Intro to deep learning

Dr. Janoś Gabler, University of Bonn

Lecture 8: Neural Networks from Scratch

Motivation

- Today we finally implement a neural network from scratch
- We look at two examples to get intuition
  - Digit recognition as in 3Blue1Brown Video
  - Even tinier problem to get intuition
- You will understand things we have already worked with
  - What are these "last hidden states"
  - What is a "classification head"
- Many pretty plots!

Topics

- What is a neural network
- What are the trainable parameters
- What are nonlinearities and why do we need them
- What does a Network do before it is trained
- Training loops from scratch

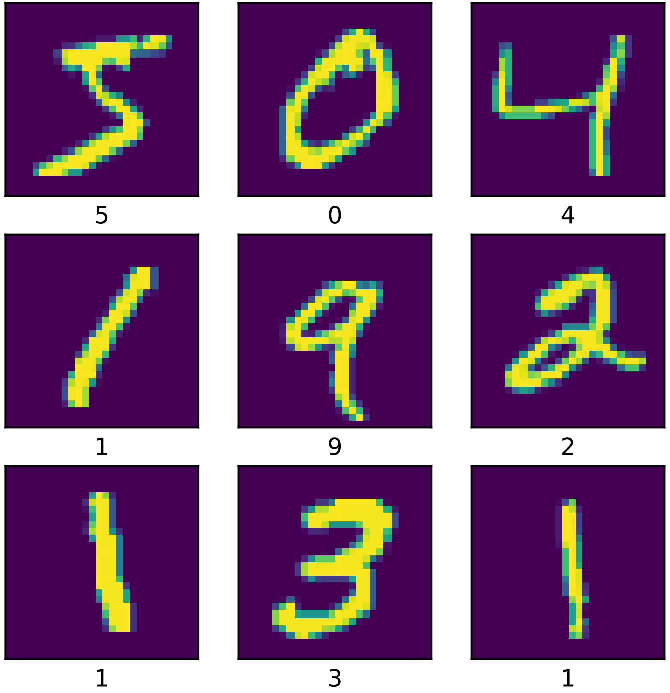
Technical topics

- Randomness in pytorch
- More advanced automatic differentiation
- Indexing tricks

Disclaimer

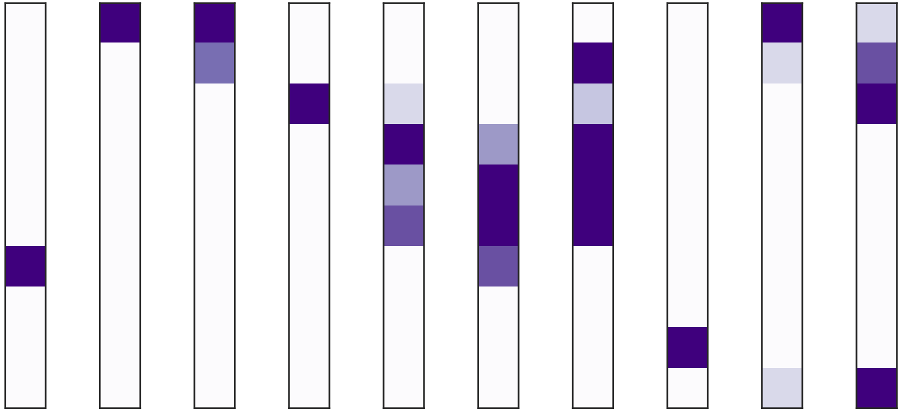
- Today we implement many things from absolute scratch
- This is so you gain understanding, how things works
- In practice, you should use higher level interfaces
- We will learn how to do that next week

Task 1: Digit recognition



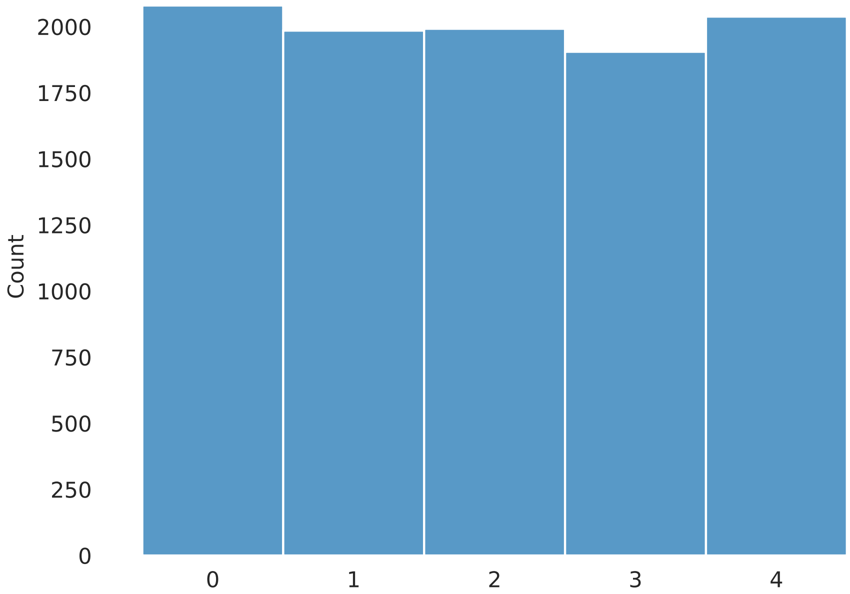
- 10 different digits
- Standard introductory example
- 28 x 28 pixels
- 255 shades of brightness
- Can be solved with very simple models
- 60 000 images with balanced class distribution

Task 2: Line length recognition

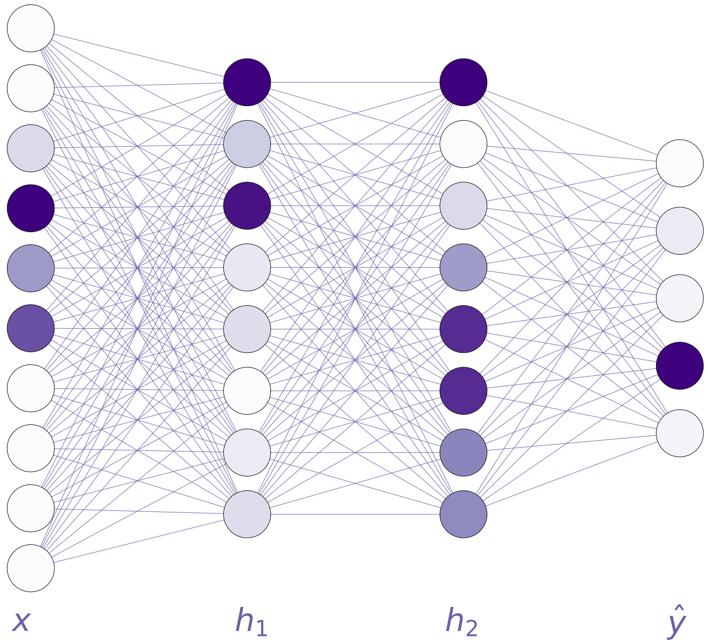


- Images of 10 x 1 Pixels with lines of length 1 to 5
- Task: Estimate the length of the line
- Can see correct result from flattened image
- Simulated sample of 10 000 images with balanced class distribution

Class balance

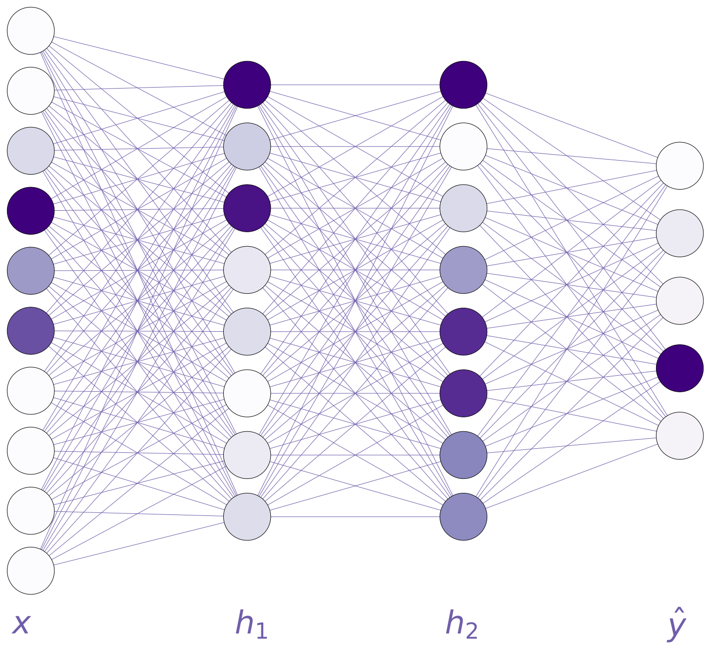


What is a neural network



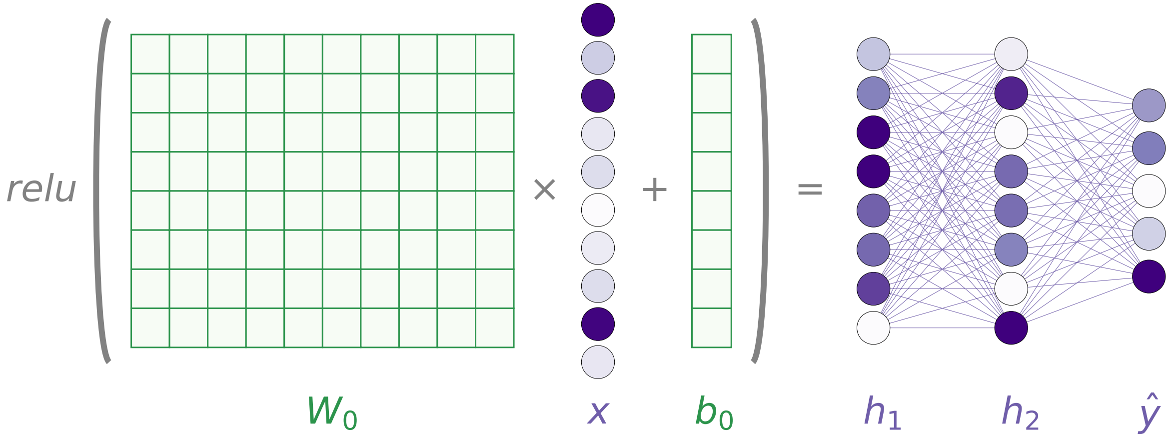
- A network consists of multiple layers of neurons
- Layer of neuron = vector of numbers
  - Input layer: just the flat image
  - hidden: transformations of image
  - Output: class probabilities
- High number -> active neuron
- Values in one layer determine values in next layer
- This model is already trained

Network architecture



- This is a Feed-Forward Network or Multi Layer Perceptron (MLP)
- Fully determined by:
  - Number of layers
  - Their dimensions
  - Activation functions
- Only dimensions of hidden layers are a choice

From x to h_1

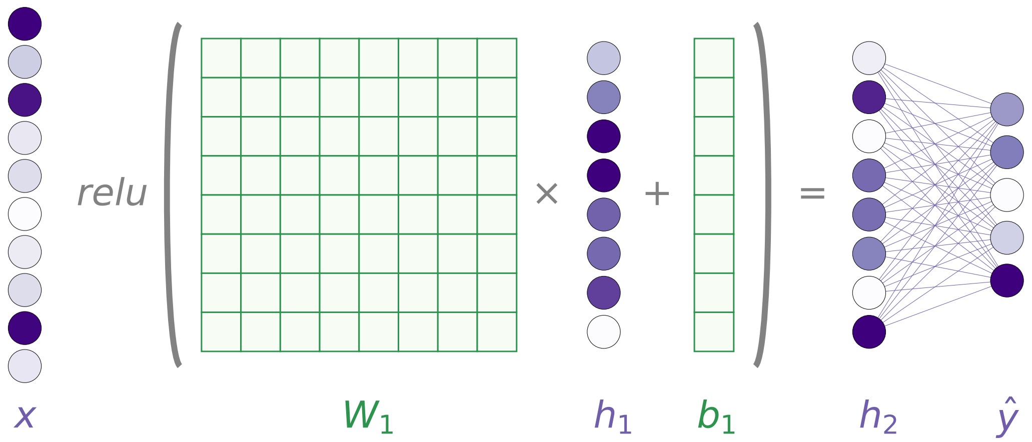


$$h_1 = relu(W_0 x + b_0)$$

Weights and biases

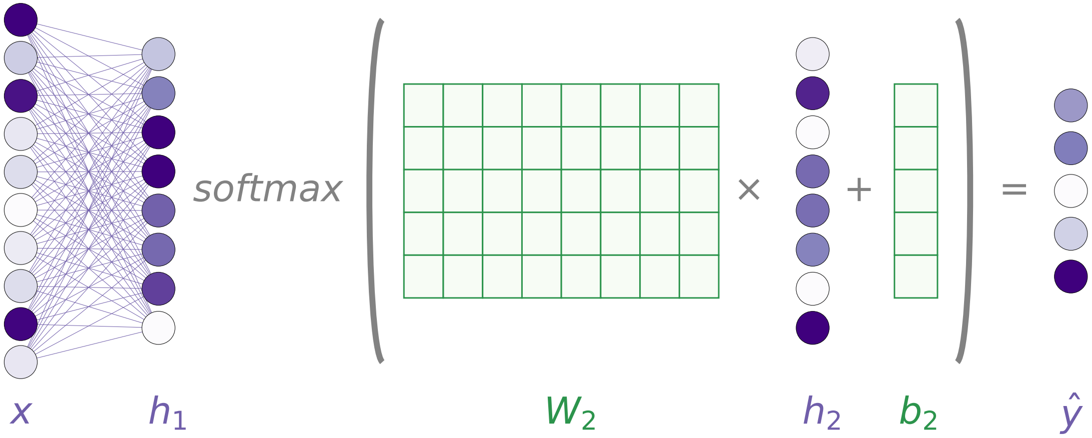
- Weights and biases are the trainable parameters
- Like β in a linear model but many more!
  - Weights are slope parameters
  - Biases are intercepts
- Weights are a matrix because as in regression with multiple outcomes

From h_1 to h_2



$$h_2 = relu(W_1 h_1 + b_1)$$

From h_2 to probabilities



$$\hat{y} = softmax(W_2 h_2 + b_2)$$

Relationship to before

- h_2 are the last hidden states we extracted in lectures 5 and 6
- The step from h_2 to $\hat{y}$ is a classification head, as in the model from lecture 7
- Of course, the models we had were:
  - deeper: Bert has 12 layers
  - larger: Bert has an input dimension of 30k and hidden dimension of 768
  - different: Transformer architecture instead of feed-forward

Task 1

5 min

Initializing parameters

- Paramters will be trained via SGD
- Need start parameters
- Simple approach: Random values close to zero, e.g. \simU[-0.5, .5]
    - Small $\rightarrow$ nothing explodes
    - Centered at zero $\rightarrow$ area of strong gradients
- There are more sophisticated methods (blogpost)

Randomness in pytorch

```
>>> torch.rand(size=(1, 3))
```

```
tensor([[0.8509, 0.1596, 0.9954]])
```

```
>>> torch.rand(size=(1, 3))
```

```
tensor([[0.6959, 0.8918, 0.3364]])
```

```
torch.manual_seed(1234)
torch.rand(size=(1, 3))
```

```
tensor([[0.0290, 0.4019, 0.2598]])
```

```
torch.rand(size=1, 3)
```

```
tensor([[0.3666, 0.0583, 0.7006]])
```

```
torch.manual_seed(1234)
torch.rand(size=(1, 3))
```

```
tensor([[0.0290, 0.4019, 0.2598]])
```

- `` `torch.rand` `` draws from $U[0, 1]$
- Each time you call it, you get different numbers
- Setting a seed, puts you in a reproducible random state
- The seed has a global effect, i.e. not just on the next drawn number but on all following numbers until the next seed

Transforming random variables

- Linear transformations of uniform random variables are uniform random variables with other bounds
- $x \sim U[0,1] \rightarrow ax + b \sim U[b, a+b]$
- Use this to generate start parameters between -0.5 and 0.5

Task 2

Why do we need nonlinearities

- Without nonlinearities, our model would be:

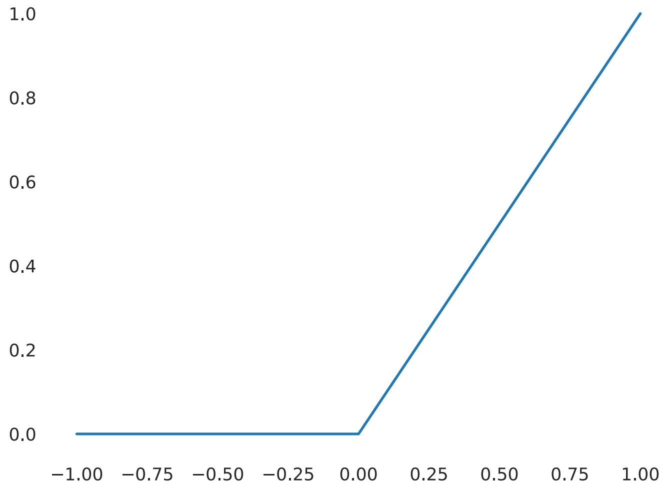
$$W_2(W_1(W_0x + b_0) + b_1) + b_2$$

- This could be simplified to:

$$Wx + b$$

- Thus we would end up with one linear model!

What is relu



- relu = rectified linear unit
- $r(x) = max(0, x)$
- Most commonly used non-linearity in neural networks
- You will see why we need non-linearities in a second

Other activation functions

- Sigmoid was used a lot historically
- Most common today is relu
- Many options out there!
- Blogpost

A brain analogy

- Neurons in the brain have a certain level of excitment
- If the excitement is above a certain level, the neuron fires
- Firing means, the neuron sends information to another neuron
- Receiving information changes that neuron’s excitement

What is softmax

- Converts any real-valued vector into a vector of valid probabilities

$$\sigma : \mathbb{R}^K \to \left\{ z \in \mathbb{R}^K | z_i \geq 0, \sum_{i=1}^K z_i = 1 \right\}$$

$$\sigma(z)_j = \frac{e^{z_j}}{\sum_{i=1}^K e^{z_i}}$$

- Our probabilities do not have frequentist interpretation
- You know this as choice probabilities in a logit model

It should be called soft argmax!

```
softmax([1, 1, 1, 1])
```

```
array([0.25, 0.25, 0.25, 0.25])
```

```
softmax([1, 1, 2, 1])
```

```
array([0.17, 0.17, 0.48, 0.17])
```

```
softmax([1, 1, 5, 1])
```

```
array([0.02, 0.02, 0.95, 0.02])
```

```
softmax([1, 1, 10, 1])
```

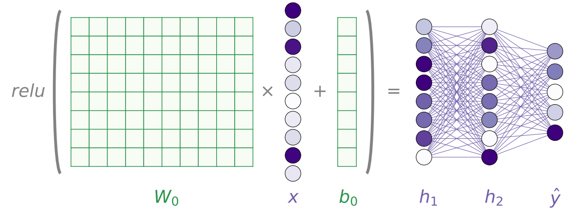
```
array([0., 0., 1., 0.])
```

- Softmax approximates an argmax
- If sizes of vector elements vary strongly, it becomes an indicator function for the largest element

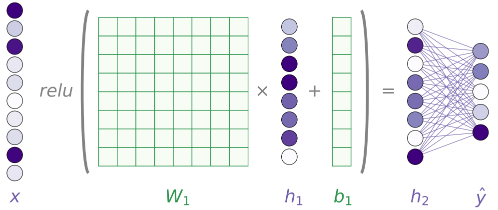
Task 3

Summary

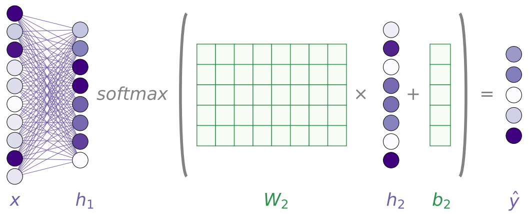
$$h_1 = relu(W_0 x + b_0)$$



$$h_2 = relu(W_1 h_1 + b_1)$$

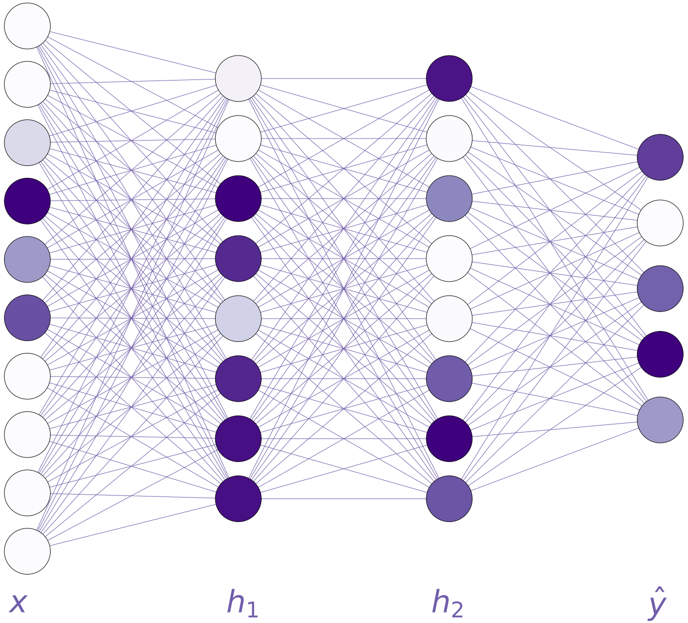


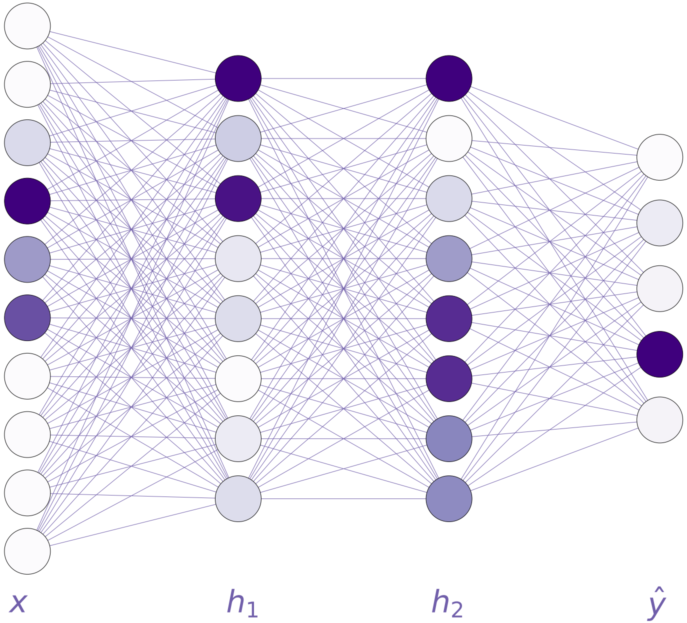
$$\hat{y} = softmax(W_2 h_2 + b_2)$$



Task 4

Goal of training





- Untrained network
- Multiple outcomes have relatively high scores

- Trained network
- Correct outcome has high score

NLL-Loss

- Negative log-likelihood loss
  - Likelihood is the score of the correct label
  - Take the log for numerical stability
  - Make negative to get something we can minimize
- Equivalent to cross-entropy loss but cross-entropy works on scores that are not yet softmaxed
- Blogpost

Batch model

```python
def batch_model(batch, weights, biases):
    n_out = len(biases[-1])
    out = torch.zeros((len(batch), n_out))
    for i, x in enumerate(batch):
        out[i] = model(x, weights, biases)
    return out
```

- For optimization we want to evaluate the model on a batch of parameters
- Since we do not care about performance, we can do this in a loop
- I give you this function in the notebook
- The result of this will go into the loss function

Indexing trick

```
>>> a = torch.arange(12).reshape(4, 3)
>>> a
```

```
tensor([[ 0,  1,  2],
        [ 3,  4,  5],
        [ 6,  7,  8],
        [ 9, 10, 11]])
```

```
>>> a[torch.arange(4), torch.tensor([0, 1, 2, 1])]
```

```
tensor([ 0,  4,  8, 10])
```

- You will need this to compute the loss function
- Replacing the arange by `:` would not work!
- Numpy has `np.choose` for this, but torch does not

Task 5

When does the magic start?

- So far, the Neural Network was disappointing
- Just three lines of code, and not even difficult ones!
- Magic comes from training!
- Analogy: It is not the linear model $y = x\beta$ that is useful but OLS!
- Now we write a training loop to make our model work!

Refresher: Pseudo code for SGD

```
for i in range(nb_epochs):
  shuffle_data(data)
  for batch in data:
    params_grad = evaluate_gradient(loss_function, batch, params)
    params = params - learning_rate * params_grad
```

- We will implement this from scratch using pytorch's autograd ability
- We look at three key ingredients before you do it!

1. Loop over random batches of data
2. Doing calculations with gradients
3. Zeroing gradients!

Looping over random batches of data

```
data = torch.arange(12).reshape(4, 3)
data
```

```
tensor([[ 0,  1,  2],
        [ 3,  4,  5],
        [ 6,  7,  8],
        [ 9, 10, 11]])
```

```
batch_size = 2
batch_indices = torch.randperm(len(data)).reshape(-1, batc
batch_indices
```

```
tensor([[3, 1],
        [2, 0]])
```

```
for idxs in batch_indices:
    batch = data[idxs]
    print(batch)
```

```
tensor([[ 9, 10, 11],
        [ 3,  4,  5]])
tensor([[6, 7, 8],
        [0, 1, 2]])
```

- Draw random permutations of an arange as long as the data
- Reshape them so rows become batch indices
- Loop over batch indices and create batches

Calculations with gradients

```
>>> def f(x):
...     return (x ** 2).sum()


>>> a = torch.tensor(
...     [1., 2., 3.],
...     requires_grad=True,
... )
>>> b = f(a)
>>> b.backward()
>>> a.grad
```

```
tensor([2., 4., 6.])
```

```
>>> a.data = a.data - 0.1 * a.grad.data
>>> a
```

```
tensor([0.8000, 1.6000, 2.4000],
       requires_grad=True)
```

- You cannot just subtract the `a.grad` from a
- Doing so, leads to wrong results
- In the second iteration it also leads to an error

```
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
Cell In[227], line 1
----> 1 a = a - 0.1 * a.grad

TypeError: unsupported operand type(s) for *: 'float' and 'NoneType'
```

Important: Zero the gradient

```
a = torch.tensor([1., 2., 3.], requires_grad=True)
b = f(a)
b.backward()
a.grad
```

```
tensor([2., 4., 6.])
```

```
c = f(a)
c.backward()
a.grad
```

```
tensor([ 4.,  8., 12.])
```

```
a = torch.tensor([1., 2., 3.], requires_grad=True)
b = f(a)
b.backward()
a.grad
```

```
tensor([2., 4., 6.])
```

```
a.grad.zero_()
c = f(a)
c.backward()
a.grad
```

```
tensor([2., 4., 6.])
```

When to zero

- There are two possible positions
  - Right before you do the forward pass (i.e. call the model)
  - Right after you do the gradient update
- Need to do this even if you use pre-implemented pytorch models and optimizers
- Gets a bit more convenient then but stays equally dangerous!

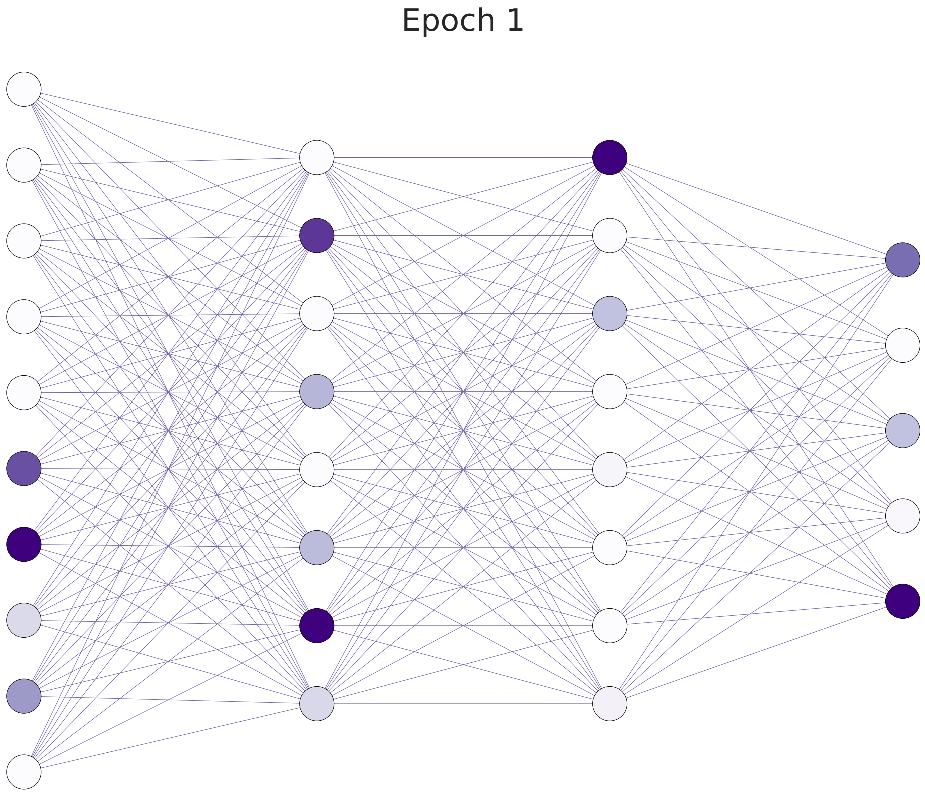
footgun:

any feature whose addition to a product results in the user shooting themselves in the foot

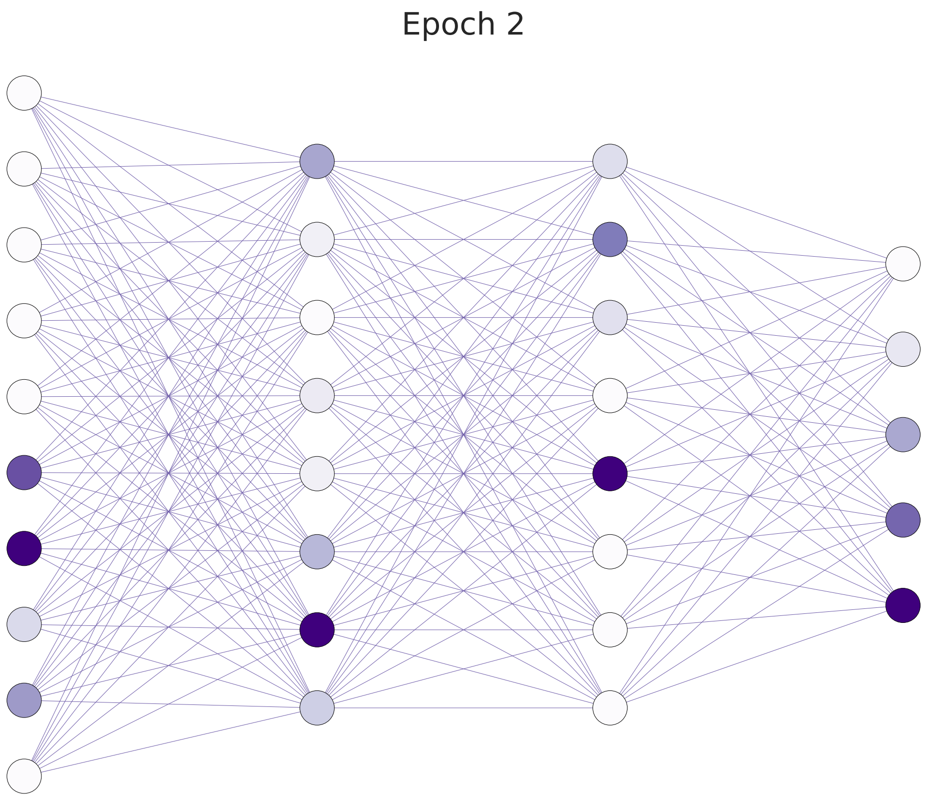
@RobTatman

Task 6

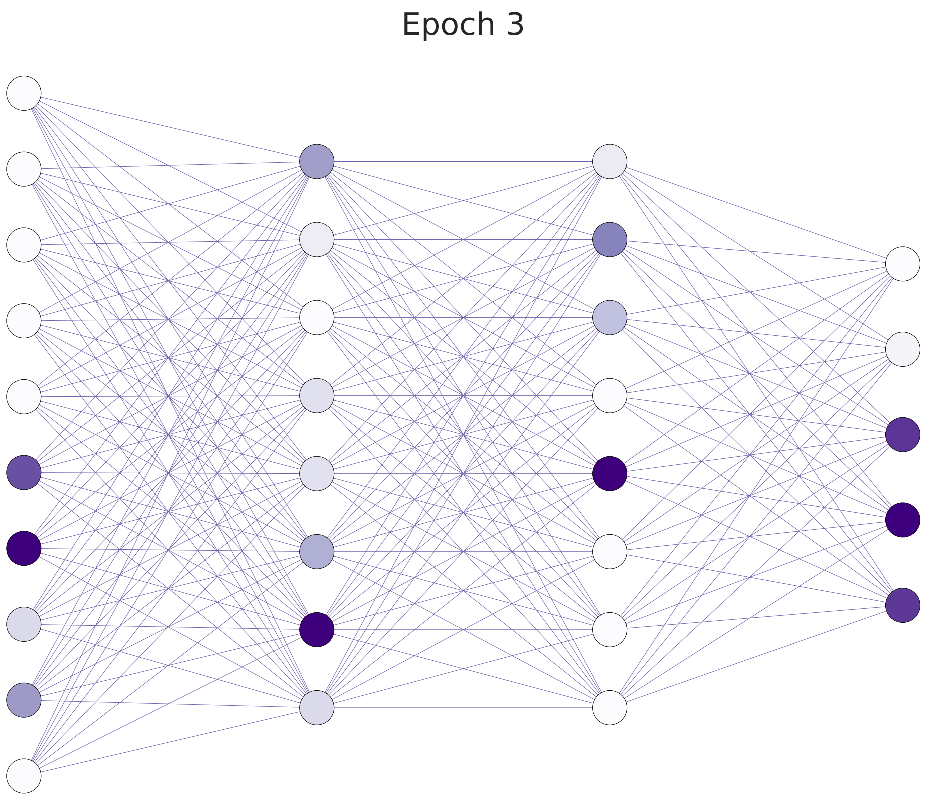
What happens during training



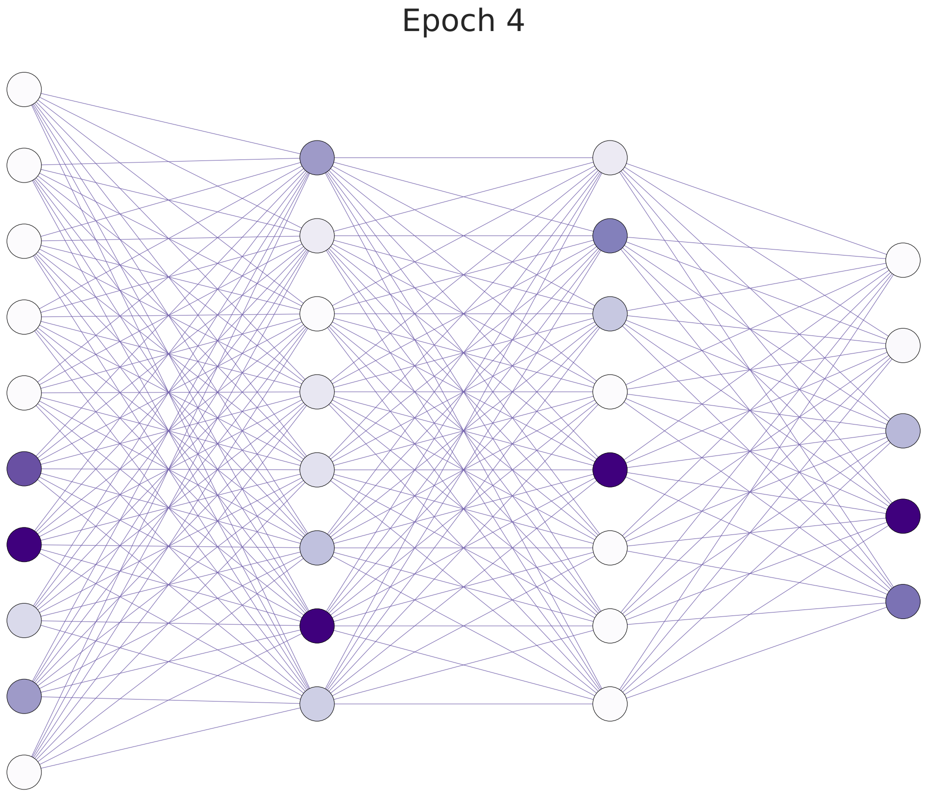
What happens during training



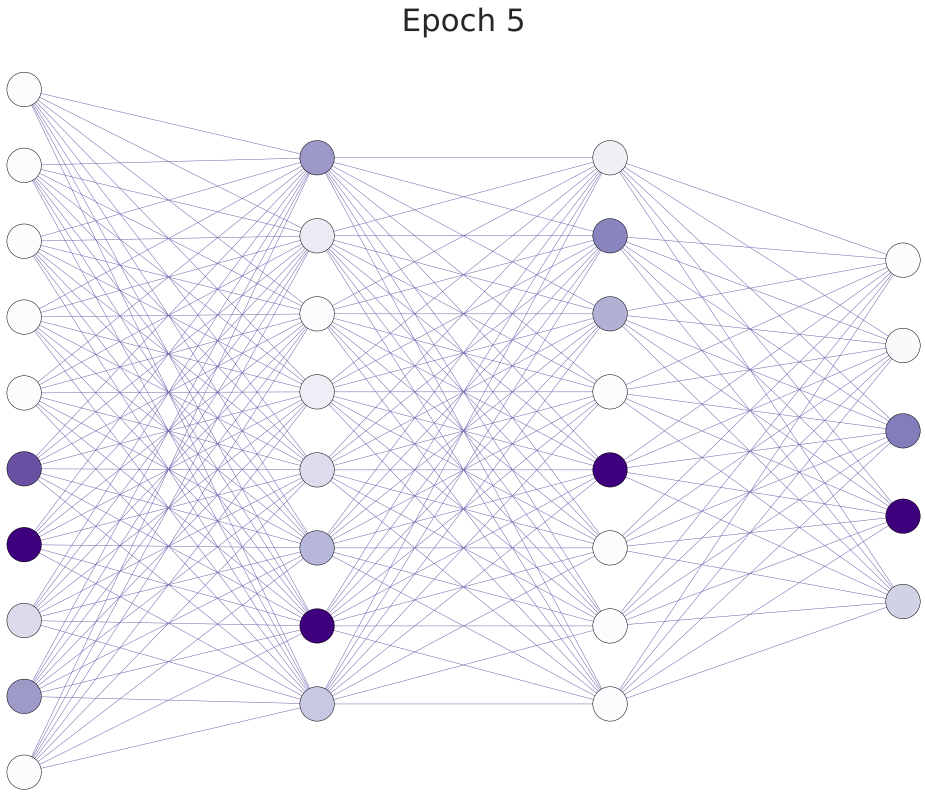
What happens during training



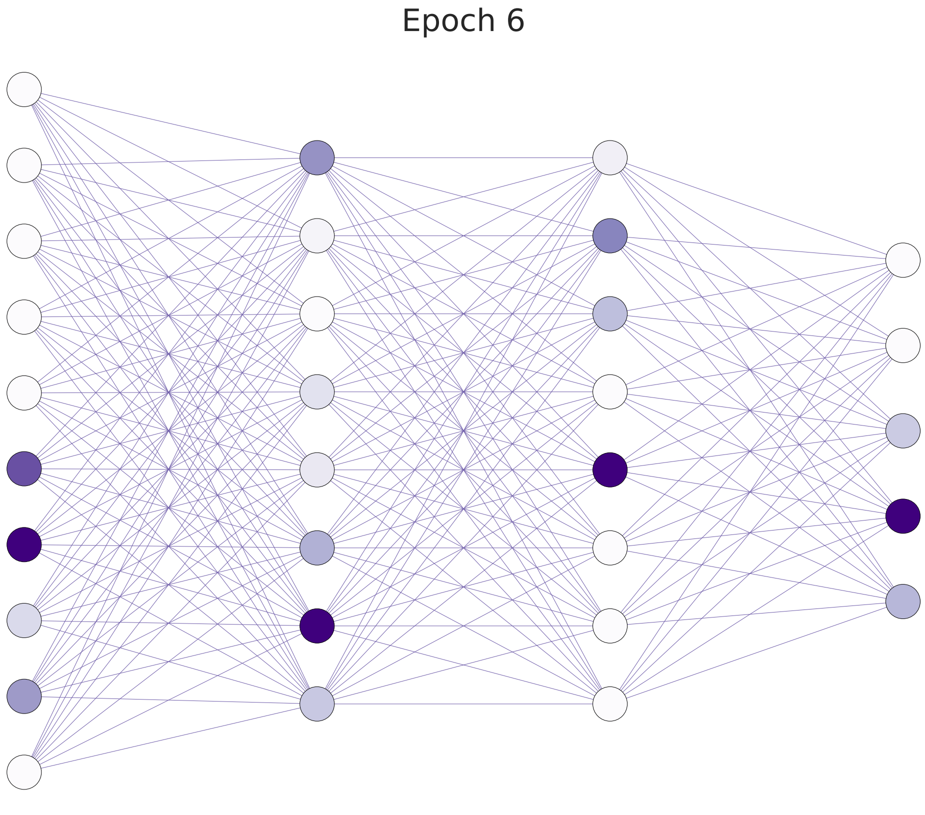
What happens during training



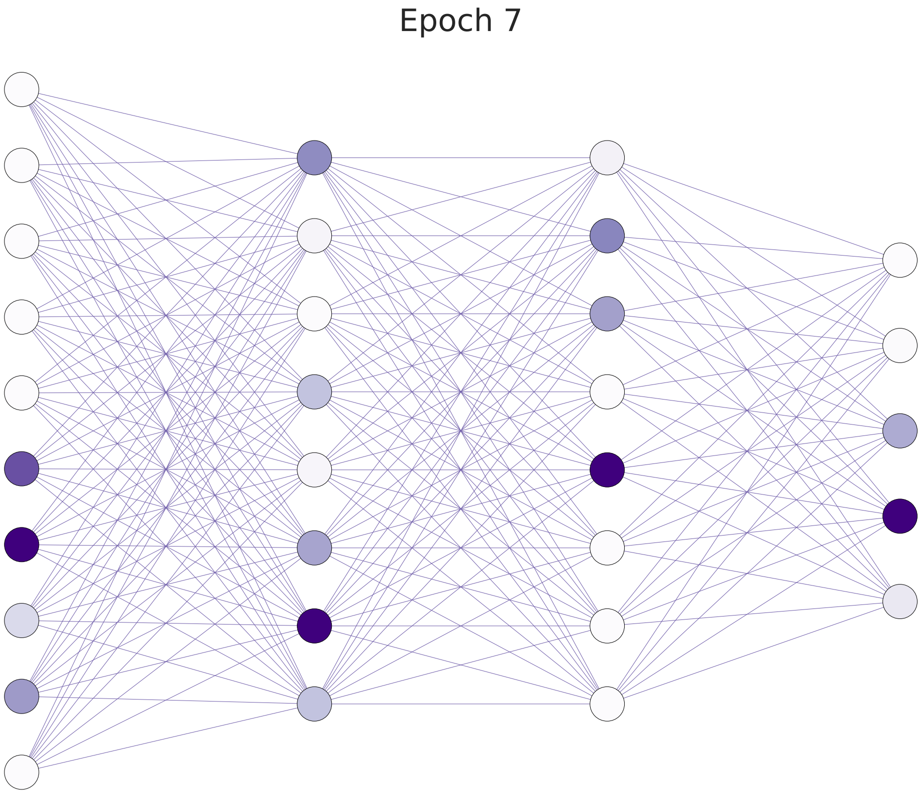
What happens during training



What happens during training



What happens during training



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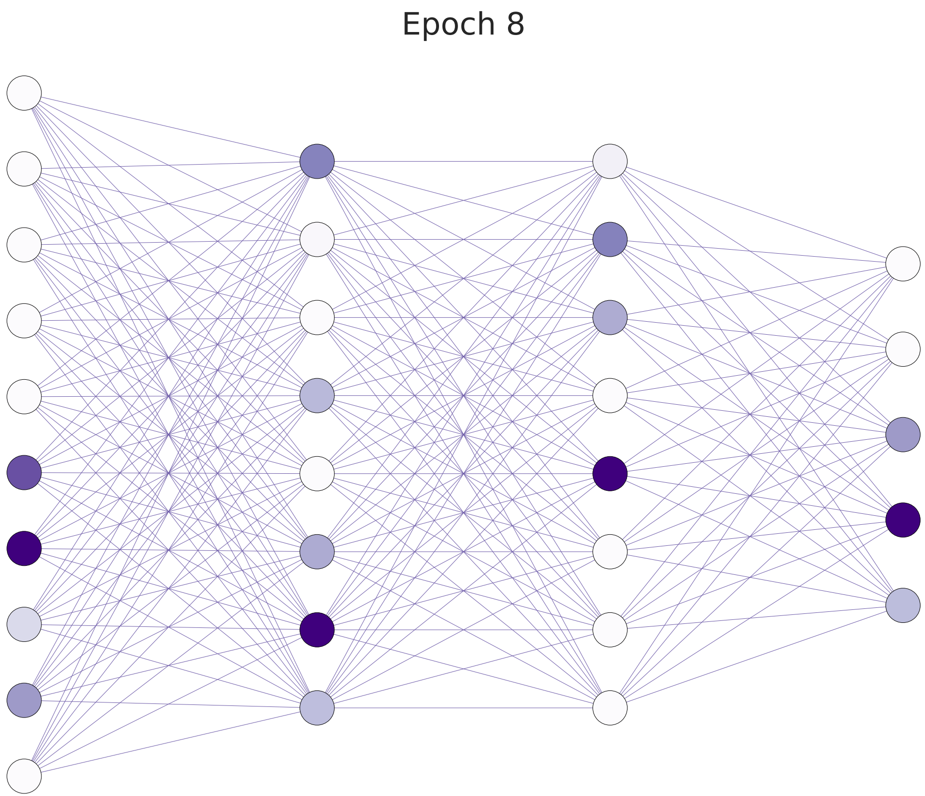
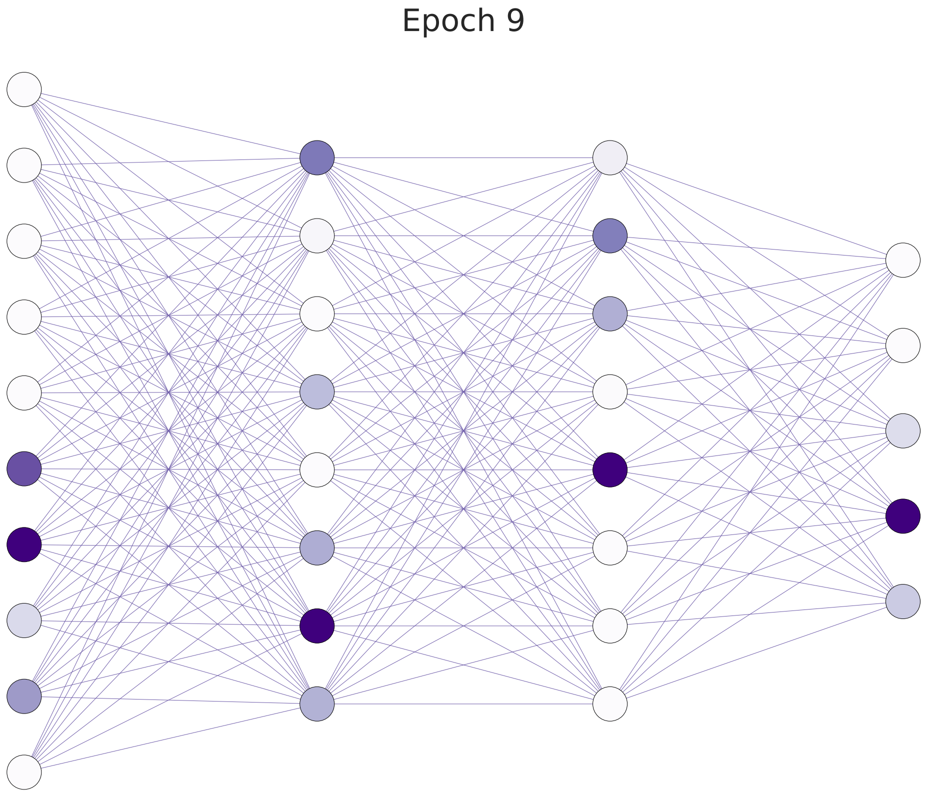


What happens during training



Limits of intuition

- Even in this small network, we only see that the network learns, not how it does that
- Different starting values lead to similar performance but different networks
- The network can switch out where it stores information
- No reason to think that bottom entries are related to bottom pixels or longer lines

Need some monitoring

- After task 7, your output of running the training should look somthing like this

```
Accuracy after epoch 0: 0.4580000042915344
Accuracy after epoch 1: 0.5734999775886536
```

- Numbers can vary, this was on the digits example

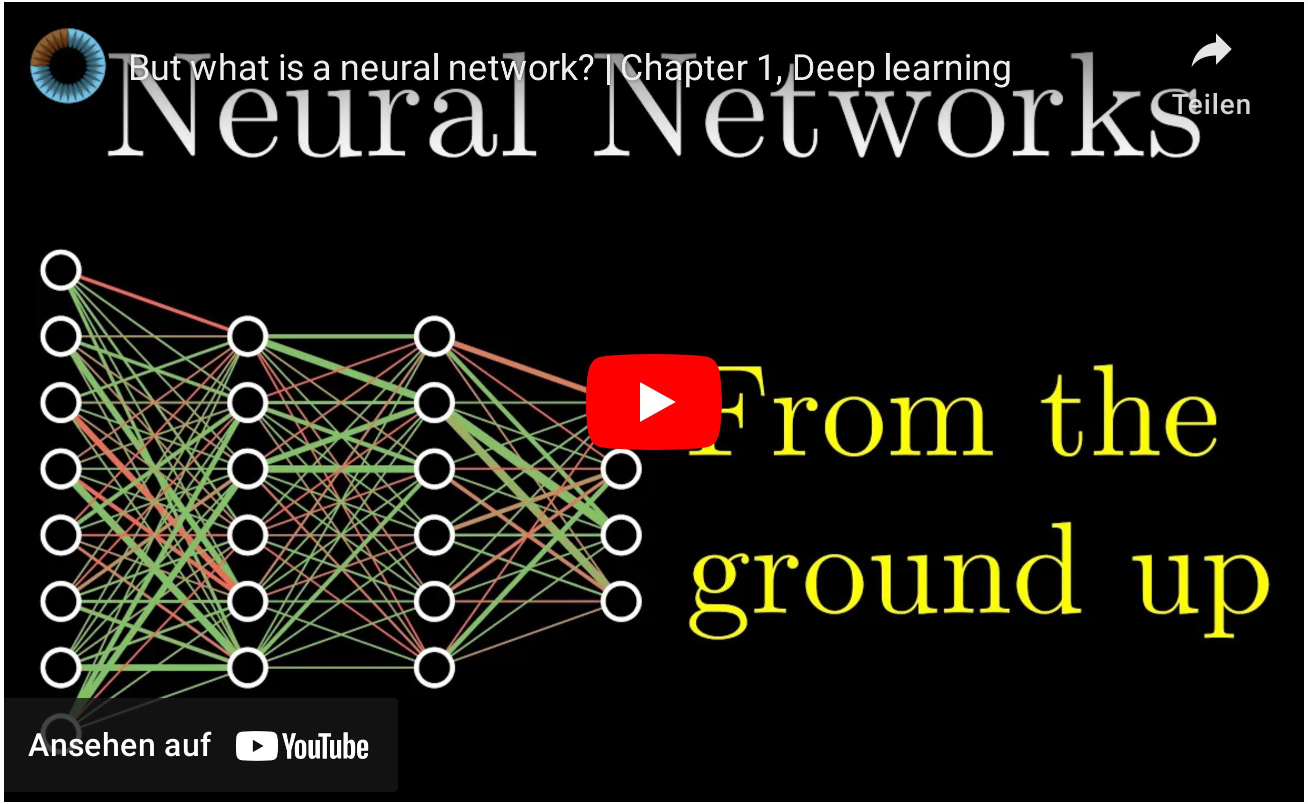
Task 7

The hyperparameters

- Learning rates
  - Want it to be as large as possible for speed
  - Too large can lead to NaNs and non-convergence
  - 0.01 is very small for such a tiny network
- Batch size
  - Want to make it as small as possible for speed
  - Too small means that update become erratic
- Number of epochs
  - For this tiny model we are not very worried about overfitting
  - Thus, more is better but do not exaggerate

Task 8

Video


But what is a neural network? | Chapter 1, Deep learning
Teilen
Neural Networks
From the
ground up
Ansehen auf YouTube