Deep Learning

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Topics

- What are artificial neural networks?
- How are they trained on data?
- Why is DL so successful?

Artificial neural networks (ANNs) are the core of deep learning

“Deep learning” means training ANNs with several hidden layers

Major successes:

- Natural language processing
- Image recognition
- Speech recognition
- Games
- LLMs

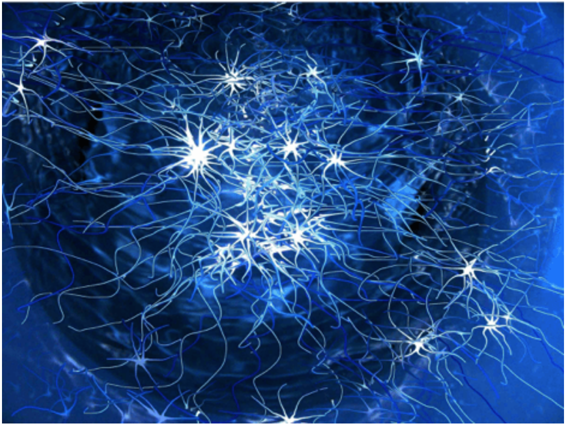
History

- 1940s: McCulloch & Pitts create mathematical model of NN
- 1950s: Rosenblatt develops the perceptron (trainable NN)
- 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 DL

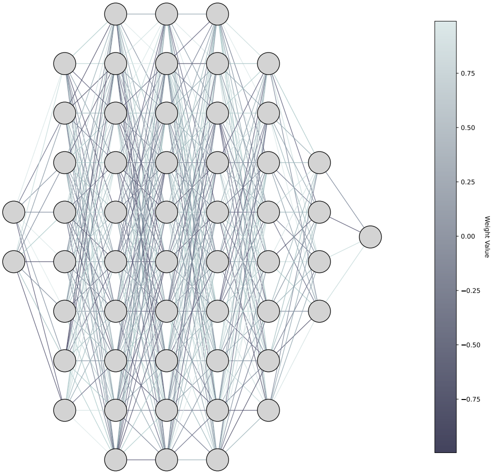
- CNNs, RNNs, LSTMs, transformers, LLMs, etc.

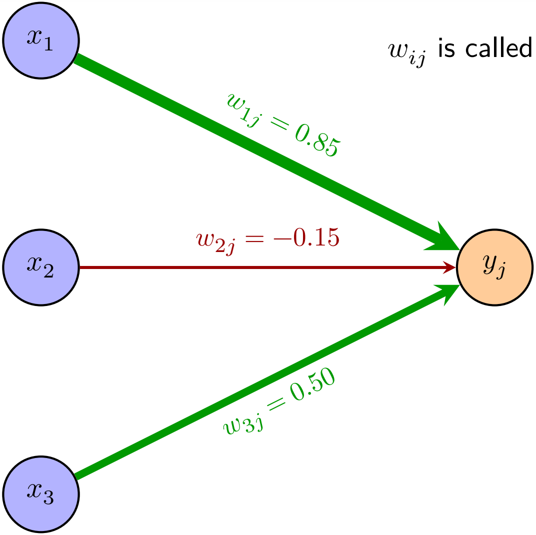
A model of the human brain



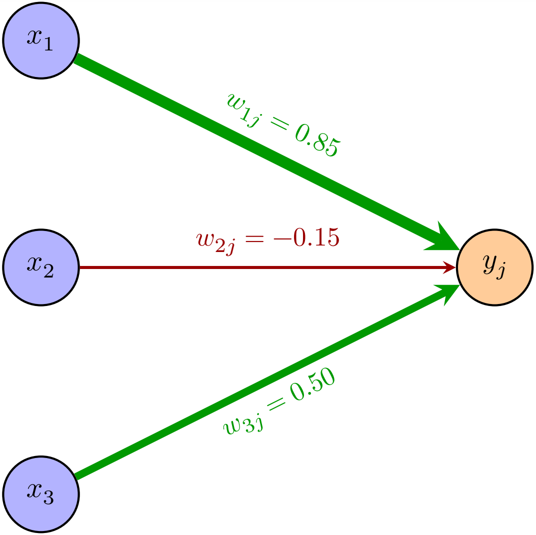
– source: Dartmouth undergraduate journal of science

A mathematical representation: directed acyclic graph

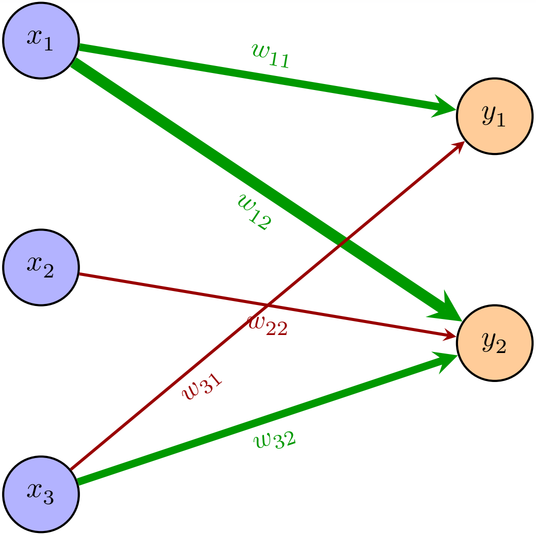




w_{ij} is called a “weight”



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



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

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

$$\implies y = xW$$

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

This is natural given our notation

- w_{ij} points from i to j
- hence $y_j = \sum_i x_i w_{ij}$ (total flow of activation to node j)
- hence $y = xW$

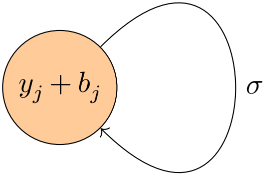
Also fine to use column vectors — just transpose W

Next steps

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

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

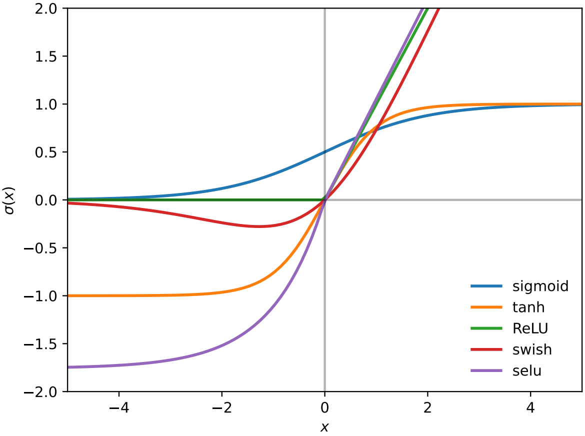
Then apply activation:

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

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

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

Common activation functions



Universal function approximation I

Theorem. (Cybenko–Hornik 1989, 1991) Let

- $K \subset \mathbb{R}^n$ be compact,
- f be a continuous functions from K to $\mathbb{R}^m$, and
- σ be a continuous map from $\mathbb{R}$ to itself

If σ is not polynomial, then, for every $\varepsilon > 0$, there exist matrices A, C and vector b such that

$$\sup_{x \in K} \| f(x) - C\sigma(Ax + b) \| < \varepsilon$$

(The function σ is applied component-wise)

Universal function approximation II

Recall that the ReLU activation has the form $\sigma(x) = \max\{x, 0\}$

Theorem. Let

- $f\colon \mathbb{R}^n \to \mathbb{R}^m$ be Borel measurable and
- $d = \max\{n+1, m\}$

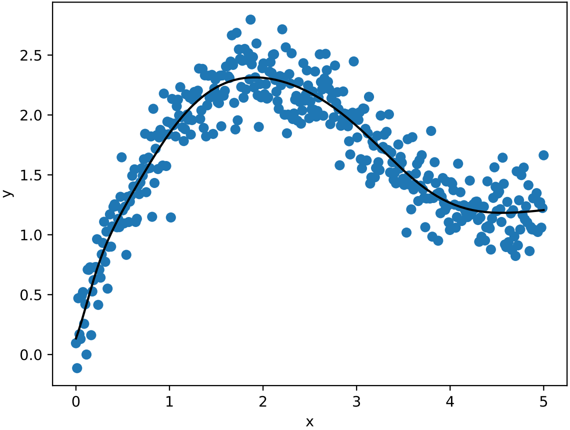
If f is Bochner–Lebesgue integrable, then, for any $\varepsilon > 0$, there exists a fully connected ReLU network g of width d satisfying

$$\int \|f(x) - g(x)\| \, \mathrm{d}x < \varepsilon$$

Before we get too excited: many function classes have the universal function approximation property

- polynomials in $C_0(K) :=$ continuous functions on compacts
- finite linear combinations of an ONS in a Hilbert space
- SVMs with RBF kernels in reproducing kernel Hilbert space
- Gaussian processes with RBF kernels in $C_0(K)$
- random forests
- etc.

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

$$f_\theta = G_m \circ G_{m-1} \circ \cdots \circ G_2 \circ G_1$$

where

- $G_\ell(x) = \sigma_\ell(xW_\ell + b_\ell)$
- $\theta := \{W_1, b_1, W_2, b_2, \dots, W_m, b_m\}$
- σ_ℓ is an activation function

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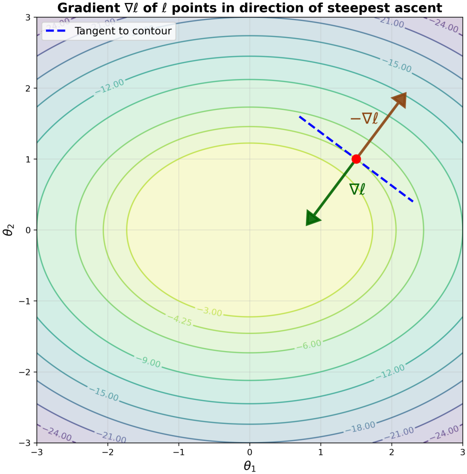
Minimizing the loss functions



Gradient descent

Algorithm: Implement $\nabla \ell$ and then update guess θ_k via

$$\theta_{k+1} = \theta_k - \lambda_k \cdot \nabla \ell(\theta_k)$$

- take a step in the opposite direction to the grad vector
- λ_k is the **learning rate**
- iterate until hit a stopping condition
- in practice replace $\ell(\theta)$ with batched loss → **SGD**

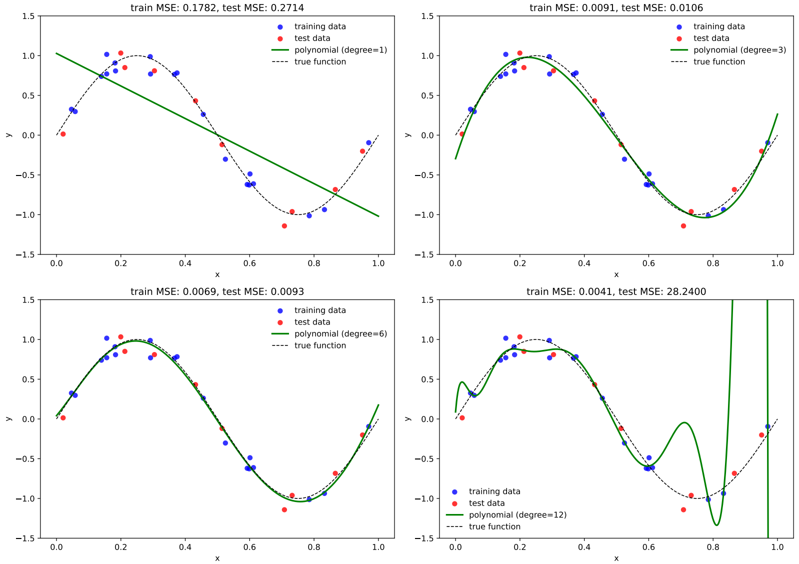
$$\frac{1}{|B|} \sum_{i \in B} (y_i - f_\theta(x_i))^2$$

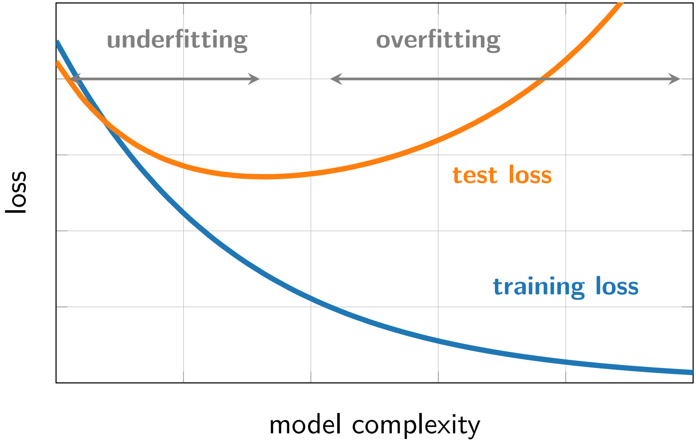
Extensions

- Many variations on SGD
- 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
polynomial (degree=3)
train MSE: 0.0069, test MSE: 0.0093
polynomial (degree=6)
train MSE: 0.0041, test MSE: 28.2400
polynomial (degree=12)
y
x
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0.0
0.2
0.4
0.6
0.8
1.0


underfitting
overfitting
test loss
training loss
loss
model complexity

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

Answer 1 Underlying relationships are complex – need complex model

Answer 2 Engineers avoid using full complexity of the model

- Early stopping halts training when test loss starts to rise
- Drop out – shut down some 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

Randomness “adds some smoothing” to a given data set

“The model must learn to be robust to these perturbations, which encourages it to find smoother, more generalizable decision boundaries rather than fitting to noise in the training data.”

Answer 4 Modern architectures have inductive biases

Examples.

- Translation invariance in CNNs
- Localization in CNNs – pixels influenced more by neighbor pixels
- Parameter sharing in RNNs – similarity of transformations across time

Injection of good priors guides learning

Summary

Why can DL successfully generalize?

CS story

Because

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

Really?

CS story

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- based on a model of the human brain!
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Really?

Claude AI

“Traditional methods typically require you to

- specify the intrinsic dimension,
- choose kernel parameters, or
- make structural assumptions about the manifold

Neural networks automatically adapt to intrinsic structure without requiring this prior knowledge”

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Really?

Alternative story

- Easy to understand with limited maths background
- Scales well to high dimensions
- Function evaluations are highly parallelizable
- Flexible – can inject inductive biases
- Smooth recursive structure suited to calculating gradients

On top of — because of — this:

- Has received massive investment from the CS community
  - algos
  - software
  - hardware
- Many incremental improvements to improve regularization
- Steady increase in injection of domain-specific knowledge
  - CNNs
  - RNNs
  - transformers, etc.

DL with JaX

JAX is more general-purpose than PyTorch or TensorFlow

- Both explicitly designed for deep learning

But DL is the most important use-case

```
@jax.jit
def f(θ, x):
    for W, b in θ:
        x = jnp.tanh(x @ W + b)
    return x

def loss(θ, x, y):
  return jnp.sum((y - f(θ, x))**2)

loss_gradient = grad(loss)

def train(θ, x_data, y_data):
    for i in range(m):
        θ = θ - λ * loss_gradient(θ, x_data, y_data)
    return θ
```

JAX PyTrees

Consider a function of the form

$$f_\theta = G_m \circ G_{m-1} \circ \cdots \circ G_2 \circ G_1$$

where

- $G_\ell x = \sigma_\ell(xW_\ell + b_\ell)$ for $\ell = 1, \ldots, m$
- θ represents the "vector" of all parameters
- σ_ℓ is a given function

The idea that the vector θ contains all parameters is conceptually useful but awkward within code...

To handle these kinds of situations we can use PyTrees

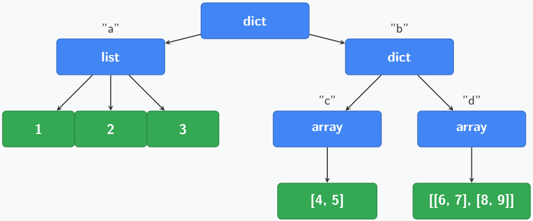
- A tree-like data structure built from Python containers
- A concept, not a data type
- Used to store parameters

Examples.

- A list of dictionaries, each dictionary contains parameters
- A dictionary of lists
- A dictionary of lists of dictionaries
- etc.

JAX PyTree Structure

```python
pytree = {
    "a": [1, 2, 3],
    "b": {"c": jnp.array([4, 5]), "d": jnp.array([[6, 7], [8, 9]])}
}
```



🟦 Container nodes (dict, list, tuple)

🟩 Leaf nodes (arrays, scalars)

JAX can

- apply functions to all leaves in a PyTree structure
- differentiate functions with respect to the leaves of PyTrees
- etc.

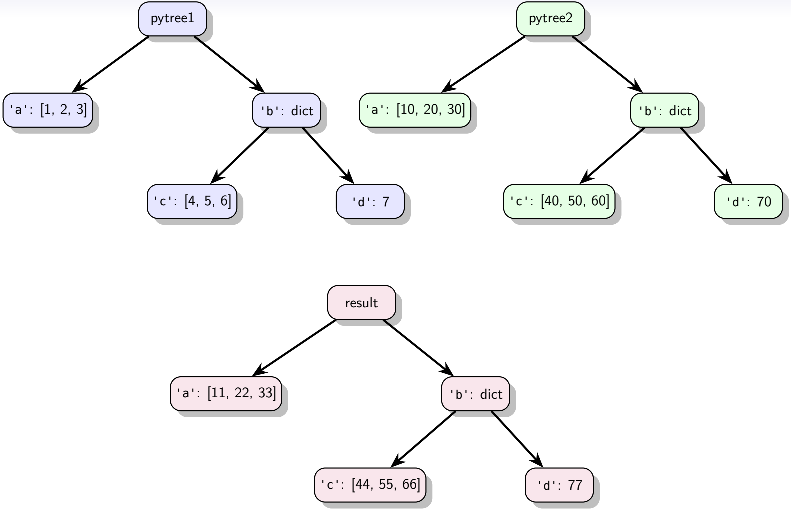


Figure: `jax.tree.map(lambda x, y: x + y, pytree1, pytree2)`

```python
# Apply gradient updates to all parameters
def sgd_update(params, grads, learning_rate):
    return jax.tree.map(
        lambda p, g: p - learning_rate * g,
        params,
        grads
    )

# Calculate gradients (PyTree with same structure as params)
loss_grad = jax.grad(loss_fn)
grads = loss_grad(params, x, y)

# Update all parameters at once
updated_params = sgd_update(params, grads, 0.01)
```