Neural Networks II

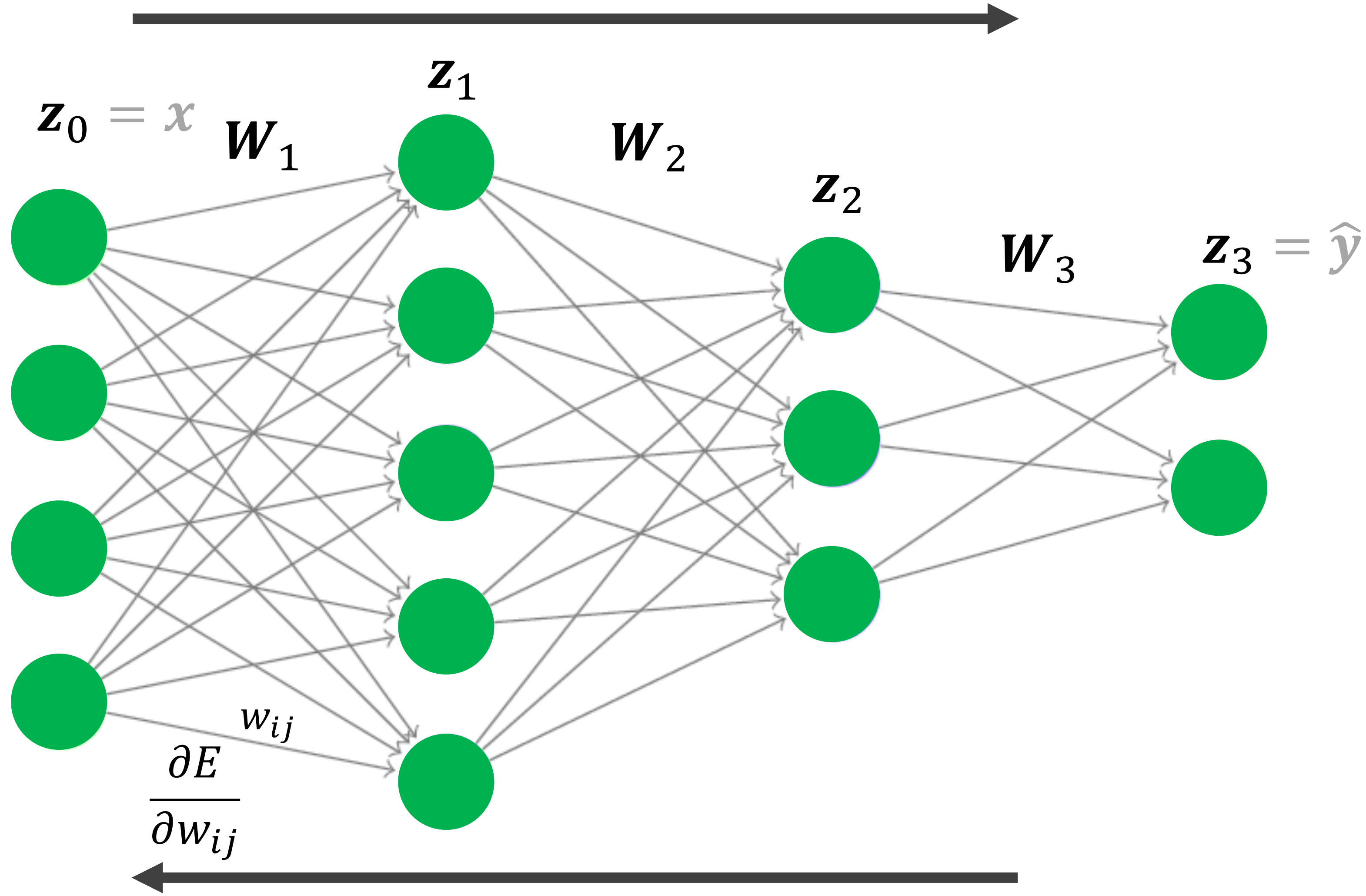
Lecture 17

What is a neural network and **how does it work**?

How do we **choose model weights**?
(i.e. how do we fit our model to data)

What are the challenges of using neural networks?

Forward propagation to create prediction and calculate training error



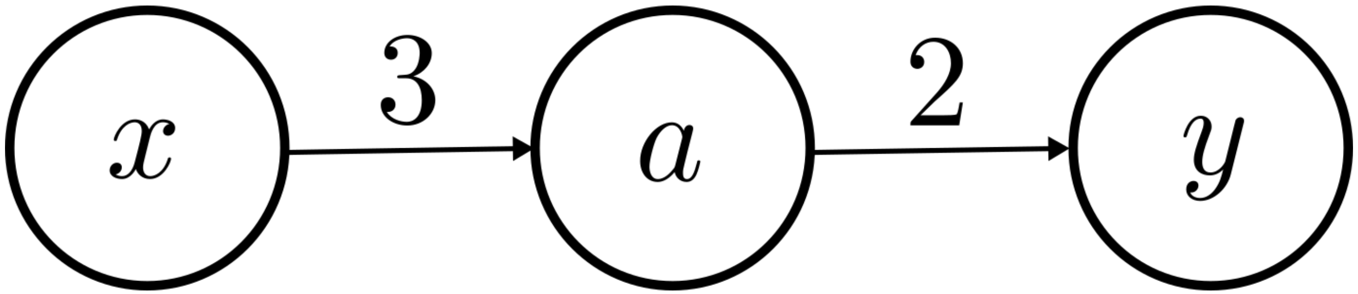
$$E = \frac{1}{2}\sum_k (\hat{y}_k - y_k)^2$$

Backpropagation lets us **assign the error** to each of the parameters so we can tune them

(gradient descent) $w_{ij} \leftarrow w_{ij} - \eta \frac{\partial E}{\partial w_{ij}}$

Backpropagation is simply the recursive application of the chain rule

Example #1



$$y = 2a \qquad \frac{\partial y}{\partial a} = 2$$

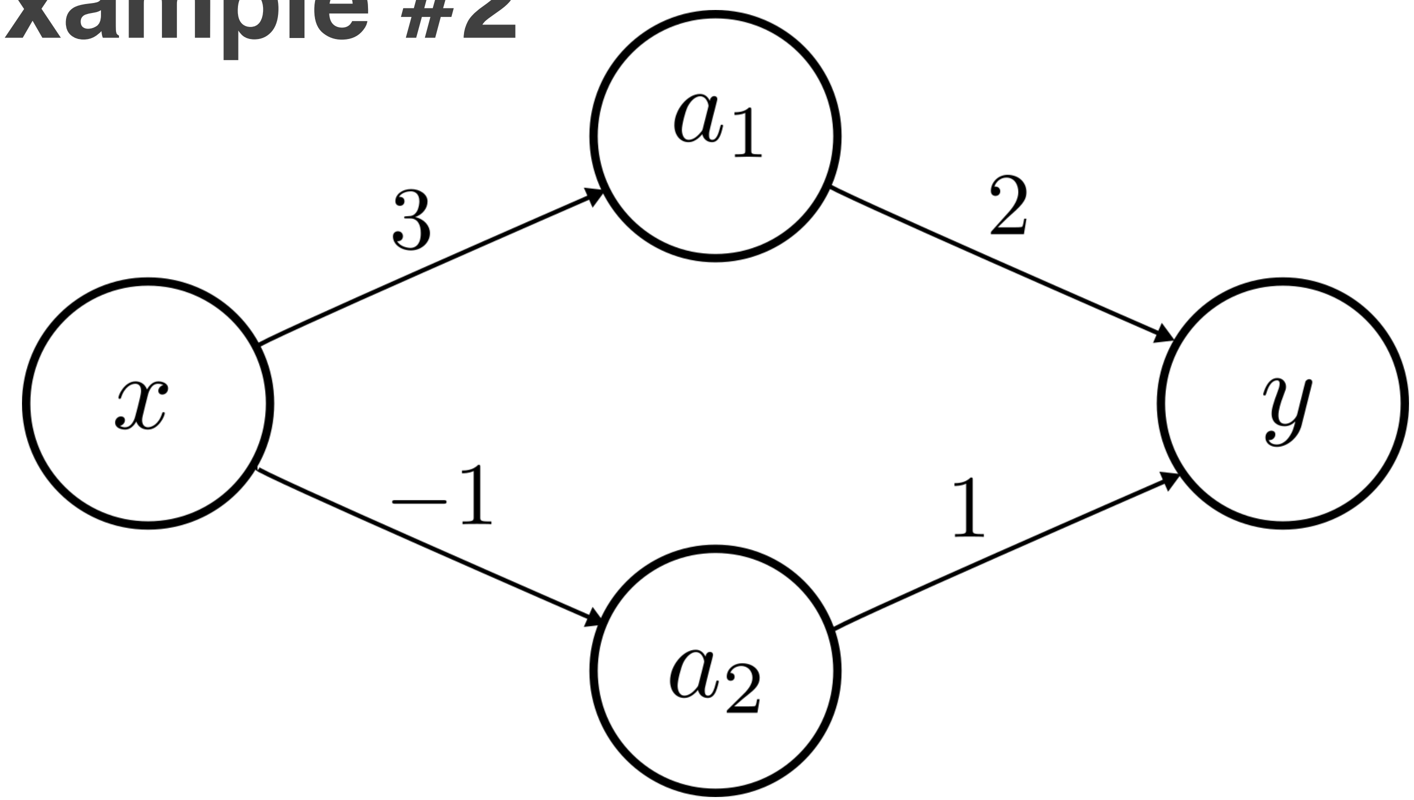
$$a = 3x \qquad \frac{\partial a}{\partial x} = 3$$

$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial a}\frac{\partial a}{\partial x} = (2)(3) = 6$$

Chain Rule

Along a path we apply the chain rule

Example #2



$$y = 2a_1 + a_2$$

$$a_1 = 3x$$

$$a_2 = -x$$

$$\frac{\partial y}{\partial x} = \frac{\partial}{\partial x}(2a_1 + 1a_2)$$

Sum Rule

Across paths we apply the sum rule

$$= (2)\frac{\partial a_1}{\partial x} + (1)\frac{\partial a_2}{\partial x}$$

Chain Rule

$$= \frac{\partial y}{\partial a_1}\frac{\partial a_1}{\partial x} + \frac{\partial y}{\partial a_2}\frac{\partial a_2}{\partial x}$$

$$= (2)(3) + (1)(-1)$$

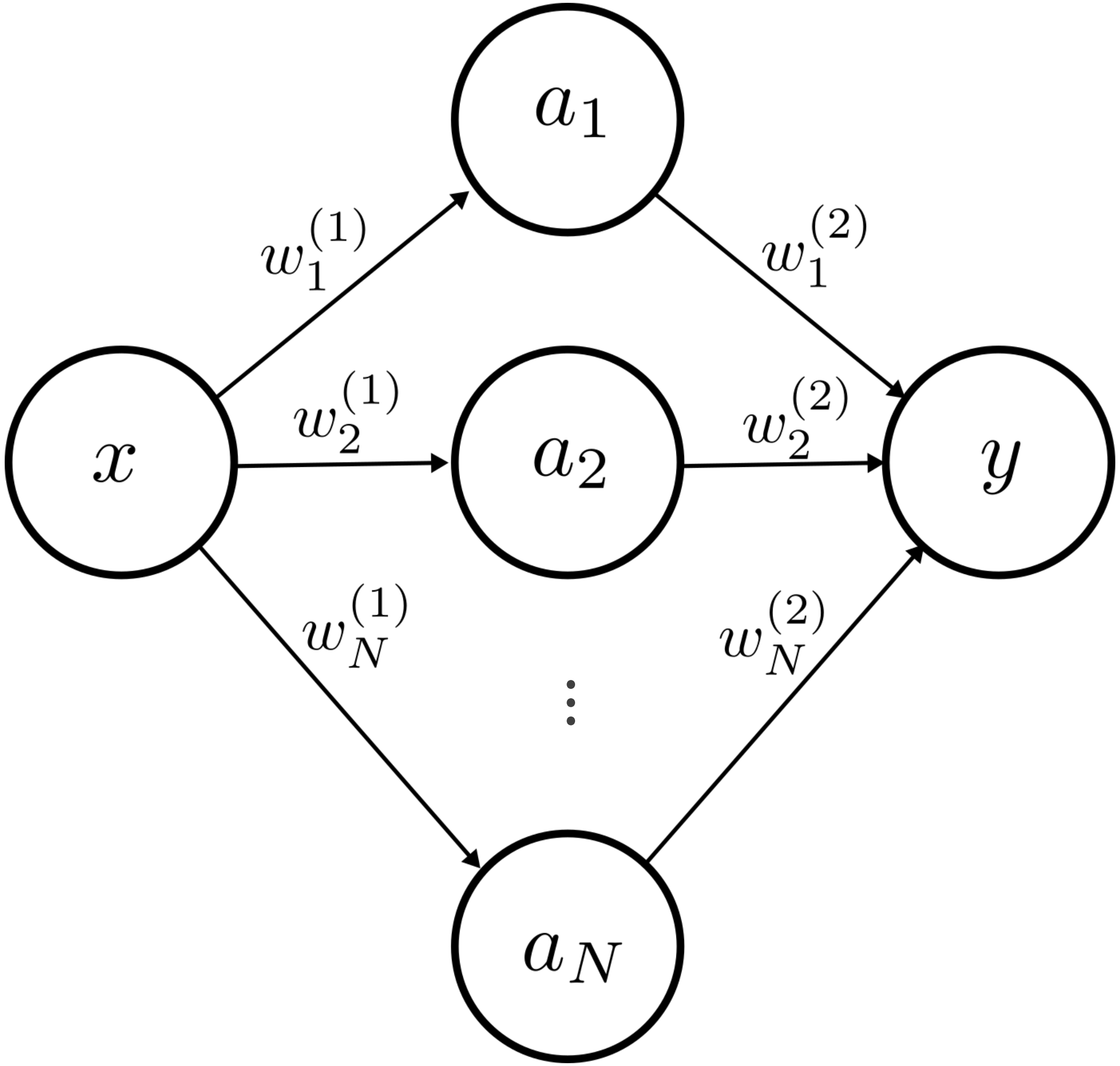
$$= 5$$

Example #3

$$y = \sum_{j=1}^{N} w_j^{(2)} a_j \qquad \frac{\partial y}{\partial a_i} = w_i^{(2)}$$

$$a_i = w_i^{(1)} x \qquad \frac{\partial a_i}{\partial x} = w_i^{(1)}$$

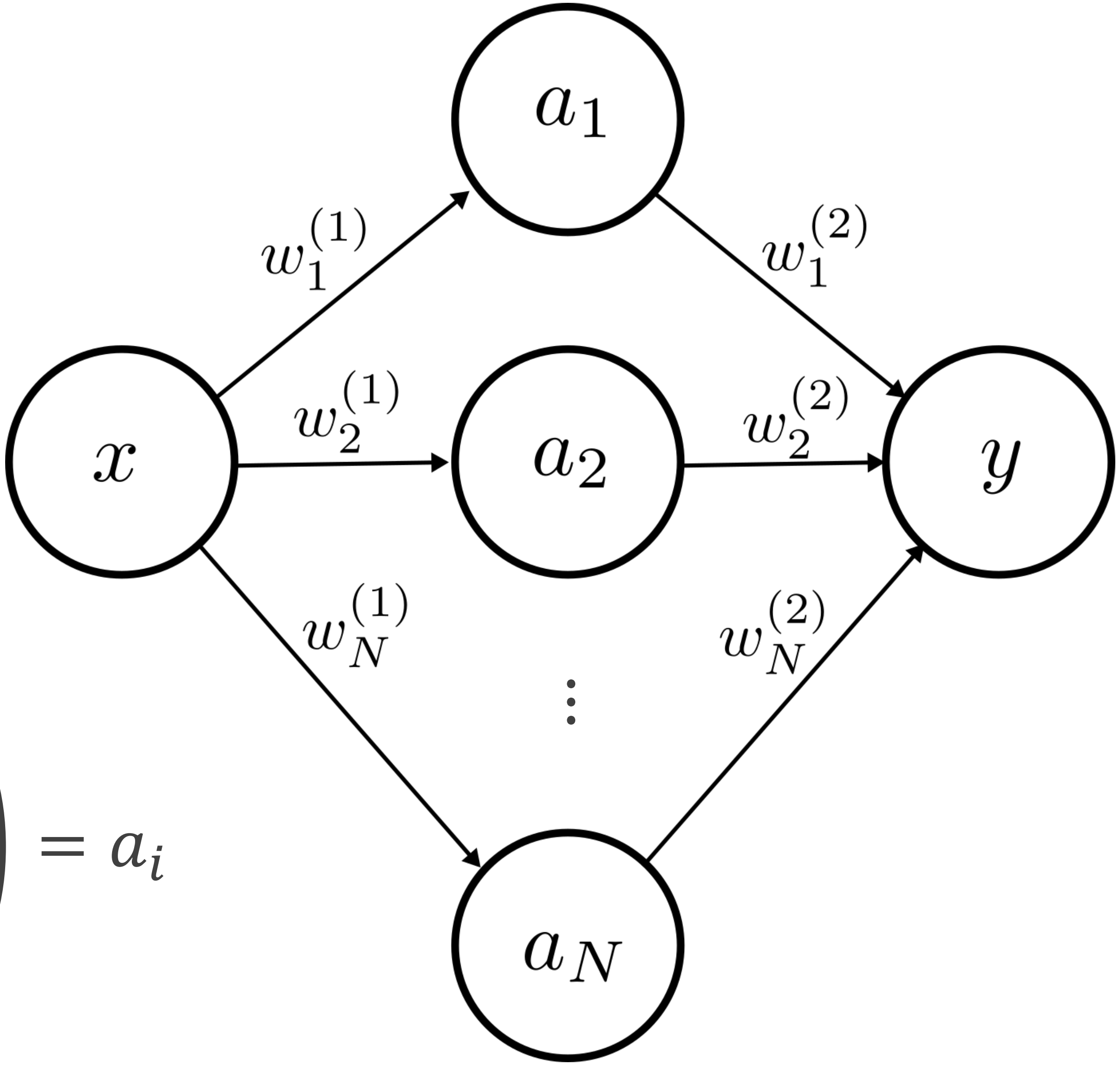
$$\frac{\partial y}{\partial x} = \sum_{j=1}^{N} \frac{\partial y}{\partial a_j} \frac{\partial a_j}{\partial x} = \sum_{j=1}^{N} w_j^{(2)} w_j^{(1)}$$



Example #3

$$y = \sum_{j=1}^{N} w_j^{(2)} a_j \qquad \frac{\partial y}{\partial a_i} = w_i^{(2)}$$

$$a_i = w_i^{(1)} x \qquad \frac{\partial a_i}{\partial x} = w_i^{(1)}$$



Derivatives with respect to the weights:

$$\frac{\partial y}{\partial w_i^{(2)}} = \frac{\partial y}{\partial y} \frac{\partial y}{\partial w_i^{(2)}} = \frac{\partial}{\partial w_i^{(2)}} \left(\sum_{j=1}^{N} w_j^{(2)} a_j \right) = a_i$$

$$\frac{\partial y}{\partial w_i^{(1)}} = \frac{\partial y}{\partial a_i} \frac{\partial a_i}{\partial w_i^{(1)}} = w_i^{(2)} x$$

Backpropagation intuitively

Consider a derivative of a complicated function that can be represented as a long chain rule application

$$\frac{\partial f}{\partial z} = \underbrace{\frac{\partial f}{\partial w}\frac{\partial w}{\partial x}}_{\frac{\partial f}{\partial x}}\frac{\partial x}{\partial y}\frac{\partial y}{\partial z}$$

Chain rule equality

This process of using the next step in the chain rule is backpropagation

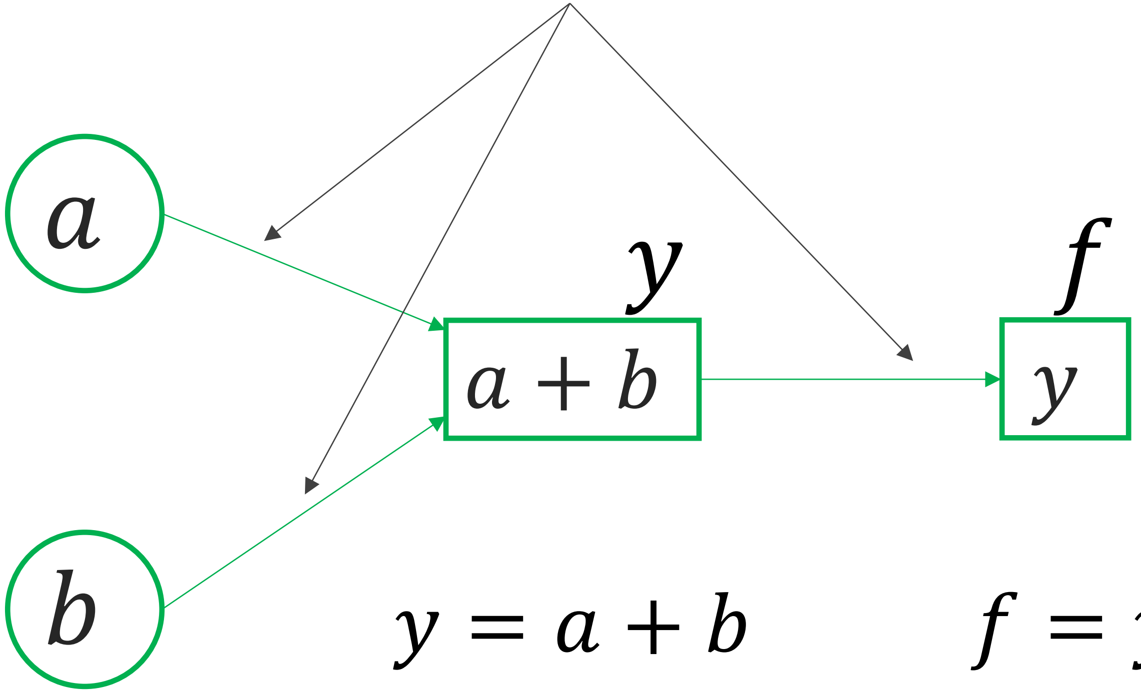
$$\frac{\partial f}{\partial z} = \underbrace{\frac{\partial f}{\partial w}\frac{\partial w}{\partial x}}_{\frac{\partial f}{\partial x}}\frac{\partial x}{\partial y}\frac{\partial y}{\partial z} = \underbrace{\frac{\partial f}{\partial x}\frac{\partial x}{\partial y}}_{\frac{\partial f}{\partial y}}\frac{\partial y}{\partial z} = \underbrace{\frac{\partial f}{\partial y}\frac{\partial y}{\partial z}}_{\frac{\partial f}{\partial z}} = \frac{\partial f}{\partial z}$$

Simple example

Edges are outputs from the last node and inputs to the next function.

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

This graph to the right represents this function



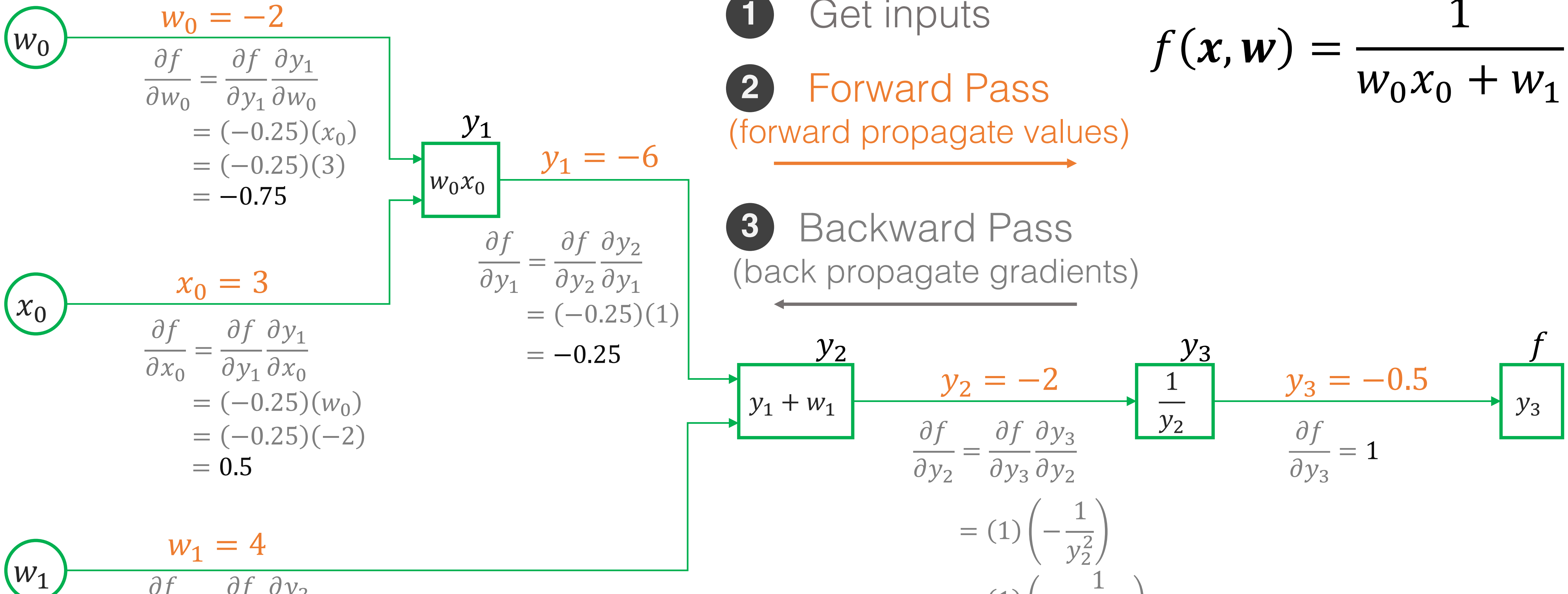
Name of the variable at that node

Operation that the node performs

Local derivatives (one for each edge input into a node): $\frac{\partial y}{\partial a} = 1, \quad \frac{\partial y}{\partial b} = 1$

1. Get inputs
2. Forward Pass
(forward propagate values)
3. Backward Pass
(back propagate gradients)

$$f(\boldsymbol{x},\boldsymbol{w}) = \frac{1}{w_0 x_0 + w_1}$$



$$\frac{\partial f}{\partial w_0} = \frac{\partial f}{\partial y_1}\frac{\partial y_1}{\partial w_0} = (-0.25)(x_0) = (-0.25)(3) = -0.75$$

$$\frac{\partial f}{\partial x_0} = \frac{\partial f}{\partial y_1}\frac{\partial y_1}{\partial x_0} = (-0.25)(w_0) = (-0.25)(-2) = 0.5$$

$$\frac{\partial f}{\partial w_1} = \frac{\partial f}{\partial y_2}\frac{\partial y_2}{\partial w_1} = (-0.25)(1) = -0.25$$

$$\frac{\partial f}{\partial y_1} = \frac{\partial f}{\partial y_2}\frac{\partial y_2}{\partial y_1} = (-0.25)(1) = -0.25$$

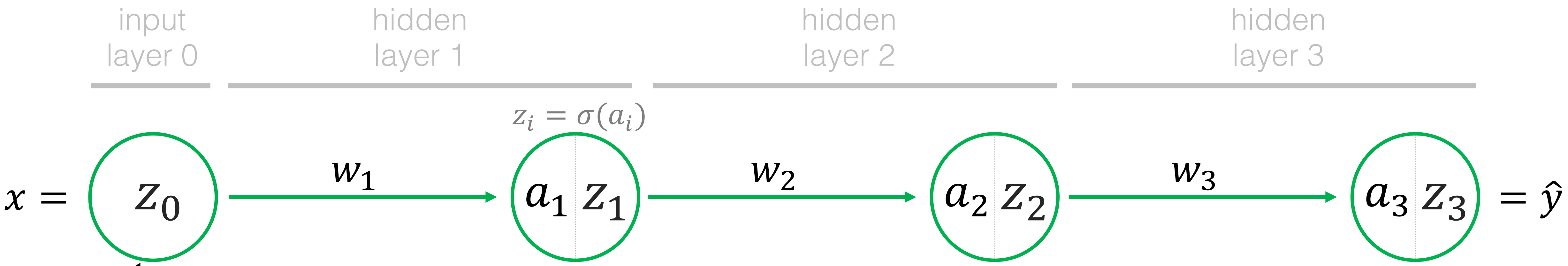
$$\frac{\partial f}{\partial y_2} = \frac{\partial f}{\partial y_3}\frac{\partial y_3}{\partial y_2} = (1)\left(-\frac{1}{y_2^2}\right) = (1)\left(-\frac{1}{(-2)^2}\right) = -0.25$$

$$\frac{\partial f}{\partial y_3} = 1$$

Local derivatives:
(one per edge)

$$\frac{\partial y_1}{\partial w_0} = x_0, \quad \frac{\partial y_1}{\partial x_0} = w_0 \qquad \frac{\partial y_2}{\partial y_1} = \frac{\partial y_2}{\partial w_1} = 1 \qquad \frac{\partial y_3}{\partial y_2} = -\frac{1}{y_2^2} \qquad \frac{\partial f}{\partial y_3} = 1$$

Let’s try an example closer to a real neural network



$$E = \frac{1}{2}(\hat{y} - y)^2$$

$$z_3 = \hat{y} = \sigma(a_3)$$

$$a_3 = w_3 z_2$$

$$z_2 = \sigma(a_2)$$

$$a_2 = w_2 z_1$$

$$z_1 = \sigma(a_1)$$

$$a_1 = w_1 z_0 \rightarrow x$$

Forward propagation

In this particular case, this could be written as a single function of z_0

$$\hat{y} = z_3 = \sigma\left(w_3 \sigma\left(w_2 \sigma(w_1 z_0)\right)\right)$$

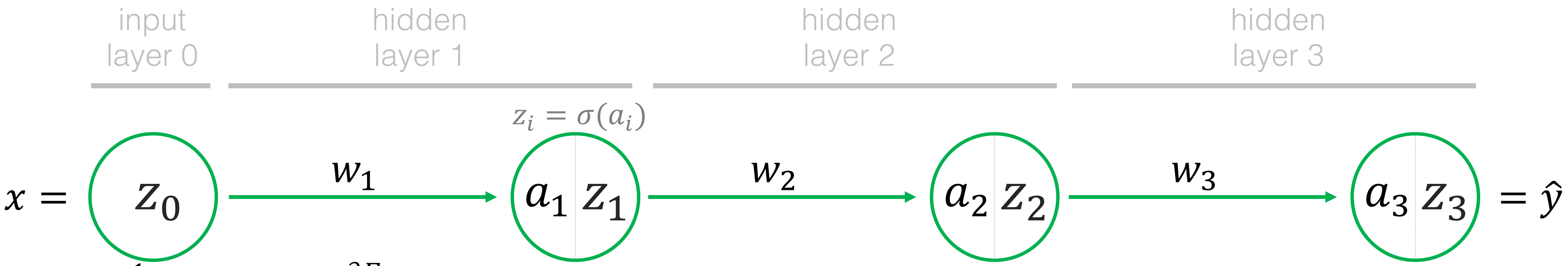
We can calculate the error:

$$E = \frac{1}{2}(\hat{y} - y)^2$$

We want to estimate the gradient with respect to each parameter

$$\frac{\partial E}{\partial w_i}$$

Backpropagation: an efficient way of calculating these values



Forward propagation

$$E = \frac{1}{2}(\hat{y} - y)^2$$

$$\hat{y} = \sigma(a_3)$$

$$a_3 = w_3 z_2$$

$$z_2 = \sigma(a_2)$$

$$a_2 = w_2 z_1$$

$$z_1 = \sigma(a_1)$$

$$a_1 = w_1 z_0$$

Backpropagation

$$\frac{\partial E}{\partial \hat{y}} = \hat{y} - \mathrm{y}$$

$$\frac{\partial \hat{y}}{\partial a_3} = \sigma'(a_3)$$

$$\frac{\partial a_3}{\partial z_2} = w_3$$

$$\frac{\partial z_2}{\partial a_2} = \sigma'(a_2)$$

$$\frac{\partial a_2}{\partial z_1} = w_2$$

$$\frac{\partial z_1}{\partial a_1} = \sigma'(a_1)$$

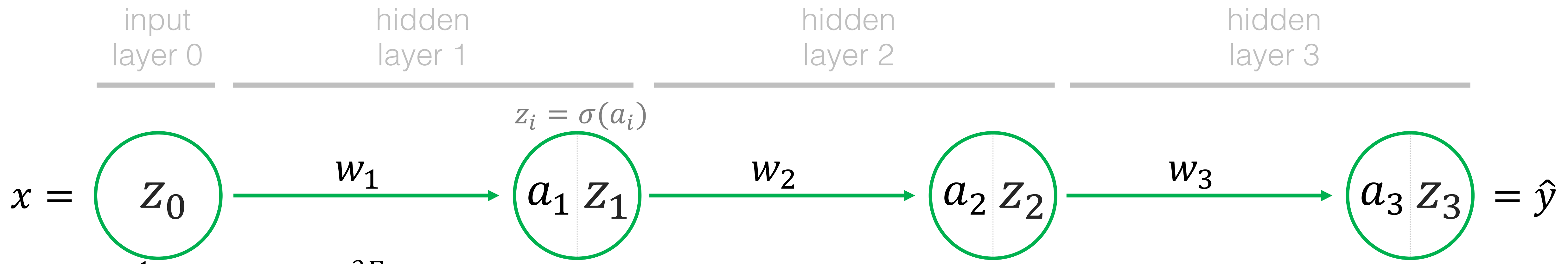
$$\frac{\partial a_1}{\partial w_1} = z_0 = x$$

Let's calculate $\frac{\partial E}{\partial w_1}$

$$\frac{\partial E}{\partial w_1} = \underline{\frac{\partial E}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a_3} \frac{\partial a_3}{\partial z_2} \frac{\partial z_2}{\partial a_2} \frac{\partial a_2}{\partial z_1} \frac{\partial z_1}{\partial a_1}} \frac{\partial a_1}{\partial w_1}$$

$$\frac{\partial E}{\partial w_1} = \underline{(\hat{y} - \mathrm{y})\sigma'(a_3) w_3 \sigma'(a_2) w_2 \sigma'(a_1)} z_0$$

We know all these quantities from forward propagation



Forward propagation

$E = \frac{1}{2}(\hat{y} - y)^2$	$\frac{\partial E}{\partial \hat{y}} = \hat{y} - y$
$\hat{y} = \sigma(a_3)$	$\frac{\partial \hat{y}}{\partial a_3} = \sigma'(a_3)$
$a_3 = w_3 z_2$	$\frac{\partial a_3}{\partial z_2} = w_3$
$z_2 = \sigma(a_2)$	$\frac{\partial z_2}{\partial a_2} = \sigma'(a_2)$
$a_2 = w_2 z_1$	$\frac{\partial a_2}{\partial z_1} = w_2$
$z_1 = \sigma(a_1)$	$\frac{\partial z_1}{\partial a_1} = \sigma'(a_1)$
$a_1 = w_1 z_0$	$\frac{\partial a_1}{\partial w_1} = z_0 = x$

Backpropagation

$$\frac{\partial E}{\partial w_1} = \underbrace{\frac{\partial E}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a_3} \frac{\partial a_3}{\partial z_2} \frac{\partial z_2}{\partial a_2} \frac{\partial a_2}{\partial z_1} \frac{\partial z_1}{\partial a_1}}_{\frac{\partial E}{\partial a_1}} \frac{\partial a_1}{\partial w_1}$$

These derivatives with respect to the activations, a_i, allow us to quickly calculate each of our parameter derivatives:

$$\frac{\partial E}{\partial w_i} = \frac{\partial E}{\partial a_i} \frac{\partial a_i}{\partial w_{i-1}} = \underbrace{\frac{\partial E}{\partial a_i}}_{\delta_i} z_{i-1}$$

δ_i (common shorthand)

Dive deeper into neural network math

5.1 Forward Propagation

Forward propagation is the iterative application of the following two equations:

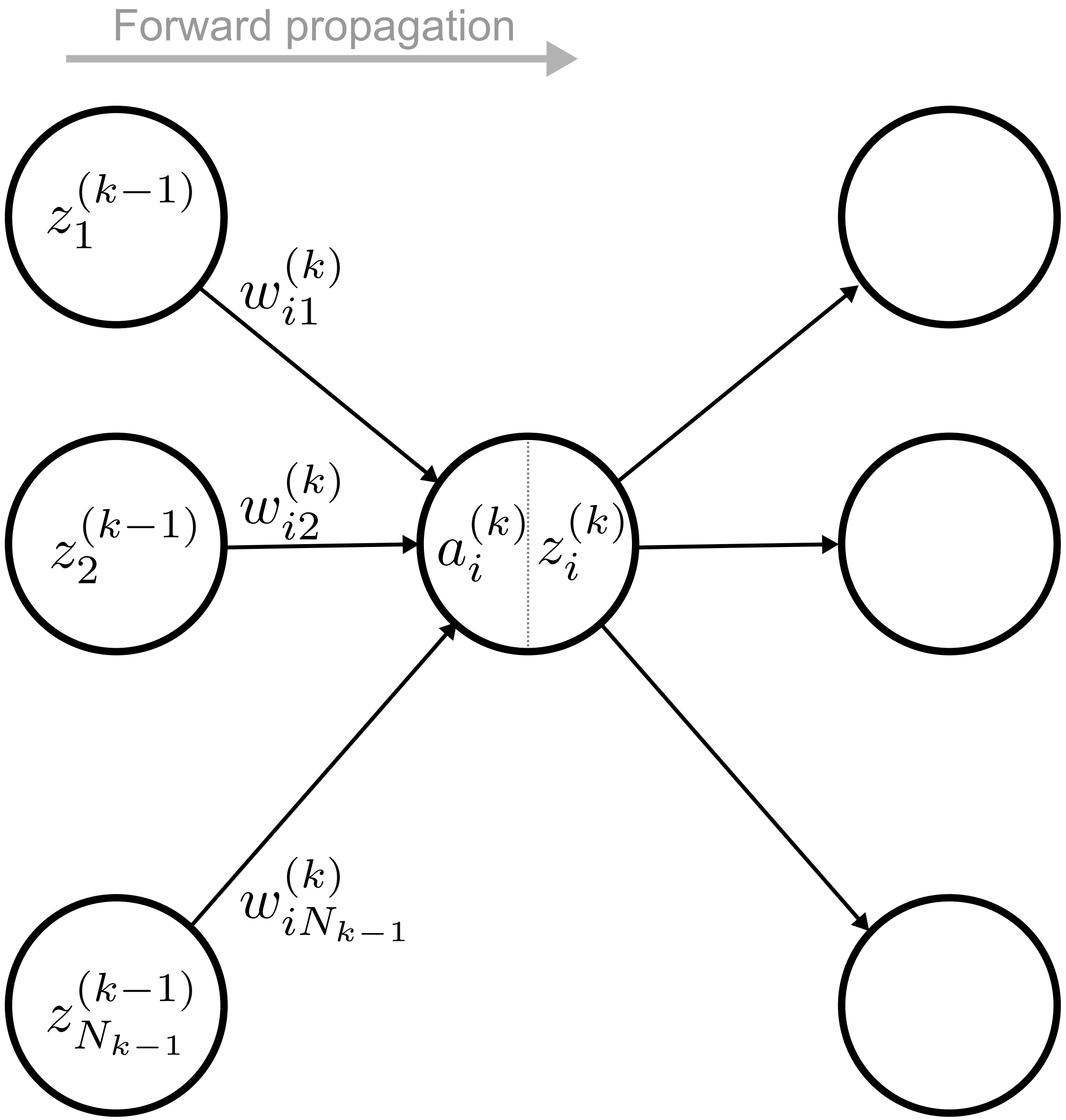
$$a_i^{(k)} = \sum_{j=1}^{N_{k-1}} w_{ij}^{(k)} z_j^{(k-1)}$$

$$z_i^{(k)} = \sigma(a_i^{(k)})$$

In matrix form those equations are:

$$\mathbf{a}^{(k)} = \mathbf{W}^{(k)}\mathbf{z}^{(k-1)}$$

$$\mathbf{z}^{(k)} = \sigma(\mathbf{a}^{(k)})$$



https://github.com/kylebradbury/neural-network-math/raw/master/neural_network_math.pdf

5.2 Backpropagation

Backpropagation begins with the calculation of the gradient of the error with respect to the final set of activations, which for mean square error with sigmoidal activation and K-layer neural network is:

$$\delta_i^{(K)} \triangleq \frac{\partial E_n}{\partial a_i^{(K)}} = (z_i^{(3)} - y_i)\sigma'(a_i^{(3)})$$

We then propagate that back through the neural network and calculate the gradients with respect to each weight along the way (for $k = K-1, \ldots 1$):

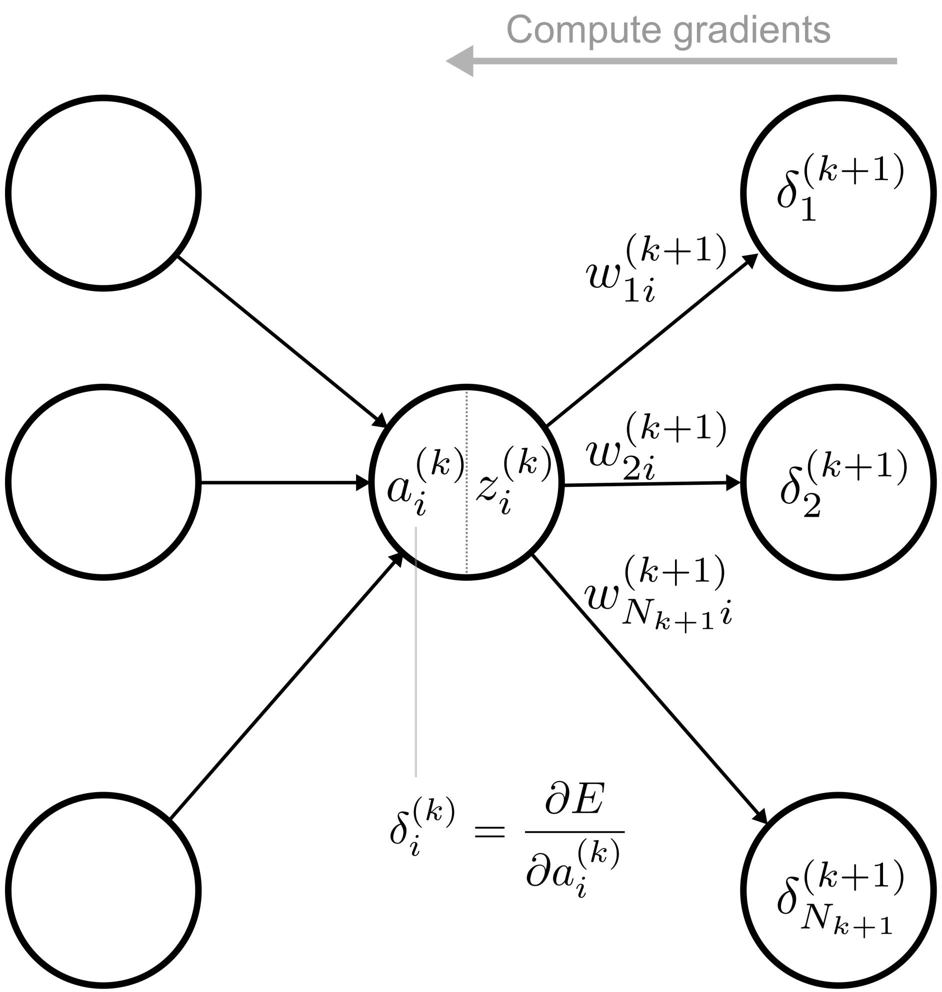
$$\delta_i^{(k)} \triangleq \frac{\partial E_n}{\partial a_i^{(k)}} = \sigma'(a_i^{(k)}) \sum_{j=1}^{N_{k+1}} \delta_j^{(k+1)} w_{ji}^{(k+1)}$$

$$\frac{\partial E_n}{\partial w_{ij}^{(k)}} = \frac{\partial E_n}{\partial a_i^{(k)}} \frac{\partial a_i^{(k)}}{\partial w_{ij}^{(k)}} = \delta_i^{(k)} z_j^{(k-1)}$$

Or in matrix form:

$$\boldsymbol{\delta}^{(k)} \triangleq \frac{\partial E_n}{\partial \mathbf{a}^{(k)}} = \mathbf{W}^{(k+1)^\top} \boldsymbol{\delta}^{(k+1)} \circ \sigma'(\mathbf{a}^{(k)})$$

$$\frac{\partial E_n}{\partial \mathbf{w}^{(k)}} = \boldsymbol{\delta}^{(k)} \mathbf{z}^{(k-1)^\top}$$



https://github.com/kylebradbury/neural-network-math/raw/master/neural_network_math.pdf

Backpropagation

1. Run forward propagation on an input and calculate all the activations, a_i

2. Evaluate $\delta_i^{(k)} = \frac{\partial E}{\partial a_i^{(k)}}$ for all nodes in the network

3. Compute the weight derivatives: $\frac{\partial E}{\partial w_{ij}^{(k)}} = \delta_i^{(k)} z_j^{(k-1)}$ for all nodes in the network

Now we have all the derivatives we need, so we can run gradient descent

Gradient Descent

Batch gradient descent

1. Calculate the gradient for each training sample and average them
2. Update all the parameters based on that average gradient
3. Repeat 1 and 2 until convergence

$$\overline{\frac{\partial E}{\partial w_{ij}}} = \frac{1}{N}\sum_{n=1}^{N}\frac{\partial E_n}{\partial w_{ij}}$$

$$w_{ij} \leftarrow w_{ij} - \eta \overline{\frac{\partial E}{\partial w_{ij}}}$$

Our loss function (E_n) is calculated for EACH training sample $n = 1,2,\ldots,N$

$$E_n = \frac{1}{2}(\hat{y}_n - y_n)^2$$

The gradient also needs to be calculated for each sample (i.e. backprop needs to be run for each sample)

Stochastic gradient descent (SGD)

1. Randomly sort the list of training samples
2. Calculate the gradient from one training sample
3. Update all the parameters based on that error
4. Repeat 2 and 3 until all training samples have been used, then repeat 1-3 until convergence

$$\frac{\partial E_n}{\partial w_{ij}}$$

$$w_{ij} \leftarrow w_{ij} - \eta \frac{\partial E_n}{\partial w_{ij}}$$

Minibatch gradient descent

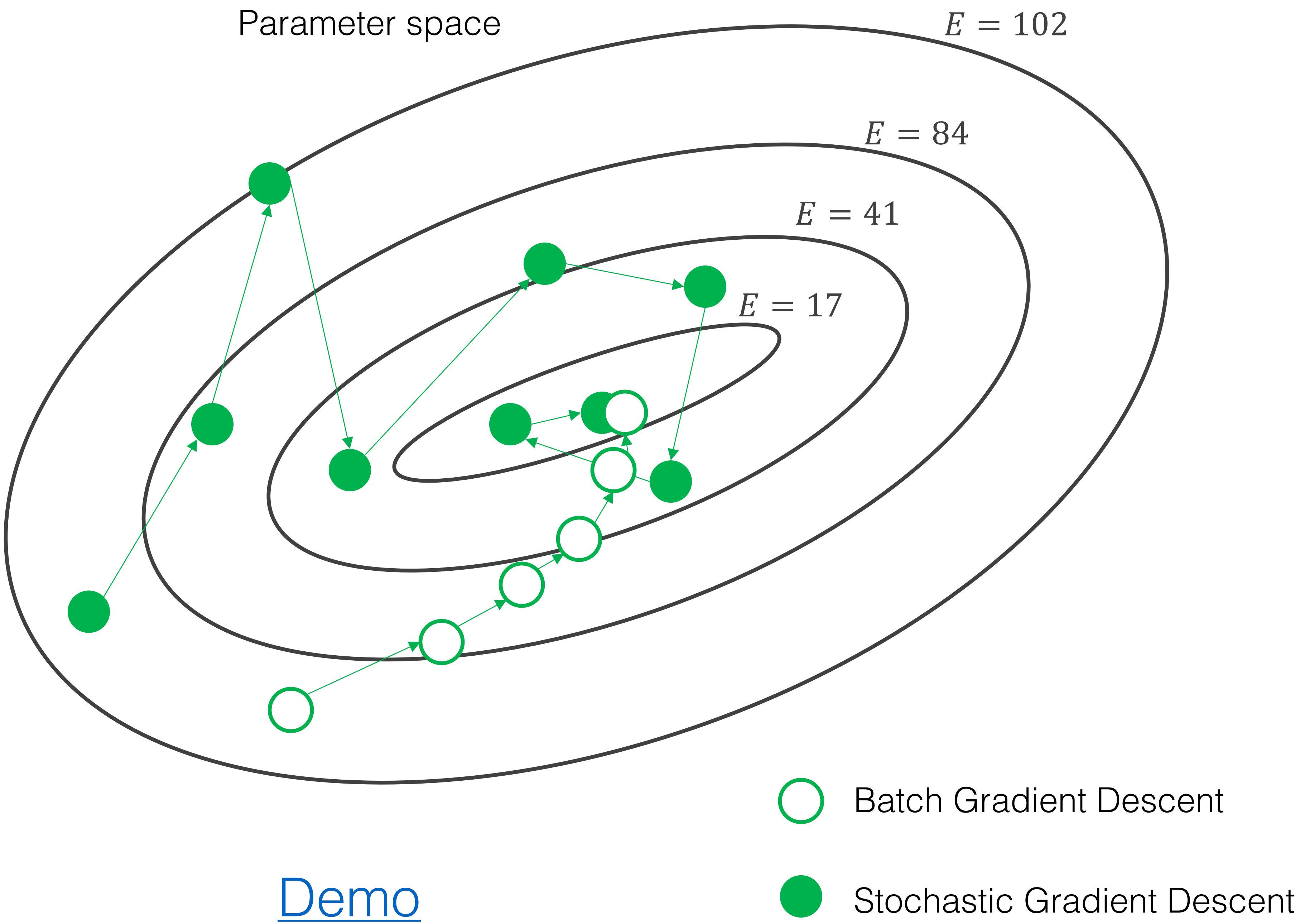
A tweak to SGD where you use a small batch of training samples rather than the whole dataset.

The average gradient across this minibatch is used for taking a gradient descent step

Batch gradient descent is rarely used in practiced because it's too computationally expensive

Stochastic gradient descent (SGD) is better at avoiding local minima

Often **minibatch** gradient descent is used (a small batch of data is used instead of a single sample in SGD)



Demo

What is a neural network and **how does it work**?

How do we **choose model weights**?
(i.e. how do we fit our model to data)

What are the challenges of using neural networks?

Successfully training neural networks

Advice from Andrej Karpathy: http://karpathy.github.io/2019/04/25/recipe/

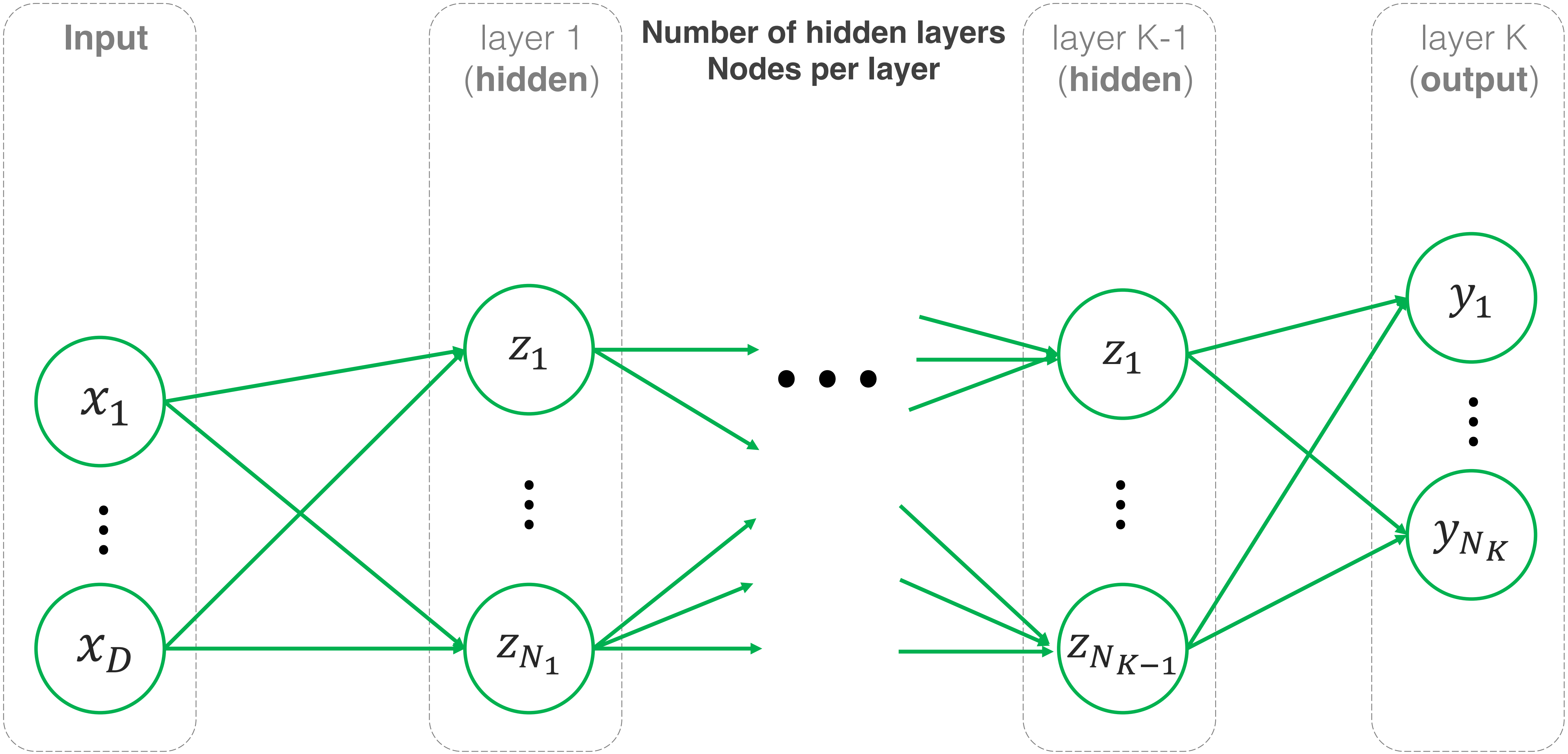
Challenges

1. Neural network training is not plug and play. You need to understand the methods.
2. It is difficult to tell when there is a mistake

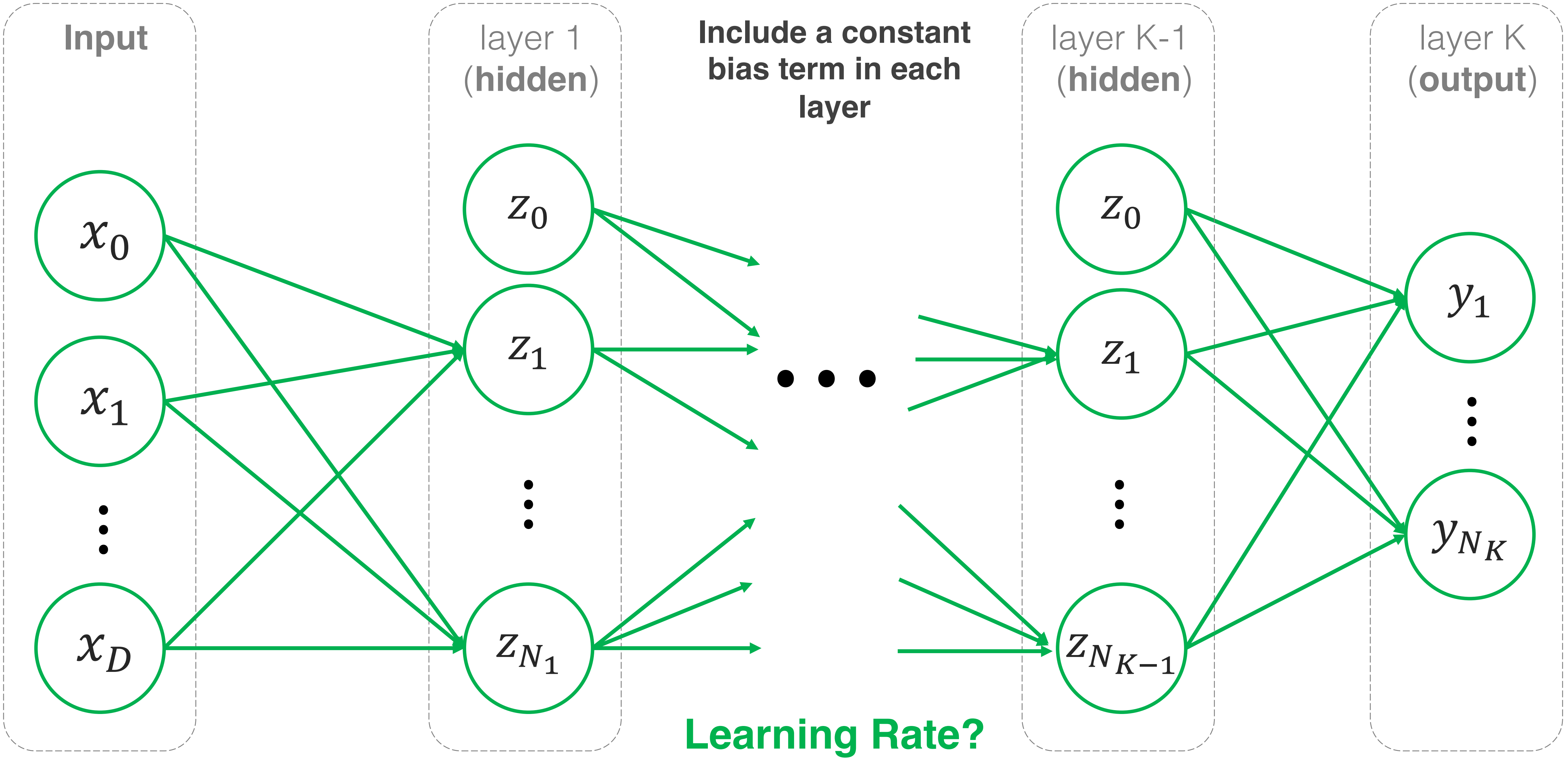
Recipe for training

1. Understand your data
2. Setup an end-to-end training/evaluation pipeline and test simple baselines
3. Overfit your model to the data to make sure you can do it
4. Regularize the model
    1. Add data
    2. Augmentation
    3. Use dropout
    4. Early stopping
5. Tune your model (identify hyperparameters)
6. “Squeeze out the juice”
    1. Model ensembles
    2. Let the model train longer

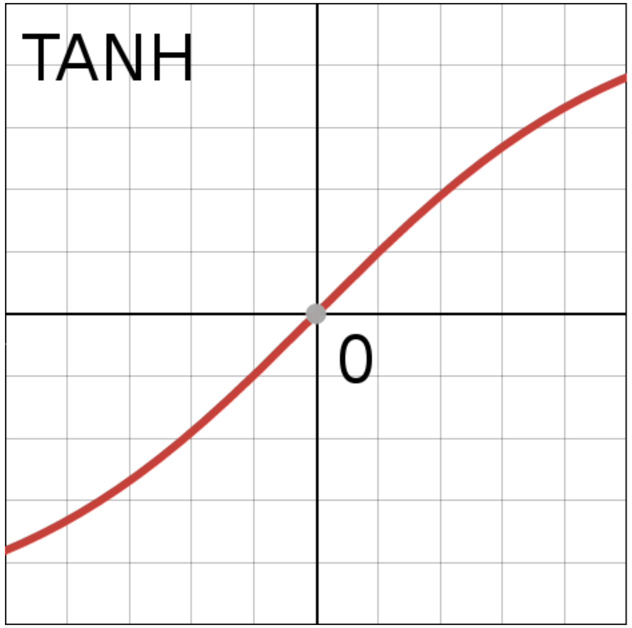
Hyperparameter / Architectural choices



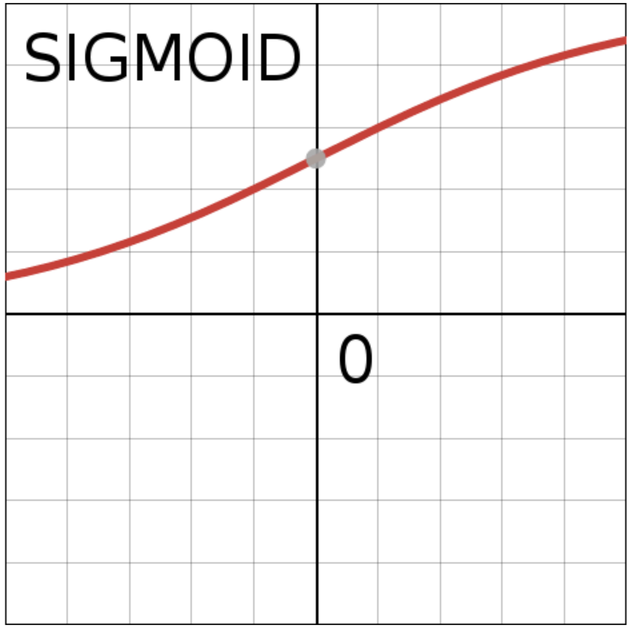
Hyperparameter / Architectural choices



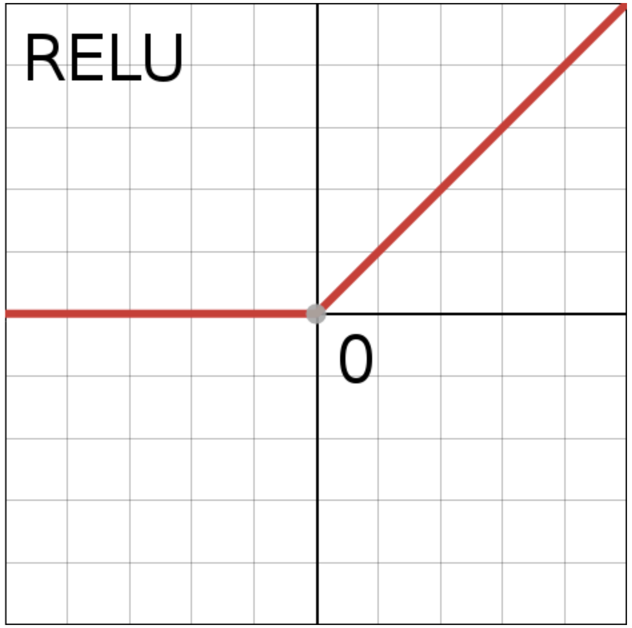
Activation Functions



Hyperbolic Tangent



Sigmoid Tangent



Rectified linear unit (ReLU)

Helps prevent vanishing gradients; adds sparsity; increases speed

Image from Danijar Hafner, Quora

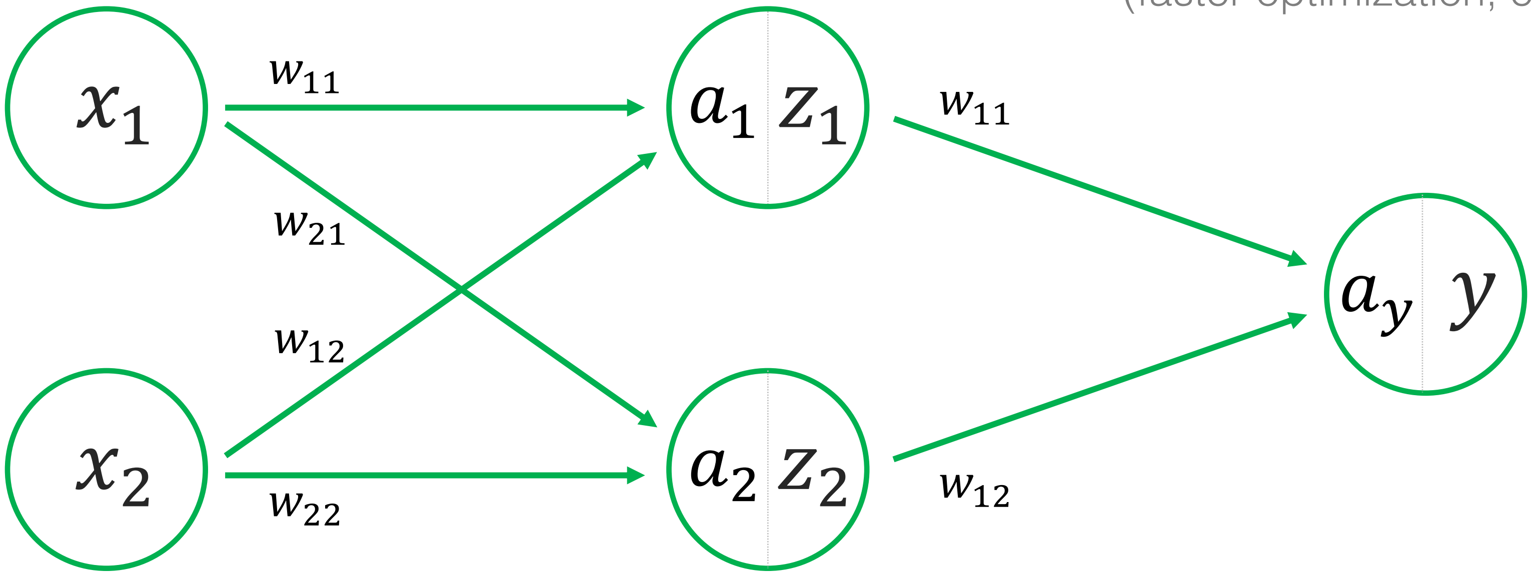
Weight initialization

Set all parameters to zeros	Bad idea: leads to too much symmetry causing many gradients to be the same and the parameters will tend to all update the same way
Random numbers	Need to be neither too small (leading to the **vanishing gradient** problem during backpropagation) nor too big (exploding gradient). A number of heuristics exist (Xavier, He, etc.)

Batch normalization

Ensures activations are unit Gaussian at each layer, improving optimization

(faster optimization, enables higher learning rates)



We calculate the activation at each later for each of the training samples in each minibatch

1. Subtract the mean of that activation value averaged across the minibatch

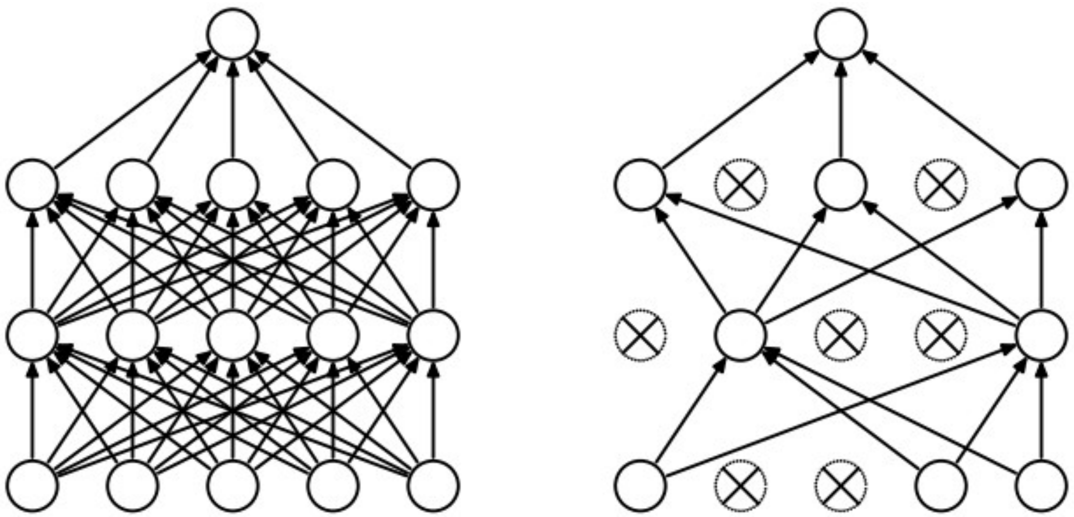
2. Divide by the standard deviation of the activation value computed across the minibatch

Regularization

L2 Regularization

L1 Regularization

Dropout



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

While training, keep a neuron active with some probability p, or setting it to zero otherwise.

Supervised Learning Techniques

Covered so far

- Linear Regression
- K-Nearest Neighbors
- Perceptron
- Logistic Regression
- Fisher's Linear Discriminant
- Linear Discriminant Analysis
- Quadratic Discriminant Analysis
- Naïve Bayes
- Decision Trees and Random Forests
- Ensemble methods (bagging, boosting, stacking)
- Neural Networks

Can be used with many machine learning techniques

Appropriate for:
- Classification
- Regression