Deep Linear Neural Networks

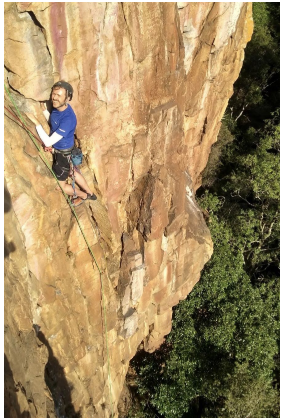
By Andrew Saxe & Saeed Salehi

neuromatch academy

Who is Andrew?

- Interested in the theory of deep learning and applications to neuroscience and psychology.

- Avid but bad rock climber
- Avid but bad singer/guitar player
- So thrilled to be learning and studying with you



Credits

A huge thank you to:

- **Saeed Salehi** for crafting the tutorials
- **Konrad Kording** for slides
- **Vladimir Haltakov**, **Spiros Chavlis**, **Polina Turishcheva**, **Anoop Kulkarni**, and **Khalid Almubarak** for content, comments & production

Welcome to Deep Linear Networks Day

We'll use the simplest possible networks to understand:

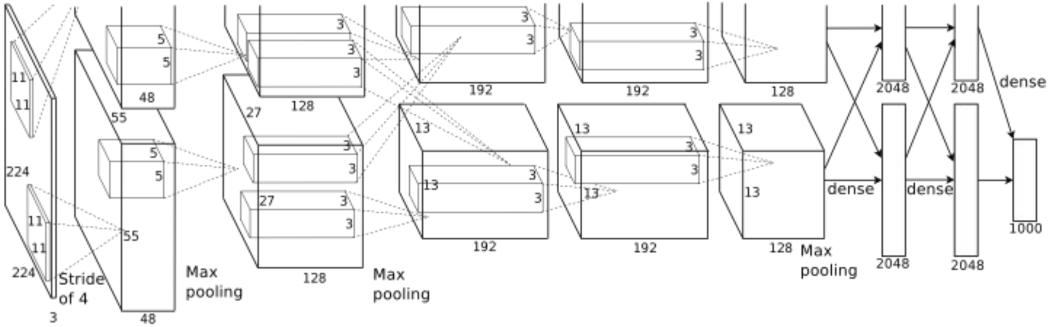
- The basics of gradient descent (Tutorial 1)
- The effect of depth on training dynamics (Tutorial 2)
- The internal representations that deep networks learn (Tutorial 3)

Gradient Descent and AutoGrad

neuromatch academy

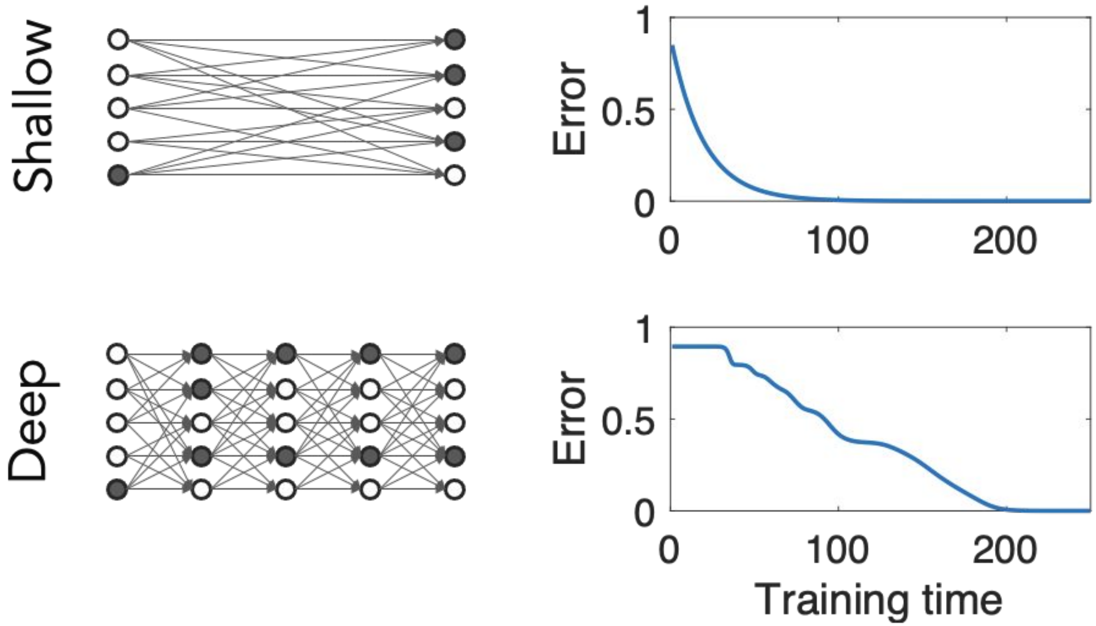
Gradient descent

How can we change parameters to make the overall system work better?

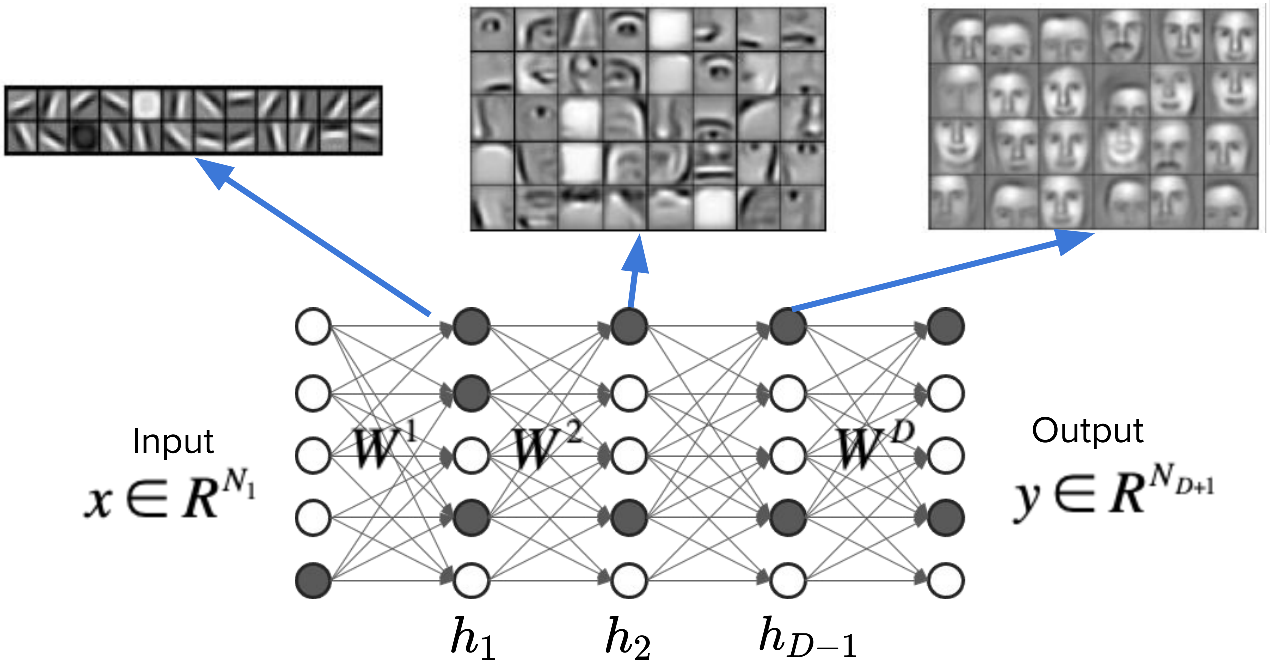


Output:
Cat
Target:
Dog

The effect of depth



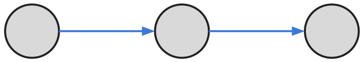
Representation learning



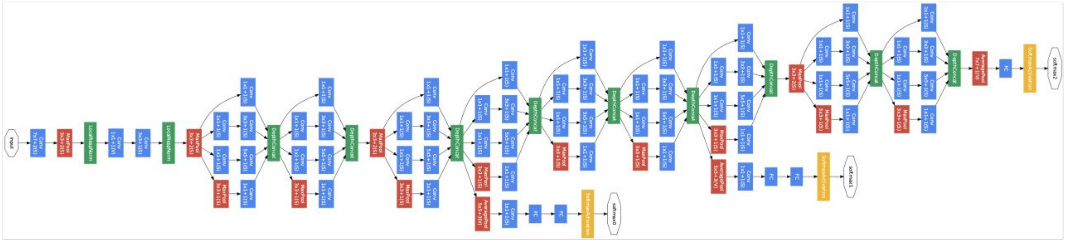
Lee et al., 2009

Simple models

Today



The rest of your career



Szegedy et al., CVPR 2015

Deep learning: key components

The designer specifies:

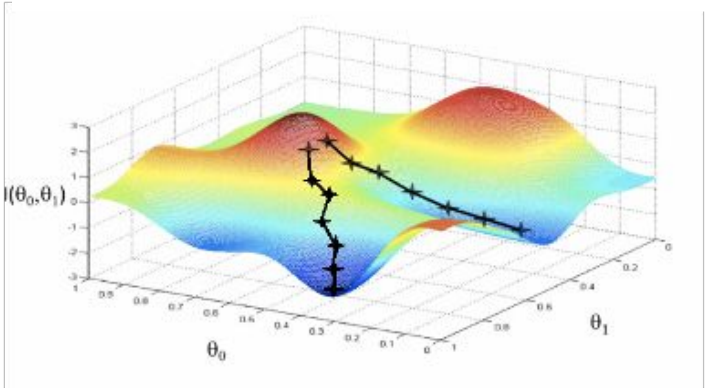
1. Objective function
2. Learning rule
3. Architecture
4. Initialisation
5. Environment

Deep learning: key components

The designer specifies:

1. **Objective function**
2. Learning rule
3. Architecture
4. Initialisation
5. Environment

What is the goal of the computation?



Deep learning: key components

The designer specifies:

1. Objective function
2. **Learning rule**
3. Architecture
4. Initialisation
5. Environment

How will weights change to improve the objective function?

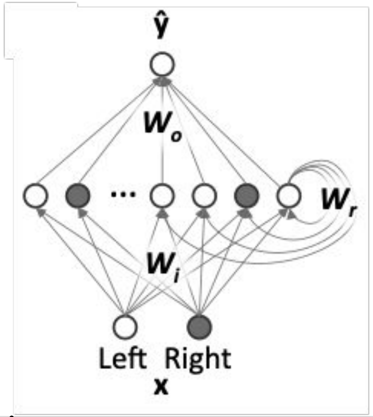
$$\Delta W = -\eta \frac{\partial L}{\partial W}$$

Deep learning: key components

The designer specifies:

1. Objective function
2. Learning rule
3. **Architecture**
4. Initialisation
5. Environment

What are the components and connectivity?



Deep learning: key components

The designer specifies:

1. Objective function
2. Learning rule
3. Architecture
4. **Initialisation**
5. Environment

What are the initial weight values?

$$W(0) \sim N(0, \sigma^2)$$

Deep learning: key components

The designer specifies:

1. Objective function
2. Learning rule
3. Architecture
4. Initialisation
5. **Environment**

What is the data provided during learning?

IMAGENET

Example

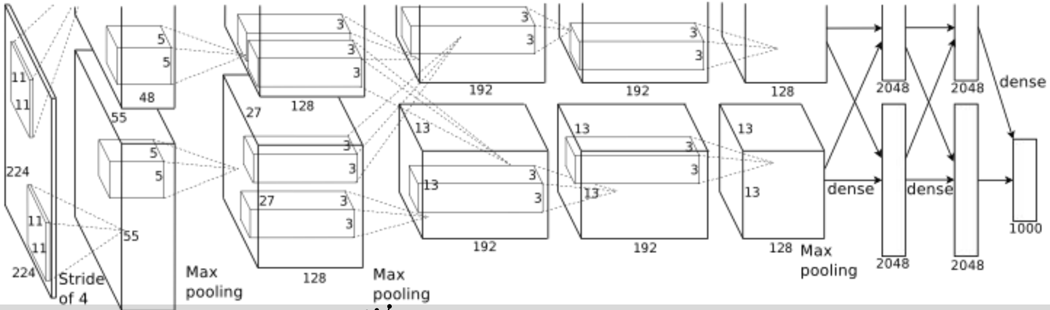
Objective function: Cross entropy loss

Learning rule: Gradient descent with momentum

Architecture: Deep convolutional ReLU network

Initialisation: He et al. (Scaled Gaussian)

Environment: ImageNet dataset



Output:
Cat
Target:
Dog

Learning as optimization

An input-output function (an ANN): $y = f_w(x)$

A loss function: $L = \ell(y, data)$

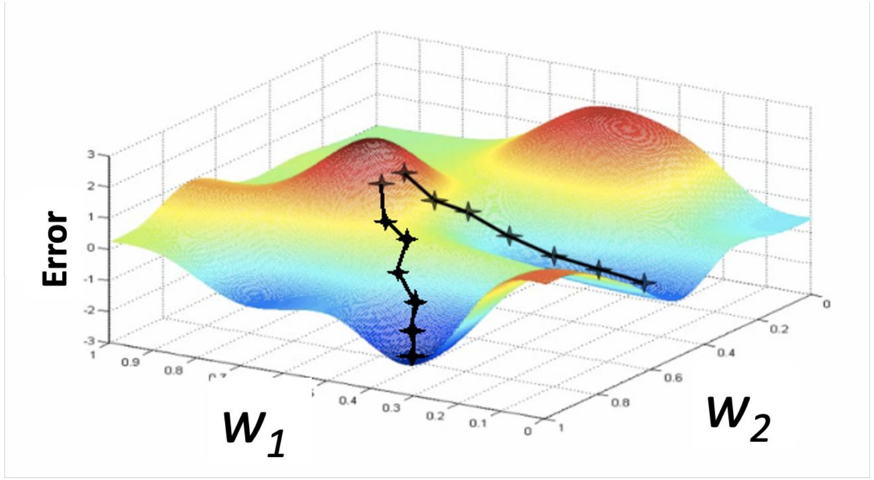
Optimization problem: $w^* = \text{argmin}_w \ell(f_w(x), data)$

The workhorse algorithm: Gradient descent

So important we will understand it at different levels:

- Conceptually
- By taking derivatives by hand (just once!)
- Through automatic differentiation in PyTorch

Gradient descent



http://blog.datumbox.com/wp-content/uploads/2013/10/gradient-descent.png

Minimize function by taking many small steps, each pointing downhill

Gradients

"how much would loss change if I changed a parameter just a tiny bit"

$$\nabla L(w) = \left[\frac{\partial L}{\partial w_1} \frac{\partial L}{\partial w_2} \cdots \frac{\partial L}{\partial w_N} \right] \Bigg|_w$$

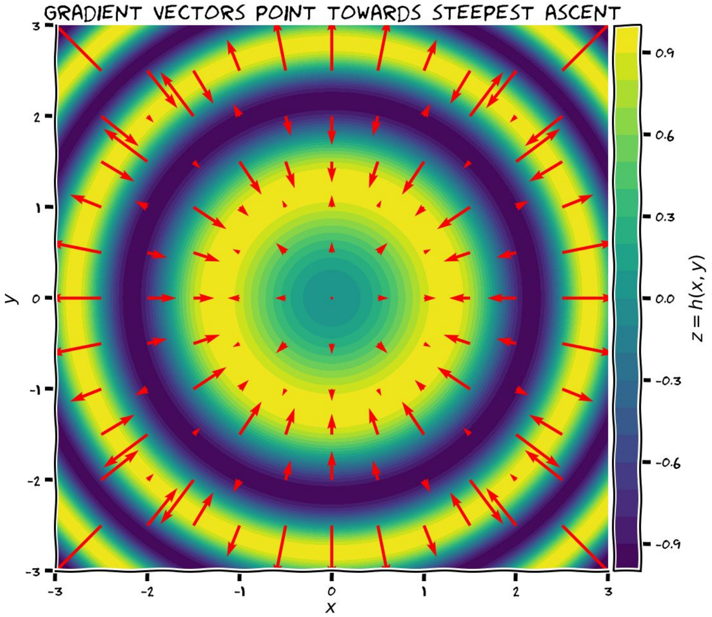
Gradients

Why are gradients useful?

Let’s start by investigating what directions the gradient points in

Derive the gradient by hand!

Gradient



The gradient points in the direction of steepest ascent.

Gradient descent

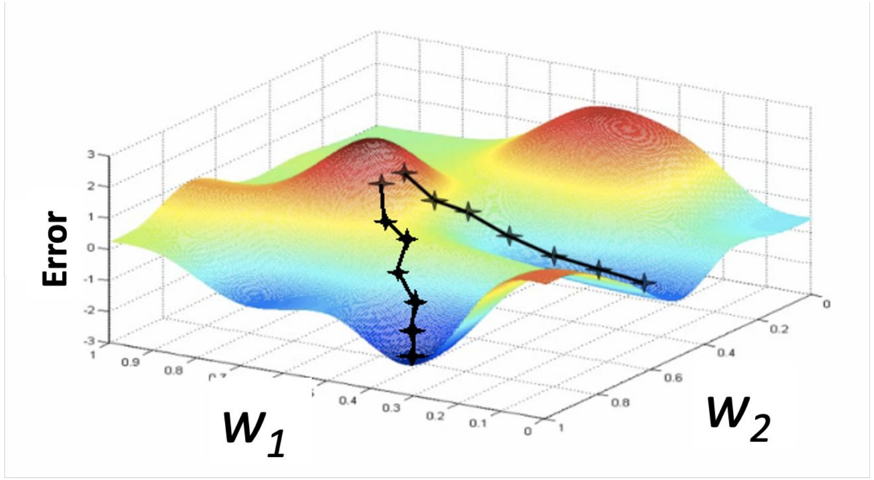
"Make small change in weights that most rapidly improves task performance"

$\Updownarrow$

Change each weight in proportion to the negative gradient of the loss

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla L(\mathbf{w}^{(t)})$$

Gradient descent



http://blog.datumbox.com/wp-content/uploads/2013/10/gradient-descent.png

Initialize: $\mathbf{w}^{(0)} = \mathbf{w}_0$

For *t=0* to *T*:

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla L(\mathbf{w}^{(t)})$$

Why gradient descent?

There are an infinite set of learning approaches that make us better

However, GD is the one that most rapidly reduces loss (for infinitesimal steps)

The core computation: Calculating the gradient

Let's try a slightly more complicated example

Because it is so fundamental, you should do it at least once

Basic tools: partial derivatives; chain rule

Derive the gradient by hand (again)!

Gradients via the computational graph

Deriving gradients ad hoc is hard and it’s easy to make mistakes

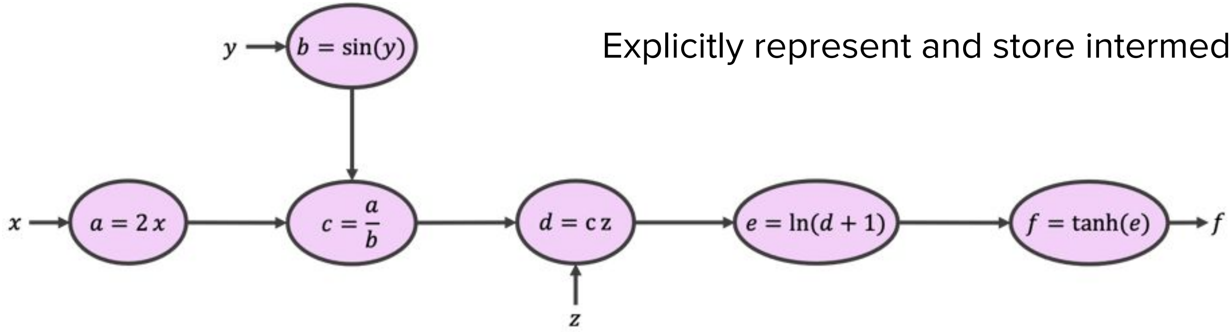
How can we simplify and systematize our approach?

Computational Graph (forward)

$$f(x, y, z) = \tanh\left(\ln\left[1 + z\frac{2x}{sin(y)}\right]\right)$$

Computational Graph (forward)

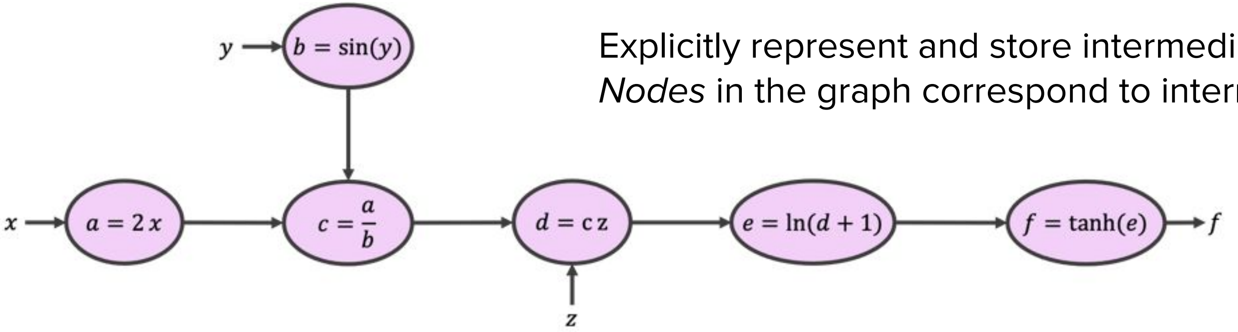
$$f(x, y, z) = \tanh\left(\ln\left[1 + z\frac{2x}{sin(y)}\right]\right)$$



Explicitly represent and store intermediate variables *a,b,c,d,e*

Computational Graph (forward)

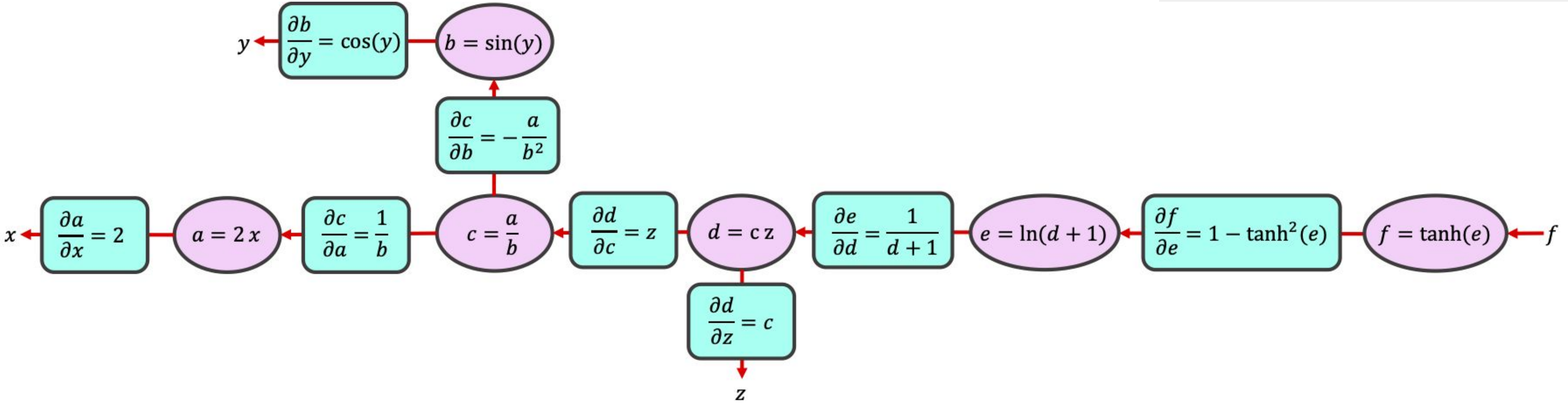
$$f(x,y,z) = \tanh\left(\ln\left[1 + z\frac{2x}{sin(y)}\right]\right)$$



Explicitly represent and store intermediate variables *a,b,c,d,e*.
Nodes in the graph correspond to intermediate variables.

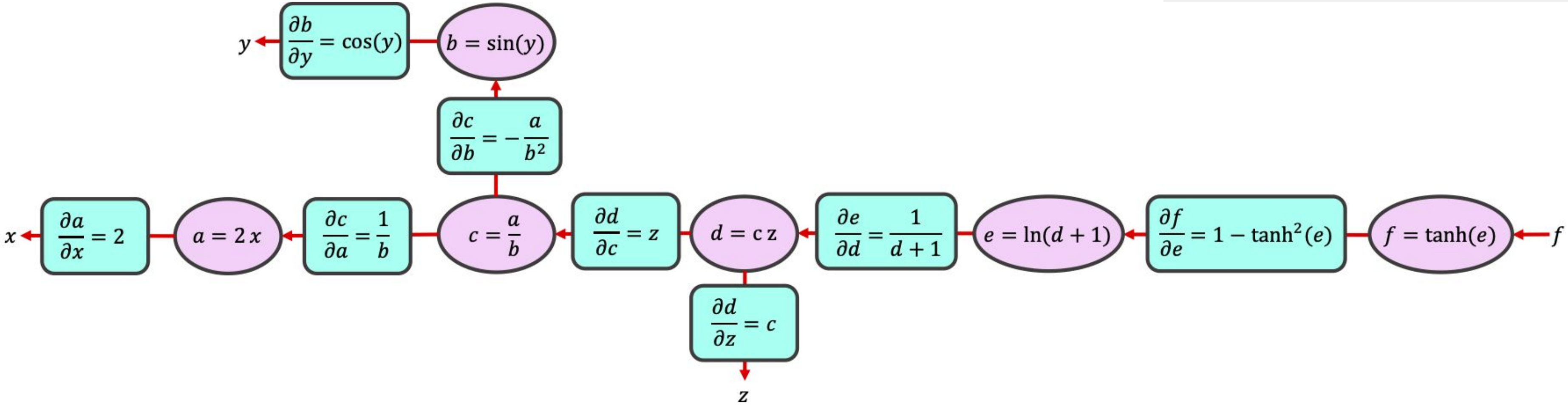
Computational Graph (backward)

Starting from the top, pass backward. Each *edge* stores partial derivative of the head of the edge with respect to the tail.



Computational Graph (backward)

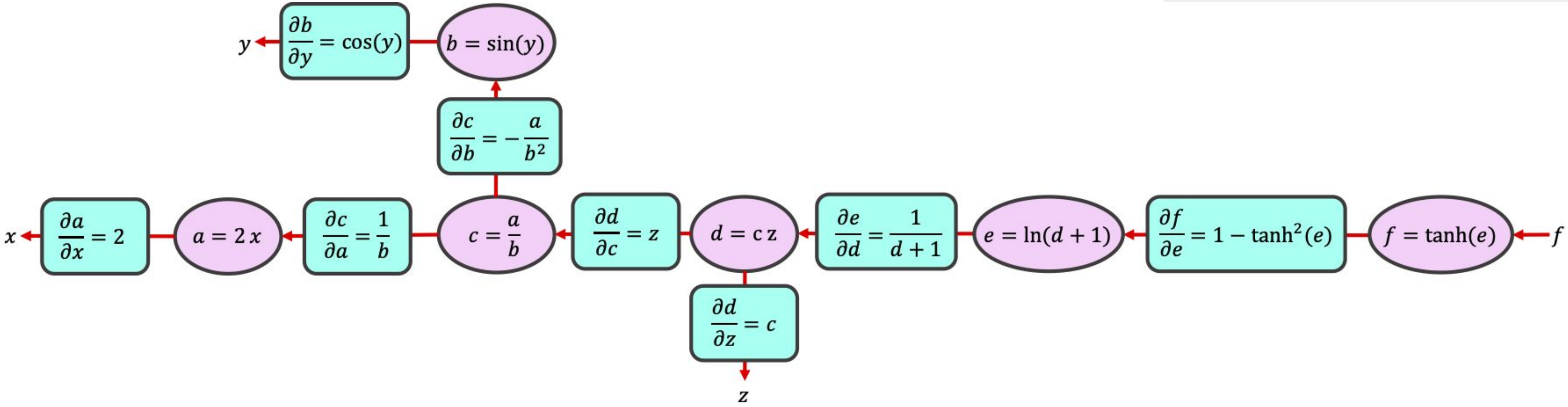
Starting from the top, pass backward. Each *edge* stores partial derivative of the head of the edge with respect to the tail.



Conveniently, the partial derivatives can often be expressed using the intermediate variables calculated in the forward pass *(a,b,c,d,e)*.

Computational Graph (gradients)

Gradients can then be easily computed using the chain rule.



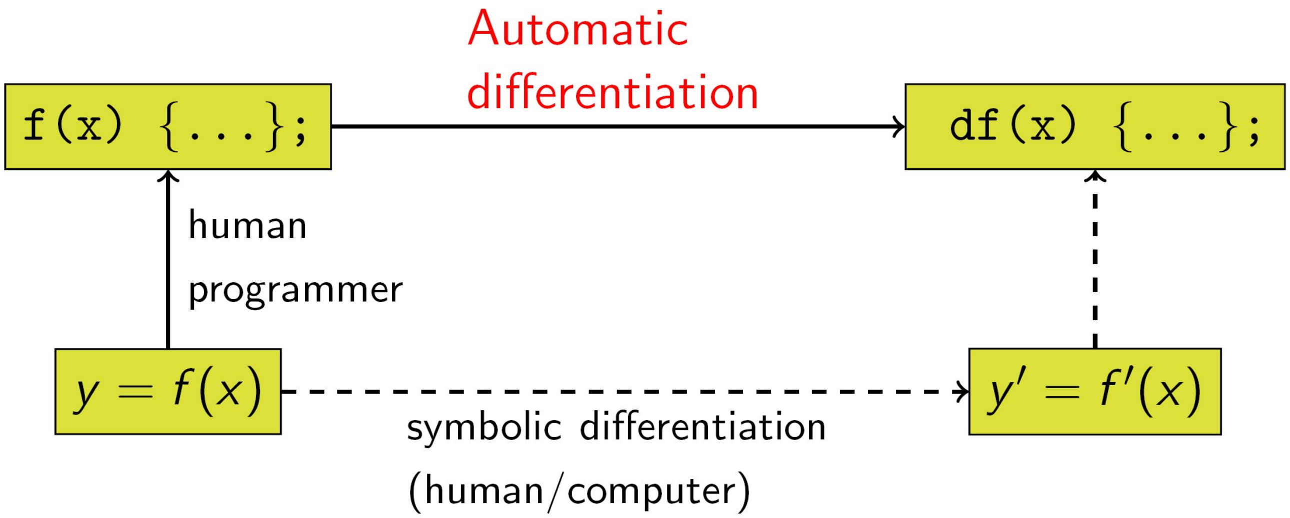
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial e}\frac{\partial e}{\partial d}\frac{\partial d}{\partial c}\frac{\partial c}{\partial a}\frac{\partial a}{\partial x} = (1 - \tanh^2(e)) \cdot \frac{1}{d+1} \cdot z \cdot \frac{1}{b} \cdot 2$$

Computational Graph (gradients)

Let’s try it: compute $\dfrac{\partial f}{\partial y}$

Derive the gradient using the graph

The magic of automatic differentiation



wikipedia

Building the computational graph

A data structure for storing intermediate values and partial derivatives needed to compute gradients.

- Node *v* represents variable
  - Stores value
  - Gradient
  - The function that created the node
- Directed edge from *v* to *u* represents the partial derivative of *u* w.r.t. *v*
- To compute the gradient $\partial L/\partial v$, find the unique path from *L* to *v* and multiply the edge weights, where L is the overall loss.

Building the computational graph

When we perform operations on PyTorch Tensors,
PyTorch does not simply calculate the output

Instead, each operation is added to the computational graph

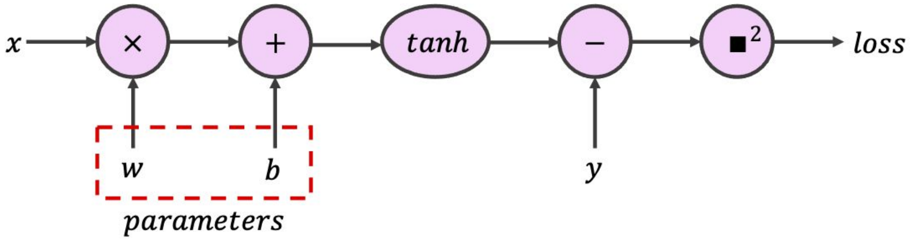
PyTorch can then do a forward and backward pass through the graph,
storing necessary intermediate variables, and yield any gradients we need

Building the computational graph

Often only some parameters are trainable and require gradients.

We indicate tensors that require gradients by setting `requires_grad=True`

$$(y - \tanh(wx + b))^2$$



Building the computational graph

PyTorch can keep adding to the graph as your code winds through functions and classes

In essence, you write code to compute the loss *L;* AutoGrad does the rest

$$(y - \tanh(wx + b))^2$$

Compute the gradient with respect to *w* and *b* the easy way!

Putting it together: a simple ANN

PyTorch can differentiate through fairly arbitrary functions

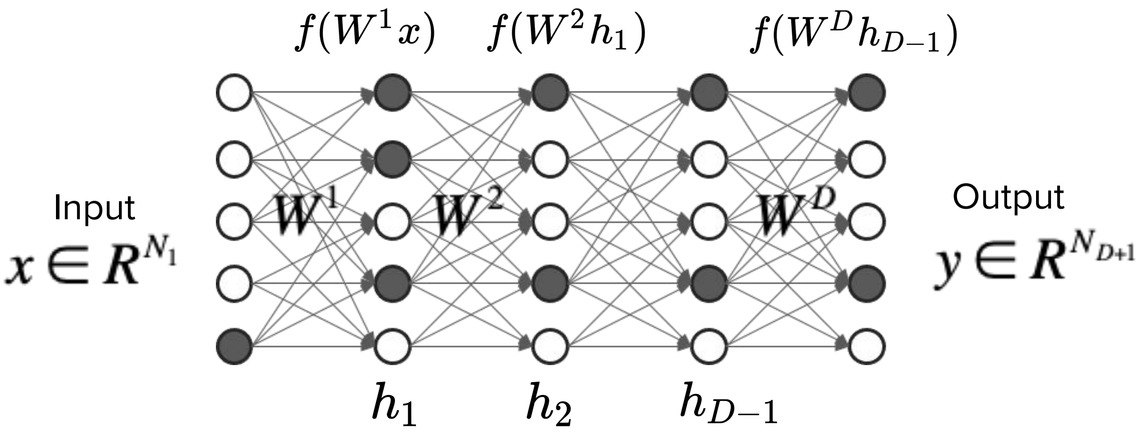
But neural networks often make use of simple building blocks

Let’s look at some ways that PyTorch makes building and training ANNs particularly simple

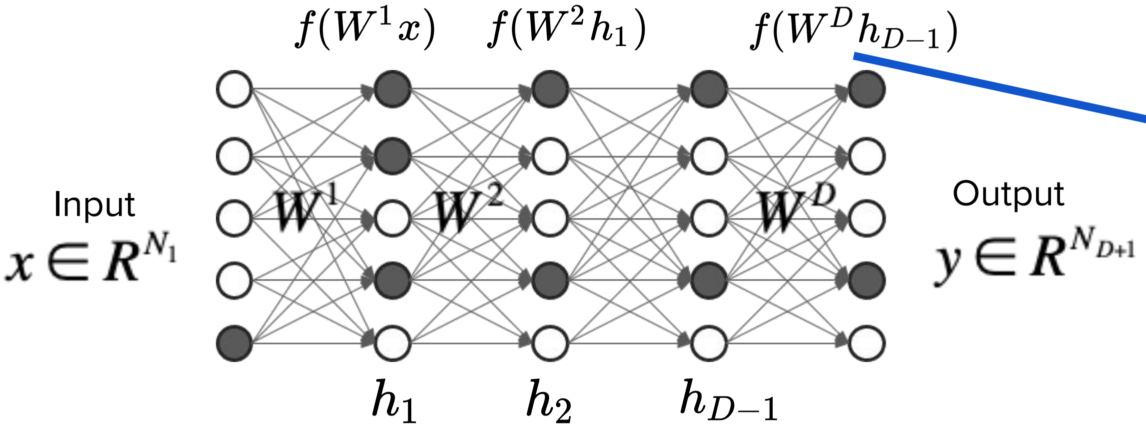
Aligning concepts and code

An input-output function (an ANN):	$y = f_w(x)$	nn.Module, nn.Sequential nn.Linear, nn.ReLU
A loss function:	$L = \ell(y, data)$	nn.MSELoss, nn.CrossEntropyLoss
Optimization problem:	$w^* = \mathrm{argmin}_w \ell(f_w(x), data)$	torch.optim.SGD, torch.optim.ADAM

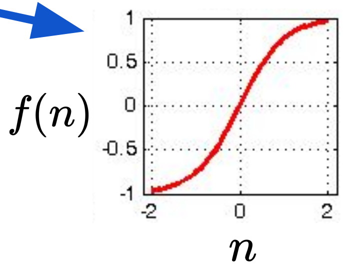
Deep Network



Deep Network



Neural nonlinearity



The canonical train loop in PyTorch

```
for i in range(n_epochs):
    optimizer.zero_grad() # Reset all gradients to zero
    prediction = neural_net(inputs) # Forward pass
    loss = loss_function(prediction, targets) # Compute the loss
    loss.backward() # Backward pass to build the graph and compute the gradients
    optimizer.step() # Update weights using gradient
```

The canonical train loop in PyTorch

Let’s use these tools!

Build a network using the nn.Module and nn components

Compute predictions for some input data

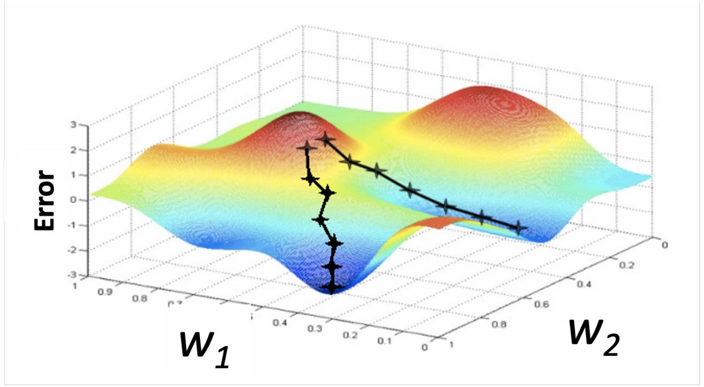
Calculate the loss

Calculate derivatives with AutoGrad

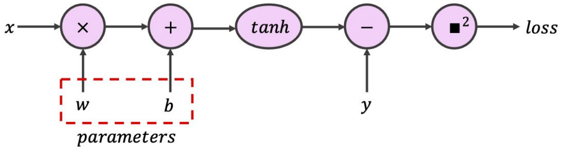
Run a step of the optimizer

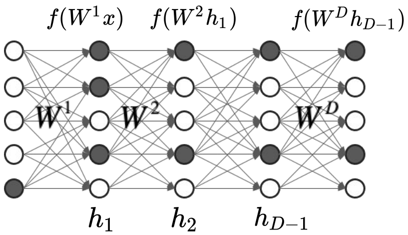
Train a neural network!

Wrap up: gradient descent



http://blog.datumbox.com/wp-content/uploads/2013/10/gradient-descent.png





Learning Hyperparameters

Andrew Saxe

The effect of depth on training

Now that we can implement a network, let's understand some core learning behaviors and tradeoffs

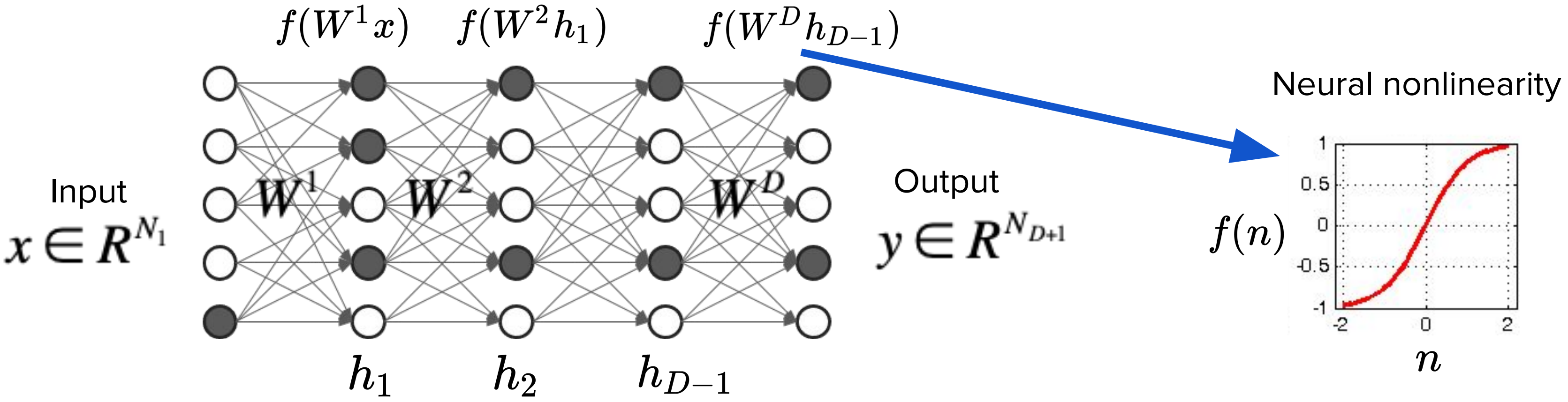
The architecture, initialization, and learning hyperparameters all can change the performance of a network dramatically

To be proficient at training deep networks, we have to build our intuition

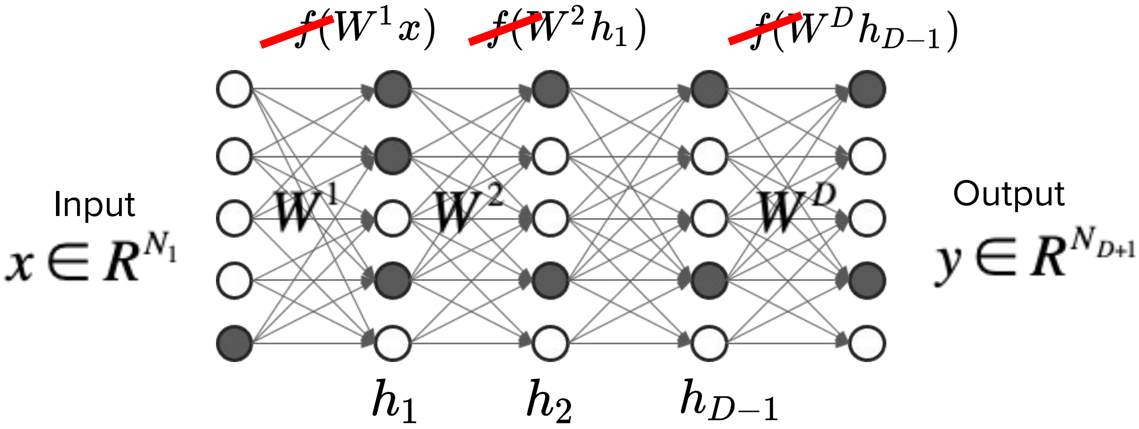
Opening the black box

Deep Network

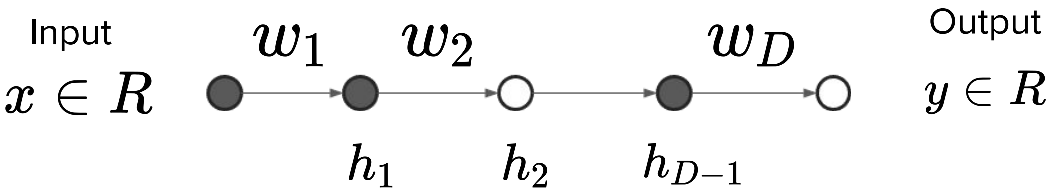
Little hope to understand full modern systems in detail



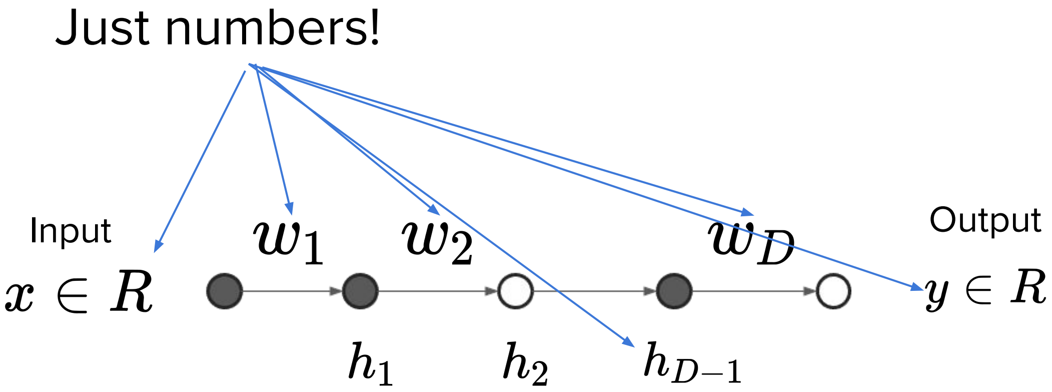
Deep *Linear* Network



Deep *Narrow* Linear Network

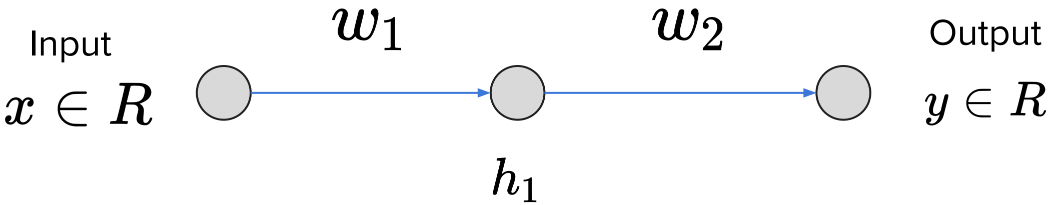


Deep *Narrow* Linear Network



$$y = w_D w_{D-1} \cdots w_1 x$$

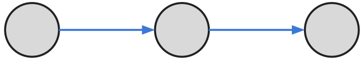
1 Layer Narrow Linear Network



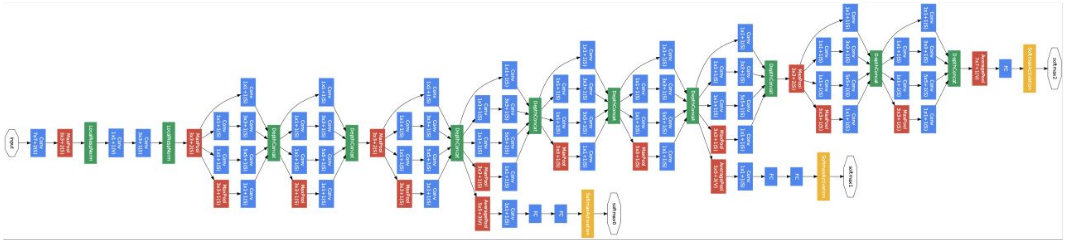
$$y = x w_1 w_2$$

Simple models

Today



The rest of your career

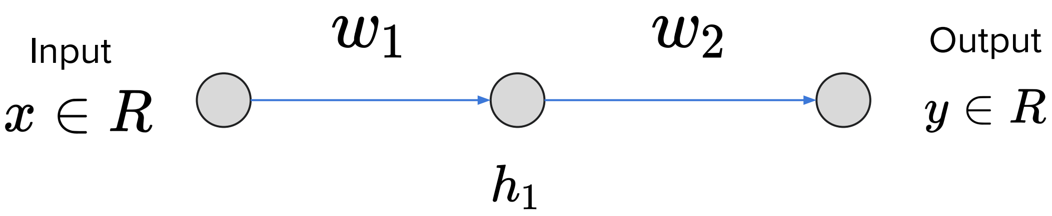


Szegedy et al., CVPR 2015

1 Layer Narrow Linear Network

Dataset: $\mathcal{D} = \{(x_1, y_1), (x_2, y_2), \cdots, (x_P, y_P)\}$

Mean squared error loss: $L(w_1, w_2) = \frac{1}{P}\sum_{p=1}^{P}(y_p - \hat{y}_p)^2$



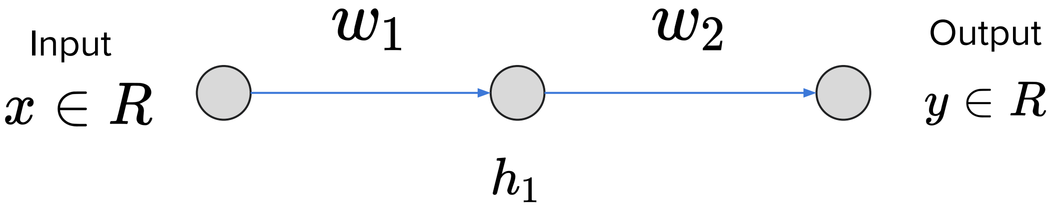
$$y = x w_1 w_2$$

Loss from one example $= \frac{1}{P}(y_p - x_p w_1 w_2)^2$

1 Layer Narrow Linear Network

Dataset: $\mathcal{D} = \{(x_1, y_1), (x_2, y_2), \cdots, (x_P, y_P)\}$

Mean squared error loss: $L(w_1, w_2) = \frac{1}{P} \sum_{p=1}^{P} (y_p - \hat{y}_p)^2$



$$y = x w_1 w_2$$

Implement gradient descent

Training landscape

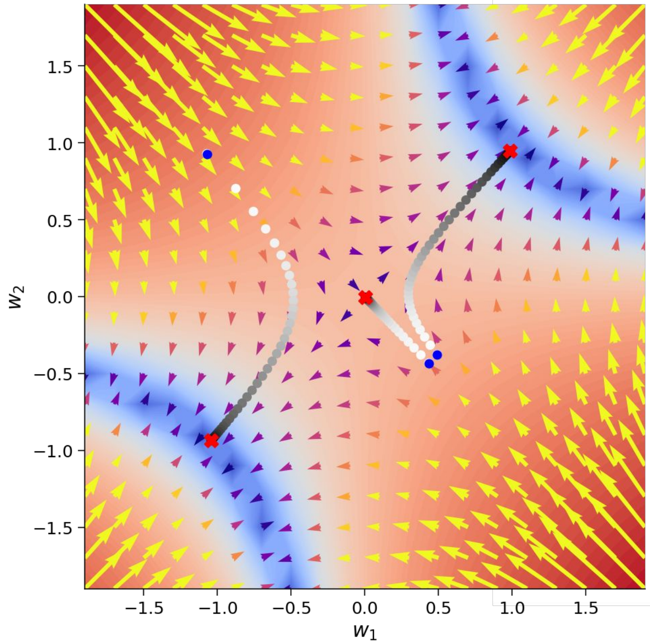
We train networks by minimizing the loss function

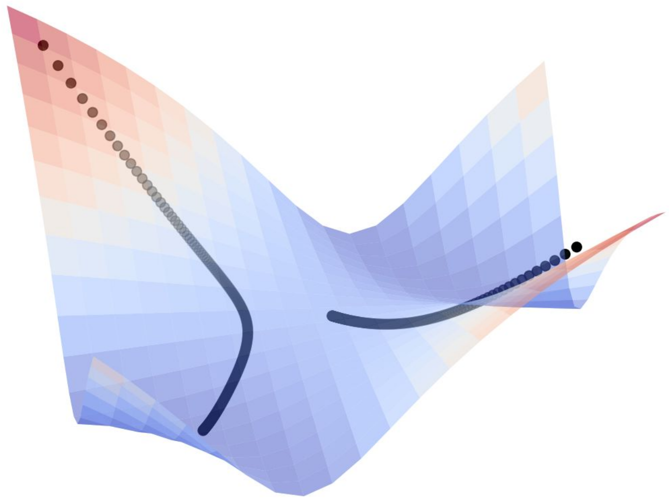
What do these loss landscapes actually look like?

Usually loss landscapes are impossible to plot because they are in high dimensions, but here we can examine it directly

Explore this loss landscape and the resulting GD trajectories

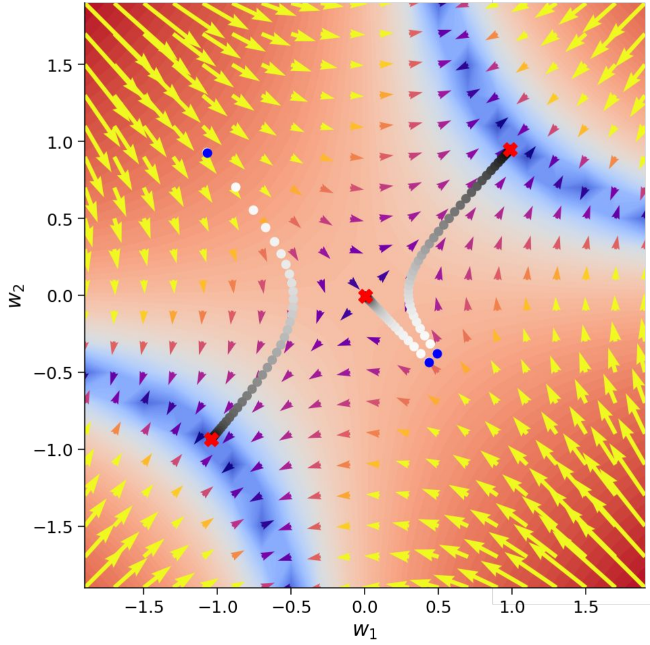
Anatomy of a landscape

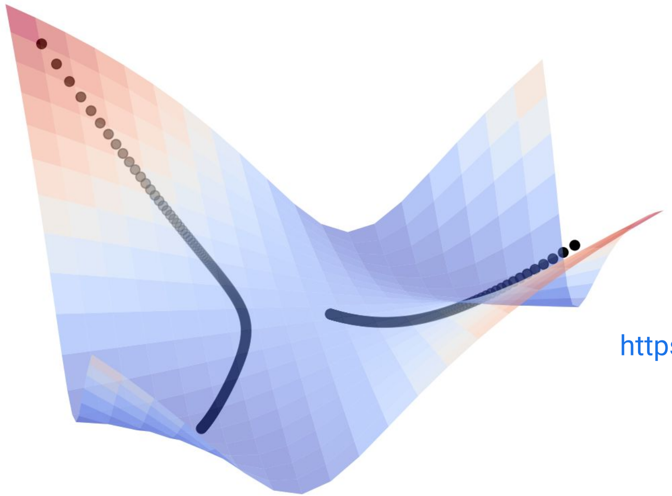




Critical points: where the gradient is zero and dynamics stop
Minimum: surrounding points are not lower
Maximum: surrounding points are not higher
Saddle point: some descent directions, some ascent directions

Anatomy of a landscape



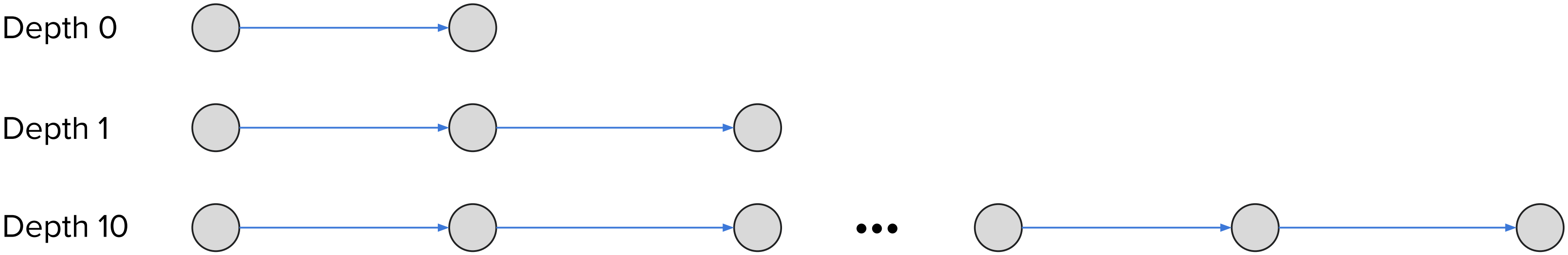


https://losslandscape.com/explorer

Critical points: where the gradient is zero and dynamics stop
Minimum: surrounding points are not lower
Maximum: surrounding points are not higher
Saddle point: some descent directions, some ascent directions

The effect of depth on training

How does network depth impact training speed, everything else being equal?



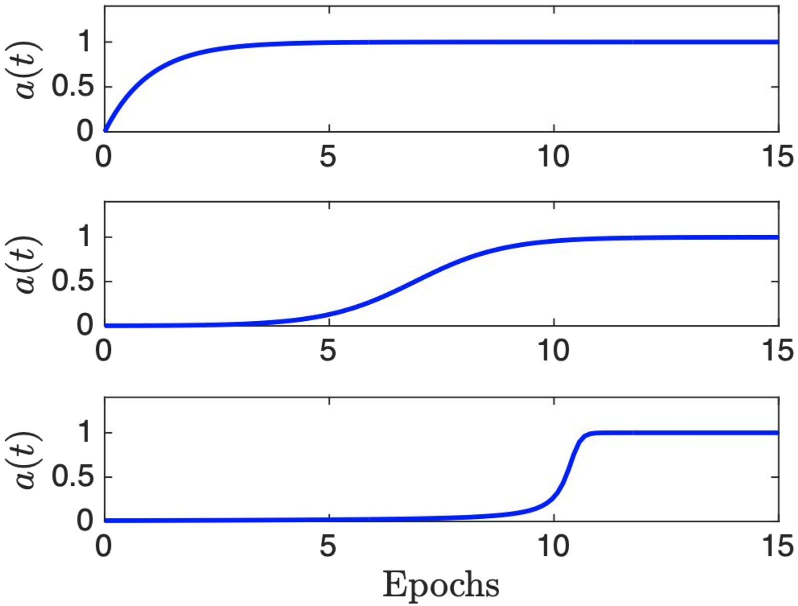
Explore how depth changes learning trajectories

The effect of depth on training

Shallow (D=0):

Deep (D=1):

V. Deep ($D \longrightarrow \infty$):



$$a(t) = w_{D+1} w_D \cdots w_2 w_1$$

Choosing a learning rate

How to pick η? $$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla L(\mathbf{w}^{(t)})$$

The gradient points in the steepest descent direction for *infinitesimal* step sizes

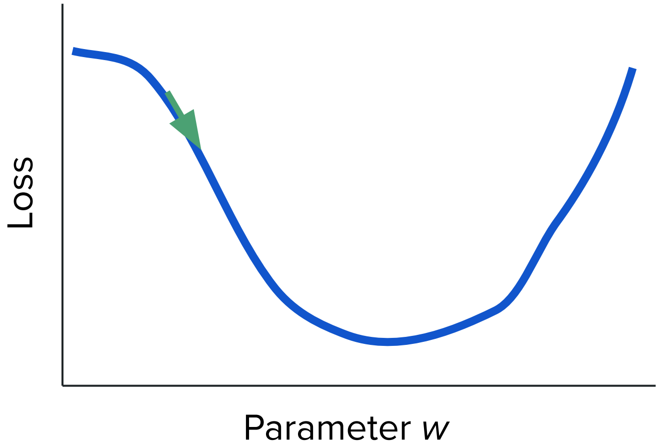
But infinitesimal step sizes don't take you very far!

Play with learning rate. Learn to diagnose issues from error curves.

Choosing a learning rate

How to pick η? $$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla L(\mathbf{w}^{(t)})$$

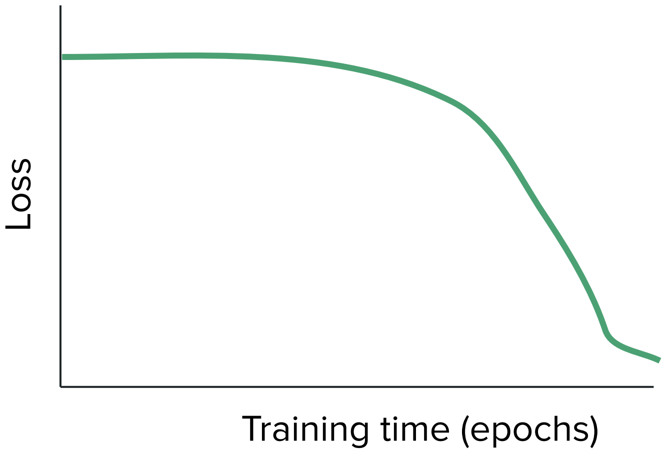
Too small:
flat line

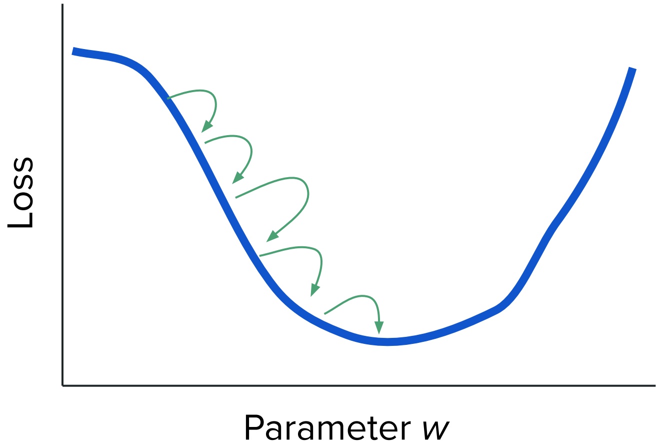


Choosing a learning rate

How to pick η? $$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla L(\mathbf{w}^{(t)})$$

Slightly too small: works but slow

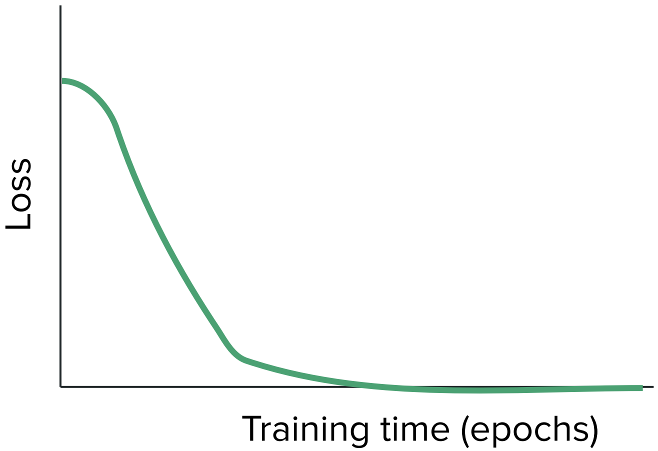


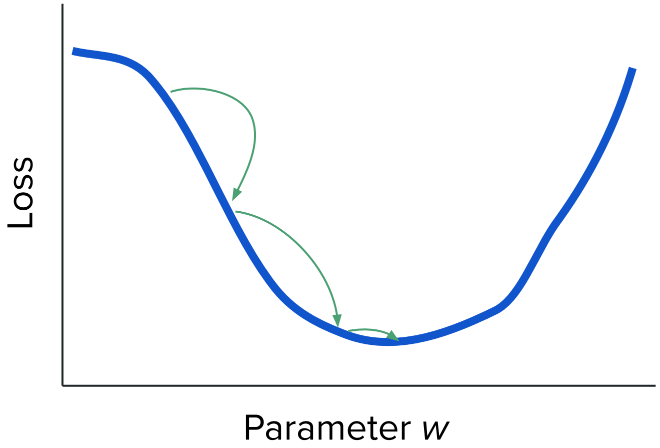


Choosing a learning rate

How to pick η? $$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla L(\mathbf{w}^{(t)})$$

Just right: converges quickly and cleanly

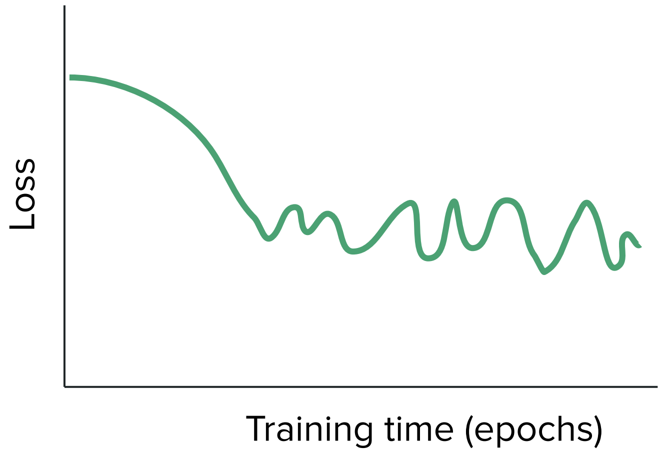


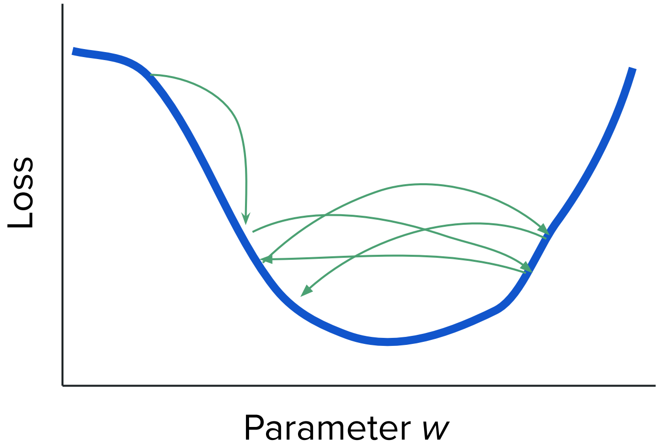


Choosing a learning rate

How to pick η? $$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla L(\mathbf{w}^{(t)})$$

Slightly too big: chaotic

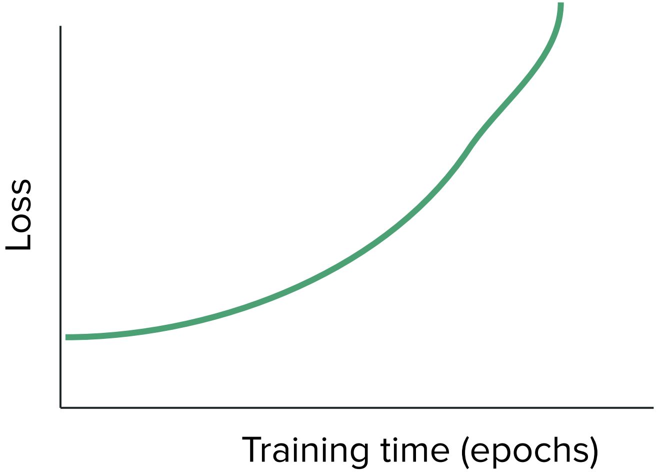


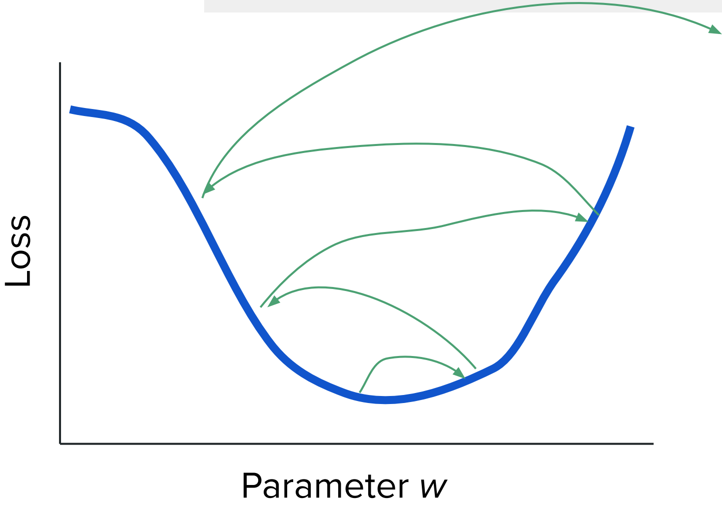


Choosing a learning rate

How to pick η? $$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla L(\mathbf{w}^{(t)})$$

Way too big:
Divergence





Choosing a learning rate

How to pick η? $$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla L(\mathbf{w}^{(t)})$$

Lesson for practice: Aim for the maximum stable learning rate

Depth and learning rate

Unfortunately, hyperparameters interact

The right learning rate for one depth may not be the right learning rate for another

Do deeper networks need larger or smaller learning rates? Are deep networks still slower to train if you optimize the learning rate for each?

Play with both depth and learning rate.

Depth and learning rate

Unfortunately, hyperparameters interact

The right learning rate for one depth may not be the right learning rate for another

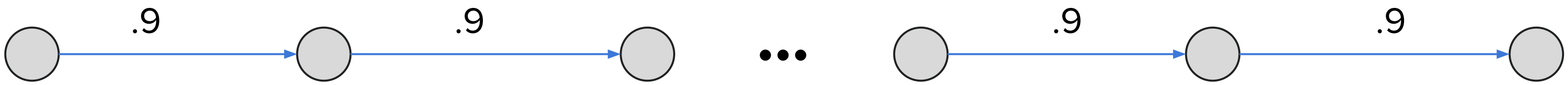
In general, deeper networks need smaller learning rates

Lesson for practice: Carefully optimise all hyperparameters for every architecture you try (this may require many computers :)

Initialisation matters

Unlike in shallow networks, learning in deep networks is exquisitely sensitive to initialisation

Basic reason: products of numbers vanish or explode $y = (\prod_{i=1}^{D} w_i)x$

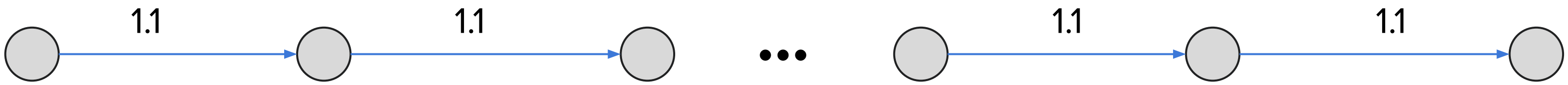


$$y = (0.9)^{100}x = 0.0000265x$$

Initialisation matters

Unlike in shallow networks, learning in deep networks is exquisitely sensitive to initialisation

Basic reason: products of numbers vanish or explode $y = (\prod_{i=1}^{D} w_i)x$

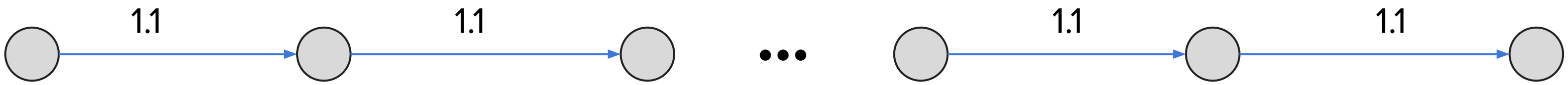


$$y = (1.1)^{100} x = 13780.6x$$

Initialisation matters

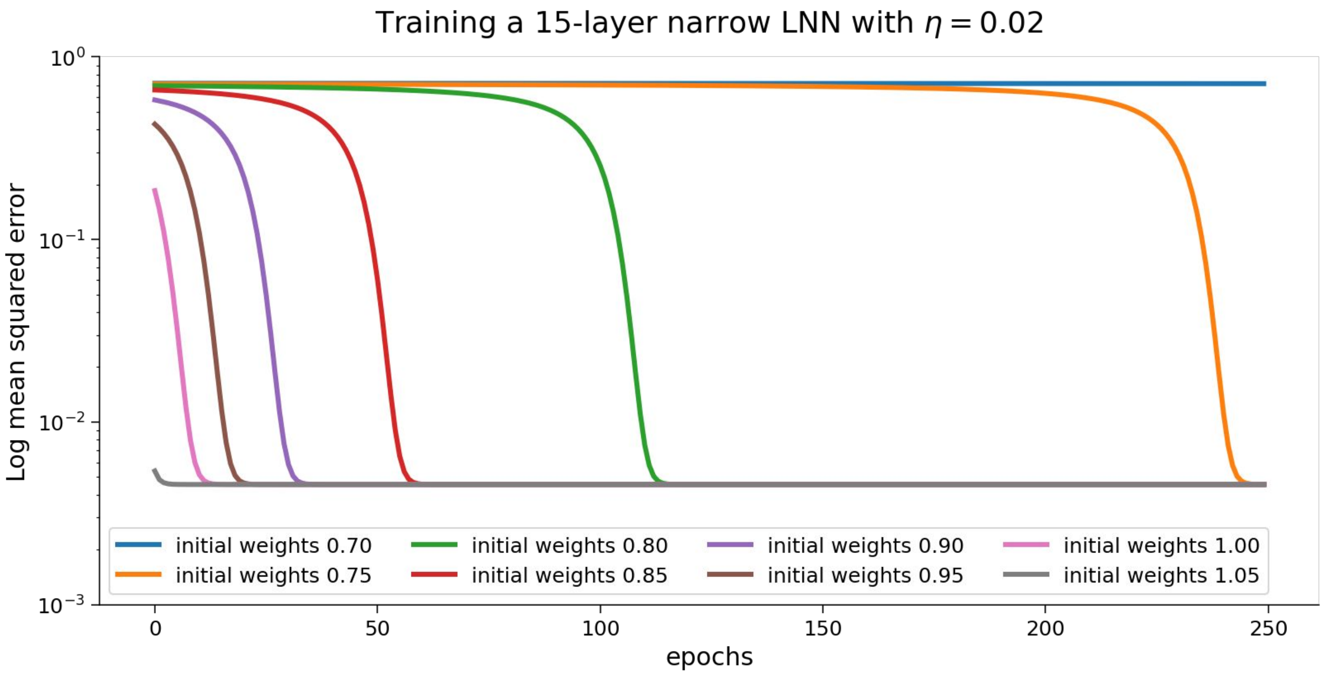
Unlike in shallow networks, learning in deep networks is exquisitely sensitive to initialisation

Basic reason: products of numbers vanish or explode $y = (\prod_{i=1}^{D} w_i)x$



Explore how initialisation impacts learning in a deep network.

Initialisation matters



Initialisation matters

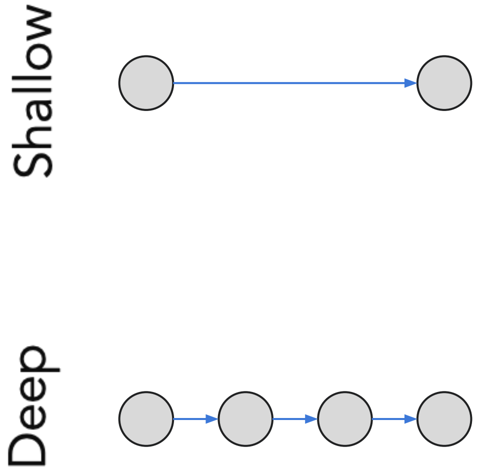
Initialisations in deep networks need to be carefully chosen so that activity and gradients have similar magnitude across the network

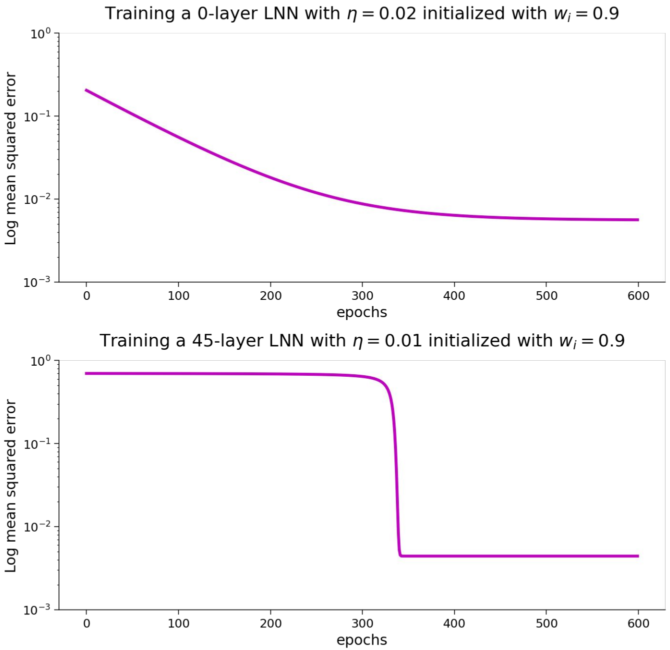
Initialisations that preserve variance across depth are known as “dynamic isometry” initialisations

For deep narrow linear network, this corresponds to weights near 1

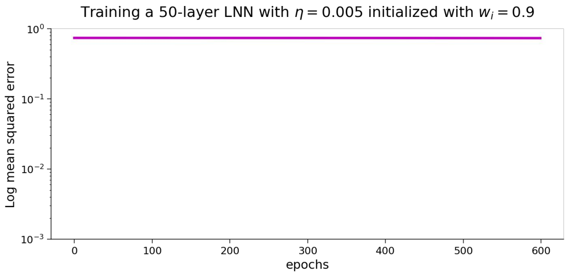
$$y = 1^{100} x = x$$

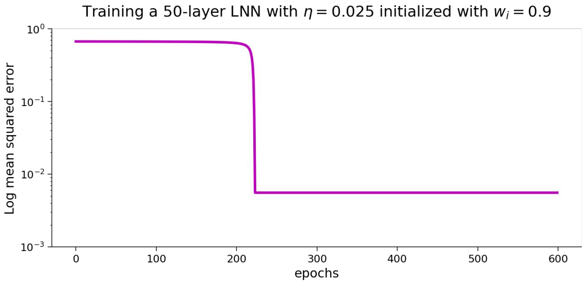
Wrap up: the effect of depth

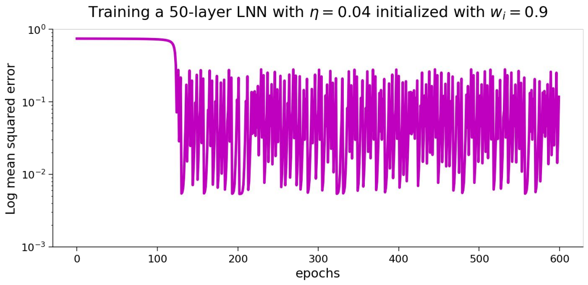




Wrap up: learning rate







Wrap up: initialization