Neural Networks

AERO 689: Machine Learning for Aerospace Engineers

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Summary

Why Neural Networks?

Motivation

Within data-driven ML, when should we use neural networks over classical methods?

Classical methods (Weeks 2–6): linear/regularized regression, logistic regression, PCA, POD, clustering

- These methods are **not inferior** — for many problems they are the right choice
- Ridge regression outperforms a NN on a 50-sample aerodynamic dataset
- Neural networks earn their place only when the problem **exceeds what the classical toolkit handles gracefully**

What Classical ML Cannot Do Easily

Limitation	Why it matters in aerospace
Fixed feature map — hand-engineering required	Wing pressure field: $O(10^5)$ DOF — no human can specify the right features
Shallow representation — hierarchical structure is expensive	Aero-acoustic noise: vortex roll-up $\rightarrow$ shear layer $\rightarrow$ far-field radiation
Does not scale — $n \times n$ matrices become intractable	Hyperspectral imagery, LiDAR, full-field strain maps
No structure sharing — inputs treated independently	Defect detection: pixel neighborhoods carry info a flat vector discards
No sequence memory — samples treated as i.i.d.	Flight dynamics, fault evolution over time, ATC commands

The Neural Network's Answer

1. Automatic feature learning — first layers extract low-level features; deeper layers compose abstractions. No domain expert needed to specify them.

2. Depth and compositionality [1], [2] — deep networks are *compact*: exponentially more efficient than shallow models for hierarchical functions.

3. Inductive biases that match physical structure

- **CNNs** — local, translation-invariant patterns (defect detection, pressure grids)
- **RNNs / LSTMs** — sequential data (flight dynamics, engine health trending)
- **GNNs** — unstructured meshes and sensor networks

4. Scaling laws [3] — classical $O(n^2)$–$O(n^3)$ methods are impractical for large n; NNs with SGD scale to billions of samples.

Why NNs Scale: SGD

Classical methods require the full dataset simultaneously:

Method	Cost per solve	Memory
Least squares	$O(np^2 + p^3)$	$O(np)$
Kernel / GP	$O(n^3)$	$O(n^2)$

SGD replaces the full gradient with a mini-batch estimate ($|\mathcal{B}| = m \ll n$):

$$\nabla_\theta \mathcal{L} \approx \frac{1}{m} \sum_{i \in \mathcal{B}} \nabla_\theta \, \ell(f_\theta(x_i),\, y_i)\,, \qquad \text{cost per step: } O(m \cdot p)$$

- Cost per update is **constant** in n — same whether $n = 10^4$ or 10^{10}
- NN loss **decomposes** as a sum over samples $\Rightarrow$ per-sample gradients are independent
- Backprop computes $\nabla_\theta \ell$ in $O(p)$ — no matrix inversion, no kernel matrix
- Mini-batch noise acts as **implicit regularization** (helps escape sharp minima)

Limitations: Optimization and Constraints

Optimization

- Loss is **non-convex** — SGD finds local minima; no global optimality guarantee
- Convergence is not guaranteed; sensitive to learning rate and initialization
- Classical methods (ridge, SVM, GP) solve *convex* problems with guaranteed global optima

Constraints

- No native constraint handling — classical methods satisfy $g(x) = 0$ exactly via KKT / Lagrange multipliers
- NNs must impose constraints via:
  - **Architecture** (hard) — output layer designed to enforce bounds or symmetry; exact but inflexible
  - **Penalty terms** (soft) — add $\lambda\, g(\theta)^2$ to the loss; satisfied only *approximately*; the weight λ requires tuning

Limitations: Data, UQ, and Hyperparameters

Data and compute

- **Data hungry** — classical methods generalize with $n \sim 10^2$; NNs typically need $n \gtrsim 10^4$
- Training large models requires GPUs and wall-clock time that classical solvers do not

Interpretability and uncertainty quantification

- **Black box** — individual weights carry no physical meaning; predictions are hard to audit
- **No built-in uncertainty** — linear regression gives exact confidence intervals; NNs require ensembles, MC dropout, or full Bayesian NNs to produce calibrated uncertainty estimates

Hyperparameters

- Architecture depth/width, learning rate, batch size, regularization strength, and optimizer must all be tuned
- No closed-form selection — typically requires cross-validation or neural architecture search (NAS)

When to Prefer Classical ML

Prefer classical methods when:

- **Small dataset** ($n \lesssim 10^3$): Ridge/Lasso generalizes better and gives exact confidence intervals
- **Smooth, low-dimensional response**: splines or polynomial regression — interpretable and sufficient
- **Interpretability required**: linear models / decision trees produce auditable rules
- **Tabular data with engineered features**: gradient boosted trees (XGBoost) consistently outperform NNs
- **Closed-form statistics needed**: linear regression gives exact confidence intervals; NNs require ensembles or dropout for uncertainty

Rule of Thumb

Use a neural network when **at least one** of the following holds:

1. Input is **raw and high-dimensional** — images, time series, fields, point clouds
2. Function is **highly nonlinear and hierarchical** — cannot be captured by a fixed kernel
3. **Sufficient data** — $n \gtrsim 10^4$, or transfer learning from a pretrained model is available
4. **Temporal or spatial structure** should be exploited automatically (RNN/LSTM, CNN)

Otherwise, start with the simplest model that works.

Neural Networks

A Neural Network as a Function

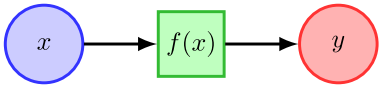


Figure 1: Simple: $y := f(x)$

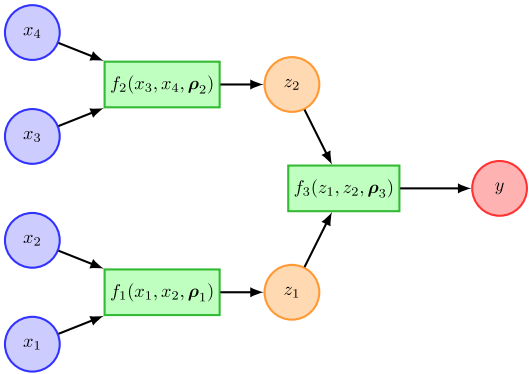
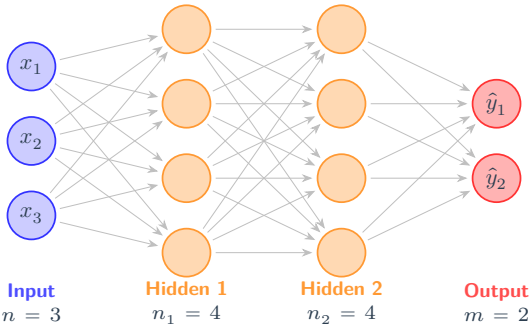


Figure 2: Complex: $y = f_3(f_1(\cdot),\ f_2(\cdot),\ \rho_3)$

In general: $y = f(x, \rho)$ where $x \in \mathcal{R}^n$ is the input and $\rho \in \mathcal{R}^p$ are the parameters.

Dense Feedforward Network

Every neuron is connected to every neuron in the next layer — hence *dense*.



Layer Operations

Each layer ℓ computes the **vector of activations**:

$$\underbrace{a^{(\ell)}}_{\text{output of layer } \ell} = \sigma\Big(W^{(\ell)}\, a^{(\ell-1)} + b^{(\ell)}\Big)$$

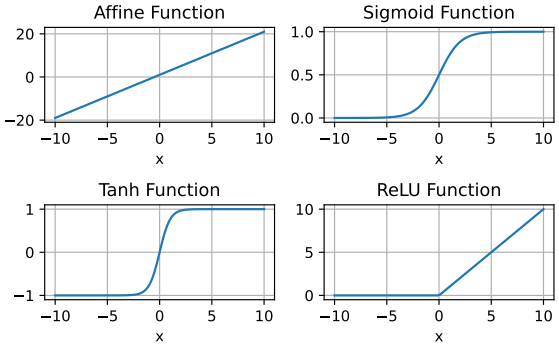
- $W^{(\ell)}$ — weight matrix; $b^{(\ell)}$ — bias vector
- σ — **activation function**, applied element-wise (broadcasting)
- "Activation of a vector" = "vector of activations" — same computation, different perspective
- The network is a *graphical architecture for composing parameterized nonlinear functions*

Activation Functions

Common Activation Functions

Name	Function
Affine	$W^T x + b$
Sigmoid	$\frac{1}{1+e^{-x}}$
Tanh	$\tanh(x)$
ReLU	$\max(0, x)$

Non-linear activations are essential: a composition of linear functions is still linear.



Building Neural Networks in Python

Framework Overview

Library	Backend	Primary use	By
TensorFlow / Keras	TF	Production, deployment	Google
PyTorch	PyTorch	Research, custom arch	Meta
scikit-learn MLP	NumPy	Rapid prototyping	Community

In practice: TensorFlow/Keras and PyTorch dominate.

TensorFlow / Keras

```
import tensorflow as tf
from keras.models import Sequential
from keras.layers import Dense

fhat = Sequential([
    Dense(2,  input_dim=1),
    Dense(10, activation="tanh"),
    Dense(5,  activation="tanh"),
    Dense(1,  activation="sigmoid"),
])

# Reverse-mode AD
x = tf.linspace(-10, 10, 100)
with tf.GradientTape() as tape:
    tape.watch(x)
    y = fhat(x)
dydx = tape.gradient(y, x)
```

PyTorch: Model Definition

```
import torch
import torch.nn as nn

class FHat(nn.Module):
    def __init__(self):
        super().__init__()
        self.net = nn.Sequential(
            nn.Linear(1, 2),
            nn.Linear(2, 10), nn.Tanh(),
            nn.Linear(10, 5), nn.Tanh(),
            nn.Linear(5, 1),  nn.Sigmoid(),
        )
    def forward(self, x):
        return self.net(x)

fhat = FHat()
```

PyTorch: Automatic Differentiation

```
x    = torch.linspace(-10, 10, 100,
                      requires_grad=True).unsqueeze(1)
y    = fhat(x)
y.sum().backward()       # dy/dx for all x simultaneously
dydx = x.grad
```

	TensorFlow / Keras	PyTorch
Training loop	`model.fit()` (hidden)	Explicit `loss.backward()`
Flexibility	High-level, concise	Fully customizable
Best for	Production / deployment	Research / custom arch

Universal Approximation Theory

Universal Approximation Theorem

Theorem (Cybenko [4]; Hornik [5]). A feedforward network with one hidden layer and finitely many neurons can approximate *any* continuous function on a compact subset of $\mathbb{R}^n$ to arbitrary accuracy.

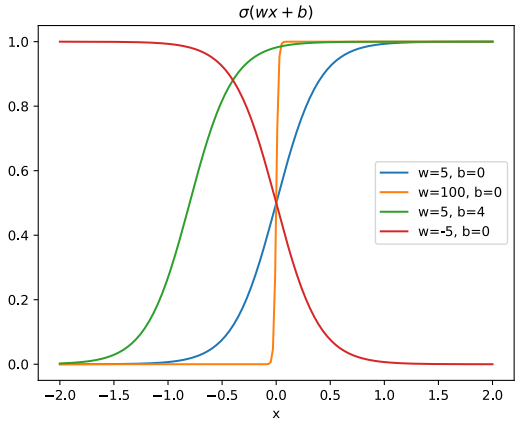
Key implications:

1. **Expressiveness** — NNs are not limited in the functions they can represent
2. **Depth efficiency** — deeper networks achieve the same accuracy with exponentially fewer parameters
3. **Non-linear activation is essential** — a composition of linear functions is still linear
4. **Does not address**: how to train, convergence speed, overfitting, or architecture choice

The theorem guarantees existence — not learnability.

Impact of Weights and Biases

Effect of Weights and Biases



Effect of w and b on $\sigma(wx + b)$.

- **Large** w, $b = 0$**:** step function — sharp transition
- **Nonzero** b**:** shifts the activation point left/right
- **Negative** w**:** deactivation — transitions from $1 \to 0$

Optimizing w and b controls the shape and location of each basis function.

Neural Basis Functions

By linearly combining sigmoid and affine functions — **locally supported functions**:

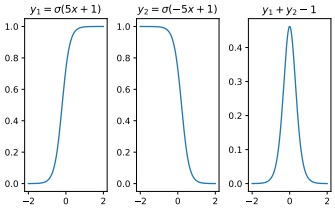


Figure 3: Bell: $y_1 + y_2 - 1$

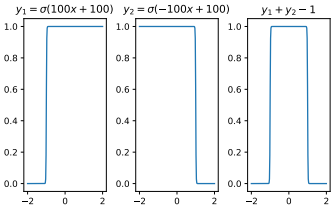


Figure 4: Box: large w

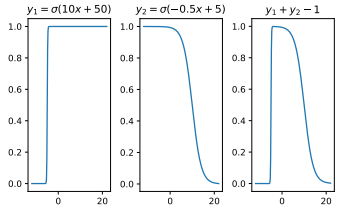


Figure 5: Asymmetric: $w_1 \neq w_2$

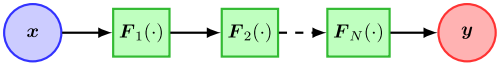
Optimizing weights and biases constructs a rich library of neural basis functions.

Deep Neural Networks

Feed-Forward Neural Network (FFNN / MLP)

$$F(x) = (F_N \circ \cdots \circ F_1)(x)$$

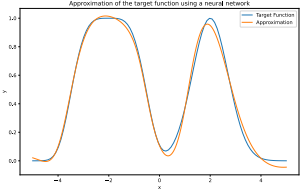
$$F_i(\cdot) = f_i(W_i\, F_{i-1}(\cdot) + b_i)$$



- W_i, b_i: weight matrix and bias of layer i
- f_i: activation function of layer i
- Well-suited for tabular data and supervised learning
- Address overfitting via weight decay or dropout
- See [6, Ch. 6] for a thorough treatment

FFNN Example: TensorFlow

```
def target_function(x):
    return np.exp(-(x-2)**2) + np.exp(-0.15*(x+2)**4)

x_train = np.linspace(-5, 5, 100).reshape(-1, 1)
y_train = target_function(x_train)

model = tf.keras.Sequential([
    tf.keras.layers.Dense(32, activation='tanh', input_shape=(1,)),
    tf.keras.layers.Dense(32, activation='tanh'),
    tf.keras.layers.Dense(32, activation='tanh'),
    tf.keras.layers.Dense(1)
])
model.compile(optimizer='adam', loss='mse')
model.fit(x_train, y_train, epochs=1000)
```



FFNN Example: PyTorch

```
class FFNN(nn.Module):
    def __init__(self):
        super().__init__()
        self.net = nn.Sequential(
            nn.Linear(1, 32), nn.Tanh(),
            nn.Linear(32, 32), nn.Tanh(),
            nn.Linear(32, 32), nn.Tanh(),
            nn.Linear(32, 1),
        )
    def forward(self, x): return self.net(x)

model     = FFNN()
optimizer = torch.optim.Adam(model.parameters(), lr=1e-3)
loss_fn   = nn.MSELoss()

for epoch in range(5000):
    optimizer.zero_grad()
    loss = loss_fn(model(x_train), y_train)
    loss.backward()
    optimizer.step()
```

Application: Aerodynamic Surrogate Modeling

Problem: Predict $\hat{C}_D(M, \alpha)$ — CFD requires hours per operating point.

Approach	Fails at	Advantage
Linear regression	Transonic drag rise ($M \approx 0.8$), stall ($\alpha > 12^\circ$)	Interpretable; fast
FFNN (2→64→64→1)	Extrapolation past training envelope	Captures strong non-linearities

Inputs: $[M, \alpha]$ **Output:** C_D **Data:** CFD sweep or wind-tunnel runs

Aerodynamic Surrogate: PyTorch

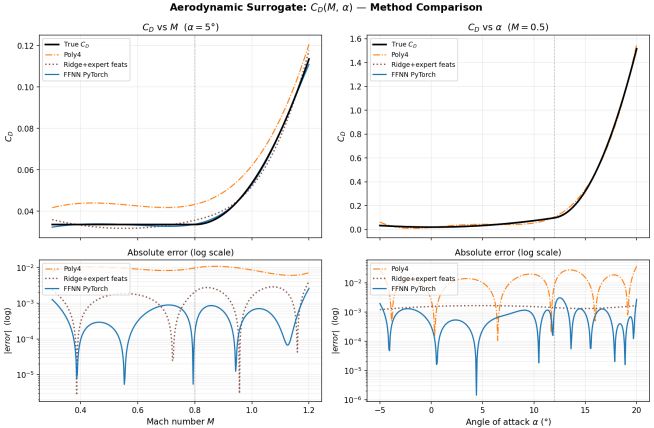
```
import torch, torch.nn as nn

class DragSurrogate(nn.Module):       # [M, alpha] -> C_D
    def __init__(self):
        super().__init__()
        self.net = nn.Sequential(
            nn.Linear(2, 64), nn.Tanh(),
            nn.Linear(64, 64), nn.Tanh(),
            nn.Linear(64, 1),
        )
    def forward(self, x): return self.net(x)

model     = DragSurrogate()
optimizer = torch.optim.Adam(model.parameters(), lr=1e-3)
loss_fn   = nn.MSELoss()

# X_train: (N, 2) [M, alpha];  y_train: (N, 1) C_D
for epoch in range(5000):
    optimizer.zero_grad()
    loss = loss_fn(model(X_train), y_train)
    loss.backward()
    optimizer.step()
```

Aerodynamic Surrogate: Accuracy Results

Method	RMSE	R^2
Polynomial (deg 4)	0.0142	0.998
Ridge + expert feats	0.0027	1.000
FFNN PyTorch	**0.0024**	**1.000**

- 2,400 train / 600 test.
- $C_D \in [0.015,\ 1.52]$.

Takeaway: expert feats beat FFNN here — NNs earn their place when features are unknown.



Top: predictions; bottom: |error| (log scale). Poly4 and expert features track well; NNs match without feature engineering.

Specific Deep Learning Architectures

Sequence Prediction: Embedding the Past

Many aerospace problems are **sequential**: given a history of observations $x_1, x_2, \ldots, x_t$, predict what happens next.

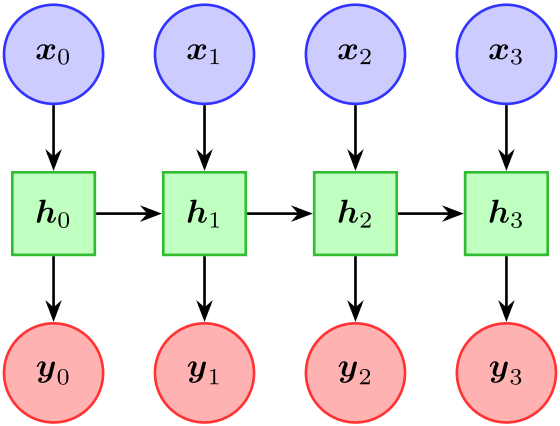
Application	Sequence (past/present)	Prediction (future)
Engine health	Sensor readings over T flights	Remaining useful life
Flight dynamics	States (α, q, V) over time	Next-step trajectory
Weather / turbulence	Gridded fields at $t_{-n} \ldots t_0$	Field at t_1

Core challenge: an FFNN takes a fixed-size input. How do we compress a variable-length sequence into a fixed representation — a **sequence embedding** — that retains the information needed for prediction?

Three approaches, each building on the last:

1. **RNN** — fold the sequence into a hidden state, one step at a time
2. **LSTM** — add gated memory so the embedding can retain long-range information
3. **Transformer** — let every step attend to every other step in parallel

Recurrent Neural Networks (RNN)



$$h_t = F(W_{xh}x_t + W_{hh}h_{t-1} + b_h)$$

$$y_t = g(W_{hy}h_t + b_y)$$

- Parameters shared across time steps
- **Hidden state** h_t is the sequence embedding — it accumulates information from $x_1, \ldots, x_t$
- At any time t, h_t is a fixed-size summary of everything seen so far

The Vanishing Gradient Problem

Training an RNN requires back-propagation through time (BPTT): gradients flow backward through every time step.

$$\frac{\partial \mathcal{L}}{\partial W_{hh}} = \sum_{t=1}^{T} \frac{\partial \mathcal{L}}{\partial h_T} \prod_{k=t+1}^{T} \frac{\partial h_k}{\partial h_{k-1}}$$

The product $\prod \frac{\partial h_k}{\partial h_{k-1}}$ involves multiplying the same weight matrix $T - t$ times:

- If eigenvalues < 1: gradients **vanish** $\Rightarrow$ early time steps are forgotten
- If eigenvalues > 1: gradients **explode** $\Rightarrow$ training diverges

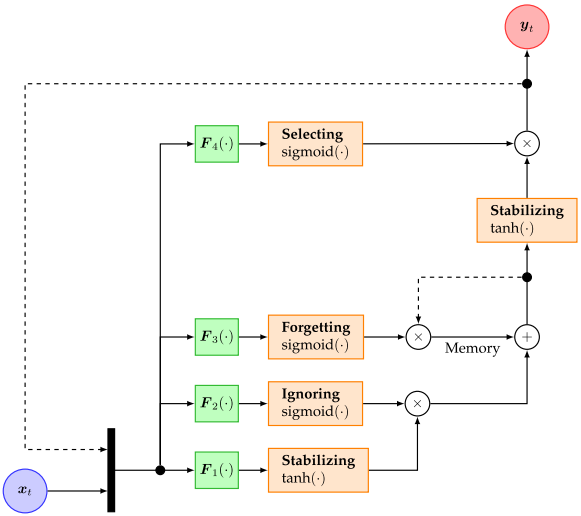
Vanishing Gradients: Consequence and Solution

Consequence: vanilla RNNs struggle to learn dependencies longer than $ $10–20 steps. The sequence embedding h_t loses early information.

Example: predicting engine failure from 200 cycles of sensor data — by the time the RNN reaches cycle 200, the gradient signal from cycle 1 has effectively disappeared.

Solution: add explicit memory with **gates** that control what to remember and what to forget $\Rightarrow$ **LSTM**.

Long Short-Term Memory (LSTM)



Three **gates** regulate memory [7]:

- **Forget gate** f_t — erases irrelevant memory
- **Input gate** i_t — writes new information
- **Output gate** o_t — controls what passes to h_t

The **cell state** c_t acts as a conveyor belt: gradients can flow through it unchanged, solving the vanishing gradient problem.

The sequence embedding is now (h_t, c_t) — richer than the RNN's h_t alone.

Periodic Forecasting Example

Goal: predict the next value of a periodic signal from a window of recent history.

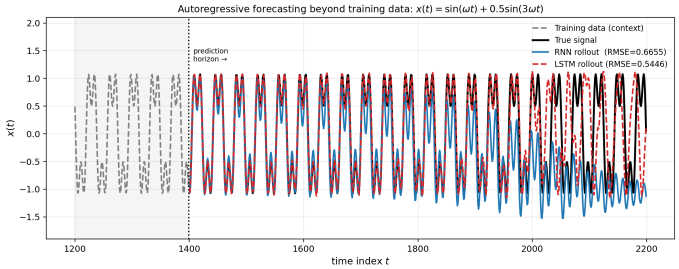
$$x_t = \sin(\omega t) + 0.5\sin(3\omega t), \quad \omega = 0.17$$

$$\hat{x}_{t+1} = f(x_{t-W+1}, \ldots, x_t), \quad W = 30$$

- Train: $t = 0, \ldots, 1399$; test rollout: $t = 1400, \ldots, 2199$
- Compare **vanilla RNN** and **LSTM** (same hidden size $= 32$)
- **Autoregressive rollout**: each prediction is fed back as the next input — no true future values used

```
def signal(t):
    return np.sin(omega * t) + 0.5 * np.sin(3 * omega * t)

X, y = make_windows(signal(t_train), window=30)

rnn  = nn.RNN(input_size=1,  hidden_size=32, batch_first=True)
lstm = nn.LSTM(input_size=1, hidden_size=32, batch_first=True)
```

Periodic Forecasting Results: RNN vs LSTM



- Gray region: last 200 training steps (context). Dashed line: end of training data.
- Both models roll out **800 steps** feeding only their own predictions — no true future values.
- Look-ahead is valid only for inputs known in advance (e.g., planned controls); using unknown future targets is leakage.
  - Valid only when future signals are genuinely available at inference time.

RNN: diverges quickly. The fixed-size hidden state h_t cannot retain phase information over many steps.

LSTM: stays accurate near the horizon, but also drifts eventually. The cell state slows error growth but cannot prevent it.

Key insight: autoregressive rollout accumulates errors at every step. Even the best recurrent model has a finite prediction horizon — this is a fundamental limitation, not just a training issue.

From Recurrence to Attention

LSTM processes the sequence **one step at a time** — step 50 must wait for steps 1–49. Two limitations:

1. **No parallelism** — training is slow on long sequences
2. **Information bottleneck** — all history must squeeze through the fixed-size state (h_t, c_t)

Key insight [8]: instead of passing information forward through a chain of hidden states, let every position in the sequence **look at every other position directly**.

Self-Attention Mechanism

Given an input sequence $x_1, \ldots, x_T$, compute three projections per position:

- $\mathbf{Q}$ (Query) — "what am I looking for?"
- $\mathbf{K}$ (Key) — "what do I contain?"
- $\mathbf{V}$ (Value) — "what information do I pass along?"

$$\text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{d_k}}\right)\mathbf{V}$$

The softmax produces a **weight matrix** over all positions — each output is a weighted combination of all inputs, where the weights are learned from data.

Dividing by $\sqrt{d_k}$ prevents dot products from growing too large in high dimensions.

Transformer Architecture

Key ideas:

- **Self-attention** — each output is an attention-weighted sum of *all* inputs
- **Multi-head attention** — h parallel heads learn different relationships simultaneously
- **Positional encoding** — injects sequence order (no recurrence)
- Scales to long sequences; backbone of modern LLMs and vision models

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}}\right)V$$

Watch: 3Blue1Brown

Attention in transformers, visually explained

https://www.youtube.com/watch?v=eMlx5fFNoYc

Self-study: Watch before the next class. We will discuss aerospace applications in lecture.

Sequence Models: Comparison

	RNN	LSTM	Transformer
Long-range memory	Poor	Good	Excellent
Parallel training	No	No	Yes
Sequence embedding	h_t	(h_t, c_t)	attention-weighted
Complexity per layer	$O(T \cdot d^2)$	$O(T \cdot d^2)$	$O(T^2 \cdot d)$

- **RNN:** simple, fast per step, but forgets early inputs
- **LSTM:** gated memory solves vanishing gradients; standard for moderate-length sequences
- **Transformer:** best for long-range dependencies and large-scale data; $O(T^2)$ cost per layer

Active research: linear attention, sparse attention, and state-space models aim to reduce the $O(T^2)$ cost while keeping the benefits of attention.

RNN Example: Frequency Estimation

```
from tensorflow.keras.layers import SimpleRNN, Dense

model = Sequential([
    SimpleRNN(50, input_shape=(50, 1), return_sequences=True),
    SimpleRNN(50),
    Dense(1)
])
model.compile(optimizer='adam', loss='mse')
model.fit(X, y, epochs=10, batch_size=32, validation_split=0.2)
```

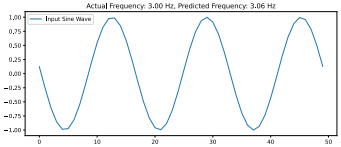


Figure 6: Frequency classification from sine-wave time series.

Application: Engine Health — NASA C-MAPSS

C-MAPSS = Commercial Modular Aero-Propulsion System Simulation [9].

NASA simulated turbofan engines running from healthy to failure under realistic conditions.

- One **cycle** = one start → operate → shutdown sequence (i.e. one flight).
- Each row in the dataset is a snapshot of all sensors during one cycle.
- Each engine has a **different initial wear** and **unknown fault onset**, so trajectories vary in length (e.g. 128–362 cycles).

Item	Description
Subset used	FD001 — single operating condition, single fault mode (HPC degradation)
Training / Test	100 / 100 engines (run-to-failure in train; cut-off in test)
Sensor channels	21 (temperatures, pressures, fan/core speeds, bypass ratio, …)
Operating settings	3 (altitude, Mach, throttle resolver angle)
Target	Remaining Useful Life (RUL) — cycles until failure, capped at 125

Free download: `https://ti.arc.nasa.gov/c/6/`

Engine Health: Problem Setup

Goal: predict how many cycles an engine has left before failure.

- **Piece-wise linear RUL:** true RUL decreases linearly (299, 298, ...), but early in life the sensors look identical — no degradation signal.
  - Capping at 125 means: any RUL > 125 is set to 125, so the model only learns the **degradation phase** where sensors actually change.
- **Rolling window ($w = 30$ cycles):** at each time step we feed the last 30 sensor readings to the model.

Inputs	Output	Why LSTM?
14 sensors + 3 settings over 30 cycles (30×17 matrix)	RUL (cycles)	Hidden state captures gradual degradation trend across the window

Engine Health: Classical Baseline

Strategy: Extract hand-crafted features from a 30-cycle window, then Ridge regression with polynomial interaction terms.

```
# For each window of 30 cycles, extract:
#   rolling mean, rolling std, trend (Δ), cycle number
# per sensor channel → 52 features per sample

from sklearn.pipeline import Pipeline
from sklearn.preprocessing import PolynomialFeatures, StandardScaler
from sklearn.linear_model import RidgeCV

ridge = Pipeline([
    ("poly", PolynomialFeatures(degree=2, interaction_only=True)),
    ("scl",  StandardScaler()),
    ("ridge", RidgeCV(alphas=[0.01, 0.1, 1.0, 10.0, 100.0])),
]).fit(X_train, y_train)
```

52 hand-crafted features $\rightarrow$ 1,378 polynomial interaction terms $\rightarrow$ Ridge selects the best linear combination.

Engine Health: Feature Engineering

A 30-cycle window of raw sensor data is a 30×17 matrix. Ridge regression needs a flat vector, so we summarize each sensor column:

Feature	What it captures
Rolling mean	Current average state of the sensor
Rolling std	How noisy / volatile the sensor is
Trend (Δ)	Is the sensor drifting up or down? (degradation direction)
Cycle number	Where in the engine's life we are

This yields $\sim$ 52 scalar features per sample — but **discards the time ordering** within the window.

Engine Health: Why Polynomial Ridge?

Polynomial interactions (`degree=2, interaction_only=True`) — creates all pairwise products of the 52 features, e.g. $\overline{T}_{30} \times \sigma_{\mathrm{P}_{15}}$.

- This lets a linear model capture nonlinear patterns like "temperature rising *while* pressure becomes noisy $\Rightarrow$ imminent failure."
- 52 features $\rightarrow$ 1,378 interaction terms

Ridge (L2) regularization prevents overfitting on 1,378 terms; `RidgeCV` auto-selects the penalty strength via cross-validation.

Key limitation: the temporal **sequence** inside each window is lost — LSTM addresses this.

Engine Health: LSTM (PyTorch)

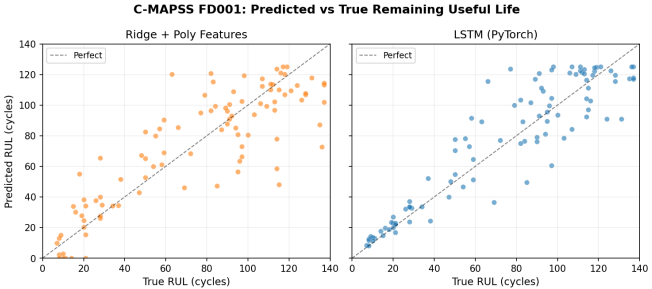
Strategy: Feed raw 30-cycle sensor sequences directly — let the LSTM learn temporal features.

```
class RULPredictor(nn.Module):
    def __init__(self, n_feat=17, h1=64, h2=32):
        super().__init__()
        self.lstm1 = nn.LSTM(n_feat, h1, batch_first=True)
        self.lstm2 = nn.LSTM(h1, h2, batch_first=True)
        self.fc    = nn.Linear(h2, 1)

    def forward(self, x):                # x: (batch, 30, 17)
        out, _ = self.lstm1(x)
        out, _ = self.lstm2(out)
        return self.fc(out[:, -1, :])    # last hidden → RUL

model     = RULPredictor()
optimizer = torch.optim.Adam(model.parameters(), lr=5e-4)
for epoch in range(80):
    for X_b, y_b in train_loader:
        optimizer.zero_grad()
        loss = nn.MSELoss()(model(X_b), y_b)
        loss.backward()
        optimizer.step()
```

Engine Health: Results

Method	RMSE	R^2
Ridge + poly feats	21.5	0.73
LSTM	**17.2**	**0.83**

- LSTM: **20% lower RMSE** — no feature engineering needed
- Ridge needs domain knowledge to build 52 hand-crafted features
- LSTM learns temporal patterns directly from raw sensors



Predicted vs true RUL (cycles). LSTM points cluster tighter around the diagonal.

Other Architrectures

Watch these videos

Watch: 3Blue1Brown

- **Word vectors:** https://youtu.be/FJtFZwbvkI4
- **Convolution:** https://youtu.be/KuXjwB4LzSA
- **Transformers:** https://youtu.be/wjZofJX0v4M
- **Attention in Tranformers:** https://www.youtube.com/watch?v=eMlx5fFNoYc

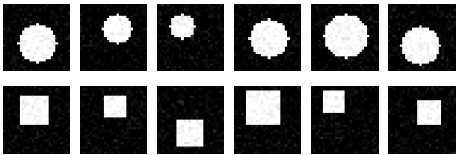
Important Architectures

Watch: 3Blue1Brown

- Convolutional Neural Networks
- Autoencoders
- Transformers

How to use them in aerospace applications?

CNN Intuition: Circles vs. Squares



2000 synthetic 28×28 images (1000 per class). Shapes at random position and size, with noise.

What separates them in pixel space?

- **Circle:** curved boundary — no right-angle gradients anywhere
- **Square:** horizontal + vertical edges, 4 sharp corners

A plain MLP sees 784 *independent* pixel values and must re-learn position from scratch.

A **CNN** slides a small window across the image and detects local patterns *wherever they appear*.

ShapeCNN: Data & Architecture

```python
import numpy as np, torch, torch.nn as nn

IMG = 28   # pixels

def make_circle():
    img = np.zeros((IMG, IMG), np.float32)
    r  = np.random.randint(5, 10)
    cx = np.random.randint(r+2, IMG-r-2)
    cy = np.random.randint(r+2, IMG-r-2)
    yy, xx = np.ogrid[:IMG, :IMG]
    img[(xx-cx)**2+(yy-cy)**2<=r**2] = 1.
    return img

def make_square():
    img = np.zeros((IMG, IMG), np.float32)
    s  = np.random.randint(8, 16)
    x0 = np.random.randint(2, IMG-s-2)
    y0 = np.random.randint(2, IMG-s-2)
    img[y0:y0+s, x0:x0+s] = 1.
    return img

circles = [make_circle() for _ in range(1000)]
squares = [make_square() for _ in range(1000)]
X = np.array(circles+squares)[:,None] # (2000,1,28,28)
y = np.array([0]*1000 + [1]*1000)
```

```python
class ShapeCNN(nn.Module):
    def __init__(self):
        super().__init__()
        self.features = nn.Sequential(
            nn.Conv2d(1, 8, 5, padding=2),
            nn.ReLU(),
            nn.MaxPool2d(2),      # 28 → 14
            nn.Conv2d(8,16,3, padding=1),
            nn.ReLU(),
            nn.MaxPool2d(2),      # 14 → 7
        )
        self.head = nn.Sequential(
            nn.Flatten(),
            nn.Linear(16*7*7, 32),
            nn.ReLU(),
            nn.Linear(32, 2),     # circle / square
        )
    def forward(self, x):
        return self.head(self.features(x))
```

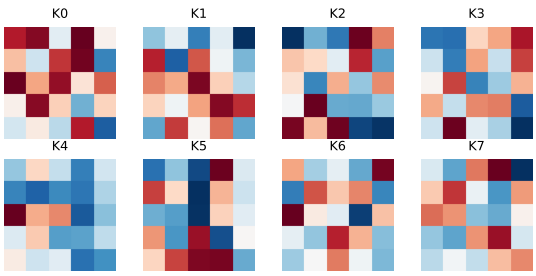
Conv2d = 2D sliding filter — the 2D analogue of the 1D C_p case.\[3pt] **MaxPool2d** = translation tolerance: the circle can be anywhere.

ShapeCNN: Training & Learned Filters

```
model   = ShapeCNN()
opt     = torch.optim.Adam(
              model.parameters(), lr=1e-3)
loss_fn = nn.CrossEntropyLoss()

for epoch in range(50):
    opt.zero_grad()
    loss = loss_fn(model(X_tr), y_tr)
    loss.backward(); opt.step()

model.eval()
with torch.no_grad():
    preds = model(X_te).argmax(1)
acc = (preds == y_te).float().mean()
print(f"Accuracy: {acc:.1%}")  # → 99.5%
```

Class	Prec.	Rec.
Circle	1.00	0.99
Square	0.99	1.00

Layer-1 learned filters (5×5, Conv2d)

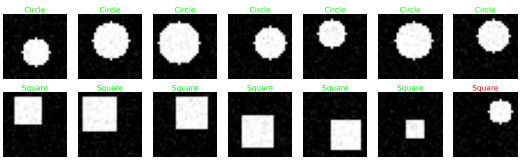


Filters emerge as **oriented edge detectors** at different angles and frequencies — the CNN automatically reinvented Sobel/Gabor filters.

Key takeaway: no one programmed "look for curves" or "look for corners." The network learned these from labeled examples alone.

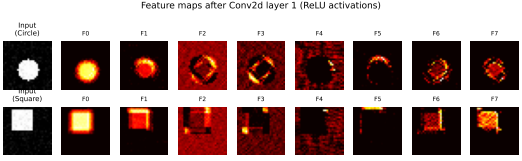
ShapeCNN: Does It Work?

Test predictions (green = correct, red = wrong)



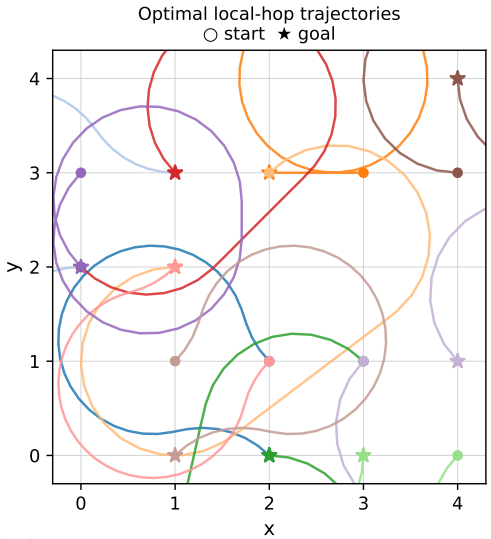
13/14 shown correct; overall test accuracy **99.5%**.

Feature maps after Conv2d layer 1



F2/F3 trace the **curved boundary** of a circle. Same filters produce **straight-edge** responses for a square — that's how the network separates the two classes.

Transformer Example: Dubins Car Path Planning



Dubins car: constant speed $v = 1$, steer with $u \in [-1, 1]$ rad/s.

Dataset: solve a **minimum-time OCP** (CasADi + IPOPT) for every local hop on a 5×5 grid $\times$ all 8×8 heading combos ;($\theta_k = k\pi/4$):

$$\min_{u(\cdot),\,T_f} \; T_f \quad \text{s.t.} \; \begin{cases} \dot{x} = v\cos\theta,\ \dot{y} = v\sin\theta,\ \dot{\theta} = u \\ |u| \le 1 \end{cases}$$

Key design: train only on **nearest-neighbour hops** — the transformer must **stitch hops** to reach distant goals (otherwise it is just a look-up table).

7573 trajectories solved in $ $288 s on 8 cores.

Transformer: State Encoding & Architecture

```
class DubinsTransformer(nn.Module):
  def __init__(self, d=64, nhead=4, nlayers=3):
    # encode each raw state R^3 -> R^d
    self.state_enc = nn.Linear(3, d)
    self.goal_enc  = nn.Linear(3, d)
    layer = nn.TransformerEncoderLayer(
        d, nhead, dim_feedforward=256,
        batch_first=True, norm_first=True)
    self.tf   = nn.TransformerEncoder(layer, nlayers)
    self.head = nn.Linear(d, 3)  # R^d -> next (x,y,th)

  def forward(self, states, goal):
    g_tok = self.goal_enc(goal).unsqueeze(1) # (B,1,d)
    s_tok = self.state_enc(states)           # (B,t,d)
    seq   = cat([g_tok, s_tok], dim=1)       # (B,t+1,d)
    mask  = causal_mask(seq)
    out   = self.tf(seq, mask=mask)
    return self.head(out[:, 1:]) # skip goal token
```

State encoding projects $\mathbf{s}_t \in \mathbb{R}^3$ into a compact $d{=}64$ space:

$$\mathbf{z}_t = W_s\,\mathbf{s}_t + \mathbf{b}_s \;\in\; \mathbb{R}^{64}$$

Goal token prepended — every state attends to the goal at all 3 layers.

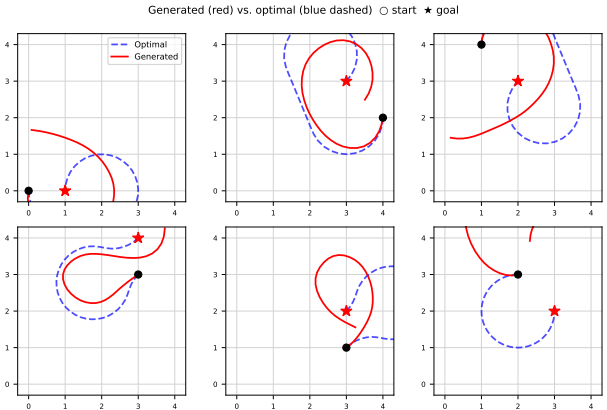
Causal mask prevents future look-ahead, enabling autoregressive rollout at test time.

Training: teacher forcing, cosine-annealed Adam, 500 epochs, batch 512:

$$\mathcal{L} = \frac{1}{T}\sum_{t=1}^{T} \|\hat{\mathbf{s}}_t - \mathbf{s}_t\|^2$$

Final loss: 1.2×10^{-4}

Transformer: Generated Trajectories



Autoregressive rollout:

$$\hat{\mathbf{s}}_{t+1} = f_\theta(\hat{\mathbf{s}}_{0:t},\, \mathbf{g})$$

No ground truth at test time — each prediction feeds back as the next input.

- Trained only on **local hops** (1-step neighbors)
- Test cases include longer hops the model never saw
- The transformer **attends to the goal token** at every layer to stay on course
- Replicates the curved, arc-shaped structure of min-time Dubins paths

Physics-Informed Neural Networks

When Data Alone Is Not Enough

Classical NNs need labeled data $\{(x_i, y_i)\}$. In many aerospace problems:

- **Data is scarce** — each CFD run or flight test is expensive
- **Physics is known** — governing equations (ODEs, PDEs) encode what we already understand
- **Extrapolation matters** — a data-only NN can predict nonsense outside the training envelope

Idea (Raissi et al., 2019): embed the governing equation directly into the loss function.

$$\mathcal{L} = \underbrace{\mathcal{L}_{\text{data}}}_{\text{fit observations}} + \lambda \underbrace{\mathcal{L}_{\text{physics}}}_{\text{satisfy PDE/ODE}}$$

The network is trained to satisfy *both* the data and the physics simultaneously.

PINN Formulation

Let $u(t;\,\theta)$ be the NN approximation of the true solution $u^*(t)$.

Data loss (initial/boundary conditions or sparse measurements):

$$\mathcal{L}_{\text{data}} = \frac{1}{N_d}\sum_{i=1}^{N_d}\big(u(t_i;\theta) - u_i^*\big)^2$$

Physics residual (evaluated at collocation points $\{t_j\}$, no labels needed):

$$\mathcal{L}_{\text{phys}} = \frac{1}{N_c}\sum_{j=1}^{N_c}\big[\mathcal{N}[u](t_j;\theta)\big]^2$$

where $\mathcal{N}[\cdot]$ is the differential operator. Gradients through $\mathcal{N}$ are computed by **automatic differentiation** — exactly the same `autograd` used for backprop.

Total loss: $\mathcal{L} = \mathcal{L}_{\text{data}} + \lambda\,\mathcal{L}_{\text{phys}}$

Application: Spring-Mass Oscillator

Problem: learn the solution $x(t)$ of the spring-mass ODE

$$\ddot{x} + \omega_n^2\, x = 0, \qquad x(0) = 1,\ \dot{x}(0) = 0, \qquad \omega_n = 2\pi \text{ rad/s}$$

- **Exact solution:** $x^*(t) = \cos(\omega_n t)$
- **Only 5 IC measurements** are given to the NN as data
- **2,000 collocation points** enforce the ODE residual
- The network takes t as input and outputs $\hat{x}(t)$
- Analogy: vibrating structure, landing gear dynamics, aeroelastic mode

```
omega_n = 2 * np.pi                        # natural frequency [rad/s]
t_ic    = torch.tensor([[0.0]])
x_ic    = torch.tensor([[1.0]])            # x(0) = 1
xdot_ic = torch.tensor([[0.0]])            # xdot(0) = 0
t_col   = torch.linspace(0, 2, 2000).unsqueeze(1).requires_grad_(True)
```

PINN: Model Definition

```
class PINN(nn.Module):
    def __init__(self):
        super().__init__()
        self.net = nn.Sequential(
            nn.Linear(1, 64), nn.Tanh(),
            nn.Linear(64, 64), nn.Tanh(),
            nn.Linear(64, 64), nn.Tanh(),
            nn.Linear(64, 1),
        )
    def forward(self, t): return self.net(t)

def ode_residual(model, t):
    """Compute x_tt + omega_n^2 * x at collocation points."""
    t = t.requires_grad_(True)
    x     = model(t)
    x_t   = torch.autograd.grad(x.sum(), t,
                                create_graph=True)[0]
    x_tt  = torch.autograd.grad(x_t.sum(), t,
                                create_graph=True)[0]
    return x_tt + omega_n**2 * x          # residual; should be 0
```

`autograd.grad` differentiates the *network output* w.r.t. the *input* t — not the weights. This is automatic differentiation used as a calculus tool.

PINN: Training Loop

```
model     = PINN()
optimizer = torch.optim.Adam(model.parameters(), lr=1e-3)
lam       = 1.0                          # physics weight

for epoch in range(10000):
    optimizer.zero_grad()

    # Data loss: initial conditions
    x_pred   = model(t_ic)
    xd_pred  = torch.autograd.grad(x_pred.sum(), t_ic,
                   create_graph=True)[0]
    L_data   = (x_pred - x_ic).pow(2).mean() \
             + (xd_pred - xdot_ic).pow(2).mean()

    # Physics loss: ODE residual at collocation points
    L_phys   = ode_residual(model, t_col).pow(2).mean()

    loss     = L_data + lam * L_phys
    loss.backward()
    optimizer.step()

print(f"Final loss: {loss.item():.6f}")
```

PINN: Results

```
t_test = torch.linspace(0, 2, 500).unsqueeze(1)
model.eval()
with torch.no_grad():
    x_pred = model(t_test).numpy()
x_exact = np.cos(omega_n * t_test.numpy())
rmse = np.sqrt(((x_pred - x_exact)**2).mean())
print(f"RMSE vs exact: {rmse:.5f}")
```

Output (typical):

```
Final loss: 0.000031
RMSE vs exact: 0.00412
```

- With **5 data points** and 2,000 collocation points, the PINN recovers $\cos(\omega_n t)$ to $< 0.5\%$ error over $[0, 2]$ s
- A data-only NN with 5 points would wildly overfit — the physics loss is the regularizer
- The same framework extends to PDEs (heat equation, Euler, Navier-Stokes) by adding spatial inputs to the network

PINN: Why Not Just Integrate the ODE?

For a simple ODE, classical integrators (RK4) are faster and more accurate. PINNs earn their place when:

Situation	Why PINN helps
Incomplete physics (unknown forcing)	Physics loss constraints what is known; data fills the gap
Inverse problems	Identify unknown parameters ω_n, c from sparse measurements
High-dimensional PDEs	Mesh-free collocation avoids the curse of dimensionality
Data + physics fusion	Sensor data and known dynamics combined in one loss

Aerospace examples: identifying structural damping from flight data, solving aeroelastic flutter equations with sparse strain gauge measurements, turbulence closure modeling.

Summary

Architecture Overview

Architecture	Best suited for	Aerospace example
FFNN / MLP	Tabular data, regression	$C_D(M, \alpha)$ surrogate; 10^4 CFD samples
RNN	Short sequences	Frequency estimation from telemetry
LSTM	Long sequences, forecasting	Engine RUL (NASA C-MAPSS); 80+ cycles
Transformer	Long-range dependencies	Turbulence intensity forecasting
CNN	Spatial / field data	$C_p(x/c)$ flow regime classification
Autoencoder	Anomaly detection, dim. red.	IMU anomaly detection without labels
PINN	Physics + sparse data	Spring-mass ODE; structural damping ID

All examples in this lecture run on a laptop CPU in under 2 minutes.

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