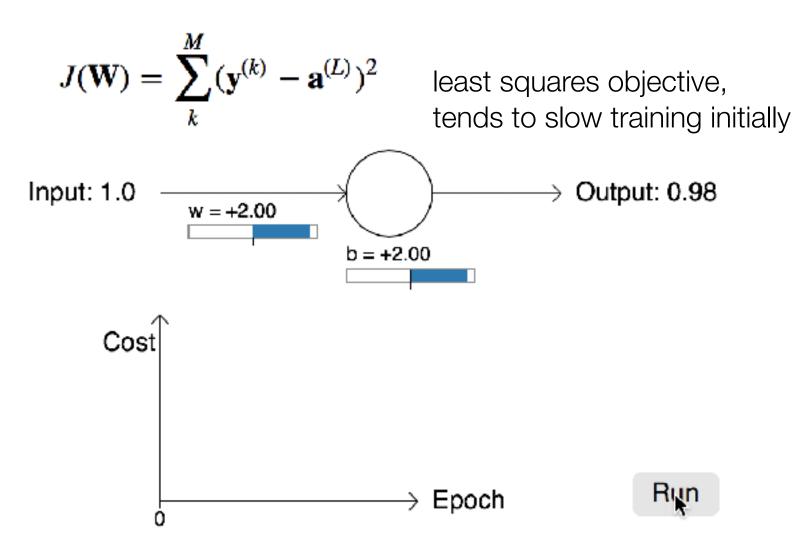
True or False: If we change the cost function, $J(\mathbf{W})$, we only need to update the final layer sensitivity calculation, $\mathbf{V}^{(2)}$, of the back propagation steps. The remainder of the algorithm is unchanged.

- A. True
- B. False

Mean squared error:



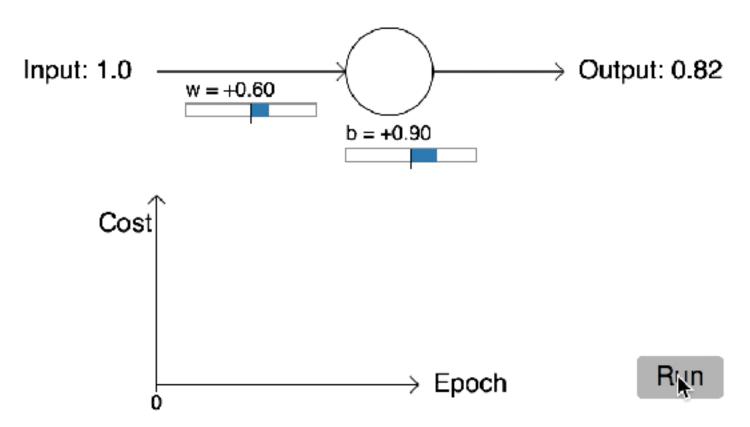
Mean squared error:



Negative of MLE: **Binary Cross entropy**

$$J(\mathbf{W}) = -\left[\mathbf{y}^{(i)}\ln([\mathbf{a}^{(L+1)}]^{(i)}) + (1 - \mathbf{y}^{(i)})\ln(1 - [\mathbf{a}^{(L+1)}]^{(i)})\right] \quad \text{speeds up}$$
initial training

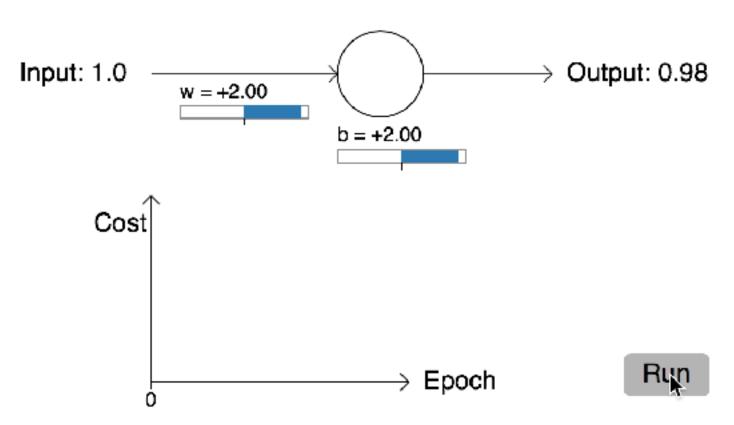
initial training



Neural Networks and Deep Learning, Michael Nielson, 2015

Negative of MLE: Binary Cross entropy

$$J(\mathbf{W}) = -\left[\mathbf{y}^{(i)} \ln([\mathbf{a}^{(L+1)}]^{(i)}) + (1 - \mathbf{y}^{(i)}) \ln(1 - [\mathbf{a}^{(L+1)}]^{(i)})\right] \quad \text{speeds up}$$
initial training



Neural Networks and Deep Learning, Michael Nielson, 2015

$$J(\mathbf{W}) = -\left[\mathbf{y}^{(i)} \ln([\mathbf{a}^{(L+1)}]^{(i)}) + (1 - \mathbf{y}^{(i)}) \ln(1 - [\mathbf{a}^{(L+1)}]^{(i)})\right] \quad \text{likely to speed up initial training}$$

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

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

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

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

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

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

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

Back to our old friend: Cross entropy

$$J(\mathbf{W}) = -\left[\mathbf{y}^{(i)} \ln([\mathbf{a}^{(L+1)}]^{(i)}) + (1 - \mathbf{y}^{(i)}) \ln(1 - [\mathbf{a}^{(L+1)}]^{(i)})\right] \quad \text{likely to speed up initial training}$$

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

$$\begin{bmatrix} \frac{\partial J(\mathbf{W})}{\partial \mathbf{z}^{(2)}} \end{bmatrix}^{(i)} = [\mathbf{a}^{(3)}]^{(i)} - \mathbf{y}^{(i)}$$
two layer network
$$\mathbf{V}^{(2)} = \mathbf{A}^{(3)} - \mathbf{Y}$$
new update

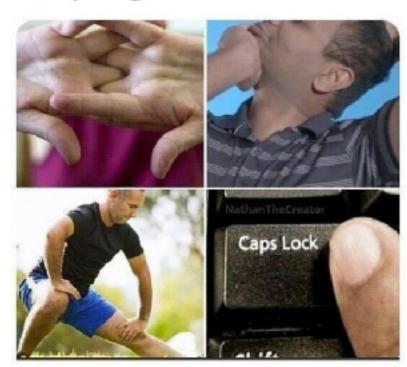
vectorized backpropagation
V2 = (A3-Y_enc) # <- this is only line t
V1 = A2*(1-A2)*(W2.T @ V2)</pre>

bp-5

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

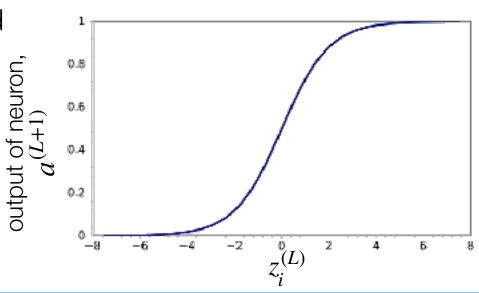
Practical Initialization of Architectures

SQL programmers be like



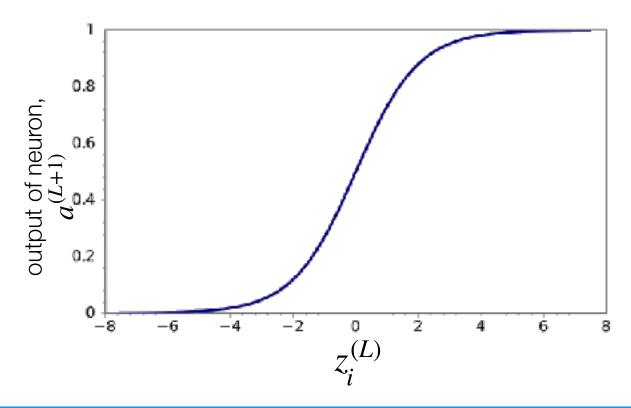
Formative Self Test

- for adding Gaussian random variables, variances add together $\mathbf{a}^{(L+1)} = \varphi(\mathbf{W}^{(L)}\mathbf{a}^{(L)}) \text{ assume each element of } \mathbf{a} \text{ is Gaussian}$
- If you initialized the weights, \mathbf{W} , with too large variance, you would expect the output of the neuron, $\mathbf{a}^{(L+1)}$, to be:
 - A. saturated to "1"
 - B. saturated to "0"
 - C. could either be saturated to "0" or "1"
 - D. would not be saturated



Formative Self Test

- for adding Gaussian distributions, variances add together $\mathbf{a}^{(L+1)} = \varphi(\mathbf{W}^{(L)}\mathbf{a}^{(L)}) \text{ assume each element of } \mathbf{a} \text{ is Gaussian}$
- What is the derivative of a saturated sigmoid neuron?
 - A. zero
 - B. one
 - C. $a \times (1 a)$
 - D. it depends



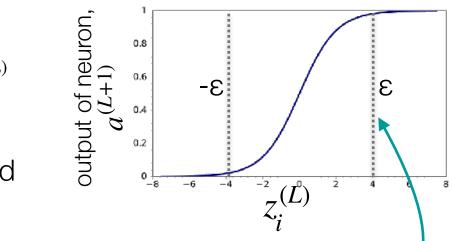
Weight initialization: try not to saturate your neurons right away!

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

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

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

each row is summed before sigmoid



want each $-\epsilon < z_i^{(L)} < \epsilon$ for no saturation, where $\epsilon = 4$ then $\sigma(z_i^{(L)}) = a_i^{(L+1)}$ is well distributed [0,1]

solution: squash initial weight magnitudes, w_{ij}

draw each $w_{ij} \sim \mathcal{N}(0,\alpha)$ from a Gaussian with **zero mean** and **specific** standard deviation such that all a variables have unit variance, $\text{Var}[a_i^{(L)}] = 1$

Glorot Weight Initialization

Understanding the difficulty of training deep feedforward neural networks

JMLR 2010 Xavier Glorot Yoshua Bengio DIRO, Université de Montréal, Montréal, Québec, Canada

Goal: We should not saturate feedforward or back propagated variance Calculate variance of each layer such that $Var[a_i^{(L+1)}] = 1$

$$|z_i^{(L)}| = \sum_{i=1}^{n^{(L)}} w_{ij} a_j^{(L)}$$
 break down feed forward by multiply in i^{th} row

$$\text{Var}[z_{i}^{(L)}] = \sum_{j}^{n^{(L)}} E[w_{ij}]^{2} \text{Var}[a_{j}^{(L)}] + \text{Var}[w_{ij}] E[a_{j}^{(L)}]^{2} + \text{Var}[w_{ij}] \text{Var}[a_{j}^{(L)}] = \sum_{j}^{n^{(L)}} \text{Var}[w_{ij}] \text{Var}[a_{j}^{(L)}]$$

$$0, \text{ if uncorrelated}$$

$$\operatorname{Var}[z_i^{(L)}] = n^{(L)} \operatorname{Var}[w_{ij}] \operatorname{Var}[a_j^{(L)}] = n^{(L)} \operatorname{Var}[w_{ij}]$$

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

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

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

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

Glorot Weight Initialization

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

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

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

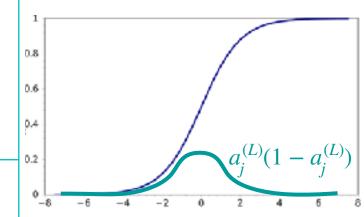
want to keep variance of v stable magnitude → stable gradient

Similar calculation for back prop.

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

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

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



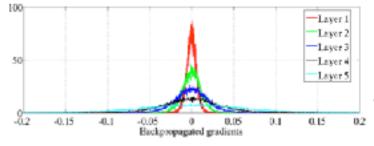
$$w_{ij}^{(L)} \sim \mathcal{N}\left(0, 4 \cdot \sqrt{\frac{2}{n^{(L)} + n^{(L+1)}}}\right)$$
 compromise

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

Glorot Weight Initialization

Understanding the difficulty of training deep feedforward neural networks

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



Starting gradient histograms per layer standard initialization

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

Demo

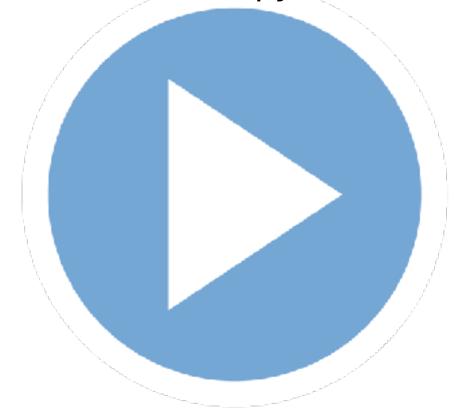
08a. Practical_NeuralNetsWithBias.ipynb

Momentum

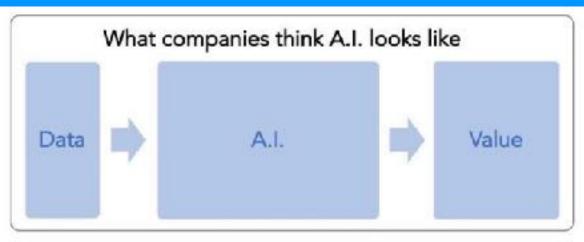
Cooling

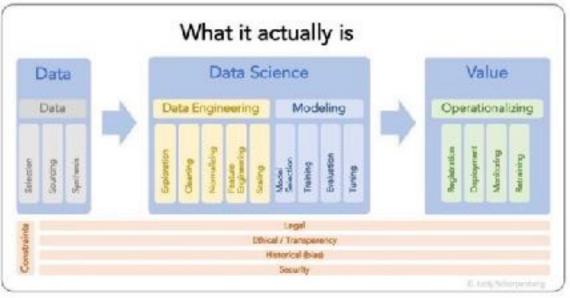
Cross Entropy

Smarter Weight Initialization



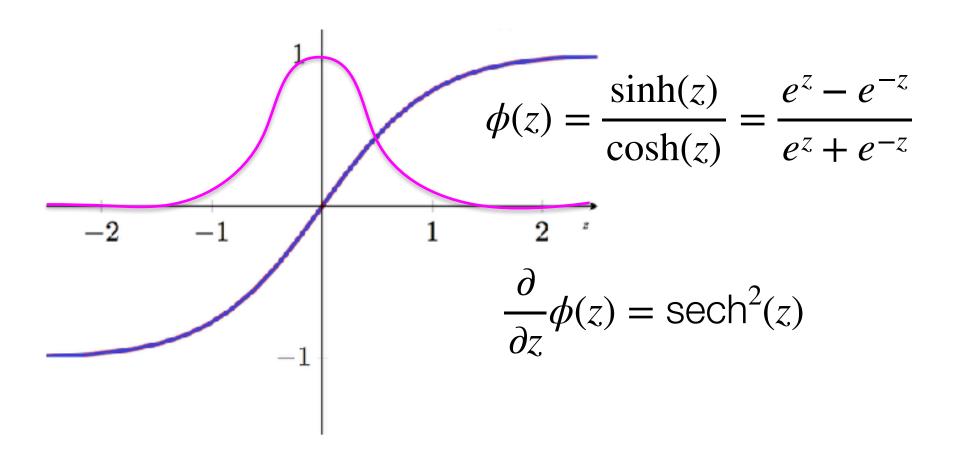
Beyond Sigmoid: Other Activations





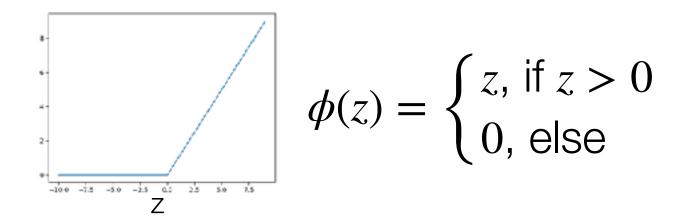
New Activation: Hyperbolic Tangent

Basically a sigmoid from -1 to 1



New Activation: ReLU

A new nonlinearity: rectified linear units



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

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

Other Activation Functions

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

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

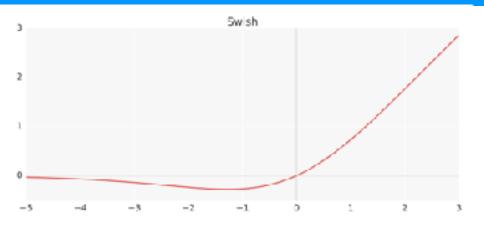


Figure 1: The Swish activation function.

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

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

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

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

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

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

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

Glorot and He Initialization

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

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

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

Summarized by Glorot and He

Activations Summary

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

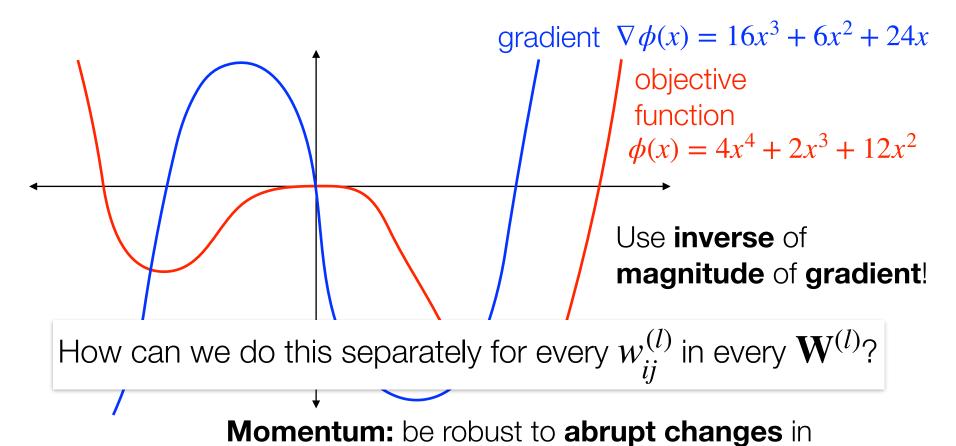


More Adaptive Optimization

Going beyond changing the learning rate

Be adaptive based on Gradient Magnitude?

- Decelerate down regions that are steep
- Accelerate on plateaus



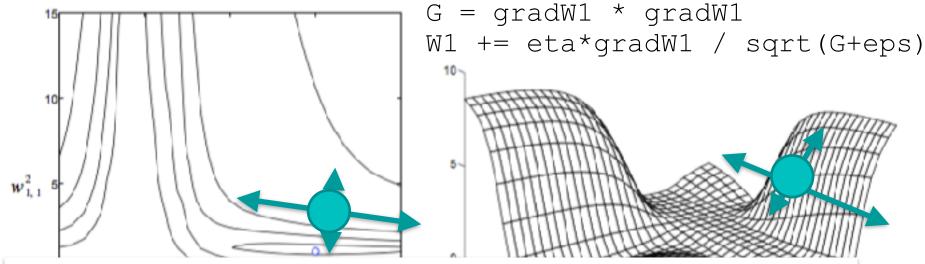
http://www.technologyuk.net/mathematics/differential-calculus/higher-derivatives.shtml 70

steepness (accumulate inverse magnitudes)

Be adaptive based on Gradient Magnitude?

Inverse magnitude of gradient in multiple directions?

$$\mathbf{W}_{k+1} \leftarrow \mathbf{W}_k + \eta \frac{1}{\sqrt{\mathbf{G}_k + \epsilon}} \odot \nabla J(\mathbf{W}_k) \qquad \mathbf{G}_k = \nabla J(\mathbf{W}_k) \odot \nabla J(\mathbf{W}_k)$$
 same size as \mathbf{W} new matrix for normalizing
$$\mathbf{G} = \operatorname{gradW1} * \operatorname{gradW1}$$



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

Note: G exists for every layer, but we will abuse layer notation

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

Adjust each element of gradient by the steepness

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

$$\begin{array}{c|c} & \text{update iteration} & k \leftarrow k+1 \\ & \text{get gradient} & \nabla J(\mathbf{W}_k) \end{array} \quad \text{for large } k, \ \hat{\mathbf{M}} \approx \mathbf{M}, \ \hat{\mathbf{V}} \approx \mathbf{V} \\ & \text{accumulated gradient} & \mathbf{M}_k \leftarrow \beta_1 \cdot \mathbf{M}_{k-1} + (1-\beta_1) \cdot \nabla J(\mathbf{W}_k) \\ & \text{accumulated squared gradient} & \mathbf{V}_k \leftarrow \beta_2 \cdot \mathbf{V}_{k-1} + (1-\beta_2) \cdot \nabla J(\mathbf{W}_k) \odot \nabla J(\mathbf{W}_k) \\ \end{array}$$

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

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

gradient with momentum

squared magnitude normalizer

Visualization of Optimization

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

Takeaways:

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

SGD

Momentum

--- NAG

Adagrad

Adadelta

Rmsprop

Demo

08a. Practical_NeuralNetsWithBias.ipynb

Momentum

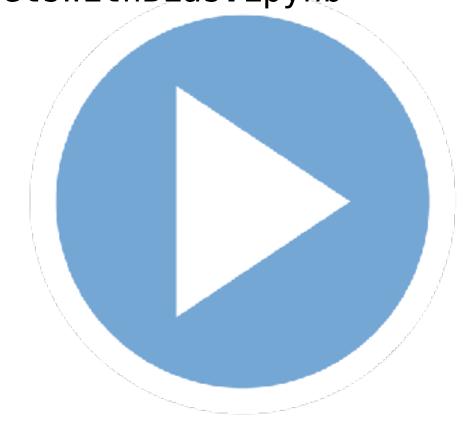
Cooling

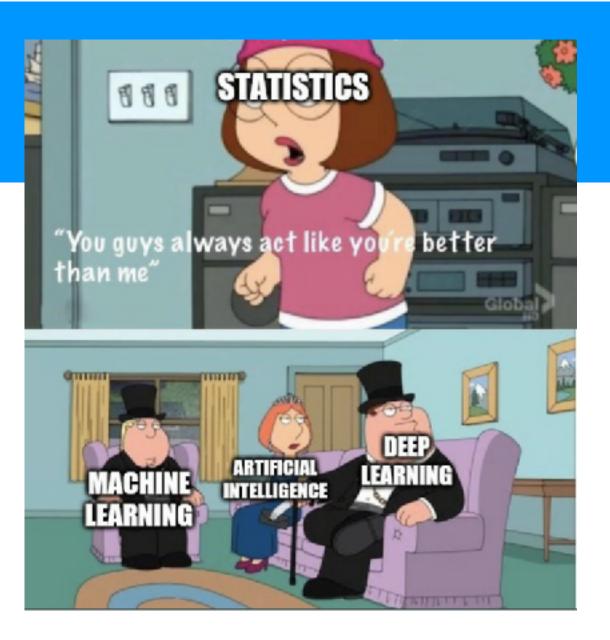
Cross Entropy

Smarter Weight Initialization

ReLU Nonlinearities

Adaptive training with AdaGrad





Review

Review

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

Cross entropy

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

new final layer update

Momentum

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

Nesterov's Accelerated Gradient

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

Mini-batching

←all data→

	batch 1	batch 2	batch 3	batch 4	batch 5	batch 6	batch 7	batch 8	batch 9
Epoch 1									
Epoch 2									
Epoch 3 Epoch 4									
Epoch 4									
•••									

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

Learning rate adaptation (eta)

$$\eta_e = \eta_0^{(1+e\cdot\epsilon)}$$
 $\eta_e = \eta_0 \cdot d^{\lfloor \frac{e}{e_d} \rfloor}$

Review: Activations Summary

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Sigmoid	$\phi(z) = \frac{1}{1 + e^{-z}}$	$\nabla \phi(z) = a(1-a)$	$w_{ij}^{(L)} \sim \pm 4\sqrt{\frac{6}{n^{(L)} + n^{(L+1)}}}$
Hyperbolic Tangent	$\phi(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$	$\nabla \phi(z) = \frac{4}{(e^z + e^{-z})^2}$	$w_{ij}^{(L)} \sim \pm \sqrt{\frac{6}{n^{(L)} + n^{(L+1)}}}$
8- 8- 9- -300 -15 -30 -23 02 22 30 25	$\phi(z) = \begin{cases} z, & \text{if } z > 0 \\ 0, & \text{else} \end{cases}$	$\nabla \phi(z) = \begin{cases} 1, & \text{if } z > 0 \\ 0, & \text{else} \end{cases}$	$w_{ij}^{(L)} \sim \pm \sqrt{2} \sqrt{\frac{6}{n^{(L)} + n^{(L+1)}}}$
SiLU	$\phi(z) = \frac{z}{1 + e^{-z}}$	$\nabla \phi(z) = \phi(z) + \sigma(z) \cdot (1 - \phi(z))$	V