DS 4400

Machine Learning and Data Mining I
Spring 2024

David Liu

Khoury College of Computer Science

Northeastern University

April 2 2024

Outline

- Training Neural Networks
  - Demo
  - Backpropagation
  - Parameter Initialization
  - Derivation for feed-forward neural network for binary classification (sigmoid activation)
- Stochastic Gradient Descent
  - Gradient descent variants
- Regularization methods for neural networks
  - Weight decay
  - Dropout

How to train Neural Networks?

- Backpropagation algorithm
- David Rumelhart, Geoffrey Hinton, Ronald Williams. "Learning representations by back-propagating errors". Nature. 323 (6088): 533–536. 1986
- Applicable to both FFNN and CNN
- Extension of Gradient Descent to multi-layer neural networks

Reminder: Logistic Regression

$$J(\theta) = -\sum_{i=1}^{N} [y_i \log h_\theta(x_i) + (1 - y_i) \log \left(1 - h_\theta(x_i)\right)]$$

- Cost of a single instance:

$$\text{loss } (h_{\boldsymbol{\theta}}(\boldsymbol{x}), y) = \begin{cases} -\log(h_{\boldsymbol{\theta}}(\boldsymbol{x})) & \text{if } y = 1 \\ -\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})) & \text{if } y = 0 \end{cases}$$

- Can re-write objective function as

$$J(\boldsymbol{\theta}) = \sum_{i=1}^{n} \text{loss } \left(h_\theta(x_i), y_i \right)$$

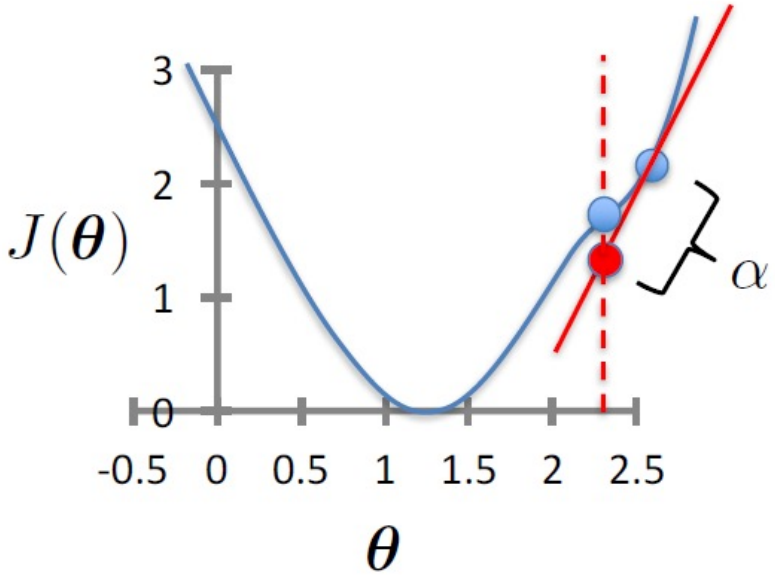
Gradient Descent

- Initialize $\boldsymbol{\theta}$ $\quad \boldsymbol{\theta} = (W, b)$
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

simultaneous update
for j = 0 ... d

learning rate (small)
e.g., α = 0.05



- Converges for convex objective
- Could get stuck in local minimum for non-convex objectives

Training Neural Networks

- Training data $x_1, y_1, \ldots x_N, y_N$
- One training example $x_i = (x_{i1}, \ldots x_{id})$, label y_i
- One forward pass through the network
  - Compute prediction $\hat{y}_i = h_\theta(x_i)$
- Loss function

Training Neural Networks

- Training data $x_1, y_1, \ldots x_N, y_N$
- Training example $x_i = (x_{i1}, \ldots x_{id})$, label y_i
- One forward pass through the network
  - Compute prediction $\hat{y}_i = h(x_i)$
- Loss function for each example
  - $L(\hat{y}, y) = -[(1 - y)\log(1 - \hat{y}) + y \log \hat{y}]$

Cross-entropy loss

- Loss function for training data
  - $J(W, b) = \frac{1}{N}\sum_i L\ (\hat{y}_i \quad , y_i)$

GD for Neural Networks

- Initialization
  - For all layers ℓ
    - Initialize $W^{[\ell]}, b^{[\ell]}$
- Backpropagation
  - Fix learning rate α
  - Repeat
    - For all layers ℓ

GD for Neural Networks

- Initialization
  - For all layers ℓ
    - Initialize $W^{[\ell]}, b^{[\ell]}$
- Backpropagation
  - Fix learning rate α
  - For all layers ℓ (starting backwards)
    - $W^{[\ell]} = W^{[\ell]} - \alpha \sum_{i=1}^{N} \frac{\partial L(\hat{y}_i, y_i)}{\partial W^{[\ell]}}$
    - $b^{[\ell]} = b^{[\ell]} - \alpha \sum_{i=1}^{N} \frac{\partial L(\hat{y}_i, y_i)}{\partial b^{[\ell]}}$

GD for Neural Networks

- Initialization
  - For all layers ℓ
    - Set $W^{[\ell]}, b^{[\ell]}$ at random
- Backpropagation
  - Fix learning rate α
  - Repeat
    - For all layers ℓ (starting backwards)

$$W^{[\ell]} = W^{[\ell]} - \alpha \sum_{i=1}^{N} \frac{\partial L(\hat{y}_i, y_i)}{\partial W^{[\ell]}}$$

$$b^{[\ell]} = b^{[\ell]} - \alpha \sum_{i=1}^{N} \frac{\partial L(\hat{y}_i, y_i)}{\partial b^{[\ell]}}$$

This is expensive!

Stochastic Gradient Descent

- Initialization
  - For all layers ℓ
    - Set $W^{[\ell]}, b^{[\ell]}$ at random
- Backpropagation
  - Fix learning rate α
  - Repeat
    - For all layers ℓ (starting backwards)
      - For all training examples x_i, y_i

$$W^{[\ell]} = W^{[\ell]} - \alpha \frac{\partial L(\hat{y}_i, y_i)}{\partial W^{[\ell]}}$$

$$b^{[\ell]} = b^{[\ell]} - \alpha \frac{\partial L(\hat{y}_i y_i)}{\partial b^{[\ell]}}$$

Incremental version of GD

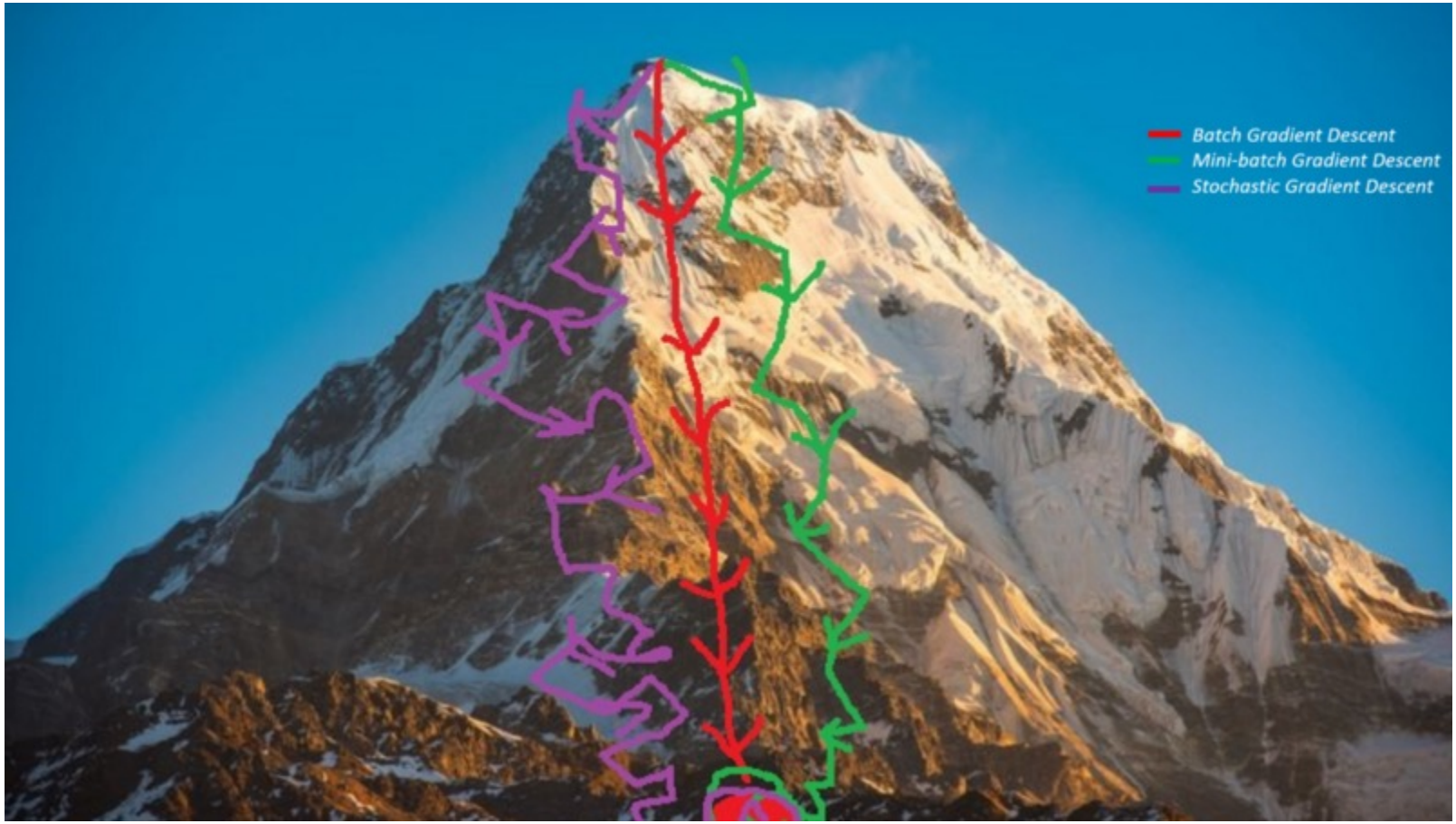
Mini-batch Gradient Descent

- Initialization
  - For all layers ℓ
    - Set $W^{[\ell]}, b^{[\ell]}$ at random
- Backpropagation
  - Fix learning rate α
  - Repeat
    - For all layers ℓ (starting backwards)
      - For all batches b of size B with training examples x_{ib}, y_{ib}

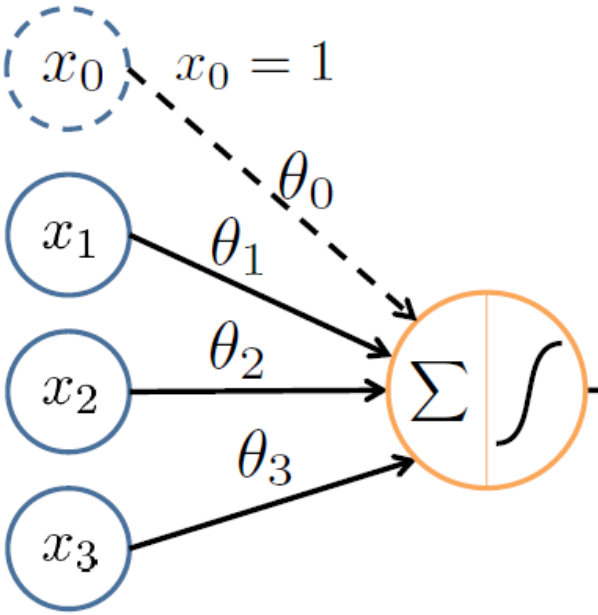
$$W^{[\ell]} = W^{[\ell]} - \alpha \sum_{i=1}^{B} \frac{\partial L(\hat{y}_{ib}, y_{ib})}{\partial W^{[\ell]}}$$

$$b^{[\ell]} = b^{[\ell]} - \alpha \sum_{i=1}^{B} \frac{\partial L(\hat{y}_{ib}, y_{ib})}{\partial b^{[\ell]}}$$

Gradient Descent Variants



Review of a Perceptron



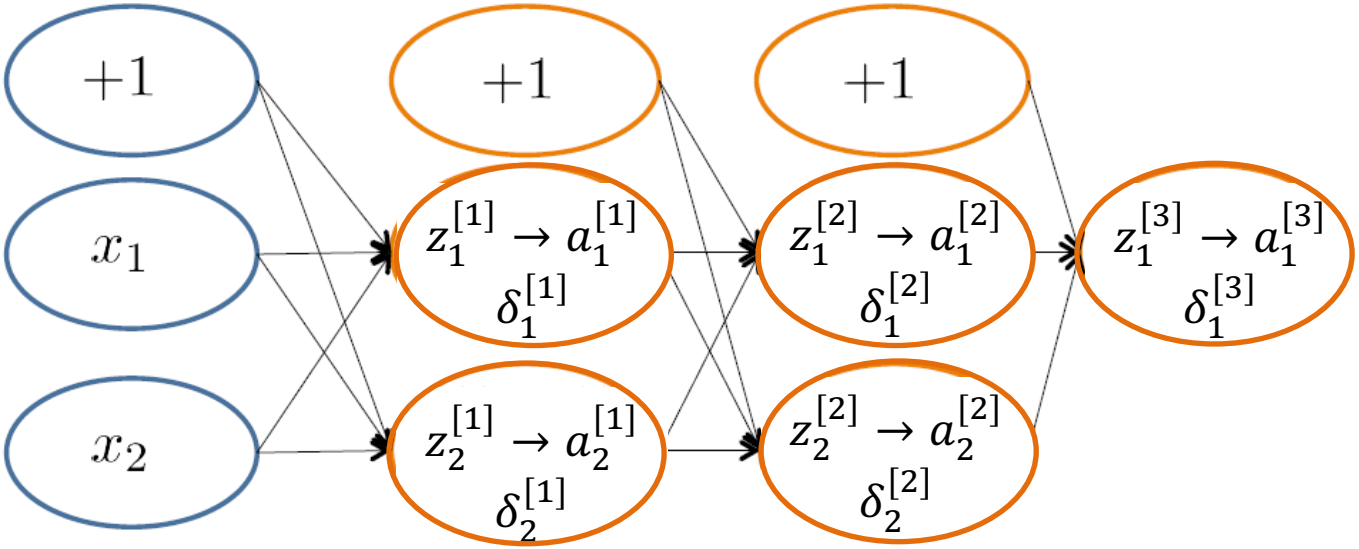
$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = g\left(\boldsymbol{\theta}^{\mathsf{T}}\mathbf{x}\right) = g(w^T x + b)$$

$$= \frac{1}{1 + e^{-\boldsymbol{\theta}^{\mathsf{T}}\mathbf{x}}}$$

Sigmoid (logistic) activation function: $g(z) = \dfrac{1}{1 + e^{-z}}$

Backpropagation Intuition

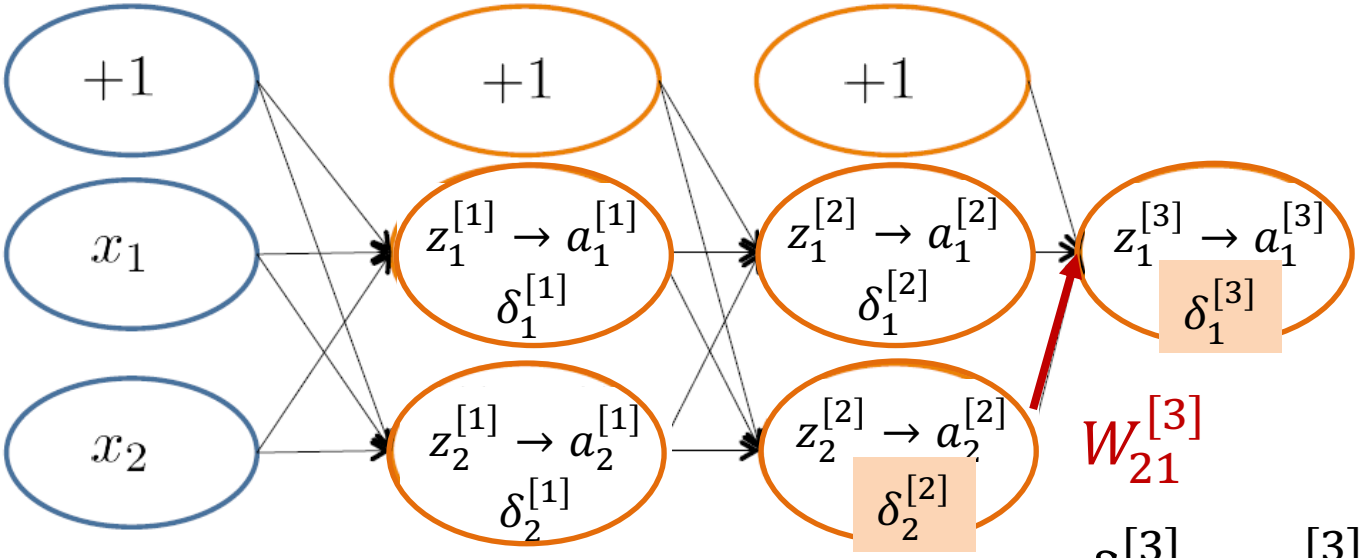


$\delta_j^{(l)}$ = "error" of node j in layer l

Formally, $\delta_j^{(l)} = \dfrac{\partial}{\partial z_j^{(l)}} \text{loss}\,(\mathbf{x}_i)$

where $\text{loss}\,(\mathbf{x}_i) = y_i \log h_\Theta(\mathbf{x}_i) + (1 - y_i) \log(1 - h_\Theta(\mathbf{x}_i))$

Backpropagation Intuition



$W_{21}^{[3]}$

$$\delta_1^{[3]} \approx a_1^{[3]} - y$$

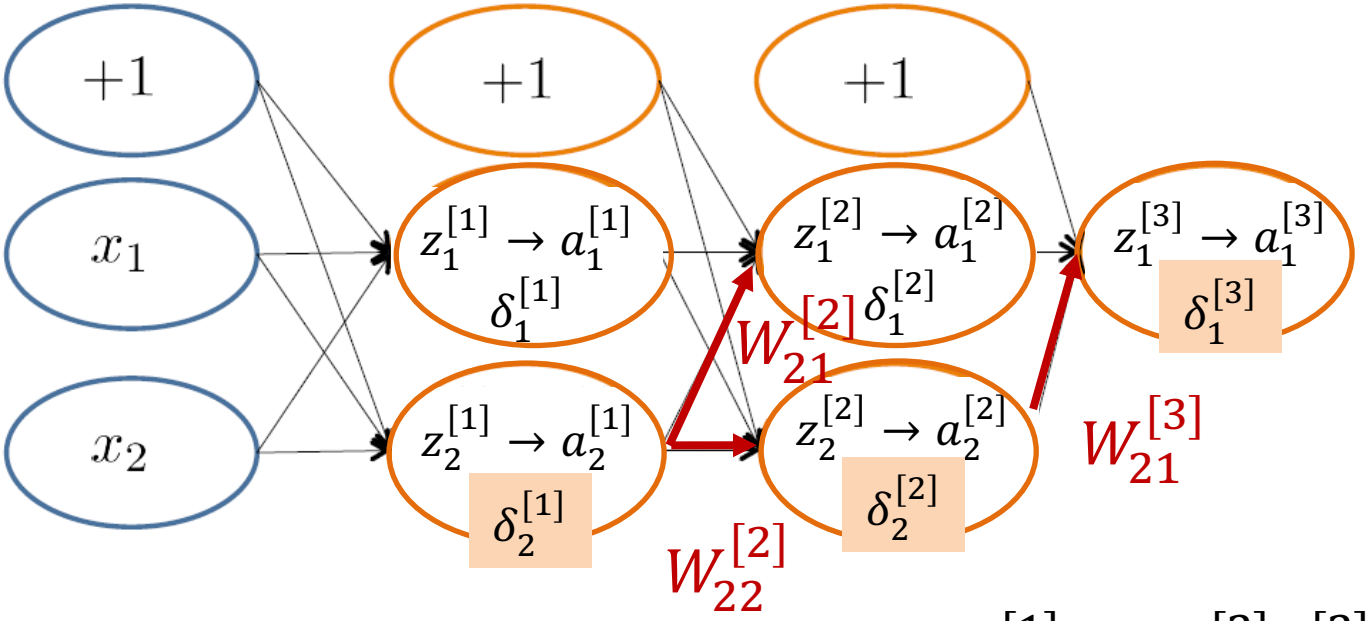
$$\delta_2^{[2]} \approx \delta_1^{[3]} \mathrm{W}_{21}^{[3]}$$

$\delta_j^{(l)}$ = "error" of node j in layer l

Formally, $\delta_j^{(l)} = \dfrac{\partial}{\partial z_j^{(l)}} \mathrm{cost}(\mathbf{x}_i)$

where $\mathrm{cost}(\mathbf{x}_i) = y_i \log h_\Theta(\mathbf{x}_i) + (1 - y_i) \log(1 - h_\Theta(\mathbf{x}_i))$

Backpropagation Intuition



$$\delta_2^{[1]} \approx W_{21}^{[2]}\delta_1^{[2]} + W_{22}^{[2]}\delta_2^{[2]}$$

$\delta_j^{(l)}$ = "error" of node j in layer l

Formally, $\delta_j^{(l)} = \dfrac{\partial}{\partial z_j^{(l)}} \text{cost}(\mathbf{x}_i)$

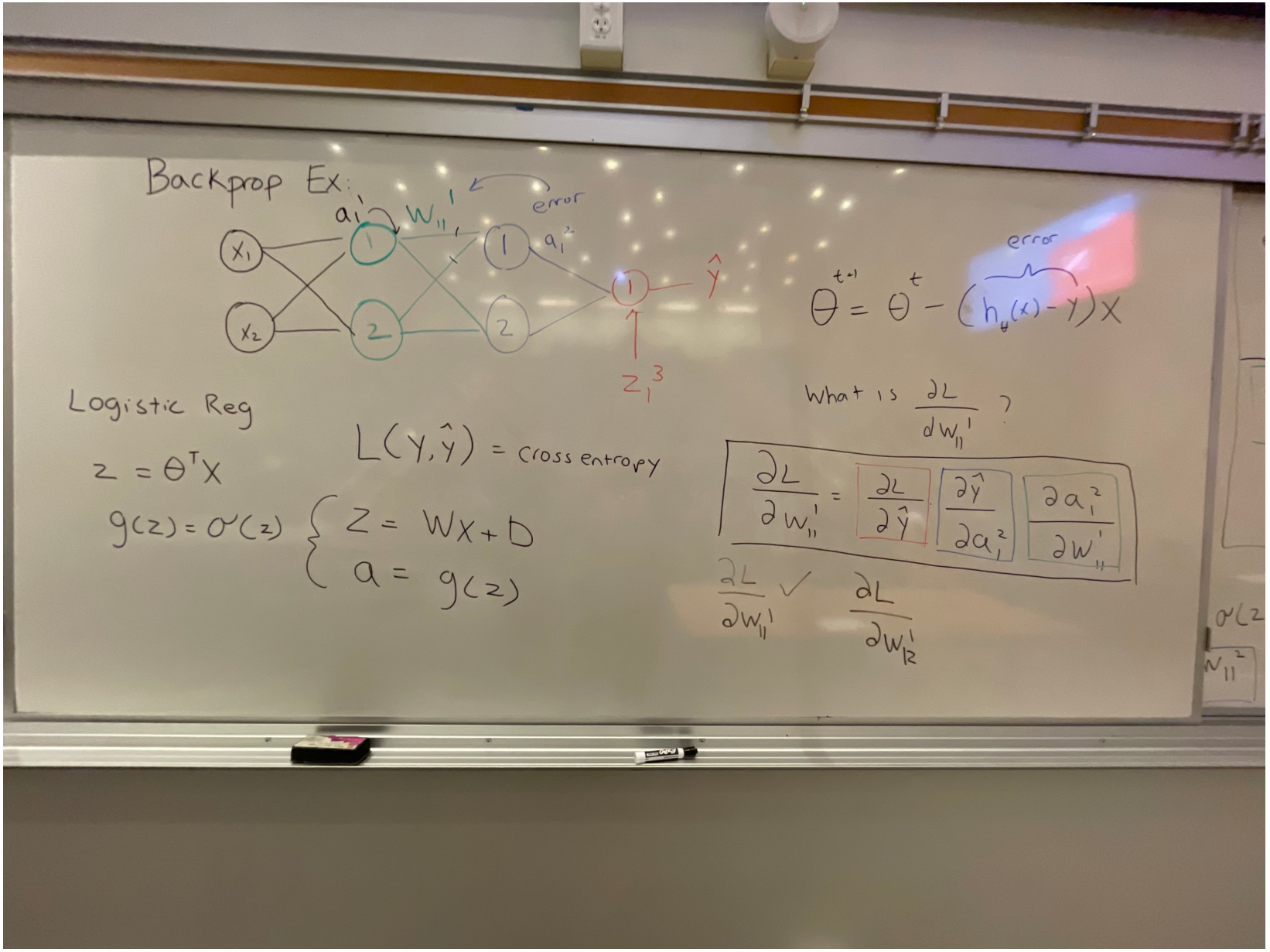
where $\text{cost}(\mathbf{x}_i) = y_i \log h_\Theta(\mathbf{x}_i) + (1 - y_i) \log(1 - h_\Theta(\mathbf{x}_i))$

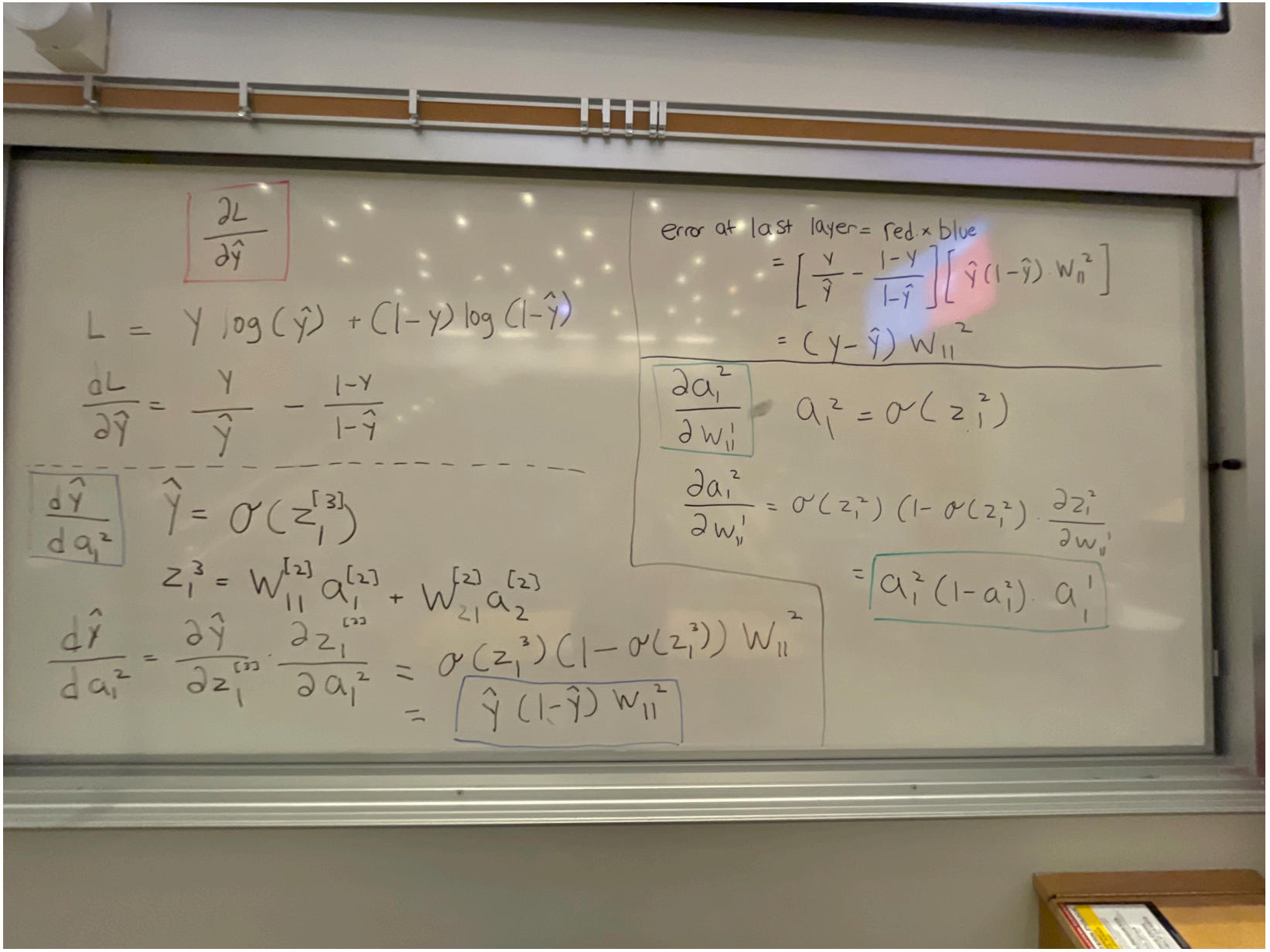
In-Class Backpropagation Example

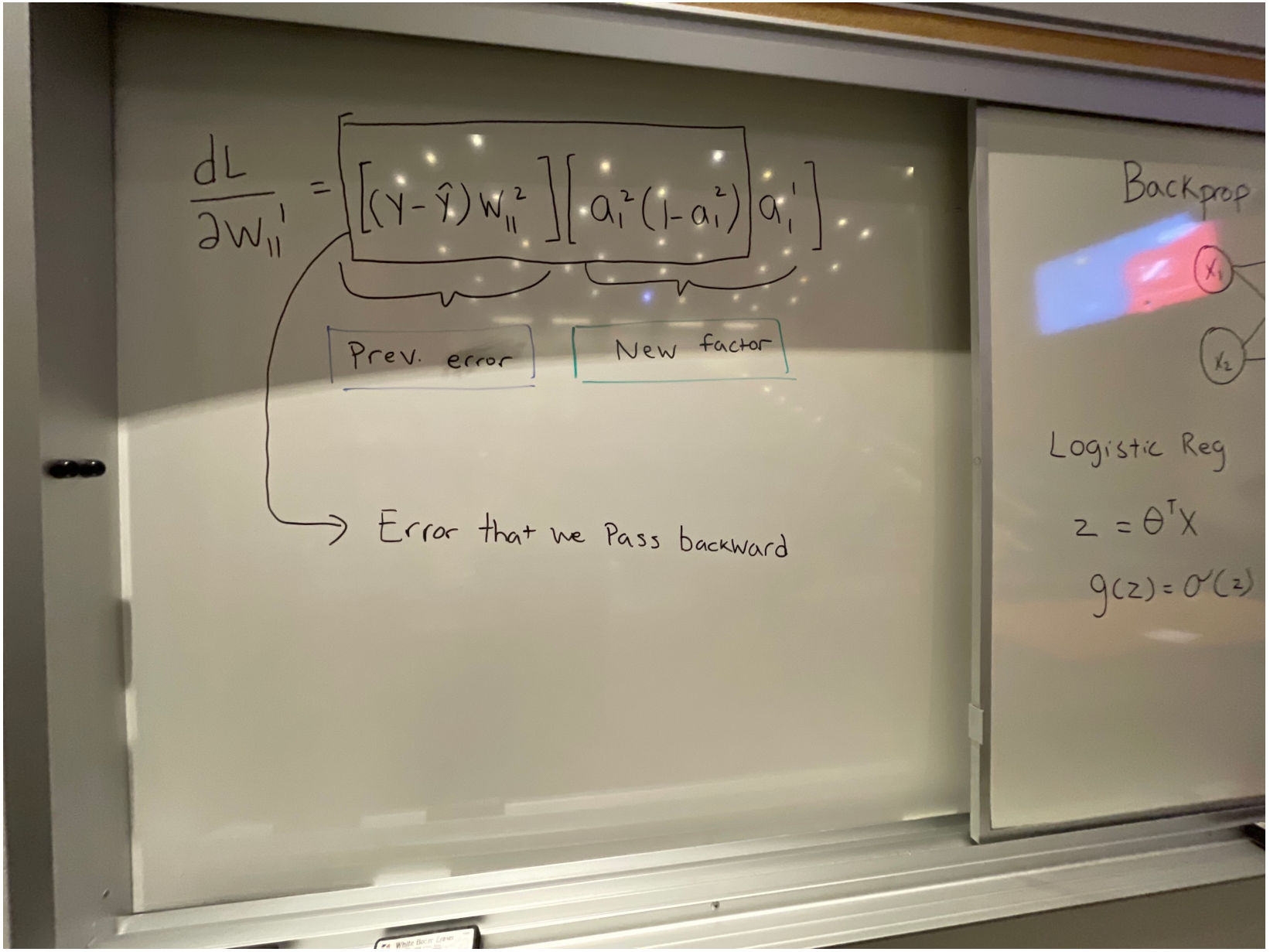
The following three whiteboard photos are from a backpropagation example done in class on Friday March 29.

The example is slightly simpler than the example that follows in the slides given that the target weight is only one layer removed from the output.

For the most part, the notation in the whiteboard example is consistent with the slides.


Backprop Ex:
error
$\hat{y}$
z_1^3
$\theta^{t+1} = \theta^t - (h_\theta(x) - y)x$
error
Logistic Reg
$z = \theta^T x$
$g(z) = \sigma(z)$
$z = Wx + b$
$a = g(z)$
$L(y, \hat{y})$ = cross entropy
What is $\frac{\partial L}{\partial w_{11}^1}$?
$\frac{\partial L}{\partial w_{11}^1} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a_1^2} \frac{\partial a_1^2}{\partial w_{11}^1}$
$\frac{\partial L}{\partial w_{11}^1}$ ✓ $\frac{\partial L}{\partial w_{12}^1}$

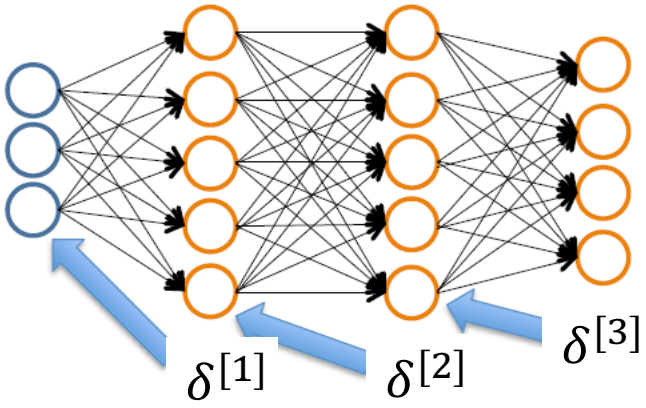

$\frac{\partial L}{\partial \hat{y}}$
$L = y \log(\hat{y}) + (1-y)\log(1-\hat{y})$
$\frac{\partial L}{\partial \hat{y}} = \frac{y}{\hat{y}} - \frac{1-y}{1-\hat{y}}$
$\frac{d\hat{y}}{da_1^2}$
$\hat{y} = \sigma(z_1^{[3]})$
$z_1^3 = W_{11}^{[2]} a_1^{[2]} + W_{21}^{[2]} a_2^{[2]}$
$\frac{d\hat{y}}{da_1^2} = \frac{\partial \hat{y}}{\partial z_1^{[3]}} \cdot \frac{\partial z_1^{[3]}}{\partial a_1^2} = \sigma(z_1^3)(1-\sigma(z_1^3)) W_{11}^2$
$= \hat{y}(1-\hat{y}) W_{11}^2$
error at last layer = red × blue
$= \left[\frac{y}{\hat{y}} - \frac{1-y}{1-\hat{y}}\right]\left[\hat{y}(1-\hat{y}) W_{11}^2\right]$
$= (y-\hat{y}) W_{11}^2$
$\frac{\partial a_1^2}{\partial w_{11}^1}$
$a_1^2 = \sigma(z_1^2)$
$\frac{\partial a_1^2}{\partial w_{11}^1} = \sigma(z_1^2)(1-\sigma(z_1^2)) \cdot \frac{\partial z_1^2}{\partial w_{11}^1}$
$= a_1^2(1-a_1^2) \cdot a_1^1$


$\frac{dL}{\partial w_{11}^{1}} = [(y-\hat{y})w_{11}^{2}][a_1^2(1-a_1^2)]a_1^1]$
Prev. error
New factor
Error that we Pass backward
Backprop
x_1
x_2
Logistic Reg
$z = \theta^T X$
$g(z) = \sigma(z)$

Backpropagation in More Depth

Let $\delta_j^{(l)}$ = "error" of node j in layer l

$$L(y, \hat{y}) = -[(1-y)\log(1-\hat{y}) + y\log\hat{y}]$$



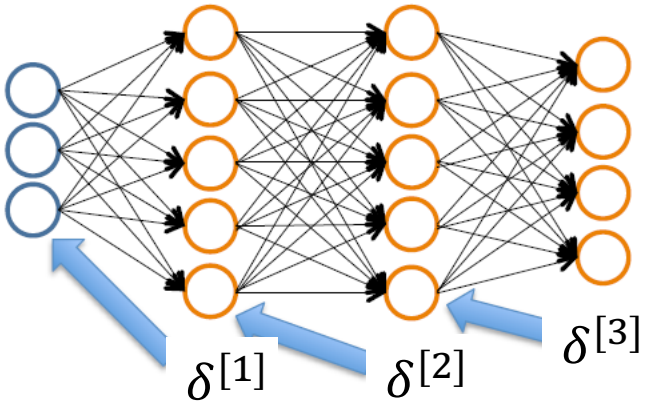
Definitions

- $z^{[\ell]} = W^{[\ell]}\, a^{[\ell-1]} + b^{[\ell]}, a^{[\ell]} = g\left(z^{[\ell]}\right)$
- $\delta^{[\ell]} = \frac{\partial L(\hat{y},y)}{\partial z^{[\ell]}}$; Output $\hat{y} = a^{[L]} = g\left(z^{[L]}\right)$

Backpropagation in More Depth

Let $\delta_j^{(l)}$ = "error" of node j in layer l

$$L(y, \hat{y}) = -[(1-y)\log(1-\hat{y}) + y\log\hat{y}]$$



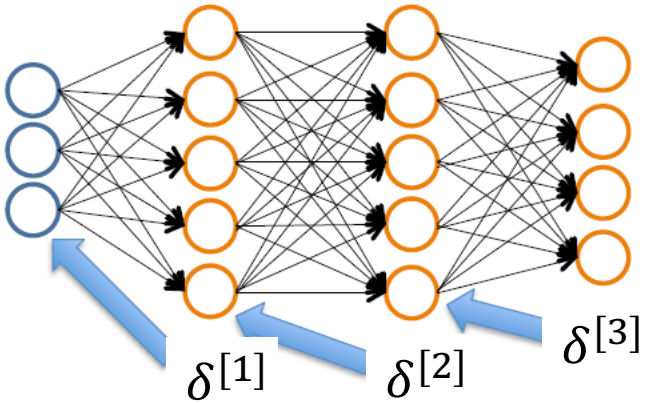
Definitions

- $z^{[\ell]} = W^{[\ell]}\, a^{[\ell-1]} + b^{[\ell]}, a^{[\ell]} = g\left(z^{[\ell]}\right)$
- $\delta^{[\ell]} = \frac{\partial L(\hat{y},y)}{\partial z^{[\ell]}}$; Output $\hat{y} = a^{[L]} = g\left(z^{[L]}\right)$

Backpropagation in More Depth

Let $\delta_j^{(l)}$ = "error" of node j in layer l

$$L(y, \hat{y}) = -[(1-y)\log(1-\hat{y}) + y\log\hat{y}]$$



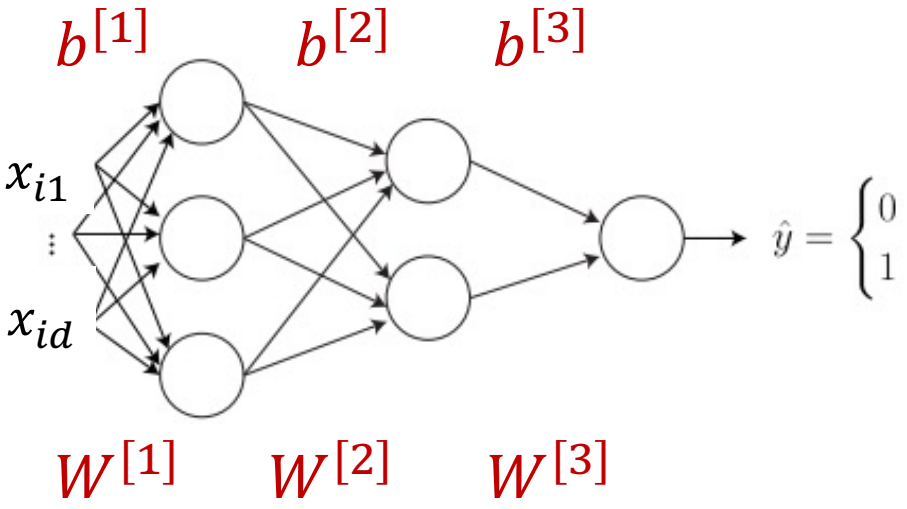
Definitions

- $z^{[\ell]} = W^{[\ell]}\, a^{[\ell-1]} + b^{[\ell]}, a^{[\ell]} = g(z^{[\ell]})$
- $\delta^{[\ell]} = \frac{\partial L(\hat{y},y)}{\partial z^{[\ell]}}$; Output $\hat{y} = a^{[L]} = g(z^{[L]})$

1. For last layer L: $\delta^{[L]} = \frac{\partial L(\hat{y},y)}{\partial z^{[L]}} = \frac{\partial L(\hat{y},y)}{\partial\, \hat{y}} \frac{\partial \hat{y}}{\partial\, z^{[L]}} = \frac{\partial L(\hat{y},y)}{\partial\, \hat{y}} g'(z^{[L]})$
2. For layer ℓ: $\delta^{[\ell]} = \frac{\partial L(\hat{y},y)}{\partial\, z^{[\ell]}} = \frac{\partial L(\hat{y},y)}{\partial\, z^{[\ell+1]}} \frac{\partial z^{[\ell+1]}}{\partial a^{[\ell]}} \frac{\partial a^{[\ell]}}{\partial z^{[\ell]}} = \delta^{[\ell+1]} W^{[\ell+1]} g'(z^{[\ell]})$
3. Compute parameter gradients
   - $\frac{\partial L(\hat{y},y)}{\partial\, W^{[\ell]}} = \frac{\partial L(\hat{y},y)}{\partial\, z^{[\ell]}} \frac{\partial z^{[\ell]}}{\partial\, W^{[\ell]}} = \delta^{[\ell]} a^{[\ell-1]T}$
   - $\frac{\partial L(\hat{y},y)}{\partial\, b^{[\ell]}} = \frac{\partial L(\hat{y},y)}{\partial\, z^{[\ell]}} \frac{\partial z^{[\ell]}}{\partial\, b^{[\ell]}} = \delta^{[\ell]}$

Example 2 Hidden Layers

Training data
Dimension d



$$z^{[1]} = W^{[1]}\ x_i + b^{[1]}$$
$$a^{[1]} = g(z^{[1]})$$
$$z^{[2]} = W^{[2]}a^{[1]} + b^{[2]}$$
$$a^{[2]} = g(z^{[2]})$$
$$z^{[3]} = W^{[3]}a^{[2]} + b^{[3]}$$
$$\hat{y}^{(i)} = a^{[3]} = g(z^{[3]})$$

Binary Classification Example

- $\delta^{[3]} = \frac{\partial L(\hat{y},y)}{\partial z^{[3]}} = \frac{\partial L(\hat{y},y)}{\partial \hat{y}} g'(z^{[3]}); \hat{y} = g(z^{[3]}) = a^{[3]}$
- $\frac{\partial L(\hat{y},y)}{\partial \hat{y}} = -\frac{\partial[(1-y)\log(1-\hat{y}) + y log\, \hat{y}]}{\partial \hat{y}} = \frac{1-y}{1-\hat{y}} - \frac{y}{\hat{y}} = \frac{\hat{y}-y}{\hat{y}(1-\hat{y})}$
- $\delta^{[3]} = \frac{\hat{y}-y}{\hat{y}(1-\hat{y})} g'(z^{[3]})$

  $= \frac{a^{[3]}-y}{g(z^{[3]})(1-g(z^{[3]}))} g(z^{[3]})\left(1 - g(z^{[3]})\right) = a^{[3]} - y$
- $\frac{\partial L(\hat{y},y)}{\partial W^{[3]}} = \delta^{[3]} a^{[2]T} = (a^{[3]} - y) a^{[2]T}$
- $\frac{\partial L(\hat{y},y)}{\partial b^{[3]}} = a^{[3]} - y$

$$g(x) = \sigma(x) = \frac{1}{1+e^{-x}}$$
$$g'(x) = \sigma'(x) = \sigma(x)(1-\sigma(x))$$

Binary Classification Example

- $\delta^{[2]} = \frac{\partial L(\hat{y},y)}{\partial z^{[2]}} = \delta^{[3]} W^{[3]} g'(z^{[2]})$

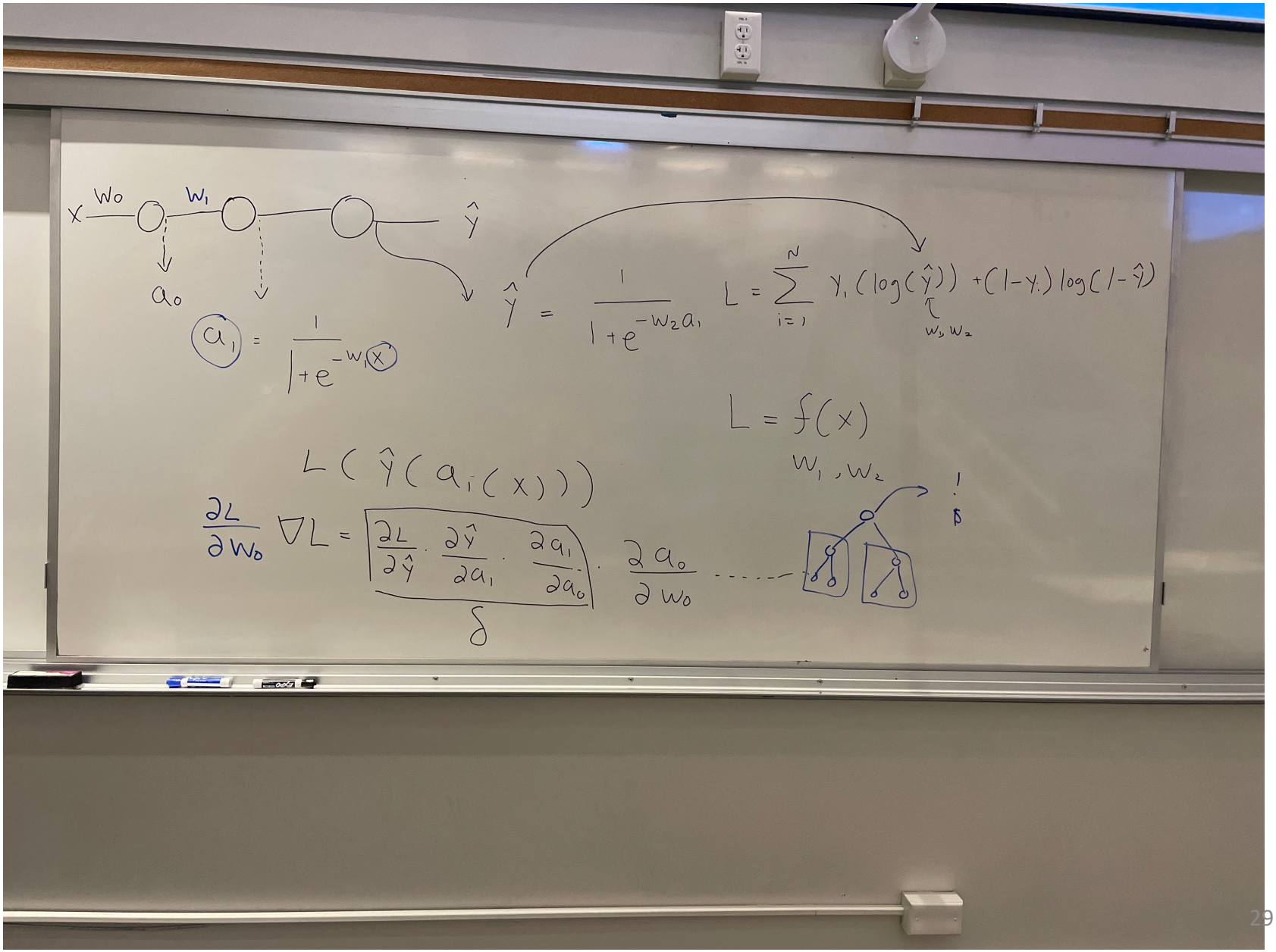
- $\frac{\partial L(\hat{y},y)}{\partial W^{[2]}} = \delta^{[2]} a^{[1]T} = \delta^{[3]} W^{[3]} g'(z^{[2]})\, a^{[1]T} =$

  $= [a^{[3]} - y] W^{[3]} g(z^{[2]})\,(1 - g(z^{[2]}))a^{[1]T}$

- $\frac{\partial L(\hat{y},y)}{\partial b^{[2]}} = [a^{[3]} - y] W^{[3]} g(z^{[2]})\,(1 - g(z^{[2]}))$

$$g(x) = \sigma(x) = \frac{1}{1 + e^{-x}}$$
$$g'(x) = \sigma'(x) = \sigma(x)(1 - \sigma(x))$$

Simpler Example For Review



Parameter Initialization

- How about we set all W and b to 0?

Parameter Initialization

- How about we set all W and b to 0?
- First layer
  - $z^{[1]} = \mathrm{W}^{[1]} x + \mathrm{b}^{[1]}$= (0,…0)
  - $a^{[1]} = \mathrm{g}\left(\mathrm{z}^{[1]}\right) = \left(\frac{1}{2}, \ldots, \frac{1}{2}\right)$
- Second layer
  - $z^{[2]} = \mathrm{W}^{[2]} x + \mathrm{b}^{[2]}$= (0,…0)
  - $a^{[2]} = \mathrm{g}\left(\mathrm{z}^{[2]}\right) = \left(\frac{1}{2}, \ldots, \frac{1}{2}\right)$
- Third layer
  - $z^{[3]} = \mathrm{W}^{[3]} x + \mathrm{b}^{[3]}$= (0,…0)
  - $a^{[3]} = \mathrm{g}\left(\mathrm{z}^{[3]}\right) = \left(\frac{1}{2}, \ldots, \frac{1}{2}\right)$ does not depend on *x*
- Initialize with random values instead!

Training NN with Backpropagation

Given training set $(x_1, y_1), \ldots, (x_N, y_N)$
Initialize all parameters $W^{[\ell]}, b^{[\ell]}$ randomly, for all layers ℓ
Loop

Set $\Delta_{ij}^{[l]} = 0$, for all layers l and indices i, j

EPOCH

For each training instance (x_k, y_k):

Compute $a^{[1]}, a^{[2]}, \ldots, a^{[L]}$ via forward propagation

Compute errors $\delta^{[L]} = a^{[L]} - y_k, \delta^{[L-1]}, \ldots \delta^{[1]}$

Compute gradients $\Delta_{ij}^{[l]} = \Delta_{ij}^{[l]} + a_j^{[l-1]} \delta_i^{[l]}$

Update weights via gradient step

- $W_{ij}^{[\ell]} = W_{ij}^{[\ell]} - \alpha \Delta_{ij}^{[\ell]}$
- Similar for $b_{ij}^{[\ell]}$

Until weights converge or maximum number of epochs is reached

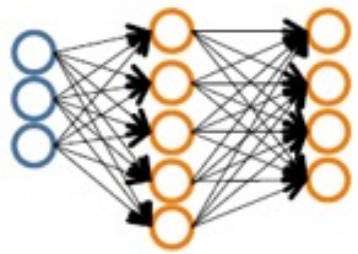
Training Neural Networks

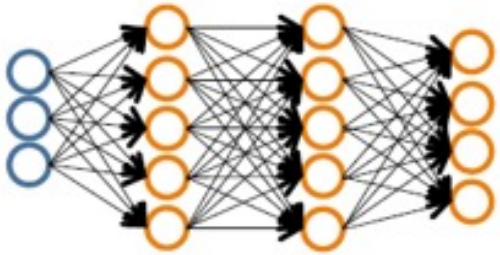
- Randomly initialize weights
- Implement forward propagation to get prediction $\hat{y}_i$ for any training instance x_i
- Compute loss function $L(\hat{y}_i, y_i)$
- Implement backpropagation to compute partial derivatives $\frac{\partial L(\hat{y}_i, y_i)}{\partial W^{[\ell]}}$ and $\frac{\partial L(\hat{y}_i, y_i)}{\partial b^{[\ell]}}$
- Use gradient descent with backpropagation to compute parameter values that optimize loss
- Can be applied to both feed-forward and convolutional nets

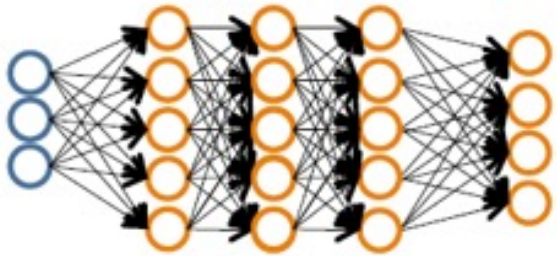
Materials

- Stanford tutorial on training Multi-Layer Neural Networks
  - http://ufldl.stanford.edu/tutorial/supervised/MultiLayerNeuralNetworks/
- Notes on backpropagation by Andrew Ng
  - http://cs229.stanford.edu/notes-spring2019/backprop.pdf
- Deep learning notes by Andrew Ng
  - http://cs229.stanford.edu/notes2020spring/cs229-notes-deep_learning.pdf

Overfitting







- The larger the network, the higher the capacity (more model parameters)
- But also more prone to overfitting!

Regularization

$$L(W) = \underbrace{\frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i)}_{\text{Data loss}} + \underbrace{\lambda R(W)}_{\text{Regularization}}$$

Data loss: Model predictions should match training data

Regularization: Prevent the model from doing *too* well on training data

λ = regularization strength (hyperparameter)

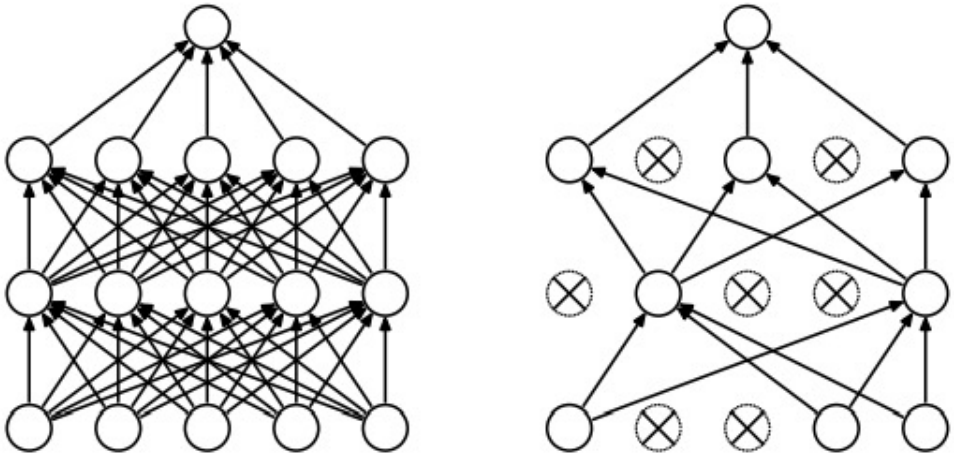
L2 regularization: $R(W) = \sum_k \sum_l W_{k,l}^2$ → Weight decay

L1 regularization: $R(W) = \sum_k \sum_l |W_{k,l}|$

Elastic net (L1 + L2): $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$

- When computing gradients of loss function, regularization term needs to be taken into account

Dropout

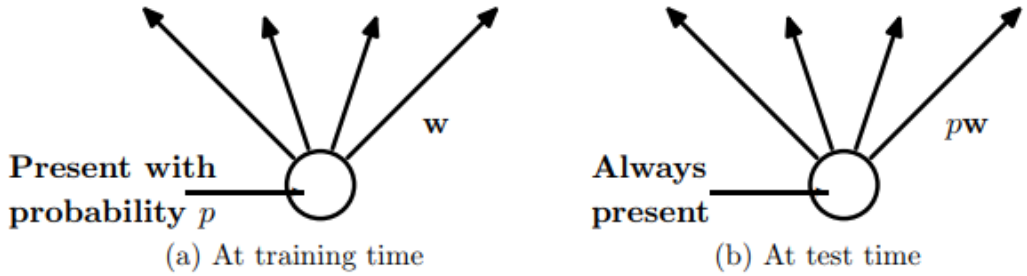


(a) Standard Neural Net (b) After applying dropout.

Figure 1: Dropout Neural Net Model. **Left**: A standard neural net with 2 hidden layers. **Right**: An example of a thinned net produced by applying dropout to the network on the left. Crossed units have been dropped.

- Regularization technique that has proven very effective for deep learning
- Srivastava et al. Dropout: A Simple Way to Prevent Neural Networks from Overfitting. Journal of Machine Learning Research 15, 2014

Dropout



(a) At training time (b) At test time

Figure 2: **Left**: A unit at training time that is present with probability p and is connected to units in the next layer with weights **w**. **Right**: At test time, the unit is always present and the weights are multiplied by p. The output at test time is same as the expected output at training time.

- At training time, sample a sub-network per epoch (batch) and learn weights
  - Keep each neuron with probability p
- At testing time, all neurons are there, but multiply weight by a factor of p

Results on MNIST

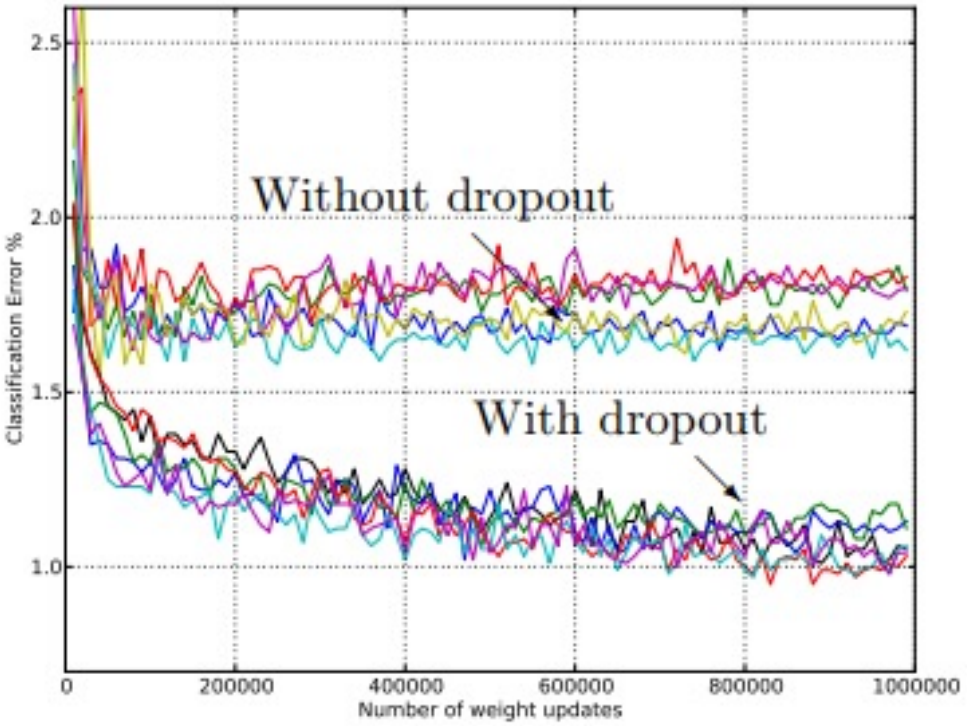


Figure 4: Test error for different architectures with and without dropout. The networks have 2 to 4 hidden layers each with 1024 to 2048 units.

Review

- Backpropagation is the standard method to train neural networks
  - Applicable to many architectures (FFNNs, CNNs, RNNs)
  - Mini batch gradient descent
  - Parameter updates are done from last layer backwards
  - Deep learning packages perform automatic differentiation (no need to compute gradients by hand)
- Neural networks tend to overfit due to over-parameterization
  - Use regularization (weight decay, dropout)

Final Project Deadlines

- Final project video < 2.5 minutes due Sunday April 14
  - What is the problem?
  - Summarize the data
  - Showcase the approach and results.
  - What did you learn in the process?

- Final project report due Friday April 19
  - 6 – 8 page report with outline on Canvas