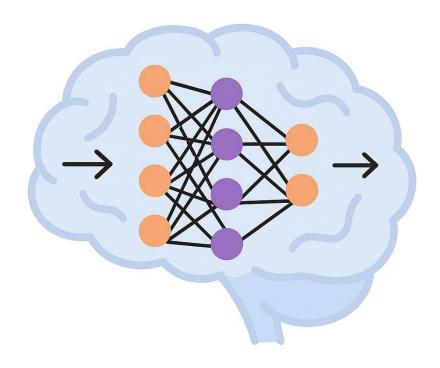
# Training Neural Networks: Tips, Tricks, and Evaluation

Mohammadtaha Bagherifard
July 2025

### 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

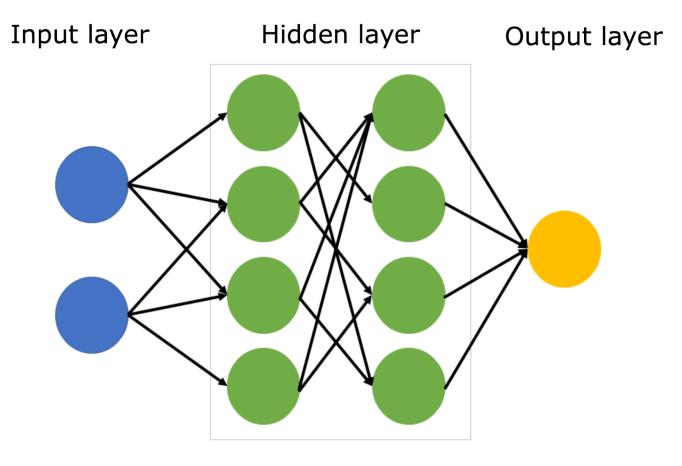
- **Output** Understanding Neural Networks What is an MLP? When & why we use it
- **Evaluating Model Performance**Accuracy, Precision, Recall, F1, Confusion Matrix
- Tuning the Model Layers, Neurons, Activations, Batch Norm, Residual Connection
- Training Tricks
  Batch size, Learning Rate, Initialization, 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





- 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

#### 

- 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<sup>2</sup> (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)	X FN (False Negative)	Recall
Actual: Negative	X 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"

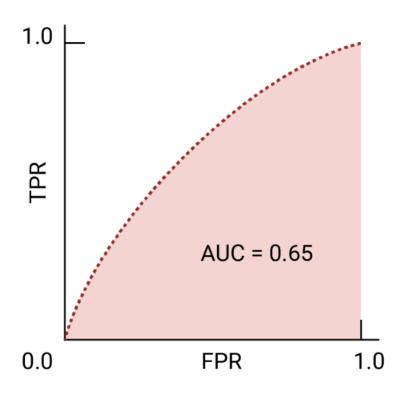
## Understanding the Confusion Matrix Examples

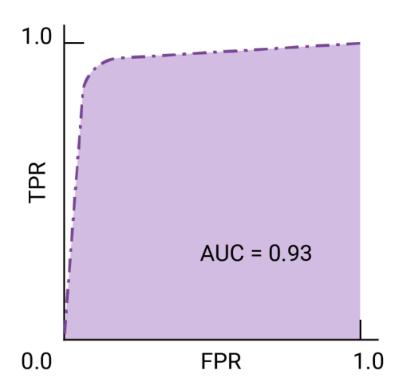
- Accuracy:
  - **Balanced datasets**, where both classes are equally important
  - **PExample**: Image classification of animals (cat vs dog)
- Precision:
  - When false positives are costly
  - **Example**: Spam detection  $\rightarrow$  we don't want to mark important emails as spam
  - **Example**: Cancer screening for expensive treatment  $\rightarrow$  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  $\approx 0.5 \rightarrow$  random guessing
- Volume of the second state of the second s
  - 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.

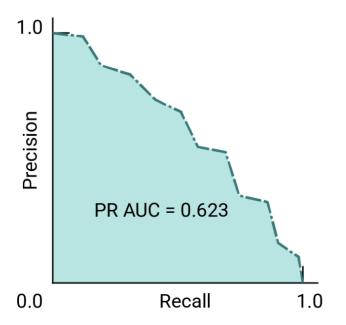
#### **Imbalanced Datasets**

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

- Probabilities (e.g., 0.91 cat, 0.23 cat, etc.)
- Sweep the classification threshold from  $0 \rightarrow 1$  (e.g., classify as positive if prob > 0.9, then 0.8, 0.7, etc.)
- IIII 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

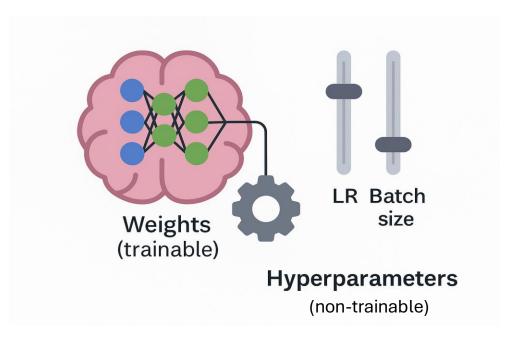
## Training Neural Networks: Parameters vs. Hyperparameters

#### 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

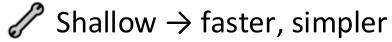
- These are manually set by the practitioner
- They define how the model is built and how it trains
- They are not learned during training
- Z Examples:
  - Model architecture: Number of layers, Neurons per layer, Activation functions (ReLU, sigmoid, etc.)
  - Training hyperparameters: Learning rate, 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



Open → 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

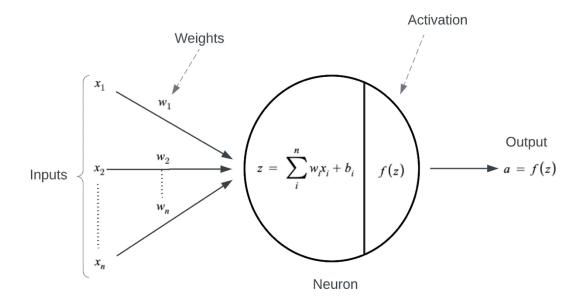
#### **Model Architecture:**

#### The Universal Approximation Theorem (UAT)

- A neural network with just one hidden layer (and enough neurons) can approximate any continuous function, given enough data.
- E Then why don't we use one huge hidden layer?
  - $\times$  Inefficient: Shallow networks may need millions of neurons to model complex functions  $\rightarrow$  slow, overfit easily.
  - $\nearrow$  Poor Generalization: Wide nets often memorize. Deep nets learn patterns (e.g., edge  $\rightarrow$  shape  $\rightarrow$  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



- 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		$f(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x \ge 0 \end{cases}$	$f'(x) = \left\{ egin{array}{ll} 0 &  ext{if } x  eq 0 \\  ext{undefined} &  ext{if } x = 0 \end{array} \right.$	{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)		$f(x) = \begin{cases} 0 & \text{if } x < 0 \\ x & \text{if } x \ge 0 \end{cases}$	$f'(x) = egin{cases} 0 &  ext{if } x < 0 \ 1 &  ext{if } x > 0 \  ext{undefined} &  ext{if } x = 0 \end{cases}$	[0, ∞) <sub>x</sub>
Softplus		$f(x) = \ln(1+e^x)$	$f'(x) = \frac{1}{1 + e^{-x}}$	(0, 1)
Leaky ReLU		$f(x) = \begin{cases} 0.01x & \text{if } x < 0 \\ x & \text{if } x \ge 0 \end{cases}$	$f'(x) = \left\{ egin{array}{ll} 0.01 &  ext{if } x < 0 \ 1 &  ext{if } x \geq 0 \end{array}  ight.$	(-1, 1)
Exponential Linear Unit(ELU)		$f(x) = \begin{cases} \alpha (e^x - 1) & \text{if } x \le 0 \\ x & \text{if } x > 0 \end{cases}$	$f^{t}(X) = \begin{cases} \alpha e^{x} & \text{if } x < 0 \\ 1 & \text{if } x > 0 \\ 1 & \text{if } x = 0 \text{ and } \alpha = 1 \end{cases}$	[0, ∞)

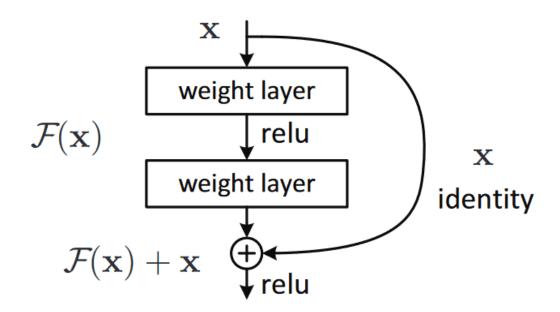
## **Model Architecture:**Residual Connection

- 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

#### **P** Benefits

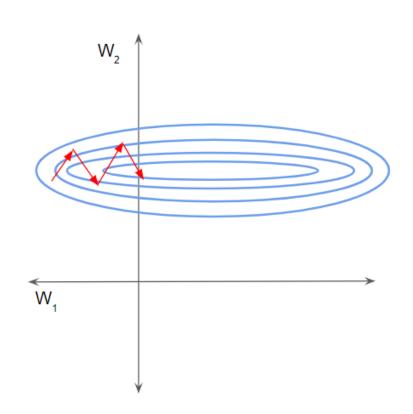
- Solves vanishing gradient problem
- Z Enables very deep architectures
- Helps with faster convergence and better generalization



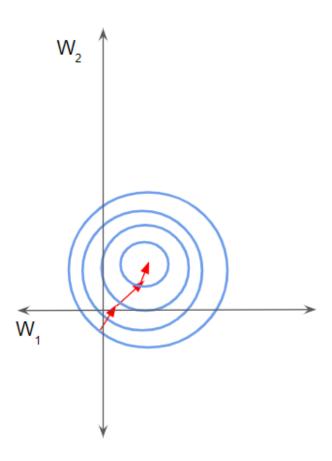
## Model Architecture: Batch Normalization

- During training, distributions of layer inputs keep shifting 7 L
  - 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)
- • O Benefits of Batch Normalization:
  - **Ø** Faster convergence
  - **@ Smoother gradients**, more stable training
  - **Less sensitive** to weight initialization & learning rate
  - **(** Acts like **regularization** → may reduce need for dropout

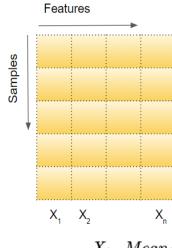
## **Model Architecture:**Batch Normalization



Loss landscape before normalisation

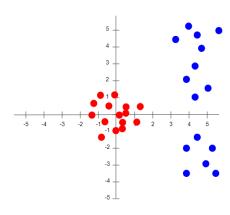


Loss landscape after normalisation



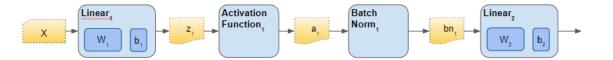
$$X_i = rac{X_i - Mean_i}{StdDev_i}$$

#### Normalisation of features

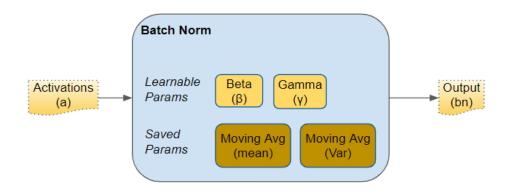


Effect of normalisation

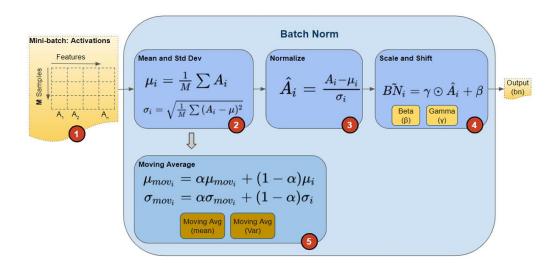
## **Model Architecture:**Batch Normalization



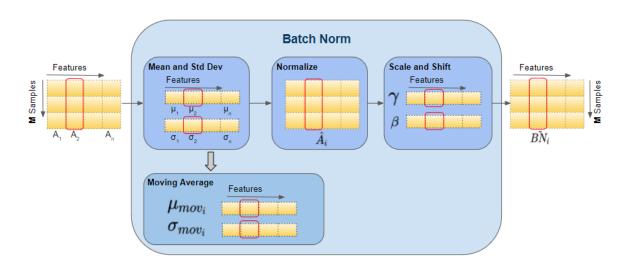
Batch norm layer's place in the network



Batch norm layer's parameters



Batch norm during training

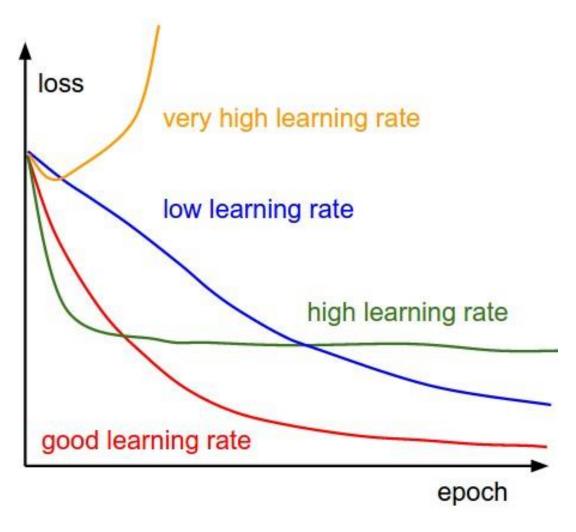


Batch norm during testing

### **Training Tricks: Learning Rate**

- Learning rate (LR) controls the size of each update to the model's weights:
  - Small LR:
    - X Slow learning, Getting stuck on local minima
    - Good for **fine-tuning / exploitation** (refining known good areas)
  - Large LR:
    - X May overshoot or diverge, Loss / gradient explosion,
    - Good for **exploration** (searching broadly across the loss landscape)
- - You can **change LR during training** using **schedulers** (e.g., cosine decay, step decay, warm-up)
  - O Some optimizers (like Adam) adjust effective LR per parameter

### **Training Tricks: Learning Rate**



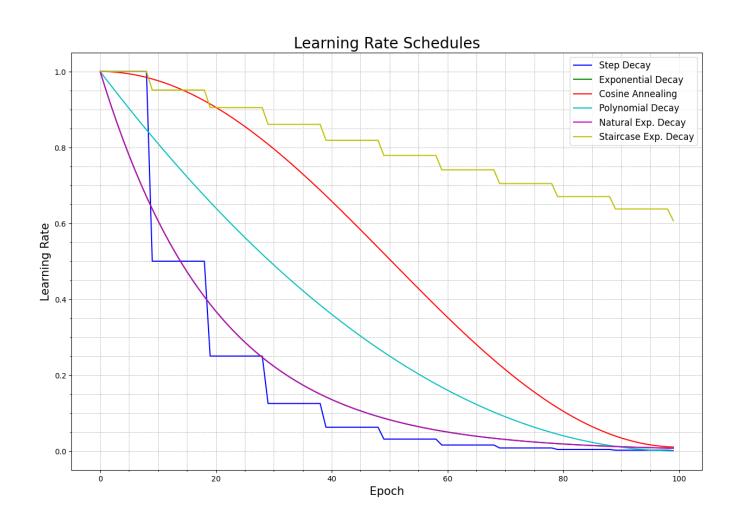
### **Training Tricks: Learning Rate Scheduling**

#### 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

### **Training Tricks: Learning Rate Scheduling**



### **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	
$\bigcirc$ Noisy gradients $\rightarrow$ $\bigcirc$ more exploration	Smoother gradients → @ more exploitation	
🞳 Slower per epoch	🜠 Faster training (more parallelism)	
Fits on less memory	X 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

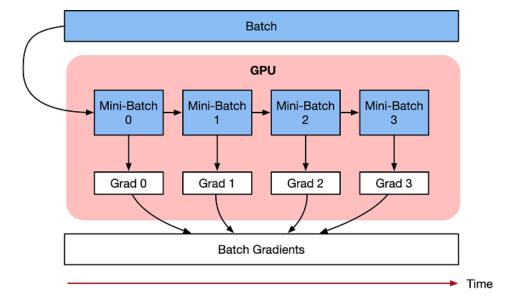
### **Training Tricks: Gradient Accumulation**

#### 🤓 Benefits:

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

#### Trade-offs:

- Slower per step (more forward/backward passes)



### **Training Tricks: Dropout**

A technique where we randomly turn off some neurons during training.

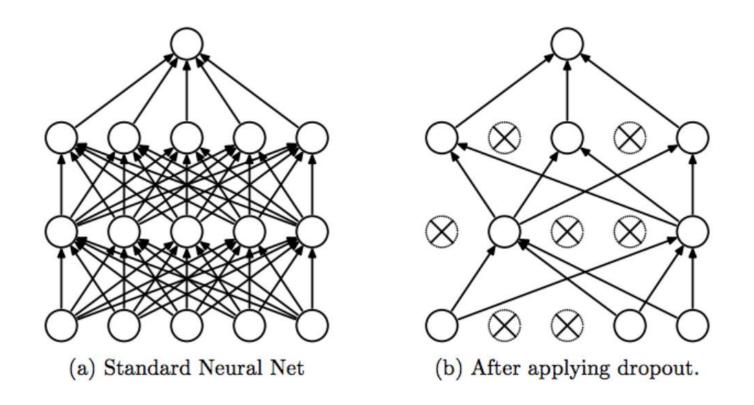
#### How it works:

- For each training step, randomly "drop" (set to 0) a fraction of neurons
- Forces the network to not rely too much on any single path
- During inference, all neurons are used.

#### Why use it?

- Prevents **co-adaptation** of neurons
- Acts as ensemble learning (many thinned networks)
- Reduces **overfitting**, especially on small datasets

# **Training Tricks: Dropout**



### **Training Tricks: Early Stopping**

☑☐ A strategy to stop training before overfitting starts — based on how the model performs on a validation set (not the training set)

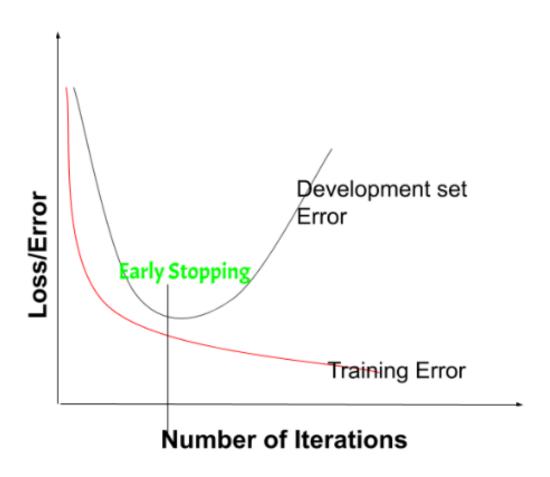
#### **Marks** How it works:

- Train the model as usual
- After each epoch (or few steps), evaluate on the validation set
- If validation performance stops improving for a number of steps (called patience) → stop training

#### Benefits:

- Prevents overfitting
- Saves training time
- Works well when you don't know the best number of epochs

# **Training Tricks: Early Stopping**



### **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
  - Name 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
- XX Symptoms:
  - Training loss becomes NaN or explodes
  - Model never converges
- Two ways to address this:
  - **Weight Initialization >** before training
  - **& Gradient Clipping**  $\rightarrow$  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)
  - **Wanishing gradients** (weights go to zero)
  - Slow or unstable learning
- - 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:

$$W_{ij} \sim U iggl[ -rac{\sqrt{6}}{\sqrt{fan_{in}+fan_{out}}}, rac{\sqrt{6}}{\sqrt{fan_{in}+fan_{out}}} iggr]$$

### **Training Tricks: He Initialization**

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

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

### **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
  - 2 Prevents instability and divergent updates
- How it works:

Let:

$$g = \|
abla \mathcal{L}( heta)\|_2$$

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

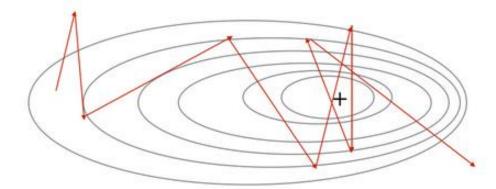
$$abla \mathcal{L} \leftarrow 
abla \mathcal{L} \cdot rac{ au}{g}$$

### **Training Tricks: Gradient Clipping**

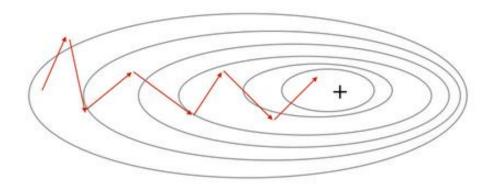
#### **Benefits:**

- 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
- X 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):

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

### **Training Tricks: Weight Decay**

#### 🤓 Benefits:

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

#### 🔽 Adam vs. AdamW:

- Adam: Adds L2 penalty to the gradients (X 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**

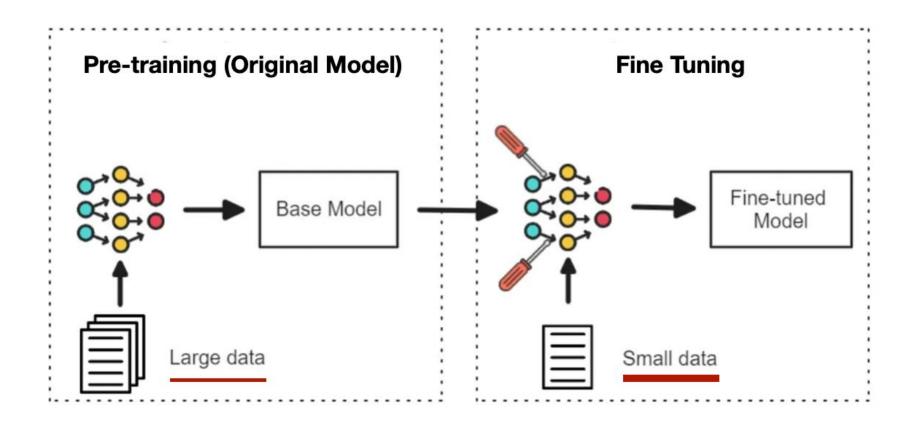
#### What does fine-tuning mean?

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



- 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