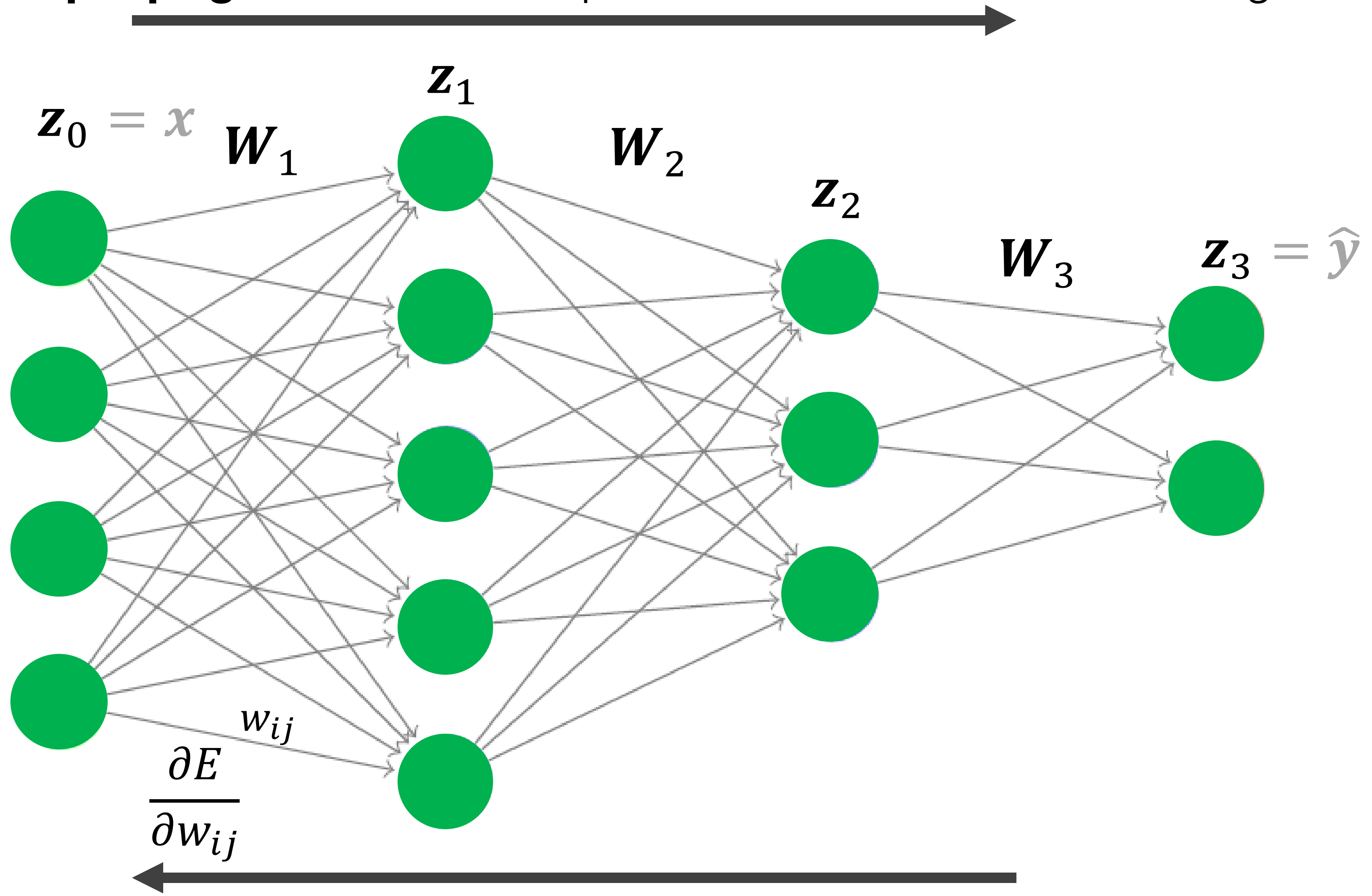
Neural Networks II

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 / cost



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

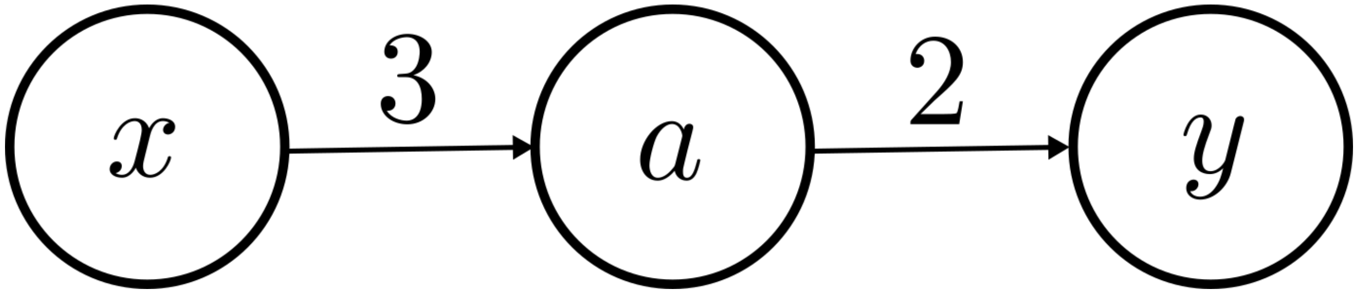
Backpropagation lets us **compute the gradient** with respect to each of the parameters so we can tune them with **gradient descent**

(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



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

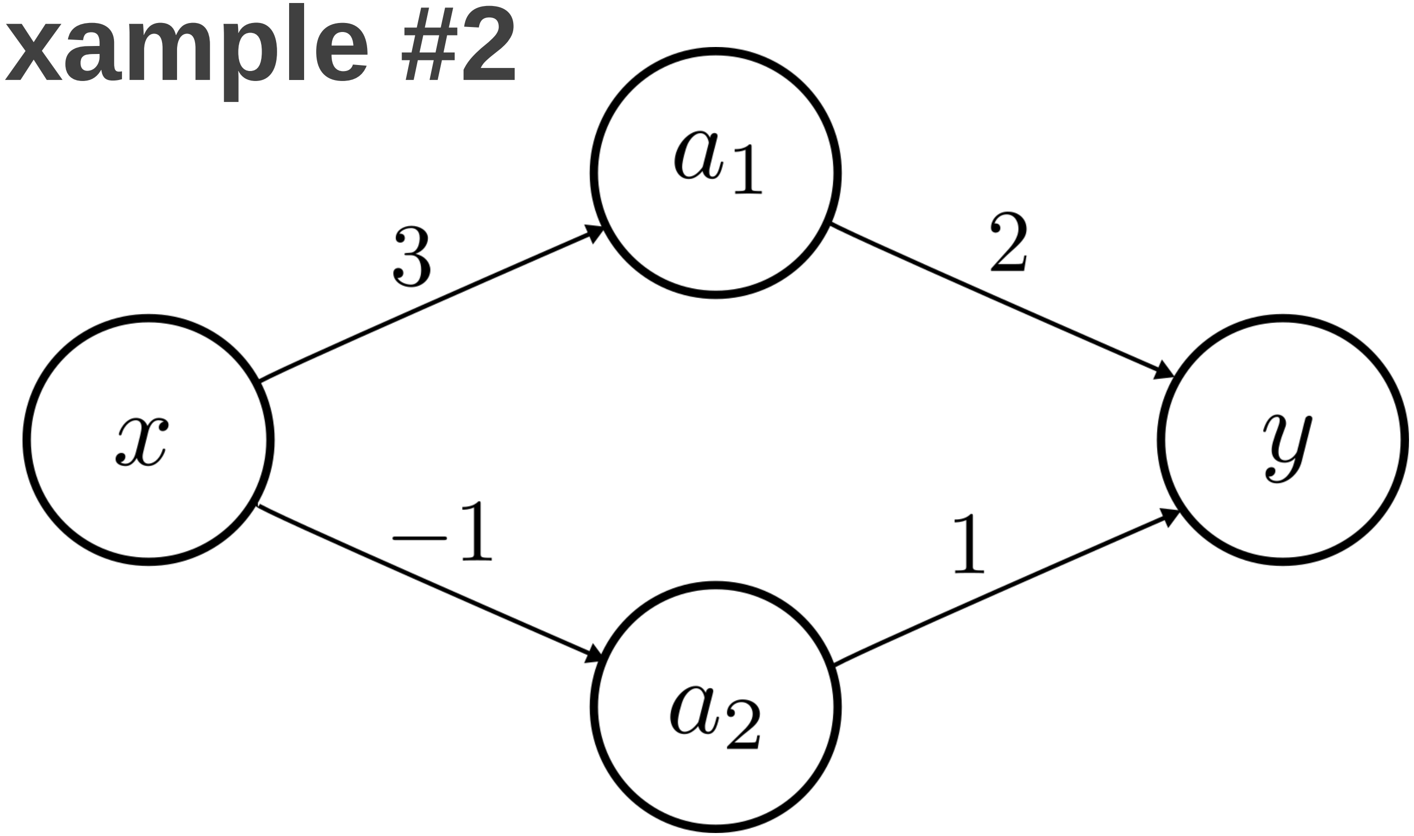
$$a = 3x \qquad \frac{\partial a}{\partial x} = 3$$

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

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

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

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

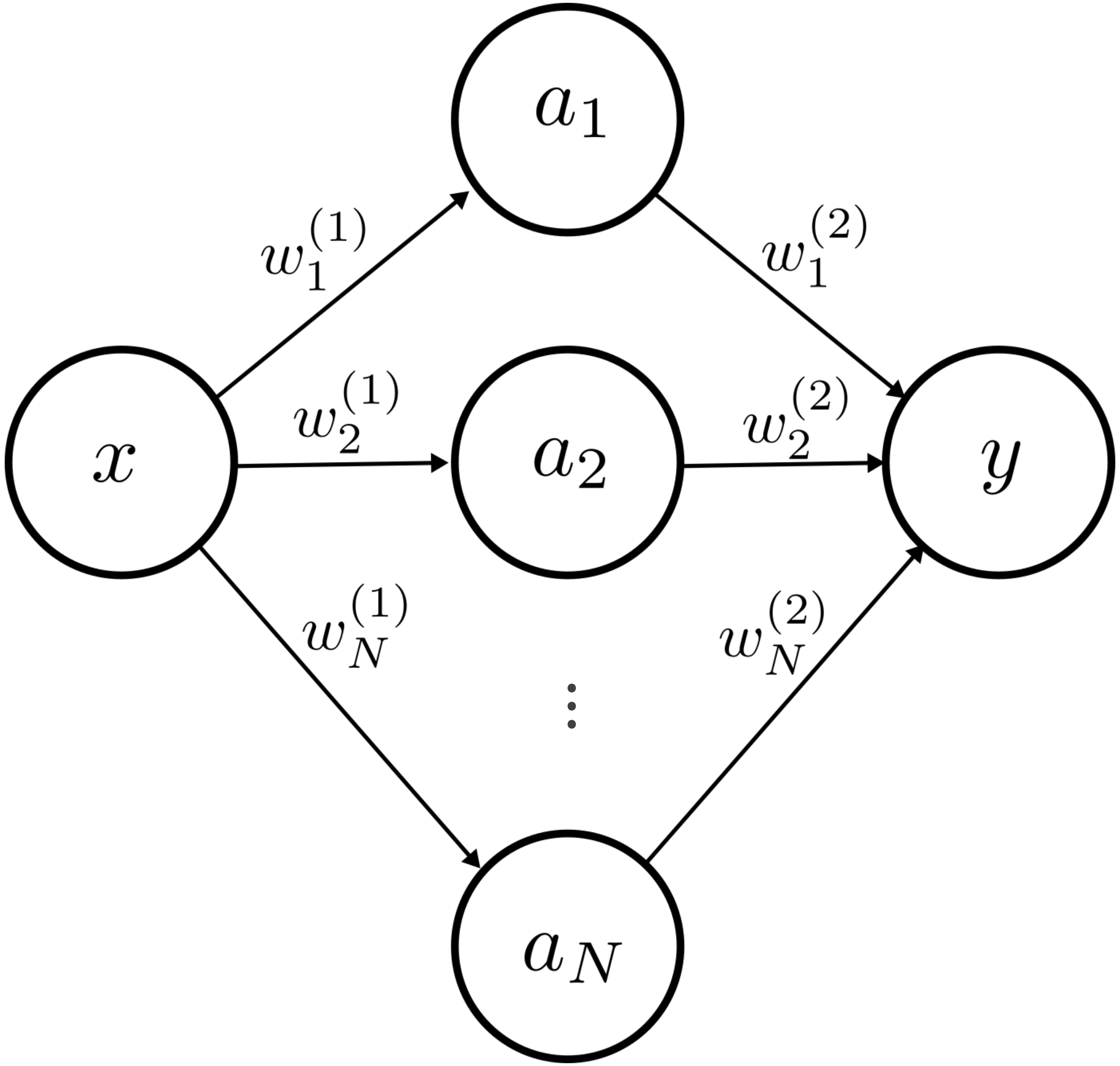
$$= 5$$

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

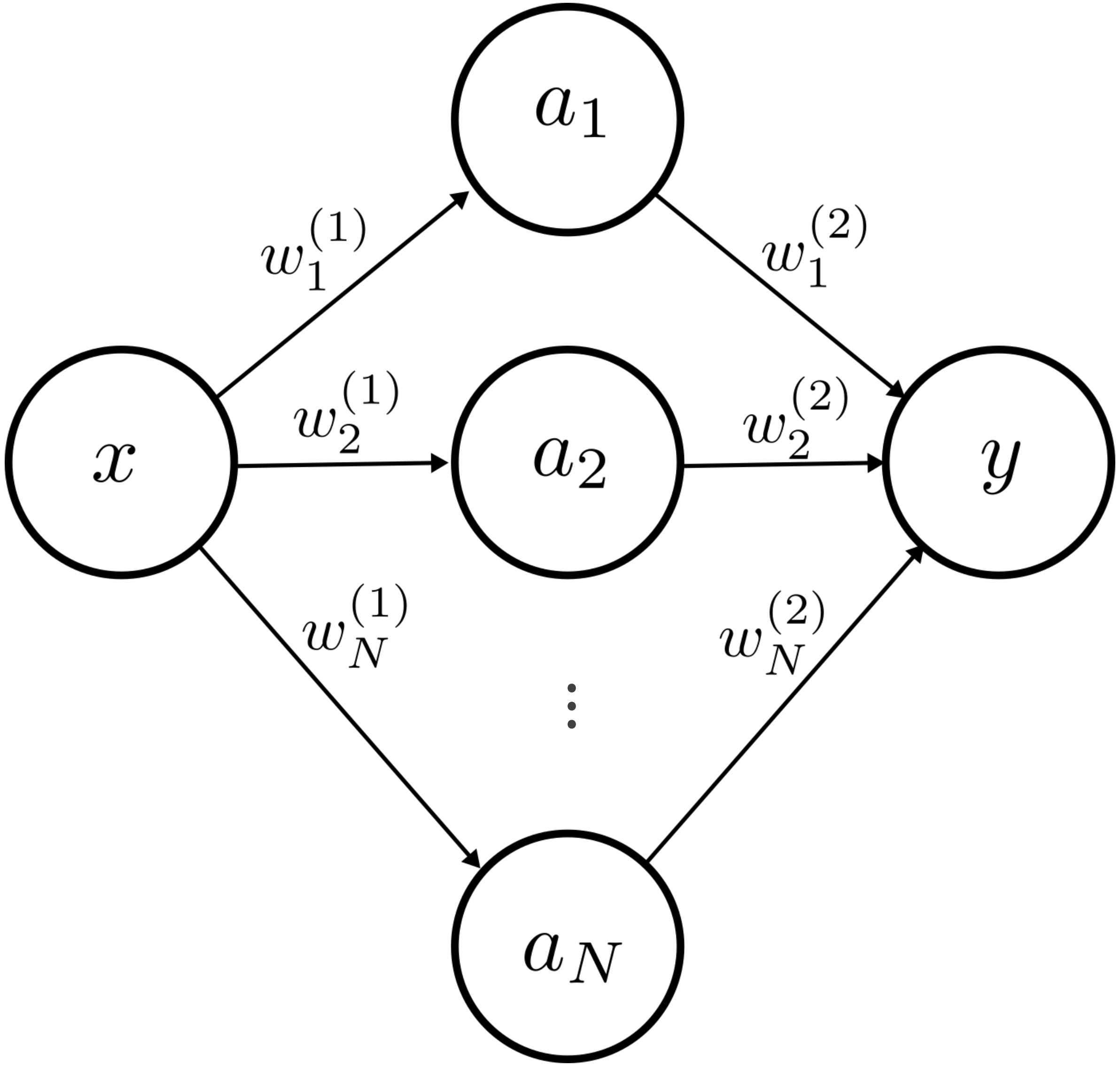
$$y = \sum_{j=1}^{N} w_j^{(2)} a_j \qquad \frac{\partial y}{\partial a_i} = w_i^{(2)}$$

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

Derivatives with respect to the weights:

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

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



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

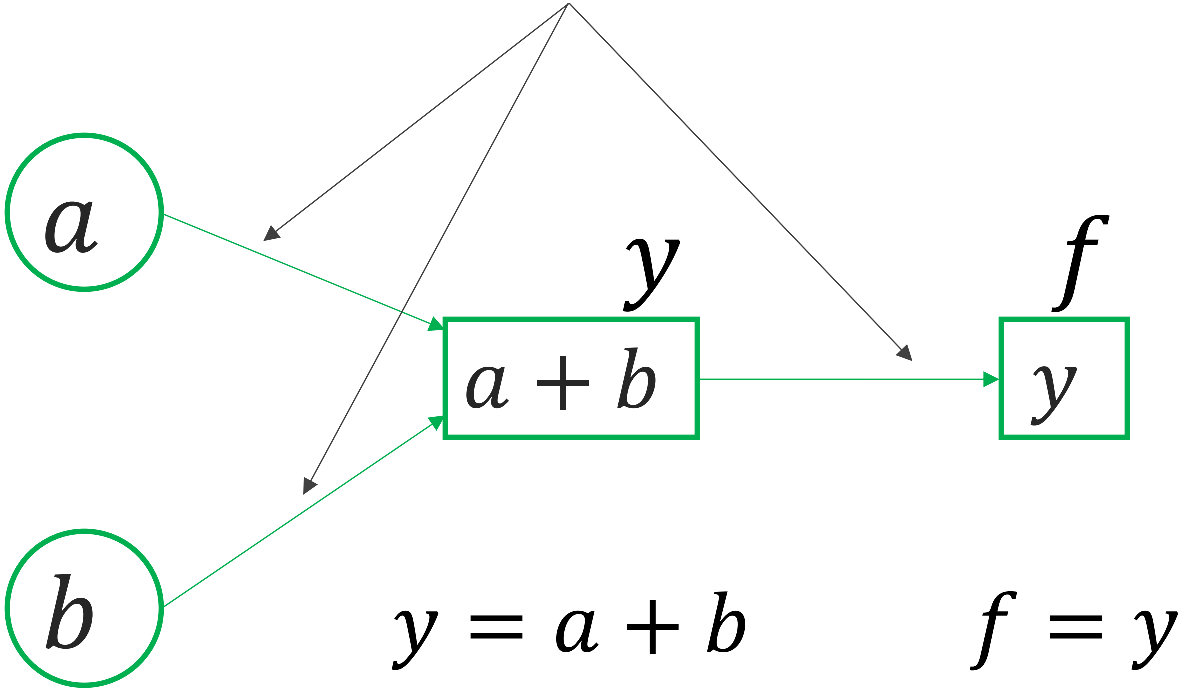
$$\frac{\partial f}{\partial z} = \underbrace{\frac{\partial f}{\partial w}\frac{\partial w}{\partial x}}_{\frac{\partial f}{\partial x}}\frac{\partial x}{\partial y}\frac{\partial y}{\partial z} = \underbrace{\frac{\partial f}{\partial x}\frac{\partial x}{\partial y}}_{\frac{\partial f}{\partial y}}\frac{\partial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

Simple example

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

This graph to the right represents this function

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



Name of the variable at that node

$$y = a + b \qquad f = y$$

Operation that the node performs

Local derivatives (one for each edge input into a node):

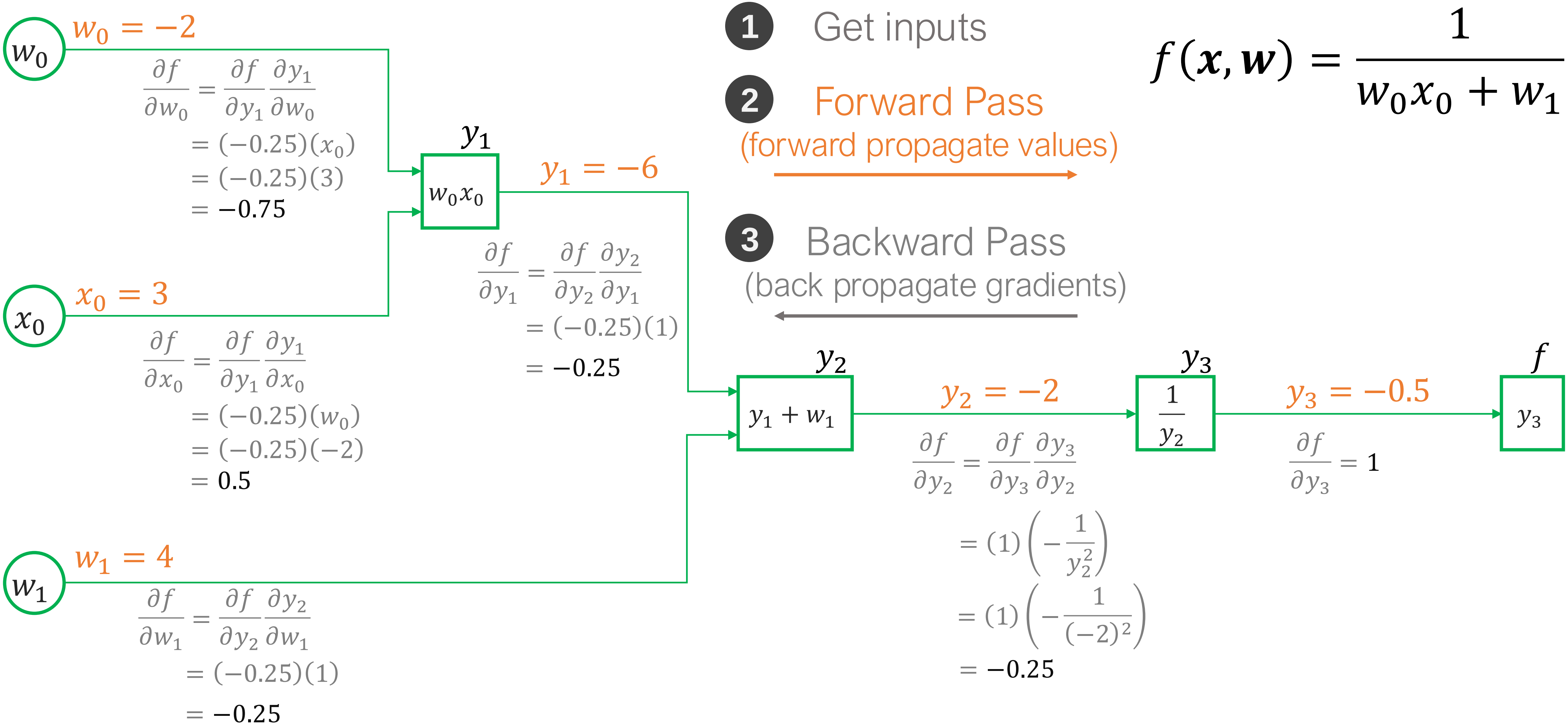
$$\frac{\partial y}{\partial a} = 1, \qquad \frac{\partial y}{\partial b} = 1$$

1 Get inputs

2 Forward Pass
(forward propagate values)

3 Backward Pass
(back propagate gradients)

$$f(\boldsymbol{x},\boldsymbol{w}) = \frac{1}{w_0x_0 + w_1}$$



$w_0 = -2$

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

$x_0 = 3$

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

$w_1 = 4$

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

$y_1 = -6$

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

$y_2 = -2$

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

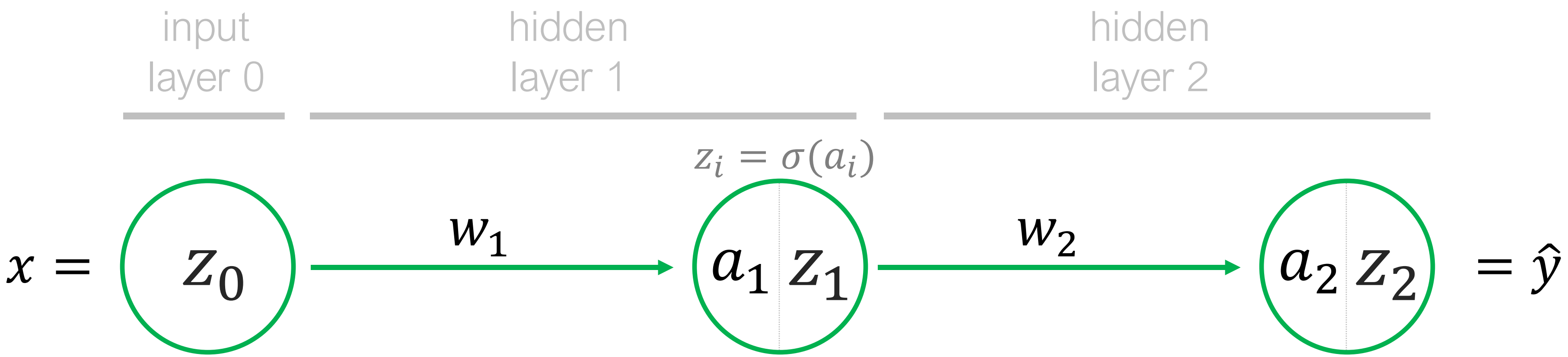
$y_3 = -0.5$

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

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



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

$$z_2 = \hat{y} = \sigma(a_2)$$

$$a_2 = w_2 z_1$$

$$z_1 = \sigma(a_1)$$

$$a_1 = w_1 z_0 \rightarrow x$$

Forward propagation

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

$$\hat{y} = z_2 = \sigma\big(w_2 \sigma(w_1 z_0)\big)$$

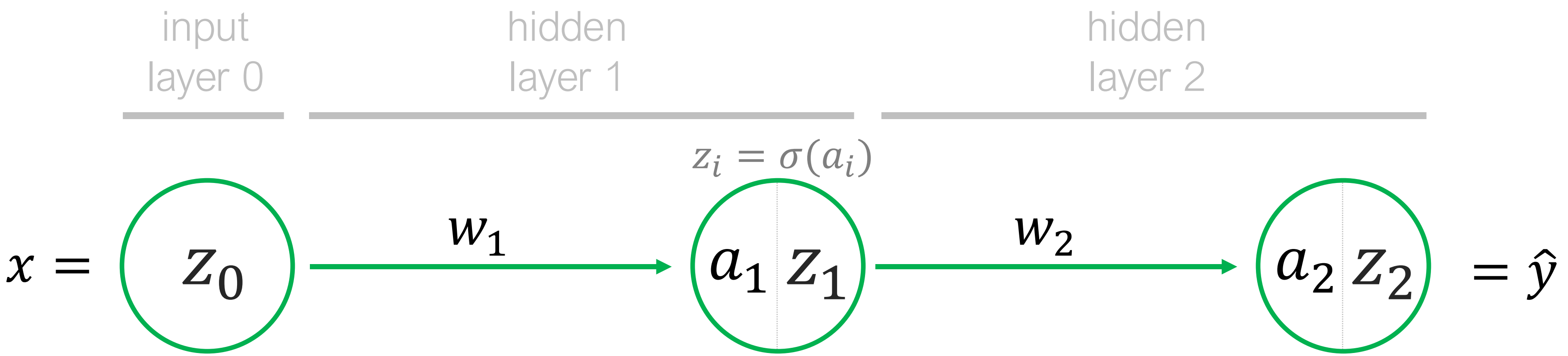
We can calculate the error:

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

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

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

$$\hat{y} = \sigma(a_2) \qquad \frac{\partial \hat{y}}{\partial a_2} = \sigma'(a_2)$$

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

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

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

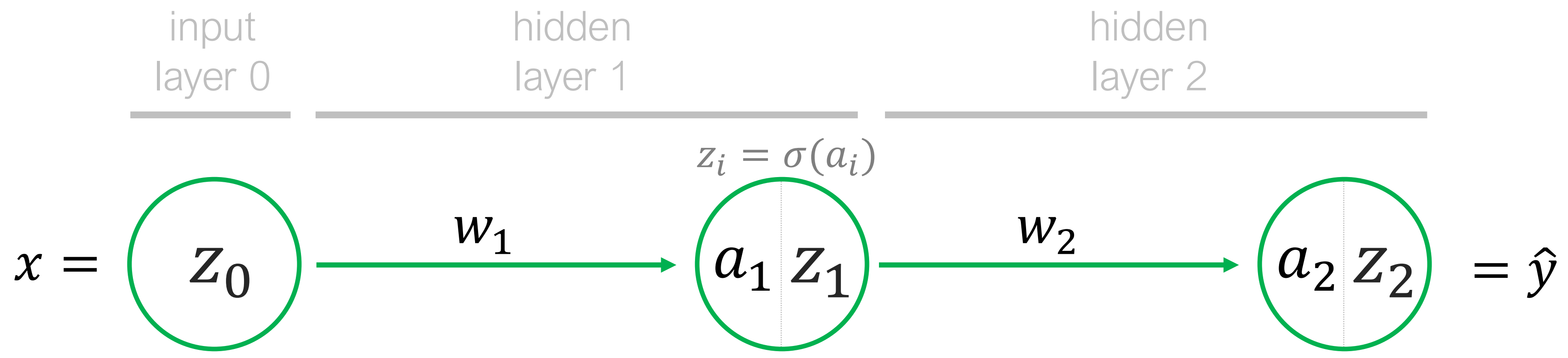
Backpropagation

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

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

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

We know all these quantities from forward propagation



Forward propagation

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

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

Backpropagation

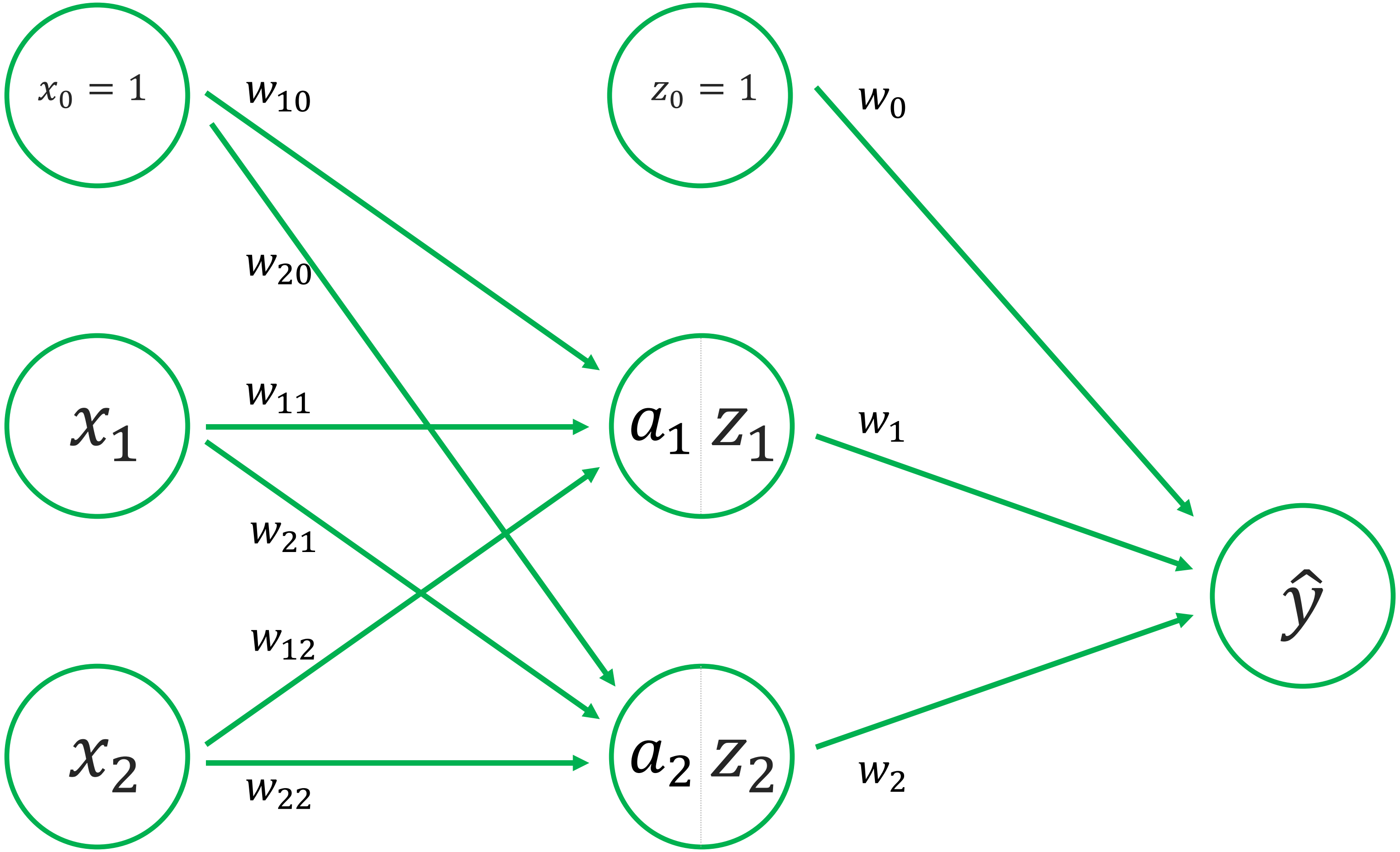
$$\frac{\partial E}{\partial w_1} = \underbrace{\frac{\partial E}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a_2} \frac{\partial a_2}{\partial z_1} \frac{\partial z_1}{\partial a_1}}_{\frac{\partial E}{\partial a_1}} \frac{\partial a_1}{\partial w_1}$$

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

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

(common shorthand)

And here's an actual mini neural network…

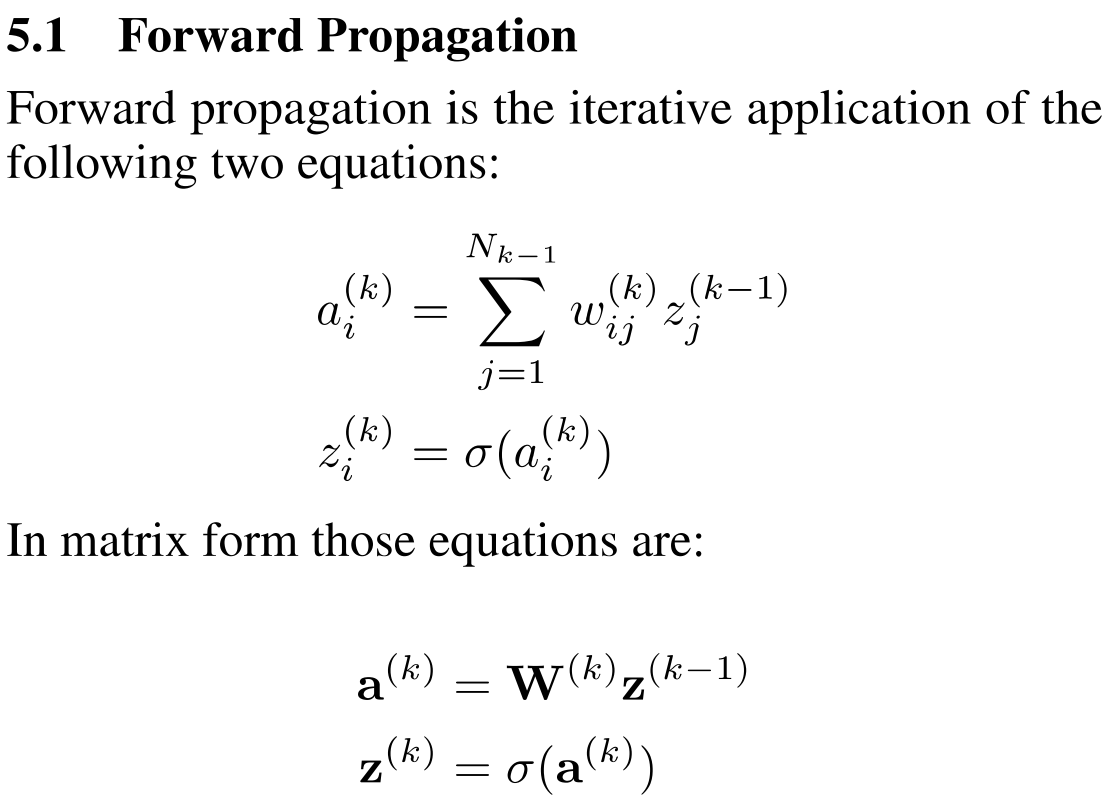


Activations in the other layer are the function $g(x)$,with derivative $g'(x)$

Linear activation for regression in the output layer

Local Relationship(s)	$a_i = w_{i0}x_0 + w_{i1}x_1 + w_{i2}x_2$	$z_i = g(a_i)$	$\hat{y} = w_0 z_0 + w_1 z_1 + w_2 z_2$		$C(y,\hat{y}) = E = \frac{1}{2}(\hat{y} - y)^2$
Local Derivative(s)	$\frac{\partial a_i}{\partial w_{ij}} = x_j$	$\frac{\partial z_i}{\partial a_i} = g'(a_i)$	$\frac{\partial \hat{y}}{\partial z_i} = w_i$	$\frac{\partial \hat{y}}{\partial w_i} = z_i$	$\frac{\partial E}{\partial \hat{y}} = \hat{y} - \mathrm{y}$
Global Derivative(s)	$\frac{\partial E}{\partial w_{ij}} = \frac{\partial E}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z_i} \frac{\partial z_i}{\partial a_i} \frac{\partial a_i}{\partial w_{ij}}$	$\frac{\partial E}{\partial a_i} = \frac{\partial E}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z_i} \frac{\partial z_i}{\partial a_i}$	$\frac{\partial E}{\partial w_i} = \frac{\partial E}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial w_i}$		$\frac{\partial E}{\partial \hat{y}} = \hat{y} - \mathrm{y}$

Quick reference for neural network math



5.1 Forward Propagation

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

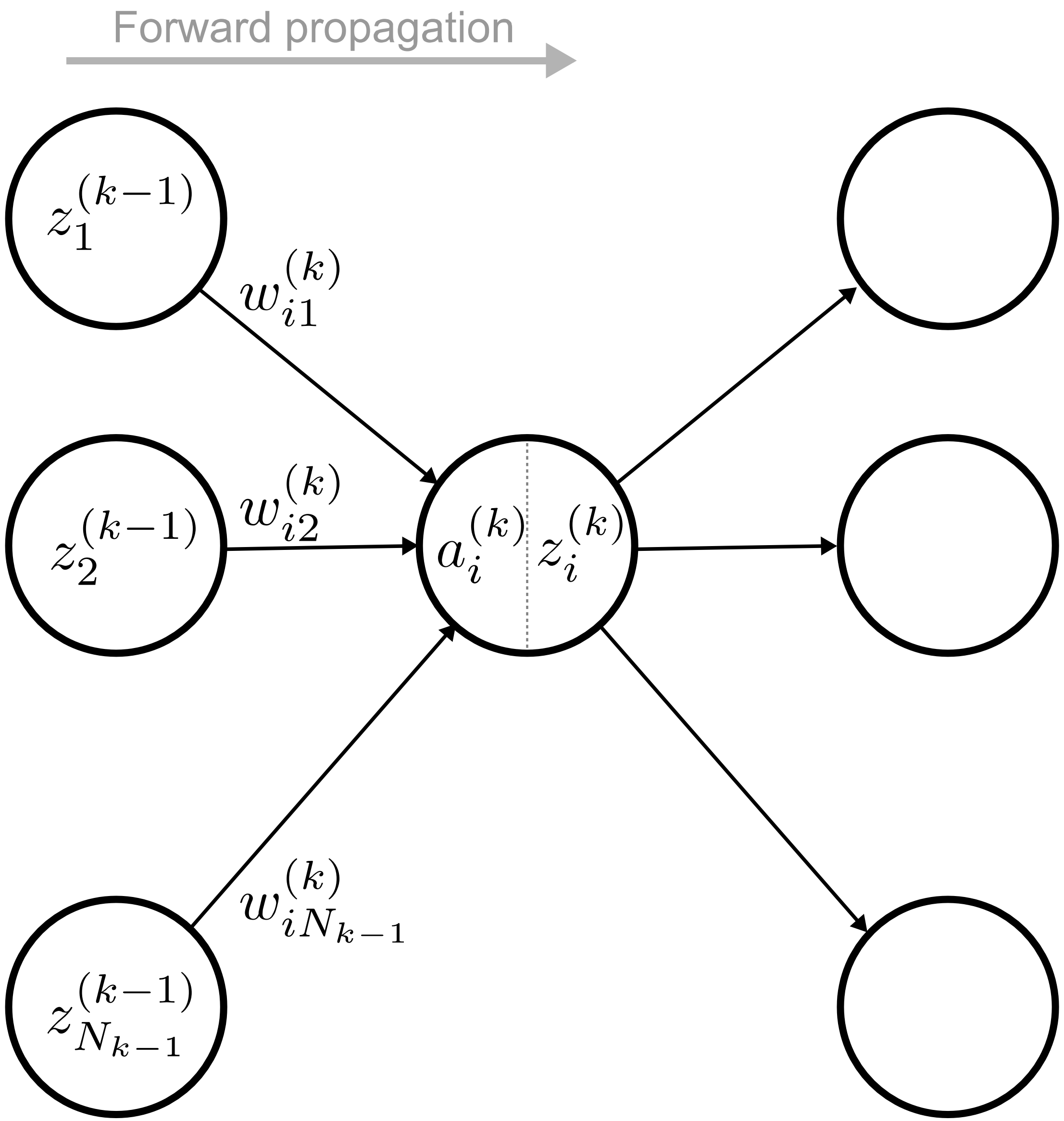
$$a_i^{(k)} = \sum_{j=1}^{N_{k-1}} w_{ij}^{(k)} z_j^{(k-1)}$$

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

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 $k = K-1, ...1$):

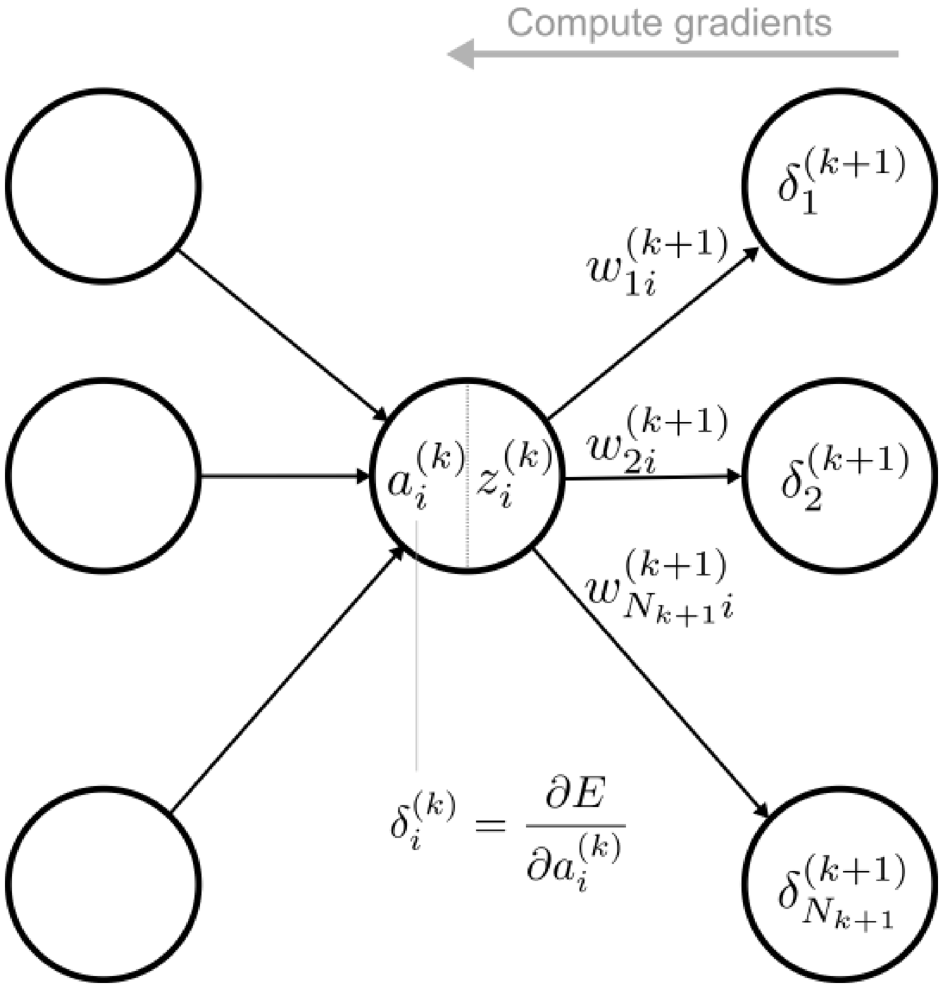
$$\delta_i^{(k)} \triangleq \frac{\partial E_n}{\partial a_i^{(k)}} = \sigma^{'}(a_i^{(k)}) \sum_{j=1}^{N_{k+1}} \delta_j^{(k+1)} w_{ji}^{(k+1)}$$

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

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 stopping criteria met

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

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

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 stopping criteria met

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

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

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

Other optimizers exist:

e.g. momentum, RMSprop, adam

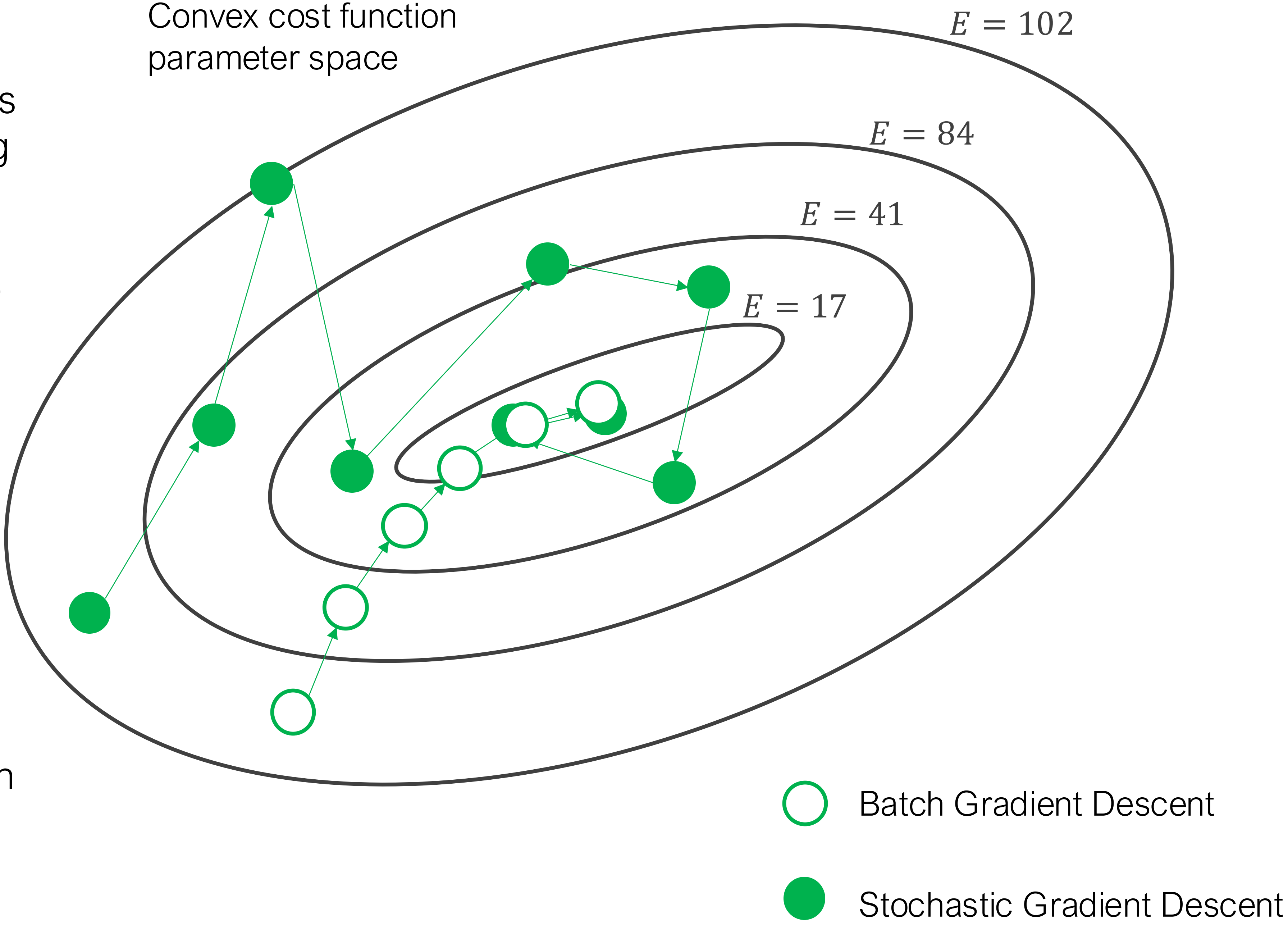
Batch gradient descent can work well if the cost function is convex (rare) and the learning rate is properly tuned

Batch gradient descent tends to converge more slowly

Stochastic gradient descent (SGD) is better at avoiding local minima, but injects noise into the training process

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

Convex cost function parameter space



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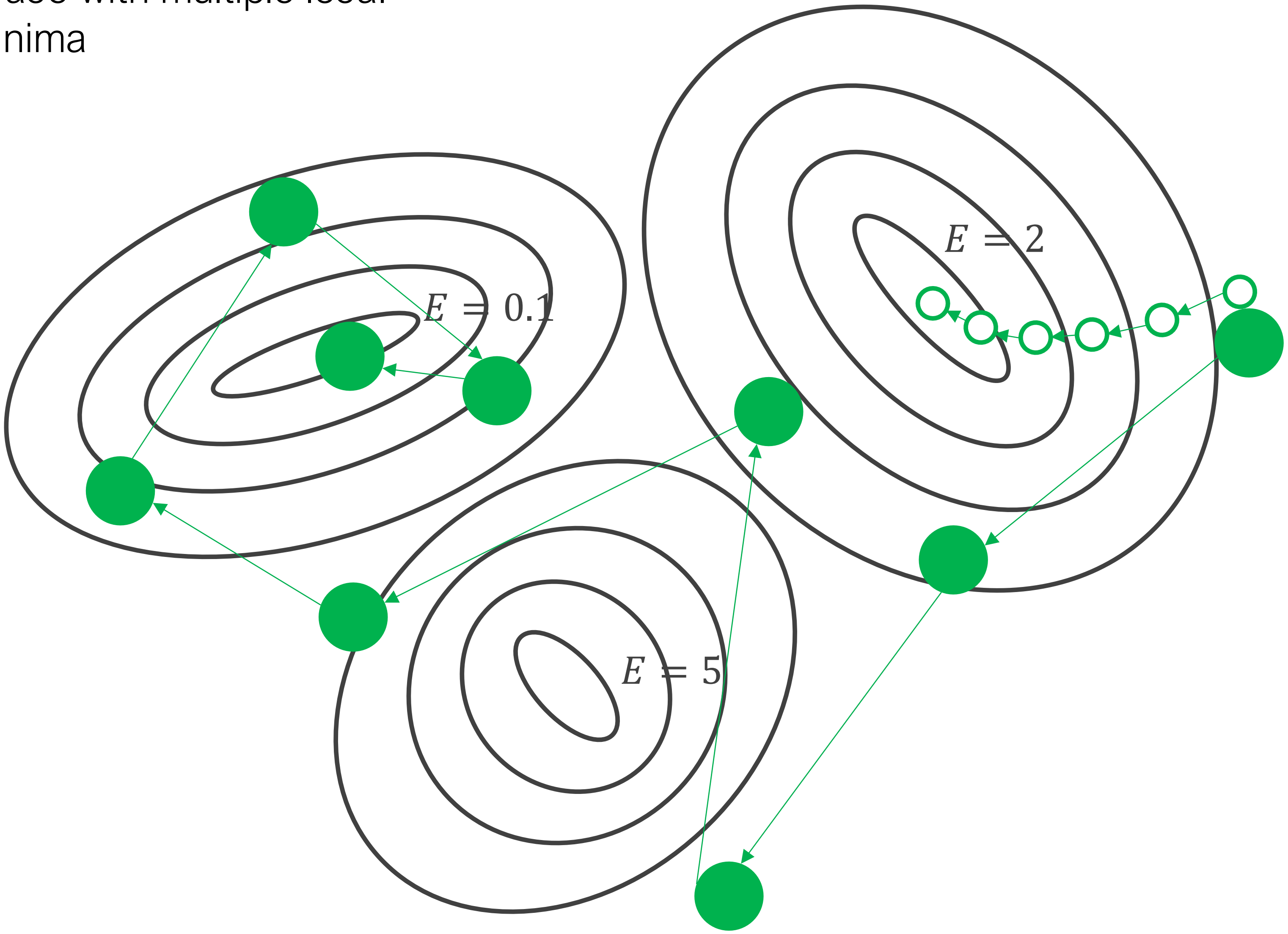
Cost function parameter space with multiple local minima



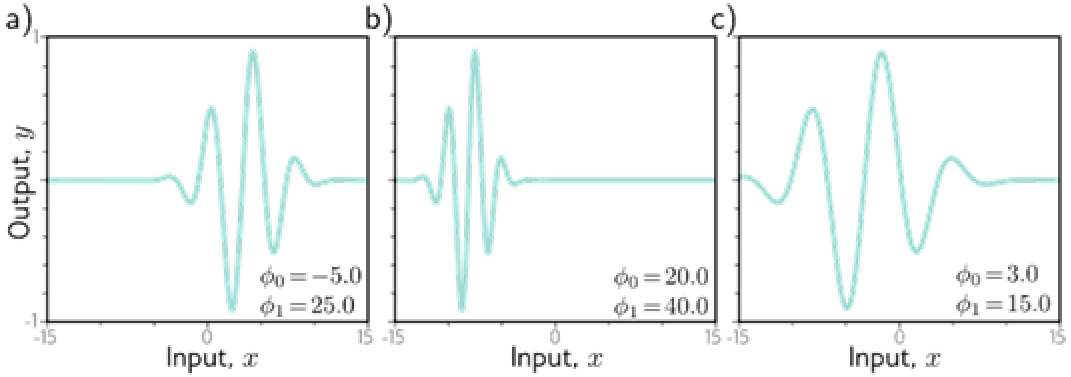
○ Batch Gradient Descent

● Stochastic Gradient Descent

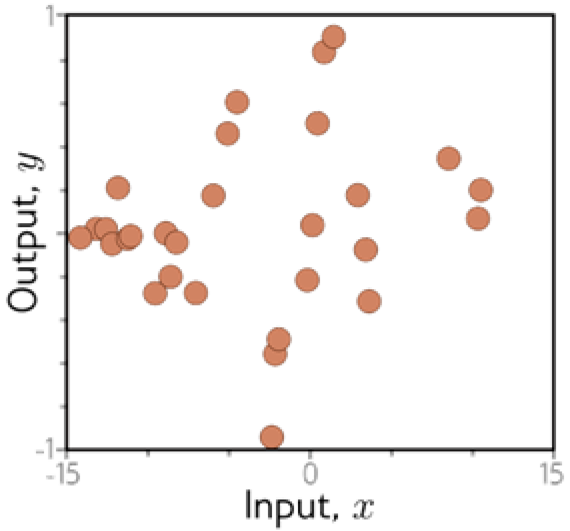
SGD Example

Gabor Model

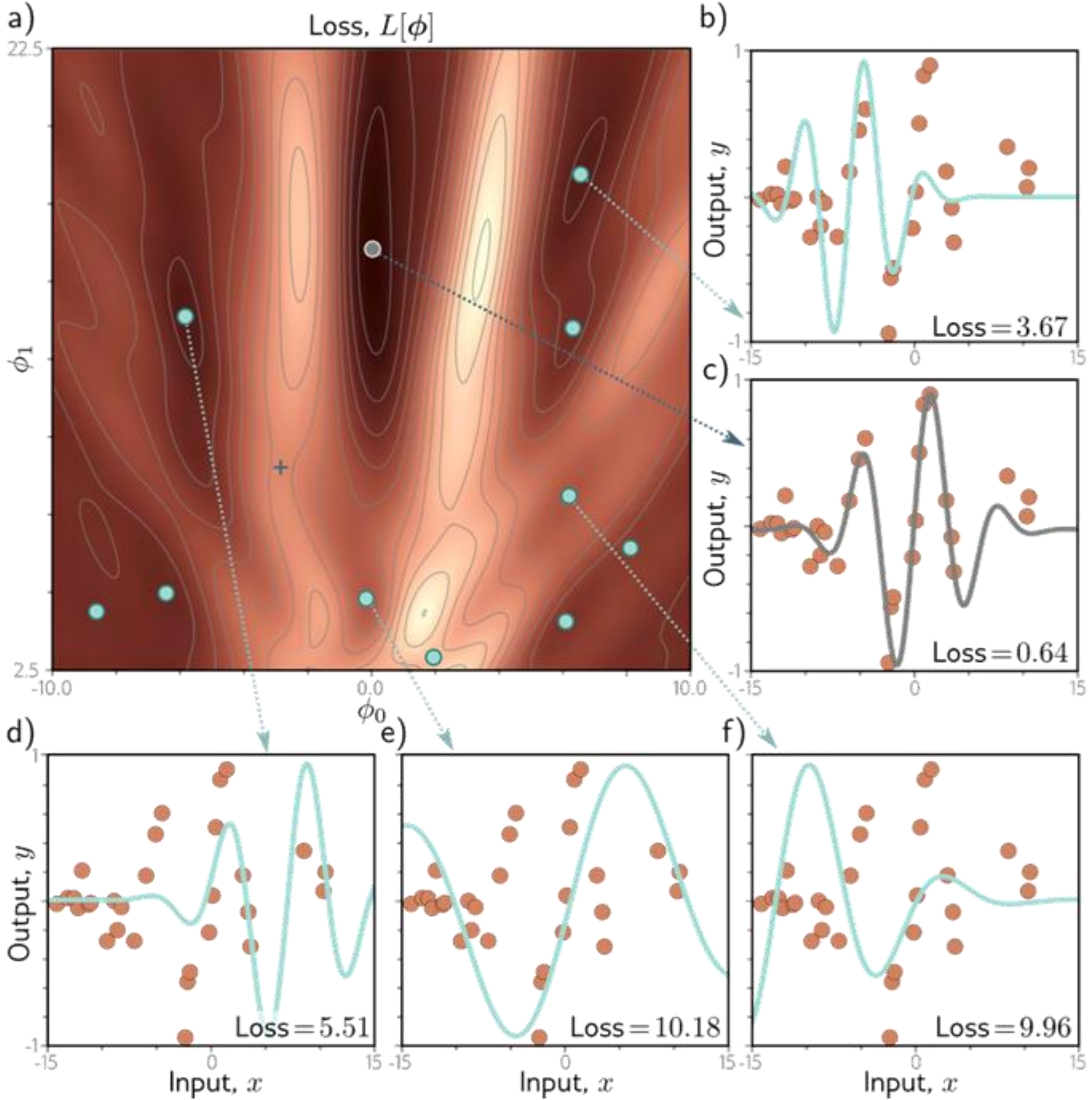
$$\mathrm{f}[x, \boldsymbol{\phi}] = \sin[\phi_0 + 0.06 \cdot \phi_1 x] \cdot \exp\left(-\frac{(\phi_0 + 0.06 \cdot \phi_1 x)^2}{32.0}\right)$$



Training Data



Global cost function for different parameter values

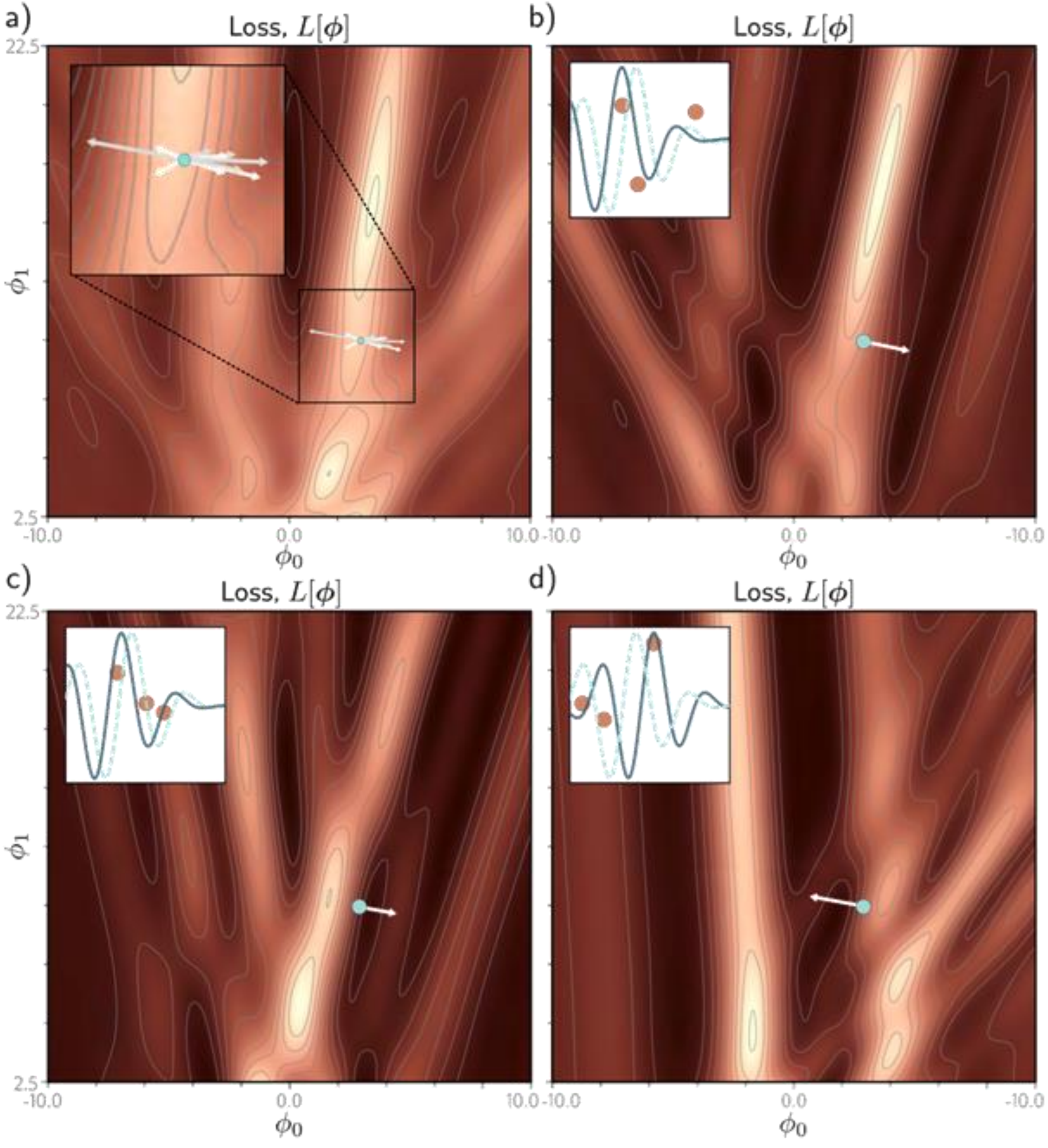


Images from Prince, Understanding Deep Learning, 2023

SGD Example

Global cost function
Cost function with the entire training dataset

Minibatch cost function 1
Cost function with minibatch



Minibatch cost function 2
Cost function with minibatch

Minibatch cost function 3
Cost function with minibatch

Images from Prince, Understanding Deep Learning, 2023

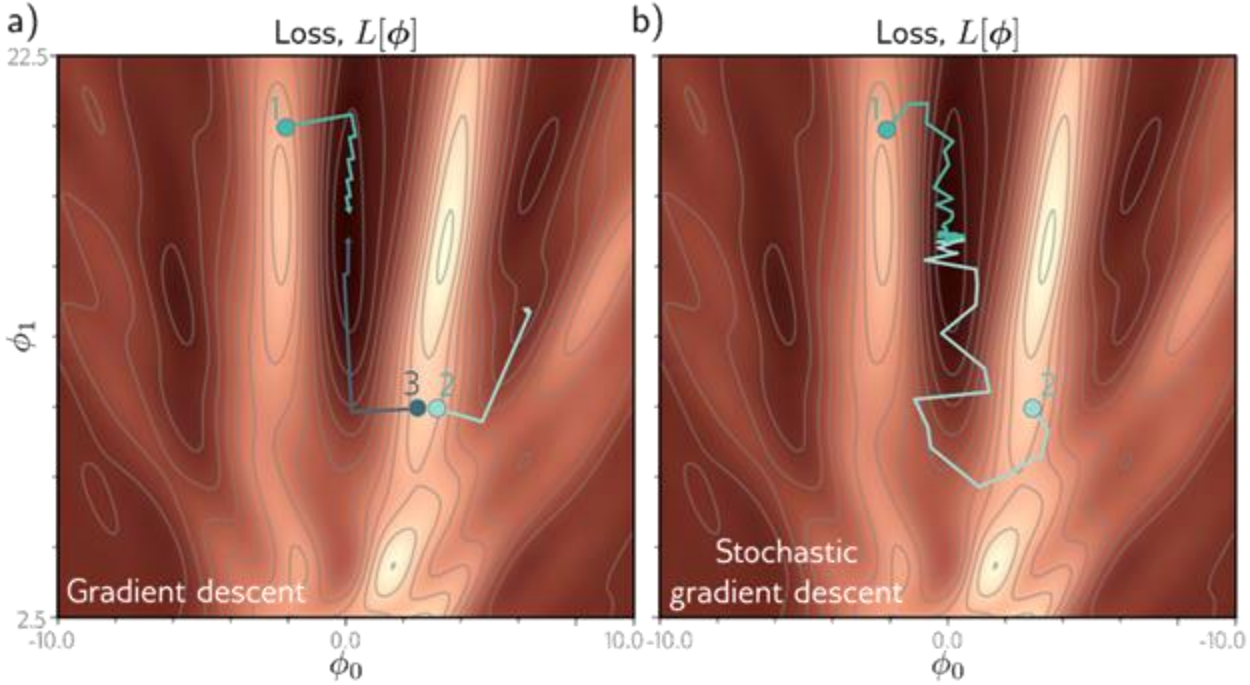
SGD Example

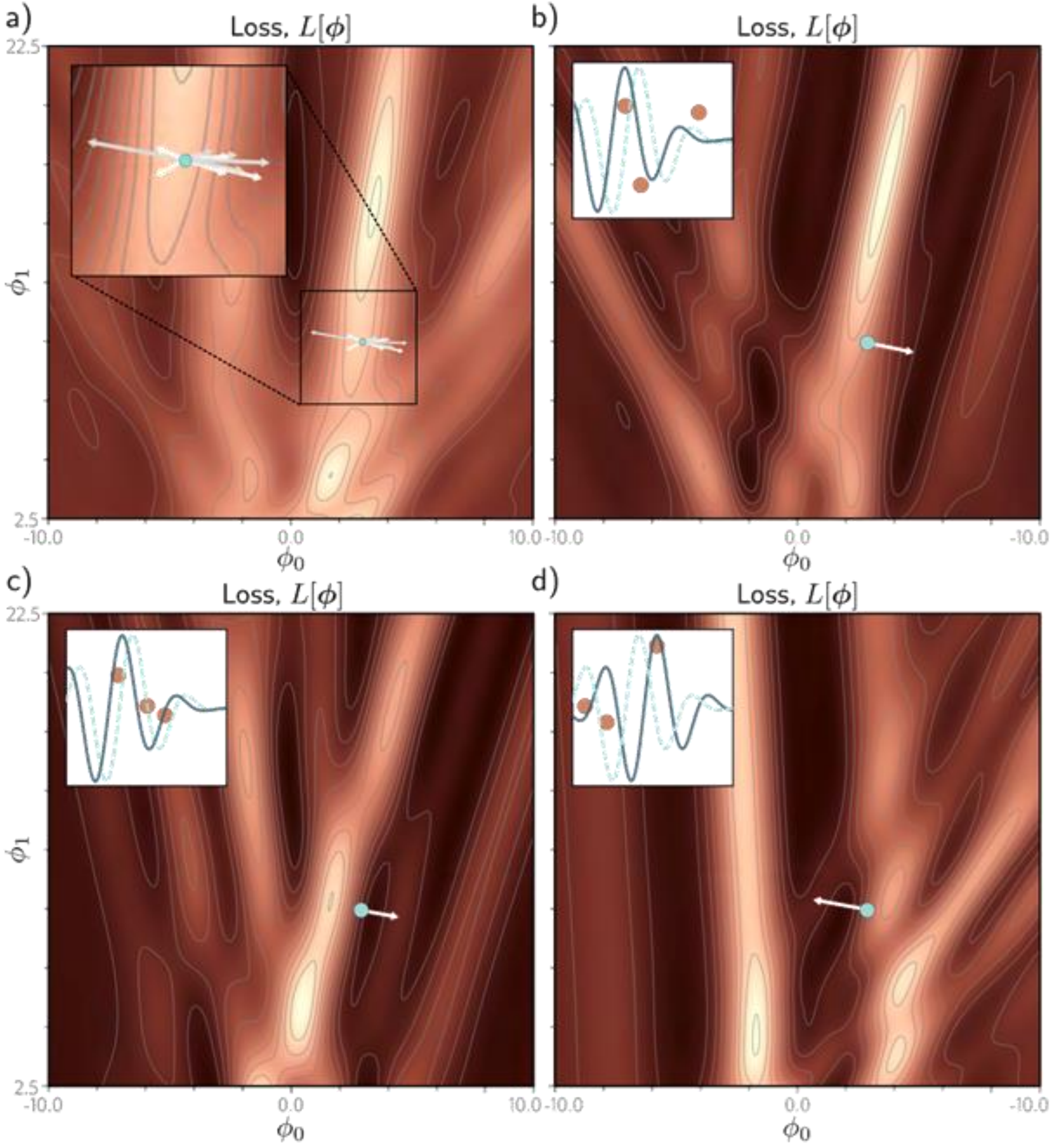
Images from Prince, Understanding Deep Learning, 2023

Gradient descent
Batch size = N

Minibatch stochastic gradient descent
1 < batch size < N

N is the number of training samples





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

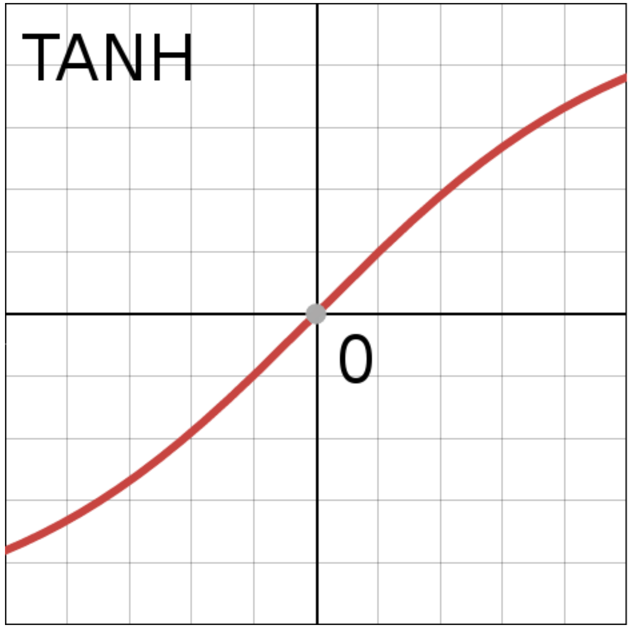
How do we **choose model weights**?
(i.e. how do we fit our model to data)

What are the challenges of using neural networks?

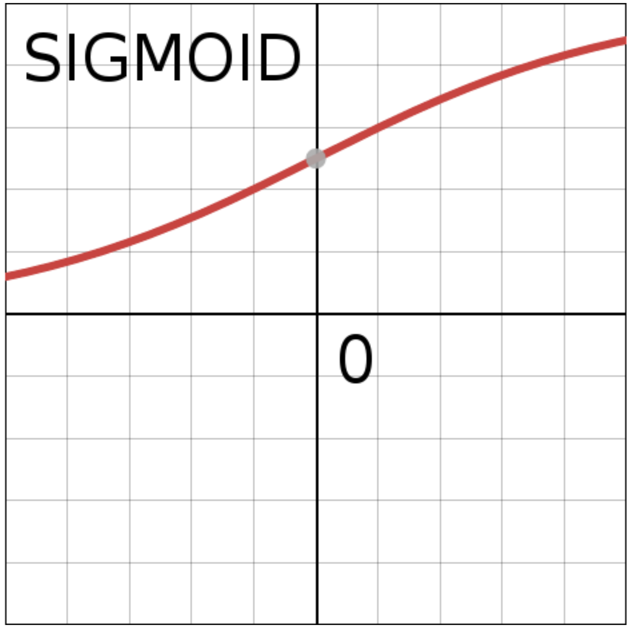
Hyperparameter / Architectural choices

- Learning Rate
- Minibatch size
- Architecture (number of nodes, number of layers, types of layers)
- Activation functions
- Weight initialization
- Regularization
- Optimizer (SGD, SGD with momentum, ADAM, etc.)
- Stopping criteria

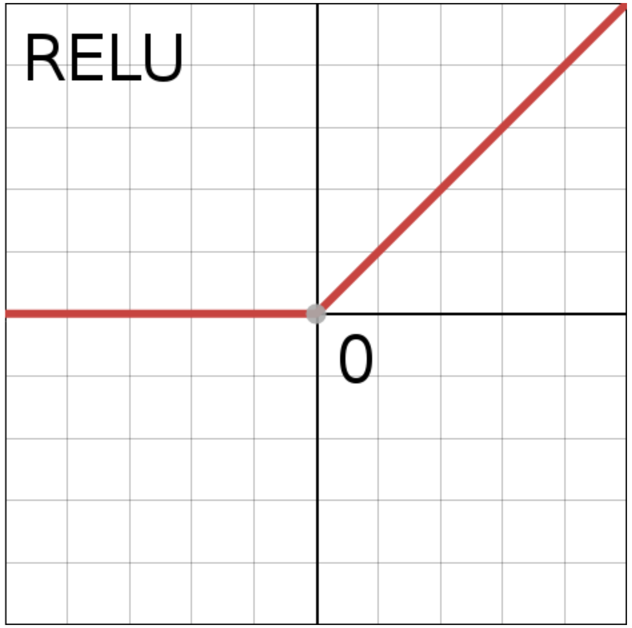
Activation Functions



Hyperbolic Tangent



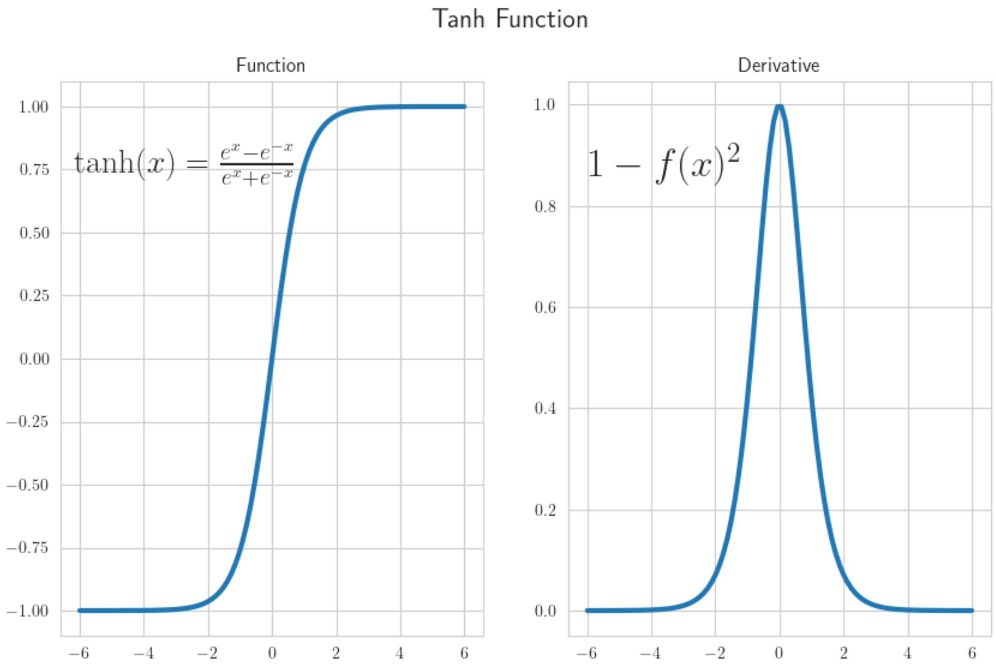
Sigmoid Tangent

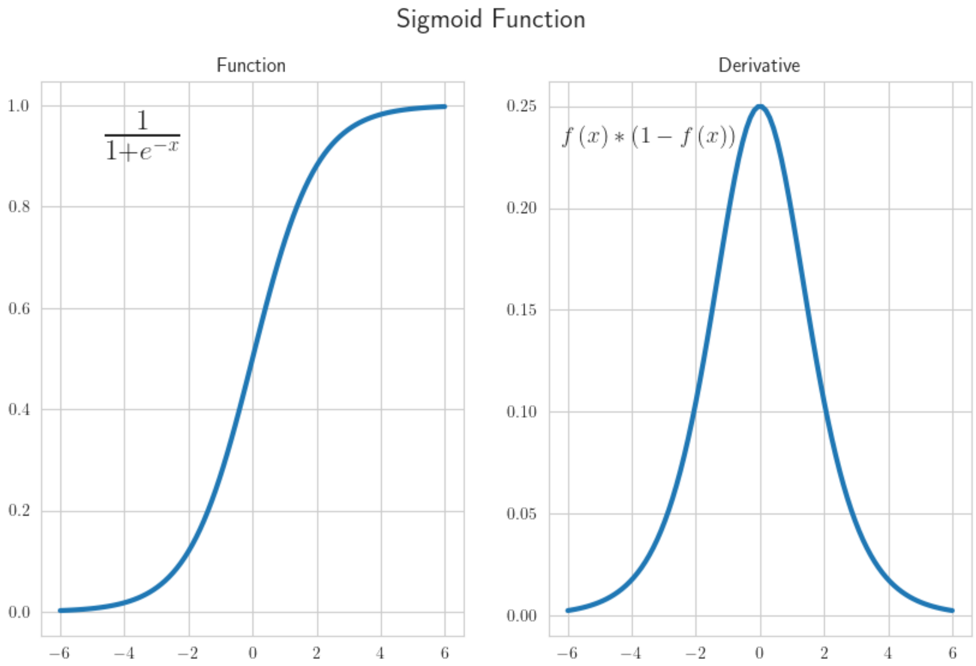


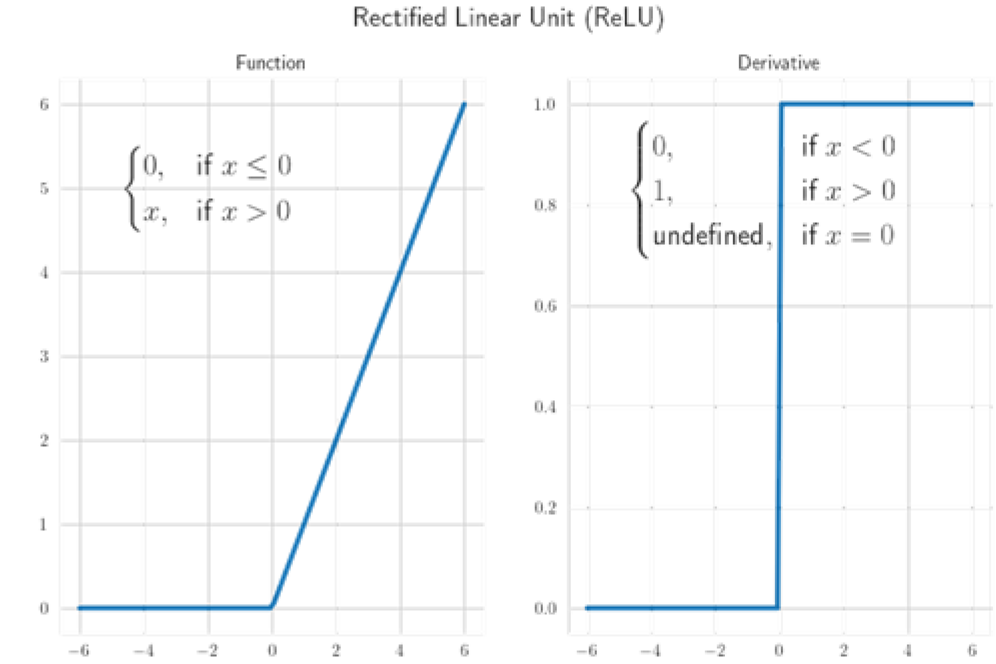
Rectified linear unit (ReLU)

Increases training/prediction speed, sparse activation, reduces vanishing gradient

Image from Danijar Hafner, Quora







Images from: https://ml-explained.com/blog/activation-functions-explained

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

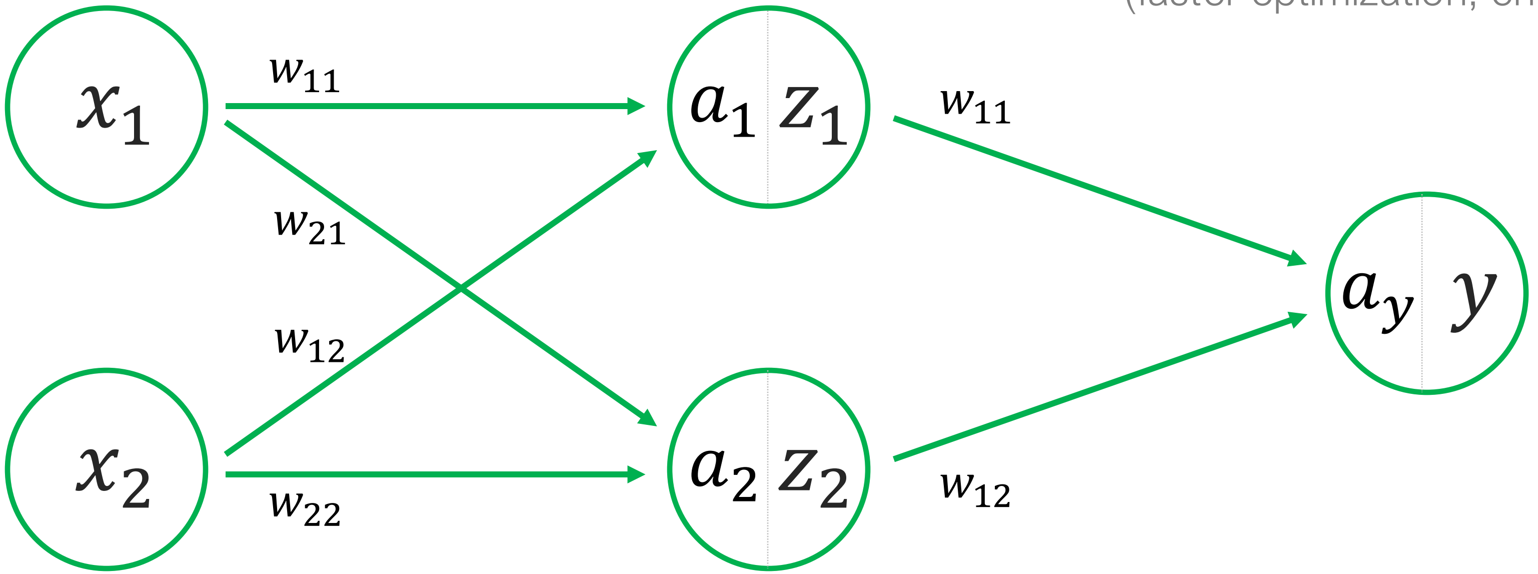
Random numbers

Need to be neither too small nor too big. 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 layer for each of the training samples in each minibatch

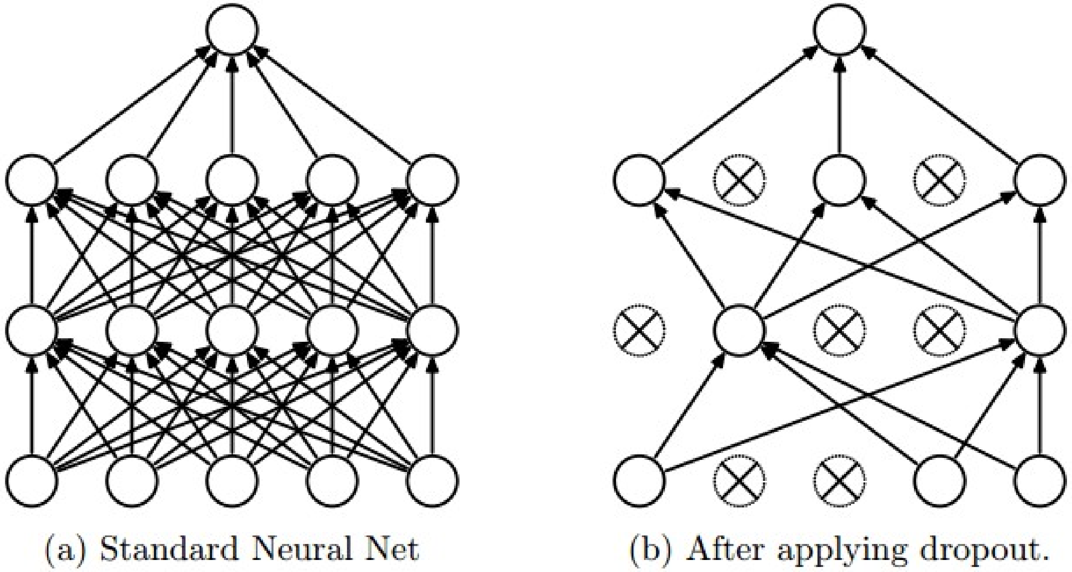
1. Subtract the mean of that activation value averaged across the minibatch

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

Regularization

L2 Regularization

L1 Regularization


(a) Standard Neural Net

(b) After applying dropout.

Dropout

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

Early Stopping

Stop the model before it has a chance to overfit
(caution: can cause underfitting)

Stanford CS231n

Watch your learning curves

Questions to ask:

- Learning anything?
- Still learning?
- Overfitting?
- Learning rate too low/high?

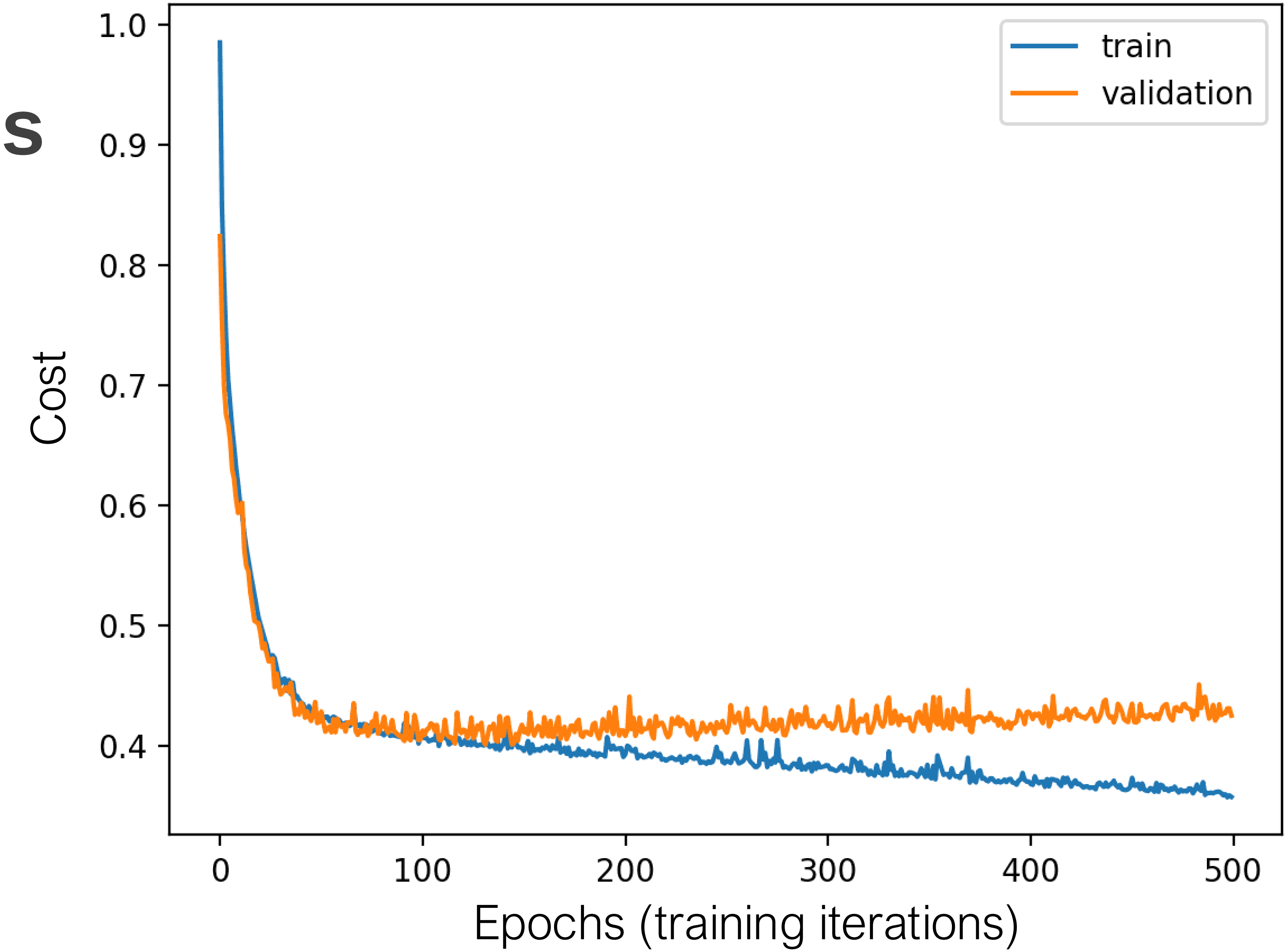


Image by Jason Brownlee

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 (ensure you CAN learn)
4. Regularize the model
    1. Add data
    2. Augmentation
    3. Use dropout
    4. Early stopping
5. Tune your model (optimize hyperparameters)

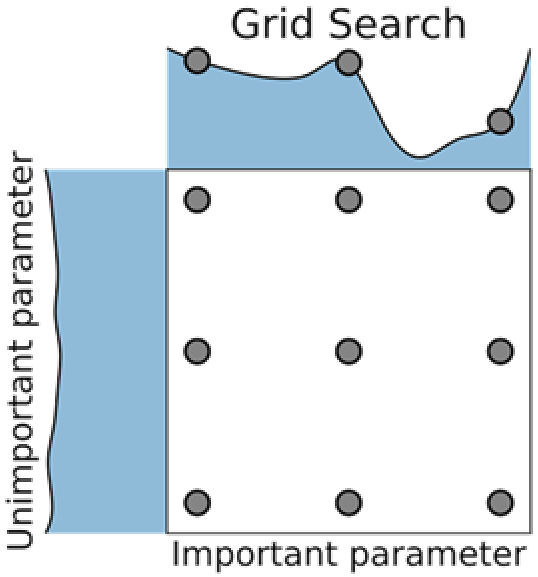
Hyperparameter tuning

- Learning Rate
- Minibatch size
- Architecture (number of nodes, number of layers, types of layers)
- Activation functions
- Weight initialization
- Regularization
- Optimizer (SGD, SGD with momentum, ADAM, etc.)
- Stopping criteria

Hyperparameter Tuning

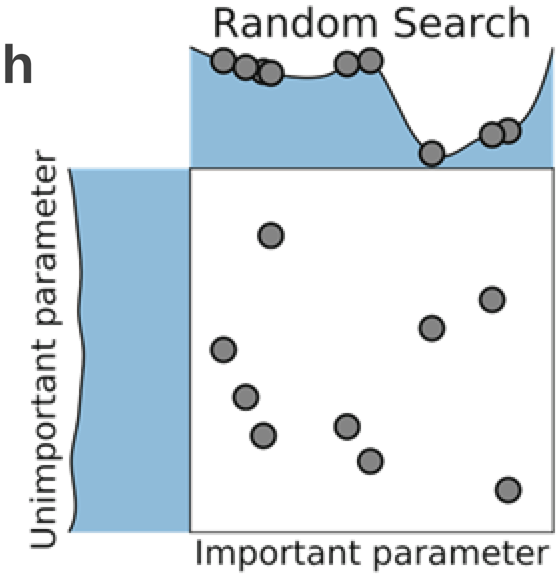
Grid Search

- Can search thoroughly
- Computationally expensive



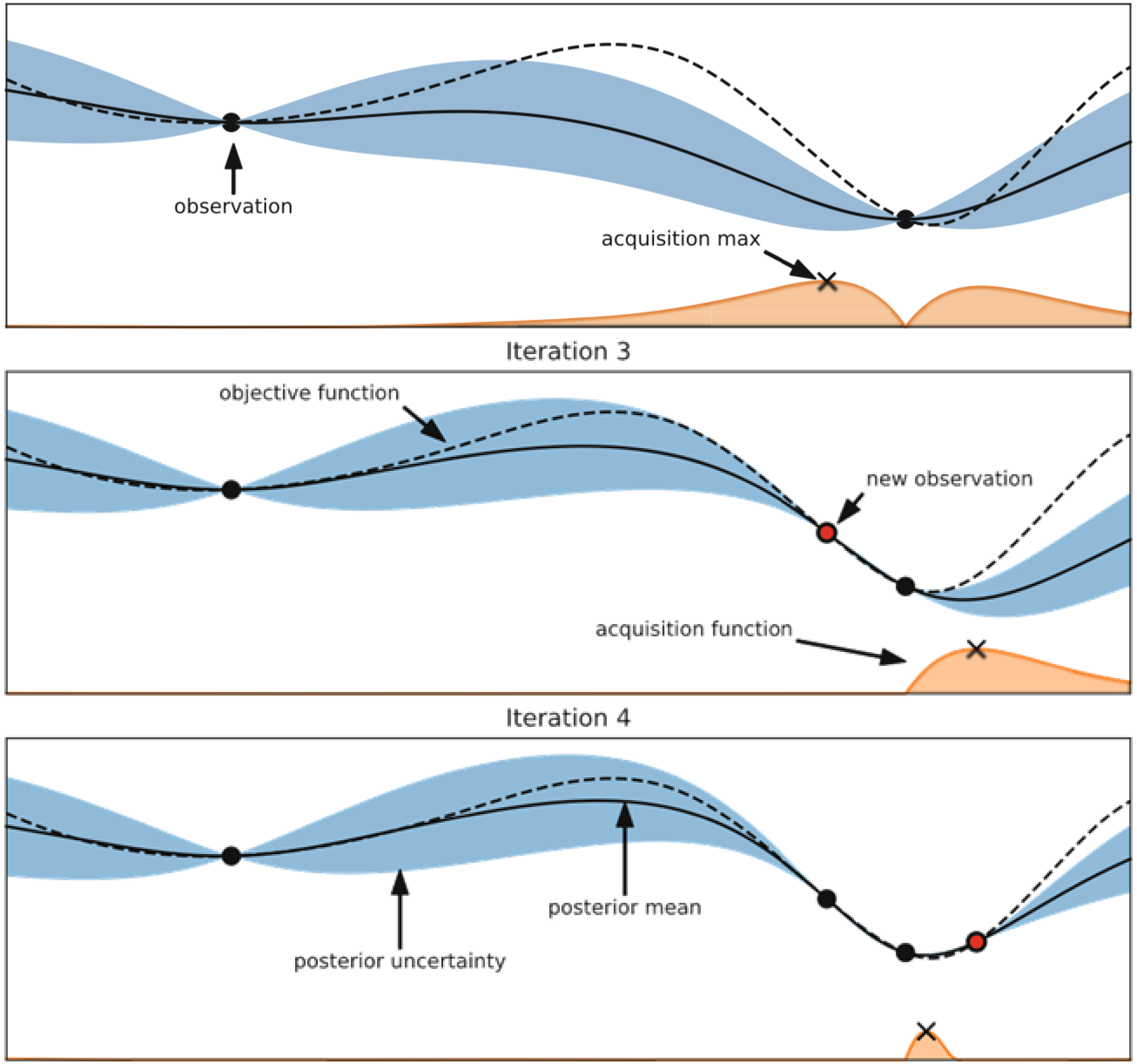
Random Search

- Works on a fixed budget and searches more quickly
- Can miss regions of the space



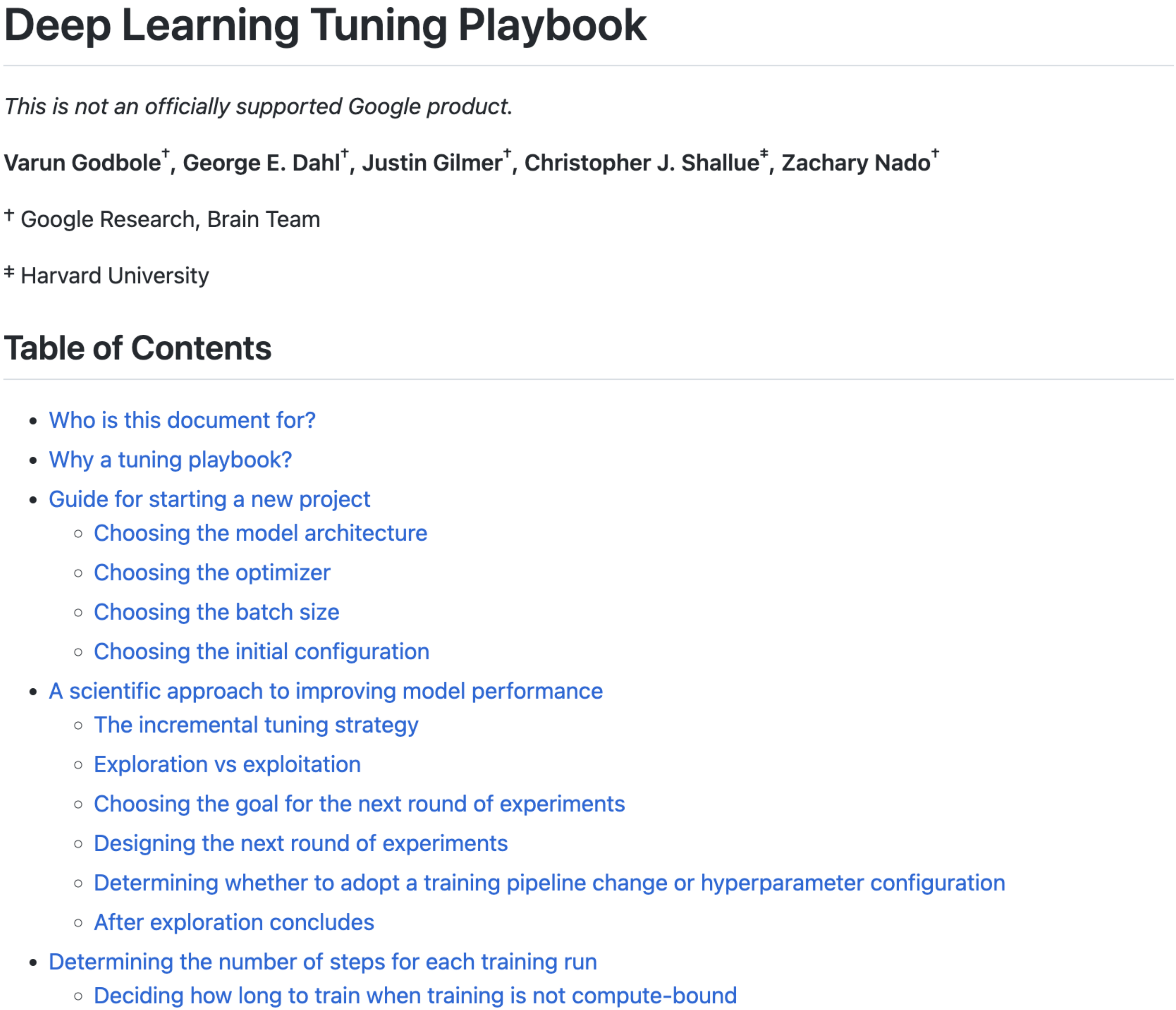
Bayesian Optimization

- Guided sampling
- Has hyperparameters of its own



Advice on using practical neural networks

[Deep Learning Tuning Playbook](#)



Deep Learning Tuning Playbook

This is not an officially supported Google product.

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