# Training Neural Networks with Gradient Descent

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University of Colorado Boulder Spring 2025



#### Review

- Last lecture:
  - Motivation for neural networks: need non-linear models
  - Neural networks' basic ingredients: hidden layers and activation units
  - Neural networks' support for diverse problems: output units
  - Objective function: what a model should learn
- Assignments (Canvas):
  - Problem set 1 due Tuesday
- Questions?

## Today's Topics

Gradient descent: how neural networks learn

Mathematical foundation of gradient descent: derivatives

Applying gradient descent to train neural networks

Training example

## Today's Topics

Gradient descent: how neural networks learn

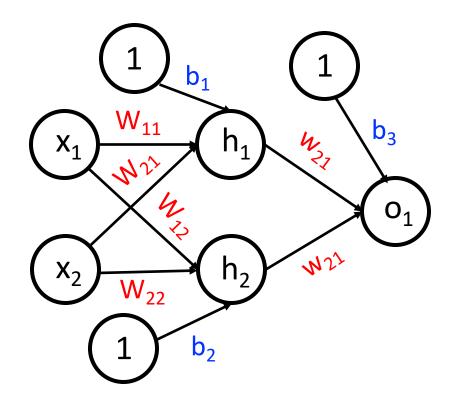
Mathematical foundation of gradient descent: derivatives

Applying gradient descent to train neural networks

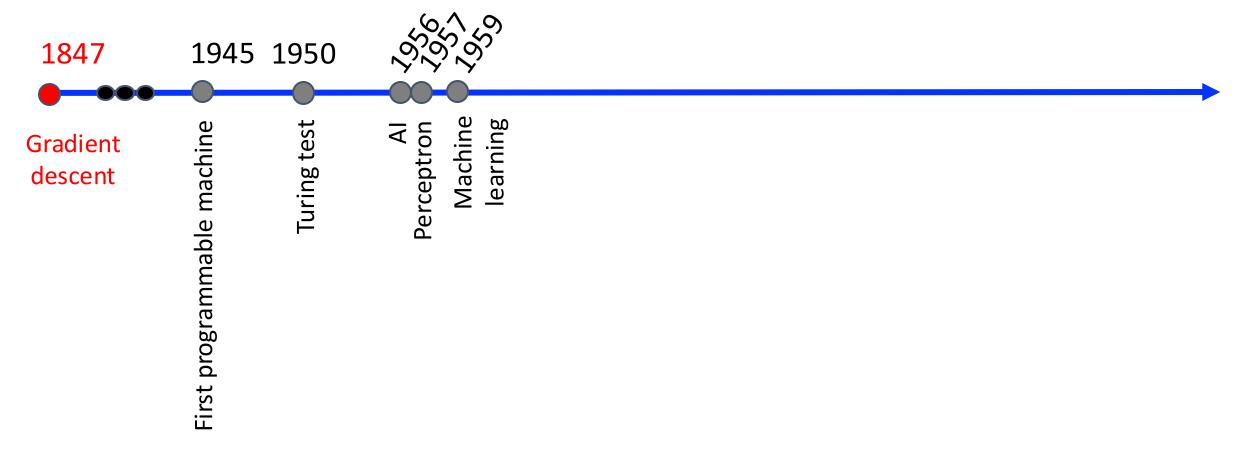
Training example

## Recall Goal: Train Neural Network to Minimize an Objective Function

 Learn model parameters that minimize an objective/loss function using gradient descent; e.g., (weights, biases)



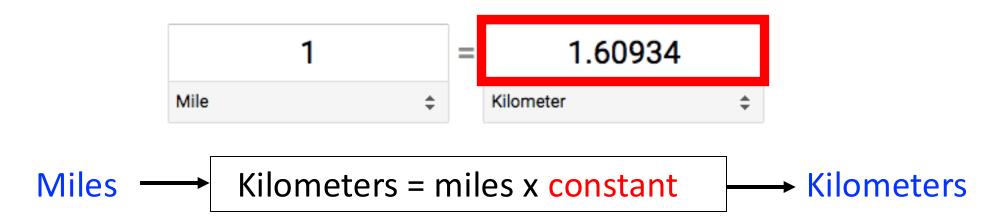
#### Approach: Gradient Descent



- Iteratively searching for better model parameters (e.g., weights and biases) that lead to smaller "losses" in the objective function
- Analogy: hike from mountains to Boulder blind or blindfolded!



- Repeat:
  - 1. Guess
  - 2. Calculate error
- e.g., learn linear model for converting kilometers to miles when only observing the input "miles" and output "kilometers"



- Repeat:
  - 1. Guess
  - 2. Calculate error
- e.g., learn constant multiplier to convert US dollars to Israeli shekels

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```
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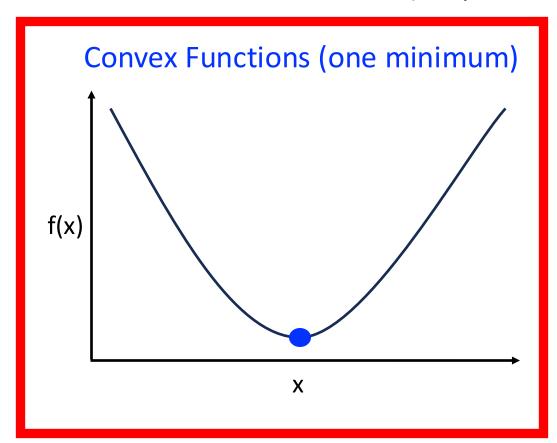
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- e.g., learn constant multiplier to convert US dollars to Israeli shekels

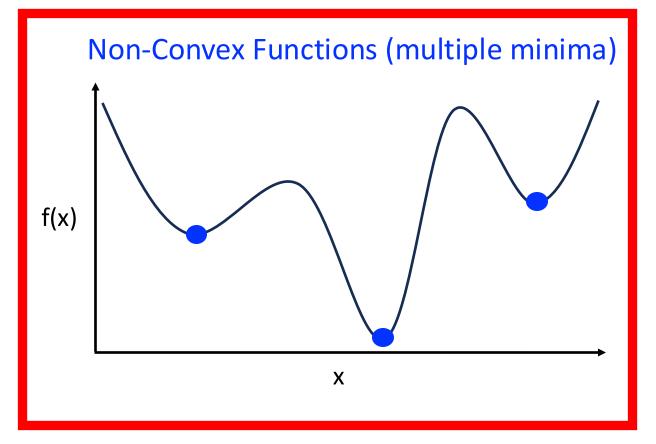
- Repeat:
  - 1. Guess
  - 2. Calculate error
- e.g., learn constant multiplier to convert US dollars to Israeli shekels

• Idea: iteratively adjust constant (i.e., model parameter) to reduce error

#### Gradient Descent: Possible Scenarios

(simple 1-dimensional plots)





Currency conversion example

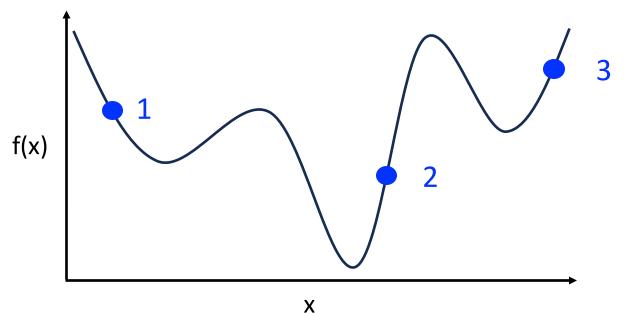
Our focus: deep learning

#### Gradient Descent: Definitions

- Gradient: a vector indicating how a slight change to each function variable in x increases the output f(x) (i.e., partial derivatives for multiple variables)
- Recall, a derivative indicates the slope (rise/run) of the function at any point

• Gradient descent: to minimize the function, iteratively step in opposite direction of gradient

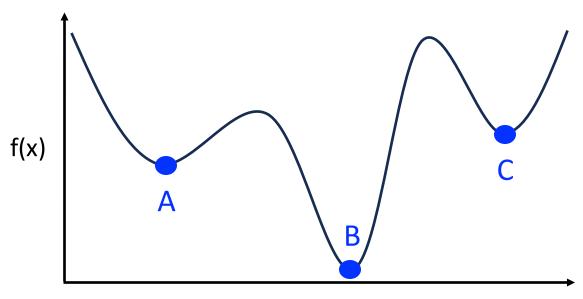
(i.e., descent rather than ascent)



- What does the derivative look like at position 1? (Class volunteer)
- Is position 1's slope positive or negative?
- From position 1, should follow opposite the gradient direction to minimize the function
- What does the derivative look like at position 2? (Class volunteer)
- Is position 2's slope positive or negative?
- From position 2, should follow opposite the gradient direction to minimize the function

#### Gradient Descent: Definitions

- Gradient: a vector indicating how a slight change to each function variable in x increases the output f(x) (i.e., partial derivatives for multiple variables)
- Recall, a derivative indicates the slope (rise/run) of the function at any point
- **Gradient descent**: to *minimize* the function, iteratively step in opposite direction of gradient (i.e., descent rather than ascent)

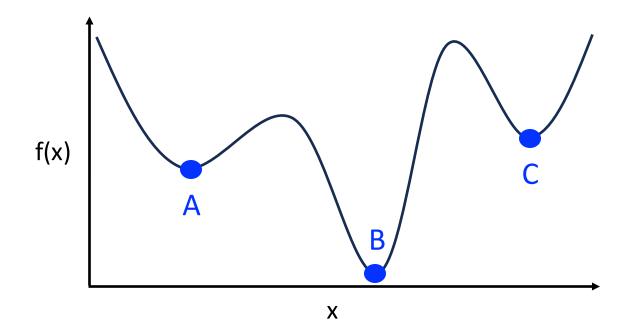


X

Which letter(s) show global minima?

Which letter(s) show local minima?

Gradient descent can arrive at a local minimum rather than global minimum, a possibility that initially deterred its adoption for neural networks



Global minima: B

Local minima: A, B, C

## Today's Topics

Gradient descent: how neural networks learn

Mathematical foundation of gradient descent: derivatives

Applying gradient descent to train neural networks

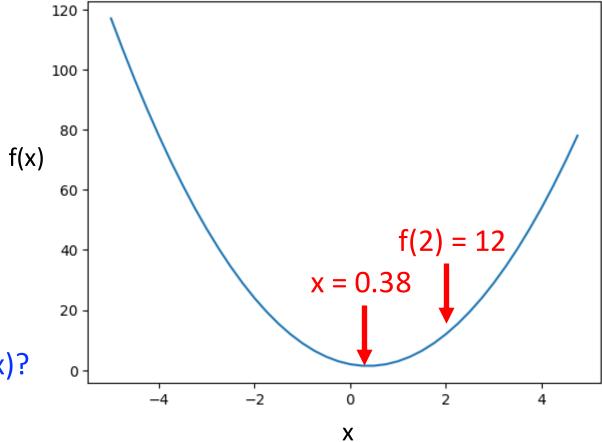
Training example

$$f(x) = 2 - 3x + 4x^2$$

Is this function convex or non-convex?

What is the value of the function at x = 2?

What is the value of x at the minimum of f(x)?



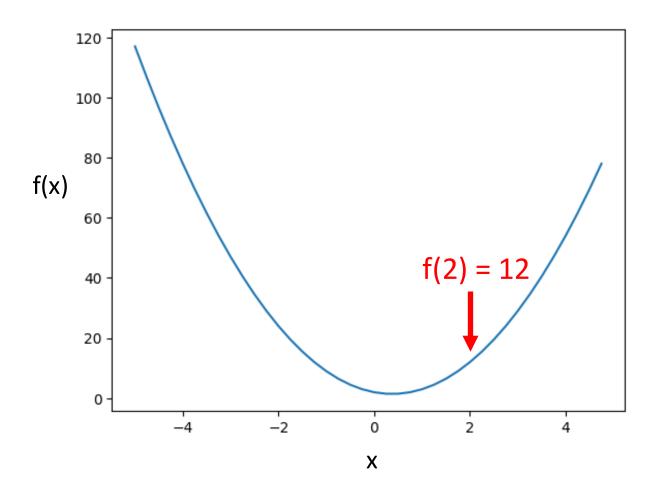
$$f(x) = 2 - 3x + 4x^2$$

Derivative indicates how a slight change (i.e., h) to every x will change the output:

slope = 
$$\frac{\text{rise}}{\text{run}} = \frac{f(x+h) - f(x)}{h}$$

If h is slightly positive, at x=2, will f(x+h) be greater than or less than 12?

By how much?



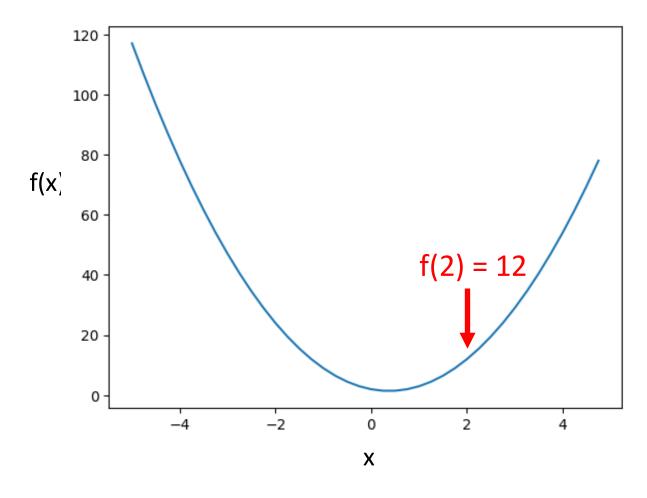
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slope = 
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e.g., at x = 2- for h = 0.01: f(x+h) = 12.1304, slope = 13.04

Increasing x by h=0.01 results in an increase of ~13.04 times that amount (13.04 \* .01)



$$f(x) = 2 - 3x + 4x^2$$

Derivative indicates how a slight change (i.e., h) to every x will change the output:

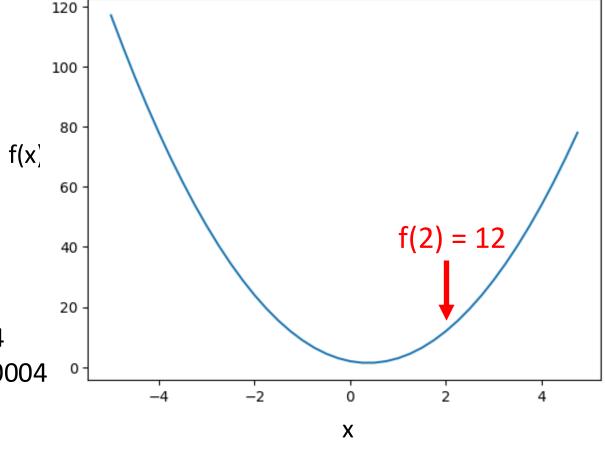
slope = 
$$\frac{\text{rise}}{\text{run}} = \frac{f(x+h) - f(x)}{h}$$

e.g., at x = 2

- for h = 0.01: f(x+h) = 12.1304, slope = 13.04
- for h = 0.001: f(x+h) = 12.013004 & slope = 13.004
- for h = 0.0001: f(x+h) = 12.0013004 & slope = 13.0004

As h gets closer to 0, slope approaches what?

Mathematically, f'(x) = -3 + 8x; f'(2) = -3 + 16 = 13



$$f(x) = 2 - 3x + 4x^2$$

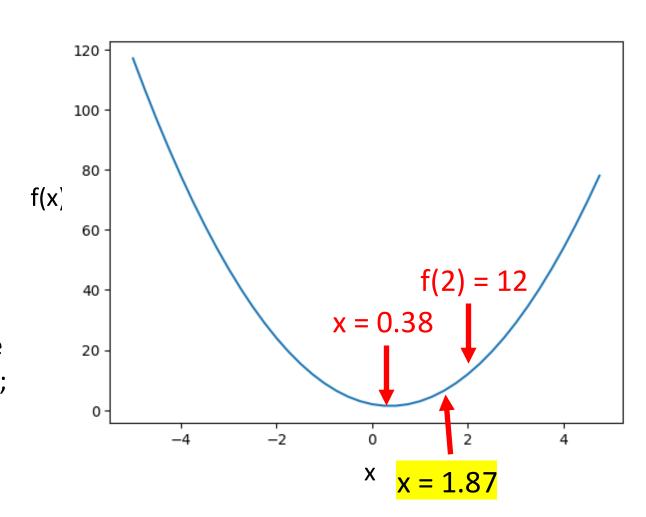
Derivative indicates how a slight change (i.e., h) to every x will change the output:

slope = 
$$\frac{\text{rise}}{\text{run}} = \frac{f(x+h) - f(x)}{h}$$

e.g., at x = 2 and df/dx = 13

Approach minimum point by stepping in opposite direction of derivative (e.g., learning rate of 0.01); what should be new value for x?

$$2 - (0.01 * 13) = 1.87$$



$$f(x) = 2 - 3x + 4x^2$$

Derivative indicates how a slight change (i.e., h) to every x will change the output:

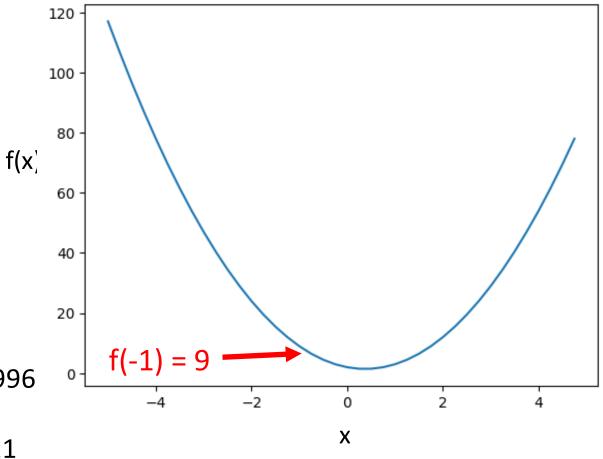
slope = 
$$\frac{\text{rise}}{\text{run}} = \frac{f(x+h) - f(x)}{h}$$

e.g., at x = -1

- for h = 0.01: f(x+h) = 8.8904, slope = -10.96
- for h = 0.001: f(x+h) = 8.989004, slope = -10.996
- for h = 0.0001: f(x+h) = 8.99890004, slope = -10.9996

As h gets closer to 0, slope approaches what?

Mathematically, f'(x) = -3 + 8x; f'(-1) = -3 + 8\*-1 = -11



$$f(x) = 2 - 3x + 4x^2$$

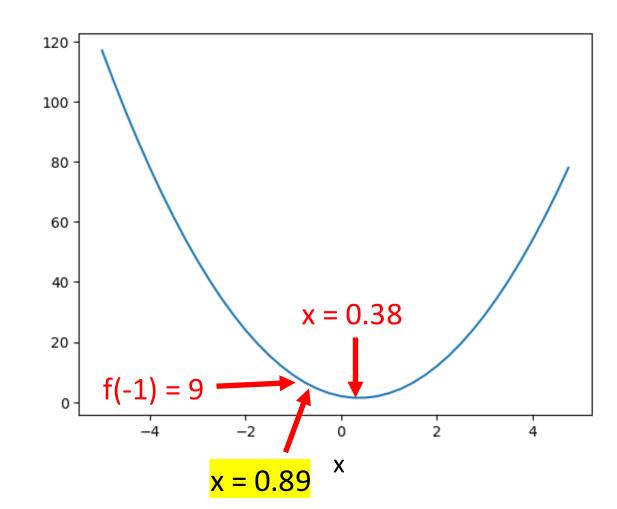
Derivative indicates how a slight change (i.e., h) to every x will change the output:

slope = 
$$\frac{\text{rise}}{\text{run}} = \frac{f(x+h) - f(x)}{h}$$

e.g., at x = -1 and df/dx = -11

Approach minimum point by stepping in opposite direction of derivative (e.g., learning rate of 0.01); what should be new value for x?

$$-1 - (0.01 * -11) = -0.89$$



f(x) = a + bc; where x is a vector with all parameters

Gradient indicates how a slight change (i.e., h) to any **input** will change the output:

slope = 
$$\frac{\text{rise}}{\text{run}} = \frac{f(\mathbf{x} + \mathbf{h}) - f(\mathbf{x})}{\mathbf{h}}$$

What is the value of the function when a = 1, b = -2, and c = 3?

If we only change a with a slightly positive h, will f(x+h) be greater than or less than -5?

By how much?

f(x) = a + bc; where x is a vector with all parameters

Gradient indicates how a slight change (i.e., h) to any **input** will change the output:

slope = 
$$\frac{\text{rise}}{\text{run}} = \frac{f(\mathbf{x} + \mathbf{h}) - f(\mathbf{x})}{\mathbf{h}}$$

e.g., at a = 1, b = -2, and c = 3 when only changing the value of a - for h = 0.01:  $f(\mathbf{x}+h) = (1+.01) + -2*3 = -4.99$ , slope = 1.000 - for h = 0.001:  $f(\mathbf{x}+h) = (1+.001) + -2*3 = -4.999$ , slope = 1.000 As h gets closer to 0, slope approaches 1

Mathematically, df/da = 1

f(x) = a + bc; where x is a vector with all parameters

Gradient indicates how a slight change (i.e., h) to any **input** will change the output:

slope = 
$$\frac{\text{rise}}{\text{run}} = \frac{f(\mathbf{x} + \mathbf{h}) - f(\mathbf{x})}{\mathbf{h}}$$

Recall the value of the function when a = 1, b = -2, and c = 3 is -5

If we change only b with a slightly positive h, will f(x+h) be greater than or less than -5?

By how much?

f(x) = a + bc; where x is a vector with all parameters

Gradient indicates how a slight change (i.e., h) to any **input** will change the output:

slope = 
$$\frac{\text{rise}}{\text{run}} = \frac{f(\mathbf{x} + \mathbf{h}) - f(\mathbf{x})}{\mathbf{h}}$$

e.g., at a = 1, b = -2, and c = 3 when only changing the value of b (rounding to 3 decimals)

- for h = 0.01: f(x+h) = 1 + (-2 + .01)\*3 = -4.970, slope = 3.000

- for h = 0.001: f(x+h) = 1 + (-2 + .001)\*3 = -4.997, slope = 3.000

As h gets closer to 0, slope approaches 3

Mathematically, df/db = c (which we set to 3)

f(x) = a + bc; where x is a vector with all parameters

Gradient indicates how a slight change (i.e., h) to any **input** will change the output:

slope = 
$$\frac{\text{rise}}{\text{run}} = \frac{f(\mathbf{x} + \mathbf{h}) - f(\mathbf{x})}{\mathbf{h}}$$

Recall the value of the function when a = 1, b = -2, and c = 3 is -5

If we change only c with a slightly positive h, will f(x+h) be greater than or less than -5?

By how much?

f(x) = a + bc; where x is a vector with all parameters

Gradient indicates how a slight change (i.e., h) to any **input** will change the output:

slope = 
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e.g., at a = 1, b = -2, and c = 3 when only changing the value of c (rounding to 3 decimals)

- for h = 0.01: f(x+h) = 1 + -2\*(3 + .01) = -5. 02, slope = -2.000

- for h = 0.001: f(x+h) = 1 + -2\*(3 + .001) = -5.002, slope = -2.000

As h gets closer to 0, slope approaches -2

Mathematically, df/dc = b (which we set to -2)

f(x) = a + bc; where x is a vector with all parameters

Gradient indicates how a slight change (i.e., h) to any **input** will change the output:

slope = 
$$\frac{\text{rise}}{\text{run}} = \frac{f(\mathbf{x} + \mathbf{h}) - f(\mathbf{x})}{\mathbf{h}}$$

In summary, gradient for any input can be computed with these equations:

$$df/da = 1;$$
  $df/db = c;$   $df/dc = b$ 

Can minimize objective function by stepping (e.g., learning rate of 0.01) in opposite direction of derivative; e.g., at a = 1, b = -2, and c = 3

a - 
$$0.01*1 = 0.99$$
; b -  $0.01*c = -2.03$ ; c -  $0.01*b = 3.02$  f(x) = -5.14

## Today's Topics

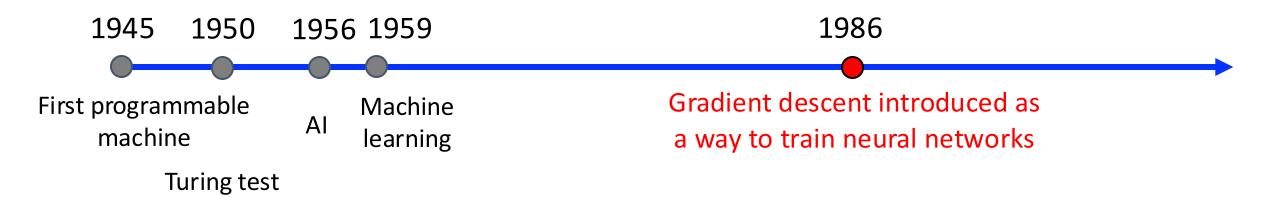
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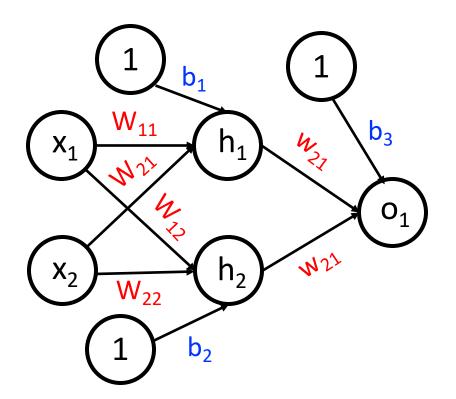
Training example

#### Training Neural Networks



#### Training Neural Networks

• Descend the loss function with gradient descent; e.g., (weights, biases)





# Gradient Descent: Implementation

- Repeat until stopping criterion met:
  - 1. Propagate training data through model to make predictions
  - Measure error of the model's predictions on training data using a loss function
  - 3. Calculate gradients to determine how each model parameter contributed to model error

Breakthrough in 1986: backpropagation used to compute the gradient

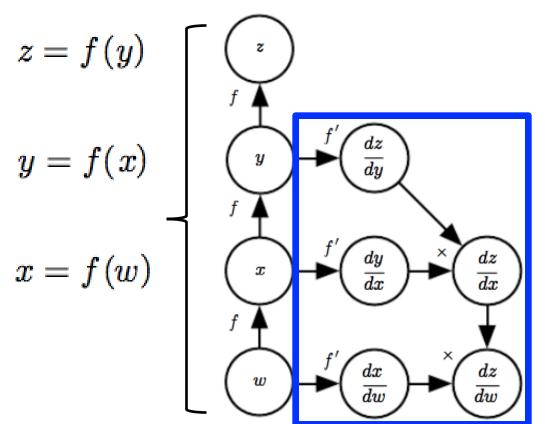
4. Update each parameter using calculated gradients

• **Key observation**: loss function is a mathematical function, that takes as input training data and model parameters (e.g., weights, biases)



Using backpropagation, we can know how to tweak all of a function's variables to minimize an error/loss function

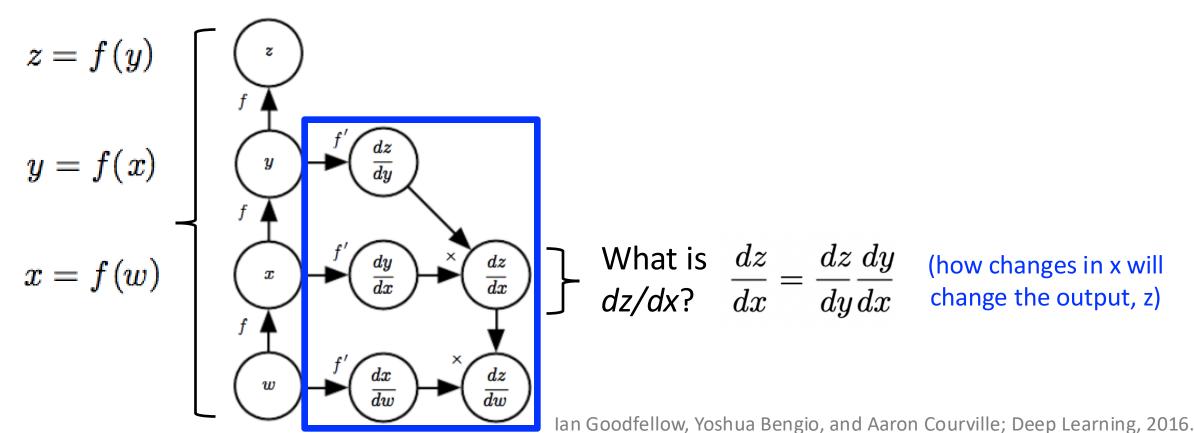
- **Key observation**: loss function is a mathematical function connected in a chain
- What we want: partial derivatives for function variables to inform how to minimize the loss function
- Backpropagation: achieves this with chain rule of calculus, which relies only on local derivatives; e.g.,



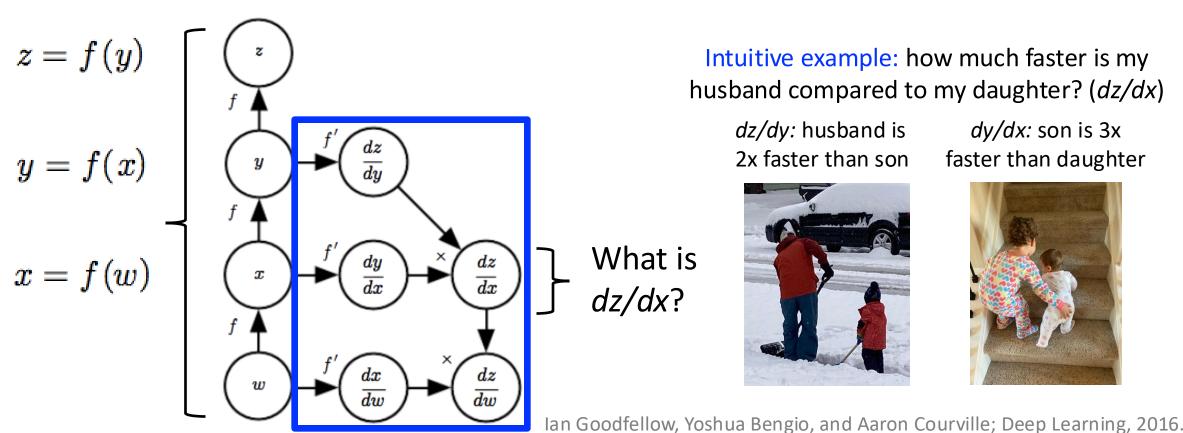
Indicates how much a small change to each variable changes the function's output

lan Goodfellow, Yoshua Bengio, and Aaron Courville; Deep Learning, 2016.

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# Gradient Descent: Implementation

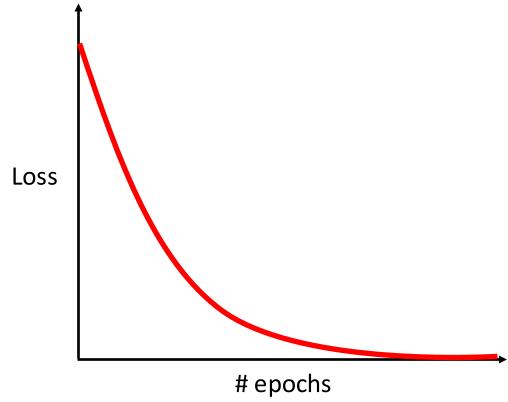
- Repeat until stopping criterion met:
  - 1. Propagate training data through model to make predictions
  - 2. Measure error of the model's predictions on training data using a loss function

We babysit this step to see how learning is going

- Calculate gradients to determine how each model parameter contributed to model error
- 4. Update each parameter using calculated gradients

# Loss Curves Signal How Well Training is Going

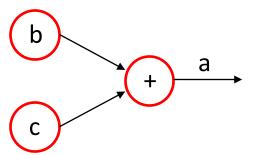
What we want to see when training:



# Abstraction for Training Neural Networks: Computational Graphs

- A directed graph expressing a mathematical expression
  - Nodes: either variables (e.g., input values) or functions (applied to the in-flowing edges)
  - Edges: values output from functions
- For example: a = b + c

OR



$$a = d^*(b + c)$$

Intermediate value stored in new variable

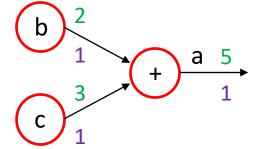
c

d

# How to Use a Computational Graph?

- Forward pass: to evaluate an expression, set input variables and then perform all sequential computational steps in the graph
- Backward pass: compute local gradient at each edge and then combine all relevant gradients for each function variable
- For example, using b=2 and c=3:

$$f(b,c) = b + c$$

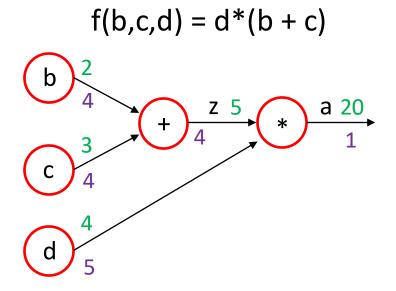


From calculus, we know:

$$-df/df = 1$$
  $-df/db = 1$   $-df/dc = 1$ 

# How to Use a Computational Graph?

- Forward pass: to evaluate an expression, set input variables and then perform all sequential computational steps in the graph
- Backward pass: compute local gradient at each edge and then combine all relevant gradients for each function variable
- For example, using b=2, c=3, and d=4:



From calculus, we know:

$$- df/df = 1 - df/dz = d - df/dd = z$$

$$- df/db = df/dz * dz/db - dz/db = 1$$

$$- df/dc = df/dz * dz/dc - df/dc = 1$$

Multiplication passes the other value through and addition passes the incoming gradient

### Motivation for Computational Graphs

- Many deep learning frameworks rely on computational graphs; why?
  - Efficient representation: modular, primitive functions can be reused and combined to build complex models
  - Efficient computation: derivatives can be calculated based on "local" derivatives of the primitive functions in the graph, which enables them to be computed in parallel and stored for later reuse
  - Interpretability: simplifies understanding, debugging, and identifying bottlenecks in the network

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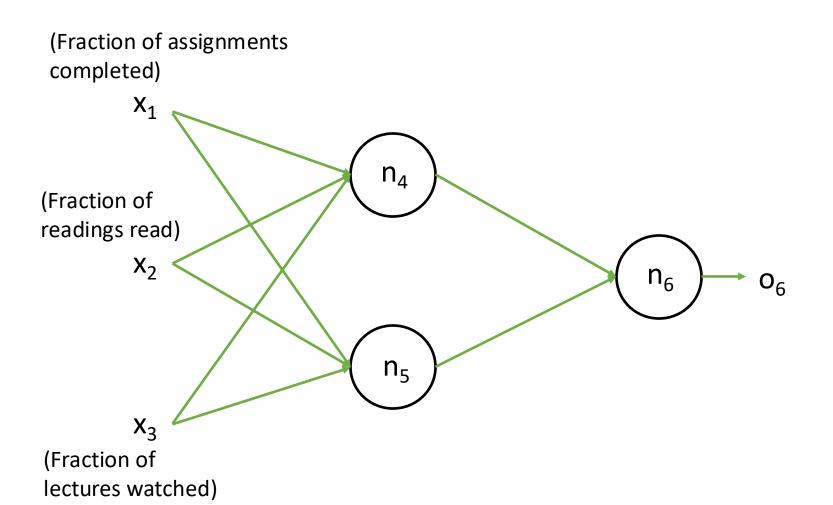
# Example

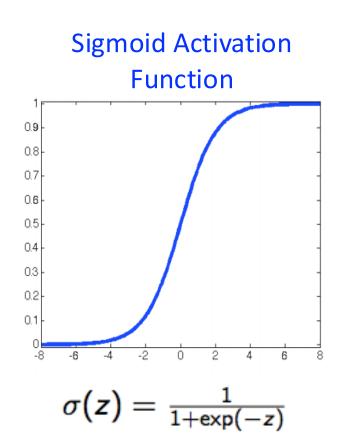
• Binary classification: predict if a student will get a B or better (minimum required for CS graduate student in this course)

### • Inputs:

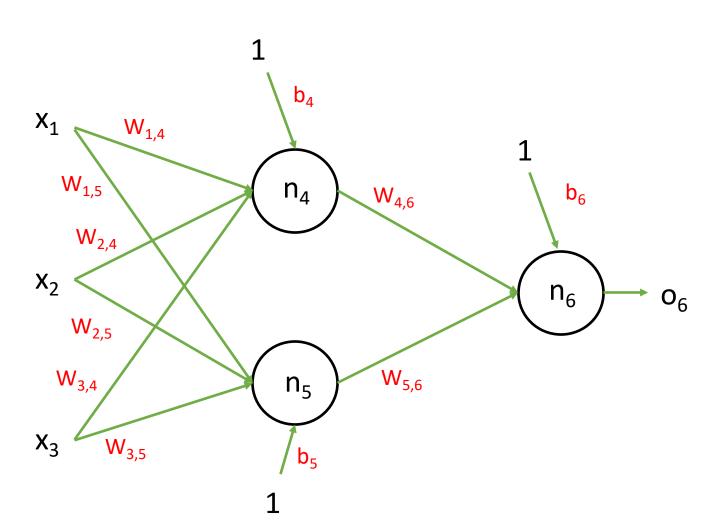
- Fraction of assignments completed
- Fraction of readings read
- Fraction of lectures watched

# Example: Choose Neural Network Architecture





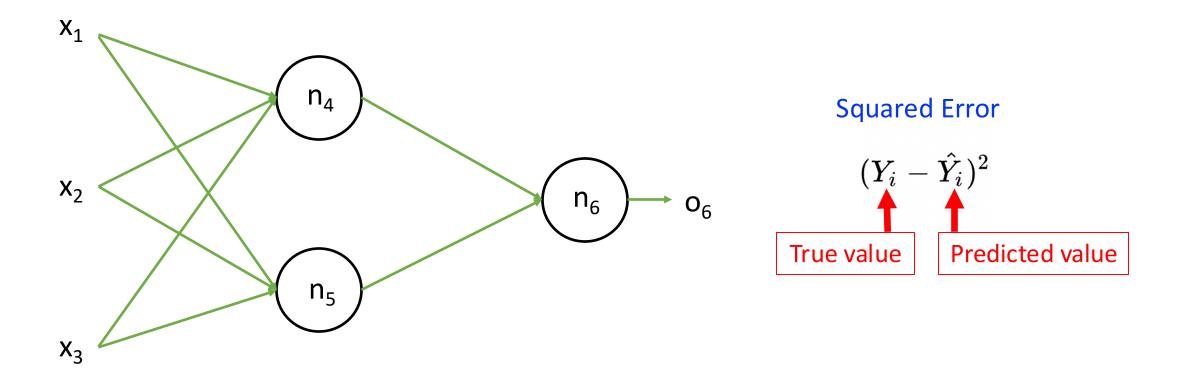
# Example: Choose Neural Network Architecture



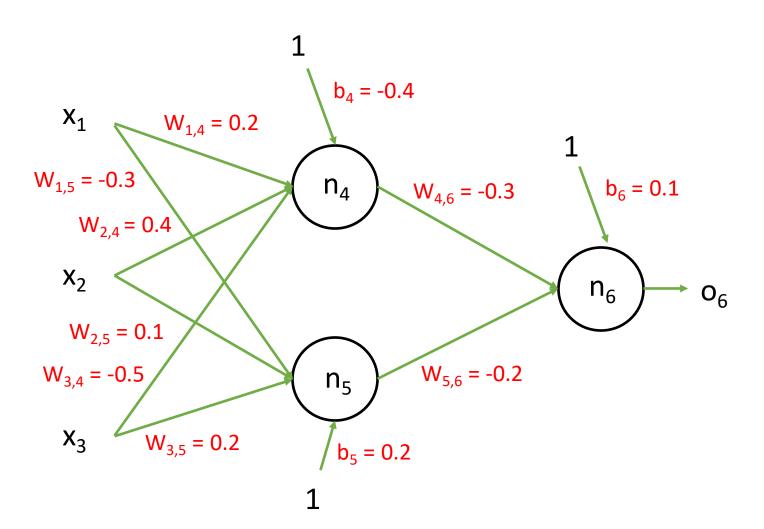
2-layer neural network 8 weights:

- Input to Hidden Layer 1:
  - 3x2 = 6
- Hidden Layer 1 to Hidden Layer 2:
  - 2x1 = 2
- 3 bias terms

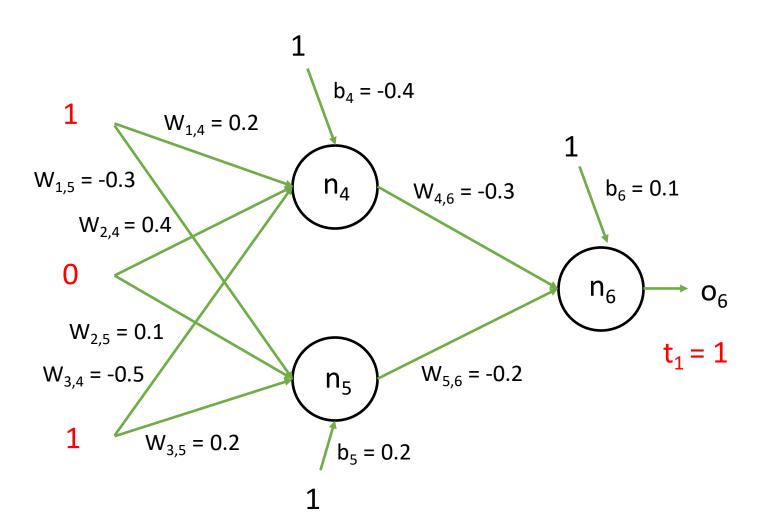
# Example: Choose Loss Function

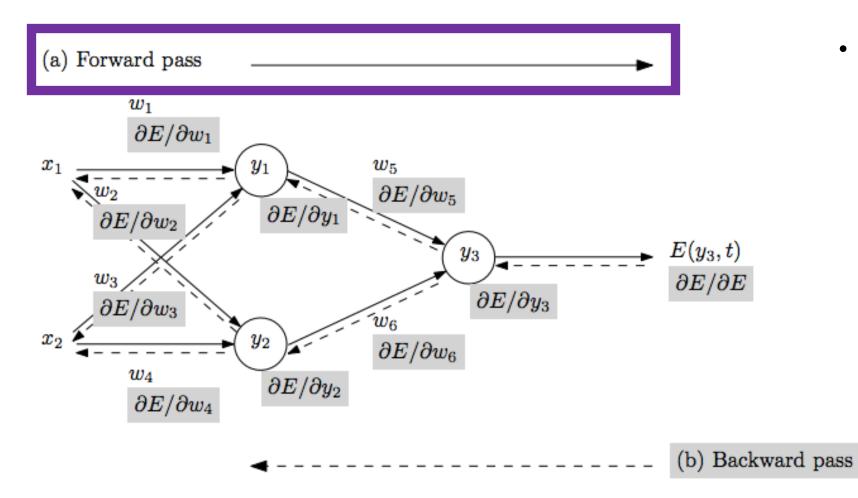


# Example: Initialize Model Parameters

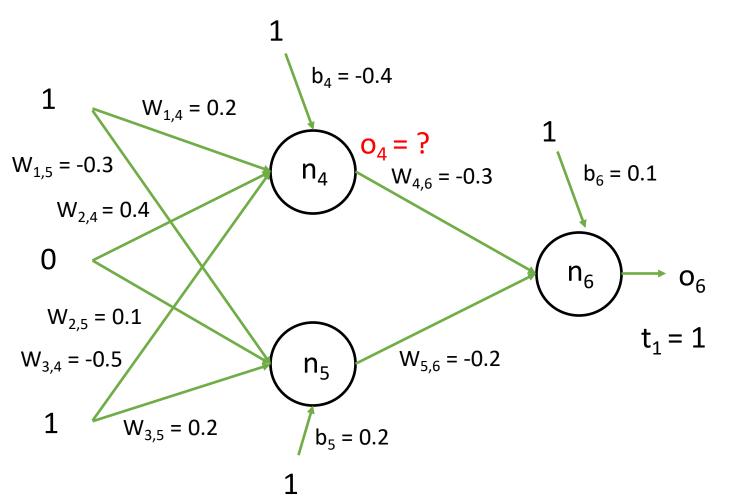


# Example: Input Training Example





- Repeat until stopping criterion met:
  - 1. Forward pass: propagate training data through model to make predictions

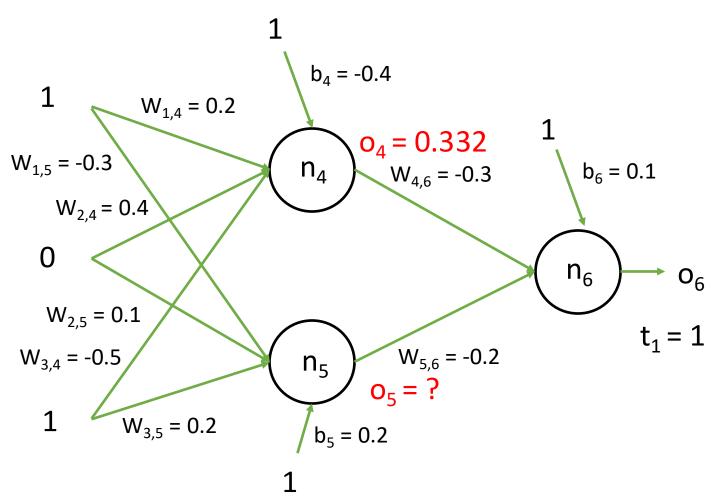


### Weighted input sum to node 4:

$$i_4 = (1 \times 0.2 + 0 \times 0.4 + 1 \times -0.5) - 0.4$$
  
 $i_4 = -0.7$ 

### Activation result from node 4:

$$o_4 = sigmoid(-0.7)$$
  
 $o_4 = 1/(1+e^{-(-0.7)})$   
 $o_4 = 0.332$ 

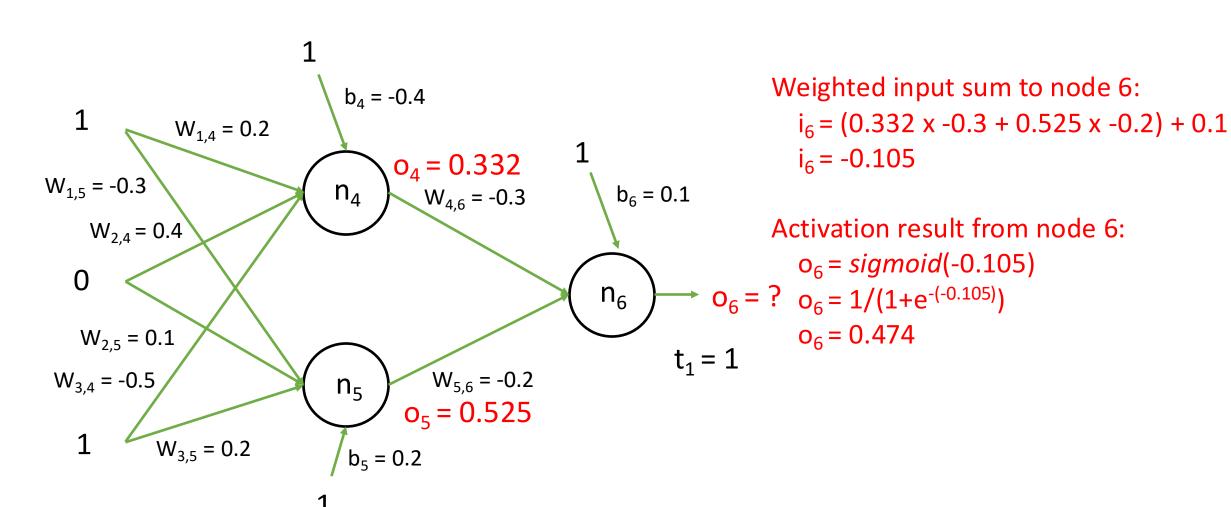


### Weighted input sum to node 5:

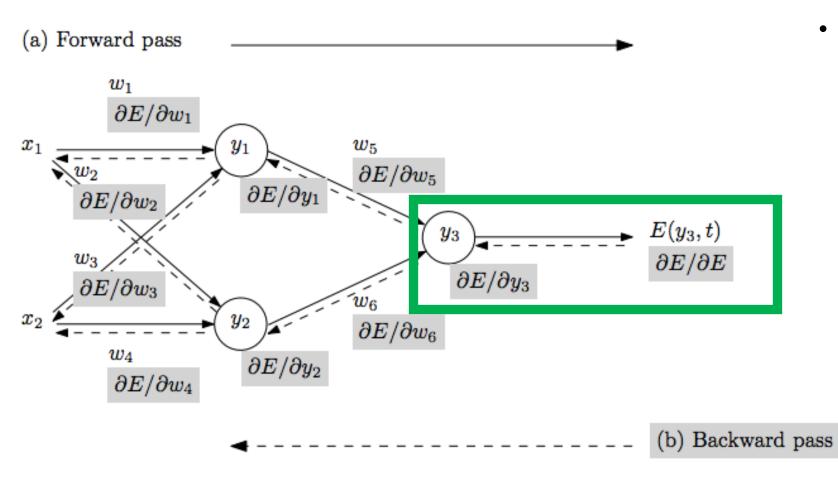
```
i_5 = (1 \times -0.3 + 0 \times 0.1 + 1 \times 0.2) + 0.2
i_5 = 0.1
```

#### Activation result from node 5:

$$o_5 = sigmoid(0.1)$$
  
 $o_5 = 1/(1+e^{-0.1})$   
 $o_5 = 0.525$ 

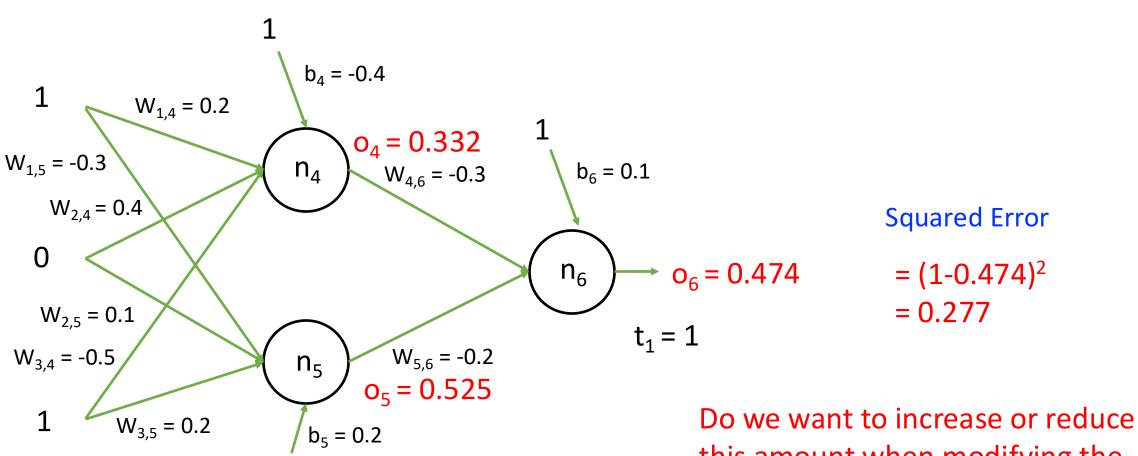


# Example: Step 2 – Calculate Error (Loss)

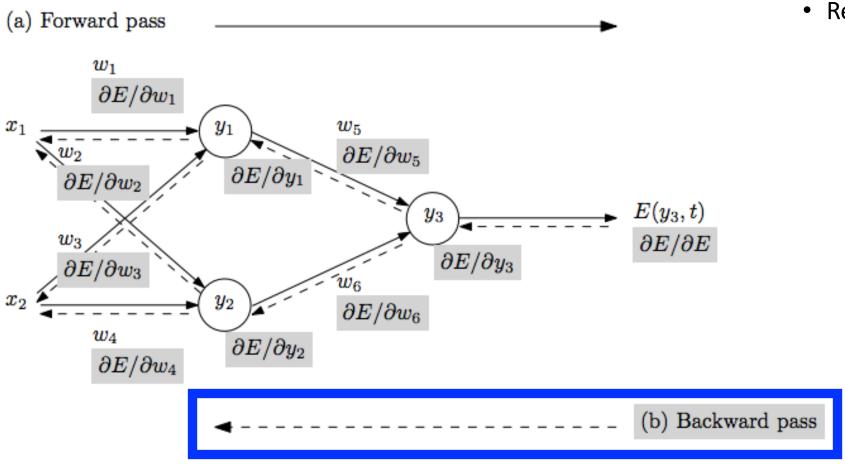


- Repeat until stopping criterion met:
  - 1. Forward pass: propagate training data through model to make predictions
  - 2. Error quantification:
    measure error of the
    model's predictions on
    training data using a loss
    function

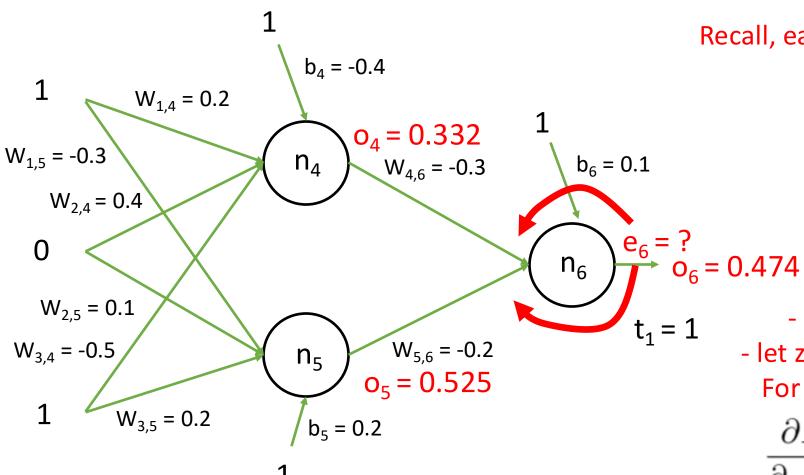
# Example: Step 2 – Calculate Error (Loss)



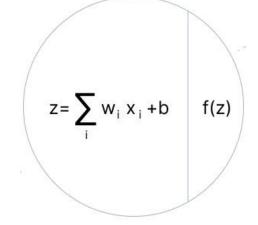
Do we want to increase or reduce this amount when modifying the model parameters during training?



- Repeat until stopping criterion met:
  - Forward pass: propagate training data through model to make predictions
  - 2. Error quantification:
    measure error of the
    model's predictions on
    training data using a loss
    function
  - 3. Backward pass: calculate gradients to determine how each model parameter contributed to model error



Recall, each node contains 2 functions:



let o<sub>k</sub> represent the activation
 let z<sub>k</sub> represent the weighted sum
 For node 6, we will first compute:

$$\frac{\partial E}{\partial z_6} = \frac{\partial E}{\partial o_6} * \frac{\partial o_6}{\partial z_6}$$

#### Loss function:

#### constant value

$$\frac{\partial E}{\partial o_6} = \frac{\partial}{\partial o_6} (t_k - o_6)^2 = -2(t_6 - o_6)$$

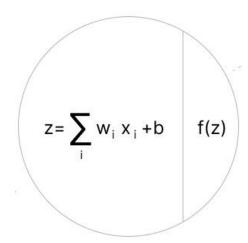
### Activation function (sigmoid):

$$\frac{\partial o_6}{\partial z_6} = \frac{\partial}{\partial z_6} \frac{1}{1 + e^{-z_6}} = (1 - \sigma(z_6)) \sigma(z_6)$$
$$= (1 - o_6)) o_6$$

### Putting them together:

$$\frac{\partial E}{\partial z_6} = -\chi (t_6 - o_6) \quad (1 - o_6) \quad o_6$$

Recall, each node contains 2 functions:



- let  $o_k$  represent the activation - let  $z_k$  represent the weighted sum For node 6, we will first compute:

$$\frac{\partial E}{\partial z_6} = \frac{\partial E}{\partial o_6} * \frac{\partial o_6}{\partial z_6}$$

Can drop constant (does not affect learning)

Loss function:

constant value

Recall, each node contains 2 functions:

Key Observation: Can compute this because both the activation function and loss function are differentiable!!!

$$\frac{\partial o_6}{\partial z_6} = \frac{\partial}{\partial z_6} \frac{1}{1 + e^{-z_6}} = (1 - \sigma(z_6)) \sigma(z_6)$$

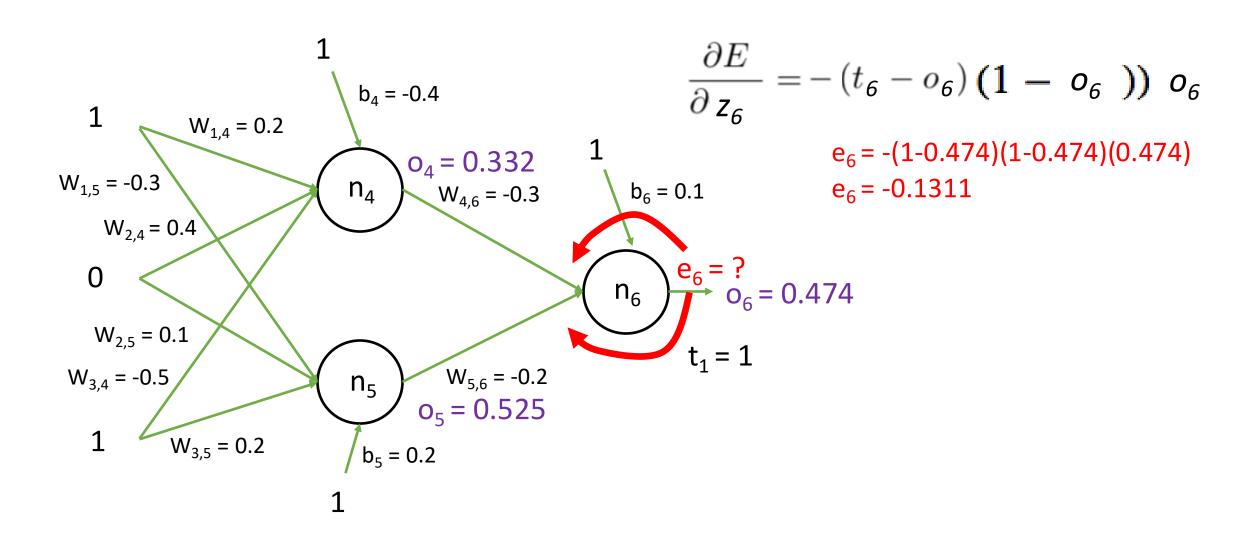
$$= (1 - o_6)) o_6$$

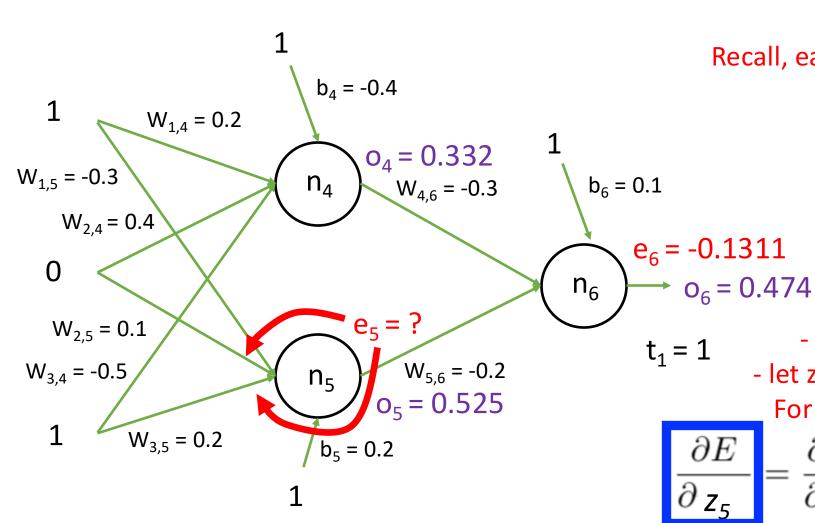
 $\frac{\partial E}{\partial z_6} = - \times (t_6 - o_6) \quad (1 - o_6)) \quad o_6$ 

let o<sub>k</sub> represent the activation
 let z<sub>k</sub> represent the weighted sum
 For node 6, we will first compute:

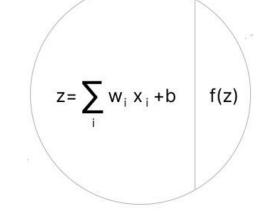
$$\frac{\partial E}{\partial z_6} = \frac{\partial E}{\partial o_6} * \frac{\partial o_6}{\partial z_6}$$

Can drop constant (does not affect learning)





Recall, each node contains 2 functions:



let o<sub>k</sub> represent the activation
 let z<sub>k</sub> represent the weighted sum
 For node 5, we will first compute:

$$\frac{\partial E}{\partial z_5} = \frac{\partial E}{\partial o_6} * \frac{\partial o_6}{\partial z_6} * \frac{\partial z_6}{\partial o_5} * \frac{\partial o_5}{\partial z_5}$$

#### Parent node:

$$\frac{\partial z_6}{\partial o_5} = \frac{\partial}{\partial o_5} \left( o_4 \, W_{4,6} + o_5 \, W_{5,6} + b_6 \right) = W_{5,6}$$

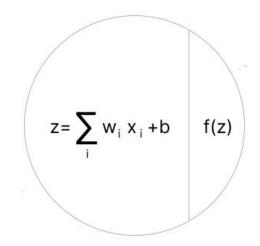
### Activation function (sigmoid):

$$\frac{\partial o_5}{\partial z_5} = \frac{\partial}{\partial z_5} \frac{1}{1 + e^{-z_5}} = (1 - \sigma(z_5)) \sigma(z_5)$$
$$= (1 - o_5)) o_5$$

### Putting them together:

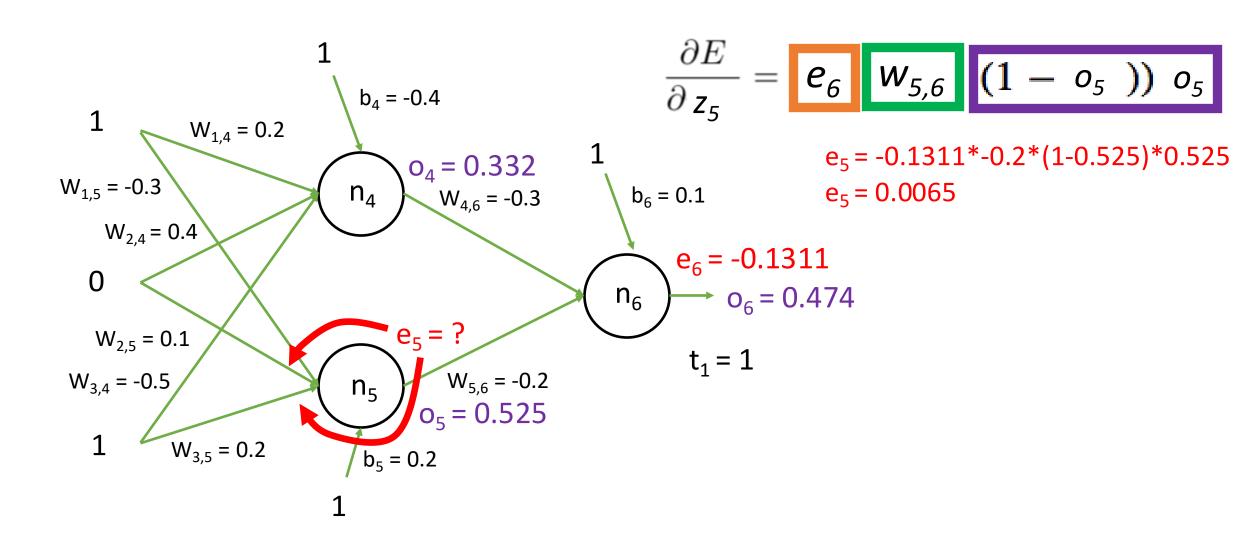
$$\frac{\partial E}{\partial z_5} = \begin{bmatrix} e_6 \end{bmatrix} W_{5,6} \quad (1 - o_5) \quad o_5$$

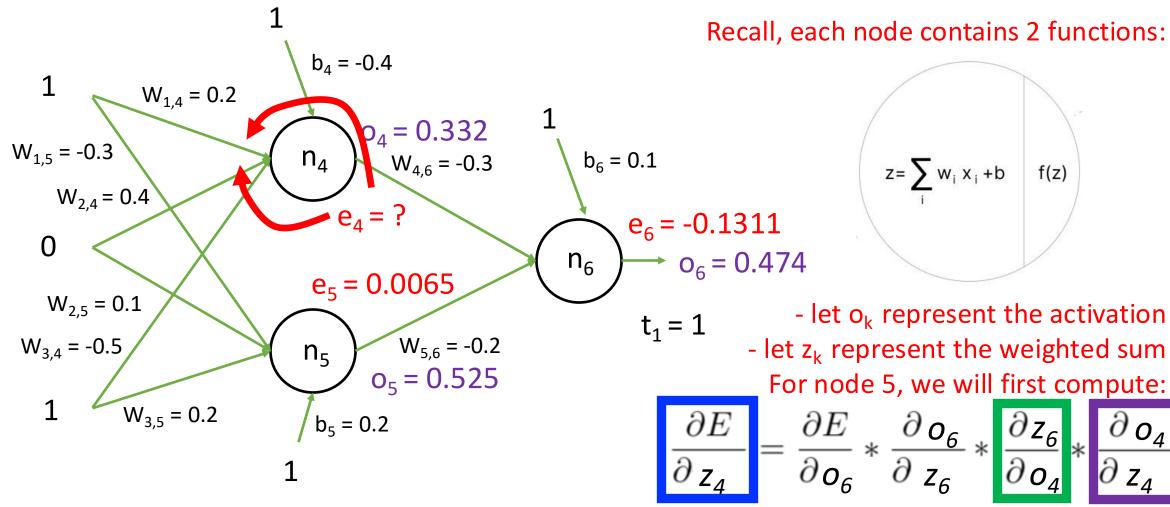
Recall, each node contains 2 functions:



- let  $o_k$  represent the activation - let  $z_k$  represent the weighted sum For node 5, we will first compute:

$$\frac{\partial E}{\partial z_5} = \frac{\partial E}{\partial o_6} * \frac{\partial o_6}{\partial z_6} * \frac{\partial z_6}{\partial o_5} * \frac{\partial o_5}{\partial z_5}$$





#### Parent node:

$$\frac{\partial z_6}{\partial o_4} = \frac{\partial}{\partial o_4} \left( o_4 \, W_{4,6} + o_5 \, W_{5,6} + b_6 \right) = W_{4,6}$$

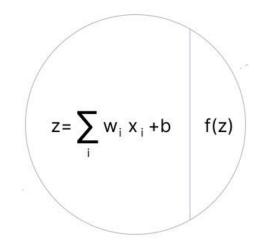
### Activation function (sigmoid):

$$\frac{\partial o_4}{\partial z_4} = \frac{\partial}{\partial z_4} \frac{1}{1 + e^{-z_4}} = (1 - \sigma(z_4)) \sigma(z_4)$$
$$= (1 - o_4)) o_4$$

### Putting them together:

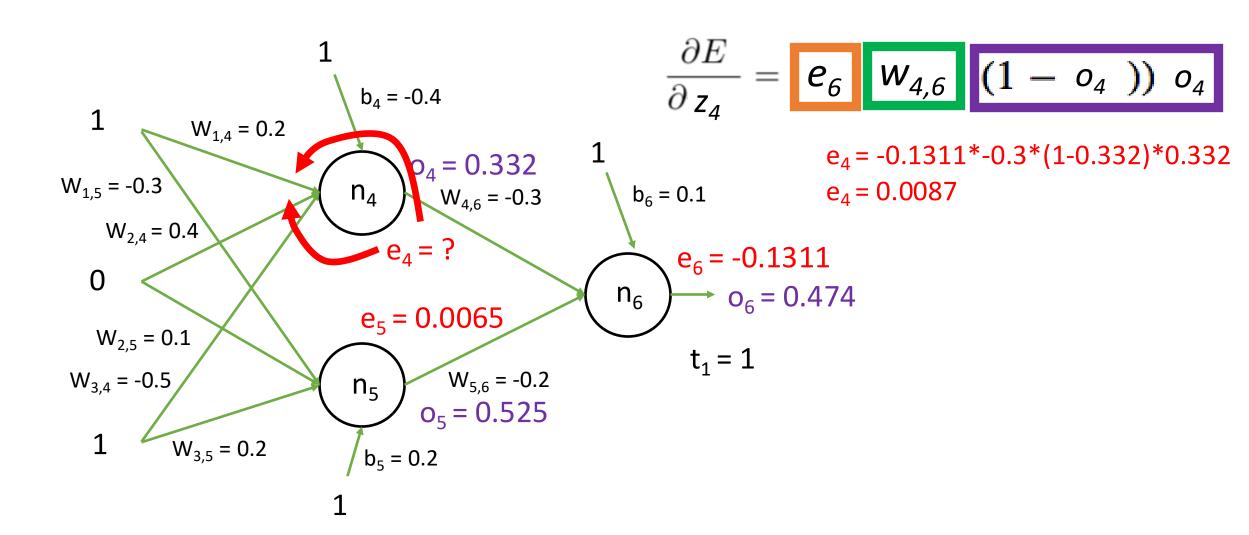
$$\frac{\partial E}{\partial z_4} = \begin{bmatrix} e_6 \end{bmatrix} W_{4,6} \quad (1 - o_4) \quad o_4$$

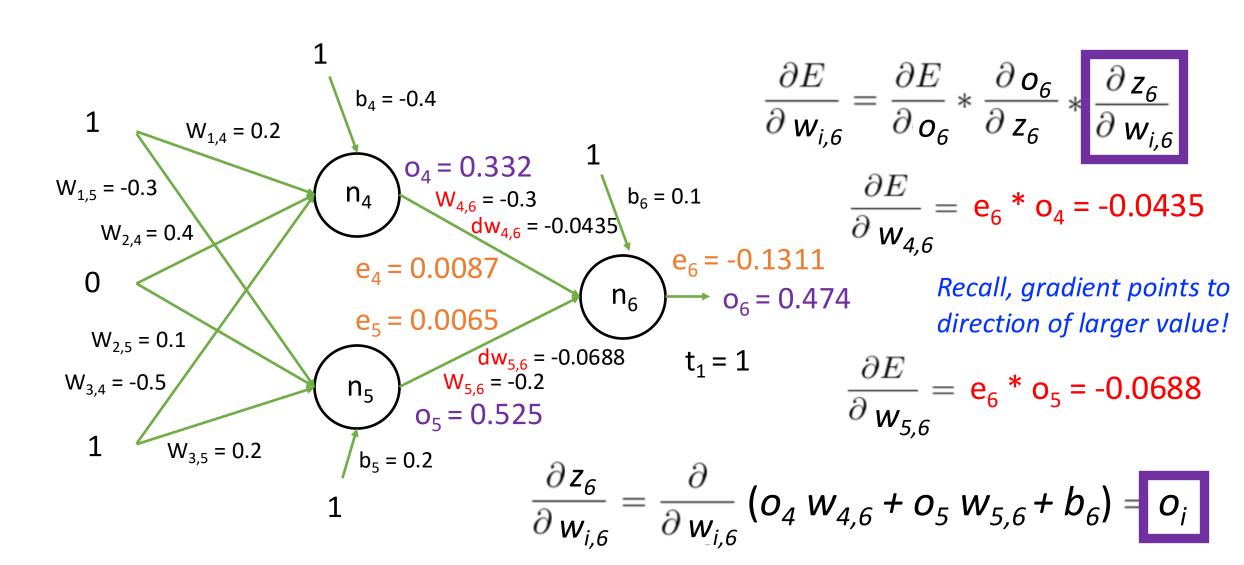
Recall, each node contains 2 functions:

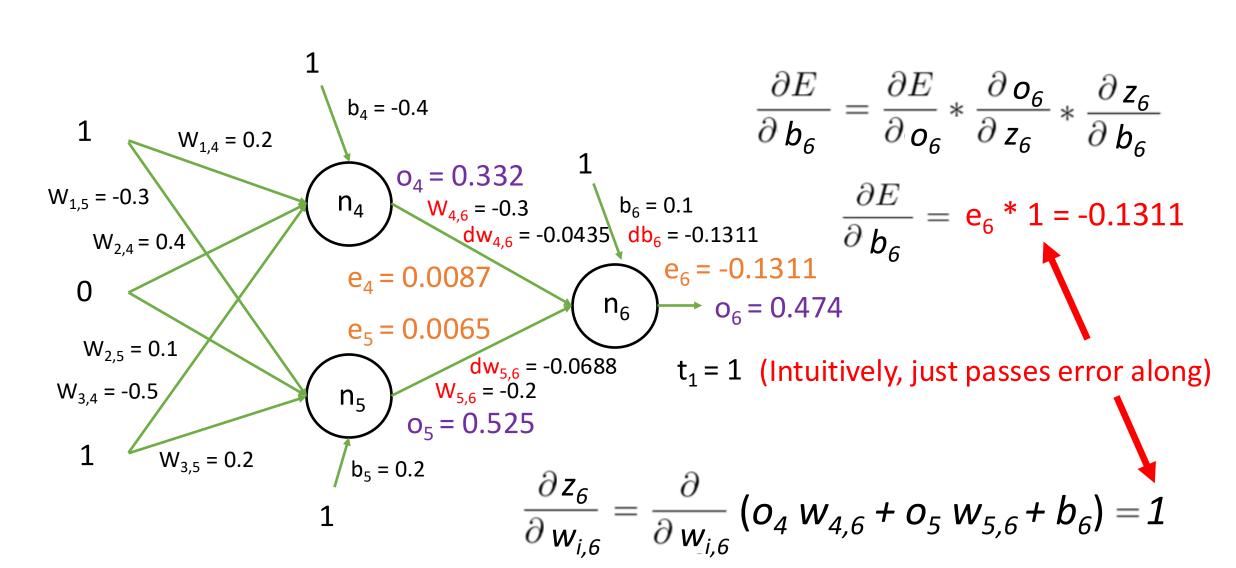


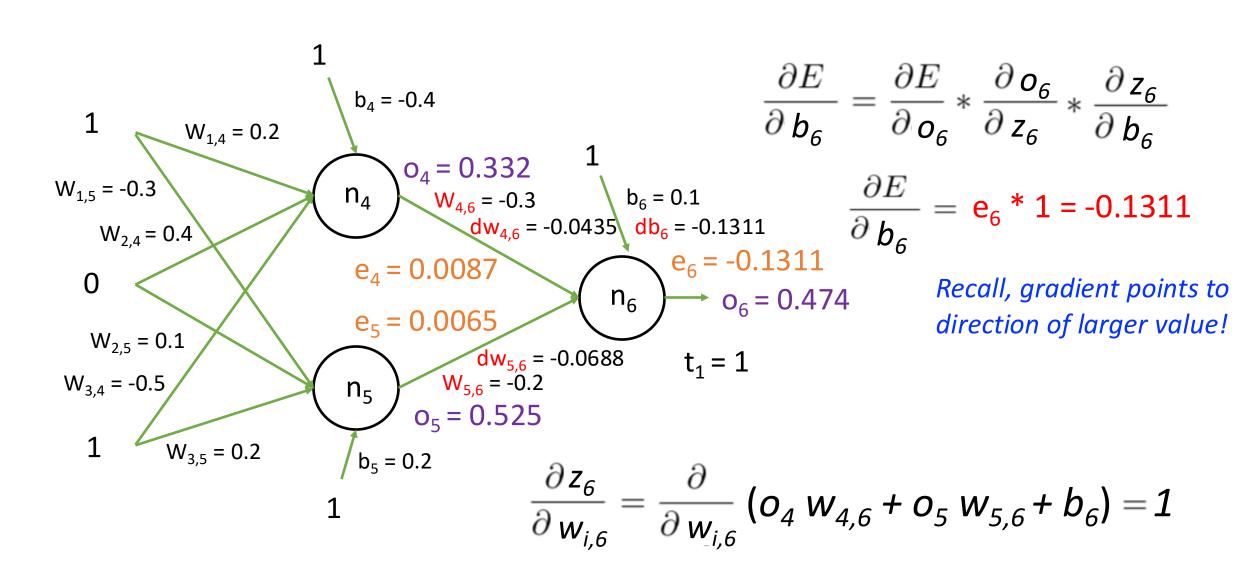
let o<sub>k</sub> represent the activation
 let z<sub>k</sub> represent the weighted sum
 For node 5, we will first compute:

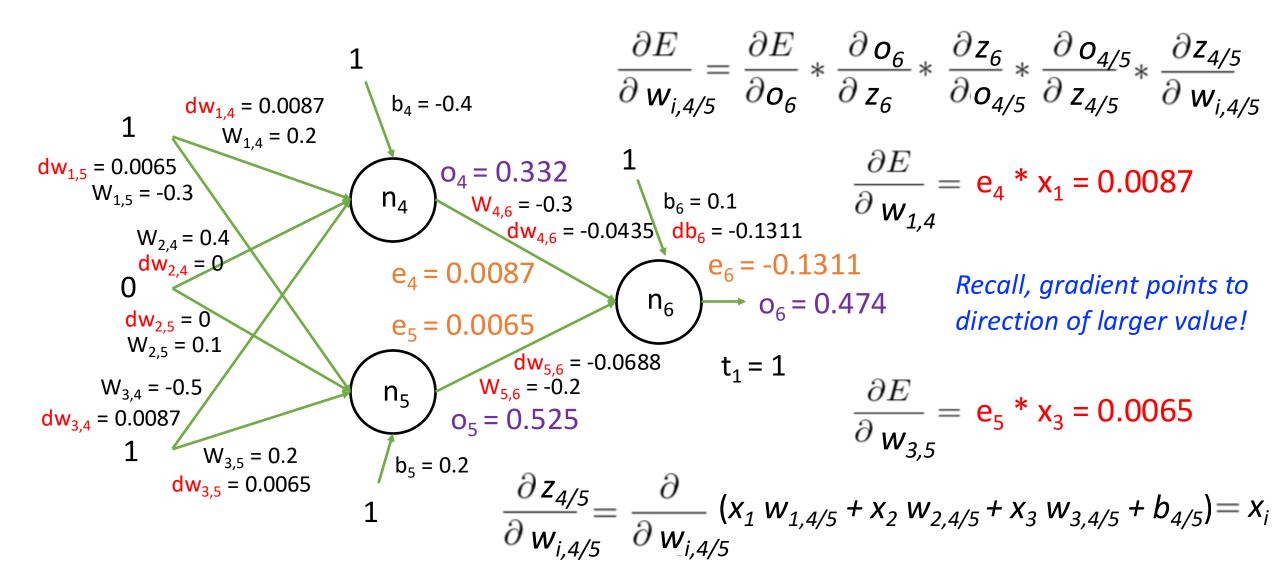
$$\frac{\partial E}{\partial z_4} = \frac{\partial E}{\partial o_6} * \frac{\partial o_6}{\partial z_6} * \frac{\partial z_6}{\partial o_4} * \frac{\partial z_6}{\partial z_4}$$

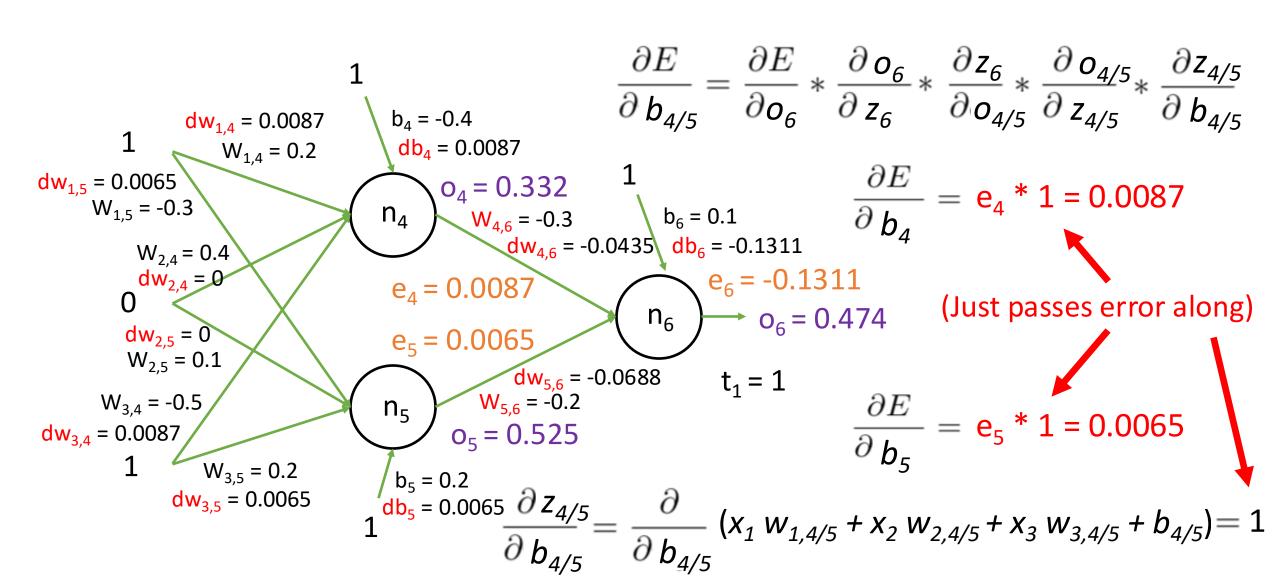


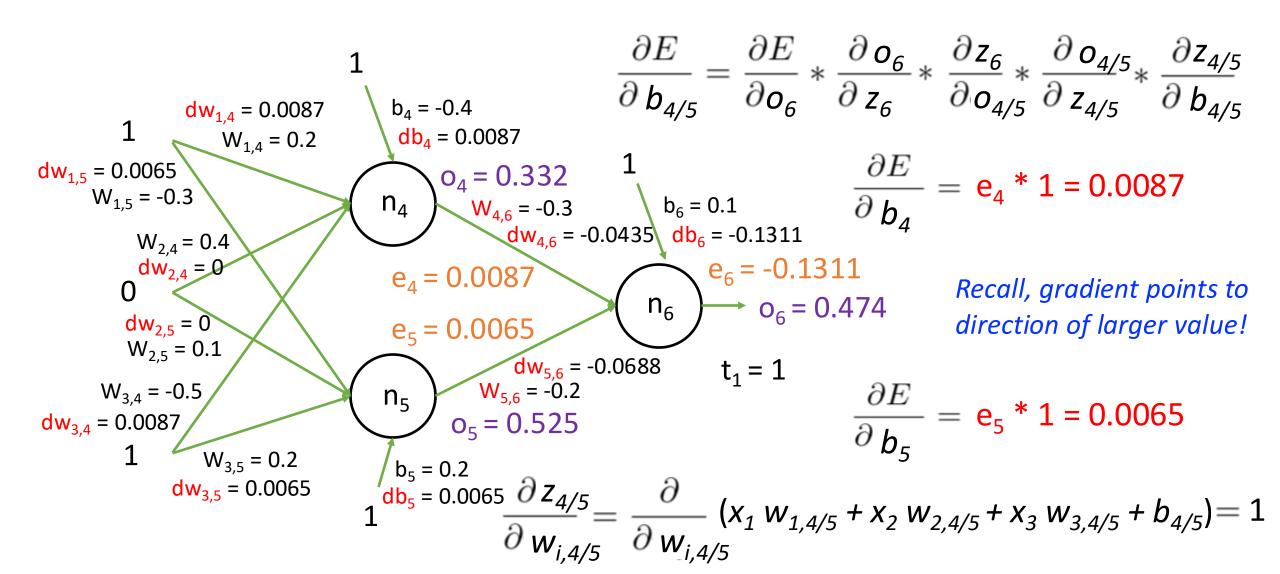


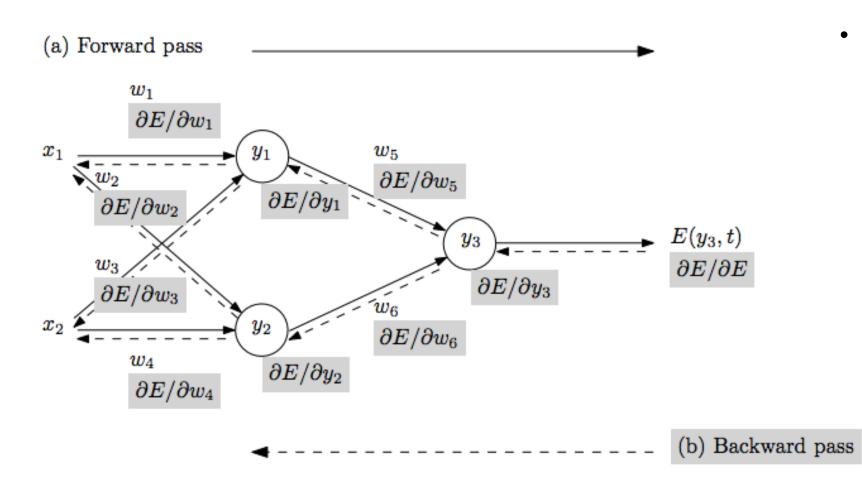




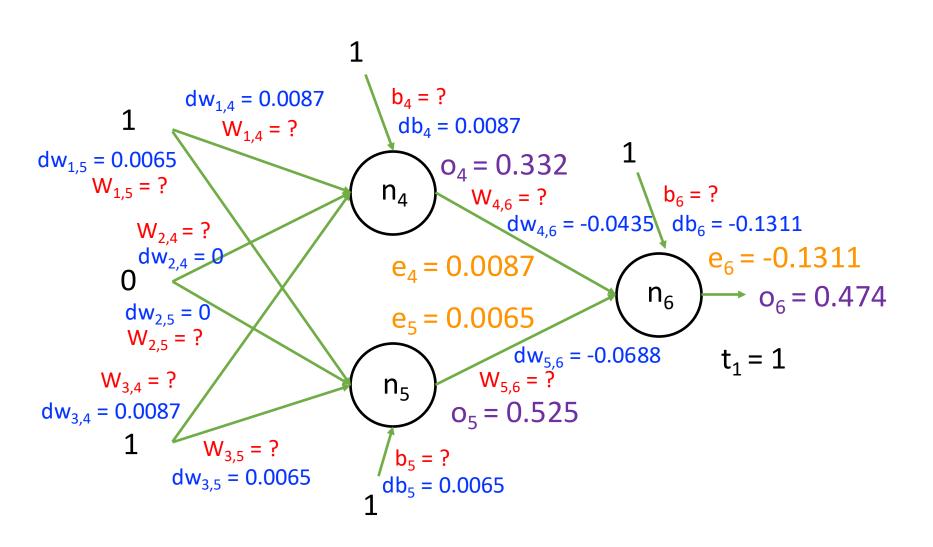


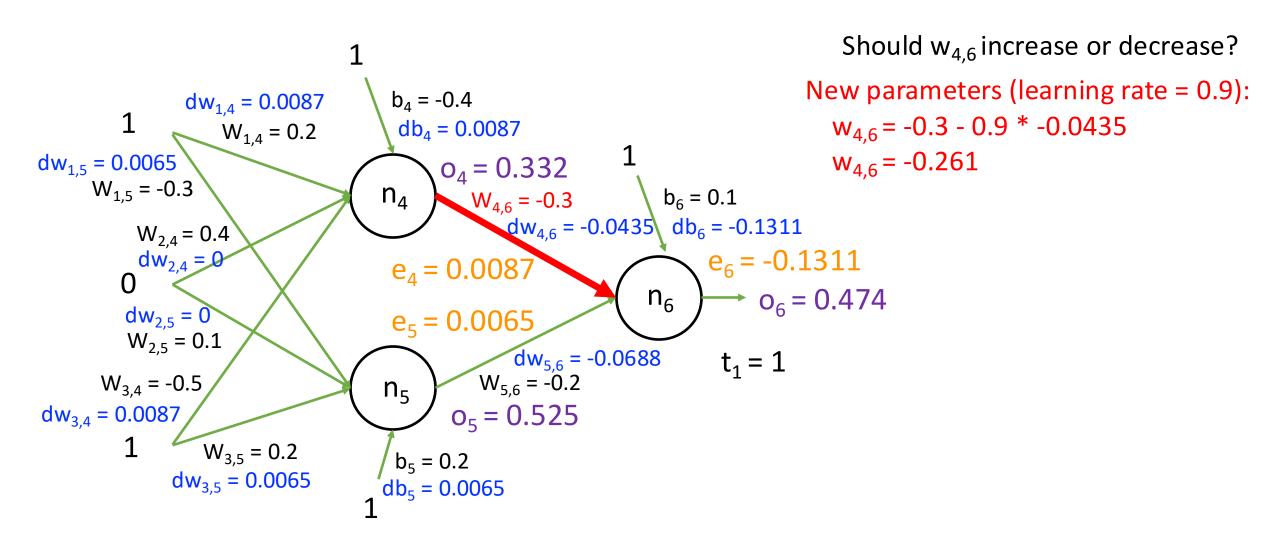


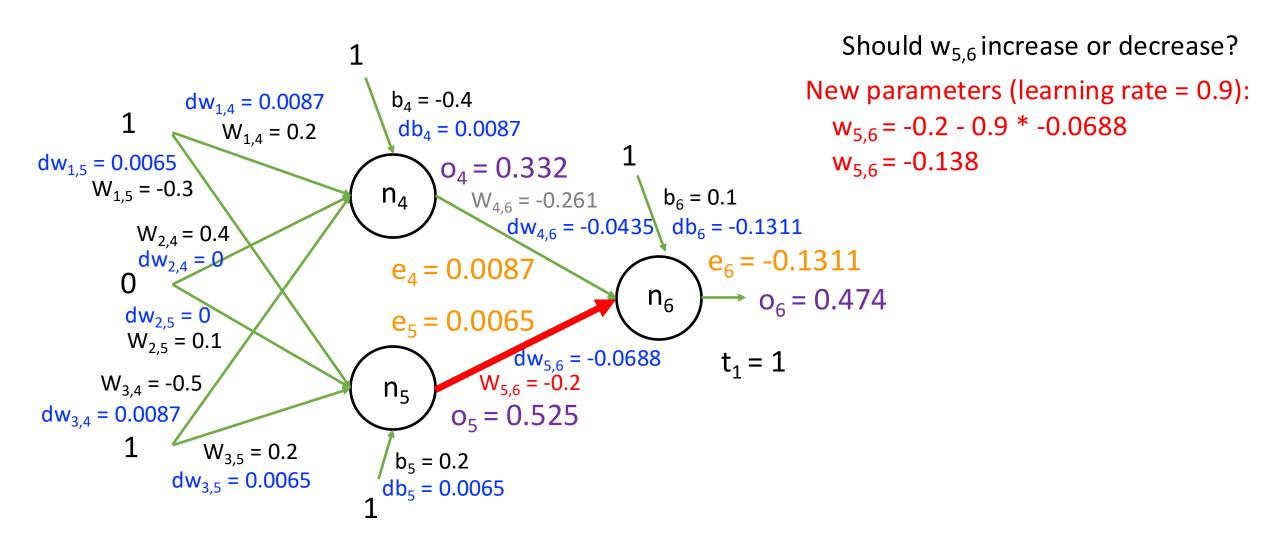


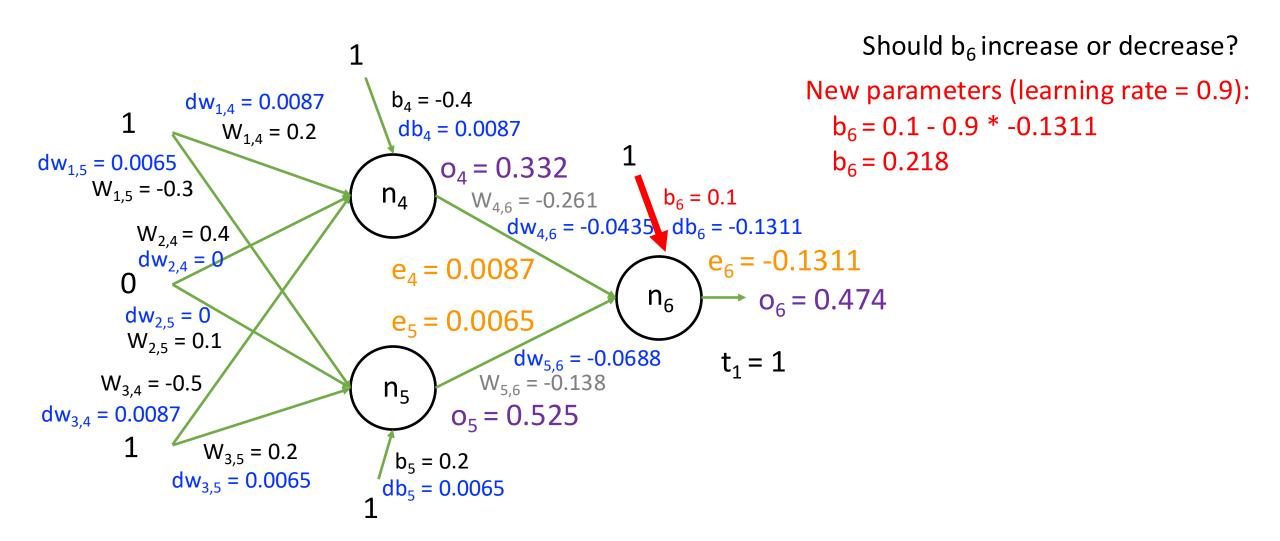


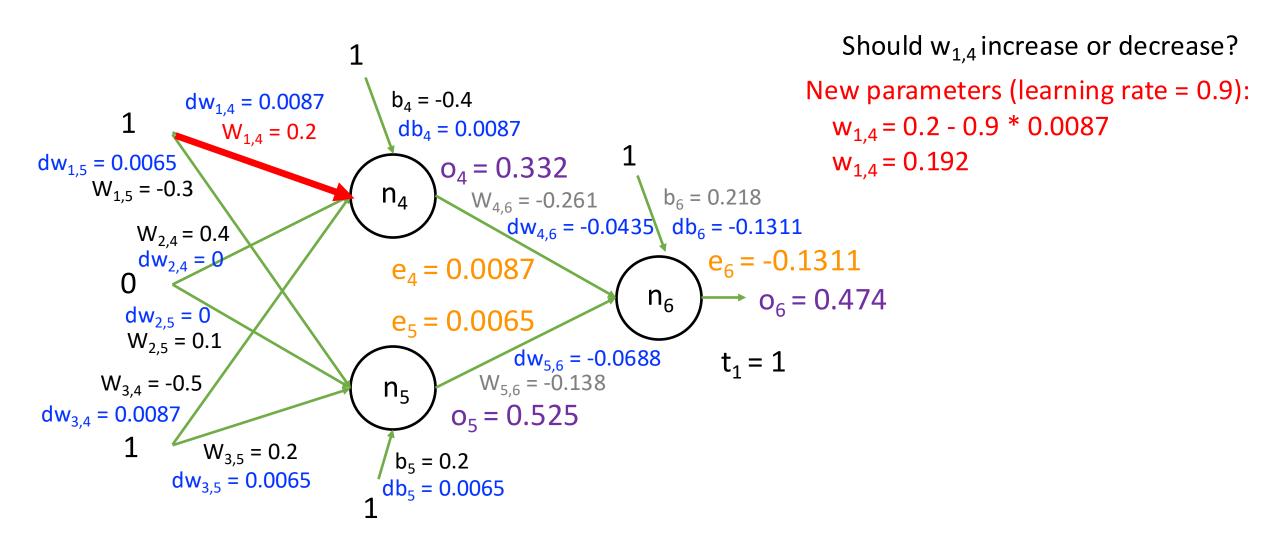
- Repeat until stopping criterion met:
  - Forward pass: propagate training data through model to make predictions
  - 2. Error quantification:
    measure error of the
    model's predictions on
    training data using a loss
    function
  - 3. Backward pass: calculate gradients to determine how each model parameter contributed to model error
  - 4. Update each parameter using calculated gradients

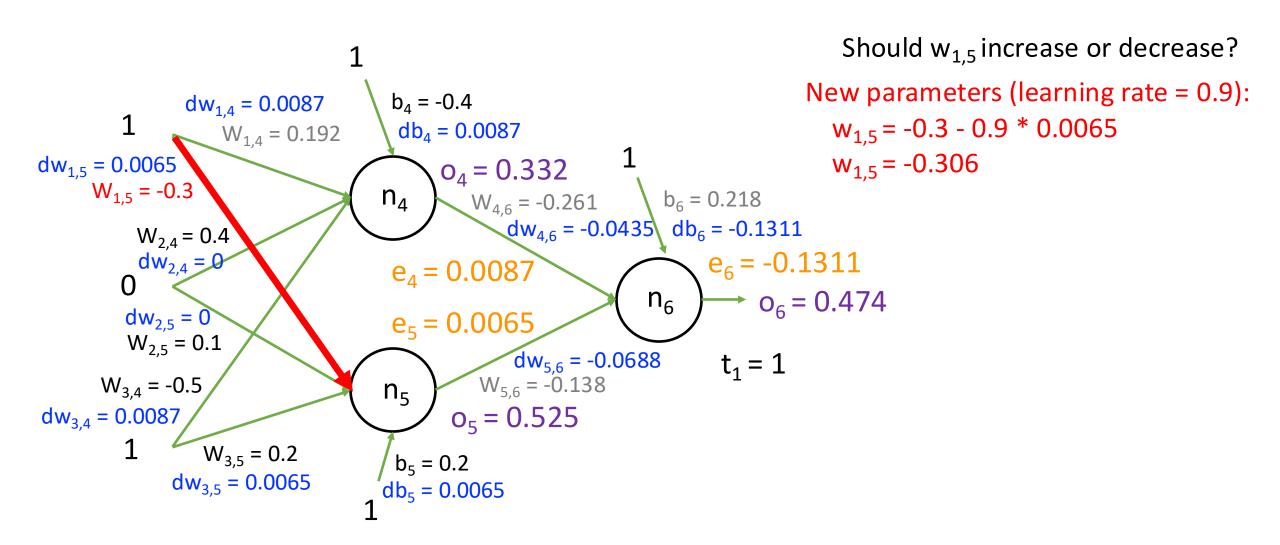


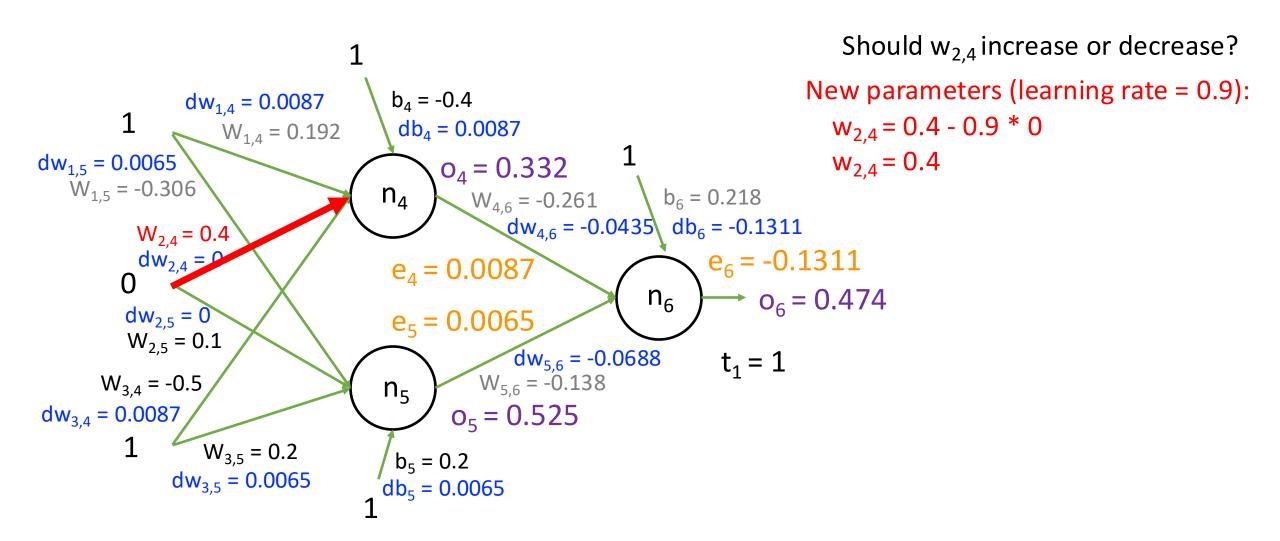


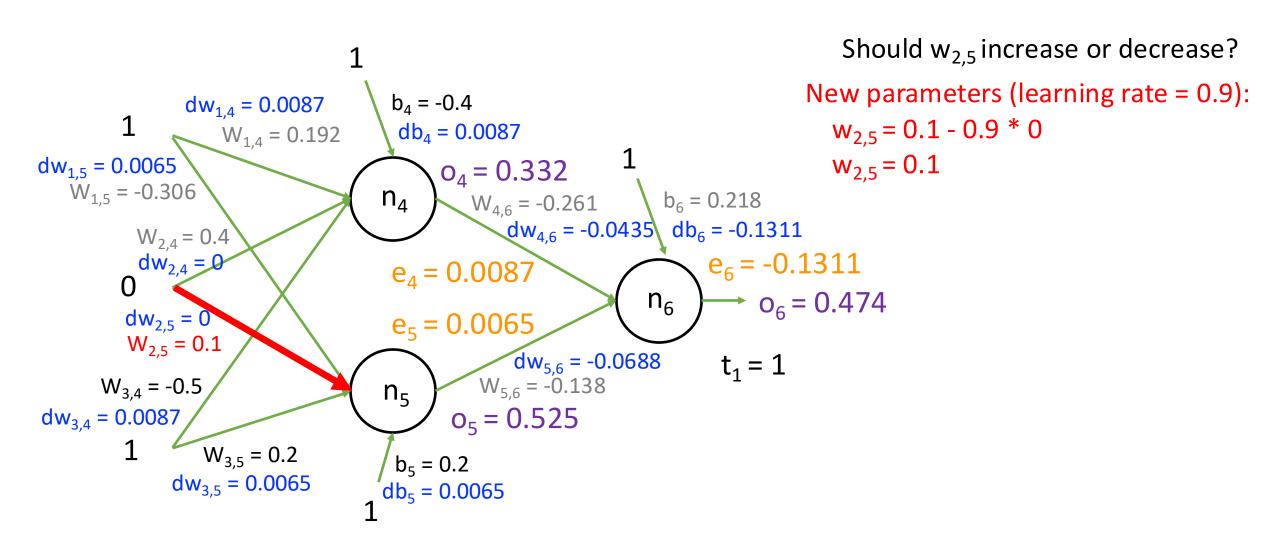


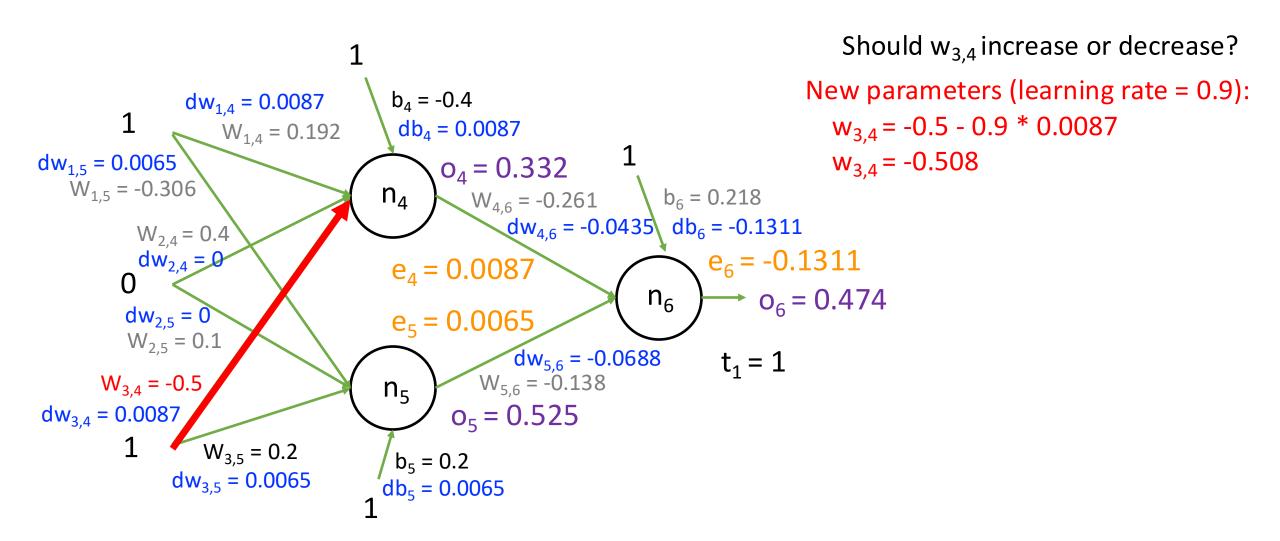


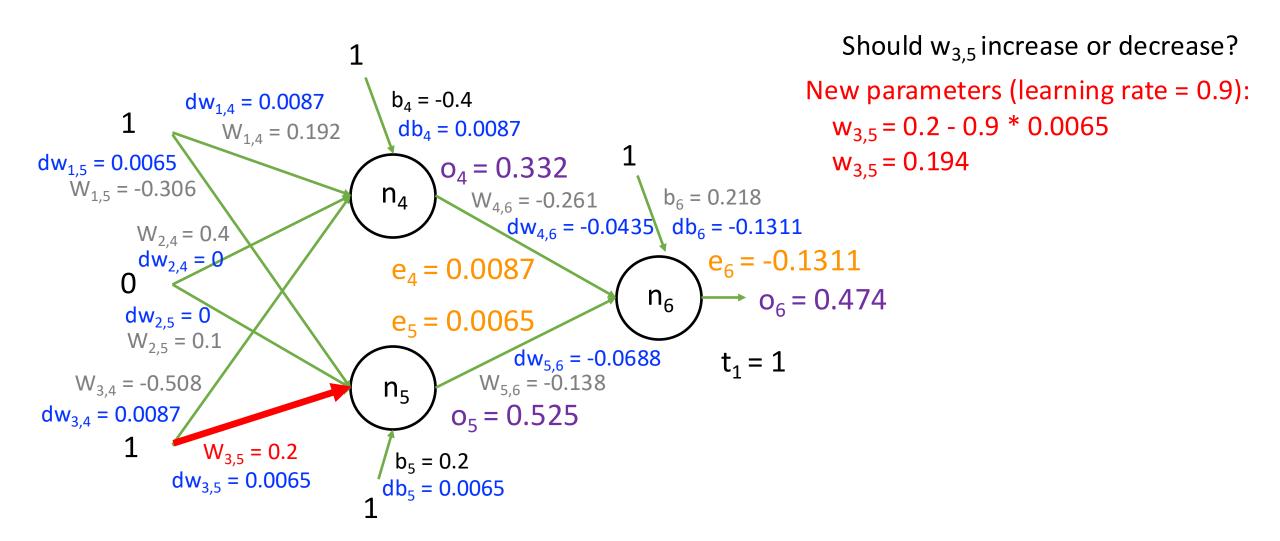


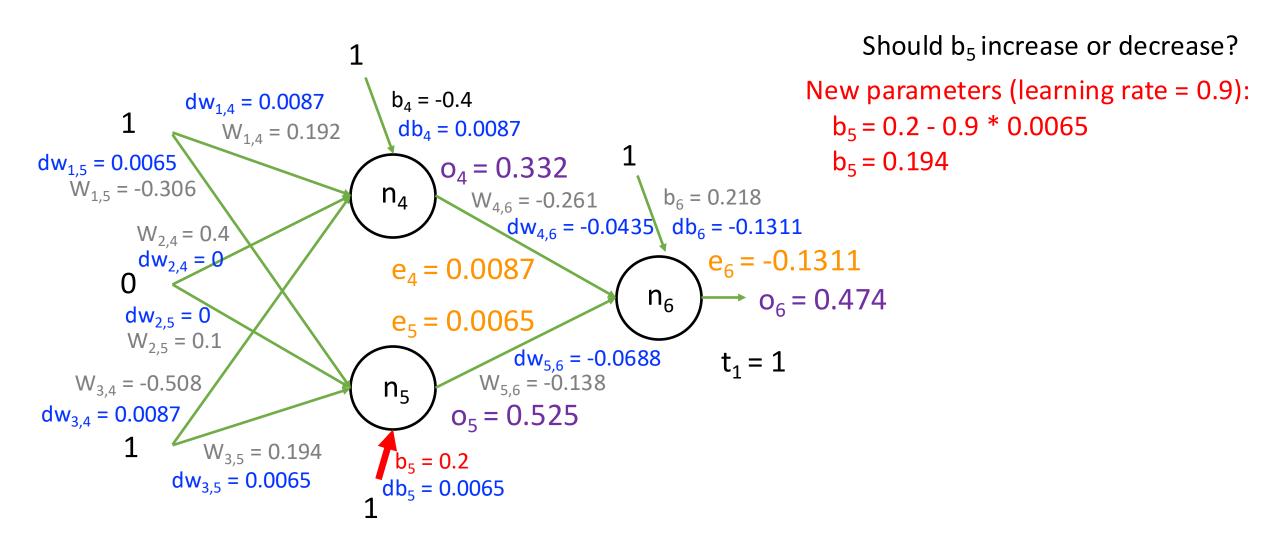


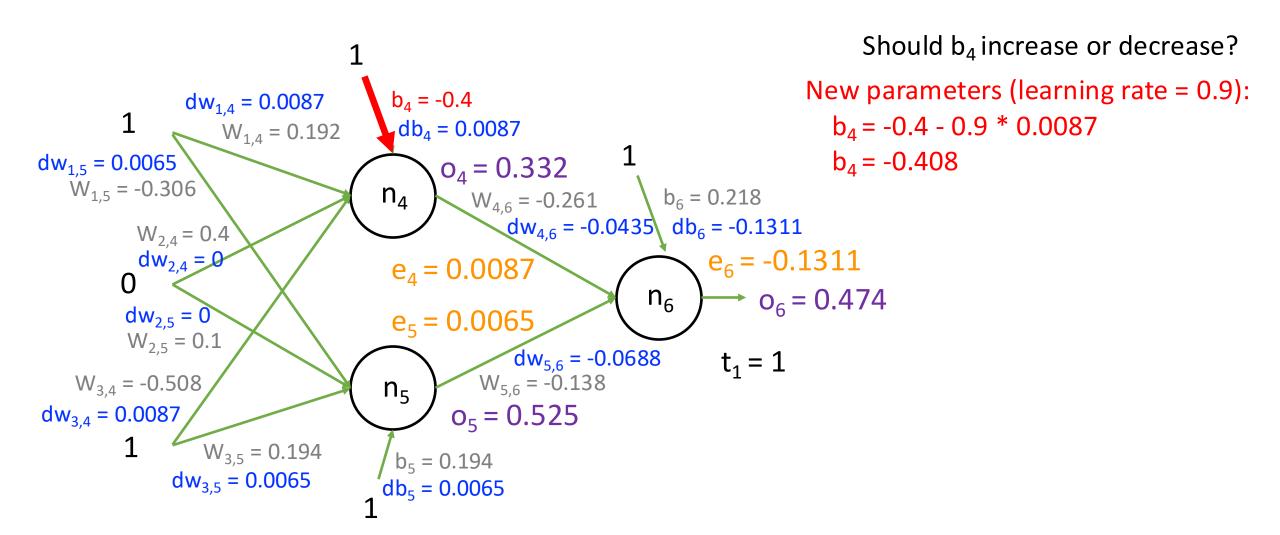




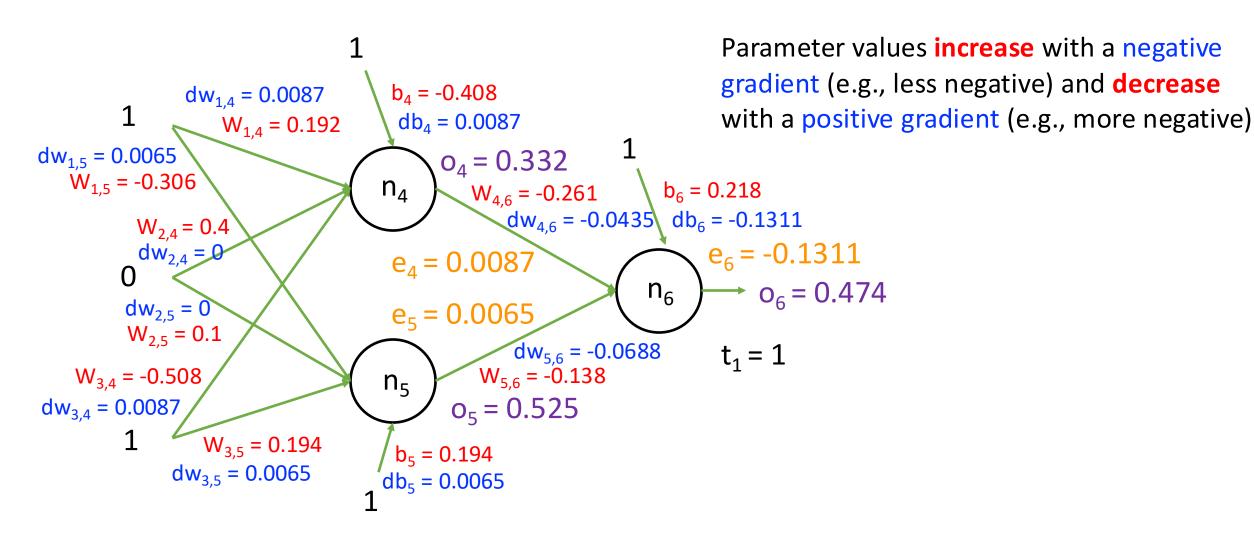








#### Example: Repeat Steps 1-4 With New Samples



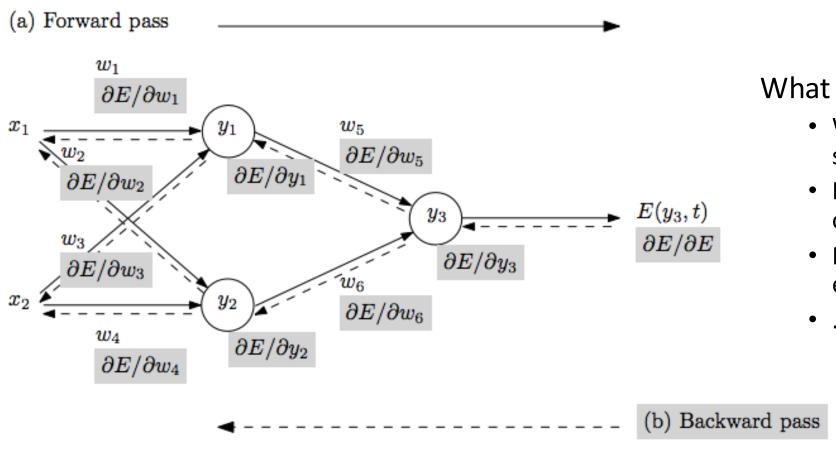
## Example: Completed Training Example For...

• Binary classification: predict if a student will get a B or better (minimum required for CS graduate student in this course)

#### • Inputs:

- Fraction of assignments completed
- Fraction of readings read
- Fraction of lectures watched

#### When to Stop Training Neural Networks?



#### What stopping criterion to use?

- Weight changes are incredibly small
- Finished a pre-specified number of epochs
- Percentage of misclassified example is below some threshold

## Training Summary: How Neural Networks Learn

Calculating gradients depends on:

- 1) Objective/loss function
  - 2) Activation functions

- Repeat until stopping criterion met:
  - 1. Forward pass: propagate training data through model to make predictions
  - 2. Error quantification:
    measure error of the
    model's predictions on
    training data using a loss
    function
  - 3. Backward pass: calculate gradients to determine how each model parameter contributed to model error
  - 4. Update each parameter using calculated gradients



## Today's Topics

Gradient descent: how neural networks learn

Mathematical foundation of gradient descent: derivatives

Applying gradient descent to train neural networks

Training example

The End