Artificial Neural Networks

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Topics

- History
- Computational graphs
- Feedforward neural networks
- Gradient descent
- Why is DL so successful?

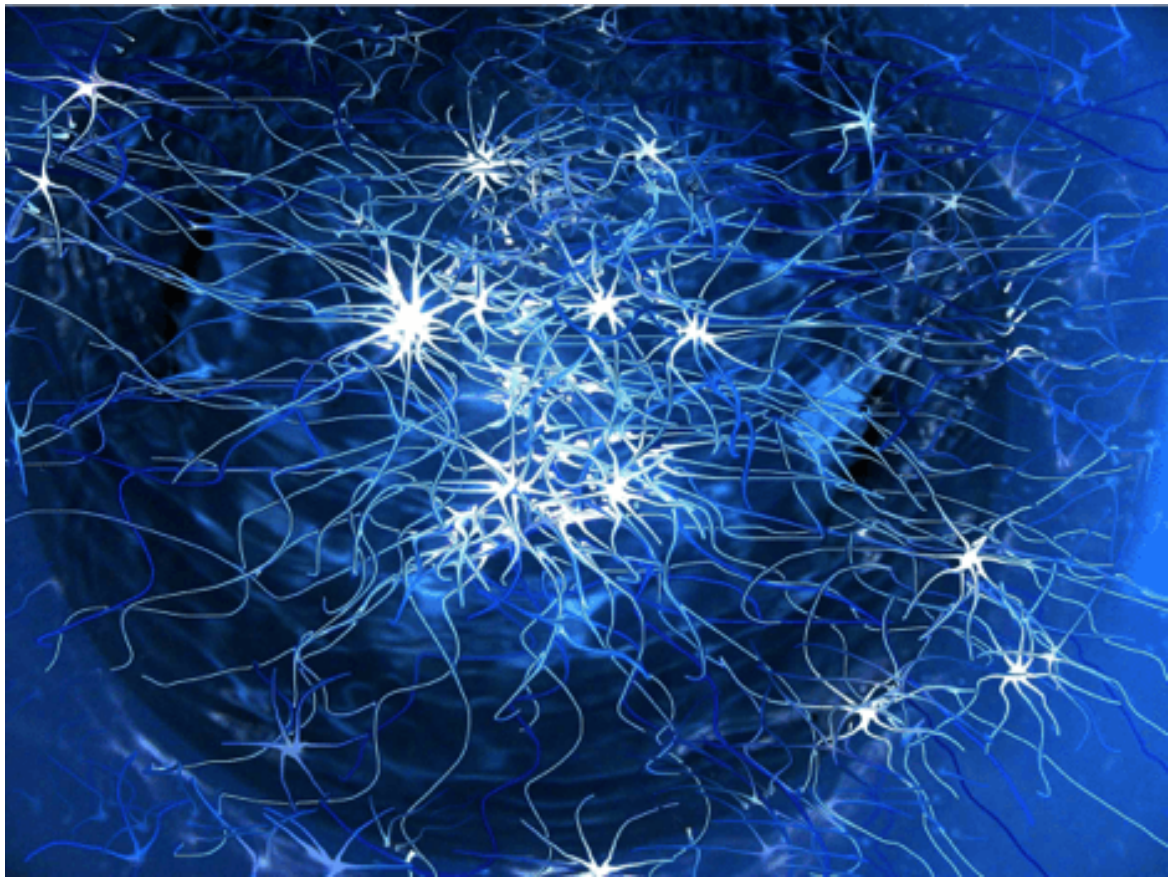
History

- 1940s: McCulloch & Pitts create mathematical model of NN
- 1950s: Rosenblatt develops the perceptron (trainable NN)
- 1960s-70s: Limited progress with single layer perceptrons
- 1980s: Backpropagation algorithm enables training of MLPs
- 1990s: SVMs temporarily overshadow ANNs in popularity
- 2000s: Deep learning finds successes in large problems

Last 10 years: Explosion of progress in deep learning

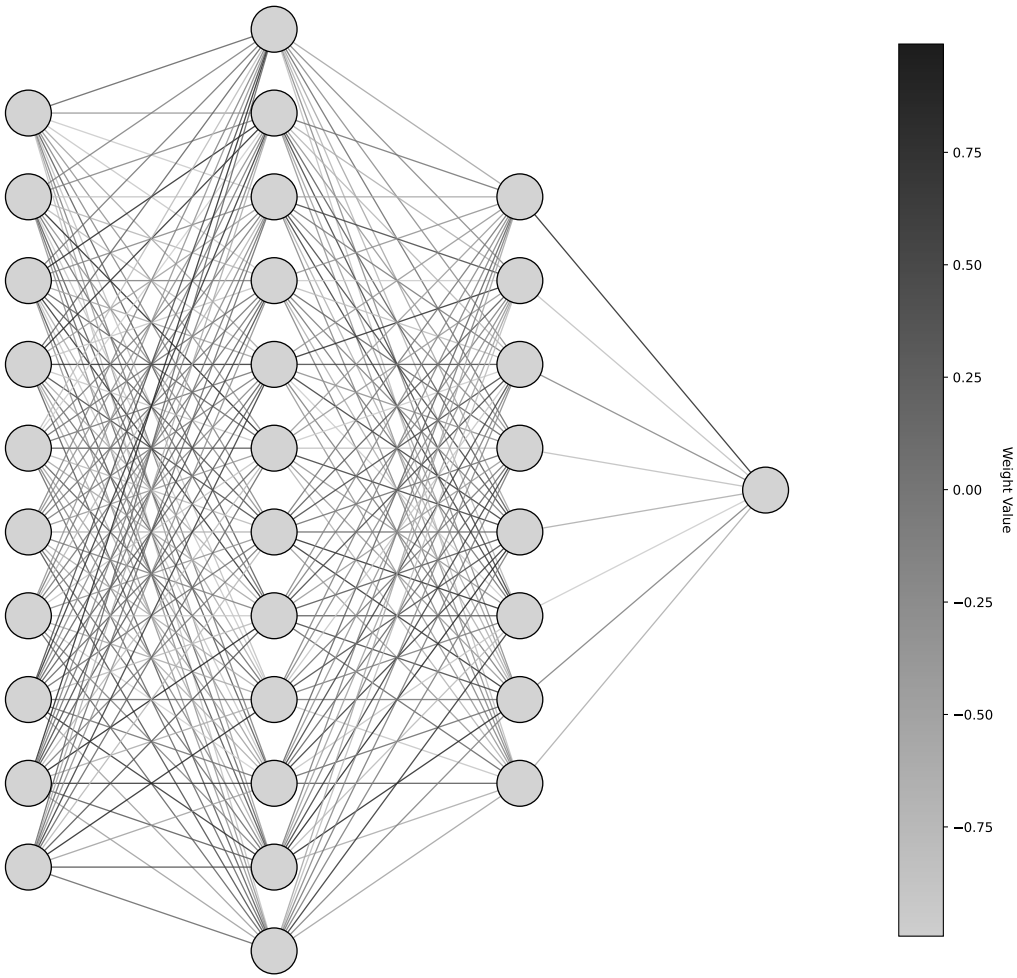
- CNNs, RNNs, LSTMs, transformers, LLMs, etc.

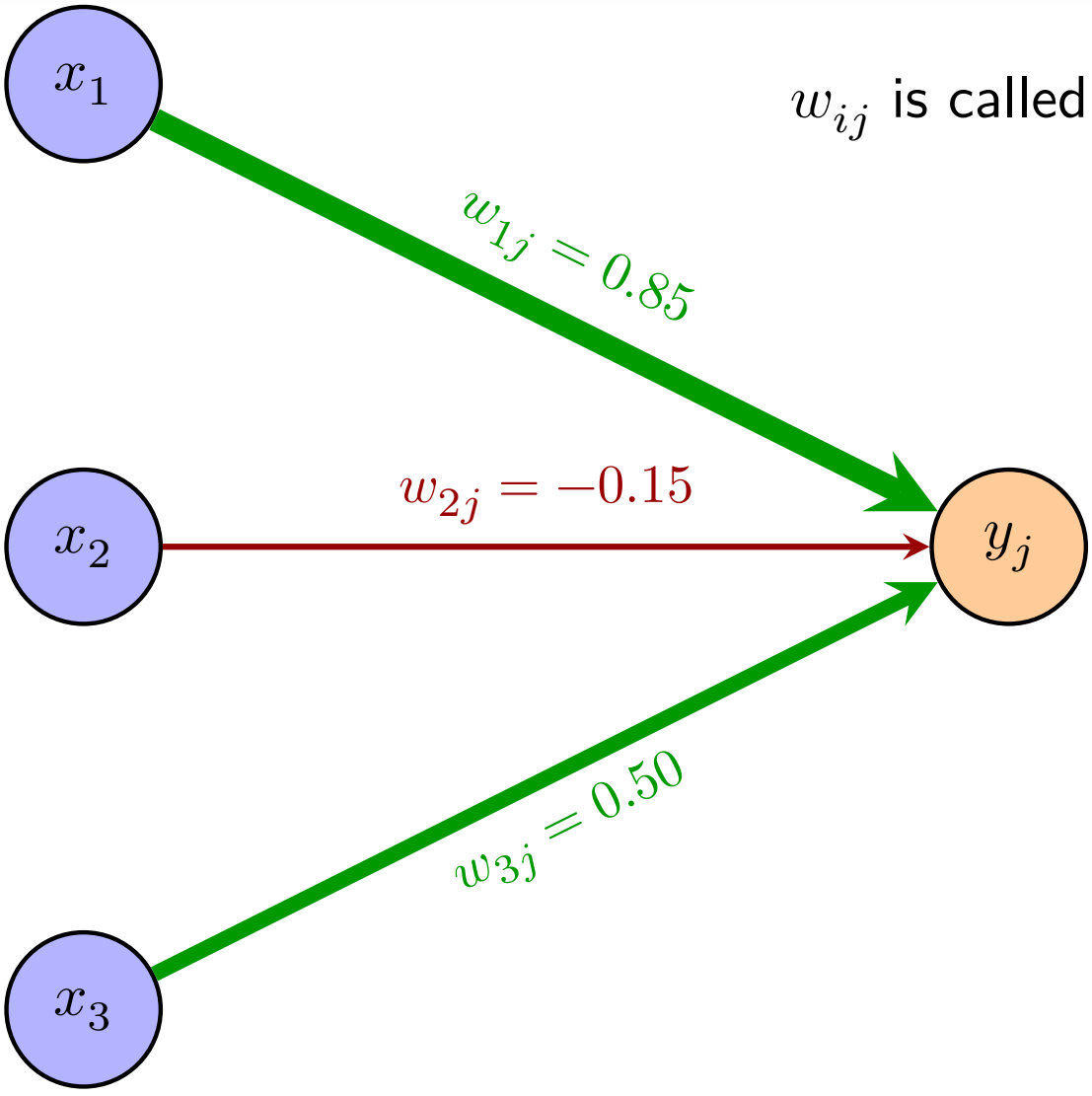
A model of the human brain



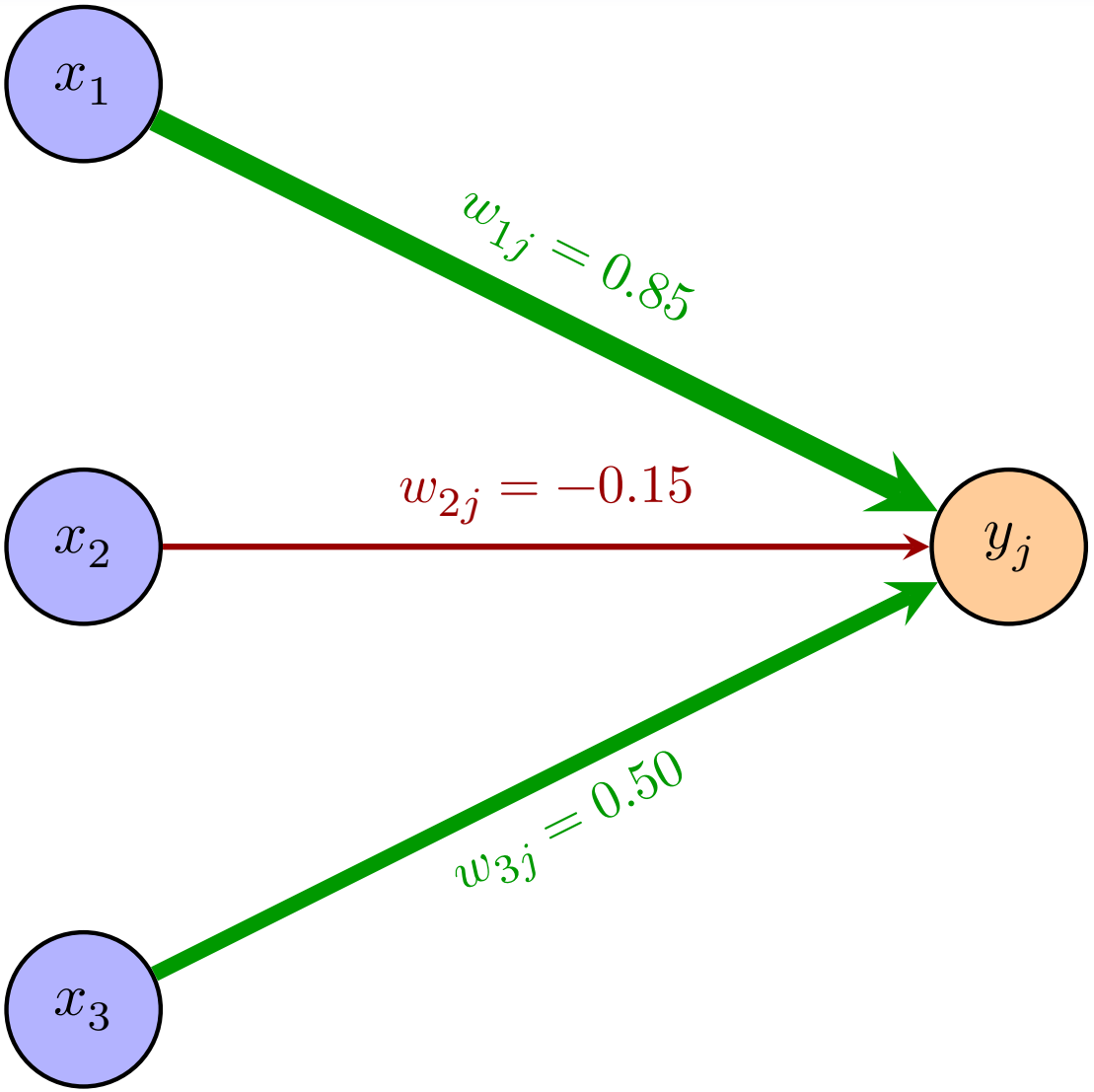
– source: Dartmouth undergraduate journal of science

A mathematical representation: directed acyclic graph

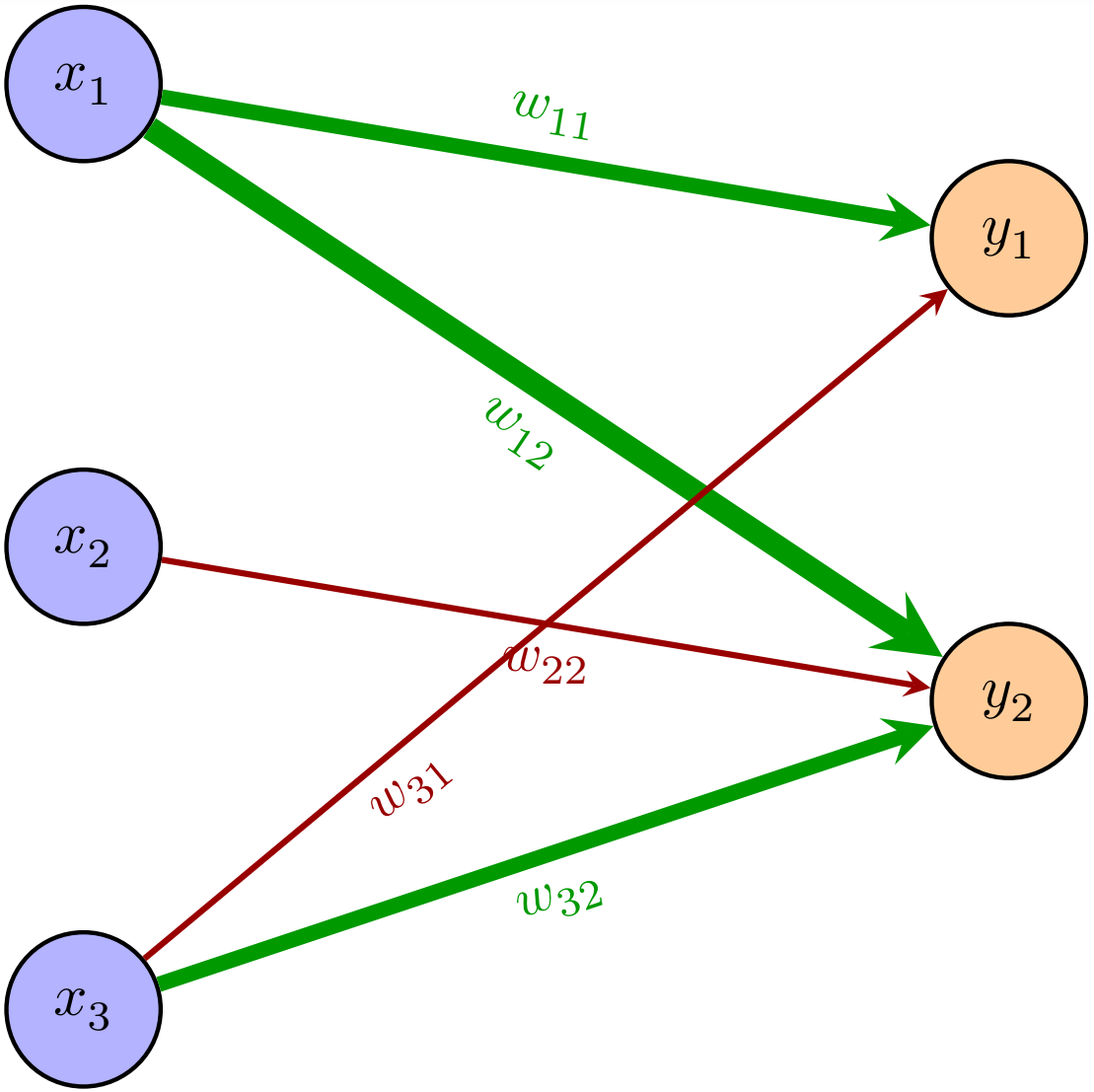




w_{ij} is called a "weight"



$$y_j = \sum_i w_{ij} x_i$$



$$y_1 = \sum_i w_{i1} x_i$$

$$y_2 = \sum_i w_{i2} x_i$$

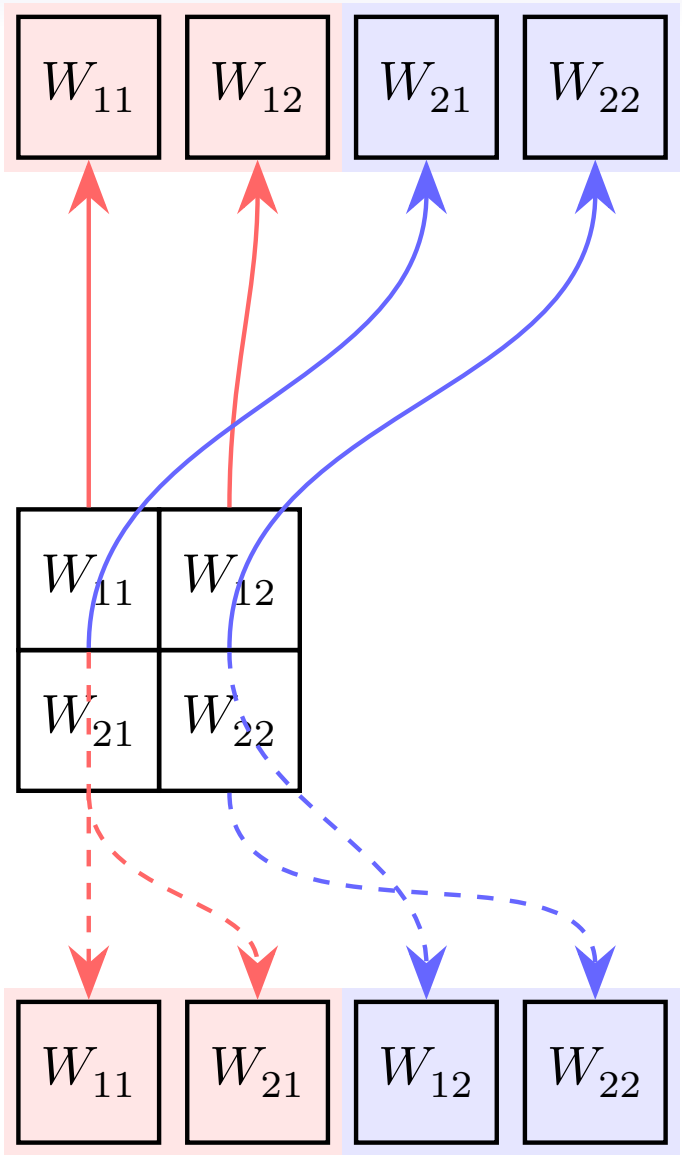
$$\Longrightarrow \; y = xW$$

Note that we are using **row vectors**: $y = xW$

This is natural given our notation

- w_{ij} points from i to j
- hence $y_j = \sum_i w_{ij} x_i$
- hence $y = xW$

But it also has another advantage ...?



row-major storage

column-major storage

Computing xW

```
for i in range(n):
    for j in range(m):
        # Access row elements of W contiguously
        y[j] += W[i, j] * x[i]
```

Computing Wx

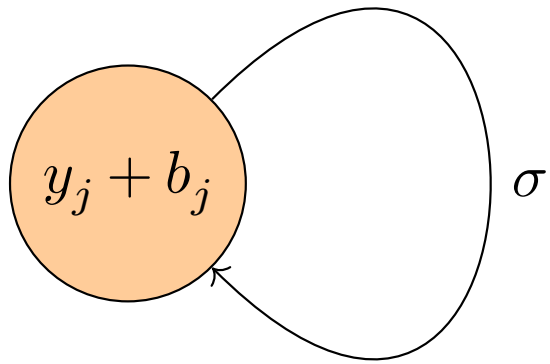
```
for j in range(n):
    for i in range(m):
        # Non-contiguous access of W
        y[i] += W[i, j] * x[j]
```

Next steps

After computing $y_j = \sum_i w_{ij} x_i$ we

1. add a bias term b_j and
2. apply a nonlinear "activation function" $\sigma \colon \mathbb{R} \to \mathbb{R}$

applying activation function



First add bias:

$$y_j = \sum_i w_{ij} x_i \qquad \rightarrow \qquad y_j = \sum_i w_{ij} x_i + b_j$$

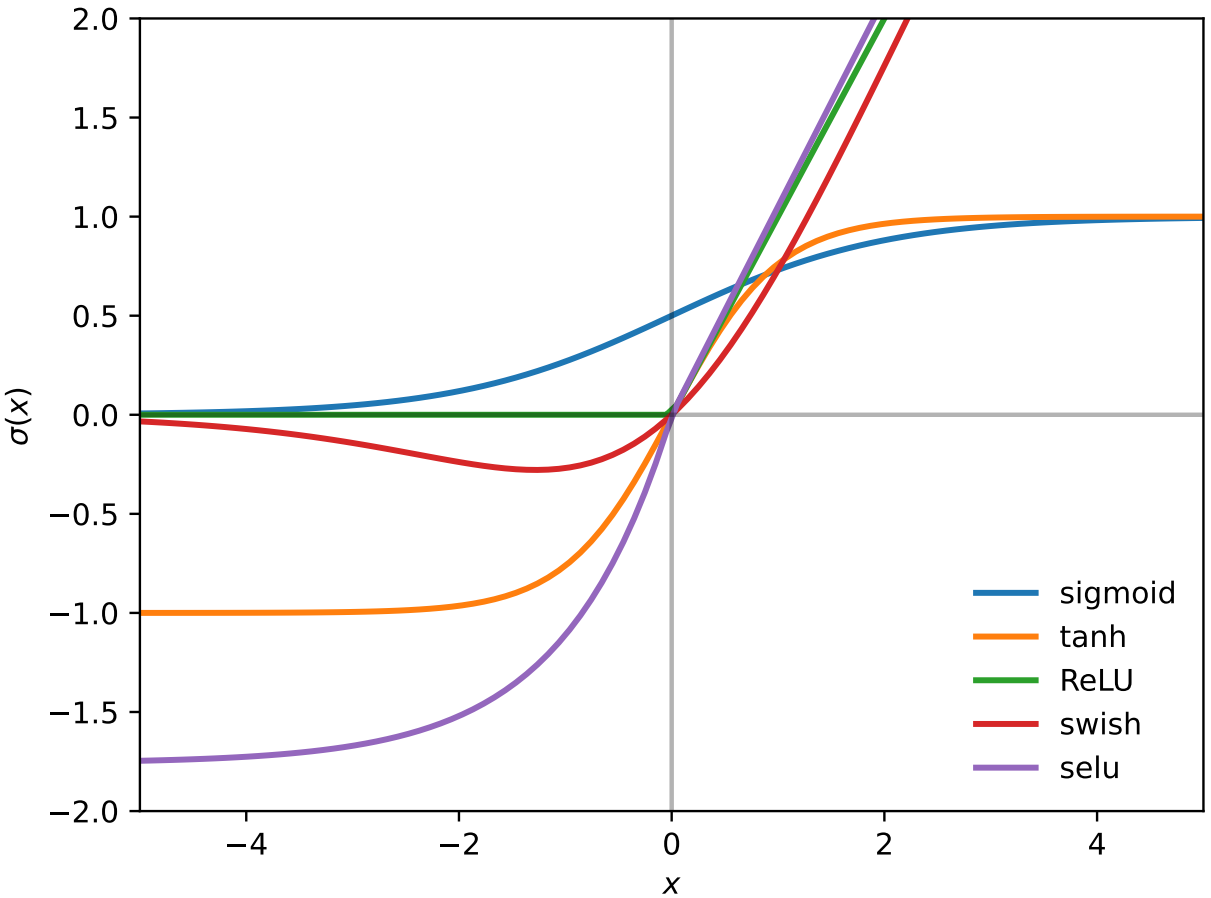
Then apply activation:

$$y_j = \sum_i w_{ij} x_i + b_j \qquad \rightarrow \qquad y_j = \sigma\left(\sum_i w_{ij} x_i + b_j\right)$$

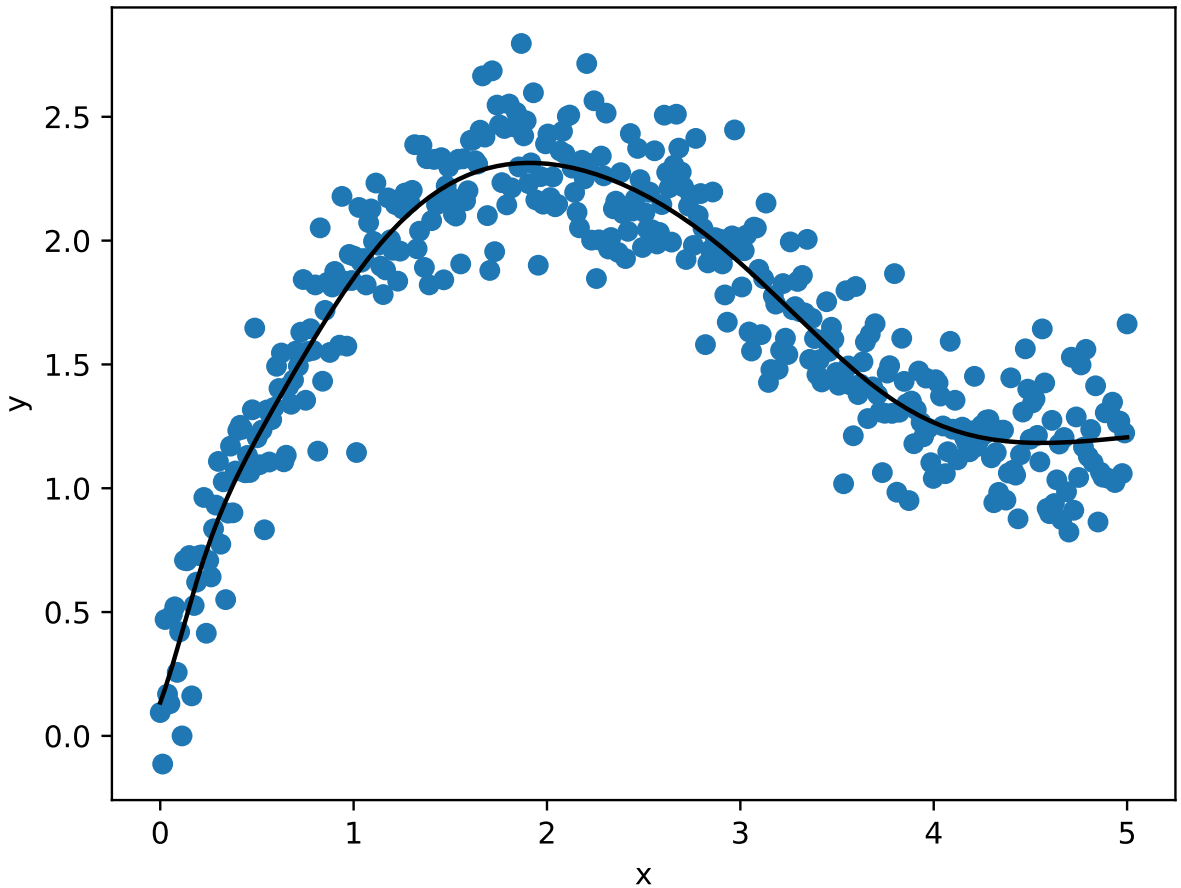
Applying σ pointwise, we can write this in vector form as

$$y = \sigma(xW + b)$$

Common activation functions



Training



Aim: Learn to predict output y from input x

- $x \in \mathbb{R}^k$
- $y \in \mathbb{R}$ (regression problem)

Examples.

- $x =$ cross section of returns, $y =$ return on oil futures tomorrow
- $x =$ weather sensor data, $y =$ max temp tomorrow

Problem:

- observe $(x_i, y_i)_{i=1}^n$ and seek f such that $y_{n+1} \approx f(x_{n+1})$

Nonlinear regression: choose model $\{f_\theta\}_{\theta \in \Theta}$ and minimize the empirical loss

$$\ell(\theta) := \frac{1}{n} \sum_{i=1}^{n} (y_i - f_\theta(x_i))^2 \quad \text{s.t.} \quad \theta \in \Theta$$

In the case of ANNs, we consider all f_θ having the form

$$f_\theta = \sigma \circ A_m \circ \cdots \circ \sigma \circ A_2 \circ \sigma \circ A_1$$

where

- $A_\ell x = x W_\ell + b_\ell$ is an affine map
- σ is a nonlinear "activation" function

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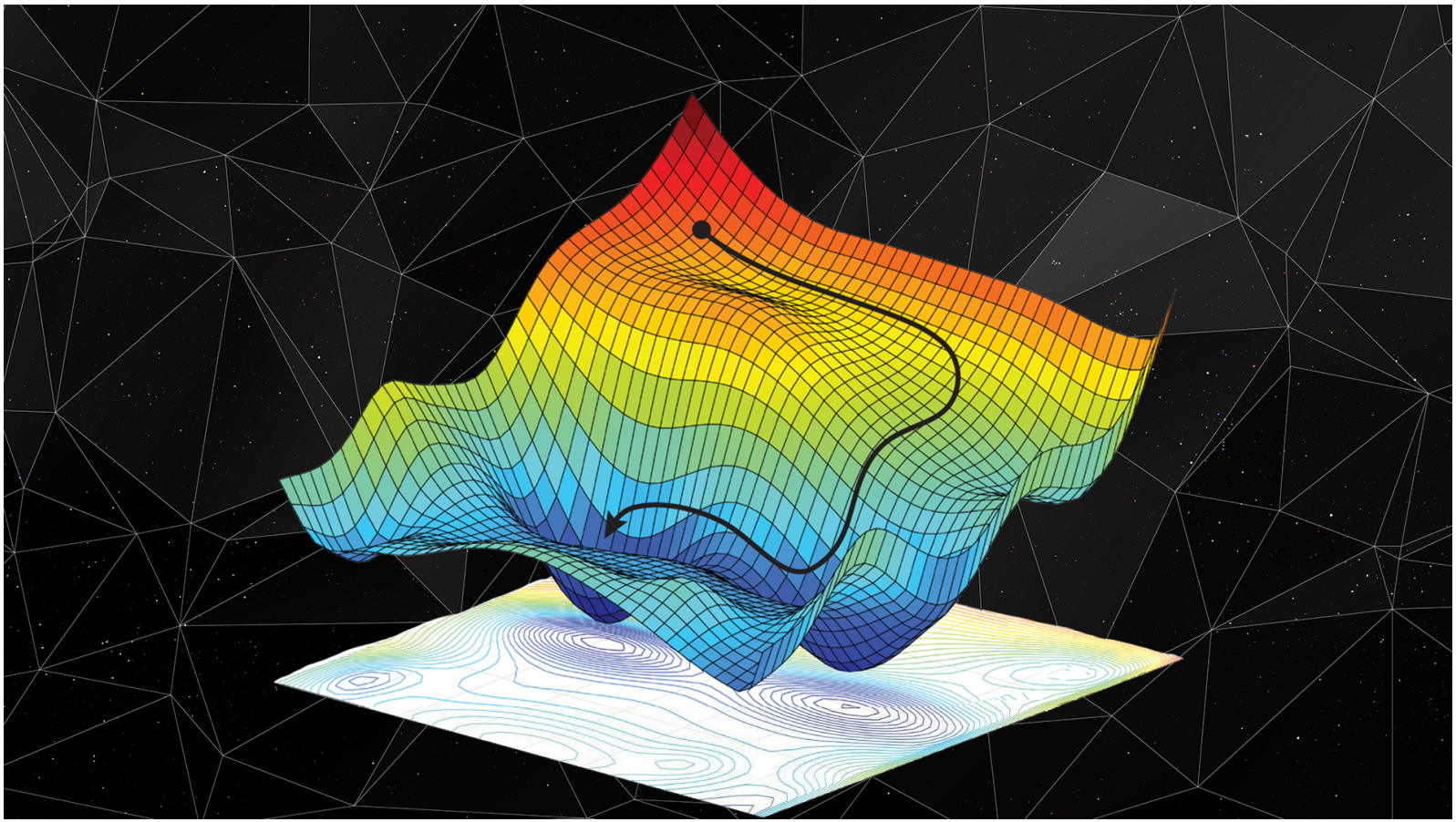
Minimizing the loss functions



Source: https://danielkhv.com/

Gradient descent

Algorithm:

$$\theta_{\text{next}} = \theta - \lambda \nabla_\theta \ell(\theta, x, y)$$

- take a step in the opposite direction to the grad vector
- λ is the **learning rate** – often changes at each step
- iterate until hit a stopping condition
- in practice replace $\ell(\theta)$ with batched loss

$$\frac{1}{|B|} \sum_{i \in B} (y_i - f_\theta(x_i))^2$$

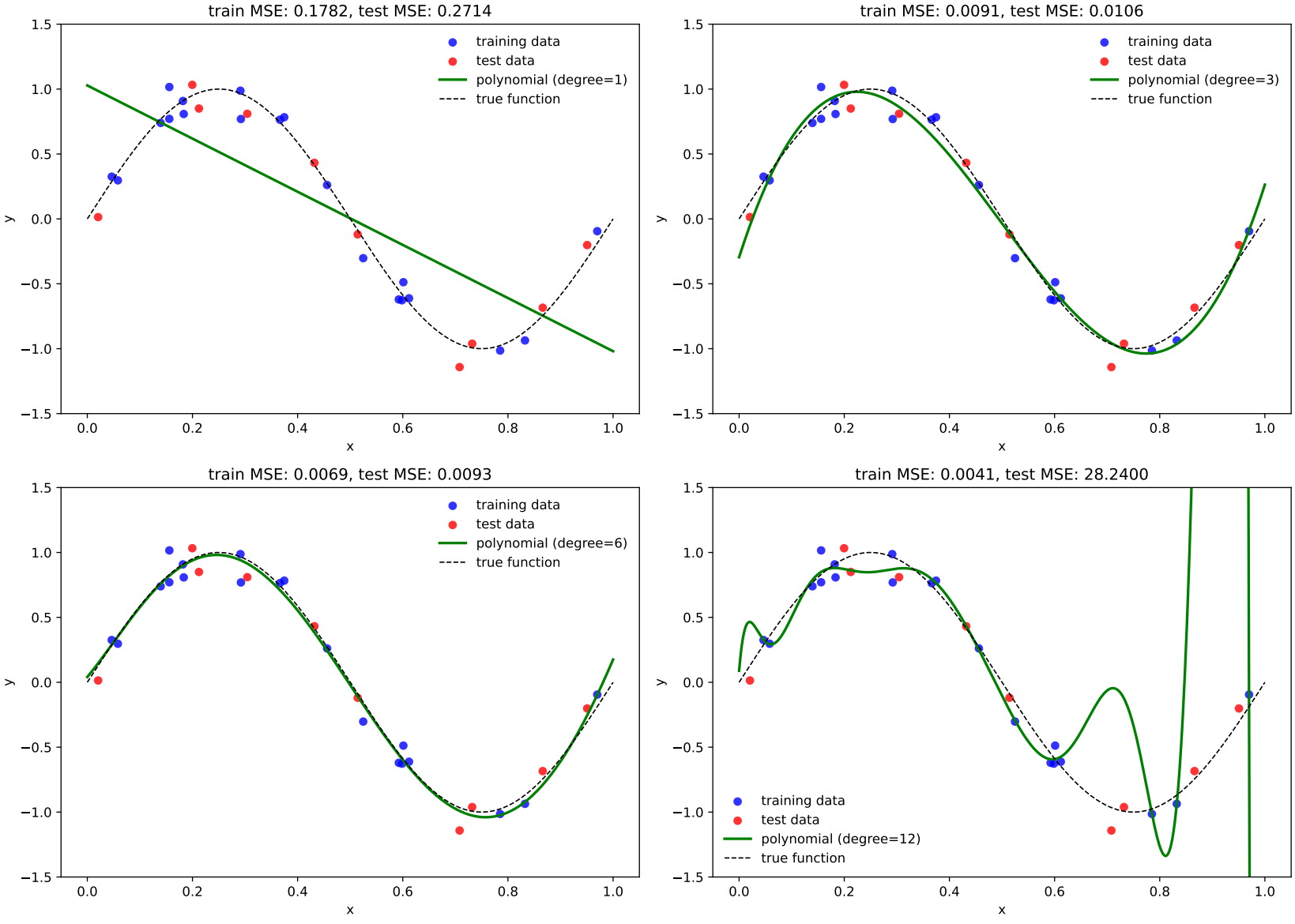
Using batches $\rightarrow$ **stochastic gradient descent**

Extensions

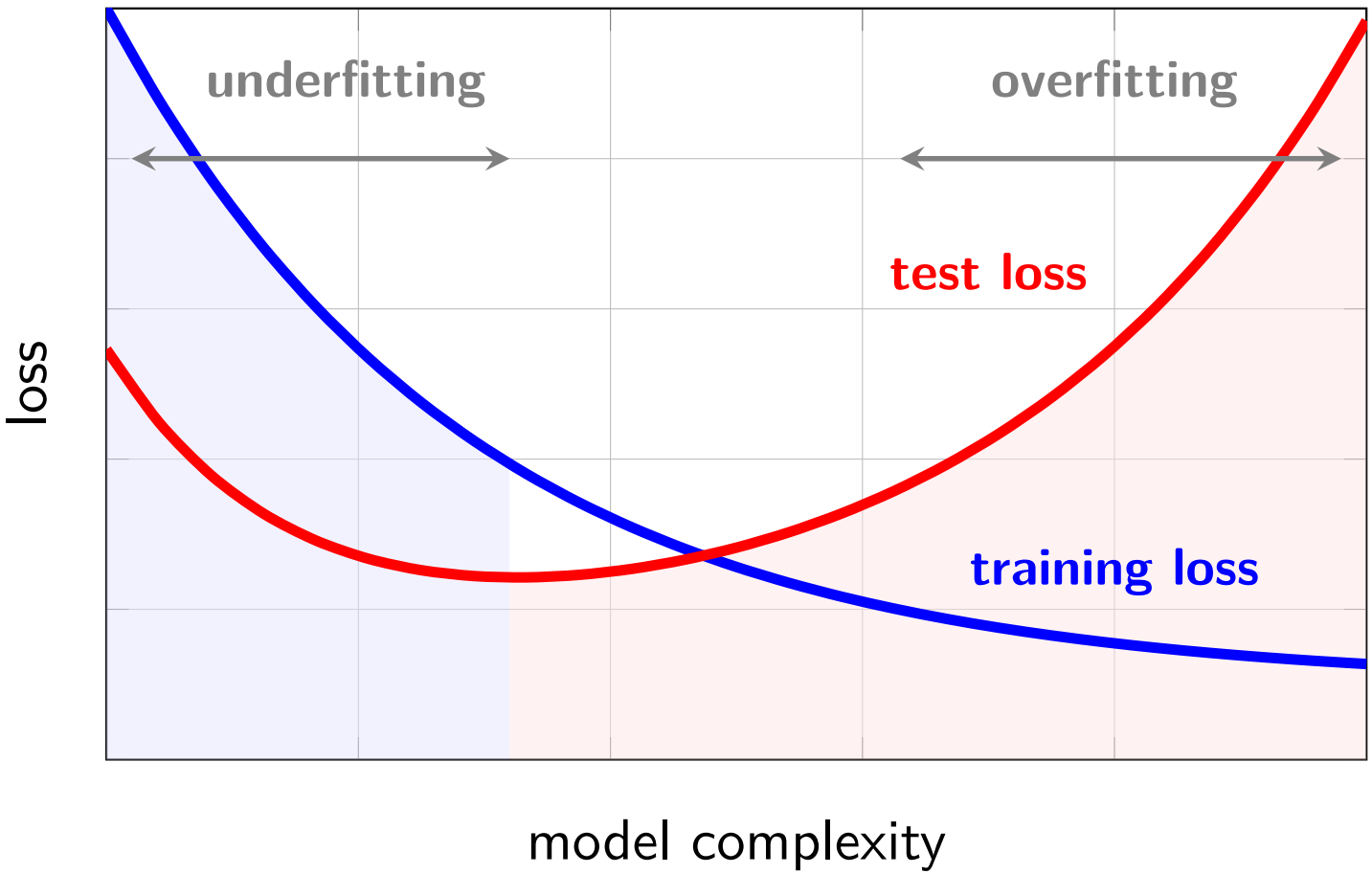
- Loss functions with regularization
- Cross-entropy loss (classification)
- Convolutional neural networks (image processing)
- Recurrent neural networks (sequential data)
- Transformers (LLMs)
- etc.

A mystery

What about overfitting?


train MSE: 0.1782, test MSE: 0.2714
training data
test data
polynomial (degree=1)
true function
train MSE: 0.0091, test MSE: 0.0106
training data
test data
polynomial (degree=3)
true function
train MSE: 0.0069, test MSE: 0.0093
training data
test data
polynomial (degree=6)
true function
train MSE: 0.0041, test MSE: 28.2400
training data
test data
polynomial (degree=12)
true function
x
y

Overfitting and underfitting



If production-level DL models are so large, why don't they overfit?

Answer 1 Data sets are large and complex – need complex model

Answer 2 Engineers avoid using full complexity of the model

- Early stopping halts training when validation performance begins to decline
- Many architectures include random drop out – randomly shut down neurons during training

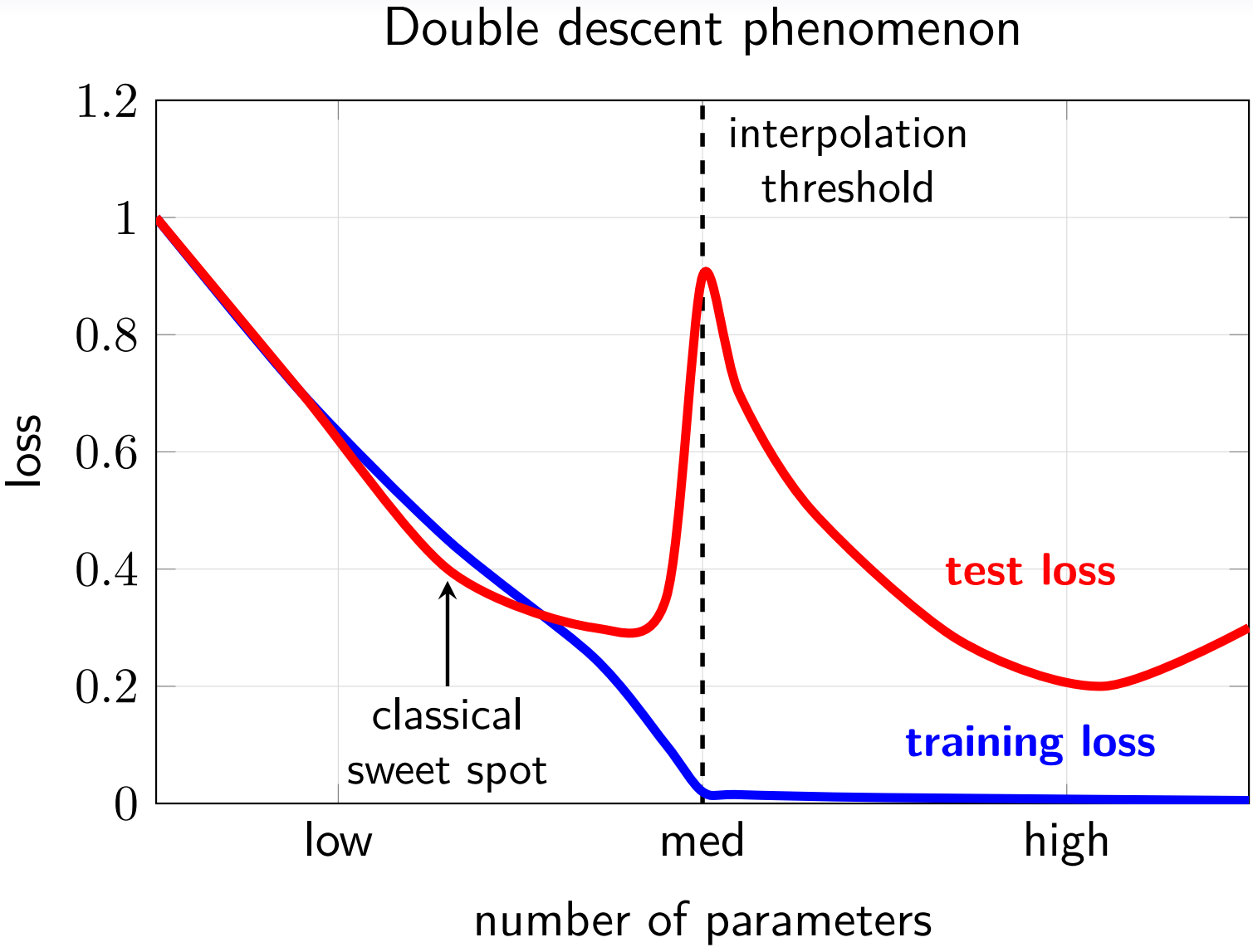
Answer 3 Adding randomization to training prevents overfitting

- Related to benefits of random dropout (randomization)
- Related techniques in DL such as DropConnect and Stochastic Depth
- Stochastic gradient descent injects randomness

Answer 4 Modern architectures have inductive biases that guide learning toward useful patterns

- translation invariance in CNNs (same pattern can be recognized anywhere in an image)
- localization in CNNs – pixels are influenced more by neighbors than pixels far away
- parameter sharing in RNNs – similarity of transformations across time
- Layer normalization and residual connections in transformers - create a bias toward stable training dynamics and information preservation across layers.

Finally, there is some evidence of "double descent" – test error starts to fall again when the number of parameters is very high


Double descent phenomenon
1.2
1
0.8
0.6
0.4
0.2
0
loss
interpolation
threshold
test loss
training loss
classical
sweet spot
low
med
high
number of parameters

Summary

Why can deep learning successfully generalize from limited observations?

Computer scientists' story

- Based on a model of the human brain!
- A universal function approximator!
- Can break the curse of dimensionality!

Alternative story (by me)

- A highly flexible function fitting technique
- Easy to understand with limited maths background
- Extends naturally to high dimensions
- Function evaluations are highly parallelizable
- Smooth recursive structure suited to calculating gradients
- Has received massive investment from the CS community
  - algorithms
  - software
  - hardware

- Many incremental improvements to improve regularization and training
- Many incremental improvements to inject domain-specific knowledge (CNNs, transformers, etc.)