Training Neural Networks: Tips, Tricks, and Evaluation

Mohammadtaha Bagherifard

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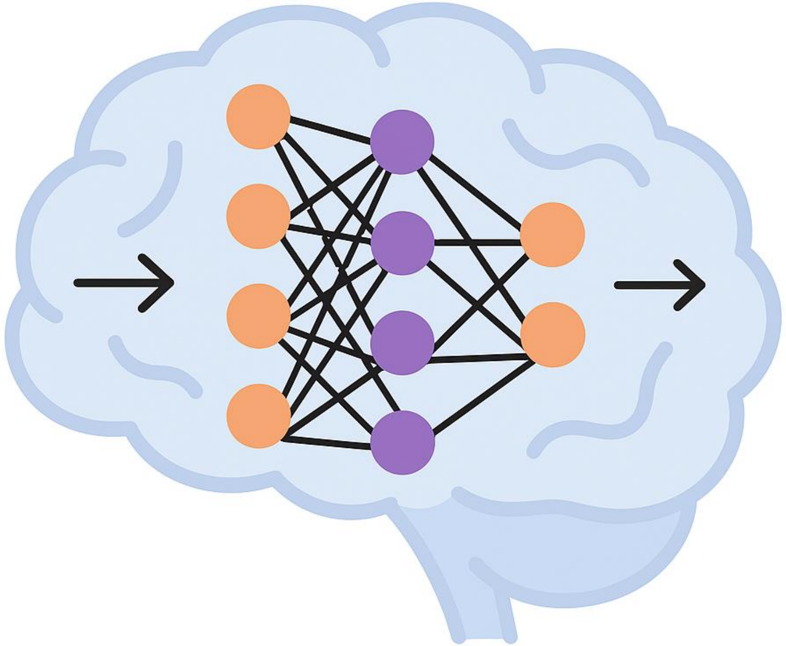
Intro

- 🎯 What you'll learn today
- 🚫 What you don't need to know
- ⏱️ Duration and format



🎯 What You'll Learn

- How to evaluate ML models beyond accuracy
- What makes training neural networks succeed or fail
- Practical tricks: learning rate, batch size, warm-up, etc.
- A peek into fine-tuning and efficient techniques.

🚫 What You Don’t Need Today

- No deep math or backpropagation formulas
- No code implementation details
- No complex derivations

⏱️ Duration and Format

- 2.5 hours of interactive lecture + 30 min Q&A
- Feel free to ask questions any time!

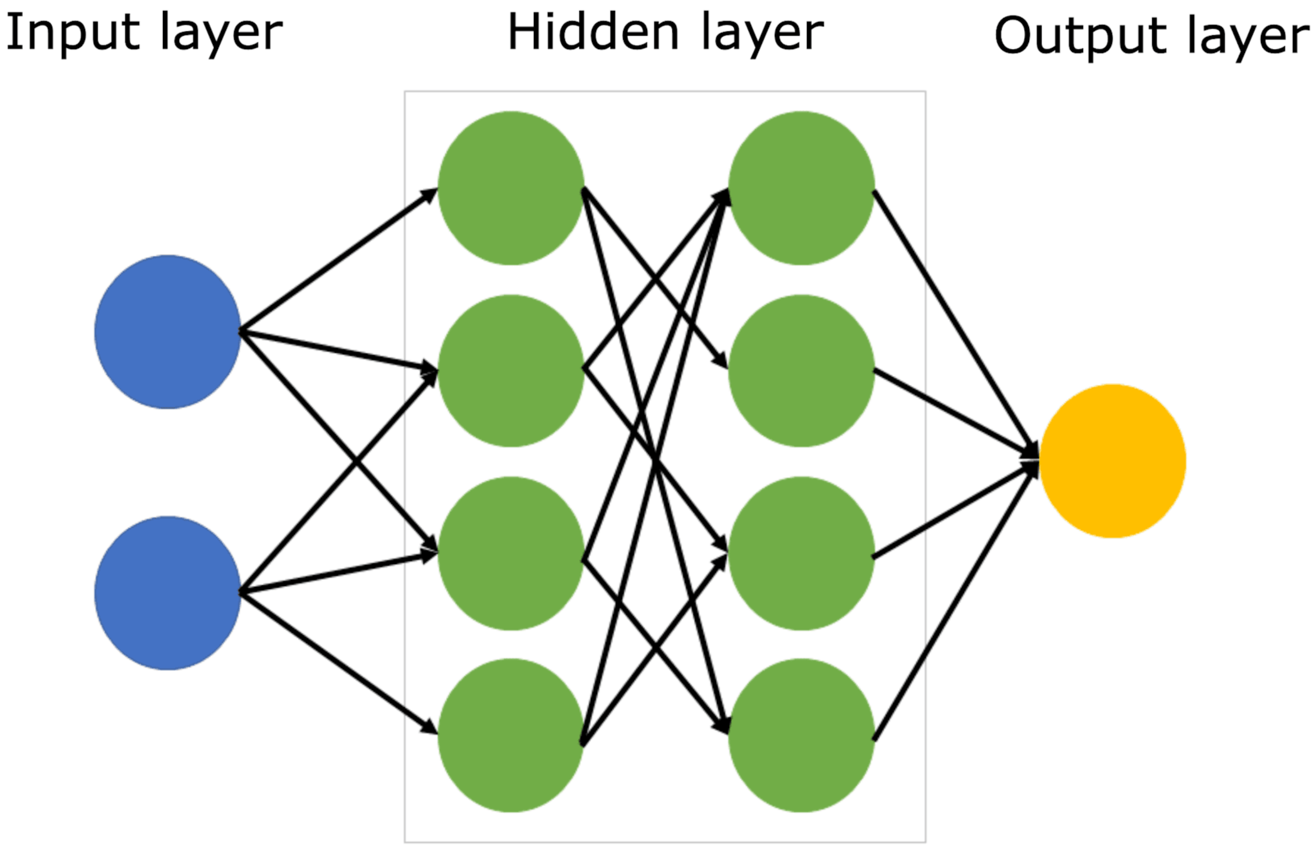
Agenda

- 🧠 **Understanding Neural Networks**
  What is an MLP? When & why we use it
- 📏 **Evaluating Model Performance**
  Accuracy, Precision, Recall, F1, Confusion Matrix
- ⚙️ **Tuning the Model**
  Layers, Neurons, Activations, Batch Norm, Residual Connection
- 🚀 **Training Tricks**
  Batch size, Learning Rate, Initialization, Gradient Clipping, Weight Decay
- 🧪 **Advanced Notes**
  Fine-tuning, Transfer learning, PEFT method (intro only)
- ❓ **Q&A + Open Discussion**
  Your questions, curiosities, and deeper dives

What is an MLP?

- A **basic type of neural network** used for classification or regression
- Made up of **layers of "neurons"** connected to each other
- Has:
  - **Input layer** (what the model sees)
  - **Hidden layers** (where learning happens)
  - **Output layer** (final prediction)
- Learns by adjusting the connections between neurons during training
- Works best with **structured/tabular data** or **simple vision/NLP tasks**
- Learns features **automatically** by stacking layers and adding non-linearity

What is an MLP?



Artificial neural networks

MLP: Classification vs Regression

- MLPs can be used for **both classification and regression**
- Only the **output layer & loss function change**
- Differences:

Task	Output Layer	Output Example
Classification	One unit per class (with Softmax / Sigmoid)	“Dog” / “Not spam”
Regression	Single unit (no activation, or ReLU if needed)	3.27, 99.5, -12.4

- MLP learns by comparing predictions to the **true label or value**

✅ Why Use MLPs? ❌ And When Not To?

✅ Pros:

- Easy to build and understand
- Great for **structured/tabular data**
- Can solve basic **NLP / vision** tasks with enough data
- Could be used in more complex architectures like Transformers

🚫 Limitations:

- Doesn’t scale well to high-dimensional input (e.g., images)
- Doesn’t model **sequences or spatial structure**
- Doesn’t assume **inductive bias**
- Has a fixed size input
- Sensitive to hyperparameters (LR, init, etc.)
- Fully connected → many parameters → **overfitting risk**
- **Not interpretable** out of the box

How Do We Evaluate ML Models?

- Evaluation depends on the **type of task**:
  - **Classification** → Accuracy, Precision, Recall, F1
  - **Regression** → MSE, MAE, R^2 (not covered here)
- Accuracy isn’t always enough — we need to understand **how the model is wrong**
- Especially important in **imbalanced datasets** (e.g., 95% healthy, 5% sick)
- We’ll focus on **classification metrics** — used in most ML competitions and practical systems

Understanding the Confusion Matrix

	Predicted: Positive	Predicted: Negative	
Actual: Positive	✓ TP (True Positive)	✗ FN (False Negative)	**Recall**
Actual: Negative	✗ FP (False Positive)	✓ TN (True Negative)	**FPR**
	Precision		

Understanding the Confusion Matrix

- **Accuracy** = (TP + TN) / (TP + TN + FP + FN)
- **Precision** = TP / (TP + FP)
  - "Of what we predicted positive, how many were actually correct?"
- **Recall** = TP / (TP + FN)
  - "Of all actual positives, how many did we catch?"
- **F1 Score** = 2 × (Precision × Recall) / (Precision + Recall)
  - "Balance between Precision & Recall"

Understanding the Confusion Matrix

Examples

- Accuracy:

  ✔ **Balanced datasets**, where both classes are equally important
  💡 **Example**: Image classification of animals (cat vs dog)

- Precision:

  ⚠ **When false positives are costly**
  💡 **Example**: Spam detection → we don’t want to mark important emails as spam
  💡 **Example**: Cancer screening for expensive treatment → avoid false alarms

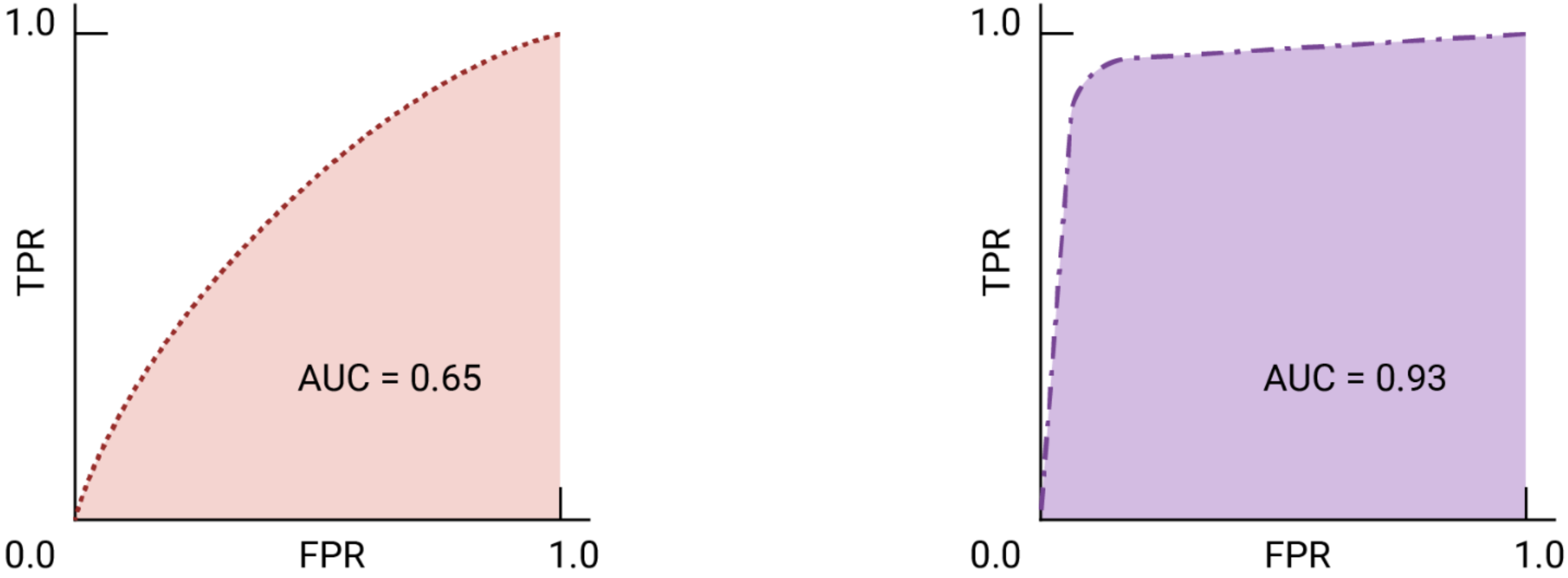
- Recall:

  🛑 **When false negatives are dangerous**
  💡 **Example**: Medical diagnosis → missing a cancer case is worse than over-alerting
  💡 **Example**: Search engines → show as many relevant results as possible

ROC Metric

- **ROC** (Receiver-operating characteristic) Curve:
  - a visual representation of model performance across all thresholds
  - X-axis: False Positive Rate (FPR)
  - Y-axis: True Positive Rate (Recall)
- **AUC** = Area under ROC curve
  - Measures how well model ranks positives over negatives
- AUC ≈ 1 → perfect classifier
- AUC ≈ 0.5 → random guessing
- ✅ Useful for comparing classifiers with **balanced datasets**.
  - FPR can look artificially low when negatives dominate

ROC Metric



ROC and AUC of two hypothetical models. The curve on the right, with a greater AUC, represents the better of the two models.

Imbalanced Datasets

- In **imbalanced datasets**, one class dominates
  - (e.g., 99% healthy, 1% sick)

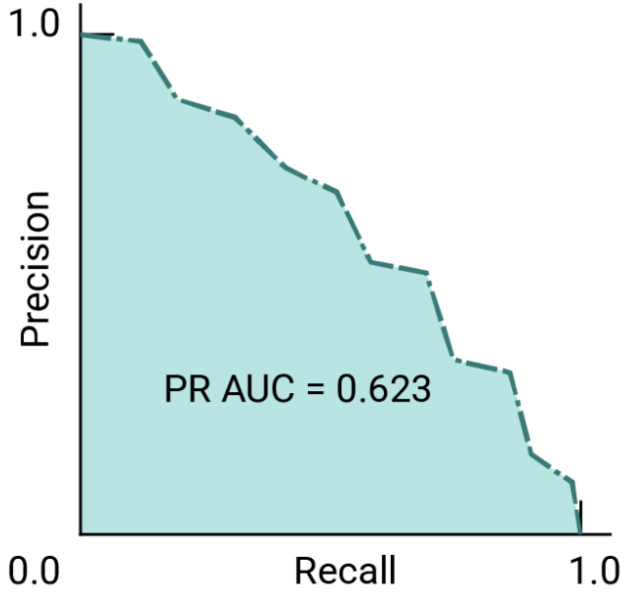
- ❌ **Accuracy is misleading**
  - A model predicting “always healthy” gets 99% accuracy → but it's useless

- We care more about **how well the model separates the classes**

- **Precision-Recall curve** is the correct metric to compare the models.

Precision-Recall Curve

- **Precision-Recall Curve** focuses only on the **positive class**:
  - Precision (how many predicted positives were correct)
  - Recall (how many actual positives we caught)

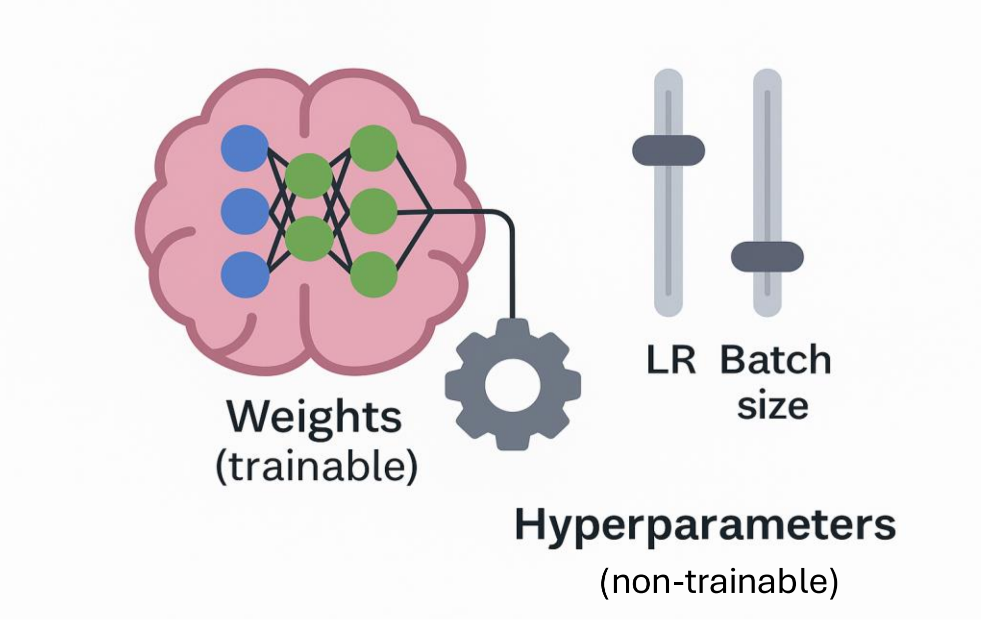


How to Plot ROC and PR Curves

- 💯 The model outputs **probabilities** (e.g., 0.91 cat, 0.23 cat, etc.)
- ➡️ Sweep the **classification threshold** from 0 → 1 (e.g., classify as positive if prob > 0.9, then 0.8, 0.7, etc.)
- 🧮 For each threshold, calculate:
  - **Confusion matrix** → then compute:
    - TPR (Recall) = TP / (TP + FN)
    - FPR = FP / (FP + TN)
    - Precision = TP / (TP + FP)
- ✅ Plot the curves:
  - **ROC**: TPR vs FPR
  - **PR**: Precision vs Recall

Training Neural Networks:
Parameters vs. Hyperparameters

1. **Trainable Parameters**
   - These are the **weights and biases** of the network
   - They are **learned automatically** via:
     - Backpropagation
     - Gradient descent (or its variants)
2. **Hyperparameters**
   - These are **manually set by the practitioner**
   - They define **how the model is built** and **how it trains**
   - They are **not learned** during training
   - ✅ **Examples:**
     - **Model architecture**: Number of layers, Neurons per layer, Activation functions (ReLU, sigmoid, etc.)
     - **Training hyperparameters**: Learning rate, Batch size, Number of epochs, Optimizer (SGD, Adam, etc.)
     - **Regularization**: Dropout rate, L2 penalty (weight decay), Early stopping



Model Architecture:

Layers and Neurons

- **Number of Layers (Depth)**
  - More layers = can learn more complex patterns
  - But also **harder to train**, more risk of overfitting

    🔧 Shallow → faster, simpler

    🧠 Deep → more expressive, but needs care
- **Neurons per Layer (Width)**
  - More neurons = more capacity
  - But also increases parameters → overfitting risk ⚠️
  - Should be **balanced** with dataset size

Model Architecture:

The Universal Approximation Theorem (UAT)

- A neural network with **just one hidden layer** (and enough neurons) can **approximate any continuous function**, given enough data.
- 🤔 Then why don’t we use one huge hidden layer?

  ❌ **Inefficient:** Shallow networks may need **millions of neurons** to model complex functions → slow, overfit easily.

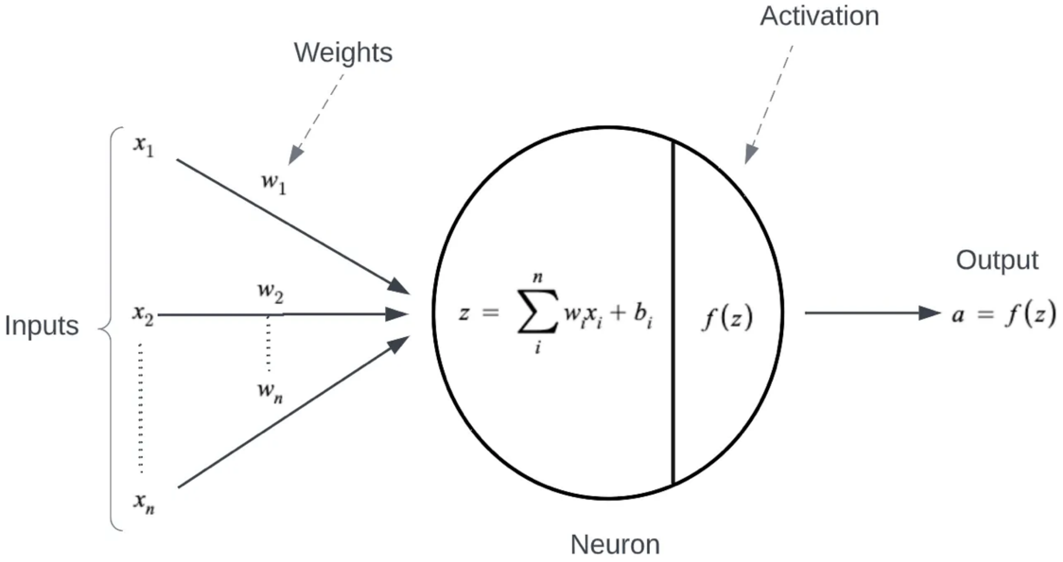
  ❌ **Poor Generalization:** Wide nets often **memorize**. Deep nets **learn patterns** (e.g., edge → shape → object).

  ❌ **Harder to Optimize:** Flat loss landscapes make training unstable. Deep nets benefit from modern tricks (e.g., batch norm, skip connections).

  ❌ **Depth = Expressiveness:** Some functions require **exponential width** in shallow nets but only **modest depth**.

Model Architecture:
Activation Function

- Without activations, neural nets are just **linear equations**
  - Stacked linear layers = still linear 😴
  - Can’t model complex relationships
- Activations introduce **non-linearity** so the network can learn curved decision boundaries



Model Architecture:

Activation Function

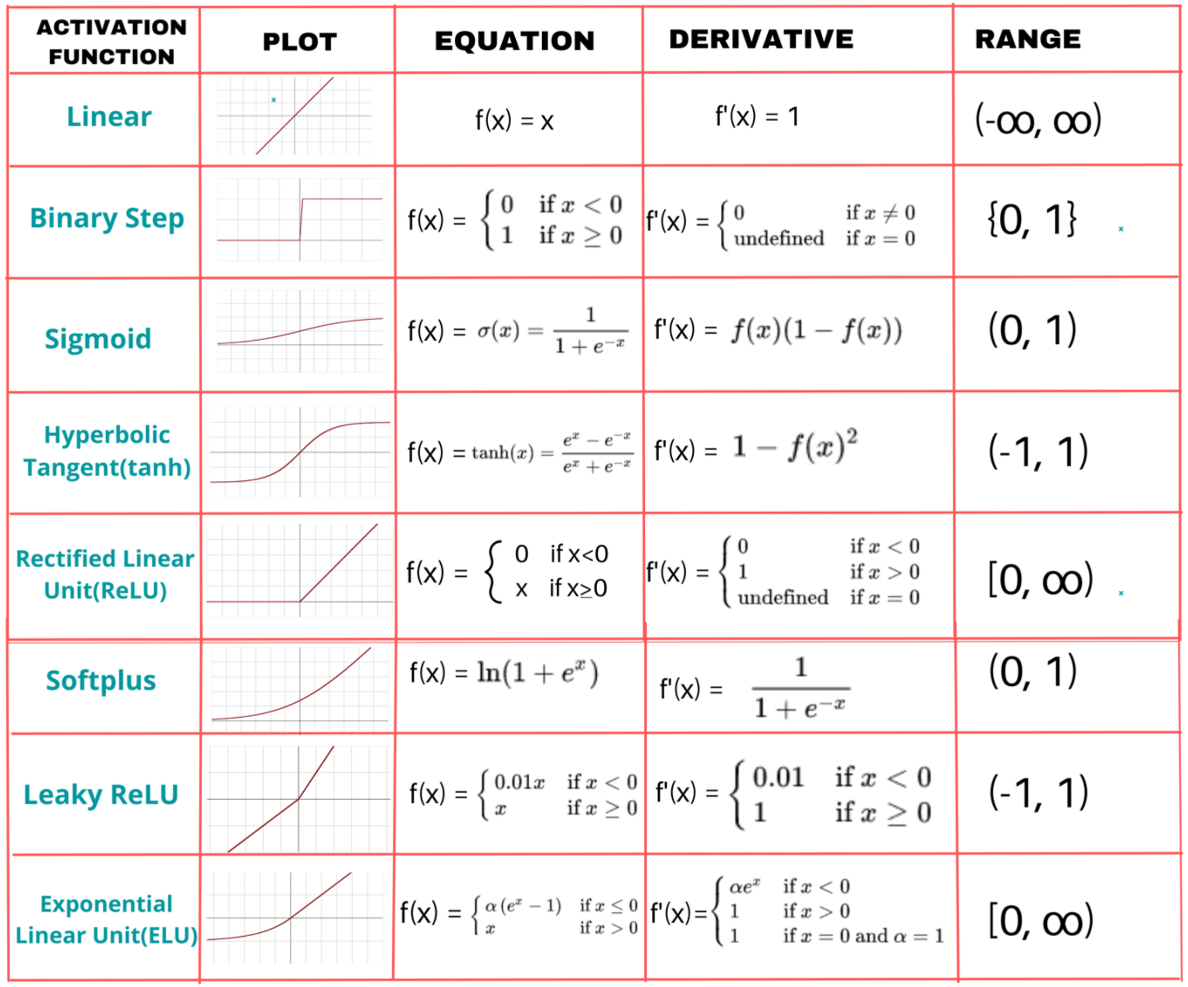
The **choice of activation** affects training behavior

🧠 **Training Effects:**

- **Sigmoid / tanh** can cause **vanishing gradients**
  - Gradients get too small → slow or stuck training
    Especially bad in deep networks
- **ReLU** avoids vanishing gradients
  - Doesn’t squeeze the output
  - Gradient is constant (1) when active
    Also sparse — many neurons output 0 → faster learning
- Some variants (e.g., Leaky ReLU, GELU) help avoid **dead neurons**

Model Architecture:

Activation Function



ACTIVATION FUNCTION	PLOT	EQUATION	DERIVATIVE	RANGE
Linear		f(x) = x	f'(x) = 1	$(-\infty, \infty)$
Binary Step		f(x) = $\begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}$	f'(x) = $\begin{cases} 0 & \text{if } x \neq 0 \\ \text{undefined} & \text{if } x = 0 \end{cases}$	{0, 1}
Sigmoid		f(x) = $\sigma(x) = \frac{1}{1+e^{-x}}$	f'(x) = $f(x)(1-f(x))$	(0, 1)
Hyperbolic Tangent(tanh)		f(x) = $\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$	f'(x) = $1 - f(x)^2$	(-1, 1)
Rectified Linear Unit(ReLU)		f(x) = $\begin{cases} 0 & \text{if } x<0 \\ x & \text{if } x\geq 0 \end{cases}$	f'(x) = $\begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x > 0 \\ \text{undefined} & \text{if } x = 0 \end{cases}$	$[0, \infty)$
Softplus		f(x) = $\ln(1+e^x)$	f'(x) = $\frac{1}{1+e^{-x}}$	(0, 1)
Leaky ReLU		f(x) = $\begin{cases} 0.01x & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases}$	f'(x) = $\begin{cases} 0.01 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}$	(-1, 1)
Exponential Linear Unit(ELU)		f(x) = $\begin{cases} \alpha(e^x - 1) & \text{if } x \leq 0 \\ x & \text{if } x > 0 \end{cases}$	f'(x)= $\begin{cases} \alpha e^x & \text{if } x < 0 \\ 1 & \text{if } x > 0 \\ 1 & \text{if } x = 0 \text{ and } \alpha = 1 \end{cases}$	$[0, \infty)$

Model Architecture:
Residual Connection

☹️ As networks get deeper, training becomes **harder**

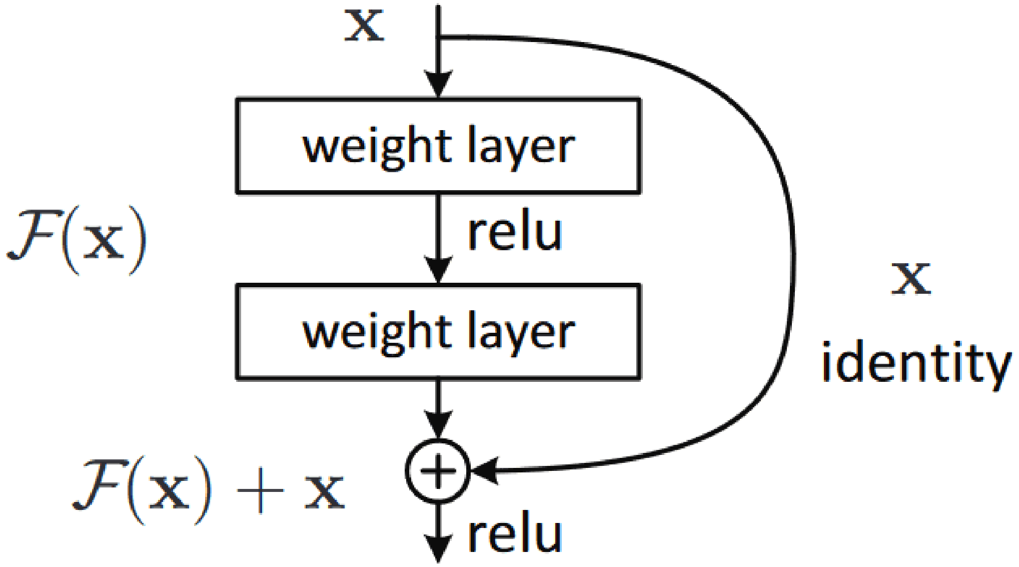
  - Vanishing gradients → layers stop learning

- **Residual Connections** (from ResNet) solve this:
  - Instead of learning F(x), the model learns a **residual**: F(x) + x
- These "skip connections" let the gradient **flow directly** to earlier layers
  - Makes it possible to train networks with **dozens or hundreds of layers**

Model Architecture:
Residual Connection

💡 Benefits

- ✅ Solves **vanishing gradient** problem
- ✅ Enables **very deep architectures**
- ✅ Helps with **faster convergence** and **better generalization**

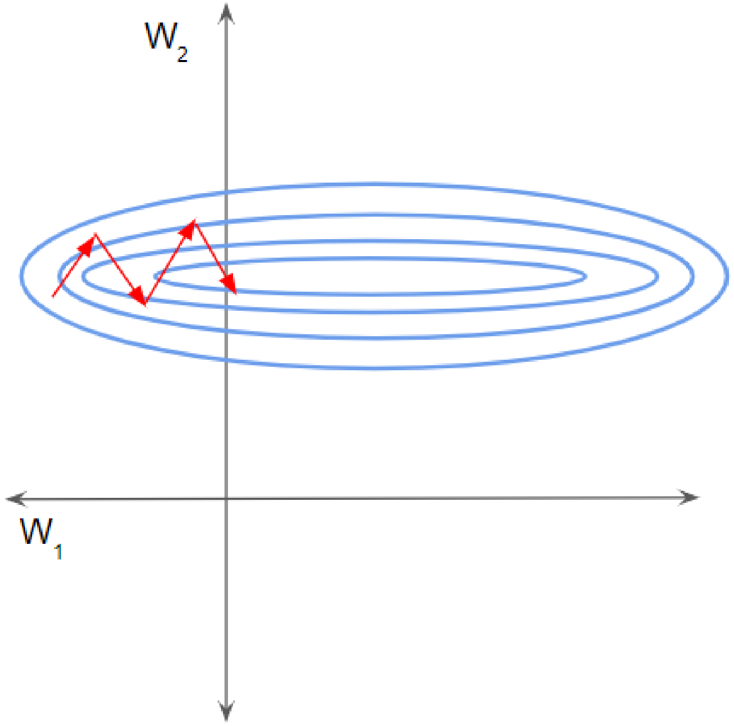


Model Architecture:
Batch Normalization

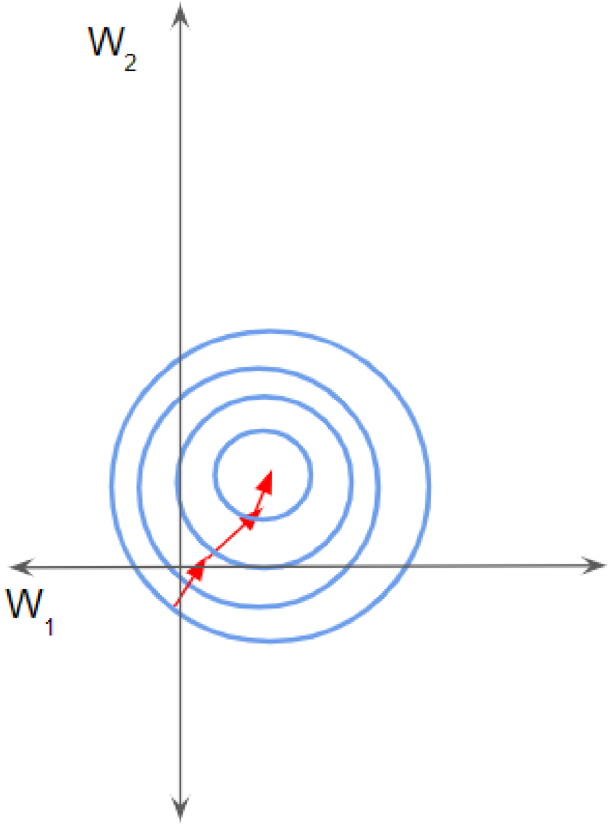
- During training, **distributions of layer inputs keep shifting ↗↙**
  - Makes training unstable and slow
  - Known as **internal covariate shift**
- **Batch Normalization (BN)** solves this by:
  - Normalizing activations in each layer
  - Rescaling & shifting them (learnable)
- 🧠 **Benefits of Batch Normalization:**
  - 🚀 **Faster convergence**
  - 🎯 **Smoother gradients**, more stable training
  - 🔧 **Less sensitive** to weight initialization & learning rate
  - 🛡️ Acts like **regularization** → may reduce need for dropout

Model Architecture:

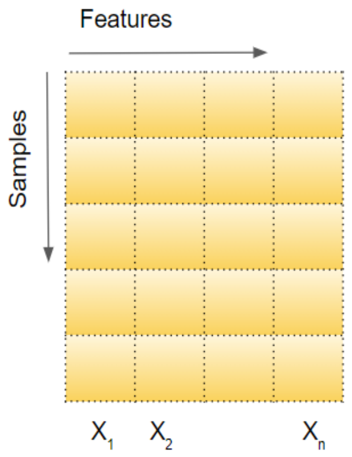
Batch Normalization



Loss landscape before normalisation

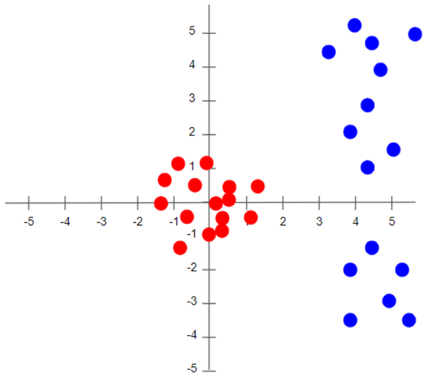


Loss landscape after normalisation



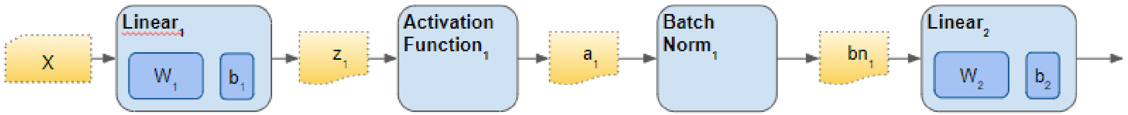
$$X_i = \frac{X_i - Mean_i}{StdDev_i}$$

Normalisation of features

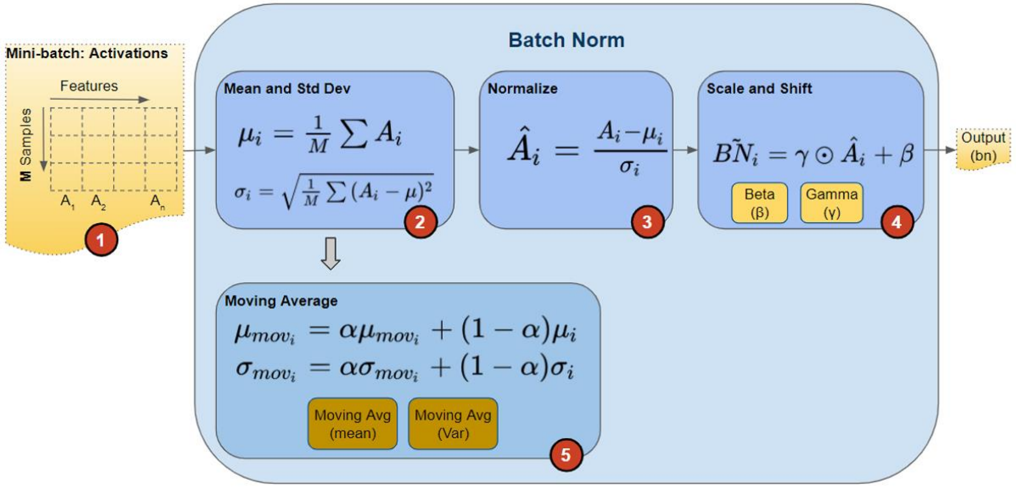


Effect of normalisation

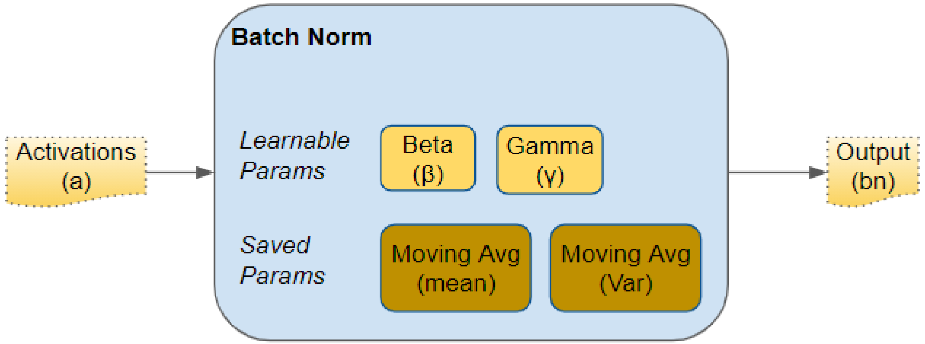
Model Architecture:
Batch Normalization



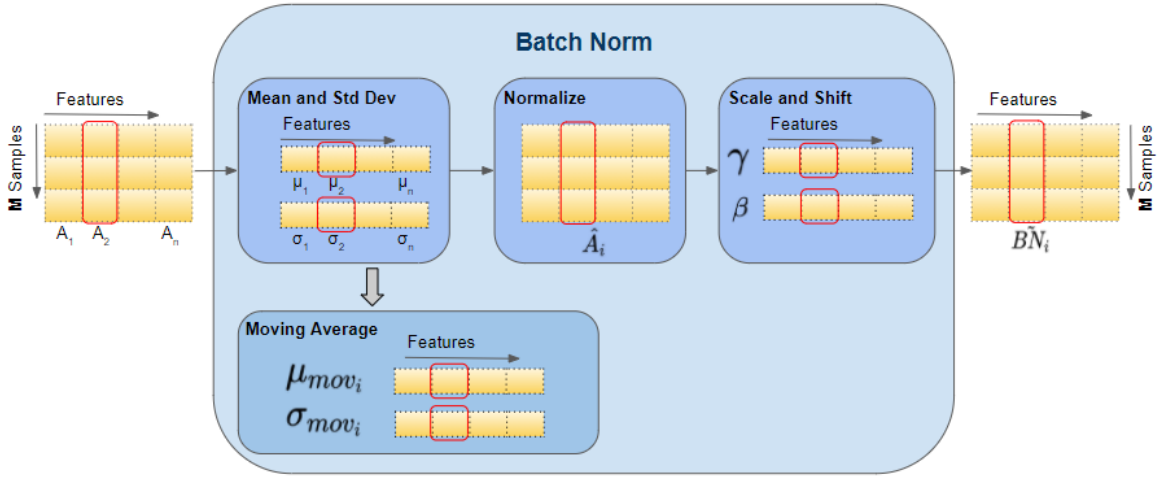
Batch norm layer’s place in the network


Mini-batch: Activations
Features
M Samples
A$_1$ A$_2$ A$_n$
1
Batch Norm
Mean and Std Dev
$\mu_i = \frac{1}{M}\sum A_i$
$\sigma_i = \sqrt{\frac{1}{M}\sum(A_i - \mu)^2}$
2
Normalize
$\hat{A}_i = \frac{A_i - \mu_i}{\sigma_i}$
3
Scale and Shift
$\tilde{BN}_i = \gamma \odot \hat{A}_i + \beta$
Beta (β)
Gamma (γ)
4
Output (bn)
Moving Average
$\mu_{mov_i} = \alpha\mu_{mov_i} + (1-\alpha)\mu_i$
$\sigma_{mov_i} = \alpha\sigma_{mov_i} + (1-\alpha)\sigma_i$
Moving Avg (mean)
Moving Avg (Var)
5

Batch norm during training



Batch norm layer’s parameters



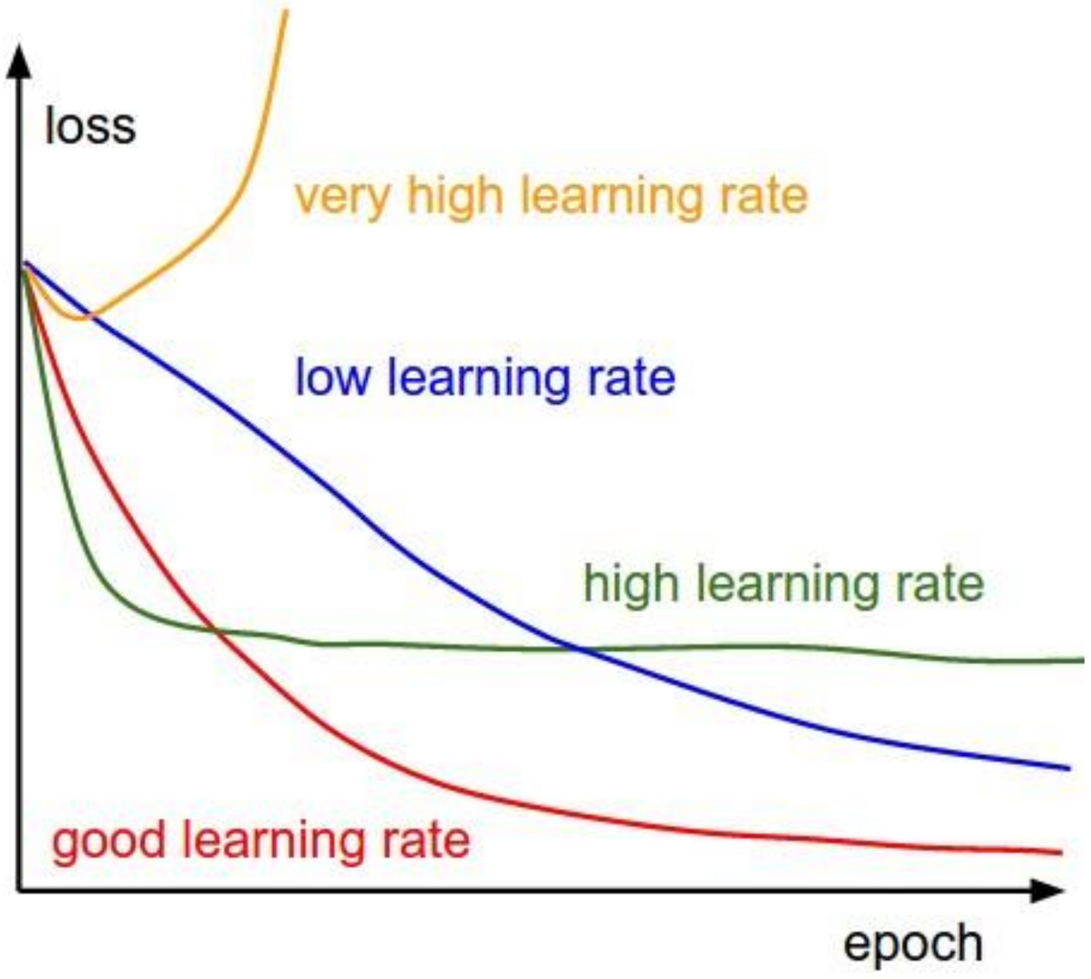
Batch norm during testing

Training Tricks: Learning Rate

- Learning rate (LR) controls the **size of each update** to the model's weights:
  - **Small LR:**
    - ❌ Slow learning, Getting stuck on local minima
    - ✅ Good for **fine-tuning / exploitation** (refining known good areas)
  - **Large LR:**
    - ❌ May overshoot or diverge, Loss / gradient explosion,
    - ✅ Good for **exploration** (searching broadly across the loss landscape)

- ⚠️ **General Notes**
  - 🔄 You can **change LR during training** using **schedulers** (e.g., cosine decay, step decay, warm-up)
  - 🧠 Some optimizers (like **Adam**) adjust effective LR **per parameter**

Training Tricks: Learning Rate



Effect of different learning rates during training

Training Tricks: Learning Rate Scheduling

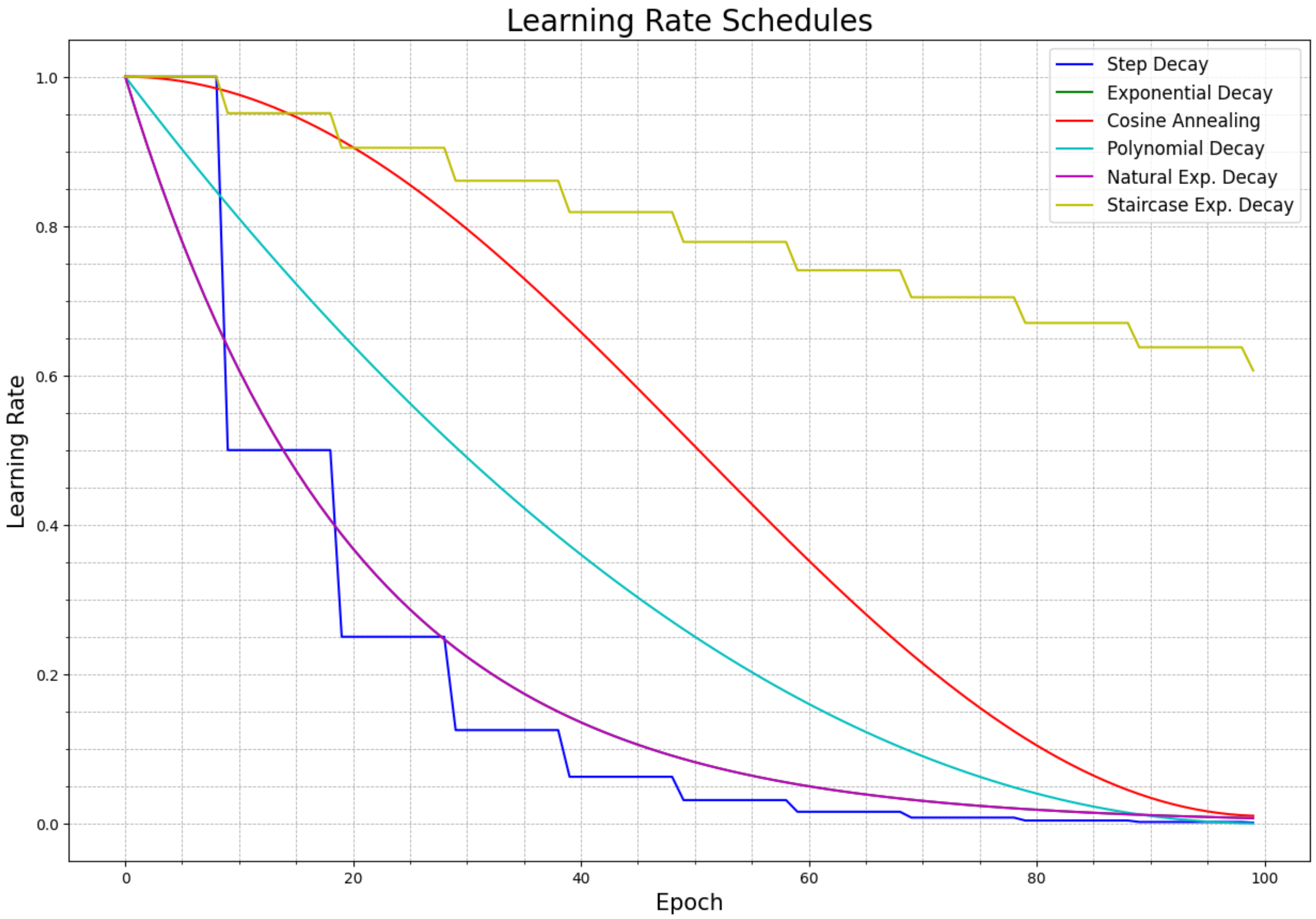
Scheduling governs the pace as you train:

- ❗Using a **constant learning rate** may not be ideal for the full training process
- 🛠️ **Schedulers** adjust the LR dynamically to improve convergence

Strategy	Idea 💡	When to Use
Step Decay	Reduce LR every N epochs	Classic; useful for staged training
Exponential / Linear Decay	LR shrinks gradually over time	Smooth convergence
Cosine Annealing	LR follows cosine curve to 0	Used in modern LLM training / fine-tuning
Warm-up	Start with small LR, then increase	Helps stabilize early training
Decay on Plateau	Reduce the LR when improvement stops	When validation loss flattens / model stalls

Common LR scheduler

Training Tricks: Learning Rate Scheduling



A visual guid to Learning Rate Schedulers in PyTorch

Training Tricks: Batch Size

- **Batch size** = number of training examples used to compute one update step
- Affects: **speed**, **stability**, **generalization**, and **memory usage**
- ⚖️ Trade-offs:

Small Batch	Large Batch
✅ Better generalization	❗ Prone to overfit
🧠 Noisy gradients → 🔍 more exploration	📉 Smoother gradients → 🎯 more exploitation
🐌 Slower per epoch	🚀 Faster training (more parallelism)
💾 Fits on less memory	❌ Needs more memory
⬅️ ➡️ Often results to flat minima (robust)	↘↗ Often results to sharp minima (sensitive)

Training Tricks: Gradient Accumulation

- Sometimes your GPU can’t handle large batch sizes due to memory limits (e.g., on big models like Transformers)
- **Gradient Accumulation** solves this by:
  - Splitting a large batch into **smaller mini-batches**
  - Computing gradients for each mini-batch
  - **Accumulating** (summing) the gradients
  - Updating weights only after **N steps**

📦 **Example:**

- You want a **batch size of 128**, but can only fit 32 in memory
  - Accumulate gradients for **4 forward-backward passes**
  - Then do **1 optimizer step**

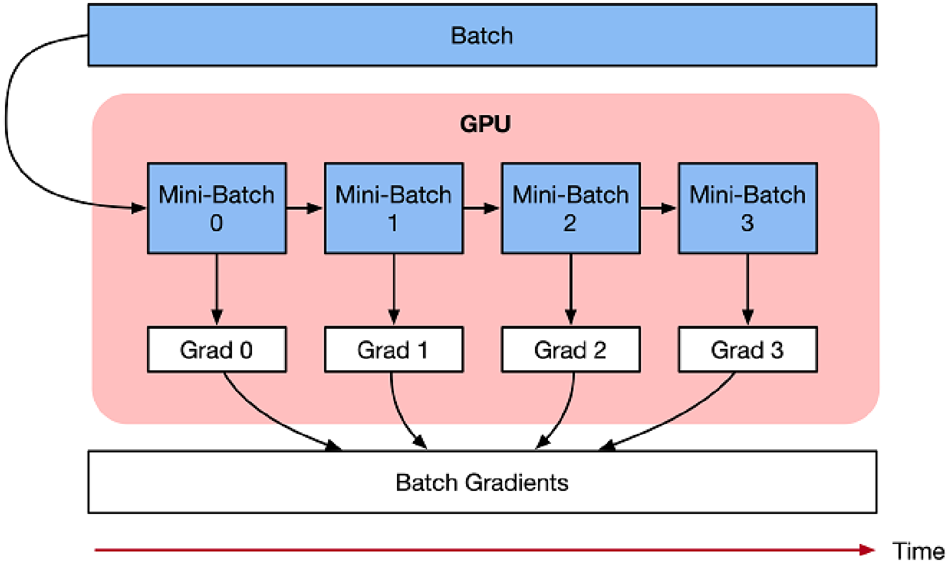
Training Tricks: Gradient Accumulation

😎 **Benefits:**

- ✅ Simulates **large batch effects**
- ✅ Works on **limited hardware**
- ✅ Helps with **more stable training**

⚖️ **Trade-offs:**

- 🐌 Slower per step (more forward/backward passes)
- ⚙️ Must handle optimizer steps carefully



Training Tricks: Gradient Explosion

- Sometimes gradients become **extremely large** during backpropagation
  - Especially in **very deep** or **recurrent** networks
  - 💣 We call this phenomenon: **“Gradient Explosion”**
- This causes:
  - 🚨 Unstable updates
  - ❌ Weights go to infinity / NaNs
  - 📉📈 Loss diverges instantly

Training Tricks: Gradient Explosion

- 🧠 **Why does it happen?**
  - Gradients **compound multiplicatively** across layers
  - If each layer amplifies even a little, it **explodes exponentially**
  - Mainly happens due to bad weight initialization
- 💥 **Symptoms:**
  - Training loss becomes **NaN** or **explodes**
  - Model **never converges**
- Two ways to address this:
  - 🎬 **Weight Initialization** → before training
  - ✂ **Gradient Clipping** → during training
  - 📉 **Weight Decay (L2-Regularization)** → during training

Training Tricks: Weight Initialization

- Neural networks start training with **random weights**
- But not all random is equal — poor initialization can cause:
  - 🔥 **Exploding gradients** (weights get huge)
  - ❄️ **Vanishing gradients** (weights go to zero)
  - 🐢 Slow or unstable learning

- 🤨 **Why does it matter?**
  - Gradients flow **backward** through the network
  - If weights are too large/small:
    - Repeated multiplications cause **gradient instability**
    - Especially in deep networks

Training Tricks: Weight Initialization

- Popular Initialization Methods:

Method	Use Case
Xavier/Glorot Initialization	For Tanh or Sigmoid activations
He Initialization	For ReLU / LeakyReLU activations
Orthogonal Initialization	Sometimes used in RNNs and CNNs

- They all aim to keep the **variance of activations and gradients stable** across layers

Training Tricks: Xavier Initialization

- ⚙️ **Designed for:** Sigmoid, Tanh
- 🎯 **Goals:**
  - Preserving activation variance during the forward pass
  - Preserving gradient variance during the backward pass
- 🔢 **Formula:**

$$W_{ij} \sim U\left[-\frac{\sqrt{6}}{\sqrt{fan_{in} + fan_{out}}}, \frac{\sqrt{6}}{\sqrt{fan_{in} + fan_{out}}}\right]$$

- 🧠 **Use when:** activations saturate easily (Tanh, Sigmoid)

Training Tricks: He Initialization

- ⚙️ **Designed for**: ReLU, Leaky ReLU
- 🎯 **Goals**:
  - Maintain **activation variance** (ReLU deactivates roughly 50% of neurons)
  - Prevent **vanishing gradients** in deep ReLU nets
- 🔢 **Formula** (for normal distribution):

$$W \sim \mathcal{N}(0, \frac{2}{N})$$

- 🧠 **Use when**: you're using **ReLU-based activations**

Training Tricks: Orthogonal Initialization

- ⚙️ **Designed for**: Stability in deep or recurrent networks
- 🎯 **Goals**:
  - Maintain **direction of gradient** (preserve norm)
  - Avoid **exploding/vanishing** gradients
- 💡 **Key idea**:
  - Initialize weights as an **orthogonal matrix**
  - This means the derivative chain is better conditioned
  - Gradients neither explode nor vanish rapidly.

- 🧠 **Use when**: working with **RNNs**, **Transformers**, or **very deep CNNs**

Training Tricks: Gradient Clipping

- What is Gradient Clipping?
  - ✂ It’s a technique to **cap the magnitude** of gradients during training
  - ⍰▯ Prevents **instability** and **divergent updates**

- ⚙ How it works:

  Let: $$g = \|\nabla \mathcal{L}(\theta)\|_2$$

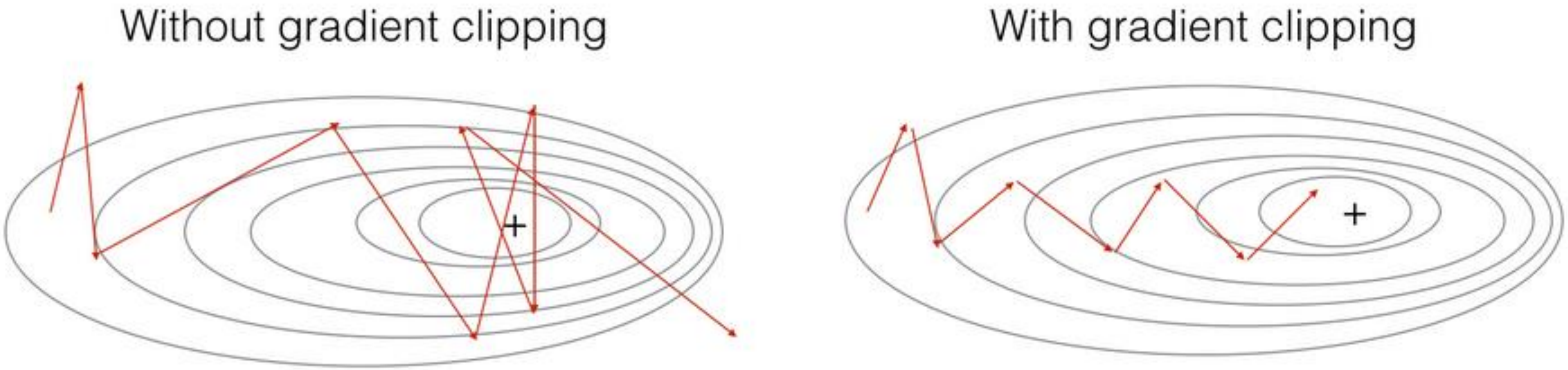
  If $g > \tau$ (a threshold), scale the gradient

  $$\nabla \mathcal{L} \leftarrow \nabla \mathcal{L} \cdot \frac{\tau}{g}$$

Training Tricks: Gradient Clipping

😎 Benefits:

- Keeps updates within a **controlled range**
- Allows training to proceed even when gradients spike
- Prevents NaNs and exploding loss
- Helps stabilize **RNNs** and **transformer-style** models
- Makes training more **robust**, especially with large learning rates



Without gradient clipping

With gradient clipping

Training Tricks: Weight Decay

💥 During training, weights can grow **too large**, especially with:

- High learning rates
- Exploding gradients
- Overfitting on small datasets

❌ Large weights = unstable training & poor generalization

🛡️ **What is Weight Decay?**

- A regularization technique that **penalizes large weights**
- Encourages the model to **keep weights small**
- Adds an L2 penalty to the loss (SGD gradient):

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{task}} + \lambda \cdot ||W||_2^2$$

Training Tricks: Weight Decay

😎 Benefits:

- ✅ Helps **prevent overfitting**
- ✅ Encourages **simpler models**
- ✅ Keeps gradients and weights more stable → fights gradient explosion

🆚 Adam vs. AdamW:

- **Adam**: Adds L2 penalty to the gradients (❌ not ideal)
- **AdamW**: Applies decay directly to weights (✅ better)

Advanced Note: Fine-tuning

🧩 **We don’t always train models from scratch.**

- Most modern ML systems start with a **pretrained model**
- Then we **fine-tune** it for a **specific task, domain, or dataset**

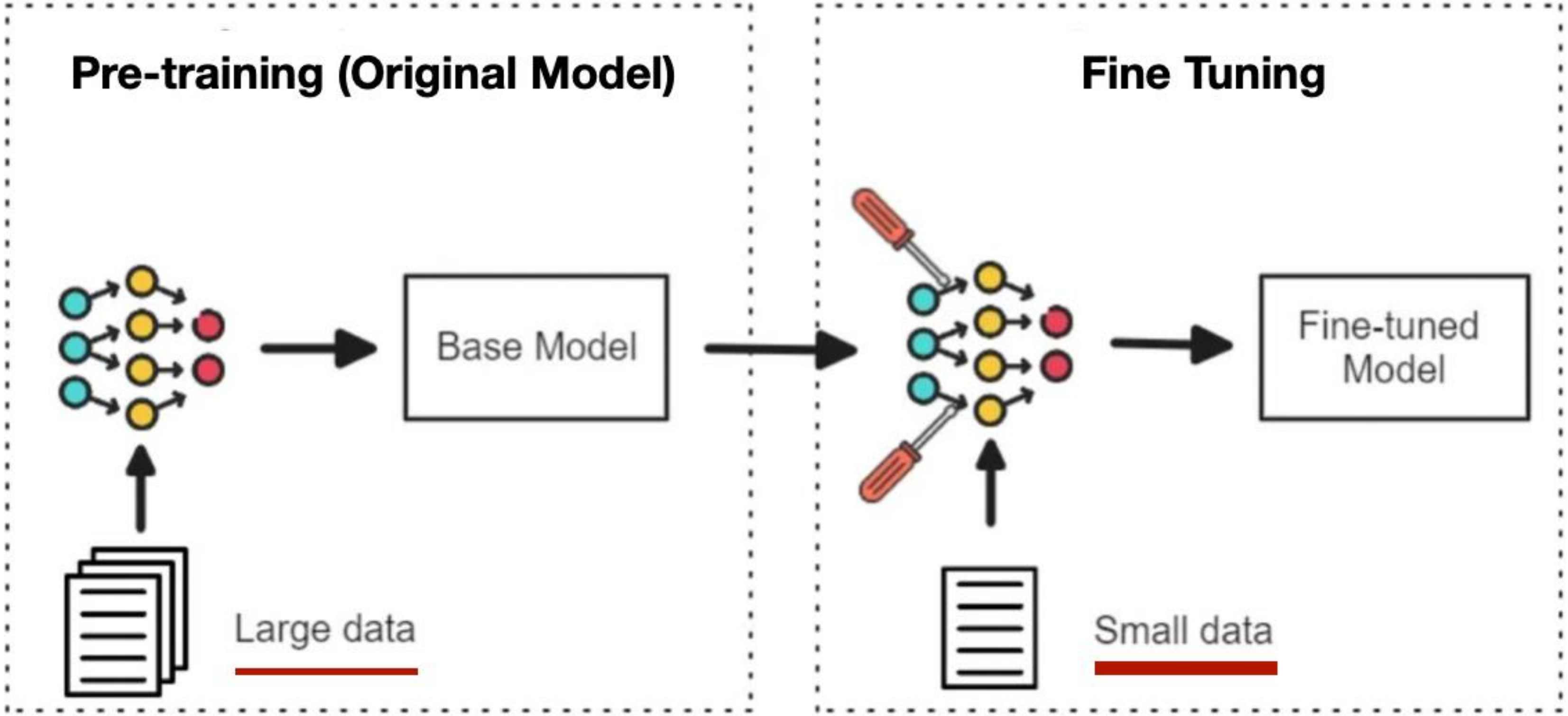
🤔 **What does fine-tuning mean?**

- Take a model that has already learned **general knowledge**, and continue training it to **specialize** in a new task.

🎯 **Why?**

- ✅ Saves compute & time
- ✅ Works well with small task-specific datasets
- ✅ Leverages **transfer learning**: reuse what's already learned

Advanced Note: Fine-tuning



Thanks for your Attention